



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 11:50 AM EDT

PDB ID : 9AU4 / pdb_00009au4
EMDB ID : EMD-43843
Title : Cryo-EM structure of a photosystem I variant containing an unusual plastoquinone derivative in its electron transfer chain
Authors : Gisriel, C.J.; Vasily, K.; Iwig, D.F.; Russell, B.P.; Vinyard, D.J.; Golbeck, J.H.; Brudvig, G.W.; Lakshmi, K.V.
Deposited on : 2024-02-28
Resolution : 2.03 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:

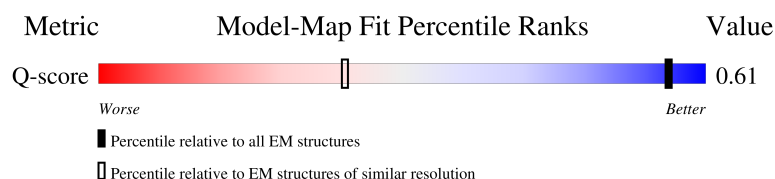
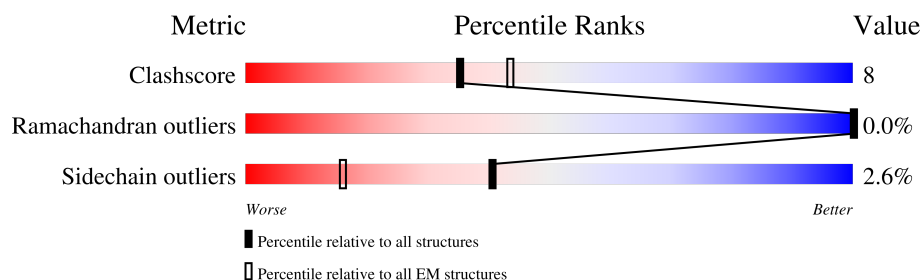
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

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 2.03 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	1771 (1.55 - 2.53)

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	751	82% 15% ..
1	G	751	82% 15% ..
1	a	751	82% 16% ..
2	B	730	84% 16%

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Mol	Chain	Length	Quality of chain
2	H	730	
2	b	730	
3	C	81	
3	N	81	
3	c	81	
4	D	141	
4	O	141	
4	d	141	
5	E	74	
5	P	74	
5	e	74	
6	F	165	
6	Q	165	
6	f	165	
7	I	40	
7	R	40	
7	i	40	
8	J	40	
8	S	40	
8	j	40	
9	K	90	
9	T	90	
9	k	90	
10	L	157	
10	U	157	

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Mol	Chain	Length	Quality of chain
10	l	157	 85% 13% •
11	M	31	 84% 13% •
11	V	31	 84% 13% •
11	m	31	 84% 13% •

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	A1AGD	A	840	X	-	-	-
13	A1AGD	B	2153	X	-	-	-
13	A1AGD	G	840	X	-	-	-
13	A1AGD	H	2153	X	-	-	-
13	A1AGD	a	840	X	-	-	-
13	A1AGD	b	2153	X	-	-	-
23	ZEX	F	205	-	X	-	-
23	ZEX	Q	205	-	X	-	-
23	ZEX	f	205	-	X	-	-

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 73866 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	G	737	Total	C	N	O	S	0	0
			5770	3780	980	983	27		
1	a	737	Total	C	N	O	S	0	0
			5770	3780	980	983	27		
1	A	737	Total	C	N	O	S	0	0
			5770	3780	980	983	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	729	Total	C	N	O	S	0	0
			5770	3798	967	990	15		
2	b	729	Total	C	N	O	S	0	0
			5770	3798	967	990	15		
2	B	729	Total	C	N	O	S	0	0
			5770	3798	967	990	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	80	Total	C	N	O	S	0	0
			600	369	103	117	11		
3	c	80	Total	C	N	O	S	0	0
			600	369	103	117	11		
3	C	80	Total	C	N	O	S	0	0
			600	369	103	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	139	Total	C	N	O	S	0	0
			1087	688	188	208	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	139	Total	C	N	O	S	0	0
			1087	688	188	208	3		
4	D	139	Total	C	N	O	S	0	0
			1087	688	188	208	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	69	Total	C	N	O		0	0
			542	340	96	106			
5	e	69	Total	C	N	O		0	0
			542	340	96	106			
5	E	69	Total	C	N	O		0	0
			542	340	96	106			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q	141	Total	C	N	O	S	0	0
			1100	711	183	201	5		
6	f	141	Total	C	N	O	S	0	0
			1100	711	183	201	5		
6	F	141	Total	C	N	O	S	0	0
			1100	711	183	201	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	40	Total	C	N	O	S	0	0
			311	209	44	55	3		
7	i	40	Total	C	N	O	S	0	0
			311	209	44	55	3		
7	I	40	Total	C	N	O	S	0	0
			311	209	44	55	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S	39	Total	C	N	O	S	0	0
			311	210	46	53	2		
8	j	39	Total	C	N	O	S	0	0
			311	210	46	53	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	39	Total	C	N	O	S	0	0
			311	210	46	53	2		

- Molecule 9 is a protein called Photosystem I reaction center subunit PsaK 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	67	Total	C	N	O	S	0	0
			484	320	77	82	5		
9	k	67	Total	C	N	O	S	0	0
			484	320	77	82	5		
9	K	67	Total	C	N	O	S	0	0
			484	320	77	82	5		

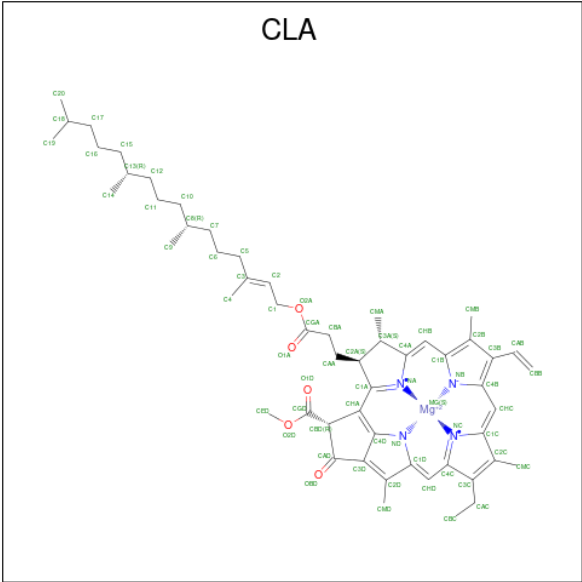
- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	154	Total	C	N	O	S	0	0
			1156	753	188	213	2		
10	l	154	Total	C	N	O	S	0	0
			1156	753	188	213	2		
10	L	154	Total	C	N	O	S	0	0
			1156	753	188	213	2		

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

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

- Molecule 12 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
12	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	G	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
12	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
12	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
12	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
12	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
12	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
12	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
12	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
12	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
12	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
12	G	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
12	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
12	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	H	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
12	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	H	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	H	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
12	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	H	1	Total 50	C 40	Mg 1	N 4	O 5	0
12	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	Q	1	Total 46	C 36	Mg 1	N 4	O 5	0
12	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
12	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
12	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
12	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
12	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
12	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
12	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
12	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
12	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
12	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
12	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	f	1	Total 46	C 36	Mg 1	N 4	O 5	0
12	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	j	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
12	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
12	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	A	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
12	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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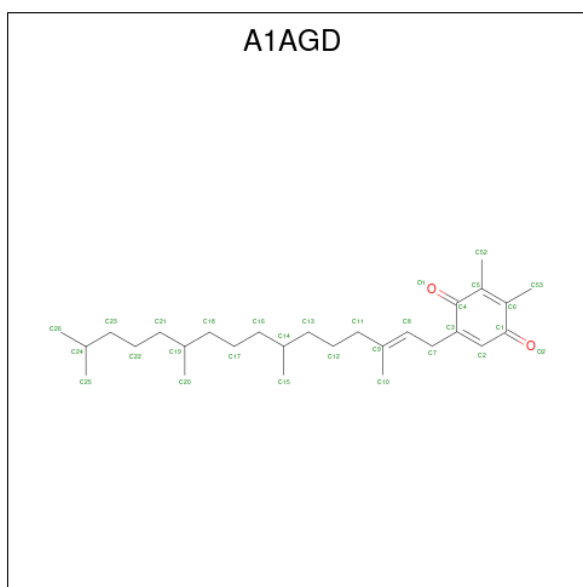
Mol	Chain	Residues	Atoms					AltConf
12	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
12	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
12	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	B	1	Total 45	C 35	Mg 1	N 4	O 5	0

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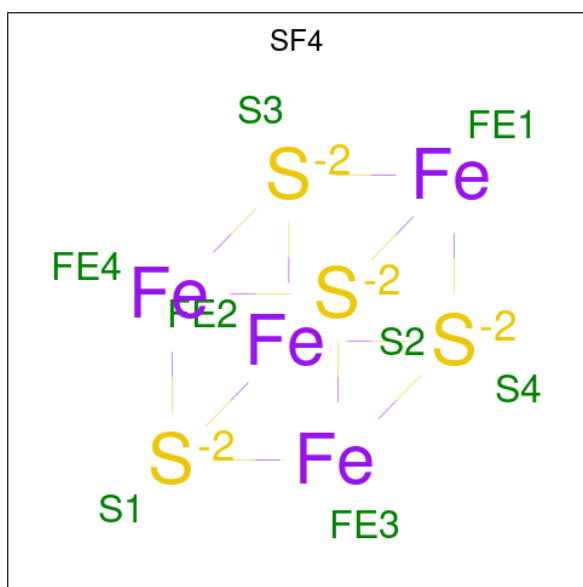
Mol	Chain	Residues	Atoms					AltConf
12	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
12	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 13 is 2,3-dimethyl-5-[(2E,7R,11R)-3,7,11,15-tetramethylhexadec-2-en-1-yl]cyclohexa-2,5-diene-1,4-dione (CCD ID: A1AGD) (formula: C₂₈H₄₆O₂).



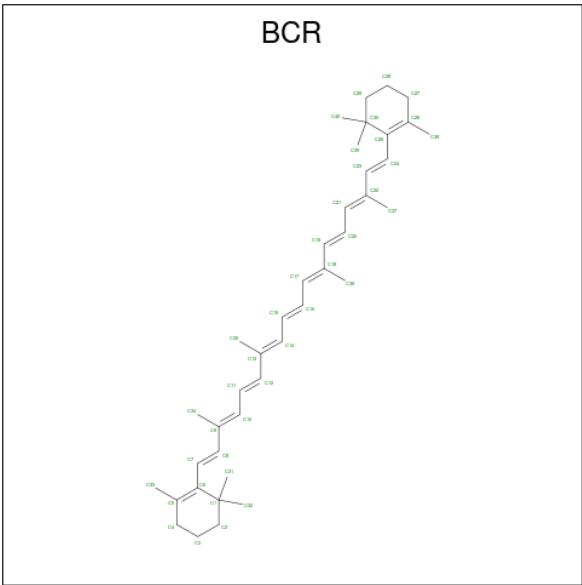
Mol	Chain	Residues	Atoms			AltConf
13	G	1	Total	C	O	0
			30	28	2	
13	H	1	Total	C	O	0
			30	28	2	
13	a	1	Total	C	O	0
			30	28	2	
13	b	1	Total	C	O	0
			30	28	2	
13	A	1	Total	C	O	0
			30	28	2	
13	B	1	Total	C	O	0
			30	28	2	

- Molecule 14 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

- Molecule 15 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms	AltConf
15	G	1	Total C 40 40	0
15	G	1	Total C 40 40	0
15	G	1	Total C 40 40	0
15	G	1	Total C 40 40	0
15	H	1	Total C 40 40	0
15	H	1	Total C 40 40	0
15	H	1	Total C 40 40	0
15	H	1	Total C 40 40	0
15	Q	1	Total C 40 40	0
15	R	1	Total C 40 40	0
15	S	1	Total C 40 40	0
15	S	1	Total C 40 40	0
15	T	1	Total C 40 40	0
15	U	1	Total C 40 40	0

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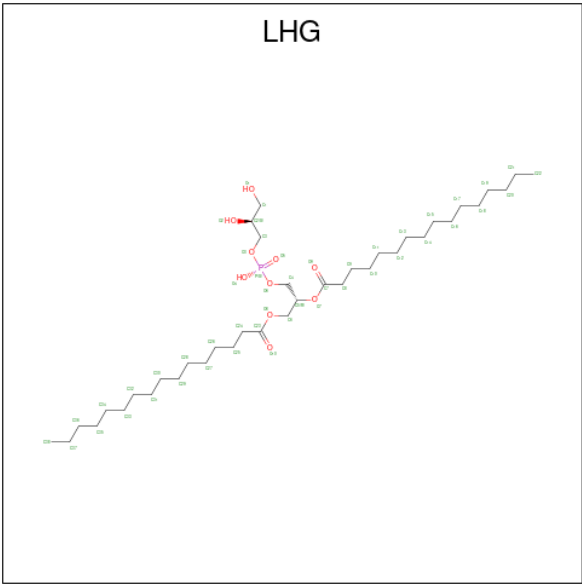
Mol	Chain	Residues	Atoms	AltConf
15	U	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	b	1	Total C 40 40	0
15	b	1	Total C 40 40	0
15	b	1	Total C 40 40	0
15	b	1	Total C 40 40	0
15	f	1	Total C 40 40	0
15	i	1	Total C 40 40	0
15	j	1	Total C 40 40	0
15	j	1	Total C 40 40	0
15	k	1	Total C 40 40	0
15	l	1	Total C 40 40	0
15	l	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	B	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms		AltConf
15	B	1	Total	C	0
			40	40	
15	B	1	Total	C	0
			40	40	
15	B	1	Total	C	0
			40	40	
15	F	1	Total	C	0
			40	40	
15	I	1	Total	C	0
			40	40	
15	J	1	Total	C	0
			40	40	
15	J	1	Total	C	0
			40	40	
15	K	1	Total	C	0
			40	40	
15	L	1	Total	C	0
			40	40	
15	L	1	Total	C	0
			40	40	

- Molecule 16 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



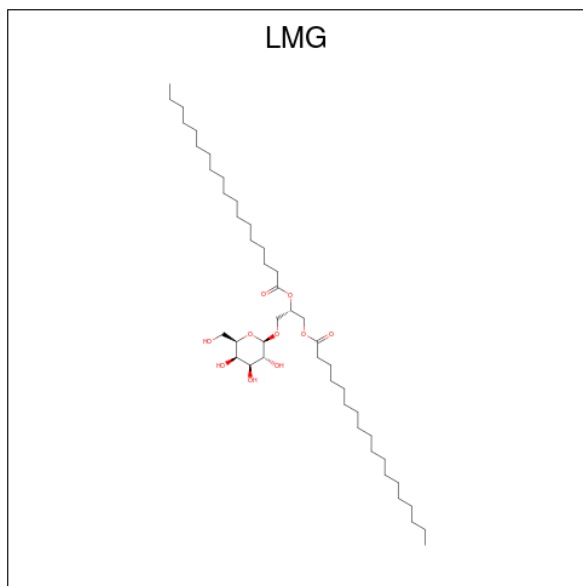
Mol	Chain	Residues	Atoms				AltConf
16	G	1	Total	C	O	P	0
			49	38	10	1	

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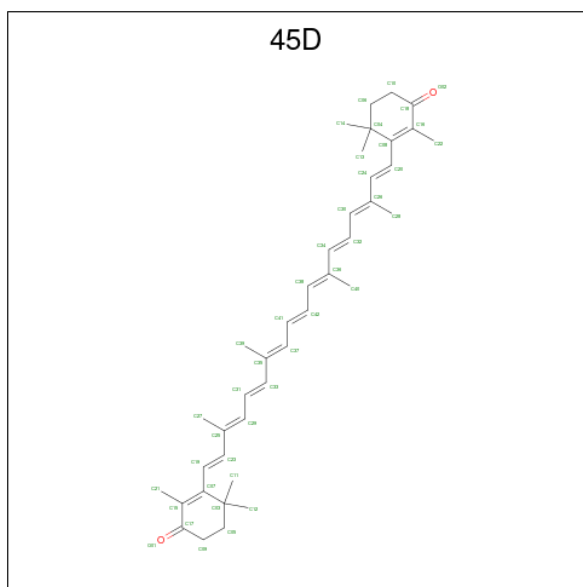
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
16	G	1	49	38	10	1	0
16	H	1	43	32	10	1	0
16	V	1	44	33	10	1	0
16	a	1	49	38	10	1	0
16	a	1	49	38	10	1	0
16	b	1	43	32	10	1	0
16	m	1	44	33	10	1	0
16	A	1	49	38	10	1	0
16	A	1	49	38	10	1	0
16	B	1	43	32	10	1	0
16	M	1	44	33	10	1	0

- Molecule 17 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
17	G	1	Total	C	O	0
			50	40	10	
17	G	1	Total	C	O	0
			32	22	10	
17	H	1	Total	C	O	0
			51	41	10	
17	a	1	Total	C	O	0
			50	40	10	
17	a	1	Total	C	O	0
			32	22	10	
17	b	1	Total	C	O	0
			51	41	10	
17	A	1	Total	C	O	0
			50	40	10	
17	A	1	Total	C	O	0
			32	22	10	
17	B	1	Total	C	O	0
			51	41	10	

- Molecule 18 is beta,beta-carotene-4,4'-dione (CCD ID: 45D) (formula: C₄₀H₅₂O₂).

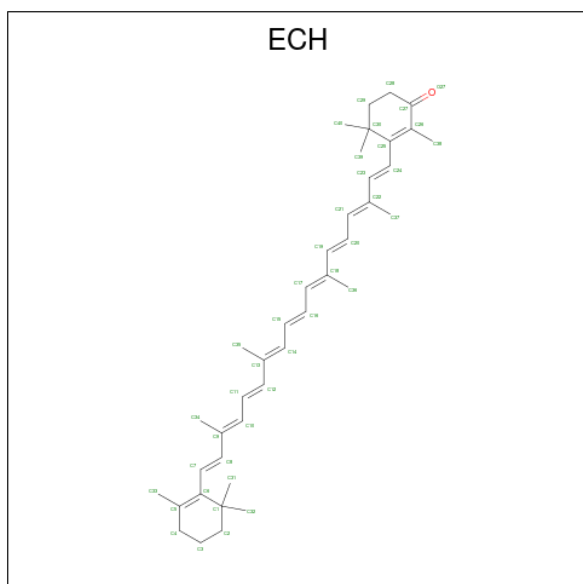


Mol	Chain	Residues	Atoms			AltConf
18	G	1	Total	C	O	0
			42	40	2	
18	a	1	Total	C	O	0
			42	40	2	
18	A	1	Total	C	O	0
			42	40	2	

- Molecule 19 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
19	G	1	Total	Cl	0
			1	1	
19	a	1	Total	Cl	0
			1	1	
19	A	1	Total	Cl	0
			1	1	

- Molecule 20 is beta,beta-caroten-4-one (CCD ID: ECH) (formula: C₄₀H₅₄O).

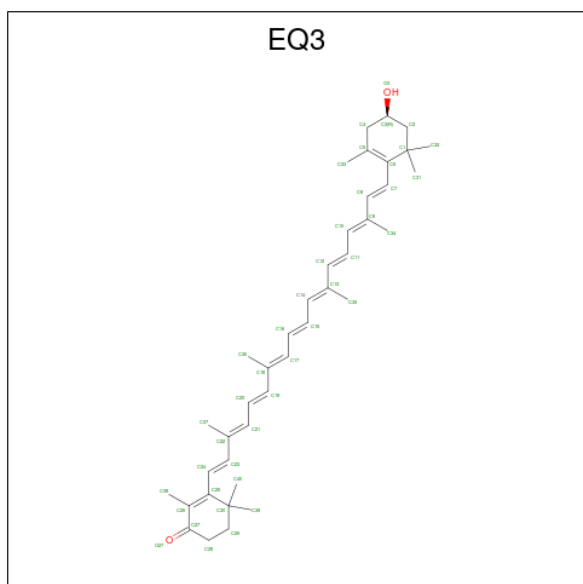


Mol	Chain	Residues	Atoms			AltConf
20	H	1	Total	C	O	0
			41	40	1	
20	V	1	Total	C	O	0
			41	40	1	
20	b	1	Total	C	O	0
			41	40	1	
20	m	1	Total	C	O	0
			41	40	1	
20	B	1	Total	C	O	0
			41	40	1	
20	M	1	Total	C	O	0
			41	40	1	

- Molecule 21 is CALCIUM ION (CCD ID: CA) (formula: Ca).

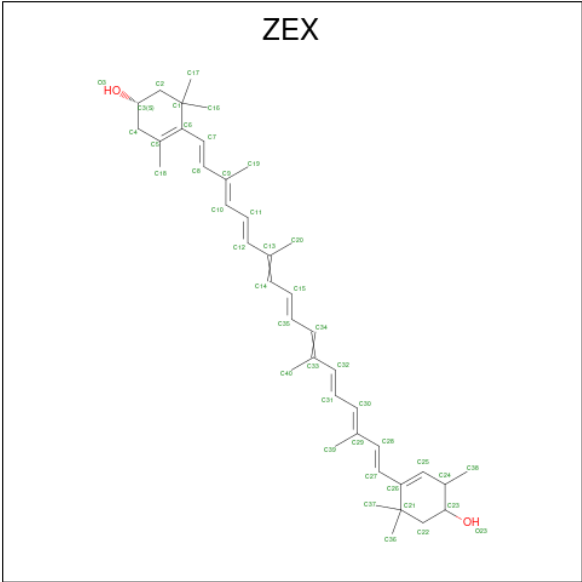
Mol	Chain	Residues	Atoms		AltConf
21	H	1	Total	Ca	0
			1	1	
21	U	1	Total	Ca	0
			1	1	
21	b	1	Total	Ca	0
			1	1	
21	l	1	Total	Ca	0
			1	1	
21	B	1	Total	Ca	0
			1	1	
21	L	1	Total	Ca	0
			1	1	

- Molecule 22 is (3'R)-3'-hydroxy-beta,beta-caroten-4-one (CCD ID: EQ3) (formula: $C_{40}H_{54}O_2$).



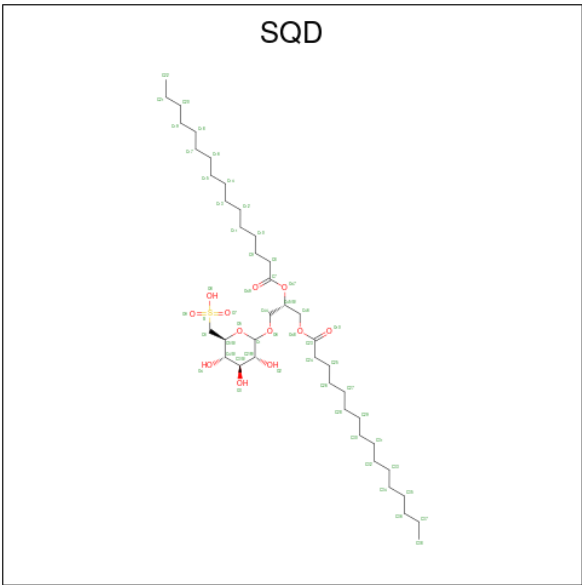
Mol	Chain	Residues	Atoms			AltConf
22	H	1	Total	C	O	0
			42	40	2	
22	b	1	Total	C	O	0
			42	40	2	
22	B	1	Total	C	O	0
			42	40	2	

- Molecule 23 is (1R,2S)-4-{(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl}-2,5,5-trimethylcyclohex-3-en-1-ol (CCD ID: ZEX) (formula: $C_{40}H_{56}O_2$).



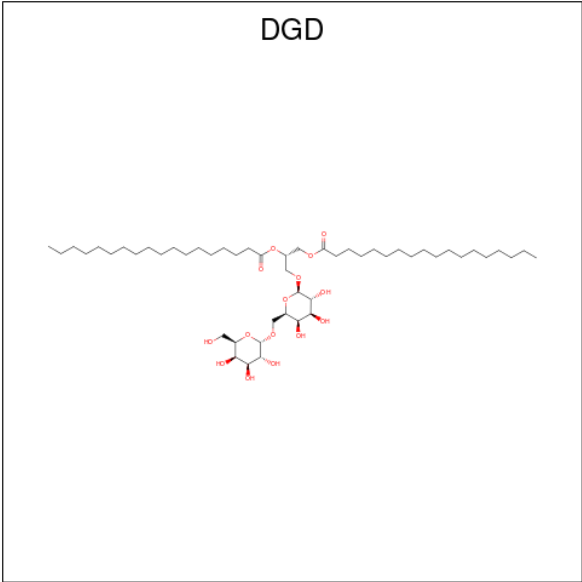
Mol	Chain	Residues	Atoms			AltConf
23	H	1	Total	C	O	0
			42	40	2	
23	Q	1	Total	C	O	0
			42	40	2	
23	b	1	Total	C	O	0
			42	40	2	
23	f	1	Total	C	O	0
			42	40	2	
23	B	1	Total	C	O	0
			42	40	2	
23	F	1	Total	C	O	0
			42	40	2	

- Molecule 24 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



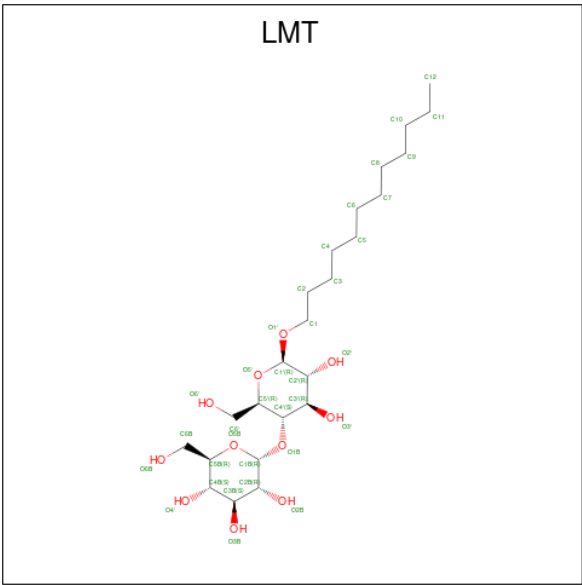
Mol	Chain	Residues	Atoms				AltConf
24	U	1	Total	C	O	S	0
			45	32	12	1	
24	V	1	Total	C	O	S	0
			54	41	12	1	
24	l	1	Total	C	O	S	0
			45	32	12	1	
24	m	1	Total	C	O	S	0
			54	41	12	1	
24	L	1	Total	C	O	S	0
			45	32	12	1	
24	M	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
25	U	1	Total	C	O	0
			49	39	10	
25	I	1	Total	C	O	0
			49	39	10	
25	L	1	Total	C	O	0
			49	39	10	

- Molecule 26 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			AltConf
26	U	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms			AltConf
26	l	1	Total	C	O	0
			35	24	11	
26	L	1	Total	C	O	0
			35	24	11	

- Molecule 27 is water.

Mol	Chain	Residues	Atoms			AltConf
27	G	90	Total	O		0
			90	90		
27	H	112	Total	O		0
			112	112		
27	N	36	Total	O		0
			36	36		
27	O	28	Total	O		0
			28	28		
27	P	7	Total	O		0
			7	7		
27	Q	2	Total	O		0
			2	2		
27	R	4	Total	O		0
			4	4		
27	U	24	Total	O		0
			24	24		
27	a	90	Total	O		0
			90	90		
27	b	112	Total	O		0
			112	112		
27	c	36	Total	O		0
			36	36		
27	d	28	Total	O		0
			28	28		
27	e	7	Total	O		0
			7	7		
27	f	2	Total	O		0
			2	2		
27	i	4	Total	O		0
			4	4		
27	l	24	Total	O		0
			24	24		
27	A	90	Total	O		0
			90	90		

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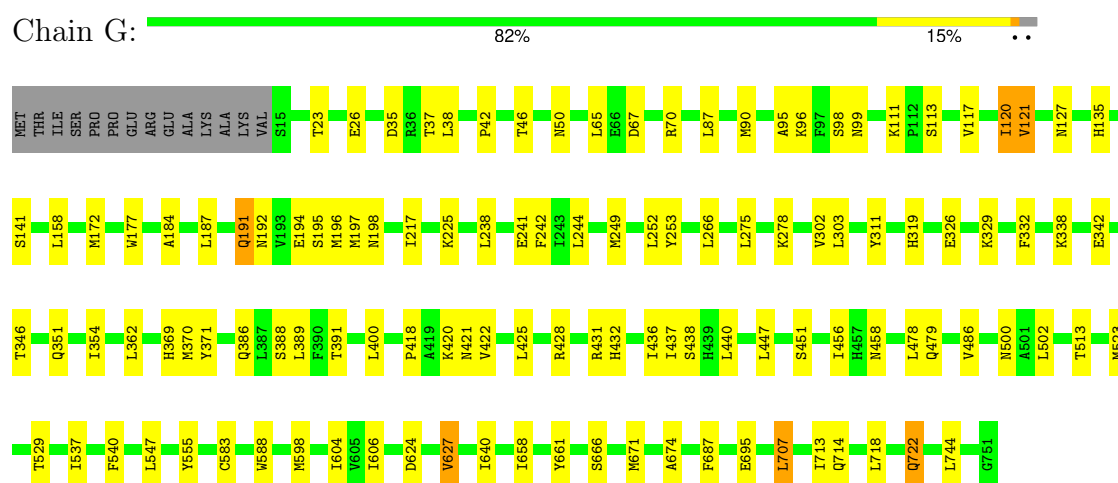
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
27	B	112	Total 112	O 112	0
27	C	36	Total 36	O 36	0
27	D	28	Total 28	O 28	0
27	E	7	Total 7	O 7	0
27	F	2	Total 2	O 2	0
27	I	4	Total 4	O 4	0
27	L	24	Total 24	O 24	0

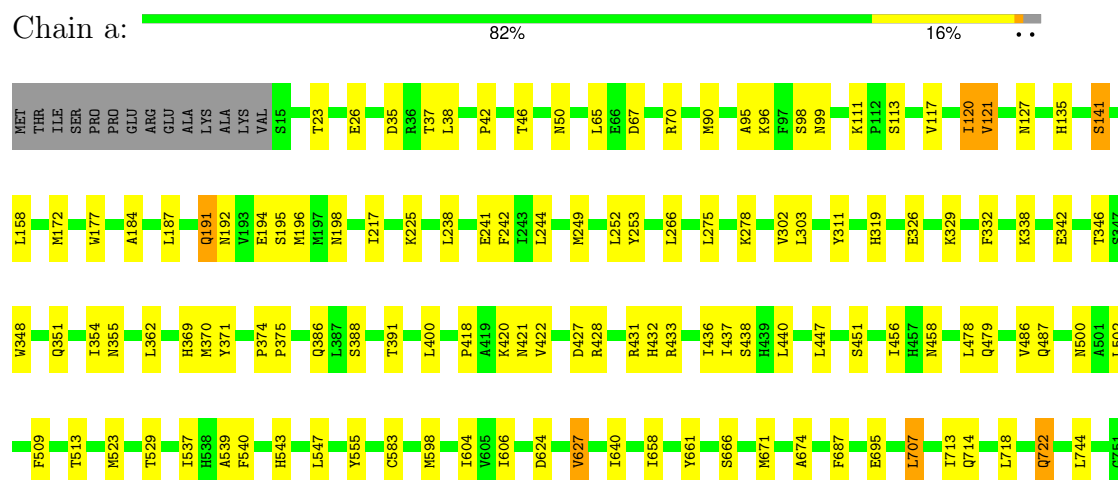
3 Residue-property plots

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

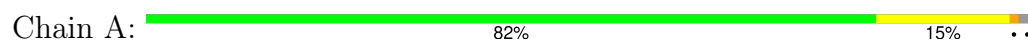
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

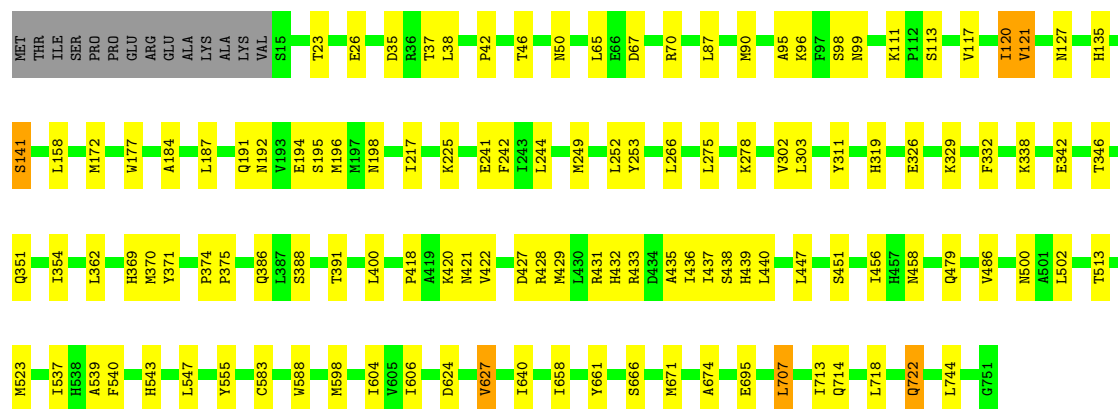


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



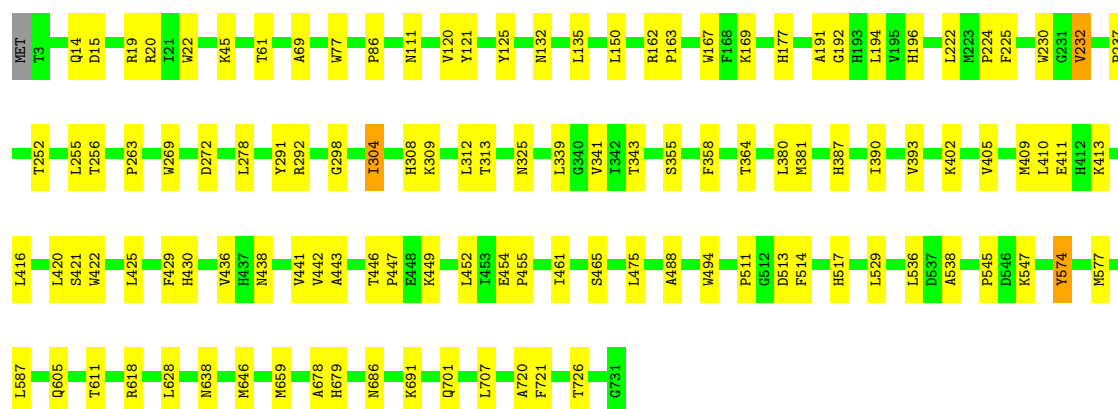
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1





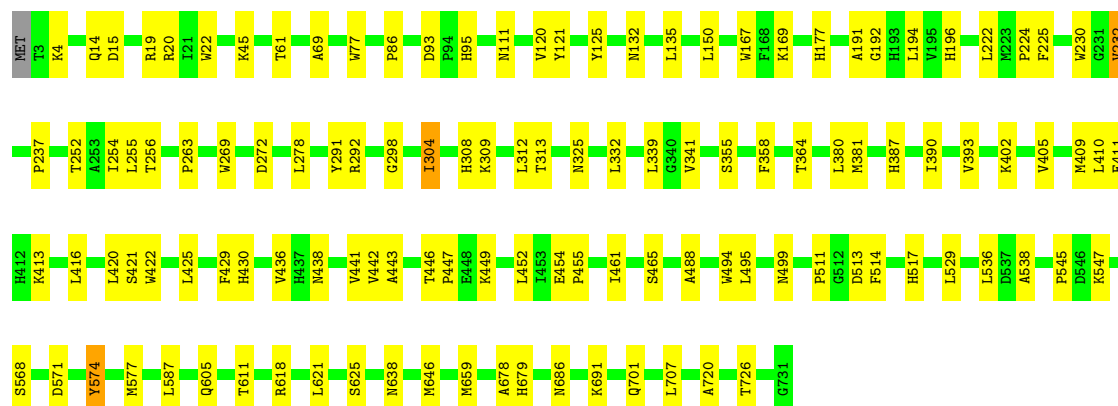
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain H: 84% 15%



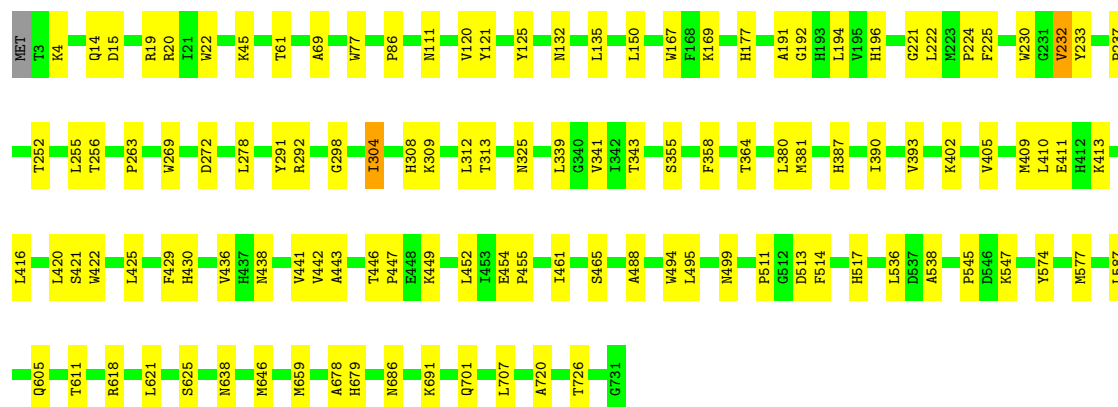
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b: 83% 16%



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 84% 16%



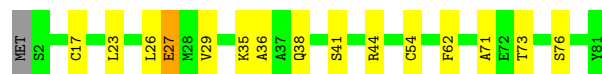
• Molecule 3: Photosystem I iron-sulfur center

Chain N: 84% 14% ..



• Molecule 3: Photosystem I iron-sulfur center

Chain c: 80% 17% ..



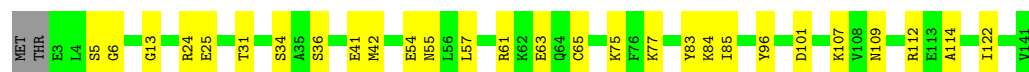
• Molecule 3: Photosystem I iron-sulfur center

Chain C: 81% 16% ..



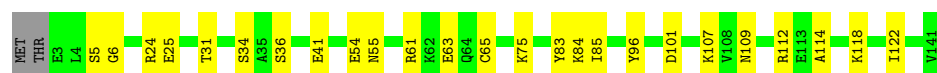
• Molecule 4: Photosystem I reaction center subunit II

Chain O: 79% 20% .



• Molecule 4: Photosystem I reaction center subunit II

Chain d: 81% 18% .



• Molecule 4: Photosystem I reaction center subunit II

MT	THR	E3	L4	S5	G6		R24	E25		T31		S34	A35	S36		E41	K42		E54	N55	L56	L57		R61	K62	E63	Q64	C65		K75	F76	K77		Y83	K84	L85		Y96			D101		K107	V108	N109		R112	E113	A114			I122		V141	
----	-----	----	----	----	----	--	-----	-----	--	-----	--	-----	-----	-----	--	-----	-----	--	-----	-----	-----	-----	--	-----	-----	-----	-----	-----	--	-----	-----	-----	--	-----	-----	-----	--	-----	--	--	------	--	------	------	------	--	------	------	------	--	--	------	--	------	--

- | MET |
|-----|
| A2 |
| V9 |
| K12 |
| R13 |
| Y17 |
| G20 |
| V28 |
| E29 |
| K30 |
| P36 |
| V56 |
| A62 |
| L66 |
| E67 |
| L68 |
| V69 |
| Q70 |
| ALA |
| ALA |
| ALA |
| LYS |

- | | | | | | | | | | | | | | | | | | | | | | |
|-----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | A2 | V9 | K12 | R13 | Y17 | G20 | V28 | E29 | K30 | P36 | V56 | A62 | L66 | E67 | L68 | V69 | Q70 | ALA | ALA | ALA | LYS |
|-----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- | | | | | | | | | | | | | | | | | | | | |
|-----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | A2 | V9 | K12 | R13 | Y17 | G20 | V28 | P36 | V56 | A62 | L66 | E67 | L68 | V69 | Q70 | ALA | ALA | ALA | LYS |
|-----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

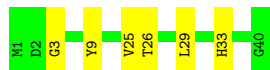
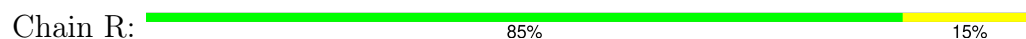
-
- | Amino Acid | Relative Abundance (approx.) |
|------------|------------------------------|
| MET | 100 |
| LYS | 10 |
| HIS | 15 |
| LEU | 15 |
| LEU | 15 |
| ALA | 15 |
| LEU | 15 |
| LEU | 15 |
| ALA | 15 |
| PHE | 15 |
| THR | 15 |
| TRP | 15 |
| PHE | 15 |
| ASN | 15 |
| PHE | 15 |
| ALA | 15 |
| PRO | 15 |
| SER | 15 |
| ALA | 15 |
| SER | 15 |
| ALA | 15 |
| ASP | 15 |
| D3 | 15 |
| P14 | 15 |
| L17 | 15 |
| L35 | 15 |
| R39 | 15 |
| Y50 | 15 |
| F51 | 15 |
| H52 | 15 |
| D56 | 15 |
| G57 | 15 |
| R58 | 15 |
| F59 | 15 |
| T60 | 15 |
| W81 | 15 |
| R84 | 15 |
| S85 | 15 |
| Y86 | 15 |
| L87 | 15 |
| E92 | 15 |
| V101 | 15 |
| M104 | 15 |
| A122 | 15 |
| T123 | 15 |

- | Residue | Score |
|---------|-------|
| MET | 1.00 |
| LYS | 0.99 |
| HIS | 0.98 |
| LEU | 0.97 |
| ALA | 0.96 |
| LEU | 0.95 |
| LEU | 0.94 |
| ALA | 0.93 |
| PHE | 0.92 |
| THR | 0.91 |
| TRP | 0.90 |
| PHE | 0.89 |
| ASN | 0.88 |
| PHE | 0.87 |
| ALA | 0.86 |
| PRO | 0.85 |
| SER | 0.84 |
| ALA | 0.83 |
| SER | 0.82 |
| ALA | 0.81 |
| ASP | 0.80 |
| D3 | 0.79 |
| P14 | 0.78 |
| L17 | 0.77 |
| I35 | 0.76 |
| R39 | 0.75 |
| Y50 | 0.74 |
| F51 | 0.73 |
| H52 | 0.72 |
| D56 | 0.71 |
| G57 | 0.70 |
| R58 | 0.69 |
| F59 | 0.68 |
| T60 | 0.67 |
| R84 | 0.66 |
| S85 | 0.65 |
| E92 | 0.64 |
| V101 | 0.63 |
| N104 | 0.62 |
| A122 | 0.61 |
| E125 | 0.60 |
| K130 | 0.59 |
| L131 | 0.58 |
| P139 | 0.57 |
| P142 | 0.56 |
| R143 | 0.55 |

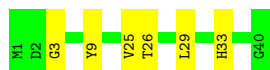
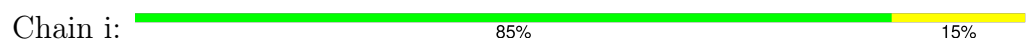
- 



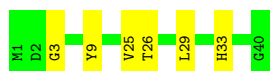
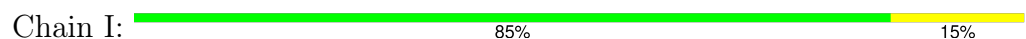
• Molecule 7: Photosystem I reaction center subunit VIII



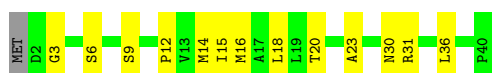
• Molecule 7: Photosystem I reaction center subunit VIII



• Molecule 7: Photosystem I reaction center subunit VIII



• Molecule 8: Photosystem I reaction center subunit IX



• Molecule 8: Photosystem I reaction center subunit IX



• Molecule 8: Photosystem I reaction center subunit IX



• Molecule 9: Photosystem I reaction center subunit PsaK 2

Chain T: 



- Molecule 9: Photosystem I reaction center subunit PsaK 2

Chain k: 



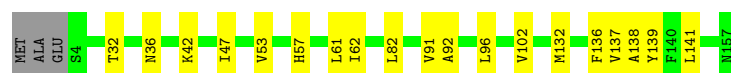
- Molecule 9: Photosystem I reaction center subunit PsaK 2

Chain K: 



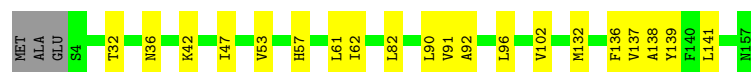
- Molecule 10: Photosystem I reaction center subunit XI

Chain U: 



- Molecule 10: Photosystem I reaction center subunit XI

Chain l: 



- Molecule 10: Photosystem I reaction center subunit XI

Chain L: 



- Molecule 11: Photosystem I reaction center subunit XII

Chain V: 



- Molecule 11: Photosystem I reaction center subunit XII

Chain m:  84% 13% •



- Molecule 11: Photosystem I reaction center subunit XII

Chain M:  84% 13% •



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	375816	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 ($e^-/\text{\AA}^2$)	40.2	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	59.972	Depositor
Minimum map value	-21.826	Depositor
Average map value	0.001	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	0.0149	Depositor
Map size ($\text{\AA}$)	266.24, 266.24, 266.24	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.83199996, 0.83199996, 0.83199996	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 45D, SQD, ZEX, CLA, LMT, EQ3, A1AGD, DGD, BCR, LMG, ECH, SF4, CL, CA, LHG

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	0.26	0/5967	0.57	3/8133 (0.0%)
1	G	0.26	0/5967	0.57	3/8133 (0.0%)
1	a	0.26	0/5967	0.57	3/8133 (0.0%)
2	B	0.26	0/5981	0.59	3/8178 (0.0%)
2	H	0.26	0/5981	0.59	3/8178 (0.0%)
2	b	0.26	0/5981	0.59	3/8178 (0.0%)
3	C	0.22	0/610	0.63	2/826 (0.2%)
3	N	0.23	0/610	0.63	2/826 (0.2%)
3	c	0.22	0/610	0.63	2/826 (0.2%)
4	D	0.19	0/1111	0.51	0/1497
4	O	0.20	0/1111	0.51	0/1497
4	d	0.19	0/1111	0.51	0/1497
5	E	0.23	0/551	0.59	2/745 (0.3%)
5	P	0.23	0/551	0.59	2/745 (0.3%)
5	e	0.23	0/551	0.59	2/745 (0.3%)
6	F	0.23	0/1130	0.58	2/1535 (0.1%)
6	Q	0.23	0/1130	0.58	2/1535 (0.1%)
6	f	0.23	0/1130	0.58	2/1535 (0.1%)
7	I	0.28	0/322	0.62	0/438
7	R	0.28	0/322	0.62	0/438
7	i	0.28	0/322	0.62	0/438
8	J	0.25	0/320	0.63	1/433 (0.2%)
8	S	0.25	0/320	0.63	1/433 (0.2%)
8	j	0.26	0/320	0.63	1/433 (0.2%)
9	K	0.27	0/492	0.71	0/661
9	T	0.27	0/492	0.71	0/661
9	k	0.27	0/492	0.71	0/661
10	L	0.25	0/1186	0.56	0/1611
10	U	0.25	0/1186	0.56	0/1611
10	l	0.25	0/1186	0.56	0/1611
11	M	0.27	0/241	0.54	0/326
11	V	0.27	0/241	0.54	0/326

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	m	0.27	0/241	0.54	0/326
All	All	0.25	0/53733	0.58	39/73149 (0.1%)

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	263	PRO	N-CD-CG	-6.99	92.72	103.20
2	B	263	PRO	N-CD-CG	-6.99	92.72	103.20
2	H	263	PRO	N-CD-CG	-6.98	92.73	103.20
2	b	263	PRO	CA-N-CD	-6.42	103.01	112.00
2	H	263	PRO	CA-N-CD	-6.41	103.02	112.00
2	B	263	PRO	CA-N-CD	-6.41	103.02	112.00
1	G	338	LYS	CA-CB-CG	5.81	125.72	114.10
1	A	338	LYS	CA-CB-CG	5.81	125.73	114.10
1	a	338	LYS	CA-CB-CG	5.81	125.71	114.10
1	G	96	LYS	CA-CB-CG	5.68	125.47	114.10
1	a	96	LYS	CA-CB-CG	5.68	125.46	114.10
1	A	96	LYS	CA-CB-CG	5.67	125.44	114.10
3	c	62	PHE	CA-C-N	5.64	129.72	121.31
3	c	62	PHE	C-N-CA	5.64	129.72	121.31
2	B	402	LYS	CA-CB-CG	5.64	125.38	114.10
3	C	62	PHE	CA-C-N	5.64	129.71	121.31
3	C	62	PHE	C-N-CA	5.64	129.71	121.31
2	b	402	LYS	CA-CB-CG	5.64	125.37	114.10
3	N	62	PHE	CA-C-N	5.63	129.70	121.31
3	N	62	PHE	C-N-CA	5.63	129.70	121.31
2	H	402	LYS	CA-CB-CG	5.61	125.33	114.10
8	J	16	MET	CB-CG-SD	5.54	129.31	112.70
8	j	16	MET	CB-CG-SD	5.53	129.30	112.70
8	S	16	MET	CB-CG-SD	5.53	129.28	112.70
6	f	104	ASN	CA-C-N	5.26	124.54	120.33
6	f	104	ASN	C-N-CA	5.26	124.54	120.33
6	F	104	ASN	CA-C-N	5.25	124.53	120.33
6	F	104	ASN	C-N-CA	5.25	124.53	120.33
6	Q	104	ASN	CA-C-N	5.19	124.48	120.33
6	Q	104	ASN	C-N-CA	5.19	124.48	120.33
5	P	13	ARG	CA-C-N	5.16	131.40	121.54
5	P	13	ARG	C-N-CA	5.16	131.40	121.54
5	E	13	ARG	CA-C-N	5.16	131.40	121.54
5	E	13	ARG	C-N-CA	5.16	131.40	121.54
5	e	13	ARG	CA-C-N	5.15	131.38	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	e	13	ARG	C-N-CA	5.15	131.38	121.54
1	G	598	MET	CA-CB-CG	5.12	124.33	114.10
1	a	598	MET	CA-CB-CG	5.11	124.33	114.10
1	A	598	MET	CA-CB-CG	5.10	124.30	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5770	0	5622	82	0
1	G	5770	0	5622	82	0
1	a	5770	0	5622	83	0
2	B	5770	0	5547	80	0
2	H	5770	0	5547	84	0
2	b	5770	0	5547	85	0
3	C	600	0	581	7	0
3	N	600	0	581	6	0
3	c	600	0	581	8	0
4	D	1087	0	1082	15	0
4	O	1087	0	1082	16	0
4	d	1087	0	1082	14	0
5	E	542	0	525	6	0
5	P	542	0	525	7	0
5	e	542	0	525	7	0
6	F	1100	0	1096	15	0
6	Q	1100	0	1096	14	0
6	f	1100	0	1096	11	0
7	I	311	0	304	6	0
7	R	311	0	304	6	0
7	i	311	0	304	6	0
8	J	311	0	316	8	0
8	S	311	0	316	10	0
8	j	311	0	316	7	0
9	K	484	0	514	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	T	484	0	514	6	0
9	k	484	0	514	6	0
10	L	1156	0	1127	14	0
10	U	1156	0	1127	15	0
10	l	1156	0	1127	16	0
11	M	238	0	260	8	0
11	V	238	0	260	7	0
11	m	238	0	260	8	0
12	A	2536	0	2594	84	0
12	B	2425	0	2404	79	0
12	F	156	0	138	5	0
12	G	2536	0	2594	84	0
12	H	2425	0	2404	82	0
12	J	90	0	66	1	0
12	K	45	0	33	0	0
12	L	260	0	288	12	0
12	Q	156	0	138	6	0
12	S	90	0	66	1	0
12	T	45	0	33	0	0
12	U	260	0	288	12	0
12	a	2536	0	2594	83	0
12	b	2425	0	2404	82	0
12	f	156	0	138	5	0
12	j	90	0	66	1	0
12	k	45	0	33	0	0
12	l	260	0	288	12	0
13	A	30	0	0	1	0
13	B	30	0	0	2	0
13	G	30	0	0	1	0
13	H	30	0	0	2	0
13	a	30	0	0	1	0
13	b	30	0	0	2	0
14	A	8	0	0	0	0
14	C	16	0	0	0	0
14	G	8	0	0	0	0
14	N	16	0	0	0	0
14	a	8	0	0	0	0
14	c	16	0	0	0	0
15	A	160	0	224	8	0
15	B	160	0	224	10	0
15	F	40	0	56	2	0
15	G	160	0	224	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	H	160	0	224	11	0
15	I	40	0	56	2	0
15	J	80	0	112	9	0
15	K	40	0	56	2	0
15	L	80	0	112	7	0
15	Q	40	0	56	2	0
15	R	40	0	56	2	0
15	S	80	0	112	9	0
15	T	40	0	56	2	0
15	U	80	0	112	5	0
15	a	160	0	224	11	0
15	b	160	0	224	8	0
15	f	40	0	56	2	0
15	i	40	0	56	1	0
15	j	80	0	112	10	0
15	k	40	0	56	2	0
15	l	80	0	112	7	0
16	A	98	0	148	8	0
16	B	43	0	59	4	0
16	G	98	0	148	8	0
16	H	43	0	59	4	0
16	M	44	0	61	2	0
16	V	44	0	61	3	0
16	a	98	0	148	8	0
16	b	43	0	59	4	0
16	m	44	0	61	2	0
17	A	82	0	107	6	0
17	B	51	0	75	0	0
17	G	82	0	107	7	0
17	H	51	0	75	0	0
17	a	82	0	107	6	0
17	b	51	0	75	0	0
18	A	42	0	52	1	0
18	G	42	0	52	1	0
18	a	42	0	52	1	0
19	A	1	0	0	0	0
19	G	1	0	0	0	0
19	a	1	0	0	0	0
20	B	41	0	54	7	0
20	H	41	0	54	6	0
20	M	41	0	54	1	0
20	V	41	0	54	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	b	41	0	54	7	0
20	m	41	0	54	1	0
21	B	1	0	0	0	0
21	H	1	0	0	0	0
21	L	1	0	0	0	0
21	U	1	0	0	0	0
21	b	1	0	0	0	0
21	l	1	0	0	0	0
22	B	42	0	0	0	0
22	H	42	0	0	0	0
22	b	42	0	0	0	0
23	B	42	0	56	2	0
23	F	42	0	55	2	0
23	H	42	0	56	3	0
23	Q	42	0	55	2	0
23	b	42	0	56	2	0
23	f	42	0	55	2	0
24	L	45	0	54	4	0
24	M	54	0	78	9	0
24	U	45	0	54	4	0
24	V	54	0	78	8	0
24	l	45	0	54	4	0
24	m	54	0	78	8	0
25	L	49	0	70	3	0
25	U	49	0	70	3	0
25	l	49	0	70	3	0
26	L	35	0	45	3	0
26	U	35	0	45	3	0
26	l	35	0	45	3	0
27	A	90	0	0	3	0
27	B	112	0	0	2	0
27	C	36	0	0	0	0
27	D	28	0	0	0	0
27	E	7	0	0	0	0
27	F	2	0	0	0	0
27	G	90	0	0	4	0
27	H	112	0	0	2	0
27	I	4	0	0	0	0
27	L	24	0	0	1	0
27	N	36	0	0	0	0
27	O	28	0	0	0	0
27	P	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	Q	2	0	0	0	0
27	R	4	0	0	0	0
27	U	24	0	0	1	0
27	a	90	0	0	3	0
27	b	112	0	0	2	0
27	c	36	0	0	0	0
27	d	28	0	0	0	0
27	e	7	0	0	0	0
27	f	2	0	0	0	0
27	i	4	0	0	0	0
27	l	24	0	0	1	0
All	All	73866	0	72915	1156	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 (1156) 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)
20:H:2143:ECH:H33B	12:a:854:CLA:HBB1	1.35	1.08
20:b:2143:ECH:H33B	12:A:854:CLA:HBB1	1.35	1.08
12:G:854:CLA:HBB1	20:B:2144:ECH:H33B	1.33	1.06
12:G:854:CLA:CBB	20:B:2144:ECH:H33B	1.86	1.05
20:b:2143:ECH:H33B	12:A:854:CLA:CBB	1.87	1.03
20:H:2143:ECH:H33B	12:a:854:CLA:CBB	1.87	1.02
12:B:2141:CLA:O1A	13:B:2153:A1AGD:C26	2.20	0.90
12:b:2140:CLA:O1A	13:b:2153:A1AGD:C26	2.20	0.90
12:H:2140:CLA:O1A	13:H:2153:A1AGD:C26	2.20	0.89
11:m:27:THR:HG23	24:m:102:SQD:O6	1.76	0.85
11:V:27:THR:HG23	24:V:102:SQD:O6	1.76	0.84
11:M:27:THR:HG23	24:M:101:SQD:O6	1.78	0.82
11:V:27:THR:CG2	24:V:102:SQD:O2	2.29	0.81
11:m:27:THR:CG2	24:m:102:SQD:O2	2.29	0.80
11:M:27:THR:CG2	24:M:101:SQD:O2	2.30	0.79
12:G:854:CLA:HBB1	20:B:2144:ECH:C33	2.12	0.78
20:H:2143:ECH:C33	12:a:854:CLA:HBB1	2.14	0.74
20:b:2143:ECH:C33	12:A:854:CLA:HBB1	2.14	0.73
12:A:851:CLA:H93	12:A:851:CLA:HBB1	1.74	0.69
12:H:2109:CLA:HBB1	12:H:2109:CLA:H71	1.75	0.69
12:B:2110:CLA:H71	12:B:2110:CLA:HBB1	1.75	0.69
12:U:205:CLA:H2	26:U:210:LMT:H42	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:l:205:CLA:H2	26:l:210:LMT:H42	1.74	0.69
12:b:2130:CLA:HBB1	16:b:2148:LHG:H301	1.75	0.68
12:H:2130:CLA:HBB1	16:H:2148:LHG:H301	1.76	0.68
7:i:33:HIS:HB2	24:L:208:SQD:H462	1.74	0.68
12:F:204:CLA:H3A	23:F:205:ZEX:H24	1.76	0.68
24:U:208:SQD:H462	7:I:33:HIS:HB2	1.74	0.68
12:a:851:CLA:H93	12:a:851:CLA:HBB1	1.74	0.68
7:R:33:HIS:HB2	24:l:208:SQD:H462	1.75	0.68
12:L:205:CLA:H2	26:L:210:LMT:H42	1.74	0.68
12:G:851:CLA:HBB1	12:G:851:CLA:H93	1.74	0.68
12:Q:204:CLA:H3A	23:Q:205:ZEX:H24	1.75	0.67
1:a:718:LEU:HB3	1:a:722:GLN:HG2	1.75	0.67
1:A:718:LEU:HB3	1:A:722:GLN:HG2	1.75	0.67
12:H:2140:CLA:O1A	13:H:2153:A1AGD:C22	2.43	0.67
12:f:204:CLA:H3A	23:f:205:ZEX:H24	1.75	0.67
12:B:2131:CLA:HBB1	16:B:2149:LHG:H301	1.76	0.67
1:G:718:LEU:HB3	1:G:722:GLN:HG2	1.75	0.67
11:V:27:THR:HG21	24:V:102:SQD:O2	1.95	0.67
12:b:2109:CLA:H71	12:b:2109:CLA:HBB1	1.75	0.67
12:b:2140:CLA:O1A	13:b:2153:A1AGD:C22	2.43	0.66
11:m:27:THR:HG21	24:m:102:SQD:O2	1.95	0.66
12:B:2141:CLA:O1A	13:B:2153:A1AGD:C22	2.43	0.66
2:B:646:MET:HG2	2:B:720:ALA:HB2	1.78	0.66
2:H:646:MET:HG2	2:H:720:ALA:HB2	1.78	0.65
1:a:420:LYS:NZ	27:a:901:HOH:O	2.29	0.65
1:G:420:LYS:NZ	27:G:901:HOH:O	2.29	0.64
11:M:27:THR:HG21	24:M:101:SQD:O2	1.97	0.64
1:A:420:LYS:NZ	27:A:901:HOH:O	2.29	0.64
2:b:646:MET:HG2	2:b:720:ALA:HB2	1.78	0.64
2:H:577:MET:HG3	2:H:707:LEU:HD21	1.80	0.64
2:B:577:MET:HG3	2:B:707:LEU:HD21	1.80	0.64
12:a:825:CLA:H91	15:a:845:BCR:H24C	1.81	0.63
12:A:825:CLA:H91	15:A:845:BCR:H24C	1.81	0.63
12:G:825:CLA:H91	15:G:845:BCR:H24C	1.81	0.63
12:a:820:CLA:H12	12:a:823:CLA:HBA2	1.81	0.63
7:R:26:THR:HG23	24:l:208:SQD:H281	1.81	0.63
2:b:577:MET:HG3	2:b:707:LEU:HD21	1.80	0.63
2:b:587:LEU:HD22	12:b:2136:CLA:HBB2	1.81	0.62
7:i:26:THR:HG23	24:L:208:SQD:H281	1.81	0.62
2:b:15:ASP:HB3	2:b:20:ARG:HB2	1.82	0.62
1:A:194:GLU:O	1:A:198:ASN:ND2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:820:CLA:H12	12:G:823:CLA:HBA2	1.81	0.61
24:U:208:SQD:H281	7:I:26:THR:HG23	1.82	0.61
12:A:820:CLA:H12	12:A:823:CLA:HBA2	1.81	0.61
2:B:15:ASP:HB3	2:B:20:ARG:HB2	1.82	0.61
1:a:194:GLU:O	1:a:198:ASN:ND2	2.33	0.61
12:a:821:CLA:HMD2	15:k:4001:BCR:H24C	1.82	0.61
12:b:2137:CLA:HBC2	23:b:2151:ZEX:H7	1.83	0.61
12:B:2138:CLA:HBC2	23:B:2152:ZEX:H7	1.82	0.61
2:H:587:LEU:HD22	12:H:2136:CLA:HBB2	1.81	0.61
12:G:821:CLA:HMD2	15:T:4001:BCR:H24C	1.82	0.61
2:H:15:ASP:HB3	2:H:20:ARG:HB2	1.81	0.60
12:H:2137:CLA:HBC2	23:H:2151:ZEX:H7	1.82	0.60
12:A:821:CLA:HMD2	15:K:4001:BCR:H24C	1.82	0.60
15:U:207:BCR:H393	10:L:132:MET:HB3	1.83	0.60
2:B:587:LEU:HD22	12:B:2137:CLA:HBB2	1.81	0.60
1:G:194:GLU:O	1:G:198:ASN:ND2	2.33	0.60
12:H:2119:CLA:H161	12:H:2126:CLA:H3A	1.84	0.59
8:S:6:SER:HA	8:S:9:SER:HB2	1.84	0.59
6:Q:84:ARG:NH1	6:Q:125:GLU:OE1	2.36	0.59
2:b:425:LEU:HD23	12:b:2102:CLA:H12	1.85	0.59
6:F:84:ARG:NH1	6:F:125:GLU:OE1	2.36	0.59
2:H:425:LEU:HD23	12:H:2102:CLA:H12	1.85	0.59
1:G:67:ASP:HA	1:G:70:ARG:HG3	1.85	0.58
2:b:339:LEU:HB3	2:b:380:LEU:HD13	1.85	0.58
12:b:2119:CLA:H161	12:b:2126:CLA:H3A	1.84	0.58
12:B:2120:CLA:H161	12:B:2127:CLA:H3A	1.84	0.58
8:J:6:SER:HA	8:J:9:SER:HB2	1.84	0.58
1:a:35:ASP:HB3	1:a:38:LEU:HB2	1.86	0.58
2:B:339:LEU:HB3	2:B:380:LEU:HD13	1.85	0.58
1:G:35:ASP:HB3	1:G:38:LEU:HB2	1.86	0.58
10:l:132:MET:HB3	15:L:207:BCR:H393	1.85	0.58
2:B:425:LEU:HD23	12:B:2103:CLA:H12	1.85	0.58
2:b:255:LEU:HD21	2:b:278:LEU:HD23	1.86	0.58
12:b:2115:CLA:HHB	20:b:2143:ECH:H24	1.86	0.58
2:H:255:LEU:HD21	2:H:278:LEU:HD23	1.85	0.58
2:H:339:LEU:HD11	12:H:2106:CLA:H51	1.86	0.58
12:H:2115:CLA:HHB	20:H:2143:ECH:H24	1.86	0.58
8:j:6:SER:HA	8:j:9:SER:HB2	1.84	0.58
2:H:339:LEU:HB3	2:H:380:LEU:HD13	1.85	0.57
2:B:339:LEU:HD11	12:B:2107:CLA:H51	1.86	0.57
12:B:2116:CLA:HHB	20:B:2144:ECH:H24	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:U:132:MET:HB3	15:l:207:BCR:H393	1.85	0.57
1:A:35:ASP:HB3	1:A:38:LEU:HB2	1.86	0.57
2:B:420:LEU:HG	12:B:2139:CLA:HBB1	1.86	0.57
2:b:420:LEU:HG	12:b:2138:CLA:HBB1	1.86	0.57
18:a:852:45D:H381	12:b:2101:CLA:H152	1.87	0.57
1:A:67:ASP:HA	1:A:70:ARG:HG3	1.85	0.57
16:G:848:LHG:H181	16:G:848:LHG:H312	1.86	0.57
1:a:67:ASP:HA	1:a:70:ARG:HG3	1.85	0.57
2:H:420:LEU:HG	12:H:2138:CLA:HBB1	1.86	0.57
2:b:339:LEU:HD11	12:b:2106:CLA:H51	1.86	0.57
16:A:848:LHG:H312	16:A:848:LHG:H181	1.86	0.57
10:U:42:LYS:NZ	24:U:208:SQD:O9	2.38	0.56
2:B:255:LEU:HD21	2:B:278:LEU:HD23	1.85	0.56
16:a:848:LHG:H312	16:a:848:LHG:H181	1.86	0.56
1:A:26:GLU:HA	8:J:3:GLY:HA3	1.87	0.56
10:l:42:LYS:NZ	24:l:208:SQD:O9	2.38	0.56
18:G:852:45D:H381	12:H:2101:CLA:H152	1.86	0.56
2:b:304:ILE:HG22	2:b:308:HIS:HE1	1.71	0.56
1:a:428:ARG:O	1:a:432:HIS:ND1	2.33	0.56
1:G:26:GLU:HA	8:S:3:GLY:HA3	1.87	0.56
1:G:117:VAL:O	1:G:127:ASN:ND2	2.38	0.56
12:H:2128:CLA:H61	15:H:2142:BCR:H23C	1.88	0.56
6:f:84:ARG:NH1	6:f:125:GLU:OE1	2.36	0.56
12:B:2138:CLA:H152	23:F:205:ZEX:H372	1.89	0.55
1:a:117:VAL:O	1:a:127:ASN:ND2	2.38	0.55
2:b:442:VAL:HG22	2:b:447:PRO:HB3	1.89	0.55
12:A:812:CLA:H203	15:A:843:BCR:H12C	1.88	0.55
2:H:442:VAL:HG22	2:H:447:PRO:HB3	1.89	0.55
1:a:26:GLU:HA	8:j:3:GLY:HA3	1.87	0.55
12:B:2129:CLA:H61	15:B:2143:BCR:H23C	1.88	0.55
1:a:418:PRO:HG3	4:d:41:GLU:HB2	1.89	0.55
2:H:465:SER:O	2:H:494:TRP:NE1	2.34	0.55
18:A:852:45D:H381	12:B:2102:CLA:H152	1.87	0.55
2:H:304:ILE:HG22	2:H:308:HIS:HE1	1.71	0.55
1:A:418:PRO:HG3	4:D:41:GLU:HB2	1.89	0.55
12:A:830:CLA:H8	12:L:204:CLA:H141	1.89	0.55
1:G:196:MET:HB2	12:G:812:CLA:HBC2	1.89	0.55
12:a:830:CLA:H8	12:l:204:CLA:H141	1.89	0.55
5:E:9:VAL:HG21	5:E:66:LEU:HD13	1.89	0.55
2:B:304:ILE:HG22	2:B:308:HIS:HE1	1.71	0.55
12:a:812:CLA:H203	15:a:843:BCR:H12C	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:9:VAL:HG21	5:e:66:LEU:HD13	1.89	0.55
2:B:192:GLY:O	2:B:196:HIS:HB2	2.07	0.55
2:B:442:VAL:HG22	2:B:447:PRO:HB3	1.88	0.55
10:L:42:LYS:NZ	24:L:208:SQD:O9	2.38	0.54
12:H:2137:CLA:H152	23:Q:205:ZEX:H372	1.88	0.54
2:b:192:GLY:O	2:b:196:HIS:HB2	2.07	0.54
12:G:812:CLA:H203	15:G:843:BCR:H12C	1.88	0.54
12:b:2137:CLA:H152	23:f:205:ZEX:H372	1.89	0.54
12:b:2128:CLA:H61	15:b:2142:BCR:H23C	1.88	0.54
1:G:418:PRO:HG3	4:O:41:GLU:HB2	1.89	0.54
4:O:84:LYS:HB3	4:O:96:TYR:HE1	1.73	0.54
1:A:196:MET:HB2	12:A:812:CLA:HBC2	1.89	0.54
2:H:224:PRO:HB2	2:H:232:VAL:HG11	1.90	0.54
1:a:99:ASN:HD21	1:a:113:SER:HB3	1.73	0.54
1:A:428:ARG:O	1:A:432:HIS:ND1	2.33	0.54
5:P:9:VAL:HG21	5:P:66:LEU:HD13	1.89	0.54
11:m:31:LYS:HE3	24:m:102:SQD:H4	1.90	0.54
12:G:825:CLA:HAB	15:G:845:BCR:H311	1.90	0.53
5:E:36:PRO:HD2	5:E:62:ALA:HA	1.91	0.53
2:H:192:GLY:O	2:H:196:HIS:HB2	2.07	0.53
1:a:127:ASN:HB3	1:a:135:HIS:HB3	1.90	0.53
1:a:192:ASN:HD22	12:a:811:CLA:HED2	1.74	0.53
8:J:20:THR:HG22	15:J:104:BCR:H17C	1.90	0.53
1:a:196:MET:HB2	12:a:812:CLA:HBC2	1.89	0.53
1:a:326:GLU:O	1:a:329:LYS:NZ	2.42	0.53
16:b:2148:LHG:H261	16:b:2148:LHG:H102	1.91	0.53
1:A:326:GLU:O	1:A:329:LYS:NZ	2.42	0.53
12:G:830:CLA:H8	12:U:204:CLA:H141	1.89	0.53
3:N:27:GLU:HG2	3:N:44:ARG:HH22	1.74	0.53
11:V:31:LYS:HE3	24:V:102:SQD:H4	1.90	0.53
4:D:84:LYS:HB3	4:D:96:TYR:HE1	1.73	0.53
16:H:2148:LHG:H261	16:H:2148:LHG:H102	1.91	0.53
11:M:31:LYS:HE3	24:M:101:SQD:H4	1.91	0.53
12:G:808:CLA:H11	15:S:104:BCR:H363	1.90	0.53
5:e:36:PRO:HD2	5:e:62:ALA:HA	1.90	0.53
7:i:9:TYR:HB2	26:L:210:LMT:H12	1.90	0.53
12:l:201:CLA:H2A	12:l:201:CLA:HED2	1.91	0.53
1:G:326:GLU:O	1:G:329:LYS:NZ	2.42	0.53
1:G:342:GLU:O	1:G:346:THR:OG1	2.23	0.53
12:a:808:CLA:H11	15:j:104:BCR:H363	1.90	0.53
2:B:224:PRO:HB2	2:B:232:VAL:HG11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:VAL:O	1:A:127:ASN:ND2	2.38	0.53
16:B:2149:LHG:H102	16:B:2149:LHG:H261	1.91	0.53
1:G:42:PRO:HB2	1:G:713:ILE:HG12	1.91	0.53
8:j:20:THR:HG22	15:j:104:BCR:H17C	1.90	0.52
4:d:84:LYS:HB3	4:d:96:TYR:HE1	1.73	0.52
12:B:2140:CLA:H143	10:L:91:VAL:HG11	1.92	0.52
12:G:805:CLA:H42	12:G:829:CLA:H51	1.91	0.52
1:a:42:PRO:HB2	1:a:713:ILE:HG12	1.91	0.52
12:a:825:CLA:HAB	15:a:845:BCR:H311	1.91	0.52
1:A:99:ASN:HD21	1:A:113:SER:HB3	1.73	0.52
12:A:805:CLA:H42	12:A:829:CLA:H51	1.91	0.52
1:G:192:ASN:HD22	12:G:811:CLA:HED2	1.74	0.52
2:B:454:GLU:OE2	6:F:52:HIS:ND1	2.42	0.52
2:H:454:GLU:OE2	6:Q:52:HIS:ND1	2.42	0.52
12:b:2139:CLA:H143	10:l:91:VAL:HG11	1.92	0.52
1:G:99:ASN:HD21	1:G:113:SER:HB3	1.73	0.52
5:P:36:PRO:HD2	5:P:62:ALA:HA	1.90	0.52
7:R:9:TYR:HB2	26:l:210:LMT:H12	1.90	0.52
10:U:32:THR:O	10:U:36:ASN:ND2	2.41	0.52
1:A:127:ASN:HB3	1:A:135:HIS:HB3	1.90	0.52
12:A:808:CLA:H11	15:J:104:BCR:H363	1.90	0.52
1:G:428:ARG:NH2	27:U:301:HOH:O	2.43	0.52
5:P:68:LEU:HD11	5:P:70:GLN:HG2	1.92	0.52
2:b:132:ASN:HA	2:b:135:LEU:HD12	1.92	0.52
2:b:454:GLU:OE2	6:f:52:HIS:ND1	2.42	0.52
1:A:192:ASN:HD22	12:A:811:CLA:HED2	1.74	0.52
12:A:825:CLA:HAB	15:A:845:BCR:H311	1.91	0.52
2:b:224:PRO:HB2	2:b:232:VAL:HG11	1.90	0.52
1:A:447:LEU:HB3	1:A:540:PHE:HB2	1.92	0.52
2:B:132:ASN:HA	2:B:135:LEU:HD12	1.92	0.52
3:C:27:GLU:HG2	3:C:44:ARG:HH22	1.74	0.52
2:H:339:LEU:O	2:H:343:THR:OG1	2.25	0.52
2:H:659:MET:HG3	12:H:2104:CLA:NC	2.25	0.52
12:H:2139:CLA:H143	10:U:91:VAL:HG11	1.92	0.52
12:A:835:CLA:H172	16:A:848:LHG:H282	1.92	0.52
2:B:659:MET:HG3	12:B:2105:CLA:NC	2.25	0.52
9:K:72:PHE:HB2	15:K:4001:BCR:H23C	1.92	0.52
12:G:835:CLA:H172	16:G:848:LHG:H282	1.92	0.52
1:a:421:ASN:ND2	27:a:919:HOH:O	2.43	0.51
3:c:27:GLU:HG2	3:c:44:ARG:HH22	1.74	0.51
12:L:201:CLA:H2A	12:L:201:CLA:HED2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:447:LEU:HB3	1:G:540:PHE:HB2	1.92	0.51
1:G:127:ASN:HB3	1:G:135:HIS:HB3	1.90	0.51
8:S:20:THR:HG22	15:S:104:BCR:H17C	1.90	0.51
2:b:659:MET:HG3	12:b:2104:CLA:NC	2.25	0.51
1:a:241:GLU:HA	1:a:244:LEU:HB2	1.92	0.51
2:H:269:TRP:HB2	2:H:272:ASP:HB2	1.92	0.51
12:U:201:CLA:HED2	12:U:201:CLA:H2A	1.91	0.51
2:B:488:ALA:HB2	12:B:2136:CLA:HED3	1.92	0.51
4:D:31:THR:HA	4:D:55:ASN:O	2.11	0.51
12:a:835:CLA:H172	16:a:848:LHG:H282	1.92	0.51
2:b:436:VAL:HG12	12:b:2133:CLA:HAC1	1.93	0.51
1:A:421:ASN:ND2	27:A:919:HOH:O	2.43	0.51
10:L:32:THR:O	10:L:36:ASN:ND2	2.41	0.51
1:G:714:GLN:NE2	5:P:17:TYR:OH	2.44	0.51
2:H:132:ASN:HA	2:H:135:LEU:HD12	1.92	0.51
12:H:2126:CLA:HBB1	12:H:2134:CLA:HAA2	1.92	0.51
26:U:210:LMT:H12	7:I:9:TYR:HB2	1.92	0.51
1:a:369:HIS:ND1	12:a:817:CLA:OBD	2.43	0.51
12:a:803:CLA:HBA2	12:a:810:CLA:H51	1.93	0.51
4:d:31:THR:HA	4:d:55:ASN:O	2.11	0.51
1:A:42:PRO:HB2	1:A:713:ILE:HG12	1.91	0.51
1:A:369:HIS:ND1	12:A:817:CLA:OBD	2.44	0.51
1:A:714:GLN:NE2	5:E:17:TYR:OH	2.44	0.51
1:G:369:HIS:ND1	12:G:817:CLA:OBD	2.44	0.51
1:G:428:ARG:O	1:G:432:HIS:ND1	2.33	0.51
12:a:805:CLA:H42	12:a:829:CLA:H51	1.91	0.51
5:e:68:LEU:HD11	5:e:70:GLN:HG2	1.92	0.51
1:A:428:ARG:NH2	27:L:301:HOH:O	2.43	0.51
1:G:421:ASN:ND2	27:G:919:HOH:O	2.43	0.51
12:G:803:CLA:HBA2	12:G:810:CLA:H51	1.93	0.51
2:H:191:ALA:HA	2:H:194:LEU:HD12	1.93	0.51
1:a:714:GLN:NE2	5:e:17:TYR:OH	2.44	0.51
12:b:2126:CLA:HBB1	12:b:2134:CLA:HAA2	1.92	0.51
10:l:62:ILE:HG13	10:l:138:ALA:HB3	1.93	0.51
1:A:241:GLU:HA	1:A:244:LEU:HB2	1.92	0.51
1:A:342:GLU:O	1:A:346:THR:OG1	2.23	0.51
12:B:2127:CLA:HBB1	12:B:2135:CLA:HAA2	1.92	0.51
10:L:62:ILE:HG13	10:L:138:ALA:HB3	1.93	0.51
1:G:311:TYR:HA	1:G:319:HIS:H	1.77	0.50
1:G:479:GLN:HB2	17:G:847:LMG:H351	1.93	0.50
2:H:488:ALA:HB2	12:H:2135:CLA:HED3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:311:TYR:HA	1:a:319:HIS:H	1.76	0.50
1:a:447:LEU:HB3	1:a:540:PHE:HB2	1.92	0.50
2:b:269:TRP:HB2	2:b:272:ASP:HB2	1.93	0.50
2:b:488:ALA:HB2	12:b:2135:CLA:HED3	1.92	0.50
5:E:68:LEU:HD11	5:E:70:GLN:HG2	1.92	0.50
1:G:241:GLU:HA	1:G:244:LEU:HB2	1.92	0.50
2:H:169:LYS:HB3	2:H:325:ASN:HD21	1.76	0.50
2:H:679:HIS:O	2:H:686:ASN:ND2	2.45	0.50
10:l:32:THR:O	10:l:36:ASN:ND2	2.41	0.50
2:B:436:VAL:HG12	12:B:2134:CLA:HAC1	1.93	0.50
2:B:679:HIS:O	2:B:686:ASN:ND2	2.44	0.50
9:k:72:PHE:HB2	15:k:4001:BCR:H23C	1.92	0.50
12:G:811:CLA:HBB1	12:G:819:CLA:HBC2	1.93	0.50
12:H:2131:CLA:HAB	12:H:2132:CLA:H202	1.94	0.50
10:U:62:ILE:HG13	10:U:138:ALA:HB3	1.93	0.50
12:A:803:CLA:HBD	12:A:810:CLA:H2	1.93	0.50
2:B:313:THR:HG21	16:B:2149:LHG:HC11	1.94	0.50
12:B:2108:CLA:H102	12:B:2108:CLA:H172	1.94	0.50
1:G:362:LEU:HD11	12:G:818:CLA:H71	1.94	0.50
12:Q:201:CLA:H102	8:S:18:LEU:HB2	1.94	0.50
1:A:722:GLN:HB2	16:A:846:LHG:HC5	1.94	0.50
12:F:201:CLA:H102	8:J:18:LEU:HB2	1.94	0.50
2:b:191:ALA:HA	2:b:194:LEU:HD12	1.93	0.50
4:d:6:GLY:HA2	4:d:54:GLU:HB3	1.94	0.50
2:B:169:LYS:HB3	2:B:325:ASN:HD21	1.76	0.50
1:G:120:ILE:HG23	1:G:121:VAL:HG13	1.93	0.50
4:O:31:THR:HA	4:O:55:ASN:O	2.11	0.50
9:T:72:PHE:HB2	15:T:4001:BCR:H23C	1.92	0.50
2:b:169:LYS:HB3	2:b:325:ASN:HD21	1.76	0.50
2:b:679:HIS:O	2:b:686:ASN:ND2	2.45	0.50
12:A:811:CLA:HBB1	12:A:819:CLA:HBC2	1.93	0.50
2:H:436:VAL:HG12	12:H:2133:CLA:HAC1	1.93	0.50
1:a:479:GLN:HB2	17:a:847:LMG:H351	1.93	0.50
12:b:2131:CLA:HAB	12:b:2132:CLA:H202	1.94	0.50
1:A:120:ILE:HG23	1:A:121:VAL:HG13	1.93	0.50
12:G:803:CLA:HBD	12:G:810:CLA:H2	1.93	0.50
1:a:120:ILE:HG23	1:a:121:VAL:HG13	1.93	0.50
1:a:722:GLN:HB2	16:a:846:LHG:HC5	1.94	0.50
12:f:201:CLA:H102	8:j:18:LEU:HB2	1.94	0.50
2:H:605:GLN:NE2	27:H:2220:HOH:O	2.45	0.49
12:a:838:CLA:HAB	12:a:838:CLA:H122	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:LEU:HD11	12:A:818:CLA:H71	1.94	0.49
12:A:803:CLA:HBA2	12:A:810:CLA:H51	1.93	0.49
2:H:545:PRO:HB3	6:Q:142:PRO:HG2	1.94	0.49
12:H:2107:CLA:H102	12:H:2107:CLA:H172	1.94	0.49
10:U:47:ILE:HD13	10:l:47:ILE:HD13	1.94	0.49
1:a:362:LEU:HD11	12:a:818:CLA:H71	1.94	0.49
2:b:545:PRO:HB3	6:f:142:PRO:HG2	1.94	0.49
2:B:120:VAL:HG13	2:B:121:TYR:HD1	1.78	0.49
2:B:191:ALA:HA	2:B:194:LEU:HD12	1.93	0.49
2:B:269:TRP:HB2	2:B:272:ASP:HB2	1.93	0.49
1:a:523:MET:HE1	1:a:627:VAL:HG11	1.94	0.49
12:a:811:CLA:HBB1	12:a:819:CLA:HBC2	1.93	0.49
1:A:479:GLN:HB2	17:A:847:LMG:H351	1.93	0.49
12:A:827:CLA:H161	15:J:101:BCR:H14C	1.95	0.49
1:G:217:ILE:HD11	1:G:275:LEU:HD21	1.94	0.49
12:G:838:CLA:H122	12:G:838:CLA:HAB	1.94	0.49
12:a:803:CLA:HBD	12:a:810:CLA:H2	1.93	0.49
12:a:827:CLA:H161	15:j:101:BCR:H14C	1.95	0.49
2:b:120:VAL:HG13	2:b:121:TYR:HD1	1.78	0.49
1:A:311:TYR:HA	1:A:319:HIS:H	1.76	0.49
2:B:291:TYR:OH	12:B:2121:CLA:O1D	2.31	0.49
2:H:291:TYR:OH	12:H:2120:CLA:O1D	2.31	0.49
1:A:98:SER:OG	1:A:99:ASN:N	2.46	0.49
4:D:61:ARG:NH2	4:D:63:GLU:OE1	2.45	0.49
2:H:120:VAL:HG13	2:H:121:TYR:HD1	1.77	0.49
1:a:46:THR:O	1:a:50:ASN:N	2.45	0.49
17:a:847:LMG:H352	17:a:847:LMG:HC92	1.94	0.49
1:A:523:MET:HE1	1:A:627:VAL:HG11	1.94	0.49
2:B:545:PRO:HB3	6:F:142:PRO:HG2	1.94	0.49
12:A:806:CLA:HMB2	15:J:101:BCR:H23C	1.95	0.49
12:A:838:CLA:HAB	12:A:838:CLA:H122	1.94	0.49
12:B:2132:CLA:HAB	12:B:2133:CLA:H202	1.94	0.49
12:G:827:CLA:H161	15:S:101:BCR:H14C	1.95	0.49
4:O:107:LYS:O	4:O:112:ARG:NH1	2.40	0.49
10:U:141:LEU:HD11	12:B:2112:CLA:H122	1.94	0.49
2:b:15:ASP:OD2	2:b:19:ARG:NH1	2.46	0.49
1:G:523:MET:HE1	1:G:627:VAL:HG11	1.94	0.49
2:H:309:LYS:H	12:H:2141:CLA:HBC2	1.78	0.49
1:G:722:GLN:HB2	16:G:846:LHG:HC5	1.94	0.49
2:b:86:PRO:HB3	2:b:121:TYR:CG	2.48	0.49
12:b:2107:CLA:H102	12:b:2107:CLA:H172	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:605:GLN:NE2	27:B:2220:HOH:O	2.45	0.49
4:D:101:ASP:OD2	4:D:109:ASN:ND2	2.43	0.49
2:H:86:PRO:HB3	2:H:121:TYR:CG	2.48	0.48
2:H:225:PHE:HA	2:H:230:TRP:HD1	1.78	0.48
1:a:217:ILE:HD11	1:a:275:LEU:HD21	1.94	0.48
12:a:811:CLA:HAB	12:a:819:CLA:H71	1.95	0.48
2:b:465:SER:O	2:b:494:TRP:NE1	2.34	0.48
12:A:811:CLA:HAB	12:A:819:CLA:H71	1.95	0.48
2:H:15:ASP:OD2	2:H:19:ARG:NH1	2.46	0.48
2:H:313:THR:HG21	16:H:2148:LHG:HC11	1.94	0.48
4:O:101:ASP:OD2	4:O:109:ASN:ND2	2.43	0.48
1:a:428:ARG:NH2	27:l:301:HOH:O	2.43	0.48
2:b:313:THR:HG21	16:b:2148:LHG:HC11	1.94	0.48
1:A:217:ILE:HD11	1:A:275:LEU:HD21	1.94	0.48
2:B:309:LYS:H	12:B:2142:CLA:HBC2	1.78	0.48
4:D:6:GLY:HA2	4:D:54:GLU:HB3	1.93	0.48
20:V:101:ECH:H40	24:V:102:SQD:H192	1.96	0.48
2:b:225:PHE:HA	2:b:230:TRP:HD1	1.78	0.48
2:b:309:LYS:H	12:b:2141:CLA:HBC2	1.78	0.48
17:A:847:LMG:H352	17:A:847:LMG:HC92	1.94	0.48
12:B:2105:CLA:H192	15:B:2146:BCR:H353	1.95	0.48
4:O:6:GLY:HA2	4:O:54:GLU:HB3	1.94	0.48
12:U:205:CLA:H122	12:B:2112:CLA:H203	1.96	0.48
2:b:393:VAL:HG23	2:b:538:ALA:HB1	1.95	0.48
2:b:605:GLN:NE2	27:b:2220:HOH:O	2.45	0.48
2:B:15:ASP:OD2	2:B:19:ARG:NH1	2.46	0.48
12:G:817:CLA:HBA2	12:G:817:CLA:H3A	1.56	0.48
17:G:847:LMG:HC92	17:G:847:LMG:H352	1.94	0.48
12:H:2111:CLA:H122	10:l:141:LEU:HD11	1.96	0.48
10:U:47:ILE:HD13	10:L:47:ILE:HD13	1.94	0.48
12:a:806:CLA:HMB2	15:j:101:BCR:H23C	1.95	0.48
10:l:47:ILE:HD13	10:L:47:ILE:HD13	1.95	0.48
1:A:46:THR:O	1:A:50:ASN:N	2.45	0.48
5:E:12:LYS:HG3	5:E:67:GLU:HG3	1.96	0.48
12:a:811:CLA:H3A	12:a:811:CLA:HBA2	1.61	0.48
2:b:291:TYR:OH	12:b:2120:CLA:O1D	2.31	0.48
4:d:65:CYS:HB3	4:d:85:ILE:HG12	1.96	0.48
5:e:12:LYS:HG3	5:e:67:GLU:HG3	1.96	0.48
12:A:805:CLA:H41	12:A:805:CLA:H62	1.63	0.48
12:A:812:CLA:H143	15:A:843:BCR:H10C	1.95	0.48
2:B:411:GLU:OE1	6:F:143:ARG:NH1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:486:VAL:HG21	12:a:835:CLA:H11	1.96	0.48
2:B:61:THR:HG21	12:B:2129:CLA:H42	1.96	0.48
1:G:70:ARG:HD3	1:G:184:ALA:HB1	1.96	0.48
1:G:388:SER:HB3	12:G:827:CLA:HMA1	1.96	0.48
2:H:61:THR:HG21	12:H:2128:CLA:H42	1.96	0.48
12:H:2136:CLA:HMB2	12:H:2138:CLA:HED1	1.96	0.48
5:P:12:LYS:HG3	5:P:67:GLU:HG3	1.96	0.48
2:b:61:THR:HG21	12:b:2128:CLA:H42	1.96	0.48
1:A:486:VAL:HG21	12:A:835:CLA:H11	1.96	0.48
12:B:2137:CLA:HMB2	12:B:2139:CLA:HED1	1.96	0.48
12:G:811:CLA:HAB	12:G:819:CLA:H71	1.95	0.48
12:H:2104:CLA:H192	15:H:2145:BCR:H353	1.95	0.48
12:H:2120:CLA:H72	12:H:2124:CLA:H142	1.95	0.48
12:b:2120:CLA:H72	12:b:2124:CLA:H142	1.96	0.48
2:B:465:SER:O	2:B:494:TRP:NE1	2.34	0.48
2:H:393:VAL:HG23	2:H:538:ALA:HB1	1.95	0.48
12:a:839:CLA:H161	8:j:23:ALA:HB2	1.96	0.48
12:b:2104:CLA:H192	15:b:2145:BCR:H353	1.95	0.48
12:b:2141:CLA:HMB3	15:b:2146:BCR:H11C	1.96	0.48
2:b:411:GLU:OE1	6:f:143:ARG:NH1	2.47	0.47
6:f:56:ASP:OD2	6:f:58:ARG:NH1	2.47	0.47
10:l:96:LEU:HD21	15:l:206:BCR:H383	1.96	0.47
20:m:101:ECH:H40	24:m:102:SQD:H192	1.96	0.47
10:L:96:LEU:HD21	15:L:206:BCR:H383	1.96	0.47
12:G:806:CLA:HMB2	15:S:101:BCR:H23C	1.95	0.47
2:H:411:GLU:OE1	6:Q:143:ARG:NH1	2.47	0.47
2:B:69:ALA:HB2	2:B:135:LEU:HB2	1.96	0.47
2:B:86:PRO:HB3	2:B:121:TYR:CG	2.48	0.47
12:B:2121:CLA:H72	12:B:2125:CLA:H142	1.96	0.47
1:G:98:SER:OG	1:G:99:ASN:N	2.46	0.47
1:a:225:LYS:HE3	1:a:252:LEU:HB3	1.96	0.47
12:a:812:CLA:H143	15:a:843:BCR:H10C	1.95	0.47
12:B:2129:CLA:H8	15:B:2143:BCR:H21C	1.96	0.47
1:G:225:LYS:HE3	1:G:252:LEU:HB3	1.96	0.47
12:G:812:CLA:HBA1	12:G:812:CLA:H3A	1.72	0.47
2:H:69:ALA:HB2	2:H:135:LEU:HB2	1.96	0.47
12:b:2128:CLA:H8	15:b:2142:BCR:H21C	1.96	0.47
1:A:225:LYS:HE3	1:A:252:LEU:HB3	1.96	0.47
1:A:388:SER:HB3	12:A:827:CLA:HMA1	1.96	0.47
12:B:2136:CLA:HBA1	12:B:2136:CLA:H3A	1.55	0.47
1:G:46:THR:O	1:G:50:ASN:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:486:VAL:HG21	12:G:835:CLA:H11	1.96	0.47
4:O:34:SER:OG	4:O:36:SER:O	2.32	0.47
1:a:342:GLU:O	1:a:346:THR:OG1	2.23	0.47
2:b:69:ALA:HB2	2:b:135:LEU:HB2	1.96	0.47
4:D:65:CYS:HB3	4:D:85:ILE:HG12	1.96	0.47
12:H:2141:CLA:HMB3	15:H:2146:BCR:H11C	1.96	0.47
4:O:65:CYS:HB3	4:O:85:ILE:HG12	1.96	0.47
10:U:96:LEU:HD21	15:U:206:BCR:H383	1.96	0.47
1:A:266:LEU:HD22	9:K:81:VAL:HG21	1.96	0.47
2:B:430:HIS:HB3	23:B:2152:ZEX:H163	1.96	0.47
4:D:34:SER:OG	4:D:36:SER:O	2.32	0.47
1:G:90:MET:HE1	12:G:807:CLA:H2A	1.96	0.47
1:G:266:LEU:HD22	9:T:81:VAL:HG21	1.96	0.47
12:H:2118:CLA:HAC1	12:H:2119:CLA:H191	1.96	0.47
12:H:2128:CLA:H8	15:H:2142:BCR:H21C	1.97	0.47
8:S:12:PRO:HA	8:S:15:ILE:HG22	1.96	0.47
1:a:70:ARG:HD3	1:a:184:ALA:HB1	1.96	0.47
1:a:266:LEU:HD22	9:k:81:VAL:HG21	1.96	0.47
3:c:73:THR:H	3:c:76:SER:HG	1.62	0.47
4:d:34:SER:OG	4:d:36:SER:O	2.32	0.47
8:j:12:PRO:HA	8:j:15:ILE:HG22	1.96	0.47
1:A:70:ARG:HD3	1:A:184:ALA:HB1	1.96	0.47
12:A:818:CLA:H92	12:A:828:CLA:H91	1.96	0.47
12:A:826:CLA:H151	12:A:833:CLA:H8	1.97	0.47
2:B:393:VAL:HG23	2:B:538:ALA:HB1	1.95	0.47
2:B:455:PRO:HG3	2:B:514:PHE:HB2	1.97	0.47
2:H:430:HIS:HB3	23:H:2151:ZEX:H163	1.96	0.47
1:a:98:SER:OG	1:a:99:ASN:N	2.46	0.47
12:b:2122:CLA:HMA1	12:b:2141:CLA:HAC2	1.97	0.47
12:A:839:CLA:H161	8:J:23:ALA:HB2	1.96	0.47
2:B:339:LEU:O	2:B:343:THR:OG1	2.25	0.47
12:B:2123:CLA:HMA1	12:B:2142:CLA:HAC2	1.97	0.47
3:C:36:ALA:HB1	3:C:38:GLN:HE21	1.79	0.47
12:L:205:CLA:HBA1	12:L:205:CLA:H3A	1.67	0.47
1:a:388:SER:HB3	12:a:827:CLA:HMA1	1.96	0.47
12:a:826:CLA:H151	12:a:833:CLA:H8	1.97	0.47
2:b:430:HIS:HB3	23:b:2151:ZEX:H163	1.96	0.47
2:b:455:PRO:HG3	2:b:514:PHE:HB2	1.97	0.47
2:b:638:ASN:ND2	27:b:2224:HOH:O	2.48	0.47
12:b:2101:CLA:H62	12:b:2101:CLA:H101	1.65	0.47
2:B:225:PHE:HA	2:B:230:TRP:HD1	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:438:SER:HB2	2:H:678:ALA:HB2	1.97	0.47
12:G:818:CLA:H92	12:G:828:CLA:H91	1.96	0.47
3:N:36:ALA:HB1	3:N:38:GLN:HE21	1.80	0.47
3:c:36:ALA:HB1	3:c:38:GLN:HE21	1.79	0.47
12:B:2142:CLA:HMB3	15:B:2147:BCR:H11C	1.96	0.47
12:G:839:CLA:H161	8:S:23:ALA:HB2	1.96	0.46
1:A:90:MET:HE1	12:A:807:CLA:H2A	1.97	0.46
12:A:817:CLA:H3A	12:A:817:CLA:HBA2	1.56	0.46
1:G:332:PHE:O	1:G:428:ARG:NH1	2.48	0.46
12:G:812:CLA:H143	15:G:843:BCR:H10C	1.95	0.46
12:G:826:CLA:H151	12:G:833:CLA:H8	1.97	0.46
1:a:687:PHE:O	2:b:574:TYR:OH	2.32	0.46
3:C:73:THR:H	3:C:76:SER:HG	1.60	0.46
15:F:202:BCR:H20C	15:F:202:BCR:H361	1.80	0.46
2:b:312:LEU:HG	16:b:2148:LHG:HC61	1.97	0.46
12:b:2108:CLA:H191	12:b:2127:CLA:H191	1.98	0.46
4:d:61:ARG:NH2	4:d:63:GLU:OE1	2.45	0.46
1:G:111:LYS:HB2	1:G:111:LYS:HE3	1.66	0.46
6:Q:81:TRP:O	6:Q:85:SER:OG	2.31	0.46
15:S:104:BCR:H20C	15:S:104:BCR:H361	1.77	0.46
2:b:222:LEU:O	2:b:225:PHE:HB3	2.16	0.46
12:b:2120:CLA:HBA2	12:b:2120:CLA:H3A	1.62	0.46
1:A:332:PHE:O	1:A:428:ARG:NH1	2.48	0.46
8:J:12:PRO:HA	8:J:15:ILE:HG22	1.96	0.46
1:G:400:LEU:HD21	12:G:805:CLA:H142	1.98	0.46
1:G:456:ILE:HG22	12:U:201:CLA:HBC2	1.98	0.46
2:H:177:HIS:HE1	12:H:2113:CLA:C1D	2.29	0.46
1:a:238:LEU:HD12	1:a:238:LEU:HA	1.85	0.46
1:a:400:LEU:HD21	12:a:805:CLA:H142	1.98	0.46
1:a:437:ILE:HG13	1:a:555:TYR:HE1	1.80	0.46
12:a:818:CLA:H92	12:a:828:CLA:H91	1.96	0.46
17:a:847:LMG:H291	17:a:847:LMG:H341	1.98	0.46
12:b:2111:CLA:H122	10:L:141:LEU:HD11	1.96	0.46
12:b:2111:CLA:H203	12:L:205:CLA:H122	1.98	0.46
4:d:101:ASP:OD2	4:d:109:ASN:ND2	2.43	0.46
1:A:438:SER:HB2	2:B:678:ALA:HB2	1.97	0.46
12:B:2119:CLA:HAC1	12:B:2120:CLA:H191	1.96	0.46
6:F:56:ASP:OD2	6:F:58:ARG:NH1	2.47	0.46
12:J:102:CLA:H3A	12:J:102:CLA:HBA2	1.73	0.46
1:G:451:SER:HB2	1:G:537:ILE:HG12	1.98	0.46
1:G:671:MET:HA	1:G:674:ALA:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:b:2118:CLA:HAC1	12:b:2119:CLA:H191	1.96	0.46
17:A:847:LMG:H291	17:A:847:LMG:H341	1.98	0.46
2:H:638:ASN:ND2	27:H:2224:HOH:O	2.48	0.46
6:Q:56:ASP:OD2	6:Q:58:ARG:NH1	2.47	0.46
1:a:671:MET:HA	1:a:674:ALA:HB3	1.97	0.46
2:b:387:HIS:HA	2:b:390:ILE:HD12	1.98	0.46
1:A:451:SER:HB2	1:A:537:ILE:HG12	1.98	0.46
2:B:222:LEU:O	2:B:225:PHE:HB3	2.16	0.46
24:M:101:SQD:H192	20:M:103:ECH:H40	1.97	0.46
12:H:2131:CLA:H91	6:Q:122:ALA:HB1	1.98	0.46
12:a:820:CLA:H61	15:a:844:BCR:H352	1.98	0.46
12:a:851:CLA:H192	10:l:61:LEU:HD21	1.98	0.46
12:b:2106:CLA:HBA1	12:b:2106:CLA:H3A	1.63	0.46
1:A:400:LEU:HD21	12:A:805:CLA:H142	1.98	0.46
2:B:177:HIS:HE1	12:B:2114:CLA:C1D	2.29	0.46
12:B:2109:CLA:H191	12:B:2128:CLA:H191	1.98	0.46
17:G:847:LMG:HC71	17:G:847:LMG:HC2	1.64	0.46
12:H:2114:CLA:H62	12:H:2114:CLA:H2	1.75	0.46
12:H:2122:CLA:HMA1	12:H:2141:CLA:HAC2	1.97	0.46
1:a:332:PHE:O	1:a:428:ARG:NH1	2.48	0.46
1:A:111:LYS:HE3	1:A:111:LYS:HB2	1.66	0.46
1:A:456:ILE:HG22	12:L:201:CLA:HBC2	1.98	0.46
12:B:2108:CLA:H72	12:B:2108:CLA:H111	1.64	0.46
1:G:437:ILE:HG13	1:G:555:TYR:HE1	1.80	0.46
2:H:312:LEU:HG	16:H:2148:LHG:HC61	1.97	0.46
2:H:387:HIS:HA	2:H:390:ILE:HD12	1.98	0.46
12:H:2128:CLA:H192	20:H:2143:ECH:H36A	1.98	0.46
12:a:824:CLA:H42	12:a:828:CLA:H193	1.98	0.46
12:b:2125:CLA:C2B	12:b:2138:CLA:H3A	2.46	0.46
12:b:2128:CLA:H192	20:b:2143:ECH:H36A	1.98	0.46
12:b:2132:CLA:H62	12:b:2132:CLA:H2	1.74	0.46
12:G:824:CLA:H42	12:G:828:CLA:H193	1.98	0.45
2:H:438:ASN:ND2	2:H:611:THR:OG1	2.49	0.45
12:H:2128:CLA:H3A	12:H:2128:CLA:HBA2	1.74	0.45
1:a:438:SER:HB2	2:b:678:ALA:HB2	1.97	0.45
12:b:2116:CLA:HBA2	12:b:2116:CLA:H3A	1.49	0.45
1:A:440:LEU:HG	1:A:547:LEU:HB2	1.98	0.45
2:B:638:ASN:ND2	27:B:2224:HOH:O	2.48	0.45
1:a:456:ILE:HG22	12:l:201:CLA:HBC2	1.98	0.45
1:a:744:LEU:HD23	1:a:744:LEU:HA	1.75	0.45
2:b:438:ASN:ND2	2:b:611:THR:OG1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:j:102:CLA:H3A	12:j:102:CLA:HBA2	1.73	0.45
3:C:26:LEU:HA	3:C:41:SER:O	2.16	0.45
2:H:455:PRO:HG3	2:H:514:PHE:HB2	1.97	0.45
2:B:422:TRP:HZ3	12:B:2139:CLA:HBC2	1.82	0.45
12:B:2111:CLA:H202	12:B:2111:CLA:H161	1.81	0.45
12:B:2115:CLA:H2	12:B:2115:CLA:H62	1.75	0.45
4:D:107:LYS:O	4:D:112:ARG:NH1	2.40	0.45
1:G:661:TYR:HD2	2:H:442:VAL:HG12	1.81	0.45
12:A:824:CLA:H42	12:A:828:CLA:H193	1.98	0.45
12:G:820:CLA:H193	12:G:823:CLA:HAC2	1.99	0.45
17:G:849:LMG:HC91	17:G:849:LMG:H312	1.99	0.45
2:H:422:TRP:HZ3	12:H:2138:CLA:HBC2	1.82	0.45
3:N:26:LEU:HA	3:N:41:SER:O	2.16	0.45
12:U:205:CLA:H203	12:U:205:CLA:H162	1.84	0.45
1:a:451:SER:HB2	1:a:537:ILE:HG12	1.98	0.45
1:a:458:ASN:HD22	1:a:640:ILE:HB	1.82	0.45
12:b:2124:CLA:H143	12:b:2124:CLA:H162	1.87	0.45
2:B:411:GLU:HA	6:F:143:ARG:HG2	1.99	0.45
2:B:438:ASN:ND2	2:B:611:THR:OG1	2.49	0.45
12:B:2126:CLA:C2B	12:B:2139:CLA:H3A	2.46	0.45
1:G:440:LEU:HG	1:G:547:LEU:HB2	1.99	0.45
12:G:804:CLA:HBA1	12:G:804:CLA:H3A	1.60	0.45
12:G:830:CLA:H93	16:G:848:LHG:H272	1.99	0.45
17:G:847:LMG:H291	17:G:847:LMG:H341	1.98	0.45
12:H:2111:CLA:H203	12:l:205:CLA:H122	1.98	0.45
1:a:90:MET:HE1	12:a:807:CLA:H2A	1.96	0.45
2:b:177:HIS:HE1	12:b:2113:CLA:C1D	2.29	0.45
10:l:53:VAL:O	10:l:57:HIS:ND1	2.46	0.45
1:A:500:ASN:HB2	12:A:834:CLA:HED2	1.99	0.45
1:A:661:TYR:HD2	2:B:442:VAL:HG12	1.81	0.45
1:A:671:MET:HA	1:A:674:ALA:HB3	1.97	0.45
12:A:851:CLA:H192	10:L:61:LEU:HD21	1.98	0.45
1:G:121:VAL:HG12	8:S:30:ASN:HD22	1.82	0.45
1:G:351:GLN:NE2	27:G:925:HOH:O	2.50	0.45
12:H:2108:CLA:H191	12:H:2127:CLA:H191	1.98	0.45
15:Q:202:BCR:H20C	15:Q:202:BCR:H361	1.81	0.45
1:a:121:VAL:HG12	8:j:30:ASN:HD22	1.82	0.45
1:a:539:ALA:O	1:a:543:HIS:ND1	2.44	0.45
12:b:2104:CLA:H111	15:b:2145:BCR:H362	1.99	0.45
12:b:2128:CLA:H43	15:b:2142:BCR:H392	1.99	0.45
3:c:26:LEU:HA	3:c:41:SER:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:PHE:HB3	1:A:249:MET:HE1	1.99	0.45
12:A:819:CLA:H102	12:A:819:CLA:H61	1.58	0.45
17:A:849:LMG:H312	17:A:849:LMG:HC91	1.99	0.45
15:J:104:BCR:H20C	15:J:104:BCR:H361	1.77	0.45
2:H:222:LEU:O	2:H:225:PHE:HB3	2.16	0.45
12:H:2112:CLA:H203	20:H:2143:ECH:H35B	1.99	0.45
12:H:2125:CLA:C2B	12:H:2138:CLA:H3A	2.46	0.45
12:H:2127:CLA:H152	12:H:2129:CLA:H152	1.98	0.45
4:O:61:ARG:NH2	4:O:63:GLU:OE1	2.45	0.45
12:U:203:CLA:H3A	12:U:203:CLA:HBA2	1.50	0.45
1:a:351:GLN:NE2	27:a:925:HOH:O	2.50	0.45
2:b:422:TRP:HZ3	12:b:2138:CLA:HBC2	1.82	0.45
12:f:201:CLA:H61	12:f:201:CLA:H41	1.72	0.45
12:l:203:CLA:HBA2	12:l:203:CLA:H3A	1.50	0.45
12:A:807:CLA:H3A	12:A:807:CLA:HBA2	1.61	0.45
2:B:312:LEU:HG	16:B:2149:LHG:HC61	1.97	0.45
12:B:2129:CLA:H192	20:B:2144:ECH:H36A	1.98	0.45
10:L:36:ASN:HB3	12:L:203:CLA:HAC1	1.99	0.45
1:a:440:LEU:HG	1:a:547:LEU:HB2	1.98	0.45
12:a:820:CLA:H193	12:a:823:CLA:HAC2	1.99	0.45
12:a:830:CLA:H93	16:a:848:LHG:H272	1.99	0.45
17:a:847:LMG:HC71	17:a:847:LMG:HC2	1.64	0.45
2:b:255:LEU:HD11	12:b:2116:CLA:HBC1	1.99	0.45
12:B:2120:CLA:HBA2	12:B:2120:CLA:H3A	1.61	0.45
12:B:2128:CLA:H152	12:B:2130:CLA:H152	1.98	0.45
12:G:820:CLA:H61	15:G:844:BCR:H352	1.98	0.45
16:G:848:LHG:H261	16:G:848:LHG:H121	1.99	0.45
2:H:256:THR:HA	12:H:2117:CLA:HED1	1.99	0.45
2:H:292:ARG:NE	2:H:298:GLY:O	2.46	0.45
10:U:36:ASN:HB3	12:U:203:CLA:HAC1	1.99	0.45
1:a:500:ASN:HB2	12:a:834:CLA:HED2	1.99	0.45
12:a:807:CLA:H3A	12:a:807:CLA:HBA2	1.61	0.45
12:a:823:CLA:HBB2	16:a:848:LHG:HC82	1.99	0.45
4:d:107:LYS:O	4:d:112:ARG:NH1	2.40	0.45
1:A:351:GLN:NE2	27:A:925:HOH:O	2.49	0.45
12:A:830:CLA:H93	16:A:848:LHG:H272	1.99	0.45
12:B:2107:CLA:H3A	12:B:2107:CLA:HBA1	1.63	0.45
12:B:2113:CLA:H203	20:B:2144:ECH:H35B	1.99	0.45
12:B:2128:CLA:H3A	12:B:2128:CLA:HBA2	1.65	0.45
12:B:2129:CLA:H43	15:B:2143:BCR:H392	1.99	0.45
12:B:2132:CLA:H91	6:F:122:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:31:THR:O	4:D:83:TYR:HA	2.17	0.45
15:L:207:BCR:H20C	15:L:207:BCR:H361	1.75	0.45
1:G:87:LEU:HD23	1:G:87:LEU:HA	1.88	0.44
1:G:249:MET:O	1:G:253:TYR:N	2.50	0.44
12:H:2107:CLA:H72	12:H:2107:CLA:H111	1.64	0.44
12:H:2128:CLA:H43	15:H:2142:BCR:H392	1.99	0.44
10:U:136:PHE:CE2	15:l:207:BCR:H391	2.52	0.44
1:A:121:VAL:HG12	8:J:30:ASN:HD22	1.82	0.44
1:A:458:ASN:HD22	1:A:640:ILE:HB	1.82	0.44
2:B:256:THR:HA	12:B:2118:CLA:HED1	1.99	0.44
2:B:387:HIS:HA	2:B:390:ILE:HD12	1.98	0.44
1:a:111:LYS:HE3	1:a:111:LYS:HB2	1.66	0.44
16:a:848:LHG:H261	16:a:848:LHG:H121	1.99	0.44
12:b:2119:CLA:H62	12:b:2119:CLA:H41	1.68	0.44
1:A:437:ILE:HG13	1:A:555:TYR:HE1	1.80	0.44
12:A:820:CLA:H193	12:A:823:CLA:HAC2	1.99	0.44
12:A:820:CLA:H61	15:A:844:BCR:H352	1.98	0.44
12:B:2124:CLA:HHB	12:B:2142:CLA:HAB	2.00	0.44
12:G:805:CLA:H12	12:G:805:CLA:HBA2	1.76	0.44
12:G:851:CLA:H192	10:U:61:LEU:HD21	1.98	0.44
12:G:851:CLA:HMC2	12:H:2139:CLA:H11	2.00	0.44
12:H:2152:CLA:HBA1	16:V:103:LHG:H122	2.00	0.44
8:S:14:MET:HE3	8:S:14:MET:HB3	1.88	0.44
1:a:355:ASN:ND2	12:a:804:CLA:OBD	2.45	0.44
2:b:256:THR:HA	12:b:2117:CLA:HED1	1.99	0.44
12:b:2108:CLA:H71	15:i:101:BCR:HC32	2.00	0.44
12:b:2127:CLA:H3A	12:b:2127:CLA:HBA2	1.65	0.44
12:b:2131:CLA:H91	6:f:122:ALA:HB1	1.98	0.44
9:k:55:LEU:HD21	9:k:58:LYS:HB3	1.99	0.44
12:L:205:CLA:H203	12:L:205:CLA:H162	1.84	0.44
1:G:458:ASN:HD22	1:G:640:ILE:HB	1.82	0.44
12:b:2127:CLA:H152	12:b:2129:CLA:H152	1.98	0.44
12:A:812:CLA:HBA1	12:A:812:CLA:H3A	1.72	0.44
12:B:2120:CLA:H41	12:B:2120:CLA:H62	1.68	0.44
9:K:55:LEU:HD21	9:K:58:LYS:HB3	1.99	0.44
1:G:500:ASN:HB2	12:G:834:CLA:HED2	1.99	0.44
24:U:208:SQD:H241	7:I:29:LEU:HB3	2.00	0.44
12:B:2102:CLA:H101	12:B:2102:CLA:H62	1.65	0.44
1:G:242:PHE:HB3	1:G:249:MET:HE1	1.99	0.44
2:H:411:GLU:HA	6:Q:143:ARG:HG2	1.99	0.44
4:O:24:ARG:NH1	4:O:25:GLU:OE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:31:THR:O	4:O:83:TYR:HA	2.17	0.44
2:b:167:TRP:CE3	12:b:2114:CLA:HAC2	2.53	0.44
4:d:75:LYS:HA	4:d:75:LYS:HD3	1.87	0.44
10:l:136:PHE:CE2	15:L:207:BCR:H391	2.53	0.44
12:l:205:CLA:H141	12:l:205:CLA:H162	1.85	0.44
12:A:804:CLA:H172	15:A:842:BCR:HC8	2.00	0.44
2:B:381:MET:HE3	2:B:381:MET:HB3	1.85	0.44
12:B:2105:CLA:H111	15:B:2146:BCR:H362	1.99	0.44
12:B:2109:CLA:H71	15:I:101:BCR:HC32	2.00	0.44
6:F:81:TRP:O	6:F:85:SER:OG	2.31	0.44
12:G:804:CLA:H172	15:G:842:BCR:HC8	2.00	0.44
12:G:818:CLA:H203	12:G:826:CLA:HAA1	2.00	0.44
2:H:167:TRP:CE3	12:H:2114:CLA:HAC2	2.53	0.44
12:H:2130:CLA:H3A	12:H:2131:CLA:OBD	2.18	0.44
7:R:25:VAL:HG22	12:l:203:CLA:H111	2.00	0.44
1:a:187:LEU:HB3	1:a:191:GLN:HE22	1.83	0.44
1:a:242:PHE:HB3	1:a:249:MET:HE1	1.99	0.44
1:a:661:TYR:HD2	2:b:442:VAL:HG12	1.81	0.44
12:a:804:CLA:H3A	12:a:804:CLA:HBA1	1.60	0.44
12:b:2130:CLA:H3A	12:b:2131:CLA:OBD	2.17	0.44
16:m:103:LHG:H292	12:A:830:CLA:H72	2.00	0.44
12:A:818:CLA:H203	12:A:826:CLA:HAA1	2.00	0.44
12:A:851:CLA:HMC2	12:B:2140:CLA:H11	2.00	0.44
2:B:167:TRP:CE3	12:B:2115:CLA:HAC2	2.53	0.44
2:B:255:LEU:HD11	12:B:2117:CLA:HBC1	1.99	0.44
12:G:829:CLA:HED2	12:G:829:CLA:H2A	2.00	0.44
12:G:832:CLA:H141	12:G:832:CLA:H162	1.83	0.44
5:P:30:LYS:HA	5:P:30:LYS:HD2	1.76	0.44
12:S:102:CLA:H3A	12:S:102:CLA:HBA2	1.73	0.44
2:b:4:LYS:NZ	11:m:30:TYR:OH	2.47	0.44
2:b:547:LYS:HB2	2:b:547:LYS:HE3	1.74	0.44
12:b:2131:CLA:HBC2	12:b:2138:CLA:HMC2	2.00	0.44
16:A:848:LHG:H261	16:A:848:LHG:H121	1.99	0.44
2:B:413:LYS:HA	2:B:416:LEU:HD12	2.00	0.44
12:B:2131:CLA:H3A	12:B:2132:CLA:OBD	2.18	0.44
11:M:30:TYR:HD1	24:M:101:SQD:H441	1.82	0.44
12:G:817:CLA:H102	12:G:834:CLA:HAA2	2.00	0.44
12:G:830:CLA:H72	16:M:102:LHG:H292	2.00	0.44
12:H:2106:CLA:HBA1	12:H:2106:CLA:H3A	1.63	0.44
9:T:55:LEU:HD21	9:T:58:LYS:HB3	1.99	0.44
1:a:374:PRO:HA	1:a:375:PRO:HD3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:a:803:CLA:HAB	12:a:807:CLA:H202	2.00	0.44
12:a:804:CLA:H172	15:a:842:BCR:HC8	2.00	0.44
2:b:411:GLU:HA	6:f:143:ARG:HG2	1.99	0.44
12:b:2112:CLA:H203	20:b:2143:ECH:H35B	1.99	0.44
12:b:2124:CLA:H142	12:b:2124:CLA:H112	1.88	0.44
12:A:807:CLA:H143	16:A:846:LHG:H223	2.00	0.44
12:A:823:CLA:HBB2	16:A:848:LHG:HC82	1.99	0.44
12:A:829:CLA:H2A	12:A:829:CLA:HED2	2.00	0.44
2:B:111:ASN:HD22	7:I:3:GLY:HA2	1.83	0.44
1:G:391:THR:HG22	1:G:606:ILE:HB	2.00	0.43
1:G:658:ILE:HD12	2:H:618:ARG:HG3	1.99	0.43
12:G:819:CLA:H61	12:G:819:CLA:H102	1.58	0.43
12:H:2104:CLA:H111	15:H:2145:BCR:H362	1.99	0.43
12:H:2127:CLA:H3A	12:H:2127:CLA:HBA2	1.65	0.43
12:a:817:CLA:H102	12:a:834:CLA:HAA2	2.00	0.43
7:i:25:VAL:HG22	12:L:203:CLA:H111	2.00	0.43
10:l:36:ASN:HB3	12:l:203:CLA:HAC1	1.99	0.43
12:A:817:CLA:H93	12:A:817:CLA:H61	1.83	0.43
4:D:24:ARG:NH1	4:D:25:GLU:OE2	2.51	0.43
12:L:203:CLA:H3A	12:L:203:CLA:HBA2	1.50	0.43
12:H:2117:CLA:H2A	12:H:2117:CLA:HED2	2.00	0.43
12:U:205:CLA:H162	12:U:205:CLA:H141	1.86	0.43
12:a:812:CLA:HBA1	12:a:812:CLA:H3A	1.71	0.43
2:b:691:LYS:HB2	12:b:2139:CLA:HED3	2.00	0.43
12:A:831:CLA:H111	12:A:831:CLA:H72	1.74	0.43
12:B:2101:CLA:HBA1	16:M:102:LHG:H122	2.00	0.43
12:B:2129:CLA:HBA2	12:B:2129:CLA:H3A	1.74	0.43
12:G:807:CLA:H143	16:G:846:LHG:H223	2.00	0.43
2:H:255:LEU:HD11	12:H:2116:CLA:HBC1	1.99	0.43
12:H:2105:CLA:H52	24:V:102:SQD:H302	2.01	0.43
12:H:2119:CLA:H3A	12:H:2119:CLA:HBA2	1.61	0.43
12:H:2123:CLA:HHB	12:H:2141:CLA:HAB	2.00	0.43
12:H:2131:CLA:HBC2	12:H:2138:CLA:HMC2	2.00	0.43
16:V:103:LHG:H292	12:a:830:CLA:H72	2.00	0.43
12:a:819:CLA:H61	12:a:819:CLA:H102	1.58	0.43
2:b:413:LYS:HA	2:b:416:LEU:HD12	2.00	0.43
12:A:839:CLA:H101	15:J:104:BCR:H362	2.00	0.43
15:B:2143:BCR:H20C	15:B:2143:BCR:H361	1.87	0.43
1:G:23:THR:HG21	1:G:177:TRP:HE1	1.84	0.43
1:G:238:LEU:HD12	1:G:238:LEU:HA	1.85	0.43
12:H:2125:CLA:HBA2	12:H:2125:CLA:H3A	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:95:ALA:HB2	1:a:158:LEU:HB2	2.01	0.43
12:a:818:CLA:H203	12:a:826:CLA:HAA1	2.00	0.43
12:b:2110:CLA:H202	12:b:2110:CLA:H161	1.81	0.43
12:b:2123:CLA:HHB	12:b:2141:CLA:HAB	2.00	0.43
25:l:209:DGD:HB81	26:l:210:LMT:H71	2.00	0.43
1:A:391:THR:HG22	1:A:606:ILE:HB	2.00	0.43
1:A:658:ILE:HD12	2:B:618:ARG:HG3	2.00	0.43
4:D:77:LYS:HA	4:D:77:LYS:HD2	1.80	0.43
12:G:831:CLA:H111	12:G:831:CLA:H72	1.74	0.43
12:H:2108:CLA:H93	12:H:2108:CLA:H61	1.85	0.43
15:H:2142:BCR:H15C	15:H:2142:BCR:H351	1.82	0.43
7:R:29:LEU:HB3	24:l:208:SQD:H241	2.00	0.43
15:R:101:BCR:H20C	15:R:101:BCR:H361	1.86	0.43
11:V:30:TYR:HD1	24:V:102:SQD:H441	1.83	0.43
12:a:833:CLA:H41	12:a:833:CLA:H62	1.71	0.43
12:b:2107:CLA:H143	12:b:2128:CLA:HBB2	2.00	0.43
12:b:2152:CLA:HBA1	16:m:103:LHG:H122	2.00	0.43
12:A:835:CLA:H193	16:A:848:LHG:H262	2.01	0.43
12:A:838:CLA:H3A	12:A:838:CLA:HBA2	1.76	0.43
12:B:2125:CLA:H142	12:B:2125:CLA:H112	1.88	0.43
12:G:823:CLA:HBB2	16:G:848:LHG:HC82	1.99	0.43
12:H:2108:CLA:H71	15:R:101:BCR:HC32	2.00	0.43
12:a:829:CLA:H2A	12:a:829:CLA:HED2	2.00	0.43
2:b:93:ASP:OD1	2:b:95:HIS:ND1	2.50	0.43
12:b:2105:CLA:H52	24:m:102:SQD:H302	2.00	0.43
1:A:87:LEU:HD23	1:A:87:LEU:HA	1.88	0.43
1:A:95:ALA:HB2	1:A:158:LEU:HB2	2.01	0.43
2:B:77:TRP:HZ3	2:B:125:TYR:HB2	1.84	0.43
12:B:2125:CLA:H143	12:B:2125:CLA:H162	1.87	0.43
12:F:201:CLA:H61	12:F:201:CLA:H41	1.72	0.43
12:G:835:CLA:H193	16:G:848:LHG:H262	2.01	0.43
12:G:839:CLA:H101	15:S:104:BCR:H362	2.00	0.43
15:H:2145:BCR:H20C	15:H:2145:BCR:H361	1.88	0.43
1:a:354:ILE:HD12	15:a:844:BCR:H342	2.00	0.43
12:a:851:CLA:HMC2	12:b:2139:CLA:H11	2.00	0.43
12:b:2126:CLA:HMB2	12:b:2134:CLA:HBA1	2.01	0.43
4:d:31:THR:O	4:d:83:TYR:HA	2.18	0.43
7:i:29:LEU:HB3	24:L:208:SQD:H241	2.00	0.43
12:B:2106:CLA:H52	24:M:101:SQD:H302	2.00	0.43
1:G:432:HIS:CE1	1:G:436:ILE:HD11	2.54	0.43
12:G:807:CLA:H142	12:G:807:CLA:H112	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:G:843:BCR:H20C	15:G:843:BCR:H361	1.84	0.43
1:a:65:LEU:HB3	1:a:187:LEU:HD11	2.01	0.43
15:a:843:BCR:H20C	15:a:843:BCR:H361	1.85	0.43
17:a:849:LMG:H312	17:a:849:LMG:HC91	1.99	0.43
2:b:14:GLN:NE2	3:c:71:ALA:HB1	2.34	0.43
12:b:2129:CLA:H161	12:b:2129:CLA:H141	1.79	0.43
3:c:17:CYS:HB2	3:c:54:CYS:HB2	2.01	0.43
4:d:24:ARG:NH1	4:d:25:GLU:OE2	2.51	0.43
1:A:65:LEU:HB3	1:A:187:LEU:HD11	2.01	0.43
1:G:95:ALA:HB2	1:G:158:LEU:HB2	2.01	0.43
12:G:805:CLA:H41	12:G:805:CLA:H62	1.63	0.43
2:H:237:PRO:HB3	2:H:256:THR:HG21	2.00	0.43
12:H:2105:CLA:H201	12:H:2108:CLA:H43	2.01	0.43
1:a:604:ILE:HD12	12:a:801:CLA:H122	2.01	0.43
1:a:658:ILE:HD12	2:b:618:ARG:HG3	2.00	0.43
12:a:833:CLA:H42	15:a:845:BCR:H23C	2.01	0.43
15:a:842:BCR:H15C	15:a:842:BCR:H351	1.93	0.43
2:b:495:LEU:O	2:b:499:ASN:ND2	2.41	0.43
12:b:2108:CLA:H61	12:b:2108:CLA:H93	1.85	0.43
3:c:29:VAL:HG21	4:d:114:ALA:HB2	2.01	0.43
1:A:249:MET:O	1:A:253:TYR:N	2.50	0.43
12:A:803:CLA:HAB	12:A:807:CLA:H202	2.00	0.43
12:A:804:CLA:HBA1	12:A:804:CLA:H3A	1.60	0.43
2:B:14:GLN:NE2	3:C:71:ALA:HB1	2.34	0.43
3:C:29:VAL:HG21	4:D:114:ALA:HB2	2.01	0.43
9:K:43:LYS:HB2	9:K:43:LYS:HE3	1.88	0.43
1:G:354:ILE:HD12	15:G:844:BCR:H342	2.00	0.43
2:H:513:ASP:O	2:H:517:HIS:ND1	2.50	0.43
2:b:77:TRP:HZ3	2:b:125:TYR:HB2	1.84	0.43
12:b:2117:CLA:HED2	12:b:2117:CLA:H2A	2.00	0.43
12:l:205:CLA:HBA1	12:l:205:CLA:H3A	1.67	0.43
11:m:30:TYR:HD1	24:m:102:SQD:H441	1.82	0.43
12:A:817:CLA:H102	12:A:834:CLA:HAA2	2.00	0.43
2:B:4:LYS:NZ	11:M:30:TYR:OH	2.47	0.43
2:B:691:LYS:HB2	12:B:2140:CLA:HED3	2.01	0.43
15:I:101:BCR:H20C	15:I:101:BCR:H361	1.86	0.43
12:G:803:CLA:HAB	12:G:807:CLA:H202	2.00	0.42
2:H:441:VAL:HB	2:H:449:LYS:HG3	2.01	0.42
12:H:2107:CLA:H143	12:H:2128:CLA:HBB2	2.00	0.42
15:S:104:BCR:H15C	15:S:104:BCR:H351	1.91	0.42
1:a:198:ASN:HD21	1:a:311:TYR:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:249:MET:O	1:a:253:TYR:N	2.50	0.42
2:b:513:ASP:O	2:b:517:HIS:ND1	2.50	0.42
12:f:201:CLA:H18	12:f:201:CLA:H151	1.86	0.42
1:A:198:ASN:HD21	1:A:311:TYR:HB2	1.84	0.42
1:A:432:HIS:CE1	1:A:436:ILE:HD11	2.54	0.42
1:A:695:GLU:OE2	2:B:547:LYS:NZ	2.52	0.42
6:F:24:LEU:O	6:F:36:ARG:NH2	2.51	0.42
9:K:20:LEU:HD12	9:K:20:LEU:HA	1.93	0.42
1:G:198:ASN:HD21	1:G:311:TYR:HB2	1.84	0.42
12:G:807:CLA:H3A	12:G:807:CLA:HBA2	1.61	0.42
2:H:77:TRP:HZ3	2:H:125:TYR:HB2	1.84	0.42
12:H:2120:CLA:HBA2	12:H:2120:CLA:H3A	1.62	0.42
12:H:2135:CLA:HBA1	12:H:2135:CLA:H3A	1.55	0.42
10:U:53:VAL:O	10:U:57:HIS:ND1	2.46	0.42
12:U:205:CLA:HAA1	25:U:209:DGD:HB42	2.01	0.42
1:a:172:MET:HE1	12:a:812:CLA:H92	2.01	0.42
1:a:432:HIS:CE1	1:a:436:ILE:HD11	2.54	0.42
12:a:805:CLA:H62	12:a:805:CLA:H41	1.63	0.42
12:a:807:CLA:H141	12:a:807:CLA:H162	1.79	0.42
12:a:818:CLA:H111	12:a:818:CLA:H72	1.76	0.42
20:b:2143:ECH:H11	20:b:2143:ECH:H8	1.80	0.42
2:B:237:PRO:HB3	2:B:256:THR:HG21	2.00	0.42
12:B:2108:CLA:H143	12:B:2129:CLA:HBB2	2.00	0.42
12:F:201:CLA:H151	12:F:201:CLA:H18	1.86	0.42
1:G:604:ILE:HD12	12:G:801:CLA:H122	2.01	0.42
12:G:836:CLA:H93	12:G:836:CLA:H112	1.91	0.42
2:H:150:LEU:HD22	11:V:22:ALA:HA	2.01	0.42
12:H:2101:CLA:H101	12:H:2101:CLA:H62	1.65	0.42
1:a:391:THR:HG22	1:a:606:ILE:HB	2.00	0.42
1:a:695:GLU:OE2	2:b:547:LYS:NZ	2.52	0.42
2:b:111:ASN:HD22	7:i:3:GLY:HA2	1.83	0.42
12:b:2107:CLA:H72	12:b:2107:CLA:H111	1.64	0.42
11:m:31:LYS:CE	24:m:102:SQD:H4	2.49	0.42
1:A:23:THR:HG21	1:A:177:TRP:HE1	1.84	0.42
12:A:825:CLA:H72	12:A:833:CLA:HAB	2.02	0.42
12:A:839:CLA:H143	12:A:839:CLA:H111	1.87	0.42
2:B:150:LEU:HD22	11:M:22:ALA:HA	2.01	0.42
12:B:2127:CLA:HMB2	12:B:2135:CLA:HBA1	2.01	0.42
15:J:104:BCR:H15C	15:J:104:BCR:H351	1.91	0.42
1:G:666:SER:HB2	2:H:443:ALA:HB1	2.01	0.42
12:G:825:CLA:H72	12:G:833:CLA:HAB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:17:CYS:HB2	3:N:54:CYS:HB2	2.01	0.42
12:U:205:CLA:HBA1	12:U:205:CLA:H3A	1.67	0.42
12:a:835:CLA:H193	16:a:848:LHG:H262	2.01	0.42
12:a:839:CLA:H101	15:j:104:BCR:H362	2.00	0.42
5:e:30:LYS:HD2	5:e:30:LYS:HA	1.75	0.42
1:A:187:LEU:HB3	1:A:191:GLN:HE22	1.83	0.42
12:A:833:CLA:H42	15:A:845:BCR:H23C	2.01	0.42
2:B:409:MET:HE2	12:B:2131:CLA:HBC3	2.01	0.42
2:B:441:VAL:HB	2:B:449:LYS:HG3	2.01	0.42
12:B:2132:CLA:HBC2	12:B:2139:CLA:HMC2	2.00	0.42
1:G:65:LEU:HB3	1:G:187:LEU:HD11	2.01	0.42
1:G:187:LEU:HB3	1:G:191:GLN:HE22	1.83	0.42
1:G:371:TYR:HA	1:G:386:GLN:HE21	1.84	0.42
2:H:14:GLN:NE2	3:N:71:ALA:HB1	2.34	0.42
2:H:111:ASN:HD22	7:R:3:GLY:HA2	1.83	0.42
2:H:691:LYS:HB2	12:H:2139:CLA:HED3	2.00	0.42
12:H:2124:CLA:H142	12:H:2124:CLA:H112	1.88	0.42
12:H:2126:CLA:HMB2	12:H:2134:CLA:HBA1	2.01	0.42
1:a:23:THR:HG21	1:a:177:TRP:HE1	1.84	0.42
12:a:807:CLA:H143	16:a:846:LHG:H223	2.00	0.42
2:b:364:THR:HG23	2:b:726:THR:HB	2.02	0.42
2:b:409:MET:HE2	12:b:2130:CLA:HBC3	2.01	0.42
1:A:172:MET:HE1	12:A:812:CLA:H92	2.01	0.42
1:A:354:ILE:HD12	15:A:844:BCR:H342	2.00	0.42
12:A:824:CLA:H143	12:A:824:CLA:H161	1.91	0.42
12:B:2106:CLA:H201	12:B:2109:CLA:H43	2.01	0.42
12:B:2119:CLA:H41	12:B:2135:CLA:HED1	2.02	0.42
1:G:278:LYS:HA	1:G:502:LEU:HB2	2.01	0.42
12:G:820:CLA:H102	12:G:823:CLA:H72	2.02	0.42
4:O:75:LYS:HA	4:O:75:LYS:HD3	1.87	0.42
2:b:237:PRO:HB3	2:b:256:THR:HG21	2.00	0.42
1:A:744:LEU:HD23	1:A:744:LEU:HA	1.75	0.42
12:B:2121:CLA:H3A	12:B:2121:CLA:HBA2	1.62	0.42
2:H:413:LYS:HA	2:H:416:LEU:HD12	2.00	0.42
12:H:2129:CLA:H141	12:H:2129:CLA:H161	1.79	0.42
12:H:2132:CLA:H2	12:H:2132:CLA:H62	1.74	0.42
10:l:92:ALA:HB1	15:l:206:BCR:H401	2.02	0.42
12:l:205:CLA:H162	12:l:205:CLA:H203	1.83	0.42
12:A:826:CLA:H141	12:A:826:CLA:H162	1.87	0.42
3:C:17:CYS:HB2	3:C:54:CYS:HB2	2.01	0.42
25:L:209:DGD:HB81	26:L:210:LMT:H71	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:339:LEU:HD23	2:H:339:LEU:HA	1.94	0.42
2:H:475:LEU:HD23	2:H:475:LEU:HA	1.94	0.42
12:a:802:CLA:H11	12:a:802:CLA:H52	1.80	0.42
12:a:820:CLA:H102	12:a:823:CLA:H72	2.02	0.42
15:l:207:BCR:H11C	15:l:207:BCR:H341	1.95	0.42
1:A:666:SER:HB2	2:B:443:ALA:HB1	2.01	0.42
12:A:820:CLA:H102	12:A:823:CLA:H72	2.02	0.42
12:B:2118:CLA:H2A	12:B:2118:CLA:HED2	2.00	0.42
12:B:2133:CLA:H2	12:B:2133:CLA:H62	1.74	0.42
12:G:811:CLA:HBA2	12:G:811:CLA:H3A	1.61	0.42
2:H:547:LYS:HE3	2:H:547:LYS:HB2	1.74	0.42
12:Q:201:CLA:H61	12:Q:201:CLA:H41	1.72	0.42
1:a:278:LYS:HA	1:a:502:LEU:HB2	2.01	0.42
1:A:371:TYR:HA	1:A:386:GLN:HE21	1.85	0.42
12:A:823:CLA:H11	12:A:823:CLA:H51	1.86	0.42
12:B:2134:CLA:HBA2	12:B:2134:CLA:H3A	1.82	0.42
20:B:2144:ECH:H11	20:B:2144:ECH:H8	1.80	0.42
2:H:413:LYS:HB2	2:H:536:LEU:HD13	2.02	0.42
3:N:29:VAL:HG21	4:O:114:ALA:HB2	2.01	0.42
2:b:420:LEU:HD13	2:b:529:LEU:HA	2.02	0.42
12:b:2105:CLA:H201	12:b:2108:CLA:H43	2.01	0.42
12:A:818:CLA:H111	12:A:818:CLA:H72	1.76	0.42
2:B:513:ASP:O	2:B:517:HIS:ND1	2.50	0.42
1:G:172:MET:HE1	12:G:812:CLA:H92	2.01	0.41
1:G:428:ARG:NH2	27:G:926:HOH:O	2.51	0.41
12:H:2112:CLA:H162	12:H:2112:CLA:H122	1.85	0.41
25:U:209:DGD:HB81	26:U:210:LMT:H71	2.00	0.41
20:V:101:ECH:H24	20:V:101:ECH:H37	1.89	0.41
13:a:840:A1AGD:C15	15:f:202:BCR:H23C	2.50	0.41
2:b:22:TRP:CG	2:b:701:GLN:HE22	2.38	0.41
1:A:278:LYS:HA	1:A:502:LEU:HB2	2.01	0.41
13:A:840:A1AGD:C15	15:F:202:BCR:H23C	2.50	0.41
2:B:621:LEU:O	2:B:625:SER:OG	2.37	0.41
6:F:87:LEU:HD23	6:F:87:LEU:HA	1.91	0.41
1:G:302:VAL:HG21	12:G:816:CLA:HAB	2.02	0.41
15:G:844:BCR:H20C	15:G:844:BCR:H361	1.88	0.41
6:Q:58:ARG:HH12	12:Q:204:CLA:HBC2	1.86	0.41
15:S:104:BCR:H24C	15:S:104:BCR:H371	1.85	0.41
9:T:67:LEU:HA	9:T:70:MET:HG3	2.03	0.41
15:U:207:BCR:H282	15:L:207:BCR:H272	2.02	0.41
12:a:802:CLA:H192	12:a:839:CLA:H143	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:118:LYS:HD2	4:d:118:LYS:HA	1.84	0.41
12:f:203:CLA:HBA1	12:f:203:CLA:H3A	1.84	0.41
15:l:206:BCR:H15C	15:l:206:BCR:H351	1.92	0.41
12:L:205:CLA:HAA1	25:L:209:DGD:HB42	2.02	0.41
12:G:824:CLA:H143	12:G:824:CLA:H161	1.91	0.41
12:G:851:CLA:H62	12:G:851:CLA:H41	1.90	0.41
2:H:420:LEU:HD13	2:H:529:LEU:HA	2.02	0.41
12:H:2118:CLA:H41	12:H:2134:CLA:HED1	2.02	0.41
4:O:77:LYS:HD2	4:O:77:LYS:HA	1.80	0.41
12:a:837:CLA:H192	12:a:837:CLA:H161	1.84	0.41
9:k:67:LEU:HA	9:k:70:MET:HG3	2.02	0.41
2:B:292:ARG:NE	2:B:298:GLY:O	2.46	0.41
2:B:364:THR:HG23	2:B:726:THR:HB	2.02	0.41
4:D:75:LYS:HA	4:D:75:LYS:HD3	1.87	0.41
9:K:67:LEU:HA	9:K:70:MET:HG3	2.02	0.41
1:G:695:GLU:OE2	2:H:547:LYS:NZ	2.52	0.41
12:G:807:CLA:H151	15:S:101:BCR:H402	2.03	0.41
1:a:707:LEU:HD11	12:b:2131:CLA:HBA1	2.03	0.41
12:a:807:CLA:H151	15:j:101:BCR:H402	2.03	0.41
12:a:836:CLA:HBB2	12:a:837:CLA:HBC3	2.03	0.41
15:a:844:BCR:H15C	15:a:844:BCR:H351	1.90	0.41
2:b:413:LYS:HB2	2:b:536:LEU:HD13	2.02	0.41
10:l:82:LEU:HD22	10:l:139:TYR:CG	2.56	0.41
12:A:807:CLA:H142	12:A:807:CLA:H112	1.82	0.41
12:A:833:CLA:H41	12:A:833:CLA:H62	1.71	0.41
2:B:22:TRP:CG	2:B:701:GLN:HE22	2.38	0.41
6:F:35:ILE:HD12	6:F:39:ARG:HH22	1.86	0.41
12:G:807:CLA:H162	12:G:807:CLA:H141	1.79	0.41
12:G:836:CLA:HBB2	12:G:837:CLA:HBC3	2.03	0.41
2:H:517:HIS:CG	12:H:2137:CLA:HED3	2.56	0.41
10:U:92:ALA:HB1	15:U:206:BCR:H401	2.02	0.41
15:U:207:BCR:H391	10:L:136:PHE:CE2	2.54	0.41
11:V:31:LYS:CE	24:V:102:SQD:H4	2.50	0.41
1:a:371:TYR:HA	1:a:386:GLN:HE21	1.84	0.41
1:a:666:SER:HB2	2:b:443:ALA:HB1	2.01	0.41
12:a:817:CLA:H93	12:a:817:CLA:H61	1.83	0.41
15:B:2147:BCR:H15C	15:B:2147:BCR:H351	1.88	0.41
4:D:42:MET:HE1	4:D:57:LEU:HD11	2.03	0.41
11:M:31:LYS:CE	24:M:101:SQD:H4	2.50	0.41
13:G:840:A1AGD:C15	15:Q:202:BCR:H23C	2.50	0.41
1:a:302:VAL:HG21	12:a:816:CLA:HAB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:a:810:CLA:H71	12:a:810:CLA:H112	1.87	0.41
12:a:825:CLA:H72	12:a:833:CLA:HAB	2.02	0.41
2:b:292:ARG:NE	2:b:298:GLY:O	2.46	0.41
2:b:517:HIS:CG	12:b:2137:CLA:HED3	2.56	0.41
2:b:568:SER:OG	2:b:571:ASP:OD2	2.38	0.41
12:b:2119:CLA:HBA2	12:b:2119:CLA:H3A	1.61	0.41
1:A:50:ASN:HD22	1:A:50:ASN:HA	1.72	0.41
12:A:812:CLA:H41	12:A:812:CLA:H61	1.90	0.41
12:A:836:CLA:HBB2	12:A:837:CLA:HBC3	2.03	0.41
15:B:2143:BCR:H15C	15:B:2143:BCR:H351	1.82	0.41
10:L:92:ALA:HB1	15:L:206:BCR:H401	2.02	0.41
12:G:833:CLA:H42	15:G:845:BCR:H23C	2.01	0.41
2:H:409:MET:HE2	12:H:2130:CLA:HBC3	2.01	0.41
12:Q:201:CLA:H18	12:Q:201:CLA:H151	1.86	0.41
12:b:2118:CLA:H41	12:b:2134:CLA:HED1	2.02	0.41
12:b:2136:CLA:HMB1	12:b:2138:CLA:HED1	2.03	0.41
15:j:104:BCR:H20C	15:j:104:BCR:H361	1.77	0.41
9:k:43:LYS:HB2	9:k:43:LYS:HE3	1.88	0.41
9:k:44:THR:OG1	9:k:45:GLY:N	2.53	0.41
12:l:205:CLA:HAA1	25:l:209:DGD:HB42	2.02	0.41
1:A:707:LEU:HD11	12:B:2132:CLA:HBA1	2.03	0.41
12:A:802:CLA:H192	12:A:839:CLA:H143	2.03	0.41
12:A:807:CLA:H151	15:J:101:BCR:H402	2.03	0.41
2:B:646:MET:HE2	15:B:2146:BCR:H333	2.02	0.41
12:G:802:CLA:H192	12:G:839:CLA:H143	2.03	0.41
12:G:839:CLA:H143	12:G:839:CLA:H111	1.87	0.41
2:H:364:THR:HG23	2:H:726:THR:HB	2.02	0.41
2:H:646:MET:HE2	15:H:2145:BCR:H333	2.02	0.41
12:a:826:CLA:H162	12:a:826:CLA:H141	1.87	0.41
17:a:847:LMG:H453	25:l:209:DGD:HAH1	2.03	0.41
2:b:452:LEU:HD23	2:b:511:PRO:HG2	2.03	0.41
12:b:2114:CLA:H62	12:b:2114:CLA:H2	1.74	0.41
6:f:35:ILE:HD12	6:f:39:ARG:HH22	1.86	0.41
1:A:604:ILE:HD12	12:A:801:CLA:H122	2.01	0.41
12:A:807:CLA:H141	12:A:807:CLA:H162	1.79	0.41
6:F:14:PRO:HA	6:F:17:LEU:HD23	2.03	0.41
15:J:104:BCR:H24C	15:J:104:BCR:H371	1.86	0.41
1:G:707:LEU:HD11	12:H:2131:CLA:HBA1	2.03	0.41
1:G:744:LEU:HD23	1:G:744:LEU:HA	1.75	0.41
17:G:849:LMG:H321	17:G:849:LMG:H291	1.89	0.41
2:H:22:TRP:CG	2:H:701:GLN:HE22	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:2124:CLA:H143	12:H:2124:CLA:H162	1.87	0.41
6:Q:14:PRO:HA	6:Q:17:LEU:HD23	2.03	0.41
6:Q:35:ILE:HD12	6:Q:39:ARG:HH22	1.86	0.41
9:T:44:THR:OG1	9:T:45:GLY:N	2.53	0.41
10:U:82:LEU:HD22	10:U:139:TYR:CG	2.56	0.41
1:a:141:SER:HA	12:a:827:CLA:HMA2	2.03	0.41
1:a:478:LEU:HB2	1:a:529:THR:HG23	2.03	0.41
12:a:807:CLA:H142	12:a:807:CLA:H112	1.82	0.41
12:a:817:CLA:HBA2	12:a:817:CLA:H3A	1.56	0.41
2:b:150:LEU:HD22	11:m:22:ALA:HA	2.01	0.41
2:b:381:MET:HE1	15:b:2144:BCR:H361	2.03	0.41
2:b:441:VAL:HB	2:b:449:LYS:HG3	2.01	0.41
1:A:374:PRO:HA	1:A:375:PRO:HD3	1.82	0.41
1:A:429:MET:HG3	12:A:820:CLA:H192	2.03	0.41
1:A:539:ALA:O	1:A:543:HIS:ND1	2.44	0.41
12:A:802:CLA:H11	12:A:802:CLA:H52	1.80	0.41
12:A:816:CLA:H11	12:A:816:CLA:H51	1.92	0.41
17:A:847:LMG:H453	25:L:209:DGD:HAH1	2.03	0.41
2:B:125:TYR:HE2	2:B:358:PHE:HE2	1.69	0.41
2:B:452:LEU:HD23	2:B:511:PRO:HG2	2.03	0.41
12:B:2132:CLA:H11	12:B:2132:CLA:H52	1.84	0.41
5:E:20:GLY:HA3	6:F:139:PRO:HA	2.03	0.41
24:M:101:SQD:H311	24:M:101:SQD:H281	1.89	0.41
15:G:845:BCR:H20C	15:G:845:BCR:H361	1.84	0.41
2:H:381:MET:HE1	15:H:2144:BCR:H361	2.03	0.41
12:H:2123:CLA:HAC1	15:H:2146:BCR:H372	2.03	0.41
12:Q:203:CLA:HBC3	8:S:18:LEU:HD22	2.03	0.41
12:U:203:CLA:H111	7:I:25:VAL:HG22	2.03	0.41
12:b:2139:CLA:H162	12:b:2139:CLA:H141	1.86	0.41
1:A:141:SER:HA	12:A:827:CLA:HMA2	2.03	0.41
17:A:847:LMG:HC2	17:A:847:LMG:HC71	1.64	0.41
9:K:44:THR:OG1	9:K:45:GLY:N	2.53	0.41
1:G:90:MET:HE1	12:G:807:CLA:C2A	2.52	0.40
1:G:431:ARG:NE	4:O:13:GLY:O	2.52	0.40
1:G:478:LEU:HB2	1:G:529:THR:HG23	2.03	0.40
2:H:447:PRO:HB2	6:Q:50:TYR:CZ	2.56	0.40
9:T:43:LYS:HB2	9:T:43:LYS:HE3	1.88	0.40
1:a:433:ARG:HA	1:a:436:ILE:HD12	2.03	0.40
12:a:810:CLA:H202	12:a:810:CLA:H161	1.92	0.40
2:b:125:TYR:HE2	2:b:358:PHE:HE2	1.69	0.40
2:b:447:PRO:HB2	6:f:50:TYR:CZ	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:b:2118:CLA:O1D	12:b:2119:CLA:HHB	2.22	0.40
5:e:20:GLY:HA3	6:f:139:PRO:HA	2.03	0.40
15:l:207:BCR:H272	15:L:207:BCR:H282	2.04	0.40
1:A:90:MET:HE1	12:A:807:CLA:C2A	2.52	0.40
1:A:427:ASP:OD2	1:A:431:ARG:NH1	2.54	0.40
1:G:197:MET:HE3	1:G:197:MET:HB3	1.82	0.40
1:G:425:LEU:HD13	12:G:823:CLA:C1C	2.52	0.40
1:G:588:TRP:CD1	12:G:829:CLA:HMD1	2.57	0.40
1:G:687:PHE:O	2:H:574:TYR:OH	2.32	0.40
12:G:802:CLA:H52	12:G:802:CLA:H8	1.90	0.40
12:G:817:CLA:H91	12:G:817:CLA:H111	1.91	0.40
2:H:341:VAL:HG21	12:H:2126:CLA:H51	2.03	0.40
12:H:2116:CLA:H3A	12:H:2116:CLA:HBA2	1.50	0.40
4:O:42:MET:HE1	4:O:57:LEU:HD11	2.03	0.40
1:a:348:TRP:HB3	12:a:804:CLA:HAC1	2.03	0.40
2:b:341:VAL:HG21	12:b:2126:CLA:H51	2.03	0.40
10:l:90:LEU:HD11	12:L:203:CLA:HAA2	2.04	0.40
12:A:832:CLA:H162	12:A:832:CLA:H141	1.83	0.40
2:B:221:GLY:O	2:B:233:TYR:OH	2.36	0.40
2:B:341:VAL:HG21	12:B:2127:CLA:H51	2.03	0.40
2:B:517:HIS:CG	12:B:2138:CLA:HED3	2.56	0.40
12:G:820:CLA:H141	12:G:820:CLA:H162	1.91	0.40
2:H:162:ARG:HA	2:H:163:PRO:HD3	1.93	0.40
2:H:381:MET:HE3	2:H:381:MET:HB3	1.85	0.40
2:H:628:LEU:HD22	2:H:721:PHE:HA	2.04	0.40
12:H:2118:CLA:O1D	12:H:2119:CLA:HHB	2.22	0.40
23:H:2151:ZEX:H363	8:S:36:LEU:HD21	2.04	0.40
16:V:103:LHG:H331	16:V:103:LHG:H151	2.03	0.40
2:b:254:ILE:HG13	2:b:255:LEU:HD12	2.04	0.40
2:b:332:LEU:HD23	2:b:332:LEU:HA	1.91	0.40
3:c:35:LYS:HE2	3:c:35:LYS:HB3	1.88	0.40
6:f:14:PRO:HA	6:f:17:LEU:HD23	2.03	0.40
15:j:101:BCR:H15C	15:j:101:BCR:H351	1.93	0.40
15:j:104:BCR:H15C	15:j:104:BCR:H351	1.91	0.40
1:A:435:ALA:O	1:A:439:HIS:ND1	2.51	0.40
12:A:818:CLA:HAB	12:A:818:CLA:H8	2.03	0.40
6:F:94:LYS:HA	6:F:94:LYS:HD3	1.99	0.40
12:F:203:CLA:HBC3	8:J:18:LEU:HD22	2.03	0.40
10:L:82:LEU:HD22	10:L:139:TYR:CG	2.56	0.40
1:G:389:LEU:HD23	1:G:389:LEU:HA	1.97	0.40
12:G:821:CLA:H11	12:G:821:CLA:H52	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:826:CLA:H162	12:G:826:CLA:H141	1.87	0.40
17:G:847:LMG:H453	25:U:209:DGD:HAH1	2.03	0.40
2:H:125:TYR:HE2	2:H:358:PHE:HE2	1.69	0.40
2:H:452:LEU:HD23	2:H:511:PRO:HG2	2.03	0.40
5:P:20:GLY:HA3	6:Q:139:PRO:HA	2.03	0.40
1:a:427:ASP:OD2	1:a:431:ARG:NH1	2.54	0.40
12:a:803:CLA:H52	12:a:810:CLA:H172	2.03	0.40
12:a:812:CLA:H111	12:a:812:CLA:H91	1.87	0.40
12:a:821:CLA:H142	12:a:821:CLA:H112	1.97	0.40
2:b:621:LEU:O	2:b:625:SER:OG	2.37	0.40
2:b:646:MET:HE2	15:b:2145:BCR:H333	2.02	0.40
12:b:2125:CLA:HBA2	12:b:2125:CLA:H3A	1.85	0.40
12:b:2140:CLA:H91	12:b:2140:CLA:H112	1.92	0.40
15:j:104:BCR:H371	15:j:104:BCR:H24C	1.86	0.40
1:A:302:VAL:HG21	12:A:816:CLA:HAB	2.02	0.40
1:A:433:ARG:HA	1:A:436:ILE:HD12	2.04	0.40
2:B:413:LYS:HB2	2:B:536:LEU:HD13	2.02	0.40
2:B:495:LEU:O	2:B:499:ASN:ND2	2.41	0.40
12:G:803:CLA:H52	12:G:810:CLA:H172	2.03	0.40
12:G:833:CLA:H91	12:G:833:CLA:H111	1.95	0.40
6:Q:87:LEU:HD23	6:Q:87:LEU:HA	1.91	0.40
1:a:375:PRO:HG2	12:a:818:CLA:HAA2	2.03	0.40
1:a:487:GLN:HG2	1:a:509:PHE:HA	2.04	0.40
12:a:838:CLA:H3A	12:a:838:CLA:HBA2	1.76	0.40
15:f:202:BCR:H20C	15:f:202:BCR:H361	1.80	0.40
1:A:588:TRP:CD1	12:A:829:CLA:HMD1	2.57	0.40
2:B:447:PRO:HB2	6:F:50:TYR:CZ	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	735/751 (98%)	701 (95%)	33 (4%)	1 (0%)	48	45
1	G	735/751 (98%)	701 (95%)	33 (4%)	1 (0%)	48	45
1	a	735/751 (98%)	701 (95%)	33 (4%)	1 (0%)	48	45
2	B	727/730 (100%)	692 (95%)	35 (5%)	0	100	100
2	H	727/730 (100%)	692 (95%)	35 (5%)	0	100	100
2	b	727/730 (100%)	692 (95%)	35 (5%)	0	100	100
3	C	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
3	N	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
3	c	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
4	D	137/141 (97%)	134 (98%)	3 (2%)	0	100	100
4	O	137/141 (97%)	134 (98%)	3 (2%)	0	100	100
4	d	137/141 (97%)	134 (98%)	3 (2%)	0	100	100
5	E	67/74 (90%)	62 (92%)	5 (8%)	0	100	100
5	P	67/74 (90%)	62 (92%)	5 (8%)	0	100	100
5	e	67/74 (90%)	62 (92%)	5 (8%)	0	100	100
6	F	139/165 (84%)	136 (98%)	3 (2%)	0	100	100
6	Q	139/165 (84%)	136 (98%)	3 (2%)	0	100	100
6	f	139/165 (84%)	136 (98%)	3 (2%)	0	100	100
7	I	38/40 (95%)	35 (92%)	3 (8%)	0	100	100
7	R	38/40 (95%)	35 (92%)	3 (8%)	0	100	100
7	i	38/40 (95%)	35 (92%)	3 (8%)	0	100	100
8	J	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
8	S	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
8	j	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
9	K	65/90 (72%)	58 (89%)	7 (11%)	0	100	100
9	T	65/90 (72%)	58 (89%)	7 (11%)	0	100	100
9	k	65/90 (72%)	58 (89%)	7 (11%)	0	100	100
10	L	152/157 (97%)	146 (96%)	6 (4%)	0	100	100
10	U	152/157 (97%)	146 (96%)	6 (4%)	0	100	100
10	l	152/157 (97%)	146 (96%)	6 (4%)	0	100	100
11	M	29/31 (94%)	29 (100%)	0	0	100	100
11	V	29/31 (94%)	29 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	m	29/31 (94%)	29 (100%)	0	0	100	100
All	All	6612/6900 (96%)	6312 (96%)	297 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	121	VAL
1	a	121	VAL
1	A	121	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	591/603 (98%)	578 (98%)	13 (2%)	45	45
1	G	591/603 (98%)	577 (98%)	14 (2%)	43	41
1	a	591/603 (98%)	577 (98%)	14 (2%)	43	41
2	B	582/583 (100%)	570 (98%)	12 (2%)	47	47
2	H	582/583 (100%)	570 (98%)	12 (2%)	47	47
2	b	582/583 (100%)	570 (98%)	12 (2%)	47	47
3	C	68/69 (99%)	66 (97%)	2 (3%)	37	34
3	N	68/69 (99%)	66 (97%)	2 (3%)	37	34
3	c	68/69 (99%)	66 (97%)	2 (3%)	37	34
4	D	114/116 (98%)	112 (98%)	2 (2%)	51	52
4	O	114/116 (98%)	112 (98%)	2 (2%)	51	52
4	d	114/116 (98%)	112 (98%)	2 (2%)	51	52
5	E	58/60 (97%)	55 (95%)	3 (5%)	21	13
5	P	58/60 (97%)	55 (95%)	3 (5%)	21	13
5	e	58/60 (97%)	55 (95%)	3 (5%)	21	13
6	F	118/137 (86%)	112 (95%)	6 (5%)	21	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	Q	118/137 (86%)	112 (95%)	6 (5%)	21	14
6	f	118/137 (86%)	112 (95%)	6 (5%)	21	14
7	I	32/32 (100%)	32 (100%)	0	100	100
7	R	32/32 (100%)	32 (100%)	0	100	100
7	i	32/32 (100%)	32 (100%)	0	100	100
8	J	34/35 (97%)	33 (97%)	1 (3%)	37	34
8	S	34/35 (97%)	33 (97%)	1 (3%)	37	34
8	j	34/35 (97%)	33 (97%)	1 (3%)	37	34
9	K	50/68 (74%)	47 (94%)	3 (6%)	17	10
9	T	50/68 (74%)	47 (94%)	3 (6%)	17	10
9	k	50/68 (74%)	47 (94%)	3 (6%)	17	10
10	L	116/118 (98%)	114 (98%)	2 (2%)	53	53
10	U	116/118 (98%)	114 (98%)	2 (2%)	53	53
10	l	116/118 (98%)	114 (98%)	2 (2%)	53	53
11	M	25/25 (100%)	23 (92%)	2 (8%)	11	5
11	V	25/25 (100%)	23 (92%)	2 (8%)	11	5
11	m	25/25 (100%)	23 (92%)	2 (8%)	11	5
All	All	5364/5538 (97%)	5224 (97%)	140 (3%)	41	38

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	37	THR
1	G	120	ILE
1	G	141	SER
1	G	191	GLN
1	G	195	SER
1	G	303	LEU
1	G	370	MET
1	G	422	VAL
1	G	513	THR
1	G	583	CYS
1	G	624	ASP
1	G	627	VAL
1	G	707	LEU
1	G	722	GLN

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Mol	Chain	Res	Type
2	H	45	LYS
2	H	232	VAL
2	H	252	THR
2	H	304	ILE
2	H	355	SER
2	H	405	VAL
2	H	410	LEU
2	H	421	SER
2	H	429	PHE
2	H	446	THR
2	H	461	ILE
2	H	574	TYR
3	N	23	LEU
3	N	27	GLU
4	O	5	SER
4	O	122	ILE
5	P	28	VAL
5	P	56	VAL
5	P	69	VAL
6	Q	60	THR
6	Q	85	SER
6	Q	92	GLU
6	Q	101	VAL
6	Q	130	LYS
6	Q	132	VAL
8	S	31	ARG
9	T	22	VAL
9	T	25	ILE
9	T	44	THR
10	U	102	VAL
10	U	137	VAL
11	V	12	LEU
11	V	27	THR
1	a	37	THR
1	a	120	ILE
1	a	141	SER
1	a	191	GLN
1	a	195	SER
1	a	303	LEU
1	a	370	MET
1	a	422	VAL
1	a	513	THR

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Mol	Chain	Res	Type
1	a	583	CYS
1	a	624	ASP
1	a	627	VAL
1	a	707	LEU
1	a	722	GLN
2	b	45	LYS
2	b	232	VAL
2	b	252	THR
2	b	304	ILE
2	b	355	SER
2	b	405	VAL
2	b	410	LEU
2	b	421	SER
2	b	429	PHE
2	b	446	THR
2	b	461	ILE
2	b	574	TYR
3	c	23	LEU
3	c	27	GLU
4	d	5	SER
4	d	122	ILE
5	e	28	VAL
5	e	56	VAL
5	e	69	VAL
6	f	60	THR
6	f	85	SER
6	f	92	GLU
6	f	101	VAL
6	f	130	LYS
6	f	132	VAL
8	j	31	ARG
9	k	22	VAL
9	k	25	ILE
9	k	44	THR
10	l	102	VAL
10	l	137	VAL
11	m	12	LEU
11	m	27	THR
1	A	37	THR
1	A	120	ILE
1	A	141	SER
1	A	195	SER

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Mol	Chain	Res	Type
1	A	303	LEU
1	A	370	MET
1	A	422	VAL
1	A	513	THR
1	A	583	CYS
1	A	624	ASP
1	A	627	VAL
1	A	707	LEU
1	A	722	GLN
2	B	45	LYS
2	B	232	VAL
2	B	252	THR
2	B	304	ILE
2	B	355	SER
2	B	405	VAL
2	B	410	LEU
2	B	421	SER
2	B	429	PHE
2	B	446	THR
2	B	461	ILE
2	B	574	TYR
3	C	23	LEU
3	C	27	GLU
4	D	5	SER
4	D	122	ILE
5	E	28	VAL
5	E	56	VAL
5	E	69	VAL
6	F	60	THR
6	F	85	SER
6	F	92	GLU
6	F	101	VAL
6	F	130	LYS
6	F	132	VAL
8	J	31	ARG
9	K	22	VAL
9	K	25	ILE
9	K	44	THR
10	L	102	VAL
10	L	137	VAL
11	M	12	LEU
11	M	27	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (124) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	19	ASN
1	G	138	GLN
1	G	192	ASN
1	G	218	HIS
1	G	351	GLN
1	G	441	ASN
1	G	637	GLN
1	G	714	GLN
2	H	14	GLN
2	H	44	GLN
2	H	102	ASN
2	H	106	GLN
2	H	111	ASN
2	H	114	ASN
2	H	158	GLN
2	H	177	HIS
2	H	229	ASN
2	H	276	HIS
2	H	306	ASN
2	H	325	ASN
2	H	331	GLN
2	H	437	HIS
2	H	438	ASN
2	H	503	ASN
2	H	605	GLN
2	H	609	ASN
2	H	624	ASN
2	H	627	GLN
2	H	686	ASN
3	N	3	HIS
3	N	38	GLN
4	O	23	ASN
5	P	4	ASN
6	Q	13	ASN
6	Q	61	HIS
8	S	30	ASN
9	T	74	HIS
10	U	5	ASN
10	U	144	ASN
10	U	157	ASN
1	a	19	ASN

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Mol	Chain	Res	Type
1	a	138	GLN
1	a	192	ASN
1	a	218	HIS
1	a	351	GLN
1	a	441	ASN
1	a	714	GLN
2	b	14	GLN
2	b	44	GLN
2	b	102	ASN
2	b	106	GLN
2	b	111	ASN
2	b	158	GLN
2	b	177	HIS
2	b	229	ASN
2	b	276	HIS
2	b	306	ASN
2	b	325	ASN
2	b	331	GLN
2	b	366	GLN
2	b	437	HIS
2	b	438	ASN
2	b	503	ASN
2	b	595	HIS
2	b	605	GLN
2	b	609	ASN
2	b	624	ASN
2	b	627	GLN
2	b	686	ASN
3	c	3	HIS
3	c	38	GLN
4	d	23	ASN
5	e	4	ASN
6	f	13	ASN
6	f	61	HIS
6	f	99	GLN
8	j	30	ASN
9	k	74	HIS
10	l	5	ASN
10	l	144	ASN
10	l	157	ASN
1	A	19	ASN
1	A	138	GLN

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Mol	Chain	Res	Type
1	A	192	ASN
1	A	218	HIS
1	A	351	GLN
1	A	441	ASN
1	A	637	GLN
1	A	714	GLN
2	B	14	GLN
2	B	44	GLN
2	B	102	ASN
2	B	106	GLN
2	B	111	ASN
2	B	158	GLN
2	B	177	HIS
2	B	229	ASN
2	B	276	HIS
2	B	306	ASN
2	B	325	ASN
2	B	331	GLN
2	B	366	GLN
2	B	437	HIS
2	B	438	ASN
2	B	503	ASN
2	B	595	HIS
2	B	605	GLN
2	B	609	ASN
2	B	624	ASN
2	B	627	GLN
2	B	686	ASN
3	C	3	HIS
3	C	38	GLN
4	D	23	ASN
5	E	4	ASN
6	F	13	ASN
6	F	61	HIS
6	F	99	GLN
8	J	30	ASN
9	K	30	ASN
9	K	74	HIS
10	L	5	ASN
10	L	144	ASN
10	L	157	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 402 ligands modelled in this entry, 9 are monoatomic - leaving 393 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	$\# Z > 2$
12	CLA	a	819	1	69,73,73	1.18	7 (10%)	82,113,113	1.32	6 (7%)
12	CLA	Q	204	-	49,53,73	1.40	6 (12%)	58,89,113	1.42	4 (6%)
12	CLA	a	810	1,12	69,73,73	1.18	8 (11%)	82,113,113	1.35	6 (7%)
12	CLA	b	2124	27	69,73,73	1.17	7 (10%)	82,113,113	1.31	8 (9%)
12	CLA	B	2122	-	59,63,73	1.26	7 (11%)	70,101,113	1.33	7 (10%)
12	CLA	G	805	1	69,73,73	1.16	8 (11%)	82,113,113	1.40	9 (10%)
12	CLA	b	2110	2	69,73,73	1.21	7 (10%)	82,113,113	1.34	5 (6%)
12	CLA	A	801	1	69,73,73	1.20	8 (11%)	82,113,113	1.30	7 (8%)
12	CLA	H	2133	2	69,73,73	1.18	7 (10%)	82,113,113	1.33	6 (7%)
12	CLA	B	2132	2	59,63,73	1.26	8 (13%)	70,101,113	1.38	7 (10%)
15	BCR	j	104	-	41,41,41	1.07	3 (7%)	56,56,56	1.27	7 (12%)
12	CLA	b	2135	-	49,53,73	1.39	8 (16%)	58,89,113	1.43	5 (8%)
12	CLA	H	2141	16	49,53,73	1.39	6 (12%)	58,89,113	1.54	7 (12%)
12	CLA	b	2140	2	69,73,73	1.18	6 (8%)	82,113,113	1.35	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	H	2129	2	69,73,73	1.20	10 (14%)	82,113,113	1.36	7 (8%)
24	SQD	L	208	-	43,45,54	1.67	8 (18%)	53,56,65	1.58	7 (13%)
12	CLA	G	804	1	69,73,73	1.15	8 (11%)	82,113,113	1.44	6 (7%)
12	CLA	H	2139	27	69,73,73	1.14	8 (11%)	82,113,113	1.35	7 (8%)
24	SQD	l	208	-	43,45,54	1.67	8 (18%)	53,56,65	1.58	7 (13%)
12	CLA	H	2124	27	69,73,73	1.17	8 (11%)	82,113,113	1.31	8 (9%)
24	SQD	m	102	-	52,54,54	1.56	7 (13%)	62,65,65	1.37	8 (12%)
12	CLA	B	2131	-	49,53,73	1.39	8 (16%)	58,89,113	1.47	4 (6%)
12	CLA	b	2112	2	69,73,73	1.18	7 (10%)	82,113,113	1.27	5 (6%)
12	CLA	G	836	1	69,73,73	1.16	9 (13%)	82,113,113	1.27	4 (4%)
12	CLA	J	103	8	49,53,73	1.40	6 (12%)	58,89,113	1.47	5 (8%)
12	CLA	b	2125	27	54,58,73	1.31	8 (14%)	64,95,113	1.45	8 (12%)
12	CLA	B	2106	2	69,73,73	1.16	7 (10%)	82,113,113	1.32	7 (8%)
15	BCR	B	2143	-	41,41,41	1.09	2 (4%)	56,56,56	1.20	5 (8%)
15	BCR	A	843	-	41,41,41	1.03	2 (4%)	56,56,56	1.27	8 (14%)
12	CLA	T	4002	9	49,53,73	1.40	8 (16%)	58,89,113	1.49	4 (6%)
12	CLA	G	829	1	69,73,73	1.18	8 (11%)	82,113,113	1.42	5 (6%)
12	CLA	H	2126	2	69,73,73	1.19	8 (11%)	82,113,113	1.28	4 (4%)
12	CLA	G	810	1,12	69,73,73	1.18	8 (11%)	82,113,113	1.35	6 (7%)
13	A1AGD	a	840	-	30,30,30	1.80	8 (26%)	38,39,39	1.93	12 (31%)
12	CLA	A	806	1	54,58,73	1.31	7 (12%)	64,95,113	1.47	6 (9%)
12	CLA	G	851	27	69,73,73	1.16	7 (10%)	82,113,113	1.33	6 (7%)
12	CLA	G	832	1	69,73,73	1.18	6 (8%)	82,113,113	1.21	5 (6%)
12	CLA	a	805	1	69,73,73	1.16	9 (13%)	82,113,113	1.40	9 (10%)
12	CLA	A	808	1	54,58,73	1.30	8 (14%)	64,95,113	1.54	8 (12%)
15	BCR	i	101	-	41,41,41	1.02	2 (4%)	56,56,56	1.32	6 (10%)
15	BCR	H	2146	-	41,41,41	1.07	2 (4%)	56,56,56	1.35	6 (10%)
12	CLA	H	2127	2	69,73,73	1.16	7 (10%)	82,113,113	1.27	7 (8%)
12	CLA	G	808	1	54,58,73	1.30	8 (14%)	64,95,113	1.54	8 (12%)
12	CLA	S	102	-	49,53,73	1.41	6 (12%)	58,89,113	1.51	6 (10%)
12	CLA	K	4002	9	49,53,73	1.40	7 (14%)	58,89,113	1.49	4 (6%)
16	LHG	B	2149	12	42,42,48	0.64	0	45,48,54	1.22	4 (8%)
12	CLA	a	836	1	69,73,73	1.16	9 (13%)	82,113,113	1.27	4 (4%)
14	SF4	c	102	3	0,12,12	-	-	-	-	-
12	CLA	b	2121	-	59,63,73	1.27	7 (11%)	70,101,113	1.33	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	j	103	8	49,53,73	1.40	6 (12%)	58,89,113	1.47	5 (8%)
17	LMG	B	2148	-	51,51,55	0.75	0	59,59,63	1.30	8 (13%)
12	CLA	H	2130	-	49,53,73	1.39	8 (16%)	58,89,113	1.47	4 (6%)
12	CLA	F	204	-	49,53,73	1.40	6 (12%)	58,89,113	1.43	4 (6%)
12	CLA	a	812	1	69,73,73	1.19	8 (11%)	82,113,113	1.26	7 (8%)
20	ECH	B	2144	-	42,42,42	0.40	0	55,58,58	1.59	7 (12%)
12	CLA	a	829	1	69,73,73	1.18	7 (10%)	82,113,113	1.43	5 (6%)
12	CLA	G	831	1	64,68,73	1.21	8 (12%)	76,107,113	1.37	7 (9%)
12	CLA	B	2135	-	49,53,73	1.38	6 (12%)	58,89,113	1.49	6 (10%)
12	CLA	l	201	1	69,73,73	1.13	7 (10%)	82,113,113	1.32	8 (9%)
12	CLA	H	2106	-	69,73,73	1.16	5 (7%)	82,113,113	1.33	8 (9%)
12	CLA	H	2152	16	54,58,73	1.28	7 (12%)	64,95,113	1.49	5 (7%)
12	CLA	A	837	1	69,73,73	1.17	7 (10%)	82,113,113	1.33	6 (7%)
25	DGD	l	209	-	49,49,67	0.95	5 (10%)	57,57,81	1.37	7 (12%)
16	LHG	m	103	-	43,43,48	0.66	1 (2%)	46,49,54	1.23	4 (8%)
12	CLA	b	2115	2	49,53,73	1.42	7 (14%)	58,89,113	1.49	4 (6%)
12	CLA	b	2106	-	69,73,73	1.16	5 (7%)	82,113,113	1.33	8 (9%)
12	CLA	A	805	1	69,73,73	1.16	8 (11%)	82,113,113	1.40	9 (10%)
15	BCR	J	104	-	41,41,41	1.06	3 (7%)	56,56,56	1.27	7 (12%)
25	DGD	U	209	-	49,49,67	0.95	5 (10%)	57,57,81	1.36	7 (12%)
12	CLA	H	2108	2	69,73,73	1.17	7 (10%)	82,113,113	1.33	5 (6%)
12	CLA	a	832	1	69,73,73	1.17	7 (10%)	82,113,113	1.20	5 (6%)
12	CLA	A	804	1	69,73,73	1.15	8 (11%)	82,113,113	1.44	6 (7%)
12	CLA	a	802	1	69,73,73	1.17	8 (11%)	82,113,113	1.25	6 (7%)
12	CLA	A	829	1	69,73,73	1.18	8 (11%)	82,113,113	1.42	5 (6%)
23	ZEX	B	2152	-	43,43,43	5.84	26 (60%)	51,60,60	10.37	30 (58%)
12	CLA	B	2120	2	69,73,73	1.17	8 (11%)	82,113,113	1.28	8 (9%)
12	CLA	b	2136	2	49,53,73	1.38	9 (18%)	58,89,113	1.54	6 (10%)
12	CLA	H	2121	-	59,63,73	1.26	7 (11%)	70,101,113	1.33	7 (10%)
12	CLA	b	2132	2	69,73,73	1.15	5 (7%)	82,113,113	1.47	8 (9%)
12	CLA	H	2114	-	69,73,73	1.19	9 (13%)	82,113,113	1.33	7 (8%)
12	CLA	H	2134	-	49,53,73	1.37	6 (12%)	58,89,113	1.48	6 (10%)
12	CLA	A	815	-	49,53,73	1.40	7 (14%)	58,89,113	1.48	4 (6%)
12	CLA	J	102	-	49,53,73	1.40	6 (12%)	58,89,113	1.52	6 (10%)
15	BCR	A	842	-	41,41,41	1.04	2 (4%)	56,56,56	1.23	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	LHG	G	846	-	48,48,48	0.67	2 (4%)	51,54,54	1.29	7 (13%)
14	SF4	a	841	1,2	0,12,12	-	-	-		
12	CLA	A	819	1	69,73,73	1.19	7 (10%)	82,113,113	1.32	6 (7%)
12	CLA	a	831	1	64,68,73	1.21	8 (12%)	76,107,113	1.38	7 (9%)
14	SF4	C	101	3	0,12,12	-	-	-		
12	CLA	Q	201	27	69,73,73	1.17	8 (11%)	82,113,113	1.26	4 (4%)
17	LMG	A	849	-	32,32,55	1.00	1 (3%)	40,40,63	1.27	4 (10%)
12	CLA	B	2142	16	49,53,73	1.39	6 (12%)	58,89,113	1.55	7 (12%)
12	CLA	B	2133	2	69,73,73	1.16	5 (7%)	82,113,113	1.47	9 (10%)
15	BCR	j	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.34	8 (14%)
12	CLA	G	816	1	59,63,73	1.25	8 (13%)	70,101,113	1.45	7 (10%)
12	CLA	A	813	1	69,73,73	1.18	5 (7%)	82,113,113	1.34	5 (6%)
22	EQ3	H	2150	-	43,43,43	4.23	24 (55%)	55,60,60	5.22	27 (49%)
12	CLA	A	831	1	64,68,73	1.21	8 (12%)	76,107,113	1.38	7 (9%)
12	CLA	B	2121	-	59,63,73	1.28	8 (13%)	70,101,113	1.40	5 (7%)
12	CLA	b	2123	2	59,63,73	1.27	7 (11%)	70,101,113	1.45	8 (11%)
12	CLA	A	809	1	54,58,73	1.33	7 (12%)	64,95,113	1.46	9 (14%)
12	CLA	B	2114	-	49,53,73	1.42	6 (12%)	58,89,113	1.44	4 (6%)
12	CLA	A	824	27	69,73,73	1.20	7 (10%)	82,113,113	1.38	10 (12%)
12	CLA	H	2137	2	69,73,73	1.14	7 (10%)	82,113,113	1.31	7 (8%)
12	CLA	b	2127	2	69,73,73	1.15	7 (10%)	82,113,113	1.26	6 (7%)
12	CLA	G	833	1	69,73,73	1.14	8 (11%)	82,113,113	1.36	5 (6%)
12	CLA	G	850	27	69,73,73	1.16	9 (13%)	82,113,113	1.26	5 (6%)
16	LHG	a	846	-	48,48,48	0.67	2 (4%)	51,54,54	1.28	7 (13%)
12	CLA	H	2118	2	54,58,73	1.34	8 (14%)	64,95,113	1.49	6 (9%)
12	CLA	B	2116	2	49,53,73	1.41	8 (16%)	58,89,113	1.49	4 (6%)
12	CLA	L	201	1	69,73,73	1.13	7 (10%)	82,113,113	1.31	7 (8%)
12	CLA	l	204	10	69,73,73	1.14	9 (13%)	82,113,113	1.33	6 (7%)
12	CLA	k	4002	9	49,53,73	1.40	7 (14%)	58,89,113	1.49	4 (6%)
12	CLA	B	2138	2	69,73,73	1.15	8 (11%)	82,113,113	1.31	7 (8%)
14	SF4	G	841	1,2	0,12,12	-	-	-		
17	LMG	H	2147	-	51,51,55	0.75	0	59,59,63	1.30	8 (13%)
15	BCR	G	843	-	41,41,41	1.04	2 (4%)	56,56,56	1.26	8 (14%)
12	CLA	a	818	1	69,73,73	1.16	8 (11%)	82,113,113	1.33	8 (9%)
12	CLA	A	816	1	59,63,73	1.25	8 (13%)	70,101,113	1.45	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	ECH	m	101	-	42,42,42	0.39	0	55,58,58	0.74	0
15	BCR	S	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.33	8 (14%)
12	CLA	H	2104	-	69,73,73	1.13	8 (11%)	82,113,113	1.53	8 (9%)
12	CLA	b	2120	-	59,63,73	1.28	8 (13%)	70,101,113	1.41	5 (7%)
12	CLA	H	2131	2	59,63,73	1.26	8 (13%)	70,101,113	1.37	7 (10%)
17	LMG	b	2147	-	51,51,55	0.75	0	59,59,63	1.30	8 (13%)
15	BCR	B	2145	-	41,41,41	1.01	2 (4%)	56,56,56	1.35	8 (14%)
15	BCR	l	207	-	41,41,41	1.07	2 (4%)	56,56,56	1.35	8 (14%)
12	CLA	B	2140	27	69,73,73	1.14	8 (11%)	82,113,113	1.35	7 (8%)
12	CLA	b	2134	-	49,53,73	1.38	6 (12%)	58,89,113	1.49	6 (10%)
12	CLA	G	801	1	69,73,73	1.20	8 (11%)	82,113,113	1.30	7 (8%)
15	BCR	U	206	-	41,41,41	1.02	2 (4%)	56,56,56	1.23	5 (8%)
12	CLA	H	2109	-	69,73,73	1.15	8 (11%)	82,113,113	1.43	7 (8%)
12	CLA	H	2138	-	49,53,73	1.36	8 (16%)	58,89,113	1.42	5 (8%)
15	BCR	b	2145	-	41,41,41	1.05	2 (4%)	56,56,56	1.14	3 (5%)
15	BCR	F	202	-	41,41,41	1.04	2 (4%)	56,56,56	1.21	5 (8%)
12	CLA	H	2102	-	69,73,73	1.13	9 (13%)	82,113,113	1.47	9 (10%)
12	CLA	B	2137	2	49,53,73	1.38	8 (16%)	58,89,113	1.54	6 (10%)
23	ZEX	F	205	-	43,43,43	5.82	27 (62%)	51,60,60	10.43	30 (58%)
17	LMG	a	847	-	50,50,55	1.00	5 (10%)	58,58,63	1.28	6 (10%)
12	CLA	a	814	-	49,53,73	1.38	7 (14%)	58,89,113	1.56	6 (10%)
16	LHG	A	848	12	48,48,48	0.63	1 (2%)	51,54,54	1.26	6 (11%)
17	LMG	G	847	-	50,50,55	1.00	5 (10%)	58,58,63	1.29	6 (10%)
12	CLA	G	854	-	59,63,73	1.27	8 (13%)	70,101,113	1.40	9 (12%)
12	CLA	F	203	-	49,53,73	1.40	8 (16%)	58,89,113	1.41	5 (8%)
12	CLA	b	2128	2	69,73,73	1.18	8 (11%)	82,113,113	1.18	6 (7%)
12	CLA	A	821	1	64,68,73	1.21	8 (12%)	76,107,113	1.32	4 (5%)
12	CLA	A	803	1,12	59,63,73	1.27	6 (10%)	70,101,113	1.39	7 (10%)
12	CLA	a	834	1	59,63,73	1.26	7 (11%)	70,101,113	1.47	11 (15%)
15	BCR	G	845	-	41,41,41	1.11	2 (4%)	56,56,56	1.28	4 (7%)
12	CLA	G	837	1	69,73,73	1.18	7 (10%)	82,113,113	1.33	6 (7%)
12	CLA	H	2110	2	69,73,73	1.21	6 (8%)	82,113,113	1.33	5 (6%)
12	CLA	A	850	27	69,73,73	1.16	8 (11%)	82,113,113	1.25	5 (6%)
14	SF4	A	841	1,2	0,12,12	-	-	-	-	-
15	BCR	T	4001	-	41,41,41	1.02	3 (7%)	56,56,56	1.31	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	H	2116	-	49,53,73	1.39	7 (14%)	58,89,113	1.49	5 (8%)
12	CLA	B	2102	27	69,73,73	1.14	8 (11%)	82,113,113	1.28	7 (8%)
15	BCR	H	2145	-	41,41,41	1.06	2 (4%)	56,56,56	1.14	3 (5%)
12	CLA	A	836	1	69,73,73	1.16	8 (11%)	82,113,113	1.27	4 (4%)
12	CLA	B	2129	2	69,73,73	1.18	8 (11%)	82,113,113	1.18	5 (6%)
14	SF4	C	102	3	0,12,12	-	-	-	-	-
13	A1AGD	H	2153	-	30,30,30	2.73	6 (20%)	38,39,39	2.83	13 (34%)
12	CLA	B	2105	-	69,73,73	1.13	8 (11%)	82,113,113	1.53	8 (9%)
12	CLA	b	2141	16	49,53,73	1.39	6 (12%)	58,89,113	1.55	7 (12%)
12	CLA	a	801	1	69,73,73	1.20	9 (13%)	82,113,113	1.30	7 (8%)
12	CLA	H	2140	2	69,73,73	1.18	6 (8%)	82,113,113	1.34	5 (6%)
12	CLA	b	2107	2	69,73,73	1.17	9 (13%)	82,113,113	1.27	4 (4%)
12	CLA	B	2108	2	69,73,73	1.18	9 (13%)	82,113,113	1.27	4 (4%)
12	CLA	B	2126	27	54,58,73	1.31	8 (14%)	64,95,113	1.45	8 (12%)
12	CLA	G	817	1	64,68,73	1.21	9 (14%)	76,107,113	1.29	8 (10%)
12	CLA	G	835	1	69,73,73	1.16	9 (13%)	82,113,113	1.29	8 (9%)
15	BCR	K	4001	-	41,41,41	1.02	2 (4%)	56,56,56	1.31	5 (8%)
12	CLA	G	825	27	64,68,73	1.21	8 (12%)	76,107,113	1.39	10 (13%)
12	CLA	B	2134	2	69,73,73	1.18	7 (10%)	82,113,113	1.33	6 (7%)
12	CLA	B	2104	2	69,73,73	1.16	7 (10%)	82,113,113	1.33	6 (7%)
12	CLA	A	832	1	69,73,73	1.17	7 (10%)	82,113,113	1.21	4 (4%)
12	CLA	G	812	1	69,73,73	1.19	8 (11%)	82,113,113	1.26	7 (8%)
12	CLA	A	839	1	69,73,73	1.18	8 (11%)	82,113,113	1.31	6 (7%)
23	ZEX	f	205	-	43,43,43	5.82	27 (62%)	51,60,60	10.43	30 (58%)
15	BCR	R	101	-	41,41,41	1.02	2 (4%)	56,56,56	1.31	6 (10%)
15	BCR	k	4001	-	41,41,41	1.01	2 (4%)	56,56,56	1.31	5 (8%)
12	CLA	a	803	1,12	59,63,73	1.27	6 (10%)	70,101,113	1.39	8 (11%)
17	LMG	A	847	-	50,50,55	1.00	5 (10%)	58,58,63	1.29	6 (10%)
15	BCR	B	2147	-	41,41,41	1.07	2 (4%)	56,56,56	1.35	6 (10%)
12	CLA	B	2136	-	49,53,73	1.39	8 (16%)	58,89,113	1.43	5 (8%)
12	CLA	B	2141	2	69,73,73	1.18	6 (8%)	82,113,113	1.34	5 (6%)
12	CLA	a	813	1	69,73,73	1.18	6 (8%)	82,113,113	1.34	5 (6%)
23	ZEX	b	2151	-	43,43,43	5.85	26 (60%)	51,60,60	10.37	30 (58%)
16	LHG	b	2148	12	42,42,48	0.63	0	45,48,54	1.22	4 (8%)
15	BCR	f	202	-	41,41,41	1.04	2 (4%)	56,56,56	1.20	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	BCR	a	842	-	41,41,41	1.04	2 (4%)	56,56,56	1.23	5 (8%)
12	CLA	H	2105	2	69,73,73	1.16	7 (10%)	82,113,113	1.32	7 (8%)
12	CLA	a	839	1	69,73,73	1.18	8 (11%)	82,113,113	1.31	6 (7%)
24	SQD	U	208	-	43,45,54	1.67	8 (18%)	53,56,65	1.58	7 (13%)
12	CLA	G	826	1	69,73,73	1.19	8 (11%)	82,113,113	1.28	6 (7%)
16	LHG	M	102	-	43,43,48	0.66	1 (2%)	46,49,54	1.23	4 (8%)
12	CLA	b	2108	2	69,73,73	1.17	7 (10%)	82,113,113	1.34	5 (6%)
12	CLA	B	2111	2	69,73,73	1.21	7 (10%)	82,113,113	1.33	5 (6%)
22	EQ3	b	2150	-	43,43,43	4.23	24 (55%)	55,60,60	5.22	27 (49%)
12	CLA	A	822	-	54,58,73	1.31	7 (12%)	64,95,113	1.40	6 (9%)
16	LHG	V	103	-	43,43,48	0.66	1 (2%)	46,49,54	1.23	4 (8%)
12	CLA	G	820	27	69,73,73	1.15	8 (11%)	82,113,113	1.37	8 (9%)
12	CLA	B	2107	-	69,73,73	1.16	5 (7%)	82,113,113	1.33	8 (9%)
12	CLA	H	2115	2	49,53,73	1.41	7 (14%)	58,89,113	1.49	4 (6%)
12	CLA	B	2123	-	49,53,73	1.40	8 (16%)	58,89,113	1.37	4 (6%)
12	CLA	B	2113	2	69,73,73	1.18	7 (10%)	82,113,113	1.27	5 (6%)
12	CLA	A	812	1	69,73,73	1.19	8 (11%)	82,113,113	1.26	7 (8%)
13	A1AGD	B	2153	-	30,30,30	2.73	6 (20%)	38,39,39	2.83	13 (34%)
12	CLA	A	811	-	49,53,73	1.39	7 (14%)	58,89,113	1.44	4 (6%)
12	CLA	H	2103	2	69,73,73	1.16	7 (10%)	82,113,113	1.32	6 (7%)
12	CLA	G	834	1	59,63,73	1.26	7 (11%)	70,101,113	1.47	11 (15%)
12	CLA	G	828	-	69,73,73	1.15	7 (10%)	82,113,113	1.27	6 (7%)
12	CLA	A	807	1	69,73,73	1.15	8 (11%)	82,113,113	1.35	8 (9%)
12	CLA	B	2139	-	49,53,73	1.36	8 (16%)	58,89,113	1.42	5 (8%)
12	CLA	H	2136	2	49,53,73	1.38	8 (16%)	58,89,113	1.53	6 (10%)
16	LHG	a	848	12	48,48,48	0.64	1 (2%)	51,54,54	1.26	6 (11%)
15	BCR	I	101	-	41,41,41	1.02	2 (4%)	56,56,56	1.31	6 (10%)
15	BCR	b	2144	-	41,41,41	1.01	2 (4%)	56,56,56	1.35	8 (14%)
12	CLA	G	830	1	59,63,73	1.26	8 (13%)	70,101,113	1.44	10 (14%)
12	CLA	B	2124	2	59,63,73	1.26	7 (11%)	70,101,113	1.45	8 (11%)
12	CLA	U	204	10	69,73,73	1.13	8 (11%)	82,113,113	1.34	6 (7%)
15	BCR	G	842	-	41,41,41	1.04	2 (4%)	56,56,56	1.23	5 (8%)
24	SQD	V	102	-	52,54,54	1.56	7 (13%)	62,65,65	1.37	8 (12%)
18	45D	a	852	-	43,43,43	0.39	0	54,60,60	0.85	0
12	CLA	B	2119	2	54,58,73	1.34	8 (14%)	64,95,113	1.49	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	a	850	27	69,73,73	1.16	9 (13%)	82,113,113	1.25	5 (6%)
12	CLA	A	818	1	69,73,73	1.16	8 (11%)	82,113,113	1.33	8 (9%)
12	CLA	a	820	27	69,73,73	1.15	8 (11%)	82,113,113	1.38	8 (9%)
22	EQ3	B	2151	-	43,43,43	4.23	23 (53%)	55,60,60	5.22	27 (49%)
15	BCR	a	845	-	41,41,41	1.11	2 (4%)	56,56,56	1.29	4 (7%)
16	LHG	A	846	-	48,48,48	0.67	2 (4%)	51,54,54	1.28	7 (13%)
12	CLA	G	807	1	69,73,73	1.14	8 (11%)	82,113,113	1.35	8 (9%)
25	DGD	L	209	-	49,49,67	0.95	5 (10%)	57,57,81	1.37	7 (12%)
12	CLA	G	818	1	69,73,73	1.15	9 (13%)	82,113,113	1.33	8 (9%)
12	CLA	b	2111	2	69,73,73	1.18	8 (11%)	82,113,113	1.57	13 (15%)
12	CLA	a	808	1	54,58,73	1.30	8 (14%)	64,95,113	1.54	8 (12%)
12	CLA	l	203	10	69,73,73	1.14	8 (11%)	82,113,113	1.36	8 (9%)
12	CLA	H	2107	2	69,73,73	1.18	9 (13%)	82,113,113	1.27	5 (6%)
15	BCR	B	2146	-	41,41,41	1.06	2 (4%)	56,56,56	1.14	3 (5%)
12	CLA	a	828	-	69,73,73	1.16	7 (10%)	82,113,113	1.28	6 (7%)
12	CLA	G	823	1	64,68,73	1.21	9 (14%)	76,107,113	1.38	7 (9%)
12	CLA	H	2123	2	59,63,73	1.26	7 (11%)	70,101,113	1.45	8 (11%)
12	CLA	A	828	-	69,73,73	1.15	7 (10%)	82,113,113	1.28	6 (7%)
12	CLA	b	2119	2	69,73,73	1.17	8 (11%)	82,113,113	1.29	8 (9%)
12	CLA	B	2112	2	69,73,73	1.18	8 (11%)	82,113,113	1.57	13 (15%)
20	ECH	M	103	-	42,42,42	0.39	0	55,58,58	0.74	0
12	CLA	b	2113	-	49,53,73	1.42	6 (12%)	58,89,113	1.44	4 (6%)
12	CLA	B	2125	27	69,73,73	1.18	7 (10%)	82,113,113	1.31	8 (9%)
12	CLA	b	2137	2	69,73,73	1.14	7 (10%)	82,113,113	1.31	7 (8%)
12	CLA	f	204	-	49,53,73	1.39	6 (12%)	58,89,113	1.43	4 (6%)
12	CLA	a	830	1	59,63,73	1.25	8 (13%)	70,101,113	1.45	10 (14%)
12	CLA	L	205	27	69,73,73	1.17	7 (10%)	82,113,113	1.30	7 (8%)
12	CLA	b	2129	2	69,73,73	1.21	11 (15%)	82,113,113	1.36	7 (8%)
12	CLA	a	826	1	69,73,73	1.19	8 (11%)	82,113,113	1.28	6 (7%)
12	CLA	a	854	-	59,63,73	1.26	7 (11%)	70,101,113	1.40	9 (12%)
12	CLA	U	205	27	69,73,73	1.17	7 (10%)	82,113,113	1.30	7 (8%)
18	45D	A	852	-	43,43,43	0.38	0	54,60,60	0.86	0
12	CLA	b	2139	27	69,73,73	1.14	8 (11%)	82,113,113	1.35	7 (8%)
15	BCR	H	2142	-	41,41,41	1.09	2 (4%)	56,56,56	1.20	5 (8%)
12	CLA	b	2105	2	69,73,73	1.16	7 (10%)	82,113,113	1.32	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	b	2101	27	69,73,73	1.14	8 (11%)	82,113,113	1.28	8 (9%)
12	CLA	H	2119	2	69,73,73	1.17	8 (11%)	82,113,113	1.28	6 (7%)
12	CLA	G	839	1	69,73,73	1.18	8 (11%)	82,113,113	1.31	6 (7%)
12	CLA	a	824	27	69,73,73	1.19	7 (10%)	82,113,113	1.37	10 (12%)
12	CLA	a	821	1	64,68,73	1.20	8 (12%)	76,107,113	1.32	4 (5%)
12	CLA	a	811	-	49,53,73	1.39	7 (14%)	58,89,113	1.44	4 (6%)
12	CLA	G	824	27	69,73,73	1.19	7 (10%)	82,113,113	1.38	10 (12%)
12	CLA	A	825	27	64,68,73	1.20	8 (12%)	76,107,113	1.39	10 (13%)
12	CLA	H	2120	-	59,63,73	1.28	8 (13%)	70,101,113	1.40	5 (7%)
15	BCR	A	844	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	7 (12%)
12	CLA	a	817	1	64,68,73	1.22	9 (14%)	76,107,113	1.29	8 (10%)
12	CLA	a	807	1	69,73,73	1.14	8 (11%)	82,113,113	1.36	8 (9%)
12	CLA	B	2127	2	69,73,73	1.18	8 (11%)	82,113,113	1.28	4 (4%)
15	BCR	G	844	-	41,41,41	1.07	2 (4%)	56,56,56	1.27	7 (12%)
12	CLA	A	814	-	49,53,73	1.38	7 (14%)	58,89,113	1.56	6 (10%)
12	CLA	H	2113	-	49,53,73	1.42	6 (12%)	58,89,113	1.43	4 (6%)
17	LMG	G	849	-	32,32,55	1.00	1 (3%)	40,40,63	1.27	4 (10%)
12	CLA	G	806	1	54,58,73	1.31	7 (12%)	64,95,113	1.46	6 (9%)
12	CLA	b	2126	2	69,73,73	1.19	8 (11%)	82,113,113	1.27	4 (4%)
12	CLA	G	814	-	49,53,73	1.38	7 (14%)	58,89,113	1.56	6 (10%)
23	ZEX	H	2151	-	43,43,43	5.84	26 (60%)	51,60,60	10.36	30 (58%)
12	CLA	A	834	1	59,63,73	1.26	7 (11%)	70,101,113	1.47	11 (15%)
12	CLA	a	825	27	64,68,73	1.21	8 (12%)	76,107,113	1.39	10 (13%)
13	A1AGD	b	2153	-	30,30,30	2.73	6 (20%)	38,39,39	2.83	13 (34%)
15	BCR	b	2146	-	41,41,41	1.07	2 (4%)	56,56,56	1.35	6 (10%)
12	CLA	H	2112	2	69,73,73	1.18	8 (11%)	82,113,113	1.27	4 (4%)
16	LHG	G	848	12	48,48,48	0.63	1 (2%)	51,54,54	1.26	6 (11%)
20	ECH	V	101	-	42,42,42	0.39	0	55,58,58	0.74	0
12	CLA	G	822	-	54,58,73	1.31	7 (12%)	64,95,113	1.41	6 (9%)
12	CLA	b	2117	2	49,53,73	1.39	5 (10%)	58,89,113	1.54	6 (10%)
12	CLA	A	851	27	69,73,73	1.16	7 (10%)	82,113,113	1.33	6 (7%)
12	CLA	G	811	-	49,53,73	1.39	6 (12%)	58,89,113	1.44	4 (6%)
12	CLA	G	819	1	69,73,73	1.19	7 (10%)	82,113,113	1.32	6 (7%)
12	CLA	G	803	1,12	59,63,73	1.27	5 (8%)	70,101,113	1.39	8 (11%)
12	CLA	L	203	10	69,73,73	1.15	8 (11%)	82,113,113	1.37	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	A	810	1,12	69,73,73	1.18	8 (11%)	82,113,113	1.35	6 (7%)
12	CLA	B	2103	-	69,73,73	1.14	9 (13%)	82,113,113	1.47	10 (12%)
15	BCR	S	104	-	41,41,41	1.07	2 (4%)	56,56,56	1.28	7 (12%)
12	CLA	U	201	1	69,73,73	1.13	7 (10%)	82,113,113	1.31	7 (8%)
12	CLA	b	2133	2	69,73,73	1.18	8 (11%)	82,113,113	1.34	6 (7%)
12	CLA	a	833	1	69,73,73	1.14	8 (11%)	82,113,113	1.35	5 (6%)
15	BCR	H	2144	-	41,41,41	1.00	2 (4%)	56,56,56	1.35	8 (14%)
12	CLA	b	2102	-	69,73,73	1.14	9 (13%)	82,113,113	1.47	10 (12%)
12	CLA	H	2125	27	54,58,73	1.31	8 (14%)	64,95,113	1.45	7 (10%)
15	BCR	b	2142	-	41,41,41	1.09	2 (4%)	56,56,56	1.19	5 (8%)
12	CLA	f	203	-	49,53,73	1.40	8 (16%)	58,89,113	1.41	5 (8%)
12	CLA	A	838	1	69,73,73	1.18	8 (11%)	82,113,113	1.36	6 (7%)
12	CLA	H	2117	2	49,53,73	1.39	5 (10%)	58,89,113	1.55	6 (10%)
12	CLA	B	2110	-	69,73,73	1.15	8 (11%)	82,113,113	1.43	7 (8%)
12	CLA	G	802	1	69,73,73	1.16	8 (11%)	82,113,113	1.26	6 (7%)
20	ECH	H	2143	-	42,42,42	0.40	0	55,58,58	1.59	7 (12%)
12	CLA	B	2128	2	69,73,73	1.15	7 (10%)	82,113,113	1.27	6 (7%)
12	CLA	b	2114	-	69,73,73	1.18	9 (13%)	82,113,113	1.33	7 (8%)
15	BCR	Q	202	-	41,41,41	1.05	2 (4%)	56,56,56	1.21	5 (8%)
15	BCR	a	843	-	41,41,41	1.03	2 (4%)	56,56,56	1.27	8 (14%)
12	CLA	B	2101	16	54,58,73	1.28	7 (12%)	64,95,113	1.49	5 (7%)
12	CLA	S	103	8	49,53,73	1.40	6 (12%)	58,89,113	1.47	5 (8%)
12	CLA	B	2115	-	69,73,73	1.19	9 (13%)	82,113,113	1.33	7 (8%)
12	CLA	a	823	1	64,68,73	1.21	8 (12%)	76,107,113	1.38	7 (9%)
12	CLA	a	806	1	54,58,73	1.31	7 (12%)	64,95,113	1.47	6 (9%)
12	CLA	U	203	10	69,73,73	1.15	8 (11%)	82,113,113	1.38	9 (10%)
12	CLA	b	2116	-	49,53,73	1.39	7 (14%)	58,89,113	1.48	5 (8%)
12	CLA	H	2135	-	49,53,73	1.39	8 (16%)	58,89,113	1.43	5 (8%)
14	SF4	N	101	3	0,12,12	-	-	-	-	-
12	CLA	G	813	1	69,73,73	1.18	6 (8%)	82,113,113	1.34	6 (7%)
12	CLA	G	838	1	69,73,73	1.18	8 (11%)	82,113,113	1.36	7 (8%)
15	BCR	L	206	-	41,41,41	1.02	2 (4%)	56,56,56	1.23	5 (8%)
15	BCR	U	207	-	41,41,41	1.07	2 (4%)	56,56,56	1.35	8 (14%)
12	CLA	L	204	10	69,73,73	1.14	8 (11%)	82,113,113	1.33	6 (7%)
12	CLA	A	833	1	69,73,73	1.14	8 (11%)	82,113,113	1.35	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	A	802	1	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
12	CLA	A	830	1	59,63,73	1.26	8 (13%)	70,101,113	1.45	10 (14%)
12	CLA	B	2117	-	49,53,73	1.39	7 (14%)	58,89,113	1.48	5 (8%)
12	CLA	a	837	1	69,73,73	1.17	7 (10%)	82,113,113	1.31	6 (7%)
12	CLA	G	815	-	49,53,73	1.39	6 (12%)	58,89,113	1.49	4 (6%)
26	LMT	L	210	-	36,36,36	1.16	5 (13%)	47,47,47	0.99	0
12	CLA	B	2118	2	49,53,73	1.39	5 (10%)	58,89,113	1.55	6 (10%)
12	CLA	H	2122	-	49,53,73	1.40	7 (14%)	58,89,113	1.37	4 (6%)
12	CLA	b	2131	2	59,63,73	1.26	8 (13%)	70,101,113	1.37	7 (10%)
15	BCR	l	206	-	41,41,41	1.02	2 (4%)	56,56,56	1.23	5 (8%)
12	CLA	H	2128	2	69,73,73	1.18	8 (11%)	82,113,113	1.17	5 (6%)
12	CLA	a	816	1	59,63,73	1.25	8 (13%)	70,101,113	1.46	7 (10%)
14	SF4	N	102	3	0,12,12	-	-	-	-	-
18	45D	G	852	-	43,43,43	0.38	0	54,60,60	0.86	0
12	CLA	Q	203	-	49,53,73	1.41	8 (16%)	58,89,113	1.40	5 (8%)
12	CLA	H	2101	27	69,73,73	1.15	8 (11%)	82,113,113	1.29	7 (8%)
15	BCR	A	845	-	41,41,41	1.11	2 (4%)	56,56,56	1.29	4 (7%)
15	BCR	J	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.33	8 (14%)
12	CLA	B	2109	2	69,73,73	1.17	7 (10%)	82,113,113	1.33	5 (6%)
12	CLA	G	809	1	54,58,73	1.34	7 (12%)	64,95,113	1.45	9 (14%)
24	SQD	M	101	-	52,54,54	1.55	7 (13%)	62,65,65	1.37	8 (12%)
12	CLA	a	804	1	69,73,73	1.16	8 (11%)	82,113,113	1.44	6 (7%)
12	CLA	f	201	27	69,73,73	1.18	8 (11%)	82,113,113	1.27	5 (6%)
12	CLA	H	2132	2	69,73,73	1.16	5 (7%)	82,113,113	1.47	8 (9%)
12	CLA	G	827	-	69,73,73	1.15	7 (10%)	82,113,113	1.30	6 (7%)
16	LHG	H	2148	12	42,42,48	0.64	0	45,48,54	1.22	4 (8%)
12	CLA	l	205	27	69,73,73	1.17	7 (10%)	82,113,113	1.30	7 (8%)
12	CLA	a	838	1	69,73,73	1.18	8 (11%)	82,113,113	1.37	6 (7%)
12	CLA	A	820	27	69,73,73	1.16	8 (11%)	82,113,113	1.38	8 (9%)
12	CLA	b	2118	2	54,58,73	1.34	8 (14%)	64,95,113	1.48	6 (9%)
12	CLA	B	2130	2	69,73,73	1.20	11 (15%)	82,113,113	1.36	7 (8%)
20	ECH	b	2143	-	42,42,42	0.40	0	55,58,58	1.59	7 (12%)
12	CLA	b	2130	-	49,53,73	1.39	8 (16%)	58,89,113	1.47	4 (6%)
12	CLA	b	2103	2	69,73,73	1.16	7 (10%)	82,113,113	1.33	6 (7%)
26	LMT	l	210	-	36,36,36	1.16	5 (13%)	47,47,47	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	LMG	a	849	-	32,32,55	1.00	1 (3%)	40,40,63	1.26	4 (10%)
12	CLA	a	815	-	49,53,73	1.40	6 (12%)	58,89,113	1.49	4 (6%)
12	CLA	A	826	1	69,73,73	1.19	8 (11%)	82,113,113	1.28	6 (7%)
12	CLA	A	854	-	59,63,73	1.26	7 (11%)	70,101,113	1.40	9 (12%)
12	CLA	F	201	27	69,73,73	1.17	8 (11%)	82,113,113	1.27	5 (6%)
23	ZEX	Q	205	-	43,43,43	5.82	27 (62%)	51,60,60	10.43	30 (58%)
12	CLA	b	2104	-	69,73,73	1.13	9 (13%)	82,113,113	1.52	8 (9%)
15	BCR	a	844	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	7 (12%)
12	CLA	a	851	27	69,73,73	1.16	7 (10%)	82,113,113	1.33	6 (7%)
12	CLA	G	821	1	64,68,73	1.21	8 (12%)	76,107,113	1.32	4 (5%)
12	CLA	b	2122	-	49,53,73	1.41	7 (14%)	58,89,113	1.38	4 (6%)
12	CLA	H	2111	2	69,73,73	1.18	8 (11%)	82,113,113	1.57	13 (15%)
12	CLA	a	835	1	69,73,73	1.16	9 (13%)	82,113,113	1.28	8 (9%)
12	CLA	a	809	1	54,58,73	1.34	8 (14%)	64,95,113	1.45	9 (14%)
15	BCR	L	207	-	41,41,41	1.07	2 (4%)	56,56,56	1.35	8 (14%)
12	CLA	b	2152	16	54,58,73	1.28	8 (14%)	64,95,113	1.49	5 (7%)
12	CLA	a	827	-	69,73,73	1.15	7 (10%)	82,113,113	1.30	6 (7%)
13	A1AGD	A	840	-	30,30,30	1.80	8 (26%)	38,39,39	1.94	12 (31%)
12	CLA	A	823	1	64,68,73	1.21	8 (12%)	76,107,113	1.37	6 (7%)
12	CLA	A	817	1	64,68,73	1.22	9 (14%)	76,107,113	1.30	8 (10%)
13	A1AGD	G	840	-	30,30,30	1.80	8 (26%)	38,39,39	1.94	12 (31%)
14	SF4	c	101	3	0,12,12	-	-	-	-	-
12	CLA	j	102	-	49,53,73	1.41	6 (12%)	58,89,113	1.51	6 (10%)
12	CLA	b	2109	-	69,73,73	1.15	8 (11%)	82,113,113	1.44	7 (8%)
12	CLA	b	2138	-	49,53,73	1.36	8 (16%)	58,89,113	1.42	5 (8%)
12	CLA	A	835	1	69,73,73	1.16	9 (13%)	82,113,113	1.28	8 (9%)
12	CLA	A	827	-	69,73,73	1.15	7 (10%)	82,113,113	1.30	6 (7%)
12	CLA	a	822	-	54,58,73	1.31	7 (12%)	64,95,113	1.40	6 (9%)
26	LMT	U	210	-	36,36,36	1.16	5 (13%)	47,47,47	1.00	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	a	819	1	-	18/39/115/115	-
12	CLA	Q	204	-	-	5/15/91/115	-
12	CLA	a	810	1,12	-	15/39/115/115	-
12	CLA	b	2124	27	-	6/39/115/115	-
12	CLA	B	2122	-	-	10/27/103/115	-
12	CLA	G	805	1	-	14/39/115/115	-
12	CLA	b	2110	2	-	14/39/115/115	-
12	CLA	A	801	1	-	5/39/115/115	-
12	CLA	H	2133	2	-	18/39/115/115	-
12	CLA	B	2132	2	-	7/27/103/115	-
15	BCR	j	104	-	-	9/29/63/63	0/2/2/2
12	CLA	b	2135	-	-	9/15/91/115	-
12	CLA	H	2141	16	-	7/15/91/115	-
12	CLA	b	2140	2	-	16/39/115/115	-
12	CLA	H	2129	2	-	13/39/115/115	-
24	SQD	L	208	-	-	15/40/60/69	0/1/1/1
12	CLA	G	804	1	-	16/39/115/115	-
12	CLA	H	2139	27	-	10/39/115/115	-
24	SQD	l	208	-	-	15/40/60/69	0/1/1/1
12	CLA	H	2124	27	-	6/39/115/115	-
24	SQD	m	102	-	-	28/49/69/69	0/1/1/1
12	CLA	B	2131	-	-	2/15/91/115	-
12	CLA	b	2112	2	-	8/39/115/115	-
12	CLA	G	836	1	-	14/39/115/115	-
12	CLA	J	103	8	-	10/15/91/115	-
12	CLA	b	2125	27	-	4/21/97/115	-
12	CLA	B	2106	2	-	9/39/115/115	-
15	BCR	B	2143	-	-	6/29/63/63	0/2/2/2
15	BCR	A	843	-	-	15/29/63/63	0/2/2/2
12	CLA	T	4002	9	-	9/15/91/115	-
12	CLA	G	829	1	-	12/39/115/115	-
12	CLA	H	2126	2	-	11/39/115/115	-
12	CLA	G	810	1,12	-	15/39/115/115	-
13	A1AGD	a	840	-	2/2/9/11	8/23/43/43	0/1/1/1
12	CLA	A	806	1	-	7/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	G	851	27	-	13/39/115/115	-
12	CLA	G	832	1	-	12/39/115/115	-
12	CLA	a	805	1	-	14/39/115/115	-
12	CLA	A	808	1	-	3/21/97/115	-
15	BCR	i	101	-	-	7/29/63/63	0/2/2/2
15	BCR	H	2146	-	-	17/29/63/63	0/2/2/2
12	CLA	H	2127	2	-	16/39/115/115	-
12	CLA	G	808	1	-	3/21/97/115	-
12	CLA	S	102	-	-	9/15/91/115	-
12	CLA	K	4002	9	-	9/15/91/115	-
16	LHG	B	2149	12	-	18/47/47/53	-
12	CLA	a	836	1	-	14/39/115/115	-
14	SF4	c	102	3	-	-	0/6/5/5
12	CLA	b	2121	-	-	10/27/103/115	-
12	CLA	j	103	8	-	10/15/91/115	-
17	LMG	B	2148	-	-	14/46/66/70	0/1/1/1
12	CLA	H	2130	-	-	2/15/91/115	-
12	CLA	F	204	-	-	5/15/91/115	-
12	CLA	a	812	1	-	13/39/115/115	-
20	ECH	B	2144	-	-	12/29/66/66	0/2/2/2
12	CLA	a	829	1	-	12/39/115/115	-
12	CLA	G	831	1	-	9/33/109/115	-
12	CLA	B	2135	-	-	4/15/91/115	-
12	CLA	l	201	1	-	15/39/115/115	-
12	CLA	H	2106	-	-	16/39/115/115	-
12	CLA	H	2152	16	-	5/21/97/115	-
12	CLA	A	837	1	-	11/39/115/115	-
25	DGD	l	209	-	-	21/44/64/95	0/1/1/2
16	LHG	m	103	-	-	24/48/48/53	-
12	CLA	b	2115	2	-	4/15/91/115	-
12	CLA	b	2106	-	-	16/39/115/115	-
12	CLA	A	805	1	-	14/39/115/115	-
15	BCR	J	104	-	-	9/29/63/63	0/2/2/2
25	DGD	U	209	-	-	21/44/64/95	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	H	2108	2	-	11/39/115/115	-
12	CLA	a	832	1	-	12/39/115/115	-
12	CLA	A	804	1	-	16/39/115/115	-
12	CLA	a	802	1	-	9/39/115/115	-
12	CLA	A	829	1	-	12/39/115/115	-
23	ZEX	B	2152	-	-	11/29/67/67	0/2/2/2
12	CLA	B	2120	2	-	16/39/115/115	-
12	CLA	b	2136	2	-	7/15/91/115	-
12	CLA	H	2121	-	-	10/27/103/115	-
12	CLA	b	2132	2	-	18/39/115/115	-
12	CLA	H	2114	-	-	18/39/115/115	-
12	CLA	H	2134	-	-	4/15/91/115	-
12	CLA	A	815	-	-	5/15/91/115	-
12	CLA	J	102	-	-	9/15/91/115	-
15	BCR	A	842	-	-	12/29/63/63	0/2/2/2
16	LHG	G	846	-	-	28/53/53/53	-
14	SF4	a	841	1,2	-	-	0/6/5/5
12	CLA	A	819	1	-	18/39/115/115	-
12	CLA	a	831	1	-	9/33/109/115	-
14	SF4	C	101	3	-	-	0/6/5/5
12	CLA	Q	201	27	-	21/39/115/115	-
17	LMG	A	849	-	-	14/26/46/70	0/1/1/1
12	CLA	B	2142	16	-	7/15/91/115	-
12	CLA	B	2133	2	-	18/39/115/115	-
15	BCR	j	101	-	-	13/29/63/63	0/2/2/2
12	CLA	G	816	1	-	4/27/103/115	-
12	CLA	A	813	1	-	14/39/115/115	-
22	EQ3	H	2150	-	-	14/29/68/68	0/2/2/2
12	CLA	A	831	1	-	9/33/109/115	-
12	CLA	B	2121	-	-	8/27/103/115	-
12	CLA	b	2123	2	-	12/27/103/115	-
12	CLA	A	809	1	-	10/21/97/115	-
12	CLA	B	2114	-	-	10/15/91/115	-
12	CLA	A	824	27	-	19/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	H	2137	2	-	7/39/115/115	-
12	CLA	b	2127	2	-	16/39/115/115	-
12	CLA	G	833	1	-	15/39/115/115	-
12	CLA	G	850	27	-	6/39/115/115	-
16	LHG	a	846	-	-	27/53/53/53	-
12	CLA	H	2118	2	-	7/21/97/115	-
12	CLA	B	2116	2	-	4/15/91/115	-
12	CLA	L	201	1	-	15/39/115/115	-
12	CLA	l	204	10	-	8/39/115/115	-
12	CLA	k	4002	9	-	9/15/91/115	-
12	CLA	B	2138	2	-	7/39/115/115	-
14	SF4	G	841	1,2	-	-	0/6/5/5
17	LMG	H	2147	-	-	14/46/66/70	0/1/1/1
15	BCR	G	843	-	-	15/29/63/63	0/2/2/2
12	CLA	a	818	1	-	11/39/115/115	-
12	CLA	A	816	1	-	4/27/103/115	-
20	ECH	m	101	-	-	10/29/66/66	0/2/2/2
15	BCR	S	101	-	-	13/29/63/63	0/2/2/2
12	CLA	H	2104	-	-	8/39/115/115	-
12	CLA	b	2120	-	-	8/27/103/115	-
12	CLA	H	2131	2	-	7/27/103/115	-
17	LMG	b	2147	-	-	14/46/66/70	0/1/1/1
15	BCR	B	2145	-	-	8/29/63/63	0/2/2/2
15	BCR	l	207	-	-	6/29/63/63	0/2/2/2
12	CLA	B	2140	27	-	10/39/115/115	-
12	CLA	b	2134	-	-	4/15/91/115	-
12	CLA	G	801	1	-	5/39/115/115	-
15	BCR	U	206	-	-	10/29/63/63	0/2/2/2
12	CLA	H	2109	-	-	13/39/115/115	-
12	CLA	H	2138	-	-	6/15/91/115	-
15	BCR	b	2145	-	-	7/29/63/63	0/2/2/2
15	BCR	F	202	-	-	13/29/63/63	0/2/2/2
12	CLA	H	2102	-	-	12/39/115/115	-
12	CLA	B	2137	2	-	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	ZEX	F	205	-	-	14/29/67/67	0/2/2/2
17	LMG	a	847	-	-	20/45/65/70	0/1/1/1
12	CLA	a	814	-	-	4/15/91/115	-
16	LHG	A	848	12	-	19/53/53/53	-
17	LMG	G	847	-	-	20/45/65/70	0/1/1/1
12	CLA	G	854	-	-	7/27/103/115	-
12	CLA	F	203	-	-	6/15/91/115	-
12	CLA	b	2128	2	-	12/39/115/115	-
12	CLA	A	821	1	-	9/33/109/115	-
12	CLA	A	803	1,12	-	2/27/103/115	-
15	BCR	T	4001	-	-	8/29/63/63	0/2/2/2
15	BCR	G	845	-	-	8/29/63/63	0/2/2/2
12	CLA	a	834	1	-	12/27/103/115	-
12	CLA	G	837	1	-	11/39/115/115	-
12	CLA	H	2110	2	-	14/39/115/115	-
12	CLA	A	850	27	-	6/39/115/115	-
14	SF4	A	841	1,2	-	-	0/6/5/5
12	CLA	H	2116	-	-	9/15/91/115	-
12	CLA	B	2102	27	-	14/39/115/115	-
15	BCR	H	2145	-	-	7/29/63/63	0/2/2/2
12	CLA	A	836	1	-	14/39/115/115	-
12	CLA	B	2129	2	-	12/39/115/115	-
14	SF4	C	102	3	-	-	0/6/5/5
13	A1AGD	H	2153	-	2/2/9/11	8/23/43/43	0/1/1/1
12	CLA	B	2105	-	-	8/39/115/115	-
12	CLA	b	2141	16	-	7/15/91/115	-
12	CLA	a	801	1	-	5/39/115/115	-
12	CLA	H	2140	2	-	16/39/115/115	-
12	CLA	b	2107	2	-	16/39/115/115	-
12	CLA	B	2108	2	-	16/39/115/115	-
12	CLA	B	2126	27	-	4/21/97/115	-
12	CLA	G	817	1	-	17/33/109/115	-
12	CLA	G	835	1	-	13/39/115/115	-
15	BCR	K	4001	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	G	825	27	-	7/33/109/115	-
12	CLA	B	2134	2	-	18/39/115/115	-
12	CLA	B	2104	2	-	17/39/115/115	-
12	CLA	A	832	1	-	12/39/115/115	-
12	CLA	G	812	1	-	13/39/115/115	-
12	CLA	A	839	1	-	10/39/115/115	-
23	ZEX	f	205	-	-	14/29/67/67	0/2/2/2
15	BCR	R	101	-	-	7/29/63/63	0/2/2/2
15	BCR	k	4001	-	-	8/29/63/63	0/2/2/2
12	CLA	a	803	1,12	-	2/27/103/115	-
17	LMG	A	847	-	-	20/45/65/70	0/1/1/1
15	BCR	B	2147	-	-	17/29/63/63	0/2/2/2
12	CLA	B	2136	-	-	9/15/91/115	-
12	CLA	B	2141	2	-	16/39/115/115	-
12	CLA	a	813	1	-	14/39/115/115	-
23	ZEX	b	2151	-	-	11/29/67/67	0/2/2/2
16	LHG	b	2148	12	-	18/47/47/53	-
15	BCR	f	202	-	-	13/29/63/63	0/2/2/2
15	BCR	a	842	-	-	11/29/63/63	0/2/2/2
12	CLA	H	2105	2	-	9/39/115/115	-
12	CLA	a	839	1	-	10/39/115/115	-
24	SQD	U	208	-	-	15/40/60/69	0/1/1/1
12	CLA	G	826	1	-	15/39/115/115	-
16	LHG	M	102	-	-	24/48/48/53	-
12	CLA	b	2108	2	-	11/39/115/115	-
12	CLA	B	2111	2	-	14/39/115/115	-
22	EQ3	b	2150	-	-	14/29/68/68	0/2/2/2
12	CLA	A	822	-	-	8/21/97/115	-
16	LHG	V	103	-	-	24/48/48/53	-
12	CLA	G	820	27	-	7/39/115/115	-
12	CLA	B	2107	-	-	16/39/115/115	-
12	CLA	H	2115	2	-	4/15/91/115	-
12	CLA	B	2123	-	-	7/15/91/115	-
12	CLA	B	2113	2	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	A	812	1	-	13/39/115/115	-
13	A1AGD	B	2153	-	2/2/9/11	8/23/43/43	0/1/1/1
12	CLA	A	811	-	-	8/15/91/115	-
12	CLA	H	2103	2	-	17/39/115/115	-
12	CLA	G	834	1	-	12/27/103/115	-
12	CLA	G	828	-	-	12/39/115/115	-
12	CLA	A	807	1	-	14/39/115/115	-
12	CLA	B	2139	-	-	6/15/91/115	-
12	CLA	H	2136	2	-	7/15/91/115	-
16	LHG	a	848	12	-	19/53/53/53	-
15	BCR	I	101	-	-	7/29/63/63	0/2/2/2
15	BCR	b	2144	-	-	8/29/63/63	0/2/2/2
12	CLA	G	830	1	-	9/27/103/115	-
12	CLA	B	2124	2	-	12/27/103/115	-
12	CLA	U	204	10	-	8/39/115/115	-
15	BCR	G	842	-	-	12/29/63/63	0/2/2/2
24	SQD	V	102	-	-	28/49/69/69	0/1/1/1
18	45D	a	852	-	-	8/29/69/69	0/2/2/2
12	CLA	B	2119	2	-	7/21/97/115	-
12	CLA	a	850	27	-	6/39/115/115	-
12	CLA	A	818	1	-	11/39/115/115	-
12	CLA	a	820	27	-	7/39/115/115	-
22	EQ3	B	2151	-	-	14/29/68/68	0/2/2/2
15	BCR	a	845	-	-	8/29/63/63	0/2/2/2
16	LHG	A	846	-	-	27/53/53/53	-
12	CLA	G	807	1	-	14/39/115/115	-
25	DGD	L	209	-	-	21/44/64/95	0/1/1/2
12	CLA	G	818	1	-	11/39/115/115	-
12	CLA	b	2111	2	-	14/39/115/115	-
12	CLA	a	808	1	-	3/21/97/115	-
12	CLA	l	203	10	-	12/39/115/115	-
12	CLA	H	2107	2	-	16/39/115/115	-
15	BCR	B	2146	-	-	7/29/63/63	0/2/2/2
12	CLA	a	828	-	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	G	823	1	-	10/33/109/115	-
12	CLA	H	2123	2	-	12/27/103/115	-
12	CLA	A	828	-	-	12/39/115/115	-
12	CLA	b	2119	2	-	16/39/115/115	-
12	CLA	B	2112	2	-	14/39/115/115	-
20	ECH	M	103	-	-	10/29/66/66	0/2/2/2
12	CLA	b	2113	-	-	10/15/91/115	-
12	CLA	B	2125	27	-	6/39/115/115	-
12	CLA	b	2137	2	-	7/39/115/115	-
12	CLA	f	204	-	-	5/15/91/115	-
12	CLA	a	830	1	-	9/27/103/115	-
12	CLA	L	205	27	-	6/39/115/115	-
12	CLA	b	2129	2	-	13/39/115/115	-
12	CLA	a	826	1	-	15/39/115/115	-
12	CLA	a	854	-	-	7/27/103/115	-
12	CLA	U	205	27	-	6/39/115/115	-
18	45D	A	852	-	-	8/29/69/69	0/2/2/2
12	CLA	b	2139	27	-	10/39/115/115	-
15	BCR	H	2142	-	-	6/29/63/63	0/2/2/2
12	CLA	b	2105	2	-	9/39/115/115	-
12	CLA	b	2101	27	-	14/39/115/115	-
12	CLA	H	2119	2	-	16/39/115/115	-
12	CLA	G	839	1	-	10/39/115/115	-
12	CLA	a	824	27	-	19/39/115/115	-
12	CLA	a	821	1	-	9/33/109/115	-
12	CLA	a	811	-	-	8/15/91/115	-
12	CLA	G	824	27	-	19/39/115/115	-
12	CLA	A	825	27	-	7/33/109/115	-
12	CLA	H	2120	-	-	8/27/103/115	-
15	BCR	A	844	-	-	8/29/63/63	0/2/2/2
12	CLA	a	817	1	-	17/33/109/115	-
12	CLA	a	807	1	-	14/39/115/115	-
12	CLA	B	2127	2	-	11/39/115/115	-
15	BCR	G	844	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	A	814	-	-	4/15/91/115	-
12	CLA	H	2113	-	-	10/15/91/115	-
17	LMG	G	849	-	-	14/26/46/70	0/1/1/1
12	CLA	G	806	1	-	7/21/97/115	-
12	CLA	b	2126	2	-	11/39/115/115	-
12	CLA	G	814	-	-	4/15/91/115	-
23	ZEX	H	2151	-	-	11/29/67/67	0/2/2/2
12	CLA	A	834	1	-	12/27/103/115	-
12	CLA	a	825	27	-	7/33/109/115	-
13	A1AGD	b	2153	-	2/2/9/11	8/23/43/43	0/1/1/1
15	BCR	b	2146	-	-	17/29/63/63	0/2/2/2
12	CLA	H	2112	2	-	8/39/115/115	-
16	LHG	G	848	12	-	18/53/53/53	-
20	ECH	V	101	-	-	10/29/66/66	0/2/2/2
12	CLA	G	822	-	-	8/21/97/115	-
12	CLA	b	2117	2	-	10/15/91/115	-
12	CLA	A	851	27	-	13/39/115/115	-
12	CLA	G	811	-	-	8/15/91/115	-
12	CLA	G	819	1	-	18/39/115/115	-
12	CLA	G	803	1,12	-	2/27/103/115	-
12	CLA	L	203	10	-	12/39/115/115	-
12	CLA	A	810	1,12	-	15/39/115/115	-
12	CLA	B	2103	-	-	12/39/115/115	-
15	BCR	S	104	-	-	9/29/63/63	0/2/2/2
12	CLA	U	201	1	-	15/39/115/115	-
12	CLA	b	2133	2	-	18/39/115/115	-
12	CLA	a	833	1	-	15/39/115/115	-
15	BCR	H	2144	-	-	8/29/63/63	0/2/2/2
12	CLA	b	2102	-	-	12/39/115/115	-
12	CLA	H	2125	27	-	4/21/97/115	-
15	BCR	b	2142	-	-	6/29/63/63	0/2/2/2
12	CLA	f	203	-	-	6/15/91/115	-
12	CLA	A	838	1	-	5/39/115/115	-
12	CLA	H	2117	2	-	10/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	B	2110	-	-	13/39/115/115	-
12	CLA	G	802	1	-	9/39/115/115	-
20	ECH	H	2143	-	-	12/29/66/66	0/2/2/2
12	CLA	B	2128	2	-	16/39/115/115	-
12	CLA	b	2114	-	-	18/39/115/115	-
15	BCR	Q	202	-	-	13/29/63/63	0/2/2/2
15	BCR	a	843	-	-	15/29/63/63	0/2/2/2
12	CLA	B	2101	16	-	5/21/97/115	-
12	CLA	S	103	8	-	10/15/91/115	-
12	CLA	B	2115	-	-	18/39/115/115	-
12	CLA	a	823	1	-	10/33/109/115	-
12	CLA	a	806	1	-	7/21/97/115	-
12	CLA	U	203	10	-	12/39/115/115	-
12	CLA	b	2116	-	-	9/15/91/115	-
12	CLA	H	2135	-	-	9/15/91/115	-
14	SF4	N	101	3	-	-	0/6/5/5
12	CLA	G	813	1	-	14/39/115/115	-
12	CLA	G	838	1	-	5/39/115/115	-
15	BCR	L	206	-	-	10/29/63/63	0/2/2/2
15	BCR	U	207	-	-	6/29/63/63	0/2/2/2
12	CLA	L	204	10	-	8/39/115/115	-
12	CLA	A	833	1	-	15/39/115/115	-
12	CLA	A	802	1	-	9/39/115/115	-
12	CLA	A	830	1	-	9/27/103/115	-
12	CLA	B	2117	-	-	9/15/91/115	-
12	CLA	a	837	1	-	11/39/115/115	-
12	CLA	G	815	-	-	5/15/91/115	-
26	LMT	L	210	-	-	12/21/61/61	0/2/2/2
12	CLA	B	2118	2	-	10/15/91/115	-
12	CLA	H	2122	-	-	7/15/91/115	-
12	CLA	b	2131	2	-	7/27/103/115	-
15	BCR	l	206	-	-	10/29/63/63	0/2/2/2
12	CLA	H	2128	2	-	12/39/115/115	-
12	CLA	a	816	1	-	4/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	SF4	N	102	3	-	-	0/6/5/5
18	45D	G	852	-	-	8/29/69/69	0/2/2/2
12	CLA	Q	203	-	-	6/15/91/115	-
12	CLA	H	2101	27	-	14/39/115/115	-
15	BCR	A	845	-	-	8/29/63/63	0/2/2/2
15	BCR	J	101	-	-	13/29/63/63	0/2/2/2
12	CLA	B	2109	2	-	11/39/115/115	-
12	CLA	G	809	1	-	10/21/97/115	-
24	SQD	M	101	-	-	28/49/69/69	0/1/1/1
12	CLA	a	804	1	-	16/39/115/115	-
12	CLA	f	201	27	-	22/39/115/115	-
12	CLA	H	2132	2	-	18/39/115/115	-
12	CLA	G	827	-	-	6/39/115/115	-
16	LHG	H	2148	12	-	18/47/47/53	-
12	CLA	l	205	27	-	6/39/115/115	-
12	CLA	a	838	1	-	5/39/115/115	-
12	CLA	A	820	27	-	7/39/115/115	-
12	CLA	b	2118	2	-	7/21/97/115	-
12	CLA	B	2130	2	-	13/39/115/115	-
20	ECH	b	2143	-	-	12/29/66/66	0/2/2/2
12	CLA	b	2130	-	-	2/15/91/115	-
12	CLA	b	2103	2	-	17/39/115/115	-
26	LMT	l	210	-	-	12/21/61/61	0/2/2/2
17	LMG	a	849	-	-	14/26/46/70	0/1/1/1
12	CLA	a	815	-	-	5/15/91/115	-
12	CLA	A	826	1	-	15/39/115/115	-
12	CLA	A	854	-	-	7/27/103/115	-
12	CLA	F	201	27	-	22/39/115/115	-
23	ZEX	Q	205	-	-	14/29/67/67	0/2/2/2
12	CLA	b	2104	-	-	8/39/115/115	-
15	BCR	a	844	-	-	8/29/63/63	0/2/2/2
12	CLA	a	851	27	-	13/39/115/115	-
12	CLA	G	821	1	-	9/33/109/115	-
12	CLA	b	2122	-	-	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	H	2111	2	-	14/39/115/115	-
12	CLA	a	835	1	-	13/39/115/115	-
12	CLA	a	809	1	-	10/21/97/115	-
15	BCR	L	207	-	-	6/29/63/63	0/2/2/2
12	CLA	b	2152	16	-	5/21/97/115	-
13	A1AGD	A	840	-	2/2/9/11	8/23/43/43	0/1/1/1
12	CLA	a	827	-	-	6/39/115/115	-
12	CLA	A	823	1	-	10/33/109/115	-
12	CLA	A	817	1	-	17/33/109/115	-
13	A1AGD	G	840	-	2/2/9/11	8/23/43/43	0/1/1/1
14	SF4	c	101	3	-	-	0/6/5/5
12	CLA	j	102	-	-	9/15/91/115	-
12	CLA	b	2109	-	-	13/39/115/115	-
12	CLA	b	2138	-	-	6/15/91/115	-
12	CLA	A	835	1	-	13/39/115/115	-
12	CLA	A	827	-	-	6/39/115/115	-
12	CLA	a	822	-	-	8/21/97/115	-
26	LMT	U	210	-	-	12/21/61/61	0/2/2/2

All (2582) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	F	205	ZEX	C25-C26	17.19	1.60	1.34
23	Q	205	ZEX	C25-C26	17.19	1.60	1.34
23	f	205	ZEX	C25-C26	17.17	1.60	1.34
23	b	2151	ZEX	C25-C26	17.17	1.60	1.34
23	B	2152	ZEX	C25-C26	17.12	1.60	1.34
23	H	2151	ZEX	C25-C26	17.07	1.60	1.34
23	B	2152	ZEX	C2-C3	-15.48	1.30	1.52
23	H	2151	ZEX	C2-C3	-15.47	1.30	1.52
23	b	2151	ZEX	C2-C3	-15.46	1.30	1.52
23	Q	205	ZEX	C2-C3	-14.77	1.31	1.52
23	f	205	ZEX	C2-C3	-14.76	1.31	1.52
23	F	205	ZEX	C2-C3	-14.72	1.31	1.52
23	F	205	ZEX	C5-C6	14.08	1.58	1.34
23	f	205	ZEX	C5-C6	14.08	1.58	1.34
23	Q	205	ZEX	C5-C6	14.05	1.58	1.34
23	H	2151	ZEX	C5-C6	13.94	1.57	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	2152	ZEX	C5-C6	13.93	1.57	1.34
23	b	2151	ZEX	C5-C6	13.93	1.57	1.34
22	b	2150	EQ3	C25-C26	12.97	1.53	1.35
22	B	2151	EQ3	C25-C26	12.97	1.53	1.35
22	H	2150	EQ3	C25-C26	12.95	1.53	1.35
22	H	2150	EQ3	C4-C3	11.70	1.72	1.52
22	B	2151	EQ3	C4-C3	11.69	1.72	1.52
22	b	2150	EQ3	C4-C3	11.68	1.72	1.52
22	H	2150	EQ3	C5-C6	11.22	1.53	1.34
22	B	2151	EQ3	C5-C6	11.17	1.53	1.34
22	b	2150	EQ3	C5-C6	11.14	1.53	1.34
23	b	2151	ZEX	C24-C23	11.12	1.67	1.52
23	B	2152	ZEX	C24-C23	11.12	1.67	1.52
23	H	2151	ZEX	C24-C23	11.08	1.67	1.52
23	Q	205	ZEX	C24-C23	10.97	1.67	1.52
23	f	205	ZEX	C24-C23	10.95	1.66	1.52
23	F	205	ZEX	C24-C23	10.94	1.66	1.52
23	f	205	ZEX	C22-C23	-10.01	1.38	1.53
23	F	205	ZEX	C22-C23	-9.98	1.38	1.53
23	Q	205	ZEX	C22-C23	-9.97	1.38	1.53
23	b	2151	ZEX	C22-C23	-9.54	1.38	1.53
23	B	2152	ZEX	C22-C23	-9.49	1.39	1.53
23	H	2151	ZEX	C22-C23	-9.47	1.39	1.53
13	b	2153	A1AGD	C3-C4	-9.19	1.35	1.49
13	B	2153	A1AGD	C3-C4	-9.18	1.35	1.49
13	H	2153	A1AGD	C3-C4	-9.17	1.35	1.49
23	H	2151	ZEX	C27-C26	9.04	1.57	1.46
23	b	2151	ZEX	C27-C26	9.02	1.57	1.46
23	B	2152	ZEX	C27-C26	9.01	1.57	1.46
23	f	205	ZEX	C4-C3	8.86	1.67	1.52
23	Q	205	ZEX	C4-C3	8.85	1.67	1.52
23	F	205	ZEX	C4-C3	8.81	1.67	1.52
23	Q	205	ZEX	C27-C26	8.76	1.57	1.46
23	F	205	ZEX	C27-C26	8.74	1.57	1.46
23	f	205	ZEX	C27-C26	8.72	1.57	1.46
23	B	2152	ZEX	C4-C3	8.56	1.67	1.52
23	b	2151	ZEX	C4-C3	8.56	1.67	1.52
23	H	2151	ZEX	C4-C3	8.54	1.67	1.52
13	H	2153	A1AGD	C2-C1	-6.62	1.27	1.44
13	B	2153	A1AGD	C2-C1	-6.61	1.27	1.44
13	b	2153	A1AGD	C2-C1	-6.59	1.27	1.44
22	b	2150	EQ3	C1-C6	-6.43	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	H	2150	EQ3	C1-C6	-6.43	1.45	1.53
22	B	2151	EQ3	C1-C6	-6.41	1.45	1.53
22	b	2150	EQ3	C2-C3	-6.27	1.43	1.52
22	B	2151	EQ3	C2-C3	-6.25	1.43	1.52
22	H	2150	EQ3	C2-C3	-6.21	1.43	1.52
23	b	2151	ZEX	C28-C29	6.04	1.58	1.46
23	B	2152	ZEX	C28-C29	6.02	1.58	1.46
23	Q	205	ZEX	C28-C29	6.01	1.58	1.46
23	H	2151	ZEX	C28-C29	6.00	1.58	1.46
23	F	205	ZEX	C28-C29	5.99	1.58	1.46
23	f	205	ZEX	C28-C29	5.96	1.58	1.46
23	b	2151	ZEX	C21-C26	-5.92	1.46	1.53
23	B	2152	ZEX	C1-C6	-5.88	1.46	1.53
23	B	2152	ZEX	C21-C26	-5.85	1.46	1.53
23	H	2151	ZEX	C1-C6	-5.84	1.46	1.53
23	b	2151	ZEX	C1-C6	-5.83	1.46	1.53
23	H	2151	ZEX	C21-C26	-5.83	1.46	1.53
23	f	205	ZEX	C1-C6	-5.76	1.46	1.53
23	F	205	ZEX	C1-C6	-5.76	1.46	1.53
23	Q	205	ZEX	C1-C6	-5.73	1.46	1.53
23	f	205	ZEX	C21-C26	-5.70	1.46	1.53
23	F	205	ZEX	C21-C26	-5.70	1.46	1.53
13	b	2153	A1AGD	C6-C1	-5.68	1.39	1.48
13	B	2153	A1AGD	C6-C1	-5.66	1.39	1.48
23	Q	205	ZEX	C21-C26	-5.66	1.46	1.53
13	H	2153	A1AGD	C6-C1	-5.66	1.39	1.48
23	Q	205	ZEX	C8-C9	5.58	1.57	1.46
23	f	205	ZEX	C8-C9	5.57	1.57	1.46
23	F	205	ZEX	C8-C9	5.56	1.57	1.46
23	H	2151	ZEX	C8-C9	5.53	1.57	1.46
23	b	2151	ZEX	C8-C9	5.51	1.57	1.46
23	B	2152	ZEX	C8-C9	5.50	1.57	1.46
23	F	205	ZEX	C12-C13	5.34	1.57	1.46
23	f	205	ZEX	C12-C13	5.33	1.57	1.46
23	Q	205	ZEX	C12-C13	5.32	1.57	1.46
22	H	2150	EQ3	C8-C9	5.26	1.57	1.46
23	B	2152	ZEX	C12-C13	5.25	1.57	1.46
22	B	2151	EQ3	C8-C9	5.24	1.57	1.46
22	b	2150	EQ3	C8-C9	5.24	1.57	1.46
23	H	2151	ZEX	C12-C13	5.24	1.57	1.46
23	b	2151	ZEX	C12-C13	5.21	1.57	1.46
23	B	2152	ZEX	C32-C33	4.97	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	2151	ZEX	C32-C33	4.97	1.56	1.46
23	H	2151	ZEX	C32-C33	4.96	1.56	1.46
22	H	2150	EQ3	C4-C5	-4.93	1.43	1.51
22	B	2151	EQ3	C4-C5	-4.92	1.43	1.51
22	b	2150	EQ3	C4-C5	-4.91	1.43	1.51
23	f	205	ZEX	C4-C5	-4.86	1.43	1.51
13	H	2153	A1AGD	C5-C4	-4.84	1.30	1.47
13	b	2153	A1AGD	C5-C4	-4.84	1.30	1.47
13	B	2153	A1AGD	C5-C4	-4.83	1.30	1.47
23	F	205	ZEX	C4-C5	-4.83	1.43	1.51
23	Q	205	ZEX	C4-C5	-4.78	1.43	1.51
24	V	102	SQD	O48-C23	4.74	1.47	1.33
24	m	102	SQD	O48-C23	4.74	1.47	1.33
23	F	205	ZEX	C32-C33	4.74	1.56	1.46
23	Q	205	ZEX	C32-C33	4.73	1.56	1.46
24	M	101	SQD	O48-C23	4.73	1.47	1.33
23	f	205	ZEX	C32-C33	4.69	1.56	1.46
23	b	2151	ZEX	C4-C5	-4.64	1.43	1.51
23	B	2152	ZEX	C4-C5	-4.64	1.43	1.51
23	H	2151	ZEX	C4-C5	-4.63	1.43	1.51
24	L	208	SQD	O48-C23	4.61	1.46	1.33
24	U	208	SQD	O48-C23	4.61	1.46	1.33
24	l	208	SQD	O48-C23	4.60	1.46	1.33
22	b	2150	EQ3	C12-C13	4.60	1.55	1.46
22	B	2151	EQ3	C12-C13	4.59	1.55	1.46
22	H	2150	EQ3	C12-C13	4.59	1.55	1.46
23	B	2152	ZEX	C35-C34	4.44	1.56	1.43
23	H	2151	ZEX	C35-C34	4.43	1.56	1.43
23	b	2151	ZEX	C35-C34	4.43	1.56	1.43
23	f	205	ZEX	C35-C34	4.40	1.56	1.43
23	F	205	ZEX	C35-C34	4.37	1.56	1.43
23	Q	205	ZEX	C35-C34	4.37	1.56	1.43
22	b	2150	EQ3	C23-C22	4.27	1.55	1.46
22	B	2151	EQ3	C23-C22	4.27	1.55	1.46
22	H	2150	EQ3	C23-C22	4.26	1.55	1.46
23	f	205	ZEX	C2-C1	4.25	1.67	1.54
23	H	2151	ZEX	C15-C14	4.24	1.56	1.43
23	F	205	ZEX	C2-C1	4.23	1.67	1.54
23	Q	205	ZEX	C2-C1	4.23	1.67	1.54
23	B	2152	ZEX	C15-C14	4.23	1.56	1.43
23	b	2151	ZEX	C15-C14	4.22	1.56	1.43
23	f	205	ZEX	C31-C30	4.15	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	2150	EQ3	C19-C18	4.15	1.54	1.46
22	B	2151	EQ3	C19-C18	4.15	1.54	1.46
22	H	2150	EQ3	C19-C18	4.14	1.54	1.46
23	Q	205	ZEX	C31-C30	4.14	1.56	1.43
12	H	2113	CLA	C1D-ND	4.14	1.43	1.37
23	F	205	ZEX	C31-C30	4.14	1.56	1.43
12	B	2114	CLA	C1D-ND	4.11	1.43	1.37
23	f	205	ZEX	C15-C14	4.10	1.55	1.43
23	b	2151	ZEX	C31-C30	4.10	1.55	1.43
22	H	2150	EQ3	C20-C21	4.10	1.55	1.43
23	b	2151	ZEX	C11-C10	4.10	1.55	1.43
23	Q	205	ZEX	C15-C14	4.10	1.55	1.43
23	B	2152	ZEX	C11-C10	4.09	1.55	1.43
23	B	2152	ZEX	C31-C30	4.09	1.55	1.43
23	H	2151	ZEX	C11-C10	4.09	1.55	1.43
23	Q	205	ZEX	C11-C10	4.09	1.55	1.43
12	b	2113	CLA	C1D-ND	4.09	1.43	1.37
22	b	2150	EQ3	C20-C21	4.09	1.55	1.43
22	B	2151	EQ3	C20-C21	4.08	1.55	1.43
23	F	205	ZEX	C15-C14	4.08	1.55	1.43
23	f	205	ZEX	C11-C10	4.08	1.55	1.43
23	H	2151	ZEX	C31-C30	4.08	1.55	1.43
23	F	205	ZEX	C11-C10	4.08	1.55	1.43
12	G	801	CLA	C1D-ND	4.03	1.43	1.37
12	a	801	CLA	C1D-ND	4.02	1.43	1.37
12	A	801	CLA	C1D-ND	4.02	1.43	1.37
13	A	840	A1AGD	C13-C14	-3.98	1.33	1.52
13	G	840	A1AGD	C13-C14	-3.98	1.33	1.52
13	a	840	A1AGD	C13-C14	-3.98	1.33	1.52
23	H	2151	ZEX	C2-C1	3.95	1.66	1.54
23	B	2152	ZEX	C2-C1	3.94	1.66	1.54
23	b	2151	ZEX	C2-C1	3.92	1.66	1.54
23	H	2151	ZEX	C22-C21	3.90	1.66	1.54
23	b	2151	ZEX	C22-C21	3.89	1.66	1.54
23	B	2152	ZEX	C22-C21	3.89	1.66	1.54
24	V	102	SQD	O47-C45	-3.81	1.37	1.46
24	M	101	SQD	O47-C45	-3.80	1.37	1.46
24	m	102	SQD	O47-C45	-3.80	1.37	1.46
22	B	2151	EQ3	C16-C17	3.79	1.54	1.43
22	H	2150	EQ3	C16-C17	3.78	1.54	1.43
22	b	2150	EQ3	C16-C17	3.77	1.54	1.43
12	S	102	CLA	C1D-ND	3.76	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	f	205	ZEX	C22-C21	3.76	1.66	1.54
23	b	2151	ZEX	C24-C25	-3.75	1.45	1.50
23	H	2151	ZEX	C24-C25	-3.75	1.45	1.50
23	B	2152	ZEX	C24-C25	-3.75	1.45	1.50
23	F	205	ZEX	C22-C21	3.75	1.66	1.54
12	b	2108	CLA	C1D-ND	3.74	1.42	1.37
23	Q	205	ZEX	C22-C21	3.73	1.66	1.54
12	a	838	CLA	C1D-ND	3.72	1.42	1.37
13	a	840	A1AGD	C18-C19	-3.72	1.34	1.52
12	B	2109	CLA	C1D-ND	3.72	1.42	1.37
12	A	838	CLA	C1D-ND	3.71	1.42	1.37
12	A	854	CLA	C1D-ND	3.71	1.42	1.37
13	A	840	A1AGD	C18-C19	-3.71	1.34	1.52
12	H	2115	CLA	C1D-ND	3.71	1.42	1.37
12	J	102	CLA	C1D-ND	3.71	1.42	1.37
12	a	854	CLA	C1D-ND	3.70	1.42	1.37
12	j	102	CLA	C1D-ND	3.70	1.42	1.37
13	G	840	A1AGD	C18-C19	-3.69	1.34	1.52
22	H	2150	EQ3	C11-C10	3.69	1.54	1.43
12	b	2112	CLA	C1D-ND	3.69	1.42	1.37
12	b	2115	CLA	C1D-ND	3.69	1.42	1.37
12	H	2108	CLA	C1D-ND	3.69	1.42	1.37
12	S	103	CLA	C1D-ND	3.69	1.42	1.37
22	b	2150	EQ3	C11-C10	3.68	1.54	1.43
12	G	809	CLA	C1D-ND	3.68	1.42	1.37
23	Q	205	ZEX	C24-C25	-3.68	1.45	1.50
23	F	205	ZEX	C24-C25	-3.68	1.45	1.50
22	B	2151	EQ3	C11-C10	3.68	1.54	1.43
12	B	2113	CLA	C1D-ND	3.68	1.42	1.37
12	G	854	CLA	C1D-ND	3.67	1.42	1.37
12	j	103	CLA	C1D-ND	3.67	1.42	1.37
12	J	103	CLA	C1D-ND	3.67	1.42	1.37
12	A	809	CLA	C1D-ND	3.67	1.42	1.37
22	H	2150	EQ3	C2-C1	3.67	1.65	1.54
22	B	2151	EQ3	C2-C1	3.67	1.65	1.54
12	Q	203	CLA	C1D-ND	3.66	1.42	1.37
22	b	2150	EQ3	C2-C1	3.66	1.65	1.54
12	H	2112	CLA	C1D-ND	3.66	1.42	1.37
12	H	2140	CLA	C1D-ND	3.66	1.42	1.37
23	f	205	ZEX	C24-C25	-3.66	1.45	1.50
12	B	2116	CLA	C1D-ND	3.66	1.42	1.37
12	G	838	CLA	C1D-ND	3.65	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	2141	CLA	C1D-ND	3.65	1.42	1.37
12	b	2140	CLA	C1D-ND	3.65	1.42	1.37
12	K	4002	CLA	C1D-ND	3.65	1.42	1.37
12	T	4002	CLA	C1D-ND	3.65	1.42	1.37
12	a	809	CLA	C1D-ND	3.65	1.42	1.37
12	G	819	CLA	C1D-ND	3.65	1.42	1.37
12	A	819	CLA	C1D-ND	3.65	1.42	1.37
12	b	2122	CLA	C1D-ND	3.64	1.42	1.37
13	G	840	A1AGD	C7-C3	-3.64	1.46	1.51
12	B	2115	CLA	C1D-ND	3.64	1.42	1.37
12	a	819	CLA	C1D-ND	3.63	1.42	1.37
12	H	2114	CLA	C1D-ND	3.63	1.42	1.37
12	b	2114	CLA	C1D-ND	3.63	1.42	1.37
12	b	2126	CLA	C1D-ND	3.62	1.42	1.37
12	Q	204	CLA	C1D-ND	3.62	1.42	1.37
13	A	840	A1AGD	C7-C3	-3.62	1.46	1.51
12	F	203	CLA	C1D-ND	3.61	1.42	1.37
12	b	2118	CLA	C1D-ND	3.61	1.42	1.37
12	k	4002	CLA	C1D-ND	3.61	1.42	1.37
12	F	204	CLA	C1D-ND	3.61	1.42	1.37
12	H	2118	CLA	C1D-ND	3.61	1.42	1.37
12	f	203	CLA	C1D-ND	3.60	1.42	1.37
12	A	814	CLA	C1D-ND	3.59	1.42	1.37
12	B	2119	CLA	C1D-ND	3.59	1.42	1.37
12	f	204	CLA	C1D-ND	3.59	1.42	1.37
12	B	2123	CLA	C1D-ND	3.59	1.42	1.37
24	l	208	SQD	O5-C1	3.59	1.51	1.41
12	b	2121	CLA	C1D-ND	3.59	1.42	1.37
24	L	208	SQD	O5-C1	3.59	1.51	1.41
12	H	2126	CLA	C1D-ND	3.58	1.42	1.37
12	G	823	CLA	C1D-ND	3.58	1.42	1.37
12	a	827	CLA	C1D-ND	3.58	1.42	1.37
13	a	840	A1AGD	C7-C3	-3.57	1.46	1.51
12	a	814	CLA	C1D-ND	3.57	1.42	1.37
12	H	2124	CLA	C1D-ND	3.57	1.42	1.37
12	B	2118	CLA	C1D-ND	3.57	1.42	1.37
12	G	822	CLA	C1D-ND	3.57	1.42	1.37
12	a	823	CLA	C1D-ND	3.57	1.42	1.37
12	H	2122	CLA	C1D-ND	3.57	1.42	1.37
12	A	823	CLA	C1D-ND	3.57	1.42	1.37
12	A	827	CLA	C1D-ND	3.57	1.42	1.37
12	G	813	CLA	C1D-ND	3.56	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	2117	CLA	C1D-ND	3.56	1.42	1.37
12	H	2117	CLA	C1D-ND	3.56	1.42	1.37
12	B	2135	CLA	C1D-ND	3.56	1.42	1.37
12	A	813	CLA	C1D-ND	3.56	1.42	1.37
12	B	2127	CLA	C1D-ND	3.56	1.42	1.37
12	G	814	CLA	C1D-ND	3.56	1.42	1.37
12	B	2125	CLA	C1D-ND	3.56	1.42	1.37
24	U	208	SQD	O5-C1	3.56	1.51	1.41
12	H	2133	CLA	C1D-ND	3.56	1.42	1.37
12	b	2116	CLA	C1D-ND	3.55	1.42	1.37
22	B	2151	EQ3	C15-C14	3.55	1.54	1.43
12	H	2120	CLA	C1D-ND	3.55	1.42	1.37
22	H	2150	EQ3	C15-C14	3.55	1.54	1.43
12	b	2117	CLA	C1D-ND	3.55	1.42	1.37
12	a	813	CLA	C1D-ND	3.55	1.42	1.37
22	b	2150	EQ3	C15-C14	3.55	1.54	1.43
12	H	2107	CLA	C1D-ND	3.55	1.42	1.37
12	G	803	CLA	C1D-ND	3.54	1.42	1.37
12	H	2119	CLA	C1D-ND	3.54	1.42	1.37
12	B	2134	CLA	C1D-ND	3.54	1.42	1.37
12	b	2141	CLA	C1D-ND	3.54	1.42	1.37
12	B	2121	CLA	C1D-ND	3.54	1.42	1.37
12	b	2133	CLA	C1D-ND	3.54	1.42	1.37
12	H	2121	CLA	C1D-ND	3.54	1.42	1.37
24	U	208	SQD	O47-C45	-3.54	1.38	1.46
12	a	834	CLA	C1D-ND	3.54	1.42	1.37
12	H	2116	CLA	C1D-ND	3.53	1.42	1.37
12	a	812	CLA	C1D-ND	3.53	1.42	1.37
12	A	812	CLA	C1D-ND	3.53	1.42	1.37
12	b	2134	CLA	C1D-ND	3.53	1.42	1.37
12	B	2122	CLA	C1D-ND	3.53	1.42	1.37
12	G	812	CLA	C1D-ND	3.53	1.42	1.37
12	L	205	CLA	C1D-ND	3.53	1.42	1.37
12	b	2124	CLA	C1D-ND	3.52	1.42	1.37
24	L	208	SQD	O47-C45	-3.52	1.38	1.46
12	H	2134	CLA	C1D-ND	3.52	1.42	1.37
24	l	208	SQD	O47-C45	-3.52	1.38	1.46
12	l	205	CLA	C1D-ND	3.52	1.42	1.37
12	H	2141	CLA	C1D-ND	3.51	1.42	1.37
12	b	2120	CLA	C1D-ND	3.51	1.42	1.37
12	U	205	CLA	C1D-ND	3.51	1.42	1.37
12	A	803	CLA	C1D-ND	3.51	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	810	CLA	C1D-ND	3.50	1.42	1.37
12	A	834	CLA	C1D-ND	3.50	1.42	1.37
12	B	2128	CLA	C1D-ND	3.50	1.42	1.37
23	H	2151	ZEX	C7-C6	3.50	1.57	1.45
12	a	811	CLA	C1D-ND	3.50	1.42	1.37
12	G	810	CLA	C1D-ND	3.50	1.42	1.37
12	B	2108	CLA	C1D-ND	3.50	1.42	1.37
12	B	2142	CLA	C1D-ND	3.50	1.42	1.37
12	G	834	CLA	C1D-ND	3.50	1.42	1.37
12	b	2107	CLA	C1D-ND	3.50	1.42	1.37
12	A	810	CLA	C1D-ND	3.50	1.42	1.37
12	G	827	CLA	C1D-ND	3.50	1.42	1.37
15	G	845	BCR	C30-C25	-3.49	1.49	1.53
12	A	815	CLA	C1D-ND	3.49	1.42	1.37
23	B	2152	ZEX	C7-C6	3.49	1.57	1.45
12	b	2119	CLA	C1D-ND	3.49	1.42	1.37
12	a	803	CLA	C1D-ND	3.49	1.42	1.37
12	B	2120	CLA	C1D-ND	3.49	1.42	1.37
23	b	2151	ZEX	C7-C6	3.49	1.57	1.45
12	b	2127	CLA	C1D-ND	3.48	1.42	1.37
12	B	2131	CLA	C1D-ND	3.48	1.42	1.37
12	a	802	CLA	C1D-ND	3.48	1.42	1.37
12	A	802	CLA	C1D-ND	3.48	1.42	1.37
12	a	815	CLA	C1D-ND	3.48	1.42	1.37
15	a	845	BCR	C30-C25	-3.48	1.49	1.53
12	A	822	CLA	C1D-ND	3.48	1.42	1.37
12	B	2136	CLA	C1D-ND	3.48	1.42	1.37
12	H	2130	CLA	C1D-ND	3.48	1.42	1.37
12	b	2130	CLA	C1D-ND	3.48	1.42	1.37
12	A	811	CLA	C1D-ND	3.47	1.42	1.37
12	b	2123	CLA	C1D-ND	3.47	1.42	1.37
12	H	2127	CLA	C1D-ND	3.47	1.42	1.37
15	A	845	BCR	C30-C25	-3.47	1.49	1.53
12	A	806	CLA	C1D-ND	3.47	1.42	1.37
12	H	2106	CLA	C1D-ND	3.46	1.42	1.37
12	f	201	CLA	C1D-ND	3.46	1.42	1.37
12	b	2135	CLA	C1D-ND	3.46	1.42	1.37
12	a	822	CLA	C1D-ND	3.46	1.42	1.37
12	b	2131	CLA	C1D-ND	3.46	1.42	1.37
23	Q	205	ZEX	C7-C6	3.46	1.56	1.45
23	f	205	ZEX	C7-C6	3.45	1.56	1.45
12	B	2107	CLA	C1D-ND	3.45	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	805	CLA	C1D-ND	3.45	1.42	1.37
12	a	806	CLA	C1D-ND	3.45	1.42	1.37
12	G	802	CLA	C1D-ND	3.45	1.42	1.37
23	F	205	ZEX	C7-C6	3.44	1.56	1.45
12	G	806	CLA	C1D-ND	3.44	1.42	1.37
15	H	2146	BCR	C30-C25	-3.44	1.49	1.53
12	H	2131	CLA	C1D-ND	3.44	1.42	1.37
12	G	815	CLA	C1D-ND	3.44	1.42	1.37
12	H	2105	CLA	C1D-ND	3.44	1.42	1.37
12	b	2103	CLA	C1D-ND	3.43	1.42	1.37
12	H	2135	CLA	C1D-ND	3.43	1.42	1.37
12	F	201	CLA	C1D-ND	3.43	1.42	1.37
12	G	805	CLA	C1D-ND	3.43	1.42	1.37
12	G	824	CLA	C1D-ND	3.43	1.42	1.37
12	G	816	CLA	C1D-ND	3.43	1.42	1.37
12	G	820	CLA	C1D-ND	3.42	1.42	1.37
12	B	2124	CLA	C1D-ND	3.42	1.42	1.37
12	H	2136	CLA	C1D-ND	3.42	1.42	1.37
12	A	805	CLA	C1D-ND	3.42	1.42	1.37
12	A	820	CLA	C1D-ND	3.42	1.42	1.37
12	H	2103	CLA	C1D-ND	3.42	1.42	1.37
12	B	2104	CLA	C1D-ND	3.42	1.42	1.37
12	b	2106	CLA	C1D-ND	3.42	1.42	1.37
15	b	2146	BCR	C30-C25	-3.42	1.49	1.53
15	B	2147	BCR	C30-C25	-3.42	1.49	1.53
12	A	817	CLA	C1D-ND	3.42	1.42	1.37
12	A	818	CLA	C1D-ND	3.42	1.42	1.37
12	B	2132	CLA	C1D-ND	3.42	1.42	1.37
24	l	208	SQD	O47-C7	3.41	1.43	1.34
12	G	811	CLA	C1D-ND	3.41	1.42	1.37
12	A	824	CLA	C1D-ND	3.41	1.42	1.37
12	a	818	CLA	C1D-ND	3.41	1.42	1.37
12	G	828	CLA	C1D-ND	3.41	1.42	1.37
12	A	816	CLA	C1D-ND	3.41	1.42	1.37
12	a	824	CLA	C1D-ND	3.40	1.42	1.37
24	L	208	SQD	O47-C7	3.40	1.43	1.34
12	H	2123	CLA	C1D-ND	3.40	1.42	1.37
12	a	817	CLA	C1D-ND	3.40	1.42	1.37
12	G	817	CLA	C1D-ND	3.40	1.42	1.37
12	Q	201	CLA	C1D-ND	3.40	1.42	1.37
12	B	2137	CLA	C1D-ND	3.40	1.42	1.37
12	G	833	CLA	C1D-ND	3.40	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	2137	CLA	C1D-ND	3.40	1.42	1.37
24	U	208	SQD	O47-C7	3.39	1.43	1.34
12	A	807	CLA	C1D-ND	3.39	1.42	1.37
12	B	2138	CLA	C1D-ND	3.39	1.42	1.37
12	G	807	CLA	C1D-ND	3.39	1.42	1.37
12	b	2136	CLA	C1D-ND	3.39	1.42	1.37
12	H	2125	CLA	C1D-ND	3.39	1.42	1.37
13	G	840	A1AGD	C3-C4	-3.38	1.44	1.49
12	a	833	CLA	C1D-ND	3.38	1.42	1.37
12	G	818	CLA	C1D-ND	3.38	1.42	1.37
12	H	2113	CLA	C4B-NB	3.38	1.42	1.37
12	B	2106	CLA	C1D-ND	3.38	1.42	1.37
12	H	2137	CLA	C1D-ND	3.38	1.42	1.37
12	a	836	CLA	C1D-ND	3.38	1.42	1.37
12	G	829	CLA	C1D-ND	3.37	1.42	1.37
12	G	836	CLA	C1D-ND	3.37	1.42	1.37
12	B	2114	CLA	C4B-NB	3.37	1.42	1.37
12	A	833	CLA	C1D-ND	3.37	1.42	1.37
13	a	840	A1AGD	C3-C4	-3.37	1.44	1.49
13	A	840	A1AGD	C3-C4	-3.37	1.44	1.49
12	b	2105	CLA	C1D-ND	3.37	1.42	1.37
12	A	828	CLA	C1D-ND	3.37	1.42	1.37
12	b	2113	CLA	C4B-NB	3.37	1.42	1.37
12	a	807	CLA	C1D-ND	3.36	1.42	1.37
12	a	820	CLA	C1D-ND	3.36	1.42	1.37
12	a	816	CLA	C1D-ND	3.36	1.42	1.37
12	A	836	CLA	C1D-ND	3.36	1.42	1.37
12	A	829	CLA	C1D-ND	3.35	1.42	1.37
12	A	832	CLA	C1D-ND	3.34	1.42	1.37
12	A	839	CLA	C1D-ND	3.34	1.42	1.37
12	G	832	CLA	C1D-ND	3.34	1.42	1.37
12	a	839	CLA	C1D-ND	3.34	1.42	1.37
12	G	837	CLA	C1D-ND	3.34	1.42	1.37
12	a	828	CLA	C1D-ND	3.34	1.42	1.37
12	B	2126	CLA	C1D-ND	3.34	1.42	1.37
12	l	201	CLA	C1D-ND	3.33	1.42	1.37
12	G	839	CLA	C1D-ND	3.33	1.42	1.37
12	H	2128	CLA	C1D-ND	3.33	1.42	1.37
12	b	2125	CLA	C1D-ND	3.33	1.42	1.37
12	a	825	CLA	C1D-ND	3.33	1.42	1.37
12	a	832	CLA	C1D-ND	3.33	1.42	1.37
12	A	830	CLA	C1D-ND	3.32	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	830	CLA	C1D-ND	3.32	1.42	1.37
12	a	829	CLA	C1D-ND	3.31	1.42	1.37
12	a	850	CLA	C1D-ND	3.31	1.42	1.37
12	L	201	CLA	C1D-ND	3.31	1.42	1.37
12	A	821	CLA	C1D-ND	3.31	1.42	1.37
12	G	850	CLA	C1D-ND	3.30	1.42	1.37
12	A	837	CLA	C1D-ND	3.30	1.42	1.37
12	B	2129	CLA	C1D-ND	3.30	1.42	1.37
12	G	831	CLA	C1D-ND	3.30	1.42	1.37
12	A	850	CLA	C1D-ND	3.30	1.42	1.37
12	A	835	CLA	C1D-ND	3.29	1.42	1.37
12	A	831	CLA	C1D-ND	3.29	1.42	1.37
12	A	825	CLA	C1D-ND	3.29	1.42	1.37
24	M	101	SQD	O5-C1	3.29	1.50	1.41
12	G	830	CLA	C1D-ND	3.29	1.42	1.37
12	G	826	CLA	C1D-ND	3.28	1.42	1.37
12	U	201	CLA	C1D-ND	3.28	1.42	1.37
15	Q	202	BCR	C30-C25	-3.28	1.49	1.53
12	A	826	CLA	C1D-ND	3.28	1.42	1.37
12	a	835	CLA	C1D-ND	3.28	1.42	1.37
24	V	102	SQD	O5-C1	3.28	1.50	1.41
12	G	821	CLA	C1D-ND	3.27	1.42	1.37
12	G	808	CLA	C1D-ND	3.27	1.42	1.37
12	a	837	CLA	C1D-ND	3.27	1.42	1.37
24	m	102	SQD	O5-C1	3.26	1.50	1.41
12	A	808	CLA	C1D-ND	3.26	1.42	1.37
15	U	207	BCR	C1-C6	-3.26	1.49	1.53
12	a	821	CLA	C1D-ND	3.26	1.42	1.37
12	b	2121	CLA	C4B-NB	3.26	1.42	1.37
12	G	825	CLA	C1D-ND	3.26	1.42	1.37
12	G	835	CLA	C1D-ND	3.26	1.42	1.37
12	b	2128	CLA	C1D-ND	3.25	1.42	1.37
12	a	831	CLA	C1D-ND	3.24	1.42	1.37
12	a	808	CLA	C1D-ND	3.24	1.42	1.37
15	L	207	BCR	C1-C6	-3.24	1.49	1.53
12	H	2121	CLA	C4B-NB	3.23	1.42	1.37
15	l	207	BCR	C1-C6	-3.23	1.49	1.53
15	F	202	BCR	C30-C25	-3.23	1.49	1.53
12	H	2110	CLA	C1D-ND	3.23	1.42	1.37
12	b	2138	CLA	C1D-ND	3.23	1.42	1.37
12	a	826	CLA	C1D-ND	3.23	1.42	1.37
12	H	2138	CLA	C1D-ND	3.23	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	2142	BCR	C1-C6	-3.22	1.49	1.53
12	B	2122	CLA	C4B-NB	3.22	1.42	1.37
12	G	810	CLA	C4B-NB	3.21	1.42	1.37
12	B	2139	CLA	C1D-ND	3.21	1.42	1.37
24	V	102	SQD	O47-C7	3.21	1.43	1.34
12	b	2111	CLA	C1D-ND	3.21	1.42	1.37
24	m	102	SQD	O47-C7	3.20	1.43	1.34
12	B	2111	CLA	C1D-ND	3.20	1.42	1.37
15	b	2142	BCR	C1-C6	-3.20	1.49	1.53
12	a	809	CLA	C4B-NB	3.20	1.42	1.37
12	B	2119	CLA	C4B-NB	3.20	1.42	1.37
15	f	202	BCR	C30-C25	-3.20	1.49	1.53
12	a	851	CLA	C1D-ND	3.19	1.42	1.37
12	H	2109	CLA	C1D-ND	3.19	1.42	1.37
12	A	809	CLA	C4B-NB	3.19	1.42	1.37
12	b	2122	CLA	C4B-NB	3.19	1.42	1.37
12	H	2122	CLA	C4B-NB	3.19	1.42	1.37
12	G	809	CLA	C4B-NB	3.18	1.42	1.37
12	H	2101	CLA	C1D-ND	3.18	1.42	1.37
12	b	2110	CLA	C1D-ND	3.18	1.42	1.37
12	b	2109	CLA	C1D-ND	3.18	1.42	1.37
15	H	2142	BCR	C30-C25	-3.18	1.49	1.53
12	H	2118	CLA	C4B-NB	3.18	1.42	1.37
12	L	203	CLA	C1D-ND	3.18	1.42	1.37
15	B	2143	BCR	C30-C25	-3.18	1.49	1.53
12	B	2111	CLA	CMB-C2B	-3.17	1.44	1.50
12	B	2112	CLA	C1D-ND	3.17	1.42	1.37
24	M	101	SQD	O47-C7	3.17	1.43	1.34
12	B	2110	CLA	C1D-ND	3.17	1.42	1.37
12	J	103	CLA	C4B-NB	3.17	1.42	1.37
12	A	851	CLA	C1D-ND	3.17	1.42	1.37
12	b	2110	CLA	CMB-C2B	-3.17	1.44	1.50
12	U	203	CLA	C1D-ND	3.17	1.42	1.37
15	b	2142	BCR	C30-C25	-3.17	1.49	1.53
12	A	826	CLA	C4B-NB	3.17	1.42	1.37
15	B	2143	BCR	C1-C6	-3.17	1.49	1.53
12	l	203	CLA	C1D-ND	3.17	1.42	1.37
12	S	103	CLA	C4B-NB	3.16	1.42	1.37
12	b	2118	CLA	C4B-NB	3.16	1.42	1.37
12	j	103	CLA	C4B-NB	3.16	1.42	1.37
12	b	2133	CLA	C4B-NB	3.16	1.42	1.37
12	G	826	CLA	C4B-NB	3.16	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	2110	CLA	CMB-C2B	-3.16	1.44	1.50
12	G	811	CLA	C4B-NB	3.15	1.42	1.37
12	b	2101	CLA	C1D-ND	3.15	1.42	1.37
12	A	811	CLA	C4B-NB	3.15	1.42	1.37
12	H	2115	CLA	C4B-NB	3.15	1.42	1.37
12	a	826	CLA	C4B-NB	3.15	1.42	1.37
12	B	2123	CLA	C4B-NB	3.15	1.42	1.37
12	G	837	CLA	C4B-NB	3.14	1.42	1.37
12	G	803	CLA	C4B-NB	3.14	1.42	1.37
12	a	810	CLA	C4B-NB	3.14	1.42	1.37
12	a	811	CLA	C4B-NB	3.14	1.42	1.37
12	b	2115	CLA	C4B-NB	3.14	1.42	1.37
12	B	2102	CLA	C1D-ND	3.14	1.42	1.37
12	B	2116	CLA	C4B-NB	3.14	1.42	1.37
12	a	804	CLA	C1D-ND	3.14	1.42	1.37
12	H	2111	CLA	C1D-ND	3.14	1.42	1.37
12	S	102	CLA	C4B-NB	3.13	1.42	1.37
12	A	803	CLA	C4B-NB	3.13	1.42	1.37
12	A	804	CLA	C1D-ND	3.13	1.42	1.37
12	A	810	CLA	C4B-NB	3.13	1.42	1.37
12	b	2117	CLA	C4B-NB	3.13	1.42	1.37
12	G	834	CLA	C4B-NB	3.13	1.42	1.37
12	B	2118	CLA	C4B-NB	3.12	1.42	1.37
12	j	102	CLA	C4B-NB	3.12	1.42	1.37
22	b	2150	EQ3	C7-C6	3.11	1.55	1.45
12	A	834	CLA	C4B-NB	3.11	1.41	1.37
22	B	2151	EQ3	C7-C6	3.11	1.55	1.45
12	A	837	CLA	C4B-NB	3.11	1.41	1.37
12	B	2133	CLA	C1D-ND	3.11	1.41	1.37
12	B	2134	CLA	C4B-NB	3.11	1.41	1.37
12	H	2117	CLA	C4B-NB	3.11	1.41	1.37
12	a	834	CLA	C4B-NB	3.11	1.41	1.37
12	G	851	CLA	C1D-ND	3.10	1.41	1.37
12	H	2141	CLA	C4B-NB	3.10	1.41	1.37
22	H	2150	EQ3	C7-C6	3.10	1.55	1.45
12	T	4002	CLA	C4B-NB	3.10	1.41	1.37
12	a	819	CLA	C4B-NB	3.09	1.41	1.37
12	A	824	CLA	C4B-NB	3.09	1.41	1.37
12	A	819	CLA	C4B-NB	3.09	1.41	1.37
12	J	102	CLA	C4B-NB	3.09	1.41	1.37
12	a	815	CLA	C4B-NB	3.09	1.41	1.37
12	H	2132	CLA	C1D-ND	3.09	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	819	CLA	C4B-NB	3.09	1.41	1.37
12	b	2120	CLA	C4B-NB	3.09	1.41	1.37
12	B	2101	CLA	C1D-ND	3.09	1.41	1.37
12	G	804	CLA	C1D-ND	3.09	1.41	1.37
12	B	2136	CLA	C4B-NB	3.09	1.41	1.37
12	H	2152	CLA	C1D-ND	3.08	1.41	1.37
12	a	806	CLA	C4B-NB	3.08	1.41	1.37
12	b	2129	CLA	C4B-NB	3.08	1.41	1.37
12	b	2152	CLA	C1D-ND	3.08	1.41	1.37
12	H	2133	CLA	C4B-NB	3.08	1.41	1.37
12	H	2129	CLA	C4B-NB	3.08	1.41	1.37
12	B	2121	CLA	C4B-NB	3.08	1.41	1.37
12	B	2130	CLA	C4B-NB	3.07	1.41	1.37
12	A	815	CLA	C4B-NB	3.07	1.41	1.37
12	a	803	CLA	C4B-NB	3.07	1.41	1.37
12	a	837	CLA	C4B-NB	3.07	1.41	1.37
12	B	2142	CLA	C4B-NB	3.07	1.41	1.37
12	b	2132	CLA	C1D-ND	3.07	1.41	1.37
15	j	104	BCR	C1-C6	-3.07	1.49	1.53
12	F	204	CLA	C4B-NB	3.06	1.41	1.37
22	H	2150	EQ3	C24-C25	3.06	1.55	1.45
12	l	205	CLA	C4B-NB	3.06	1.41	1.37
12	k	4002	CLA	C4B-NB	3.06	1.41	1.37
12	L	205	CLA	C4B-NB	3.06	1.41	1.37
15	J	104	BCR	C1-C6	-3.05	1.49	1.53
12	b	2125	CLA	C4B-NB	3.05	1.41	1.37
12	Q	204	CLA	C4B-NB	3.05	1.41	1.37
12	K	4002	CLA	C4B-NB	3.05	1.41	1.37
12	G	806	CLA	C4B-NB	3.05	1.41	1.37
12	A	806	CLA	C4B-NB	3.05	1.41	1.37
12	B	2113	CLA	C4B-NB	3.05	1.41	1.37
22	B	2151	EQ3	C24-C25	3.04	1.55	1.45
12	B	2104	CLA	C1B-C2B	3.04	1.50	1.43
12	a	817	CLA	C4B-NB	3.04	1.41	1.37
12	B	2126	CLA	C4B-NB	3.04	1.41	1.37
15	S	104	BCR	C1-C6	-3.04	1.49	1.53
12	a	824	CLA	C4B-NB	3.04	1.41	1.37
12	H	2135	CLA	C4B-NB	3.04	1.41	1.37
22	b	2150	EQ3	C24-C25	3.04	1.55	1.45
12	b	2112	CLA	C4B-NB	3.04	1.41	1.37
12	b	2129	CLA	CMD-C2D	-3.04	1.44	1.50
12	H	2112	CLA	C4B-NB	3.04	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	S	101	BCR	C30-C25	-3.04	1.49	1.53
12	f	204	CLA	C4B-NB	3.04	1.41	1.37
12	b	2103	CLA	C1B-C2B	3.04	1.50	1.43
12	B	2130	CLA	CMD-C2D	-3.04	1.44	1.50
12	G	813	CLA	C4B-NB	3.04	1.41	1.37
12	H	2138	CLA	C4B-NB	3.04	1.41	1.37
12	B	2132	CLA	C4B-NB	3.03	1.41	1.37
12	b	2135	CLA	C4B-NB	3.03	1.41	1.37
12	H	2131	CLA	C4B-NB	3.03	1.41	1.37
12	H	2103	CLA	C1B-C2B	3.03	1.50	1.43
12	H	2129	CLA	CMD-C2D	-3.03	1.44	1.50
12	G	824	CLA	C4B-NB	3.03	1.41	1.37
12	b	2131	CLA	C4B-NB	3.03	1.41	1.37
12	b	2126	CLA	C4B-NB	3.03	1.41	1.37
12	A	813	CLA	C4B-NB	3.03	1.41	1.37
12	A	829	CLA	C4B-NB	3.03	1.41	1.37
12	H	2125	CLA	C4B-NB	3.02	1.41	1.37
12	a	829	CLA	C4B-NB	3.02	1.41	1.37
12	b	2116	CLA	C4B-NB	3.02	1.41	1.37
12	b	2141	CLA	C4B-NB	3.02	1.41	1.37
15	J	101	BCR	C30-C25	-3.02	1.49	1.53
15	j	101	BCR	C30-C25	-3.02	1.49	1.53
12	G	829	CLA	C4B-NB	3.02	1.41	1.37
12	A	839	CLA	C4B-NB	3.02	1.41	1.37
12	b	2138	CLA	C4B-NB	3.02	1.41	1.37
12	H	2104	CLA	CMC-C2C	-3.02	1.44	1.50
12	U	205	CLA	C4B-NB	3.02	1.41	1.37
12	B	2139	CLA	C4B-NB	3.02	1.41	1.37
12	B	2135	CLA	C4B-NB	3.01	1.41	1.37
12	H	2120	CLA	C4B-NB	3.01	1.41	1.37
12	B	2127	CLA	C4B-NB	3.01	1.41	1.37
12	a	839	CLA	C4B-NB	3.01	1.41	1.37
12	A	801	CLA	C1B-C2B	3.01	1.50	1.43
12	H	2126	CLA	C4B-NB	3.01	1.41	1.37
12	B	2105	CLA	CMC-C2C	-3.01	1.44	1.50
12	G	815	CLA	C4B-NB	3.01	1.41	1.37
12	a	813	CLA	C4B-NB	3.01	1.41	1.37
12	G	839	CLA	C4B-NB	3.01	1.41	1.37
12	B	2129	CLA	C4B-NB	3.01	1.41	1.37
12	H	2128	CLA	C4B-NB	3.01	1.41	1.37
12	b	2134	CLA	C4B-NB	3.00	1.41	1.37
12	b	2128	CLA	C4B-NB	3.00	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	817	CLA	C4B-NB	3.00	1.41	1.37
15	G	842	BCR	C30-C25	-3.00	1.49	1.53
12	a	801	CLA	C1B-C2B	3.00	1.50	1.43
12	B	2117	CLA	C4B-NB	3.00	1.41	1.37
12	b	2107	CLA	C4B-NB	3.00	1.41	1.37
15	B	2146	BCR	C30-C25	-2.99	1.50	1.53
12	H	2152	CLA	C4B-NB	2.99	1.41	1.37
12	b	2104	CLA	CMC-C2C	-2.99	1.44	1.50
12	b	2140	CLA	C4B-NB	2.99	1.41	1.37
12	G	801	CLA	C1B-C2B	2.99	1.50	1.43
15	S	104	BCR	C30-C25	-2.99	1.50	1.53
12	b	2123	CLA	C4B-NB	2.99	1.41	1.37
22	b	2150	EQ3	O3-C3	-2.99	1.34	1.43
24	M	101	SQD	C24-C23	2.98	1.59	1.50
24	m	102	SQD	C24-C23	2.98	1.59	1.50
12	a	812	CLA	C4B-NB	2.98	1.41	1.37
24	V	102	SQD	C24-C23	2.98	1.59	1.50
15	a	844	BCR	C30-C25	-2.98	1.50	1.53
12	H	2134	CLA	C4B-NB	2.98	1.41	1.37
12	H	2123	CLA	C4B-NB	2.98	1.41	1.37
12	H	2106	CLA	C4B-NB	2.98	1.41	1.37
12	B	2141	CLA	C4B-NB	2.98	1.41	1.37
15	G	844	BCR	C30-C25	-2.97	1.50	1.53
12	H	2132	CLA	C4B-NB	2.97	1.41	1.37
12	a	821	CLA	C4B-NB	2.97	1.41	1.37
12	G	821	CLA	C4B-NB	2.97	1.41	1.37
12	B	2108	CLA	C4B-NB	2.97	1.41	1.37
15	A	843	BCR	C1-C6	-2.97	1.50	1.53
12	a	822	CLA	C4B-NB	2.97	1.41	1.37
12	A	802	CLA	C4B-NB	2.97	1.41	1.37
12	H	2111	CLA	C4B-NB	2.97	1.41	1.37
22	B	2151	EQ3	O3-C3	-2.97	1.34	1.43
12	A	812	CLA	C4B-NB	2.97	1.41	1.37
12	B	2124	CLA	C4B-NB	2.97	1.41	1.37
15	a	842	BCR	C30-C25	-2.97	1.50	1.53
15	b	2145	BCR	C30-C25	-2.97	1.50	1.53
12	H	2107	CLA	C4B-NB	2.96	1.41	1.37
12	b	2111	CLA	C4B-NB	2.96	1.41	1.37
12	f	201	CLA	C4B-NB	2.96	1.41	1.37
24	L	208	SQD	C24-C23	2.96	1.59	1.50
12	H	2109	CLA	C4B-NB	2.96	1.41	1.37
12	Q	201	CLA	C4B-NB	2.96	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	832	CLA	C4B-NB	2.96	1.41	1.37
12	A	821	CLA	C4B-NB	2.96	1.41	1.37
15	G	843	BCR	C1-C6	-2.96	1.50	1.53
12	H	2116	CLA	C4B-NB	2.96	1.41	1.37
24	l	208	SQD	C24-C23	2.96	1.59	1.50
24	U	208	SQD	C24-C23	2.96	1.59	1.50
12	a	802	CLA	C4B-NB	2.96	1.41	1.37
12	G	817	CLA	C4B-NB	2.96	1.41	1.37
12	b	2105	CLA	C4B-NB	2.96	1.41	1.37
12	A	832	CLA	C4B-NB	2.96	1.41	1.37
12	F	201	CLA	C4B-NB	2.96	1.41	1.37
15	G	844	BCR	C1-C6	-2.95	1.50	1.53
15	A	842	BCR	C30-C25	-2.95	1.50	1.53
12	B	2112	CLA	C4B-NB	2.95	1.41	1.37
15	H	2145	BCR	C30-C25	-2.95	1.50	1.53
12	G	812	CLA	C4B-NB	2.95	1.41	1.37
12	H	2140	CLA	C4B-NB	2.95	1.41	1.37
15	a	843	BCR	C1-C6	-2.95	1.50	1.53
12	b	2152	CLA	C4B-NB	2.95	1.41	1.37
12	H	2139	CLA	C1D-ND	2.95	1.41	1.37
22	H	2150	EQ3	O3-C3	-2.95	1.34	1.43
12	A	822	CLA	C4B-NB	2.95	1.41	1.37
12	a	808	CLA	C4B-NB	2.95	1.41	1.37
15	A	844	BCR	C30-C25	-2.94	1.50	1.53
12	A	808	CLA	C4B-NB	2.94	1.41	1.37
15	a	844	BCR	C1-C6	-2.94	1.50	1.53
23	H	2151	ZEX	C40-C33	2.94	1.56	1.50
15	J	104	BCR	C30-C25	-2.94	1.50	1.53
12	G	827	CLA	C4B-NB	2.94	1.41	1.37
12	B	2133	CLA	C4B-NB	2.93	1.41	1.37
12	b	2132	CLA	C4B-NB	2.93	1.41	1.37
12	G	802	CLA	C4B-NB	2.93	1.41	1.37
12	a	832	CLA	C4B-NB	2.93	1.41	1.37
12	b	2109	CLA	C4B-NB	2.93	1.41	1.37
12	B	2110	CLA	C4B-NB	2.93	1.41	1.37
15	a	845	BCR	C1-C6	-2.93	1.50	1.53
23	b	2151	ZEX	C40-C33	2.93	1.56	1.50
23	B	2152	ZEX	C40-C33	2.92	1.56	1.50
12	b	2106	CLA	C4B-NB	2.92	1.41	1.37
12	B	2125	CLA	C4B-NB	2.92	1.41	1.37
12	H	2124	CLA	C4B-NB	2.92	1.41	1.37
12	B	2107	CLA	C4B-NB	2.91	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	2115	CLA	C4B-NB	2.91	1.41	1.37
12	H	2114	CLA	C4B-NB	2.91	1.41	1.37
15	A	845	BCR	C1-C6	-2.91	1.50	1.53
12	b	2124	CLA	C4B-NB	2.91	1.41	1.37
12	A	820	CLA	C4B-NB	2.91	1.41	1.37
15	j	101	BCR	C1-C6	-2.91	1.50	1.53
15	A	844	BCR	C1-C6	-2.91	1.50	1.53
12	Q	203	CLA	C4B-NB	2.91	1.41	1.37
12	B	2140	CLA	C1D-ND	2.91	1.41	1.37
15	G	845	BCR	C1-C6	-2.90	1.50	1.53
15	J	101	BCR	C1-C6	-2.90	1.50	1.53
12	a	820	CLA	C4B-NB	2.90	1.41	1.37
12	a	827	CLA	C4B-NB	2.90	1.41	1.37
15	j	104	BCR	C30-C25	-2.90	1.50	1.53
12	b	2129	CLA	C1D-ND	2.90	1.41	1.37
12	G	808	CLA	C4B-NB	2.90	1.41	1.37
12	A	827	CLA	C4B-NB	2.89	1.41	1.37
12	A	805	CLA	C4B-NB	2.89	1.41	1.37
12	F	203	CLA	C4B-NB	2.89	1.41	1.37
12	G	822	CLA	C4B-NB	2.89	1.41	1.37
12	G	820	CLA	C4B-NB	2.89	1.41	1.37
12	a	836	CLA	C4B-NB	2.88	1.41	1.37
12	B	2101	CLA	C4B-NB	2.88	1.41	1.37
12	B	2106	CLA	C4B-NB	2.88	1.41	1.37
15	S	101	BCR	C1-C6	-2.88	1.50	1.53
12	H	2127	CLA	C4B-NB	2.88	1.41	1.37
12	b	2114	CLA	C4B-NB	2.87	1.41	1.37
12	a	851	CLA	C4B-NB	2.87	1.41	1.37
12	f	203	CLA	C4B-NB	2.87	1.41	1.37
12	B	2141	CLA	C1B-C2B	2.87	1.49	1.43
12	B	2130	CLA	C1D-ND	2.87	1.41	1.37
12	G	831	CLA	C4B-NB	2.87	1.41	1.37
12	G	851	CLA	C4B-NB	2.87	1.41	1.37
12	a	805	CLA	C4B-NB	2.87	1.41	1.37
12	a	824	CLA	C1B-C2B	2.87	1.49	1.43
12	b	2140	CLA	C1B-C2B	2.86	1.49	1.43
12	H	2140	CLA	C1B-C2B	2.86	1.49	1.43
12	G	825	CLA	C4B-NB	2.86	1.41	1.37
12	a	831	CLA	C4B-NB	2.86	1.41	1.37
12	a	825	CLA	C4B-NB	2.86	1.41	1.37
12	A	831	CLA	C4B-NB	2.86	1.41	1.37
12	G	805	CLA	C4B-NB	2.86	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	2105	CLA	C4B-NB	2.86	1.41	1.37
12	b	2127	CLA	C4B-NB	2.85	1.41	1.37
12	A	838	CLA	C4B-NB	2.85	1.41	1.37
12	A	825	CLA	C4B-NB	2.85	1.41	1.37
23	f	205	ZEX	C40-C33	2.85	1.56	1.50
12	B	2111	CLA	C4B-NB	2.85	1.41	1.37
12	a	818	CLA	C4B-NB	2.85	1.41	1.37
15	l	206	BCR	C1-C6	-2.85	1.50	1.53
12	b	2110	CLA	C4B-NB	2.85	1.41	1.37
12	b	2139	CLA	C1D-ND	2.85	1.41	1.37
12	L	204	CLA	C4B-NB	2.85	1.41	1.37
12	H	2129	CLA	C1D-ND	2.84	1.41	1.37
12	B	2120	CLA	C4B-NB	2.84	1.41	1.37
12	G	818	CLA	C4B-NB	2.84	1.41	1.37
12	b	2119	CLA	C4B-NB	2.84	1.41	1.37
17	a	847	LMG	C4-C5	2.84	1.59	1.53
12	a	838	CLA	C4B-NB	2.84	1.41	1.37
12	A	836	CLA	C4B-NB	2.84	1.41	1.37
12	A	824	CLA	C1B-C2B	2.83	1.49	1.43
12	H	2110	CLA	C4B-NB	2.83	1.41	1.37
12	A	818	CLA	C4B-NB	2.83	1.41	1.37
12	b	2107	CLA	C1B-C2B	2.83	1.49	1.43
12	A	819	CLA	C1B-C2B	2.83	1.49	1.43
23	Q	205	ZEX	C40-C33	2.83	1.56	1.50
12	G	816	CLA	C4B-NB	2.83	1.41	1.37
12	b	2129	CLA	CMB-C2B	-2.83	1.45	1.50
12	G	838	CLA	C4B-NB	2.83	1.41	1.37
17	A	847	LMG	C4-C5	2.83	1.59	1.53
12	U	204	CLA	C4B-NB	2.83	1.41	1.37
12	L	204	CLA	C1D-ND	2.82	1.41	1.37
12	A	851	CLA	C4B-NB	2.82	1.41	1.37
12	B	2108	CLA	C1B-C2B	2.82	1.49	1.43
23	F	205	ZEX	C40-C33	2.82	1.56	1.50
12	B	2130	CLA	CMB-C2B	-2.82	1.45	1.50
15	H	2145	BCR	C1-C6	-2.82	1.50	1.53
12	A	816	CLA	C4B-NB	2.82	1.41	1.37
12	a	809	CLA	C1B-C2B	2.82	1.49	1.43
12	a	802	CLA	C1B-C2B	2.82	1.49	1.43
12	B	2128	CLA	C4B-NB	2.82	1.41	1.37
12	a	801	CLA	C4B-NB	2.82	1.41	1.37
15	U	206	BCR	C1-C6	-2.82	1.50	1.53
12	a	819	CLA	C1B-C2B	2.81	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	819	CLA	C1B-C2B	2.81	1.49	1.43
12	H	2133	CLA	C1B-C2B	2.81	1.49	1.43
12	a	807	CLA	C4B-NB	2.81	1.41	1.37
12	l	204	CLA	C1D-ND	2.81	1.41	1.37
12	H	2130	CLA	C4B-NB	2.81	1.41	1.37
12	b	2141	CLA	C1B-C2B	2.81	1.49	1.43
12	U	204	CLA	C1D-ND	2.81	1.41	1.37
17	G	847	LMG	C4-C5	2.81	1.59	1.53
12	A	802	CLA	C1B-C2B	2.81	1.49	1.43
12	b	2118	CLA	C1B-C2B	2.81	1.49	1.43
12	G	801	CLA	C4B-NB	2.81	1.41	1.37
12	B	2119	CLA	C1B-C2B	2.80	1.49	1.43
12	a	816	CLA	C1B-C2B	2.80	1.49	1.43
12	A	804	CLA	C4B-NB	2.80	1.41	1.37
12	G	824	CLA	C1B-C2B	2.80	1.49	1.43
12	A	809	CLA	C1B-C2B	2.80	1.49	1.43
12	J	103	CLA	C1B-C2B	2.80	1.49	1.43
12	j	103	CLA	C1B-C2B	2.80	1.49	1.43
12	G	816	CLA	C1B-C2B	2.80	1.49	1.43
12	S	103	CLA	C1B-C2B	2.80	1.49	1.43
12	a	816	CLA	C4B-NB	2.80	1.41	1.37
12	B	2131	CLA	C4B-NB	2.80	1.41	1.37
12	H	2107	CLA	C1B-C2B	2.80	1.49	1.43
12	H	2102	CLA	C4B-NB	2.80	1.41	1.37
12	H	2141	CLA	C1B-C2B	2.80	1.49	1.43
12	A	816	CLA	C1B-C2B	2.80	1.49	1.43
15	L	206	BCR	C1-C6	-2.80	1.50	1.53
12	b	2134	CLA	C1B-C2B	2.79	1.49	1.43
12	a	804	CLA	C4B-NB	2.79	1.41	1.37
12	B	2128	CLA	C1B-C2B	2.79	1.49	1.43
12	b	2127	CLA	C1B-C2B	2.79	1.49	1.43
12	G	809	CLA	C1B-C2B	2.79	1.49	1.43
12	A	807	CLA	C4B-NB	2.79	1.41	1.37
12	H	2118	CLA	C1B-C2B	2.79	1.49	1.43
12	G	807	CLA	C4B-NB	2.79	1.41	1.37
12	H	2129	CLA	CMB-C2B	-2.79	1.45	1.50
12	B	2142	CLA	C1B-C2B	2.79	1.49	1.43
12	G	854	CLA	C4B-NB	2.79	1.41	1.37
12	H	2114	CLA	C1B-C2B	2.79	1.49	1.43
12	H	2119	CLA	C4B-NB	2.78	1.41	1.37
12	A	823	CLA	C4B-NB	2.78	1.41	1.37
12	B	2134	CLA	C1B-C2B	2.78	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	l	204	CLA	C4B-NB	2.78	1.41	1.37
12	G	802	CLA	C1B-C2B	2.78	1.49	1.43
12	G	823	CLA	C4B-NB	2.78	1.41	1.37
12	f	204	CLA	C1B-C2B	2.78	1.49	1.43
13	a	840	A1AGD	C23-C24	-2.78	1.34	1.51
12	a	854	CLA	C4B-NB	2.78	1.41	1.37
12	b	2133	CLA	C1B-C2B	2.78	1.49	1.43
12	B	2115	CLA	C1B-C2B	2.78	1.49	1.43
12	H	2106	CLA	C1B-C2B	2.78	1.49	1.43
12	b	2126	CLA	C1B-C2B	2.78	1.49	1.43
13	G	840	A1AGD	C23-C24	-2.77	1.34	1.51
12	H	2127	CLA	C1B-C2B	2.77	1.49	1.43
12	b	2114	CLA	C1B-C2B	2.77	1.49	1.43
13	G	840	A1AGD	C52-C5	-2.77	1.45	1.50
13	A	840	A1AGD	C23-C24	-2.77	1.34	1.51
12	b	2130	CLA	C4B-NB	2.77	1.41	1.37
12	B	2135	CLA	C1B-C2B	2.77	1.49	1.43
12	b	2106	CLA	C1B-C2B	2.77	1.49	1.43
12	A	801	CLA	C4B-NB	2.77	1.41	1.37
12	G	836	CLA	C4B-NB	2.76	1.41	1.37
12	a	823	CLA	C4B-NB	2.76	1.41	1.37
12	B	2103	CLA	C4B-NB	2.76	1.41	1.37
12	G	814	CLA	C4B-NB	2.76	1.41	1.37
15	b	2145	BCR	C1-C6	-2.76	1.50	1.53
12	A	854	CLA	C4B-NB	2.76	1.41	1.37
15	B	2146	BCR	C1-C6	-2.76	1.50	1.53
12	a	805	CLA	C1B-C2B	2.76	1.49	1.43
12	b	2115	CLA	C1B-C2B	2.76	1.49	1.43
12	a	814	CLA	C4B-NB	2.76	1.41	1.37
12	F	204	CLA	C1B-C2B	2.76	1.49	1.43
12	A	814	CLA	C4B-NB	2.76	1.41	1.37
12	F	201	CLA	C1B-C2B	2.75	1.49	1.43
12	B	2127	CLA	C1B-C2B	2.75	1.49	1.43
12	f	201	CLA	C1B-C2B	2.75	1.49	1.43
12	H	2134	CLA	C1B-C2B	2.75	1.49	1.43
12	A	805	CLA	C1B-C2B	2.75	1.49	1.43
12	H	2115	CLA	C1B-C2B	2.75	1.49	1.43
12	G	805	CLA	C1B-C2B	2.75	1.49	1.43
13	A	840	A1AGD	C52-C5	-2.75	1.45	1.50
12	B	2107	CLA	C1B-C2B	2.75	1.49	1.43
22	H	2150	EQ3	C35-C13	2.74	1.56	1.50
22	b	2150	EQ3	C35-C13	2.74	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	804	CLA	C4B-NB	2.74	1.41	1.37
12	j	102	CLA	C1B-C2B	2.74	1.49	1.43
12	U	203	CLA	C4B-NB	2.74	1.41	1.37
12	Q	204	CLA	C1B-C2B	2.74	1.49	1.43
22	B	2151	EQ3	C35-C13	2.74	1.56	1.50
12	b	2113	CLA	C1B-C2B	2.74	1.49	1.43
12	A	826	CLA	CHC-C1C	2.74	1.44	1.38
12	G	826	CLA	CHC-C1C	2.74	1.44	1.38
12	a	829	CLA	C1B-C2B	2.74	1.49	1.43
12	a	806	CLA	C1B-C2B	2.74	1.49	1.43
12	A	806	CLA	C1B-C2B	2.74	1.49	1.43
12	B	2116	CLA	C1B-C2B	2.73	1.49	1.43
12	H	2126	CLA	C1B-C2B	2.73	1.49	1.43
12	a	826	CLA	C3B-C4B	2.73	1.50	1.42
12	G	829	CLA	C1B-C2B	2.73	1.49	1.43
12	T	4002	CLA	C1B-C2B	2.73	1.49	1.43
12	B	2114	CLA	C1B-C2B	2.73	1.49	1.43
12	a	832	CLA	C1B-C2B	2.73	1.49	1.43
12	G	813	CLA	C1B-C2B	2.73	1.49	1.43
12	S	102	CLA	C1B-C2B	2.73	1.49	1.43
12	a	826	CLA	CHC-C1C	2.73	1.44	1.38
12	b	2121	CLA	C1B-C2B	2.73	1.49	1.43
13	a	840	A1AGD	C52-C5	-2.73	1.45	1.50
12	G	826	CLA	C3B-C4B	2.73	1.50	1.42
12	a	814	CLA	C1B-C2B	2.73	1.49	1.43
12	A	829	CLA	C1B-C2B	2.73	1.49	1.43
12	Q	201	CLA	C1B-C2B	2.73	1.49	1.43
12	A	814	CLA	C1B-C2B	2.72	1.49	1.43
12	H	2113	CLA	C1B-C2B	2.72	1.49	1.43
12	G	832	CLA	C1B-C2B	2.72	1.49	1.43
12	H	2117	CLA	C1B-C2B	2.72	1.49	1.43
12	G	806	CLA	C1B-C2B	2.72	1.49	1.43
12	G	814	CLA	C1B-C2B	2.72	1.49	1.43
12	H	2123	CLA	C1B-C2B	2.72	1.49	1.43
12	J	102	CLA	C1B-C2B	2.72	1.49	1.43
12	b	2102	CLA	C4B-NB	2.72	1.41	1.37
12	K	4002	CLA	C1B-C2B	2.71	1.49	1.43
12	G	854	CLA	C1B-C2B	2.71	1.49	1.43
12	A	826	CLA	C3B-C4B	2.71	1.50	1.42
12	a	823	CLA	C1B-C2B	2.71	1.49	1.43
12	B	2118	CLA	C1B-C2B	2.71	1.49	1.43
12	a	804	CLA	C1B-C2B	2.71	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	2123	CLA	C1B-C2B	2.71	1.49	1.43
12	G	823	CLA	C1B-C2B	2.71	1.49	1.43
12	G	822	CLA	C1B-C2B	2.71	1.49	1.43
12	A	832	CLA	C1B-C2B	2.71	1.49	1.43
12	b	2102	CLA	C1D-ND	2.71	1.41	1.37
12	A	835	CLA	C1B-C2B	2.71	1.49	1.43
12	G	804	CLA	C1B-C2B	2.71	1.49	1.43
12	B	2103	CLA	C1D-ND	2.70	1.41	1.37
12	k	4002	CLA	C1B-C2B	2.70	1.49	1.43
12	A	854	CLA	C1B-C2B	2.70	1.49	1.43
12	b	2139	CLA	C4B-NB	2.70	1.41	1.37
12	a	835	CLA	C1B-C2B	2.70	1.49	1.43
12	B	2124	CLA	C1B-C2B	2.70	1.49	1.43
12	H	2152	CLA	C1B-C2B	2.70	1.49	1.43
12	A	813	CLA	C1B-C2B	2.70	1.49	1.43
12	H	2121	CLA	C1B-C2B	2.70	1.49	1.43
12	A	823	CLA	C1B-C2B	2.70	1.49	1.43
12	A	804	CLA	C1B-C2B	2.70	1.49	1.43
15	A	842	BCR	C1-C6	-2.70	1.50	1.53
12	H	2102	CLA	C1D-ND	2.70	1.41	1.37
12	f	203	CLA	C1B-C2B	2.70	1.49	1.43
15	a	842	BCR	C1-C6	-2.70	1.50	1.53
12	A	837	CLA	C3B-C4B	2.70	1.50	1.42
12	b	2117	CLA	C1B-C2B	2.70	1.49	1.43
12	G	815	CLA	C1B-C2B	2.69	1.49	1.43
12	b	2122	CLA	C1B-C2B	2.69	1.49	1.43
12	l	203	CLA	C4B-NB	2.69	1.41	1.37
12	A	822	CLA	C1B-C2B	2.69	1.49	1.43
12	B	2137	CLA	C4B-NB	2.69	1.41	1.37
12	a	831	CLA	C1B-C2B	2.69	1.49	1.43
12	B	2117	CLA	C1B-C2B	2.69	1.49	1.43
12	B	2122	CLA	C1B-C2B	2.69	1.49	1.43
15	T	4001	BCR	C1-C6	-2.69	1.50	1.53
12	G	835	CLA	C1B-C2B	2.69	1.49	1.43
12	l	201	CLA	C1B-C2B	2.69	1.49	1.43
12	A	821	CLA	C1B-C2B	2.69	1.49	1.43
12	G	838	CLA	C1B-C2B	2.69	1.49	1.43
12	A	827	CLA	C1B-C2B	2.69	1.49	1.43
12	H	2116	CLA	C1B-C2B	2.69	1.49	1.43
12	a	837	CLA	C3B-C4B	2.69	1.50	1.42
12	G	821	CLA	C1B-C2B	2.69	1.49	1.43
12	a	854	CLA	C1B-C2B	2.69	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	821	CLA	C1B-C2B	2.68	1.49	1.43
12	a	822	CLA	C1B-C2B	2.68	1.49	1.43
12	a	813	CLA	C1B-C2B	2.68	1.49	1.43
12	B	2113	CLA	C1B-C2B	2.68	1.49	1.43
12	F	203	CLA	C1B-C2B	2.68	1.49	1.43
12	H	2112	CLA	C1B-C2B	2.68	1.49	1.43
12	A	815	CLA	C1B-C2B	2.68	1.49	1.43
12	H	2139	CLA	C4B-NB	2.68	1.41	1.37
12	B	2140	CLA	C4B-NB	2.68	1.41	1.37
12	L	203	CLA	C4B-NB	2.68	1.41	1.37
15	H	2146	BCR	C1-C6	-2.68	1.50	1.53
12	b	2152	CLA	C1B-C2B	2.68	1.49	1.43
12	G	837	CLA	C3B-C4B	2.68	1.50	1.42
12	B	2101	CLA	C1B-C2B	2.68	1.49	1.43
12	b	2136	CLA	C4B-NB	2.67	1.41	1.37
12	b	2112	CLA	C1B-C2B	2.67	1.49	1.43
12	a	838	CLA	C1B-C2B	2.67	1.49	1.43
12	A	812	CLA	C1B-C2B	2.67	1.49	1.43
12	b	2124	CLA	C1B-C2B	2.67	1.49	1.43
12	B	2123	CLA	C1B-C2B	2.67	1.49	1.43
12	A	838	CLA	C1B-C2B	2.67	1.49	1.43
12	H	2108	CLA	C1B-C2B	2.67	1.49	1.43
12	b	2116	CLA	C1B-C2B	2.67	1.49	1.43
12	Q	203	CLA	C1B-C2B	2.67	1.49	1.43
12	L	201	CLA	C1B-C2B	2.67	1.49	1.43
12	H	2137	CLA	C1B-C2B	2.67	1.49	1.43
12	A	831	CLA	C1B-C2B	2.67	1.49	1.43
12	G	831	CLA	C1B-C2B	2.66	1.49	1.43
12	a	815	CLA	C1B-C2B	2.66	1.49	1.43
12	G	827	CLA	C1B-C2B	2.66	1.49	1.43
15	B	2147	BCR	C1-C6	-2.66	1.50	1.53
15	K	4001	BCR	C1-C6	-2.66	1.50	1.53
15	G	842	BCR	C1-C6	-2.66	1.50	1.53
12	G	812	CLA	C1B-C2B	2.66	1.49	1.43
12	B	2138	CLA	C1B-C2B	2.65	1.49	1.43
15	k	4001	BCR	C1-C6	-2.65	1.50	1.53
12	a	827	CLA	C1B-C2B	2.65	1.49	1.43
12	B	2125	CLA	C1B-C2B	2.65	1.49	1.43
12	H	2136	CLA	C4B-NB	2.65	1.41	1.37
12	a	812	CLA	C1B-C2B	2.65	1.49	1.43
12	b	2108	CLA	C1B-C2B	2.65	1.49	1.43
12	b	2138	CLA	C1B-C2B	2.64	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	2109	CLA	C1B-C2B	2.64	1.49	1.43
22	b	2150	EQ3	C33-C5	2.64	1.55	1.50
12	b	2119	CLA	C1B-C2B	2.64	1.49	1.43
12	H	2122	CLA	C1B-C2B	2.64	1.49	1.43
12	A	850	CLA	C4B-NB	2.64	1.41	1.37
22	B	2151	EQ3	C33-C5	2.64	1.55	1.50
12	H	2119	CLA	C1B-C2B	2.64	1.49	1.43
15	b	2146	BCR	C1-C6	-2.64	1.50	1.53
15	l	207	BCR	C30-C25	-2.64	1.50	1.53
12	l	204	CLA	C1B-C2B	2.64	1.49	1.43
12	H	2124	CLA	C1B-C2B	2.63	1.49	1.43
15	L	207	BCR	C30-C25	-2.63	1.50	1.53
12	U	201	CLA	C1B-C2B	2.63	1.49	1.43
12	B	2120	CLA	C1B-C2B	2.63	1.49	1.43
12	a	811	CLA	C3B-C4B	2.63	1.50	1.42
12	A	833	CLA	C4B-NB	2.63	1.41	1.37
12	L	204	CLA	C1B-C2B	2.63	1.49	1.43
12	b	2137	CLA	C1B-C2B	2.63	1.49	1.43
12	G	851	CLA	C1B-C2B	2.62	1.49	1.43
12	a	850	CLA	C4B-NB	2.62	1.41	1.37
12	a	851	CLA	C1B-C2B	2.62	1.49	1.43
12	A	851	CLA	C1B-C2B	2.62	1.49	1.43
15	U	207	BCR	C30-C25	-2.62	1.50	1.53
22	H	2150	EQ3	C33-C5	2.62	1.55	1.50
12	a	833	CLA	C4B-NB	2.62	1.41	1.37
12	A	828	CLA	C4B-NB	2.62	1.41	1.37
12	b	2131	CLA	C1B-C2B	2.62	1.49	1.43
15	b	2144	BCR	C1-C6	-2.61	1.50	1.53
12	G	833	CLA	C4B-NB	2.61	1.41	1.37
12	a	828	CLA	C4B-NB	2.61	1.41	1.37
12	U	204	CLA	C1B-C2B	2.61	1.49	1.43
12	B	2138	CLA	C4B-NB	2.61	1.41	1.37
12	G	811	CLA	C3B-C4B	2.61	1.50	1.42
12	b	2137	CLA	C4B-NB	2.61	1.41	1.37
12	G	850	CLA	C4B-NB	2.61	1.41	1.37
12	B	2137	CLA	C1B-C2B	2.60	1.49	1.43
12	A	811	CLA	C3B-C4B	2.60	1.50	1.42
12	H	2103	CLA	C4B-NB	2.60	1.41	1.37
12	H	2136	CLA	C1B-C2B	2.60	1.49	1.43
15	i	101	BCR	C1-C6	-2.60	1.50	1.53
12	B	2139	CLA	C1B-C2B	2.60	1.49	1.43
12	G	828	CLA	C4B-NB	2.60	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	2138	CLA	C1B-C2B	2.60	1.49	1.43
12	b	2120	CLA	CMB-C2B	-2.60	1.45	1.50
12	H	2101	CLA	C4B-NB	2.60	1.41	1.37
12	a	810	CLA	C1B-C2B	2.60	1.49	1.43
12	B	2121	CLA	CMB-C2B	-2.60	1.45	1.50
12	H	2120	CLA	CMB-C2B	-2.60	1.45	1.50
12	b	2136	CLA	C1B-C2B	2.59	1.49	1.43
15	B	2145	BCR	C1-C6	-2.59	1.50	1.53
12	b	2102	CLA	CMC-C2C	-2.59	1.45	1.50
12	a	817	CLA	C1B-C2B	2.59	1.49	1.43
12	G	803	CLA	C1B-C2B	2.59	1.49	1.43
12	B	2132	CLA	C1B-C2B	2.59	1.49	1.43
13	G	840	A1AGD	C6-C1	-2.59	1.44	1.48
12	U	201	CLA	C4B-NB	2.59	1.41	1.37
12	l	201	CLA	C4B-NB	2.58	1.41	1.37
13	A	840	A1AGD	C6-C1	-2.58	1.44	1.48
12	B	2102	CLA	C4B-NB	2.58	1.41	1.37
12	A	803	CLA	C1B-C2B	2.58	1.49	1.43
12	b	2101	CLA	C4B-NB	2.58	1.41	1.37
12	a	803	CLA	C1B-C2B	2.58	1.49	1.43
15	R	101	BCR	C1-C6	-2.58	1.50	1.53
12	G	836	CLA	C1B-C2B	2.58	1.49	1.43
12	H	2109	CLA	C1B-C2B	2.58	1.49	1.43
12	H	2131	CLA	C1B-C2B	2.58	1.49	1.43
12	A	817	CLA	C1B-C2B	2.58	1.49	1.43
12	B	2109	CLA	C4B-NB	2.58	1.41	1.37
12	L	201	CLA	C4B-NB	2.58	1.41	1.37
12	A	810	CLA	C1B-C2B	2.58	1.49	1.43
12	B	2126	CLA	C1B-C2B	2.58	1.49	1.43
12	B	2103	CLA	CMC-C2C	-2.57	1.45	1.50
12	H	2132	CLA	C1B-C2B	2.57	1.49	1.43
15	I	101	BCR	C1-C6	-2.57	1.50	1.53
12	b	2125	CLA	C1B-C2B	2.57	1.49	1.43
12	a	811	CLA	C1B-C2B	2.57	1.49	1.43
12	H	2128	CLA	C1B-C2B	2.57	1.49	1.43
12	B	2129	CLA	C1B-C2B	2.57	1.49	1.43
12	B	2110	CLA	C1B-C2B	2.57	1.49	1.43
12	b	2108	CLA	C4B-NB	2.57	1.41	1.37
12	G	835	CLA	C4B-NB	2.57	1.41	1.37
12	A	811	CLA	C1B-C2B	2.56	1.49	1.43
12	L	205	CLA	C1B-C2B	2.56	1.49	1.43
22	H	2150	EQ3	C34-C9	2.56	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	834	CLA	C1B-C2B	2.56	1.49	1.43
15	H	2144	BCR	C1-C6	-2.56	1.50	1.53
12	b	2128	CLA	C1B-C2B	2.56	1.49	1.43
12	A	807	CLA	C1B-C2B	2.56	1.49	1.43
12	A	808	CLA	C1B-C2B	2.56	1.49	1.43
12	B	2104	CLA	C4B-NB	2.56	1.41	1.37
12	a	807	CLA	C1B-C2B	2.56	1.49	1.43
12	H	2104	CLA	C1D-ND	2.56	1.41	1.37
12	a	808	CLA	C1B-C2B	2.56	1.49	1.43
12	b	2109	CLA	C1B-C2B	2.56	1.49	1.43
12	G	811	CLA	C1B-C2B	2.56	1.49	1.43
12	G	834	CLA	C1B-C2B	2.56	1.49	1.43
12	G	808	CLA	C1B-C2B	2.55	1.49	1.43
12	B	2133	CLA	C1B-C2B	2.55	1.49	1.43
12	B	2105	CLA	C1D-ND	2.55	1.41	1.37
12	U	205	CLA	C1B-C2B	2.55	1.49	1.43
12	b	2103	CLA	C4B-NB	2.55	1.41	1.37
13	a	840	A1AGD	C6-C1	-2.55	1.44	1.48
12	a	850	CLA	MG-NB	-2.55	2.00	2.05
22	B	2151	EQ3	C34-C9	2.55	1.56	1.50
12	A	834	CLA	C1B-C2B	2.55	1.49	1.43
12	G	810	CLA	C1B-C2B	2.55	1.49	1.43
12	H	2137	CLA	C4B-NB	2.55	1.41	1.37
12	A	830	CLA	C4B-NB	2.55	1.41	1.37
12	a	824	CLA	CMD-C2D	-2.55	1.45	1.50
12	A	824	CLA	CMD-C2D	-2.55	1.45	1.50
12	H	2125	CLA	C1B-C2B	2.54	1.49	1.43
12	A	836	CLA	C1B-C2B	2.54	1.49	1.43
12	a	836	CLA	C1B-C2B	2.54	1.49	1.43
12	G	807	CLA	C1B-C2B	2.54	1.49	1.43
12	G	817	CLA	C1B-C2B	2.54	1.49	1.43
12	a	803	CLA	C3B-C4B	2.54	1.50	1.42
12	b	2104	CLA	C1D-ND	2.54	1.41	1.37
12	l	205	CLA	C1B-C2B	2.54	1.49	1.43
26	l	210	LMT	O3'-C3'	-2.54	1.36	1.43
12	H	2102	CLA	CMC-C2C	-2.54	1.45	1.50
22	b	2150	EQ3	C34-C9	2.54	1.56	1.50
12	G	826	CLA	CMC-C2C	-2.54	1.45	1.50
12	H	2111	CLA	C1B-C2B	2.54	1.49	1.43
12	B	2112	CLA	C1B-C2B	2.54	1.49	1.43
12	G	803	CLA	CHC-C1C	2.54	1.43	1.38
12	a	835	CLA	C4B-NB	2.53	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	2132	CLA	C1B-C2B	2.53	1.49	1.43
12	H	2128	CLA	CMD-C2D	-2.53	1.45	1.50
12	G	830	CLA	C4B-NB	2.53	1.41	1.37
12	H	2108	CLA	C4B-NB	2.53	1.41	1.37
12	A	835	CLA	C4B-NB	2.53	1.41	1.37
12	a	803	CLA	CHC-C1C	2.53	1.43	1.38
12	U	203	CLA	C1B-C2B	2.53	1.49	1.43
12	B	2129	CLA	CMD-C2D	-2.53	1.45	1.50
13	b	2153	A1AGD	C53-C6	-2.53	1.45	1.50
13	H	2153	A1AGD	C53-C6	-2.53	1.45	1.50
12	a	829	CLA	CMB-C2B	-2.53	1.45	1.50
26	L	210	LMT	O3'-C3'	-2.52	1.36	1.43
12	H	2104	CLA	C4B-NB	2.52	1.41	1.37
12	G	824	CLA	CMD-C2D	-2.52	1.45	1.50
17	a	847	LMG	O1-C1	2.52	1.44	1.40
15	G	843	BCR	C30-C25	-2.52	1.50	1.53
12	A	850	CLA	MG-NB	-2.52	2.00	2.05
12	L	203	CLA	C1B-C2B	2.52	1.49	1.43
12	A	803	CLA	C3B-C4B	2.51	1.50	1.42
15	A	843	BCR	C30-C25	-2.51	1.50	1.53
12	a	826	CLA	CMC-C2C	-2.51	1.45	1.50
12	A	826	CLA	CMC-C2C	-2.51	1.45	1.50
13	B	2153	A1AGD	C53-C6	-2.51	1.45	1.50
12	b	2128	CLA	CMD-C2D	-2.51	1.45	1.50
12	G	829	CLA	CMB-C2B	-2.51	1.45	1.50
12	B	2112	CLA	C3B-C4B	2.51	1.50	1.42
12	G	850	CLA	MG-NB	-2.51	2.00	2.05
12	l	203	CLA	C1B-C2B	2.51	1.49	1.43
12	G	803	CLA	C3B-C4B	2.51	1.50	1.42
12	G	817	CLA	CHC-C1C	2.51	1.43	1.38
12	A	803	CLA	CHC-C1C	2.51	1.43	1.38
12	A	829	CLA	CMB-C2B	-2.50	1.45	1.50
26	U	210	LMT	O3'-C3'	-2.50	1.36	1.43
17	A	847	LMG	O1-C1	2.50	1.44	1.40
12	b	2135	CLA	C1B-C2B	2.50	1.49	1.43
12	B	2136	CLA	C1B-C2B	2.50	1.49	1.43
12	b	2111	CLA	C3B-C4B	2.50	1.50	1.42
12	H	2111	CLA	C3B-C4B	2.50	1.50	1.42
12	B	2106	CLA	C1B-C2B	2.50	1.49	1.43
12	b	2111	CLA	C1B-C2B	2.50	1.49	1.43
15	R	101	BCR	C30-C25	-2.50	1.50	1.53
12	H	2135	CLA	C1B-C2B	2.50	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	837	CLA	C1B-C2B	2.49	1.49	1.43
12	A	837	CLA	C1B-C2B	2.49	1.49	1.43
12	B	2105	CLA	C4B-NB	2.49	1.41	1.37
12	a	837	CLA	C1B-C2B	2.49	1.49	1.43
12	b	2105	CLA	C1B-C2B	2.49	1.49	1.43
12	a	834	CLA	C3B-C4B	2.49	1.50	1.42
12	H	2105	CLA	C3B-C4B	2.49	1.50	1.42
12	B	2106	CLA	C3B-C4B	2.49	1.50	1.42
12	a	826	CLA	C1B-C2B	2.49	1.49	1.43
12	b	2120	CLA	C1B-C2B	2.49	1.49	1.43
12	H	2132	CLA	C3B-C4B	2.48	1.50	1.42
12	b	2132	CLA	C3B-C4B	2.48	1.50	1.42
12	b	2109	CLA	CMD-C2D	-2.48	1.45	1.50
12	b	2104	CLA	C4B-NB	2.48	1.41	1.37
12	b	2131	CLA	C3B-C4B	2.48	1.50	1.42
12	A	834	CLA	C3B-C4B	2.48	1.50	1.42
12	G	834	CLA	C3B-C4B	2.48	1.49	1.42
12	a	830	CLA	MG-NB	-2.48	2.00	2.05
12	H	2109	CLA	CMD-C2D	-2.48	1.45	1.50
12	a	830	CLA	C4B-NB	2.48	1.41	1.37
12	H	2120	CLA	C1B-C2B	2.48	1.48	1.43
12	b	2109	CLA	CMC-C2C	-2.47	1.45	1.50
25	L	209	DGD	O2G-C2G	-2.47	1.40	1.46
12	H	2105	CLA	C1B-C2B	2.47	1.48	1.43
12	a	836	CLA	C3B-C4B	2.47	1.49	1.42
25	l	209	DGD	O2G-C2G	-2.47	1.40	1.46
22	H	2150	EQ3	C27-C26	2.47	1.53	1.47
12	B	2133	CLA	C3B-C4B	2.47	1.49	1.42
12	B	2110	CLA	CMD-C2D	-2.47	1.45	1.50
12	A	830	CLA	MG-NB	-2.47	2.00	2.05
12	A	833	CLA	C1B-C2B	2.47	1.48	1.43
15	I	101	BCR	C30-C25	-2.47	1.50	1.53
12	A	817	CLA	CHC-C1C	2.47	1.43	1.38
12	b	2105	CLA	C3B-C4B	2.47	1.49	1.42
22	B	2151	EQ3	C27-C26	2.47	1.53	1.47
12	A	836	CLA	C3B-C4B	2.46	1.49	1.42
12	B	2132	CLA	C3B-C4B	2.46	1.49	1.42
25	U	209	DGD	O2G-C2G	-2.46	1.40	1.46
12	H	2109	CLA	CMC-C2C	-2.46	1.45	1.50
12	G	836	CLA	C3B-C4B	2.46	1.49	1.42
12	a	833	CLA	C1B-C2B	2.46	1.48	1.43
12	G	830	CLA	MG-NB	-2.46	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	825	CLA	C3B-C4B	2.46	1.49	1.42
17	G	847	LMG	O1-C1	2.46	1.44	1.40
12	a	817	CLA	CHC-C1C	2.46	1.43	1.38
15	i	101	BCR	C30-C25	-2.46	1.50	1.53
12	A	826	CLA	C1B-C2B	2.46	1.48	1.43
25	l	209	DGD	O1G-C1G	-2.46	1.39	1.45
22	b	2150	EQ3	C27-C26	2.46	1.53	1.47
12	B	2110	CLA	CMC-C2C	-2.46	1.45	1.50
12	B	2121	CLA	C1B-C2B	2.45	1.48	1.43
15	a	843	BCR	C30-C25	-2.45	1.50	1.53
12	a	839	CLA	C1B-C2B	2.45	1.48	1.43
25	L	209	DGD	O1G-C1G	-2.45	1.39	1.45
12	G	839	CLA	C1B-C2B	2.45	1.48	1.43
12	j	102	CLA	C3B-C4B	2.45	1.49	1.42
12	G	826	CLA	C1B-C2B	2.45	1.48	1.43
12	b	2106	CLA	C3B-C4B	2.45	1.49	1.42
12	B	2107	CLA	C3B-C4B	2.44	1.49	1.42
12	G	828	CLA	C1B-C2B	2.44	1.48	1.43
12	A	839	CLA	C1B-C2B	2.44	1.48	1.43
12	l	205	CLA	C3B-C4B	2.44	1.49	1.42
25	U	209	DGD	O1G-C1G	-2.44	1.39	1.45
12	H	2131	CLA	C3B-C4B	2.44	1.49	1.42
12	G	833	CLA	C1B-C2B	2.44	1.48	1.43
12	S	102	CLA	C3B-C4B	2.44	1.49	1.42
12	H	2106	CLA	C3B-C4B	2.44	1.49	1.42
12	b	2105	CLA	CHC-C1C	2.44	1.43	1.38
12	L	205	CLA	C3B-C4B	2.43	1.49	1.42
23	f	205	ZEX	C19-C9	2.43	1.55	1.50
23	F	205	ZEX	C19-C9	2.43	1.55	1.50
12	B	2106	CLA	CHC-C1C	2.43	1.43	1.38
12	A	851	CLA	CMB-C2B	-2.43	1.45	1.50
12	b	2128	CLA	C3B-C4B	2.43	1.49	1.42
12	J	102	CLA	C3B-C4B	2.43	1.49	1.42
12	H	2106	CLA	CHC-C1C	2.43	1.43	1.38
12	b	2102	CLA	C1B-C2B	2.43	1.48	1.43
12	U	205	CLA	C3B-C4B	2.43	1.49	1.42
12	a	825	CLA	C3B-C4B	2.43	1.49	1.42
12	A	825	CLA	C3B-C4B	2.43	1.49	1.42
16	a	848	LHG	O7-C5	-2.43	1.40	1.46
12	G	822	CLA	C3B-C4B	2.42	1.49	1.42
12	a	832	CLA	C3B-C4B	2.42	1.49	1.42
12	H	2128	CLA	C3B-C4B	2.42	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	820	CLA	C3B-C4B	2.42	1.49	1.42
12	G	820	CLA	C3B-C4B	2.42	1.49	1.42
12	A	832	CLA	C3B-C4B	2.42	1.49	1.42
23	Q	205	ZEX	C19-C9	2.42	1.55	1.50
12	a	827	CLA	C3B-C4B	2.42	1.49	1.42
12	A	828	CLA	C1B-C2B	2.42	1.48	1.43
12	B	2129	CLA	C3B-C4B	2.42	1.49	1.42
12	B	2107	CLA	CHC-C1C	2.42	1.43	1.38
26	U	210	LMT	O2B-C2B	-2.42	1.37	1.43
23	H	2151	ZEX	C19-C9	2.42	1.55	1.50
12	G	808	CLA	C3B-C4B	2.42	1.49	1.42
12	A	822	CLA	C3B-C4B	2.42	1.49	1.42
12	H	2105	CLA	CHC-C1C	2.42	1.43	1.38
12	a	828	CLA	C3B-C4B	2.42	1.49	1.42
12	b	2106	CLA	CHC-C1C	2.42	1.43	1.38
12	a	820	CLA	C3B-C4B	2.41	1.49	1.42
12	a	828	CLA	C1B-C2B	2.41	1.48	1.43
12	A	808	CLA	C3B-C4B	2.41	1.49	1.42
12	b	2110	CLA	MG-NB	-2.41	2.01	2.05
12	B	2135	CLA	C3B-C4B	2.41	1.49	1.42
12	L	205	CLA	CHC-C1C	2.41	1.43	1.38
16	G	848	LHG	O7-C5	-2.41	1.40	1.46
12	a	824	CLA	C3B-C4B	2.41	1.49	1.42
12	H	2104	CLA	CHC-C1C	2.41	1.43	1.38
12	b	2134	CLA	C3B-C4B	2.41	1.49	1.42
12	B	2105	CLA	CHC-C1C	2.41	1.43	1.38
12	a	851	CLA	CMB-C2B	-2.41	1.45	1.50
12	G	832	CLA	C3B-C4B	2.41	1.49	1.42
12	a	808	CLA	C3B-C4B	2.41	1.49	1.42
12	a	809	CLA	C3B-C4B	2.41	1.49	1.42
12	A	824	CLA	C3B-C4B	2.41	1.49	1.42
12	G	838	CLA	C3B-C4B	2.40	1.49	1.42
12	B	2103	CLA	C1B-C2B	2.40	1.48	1.43
12	b	2123	CLA	C3B-C4B	2.40	1.49	1.42
12	U	205	CLA	CHC-C1C	2.40	1.43	1.38
23	B	2152	ZEX	C19-C9	2.40	1.55	1.50
12	A	825	CLA	CHC-C1C	2.40	1.43	1.38
12	b	2104	CLA	CHC-C1C	2.40	1.43	1.38
17	A	847	LMG	C7-C8	2.40	1.58	1.50
12	G	827	CLA	C3B-C4B	2.40	1.49	1.42
12	b	2121	CLA	C3B-C4B	2.40	1.49	1.42
12	A	827	CLA	C3B-C4B	2.40	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	203	CLA	C3B-C4B	2.40	1.49	1.42
12	G	851	CLA	CMB-C2B	-2.40	1.45	1.50
12	G	824	CLA	C3B-C4B	2.40	1.49	1.42
12	A	838	CLA	C3B-C4B	2.40	1.49	1.42
16	A	848	LHG	O7-C5	-2.40	1.41	1.46
12	A	807	CLA	C3B-C4B	2.40	1.49	1.42
12	l	205	CLA	CHC-C1C	2.40	1.43	1.38
12	H	2134	CLA	C3B-C4B	2.40	1.49	1.42
12	G	807	CLA	C3B-C4B	2.39	1.49	1.42
26	L	210	LMT	O2B-C2B	-2.39	1.37	1.43
12	H	2110	CLA	MG-NB	-2.39	2.01	2.05
26	l	210	LMT	O2B-C2B	-2.39	1.37	1.43
12	B	2111	CLA	C1B-C2B	2.39	1.48	1.43
17	G	847	LMG	C7-C8	2.39	1.58	1.50
12	A	809	CLA	C3B-C4B	2.39	1.49	1.42
12	G	809	CLA	C3B-C4B	2.39	1.49	1.42
12	b	2116	CLA	C3B-C4B	2.39	1.49	1.42
12	H	2123	CLA	C3B-C4B	2.39	1.49	1.42
12	a	820	CLA	CHC-C1C	2.39	1.43	1.38
12	a	822	CLA	C3B-C4B	2.39	1.49	1.42
12	A	828	CLA	C3B-C4B	2.39	1.49	1.42
12	G	835	CLA	CMD-C2D	-2.39	1.45	1.50
12	H	2102	CLA	C1B-C2B	2.39	1.48	1.43
12	a	838	CLA	C3B-C4B	2.39	1.49	1.42
12	B	2124	CLA	C3B-C4B	2.39	1.49	1.42
12	b	2131	CLA	CHC-C1C	2.39	1.43	1.38
12	H	2116	CLA	C3B-C4B	2.38	1.49	1.42
12	l	203	CLA	C3B-C4B	2.38	1.49	1.42
12	a	835	CLA	CMD-C2D	-2.38	1.45	1.50
12	a	807	CLA	CHC-C1C	2.38	1.43	1.38
12	b	2101	CLA	MG-NB	-2.38	2.01	2.05
12	U	203	CLA	C3B-C4B	2.38	1.49	1.42
12	a	825	CLA	CHC-C1C	2.38	1.43	1.38
12	G	828	CLA	C3B-C4B	2.38	1.49	1.42
12	H	2101	CLA	MG-NB	-2.38	2.01	2.05
12	B	2111	CLA	MG-NB	-2.38	2.01	2.05
12	b	2102	CLA	C3B-C4B	2.38	1.49	1.42
15	f	202	BCR	C1-C6	-2.38	1.50	1.53
12	B	2117	CLA	C3B-C4B	2.38	1.49	1.42
12	B	2122	CLA	C3B-C4B	2.38	1.49	1.42
12	a	807	CLA	C3B-C4B	2.38	1.49	1.42
12	b	2110	CLA	C1B-C2B	2.38	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	835	CLA	CMD-C2D	-2.38	1.45	1.50
12	b	2130	CLA	C1B-C2B	2.37	1.48	1.43
12	H	2135	CLA	C3B-C4B	2.37	1.49	1.42
12	H	2130	CLA	C1B-C2B	2.37	1.48	1.43
12	G	825	CLA	CHC-C1C	2.37	1.43	1.38
12	a	818	CLA	CHC-C1C	2.37	1.43	1.38
17	a	847	LMG	C7-C8	2.37	1.58	1.50
12	a	816	CLA	C3B-C4B	2.37	1.49	1.42
12	b	2104	CLA	C1B-C2B	2.37	1.48	1.43
12	A	818	CLA	C1B-C2B	2.37	1.48	1.43
12	H	2138	CLA	C3B-C4B	2.37	1.49	1.42
12	B	2103	CLA	C3B-C4B	2.37	1.49	1.42
12	A	807	CLA	CHC-C1C	2.37	1.43	1.38
12	a	818	CLA	C1B-C2B	2.37	1.48	1.43
23	b	2151	ZEX	C19-C9	2.37	1.55	1.50
12	b	2122	CLA	C3B-C4B	2.37	1.49	1.42
12	b	2113	CLA	C3B-C4B	2.37	1.49	1.42
12	B	2105	CLA	C1B-C2B	2.36	1.48	1.43
12	a	830	CLA	C1B-C2B	2.36	1.48	1.43
12	G	818	CLA	CHC-C1C	2.36	1.43	1.38
12	B	2131	CLA	C1B-C2B	2.36	1.48	1.43
24	U	208	SQD	O5-C5	2.36	1.50	1.44
24	L	208	SQD	O5-C5	2.36	1.50	1.44
12	B	2105	CLA	C3B-C4B	2.36	1.49	1.42
12	b	2129	CLA	MG-NB	-2.36	2.01	2.05
12	a	839	CLA	CHC-C1C	2.36	1.43	1.38
12	H	2131	CLA	CHC-C1C	2.36	1.43	1.38
12	H	2122	CLA	C3B-C4B	2.36	1.49	1.42
12	b	2104	CLA	C3B-C4B	2.36	1.49	1.42
12	H	2104	CLA	C3B-C4B	2.36	1.49	1.42
12	A	820	CLA	CHC-C1C	2.36	1.43	1.38
12	B	2132	CLA	CHC-C1C	2.36	1.43	1.38
12	H	2104	CLA	C1B-C2B	2.36	1.48	1.43
12	H	2124	CLA	C3B-C4B	2.36	1.49	1.42
12	B	2139	CLA	C3B-C4B	2.35	1.49	1.42
12	A	830	CLA	C1B-C2B	2.35	1.48	1.43
12	H	2129	CLA	MG-NB	-2.35	2.01	2.05
12	A	816	CLA	C3B-C4B	2.35	1.49	1.42
12	B	2123	CLA	C3B-C4B	2.35	1.49	1.42
12	b	2115	CLA	C3B-C4B	2.35	1.49	1.42
12	H	2110	CLA	C1B-C2B	2.35	1.48	1.43
12	G	821	CLA	C3B-C4B	2.35	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	2114	CLA	C3B-C4B	2.35	1.49	1.42
12	B	2102	CLA	MG-NB	-2.35	2.01	2.05
16	a	846	LHG	O7-C5	-2.35	1.41	1.46
12	H	2102	CLA	C3B-C4B	2.35	1.49	1.42
12	H	2121	CLA	C3B-C4B	2.35	1.49	1.42
12	A	818	CLA	CHC-C1C	2.35	1.43	1.38
15	F	202	BCR	C1-C6	-2.35	1.50	1.53
12	a	806	CLA	C3B-C4B	2.35	1.49	1.42
12	G	818	CLA	C1B-C2B	2.35	1.48	1.43
12	G	830	CLA	C1B-C2B	2.35	1.48	1.43
12	a	818	CLA	C3B-C4B	2.35	1.49	1.42
12	B	2136	CLA	C3B-C4B	2.35	1.49	1.42
12	G	807	CLA	CHC-C1C	2.35	1.43	1.38
12	B	2130	CLA	MG-NB	-2.35	2.01	2.05
12	G	820	CLA	CHC-C1C	2.35	1.43	1.38
12	A	806	CLA	C3B-C4B	2.35	1.49	1.42
12	A	818	CLA	C3B-C4B	2.35	1.49	1.42
12	b	2138	CLA	C3B-C4B	2.35	1.49	1.42
12	G	834	CLA	CHC-C1C	2.34	1.43	1.38
12	B	2125	CLA	C3B-C4B	2.34	1.49	1.42
12	G	816	CLA	C3B-C4B	2.34	1.49	1.42
12	f	204	CLA	C3B-C4B	2.34	1.49	1.42
15	L	206	BCR	C30-C25	-2.34	1.50	1.53
12	F	204	CLA	C3B-C4B	2.34	1.49	1.42
12	b	2112	CLA	C3B-C4B	2.34	1.49	1.42
12	b	2124	CLA	C3B-C4B	2.34	1.49	1.42
12	b	2132	CLA	CHC-C1C	2.34	1.43	1.38
15	l	206	BCR	C30-C25	-2.34	1.50	1.53
12	B	2101	CLA	C3B-C4B	2.34	1.49	1.42
24	l	208	SQD	O5-C5	2.34	1.50	1.44
12	a	822	CLA	CHC-C1C	2.34	1.43	1.38
12	a	832	CLA	CHC-C1C	2.34	1.43	1.38
12	H	2113	CLA	C3B-C4B	2.34	1.49	1.42
12	b	2135	CLA	C3B-C4B	2.34	1.49	1.42
12	A	839	CLA	C3B-C4B	2.34	1.49	1.42
12	H	2111	CLA	C3C-C2C	2.34	1.41	1.36
15	U	206	BCR	C30-C25	-2.34	1.50	1.53
12	G	812	CLA	CMB-C2B	-2.33	1.46	1.50
12	a	812	CLA	CMB-C2B	-2.33	1.46	1.50
12	G	806	CLA	C3B-C4B	2.33	1.49	1.42
12	K	4002	CLA	C3B-C4B	2.33	1.49	1.42
12	a	828	CLA	CHC-C1C	2.33	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	839	CLA	C3B-C4B	2.33	1.49	1.42
12	H	2115	CLA	C3B-C4B	2.33	1.49	1.42
12	G	851	CLA	MG-NB	-2.33	2.01	2.05
12	b	2141	CLA	C3B-C4B	2.33	1.49	1.42
12	G	818	CLA	C3B-C4B	2.33	1.49	1.42
12	A	812	CLA	CMB-C2B	-2.33	1.46	1.50
12	G	817	CLA	C3B-C4B	2.33	1.49	1.42
12	Q	204	CLA	C3B-C4B	2.33	1.49	1.42
12	b	2111	CLA	C3C-C2C	2.33	1.41	1.36
12	B	2133	CLA	CHC-C1C	2.33	1.43	1.38
12	H	2134	CLA	CHC-C1C	2.33	1.43	1.38
12	a	839	CLA	C3B-C4B	2.33	1.49	1.42
12	B	2112	CLA	C3C-C2C	2.33	1.41	1.36
12	B	2116	CLA	C3B-C4B	2.33	1.49	1.42
12	A	828	CLA	CHC-C1C	2.33	1.43	1.38
12	a	808	CLA	CHC-C1C	2.33	1.43	1.38
12	a	813	CLA	C3B-C4B	2.33	1.49	1.42
16	A	846	LHG	O7-C5	-2.33	1.41	1.46
12	A	834	CLA	CHC-C1C	2.32	1.43	1.38
12	a	830	CLA	CMD-C2D	-2.32	1.46	1.50
12	A	830	CLA	CMD-C2D	-2.32	1.46	1.50
12	b	2117	CLA	C3B-C4B	2.32	1.49	1.42
12	H	2117	CLA	C3B-C4B	2.32	1.49	1.42
12	A	821	CLA	C3B-C4B	2.32	1.49	1.42
12	B	2142	CLA	C3B-C4B	2.32	1.49	1.42
12	H	2114	CLA	CMC-C2C	-2.32	1.46	1.50
12	A	851	CLA	MG-NB	-2.32	2.01	2.05
12	B	2135	CLA	CHC-C1C	2.32	1.43	1.38
15	T	4001	BCR	C30-C25	-2.32	1.50	1.53
12	a	815	CLA	C3B-C4B	2.32	1.49	1.42
12	b	2129	CLA	C1B-C2B	2.32	1.48	1.43
12	T	4002	CLA	C3B-C4B	2.32	1.49	1.42
12	B	2104	CLA	CMD-C2D	-2.32	1.46	1.50
12	B	2137	CLA	C3B-C4B	2.32	1.49	1.42
12	a	821	CLA	C3B-C4B	2.32	1.49	1.42
12	H	2141	CLA	C3B-C4B	2.32	1.49	1.42
12	A	808	CLA	CHC-C1C	2.32	1.43	1.38
12	F	203	CLA	CHC-C1C	2.32	1.43	1.38
12	G	817	CLA	CMC-C2C	-2.32	1.46	1.50
12	G	808	CLA	CHC-C1C	2.32	1.43	1.38
12	Q	203	CLA	CHC-C1C	2.31	1.43	1.38
12	a	811	CLA	CHC-C1C	2.31	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	2136	CLA	CHC-C1C	2.31	1.43	1.38
12	f	203	CLA	CHC-C1C	2.31	1.43	1.38
12	H	2129	CLA	C3B-C4B	2.31	1.49	1.42
12	b	2103	CLA	CMD-C2D	-2.31	1.46	1.50
12	H	2136	CLA	C3B-C4B	2.31	1.49	1.42
12	A	813	CLA	C3B-C4B	2.31	1.49	1.42
12	A	839	CLA	CHC-C1C	2.31	1.43	1.38
12	b	2136	CLA	C3B-C4B	2.31	1.49	1.42
12	a	851	CLA	MG-NB	-2.31	2.01	2.05
12	a	823	CLA	C3B-C4B	2.31	1.49	1.42
12	H	2132	CLA	CHC-C1C	2.31	1.43	1.38
12	A	817	CLA	C3B-C4B	2.31	1.49	1.42
25	l	209	DGD	C3D-C2D	2.31	1.58	1.52
12	G	831	CLA	C3B-C4B	2.31	1.49	1.42
12	a	817	CLA	CMC-C2C	-2.31	1.46	1.50
12	G	839	CLA	CHC-C1C	2.31	1.43	1.38
12	a	812	CLA	CMD-C2D	-2.31	1.46	1.50
25	U	209	DGD	C3D-C2D	2.31	1.58	1.52
12	A	831	CLA	C3B-C4B	2.31	1.49	1.42
12	B	2113	CLA	C3B-C4B	2.31	1.49	1.42
12	G	832	CLA	CHC-C1C	2.31	1.43	1.38
12	A	821	CLA	CHC-C1C	2.31	1.43	1.38
12	B	2137	CLA	CHC-C1C	2.31	1.43	1.38
12	G	822	CLA	CHC-C1C	2.31	1.43	1.38
12	H	2136	CLA	CHC-C1C	2.31	1.43	1.38
12	G	815	CLA	C3B-C4B	2.31	1.49	1.42
12	a	834	CLA	CHC-C1C	2.31	1.43	1.38
12	B	2115	CLA	CMC-C2C	-2.31	1.46	1.50
12	b	2129	CLA	C3B-C4B	2.31	1.49	1.42
12	G	828	CLA	CHC-C1C	2.31	1.43	1.38
12	G	812	CLA	CMD-C2D	-2.31	1.46	1.50
12	A	827	CLA	CHC-C1C	2.31	1.43	1.38
12	A	820	CLA	C1B-C2B	2.31	1.48	1.43
12	b	2130	CLA	C3B-C4B	2.31	1.49	1.42
16	G	846	LHG	O7-C5	-2.31	1.41	1.46
12	b	2152	CLA	C3B-C4B	2.31	1.49	1.42
15	Q	202	BCR	C1-C6	-2.30	1.50	1.53
12	A	823	CLA	C3B-C4B	2.30	1.49	1.42
12	H	2103	CLA	CMD-C2D	-2.30	1.46	1.50
12	A	812	CLA	CMD-C2D	-2.30	1.46	1.50
12	a	817	CLA	C3B-C4B	2.30	1.49	1.42
12	A	832	CLA	CHC-C1C	2.30	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	2109	CLA	C3B-C4B	2.30	1.49	1.42
12	a	821	CLA	CHC-C1C	2.30	1.43	1.38
12	b	2134	CLA	CHC-C1C	2.30	1.43	1.38
12	A	815	CLA	C3B-C4B	2.30	1.49	1.42
25	U	209	DGD	C4D-C5D	2.30	1.57	1.53
12	B	2118	CLA	C3B-C4B	2.30	1.49	1.42
12	B	2131	CLA	C3B-C4B	2.30	1.49	1.42
12	A	822	CLA	CHC-C1C	2.30	1.43	1.38
12	G	813	CLA	C3B-C4B	2.30	1.49	1.42
25	L	209	DGD	C3D-C2D	2.30	1.58	1.52
12	G	830	CLA	CMD-C2D	-2.30	1.46	1.50
12	H	2152	CLA	C3B-C4B	2.30	1.49	1.42
15	K	4001	BCR	C30-C25	-2.30	1.50	1.53
12	k	4002	CLA	C3B-C4B	2.30	1.49	1.42
12	A	839	CLA	CMB-C2B	-2.30	1.46	1.50
12	H	2101	CLA	C1B-C2B	2.30	1.48	1.43
12	B	2130	CLA	C1B-C2B	2.30	1.48	1.43
12	a	801	CLA	CMD-C2D	-2.29	1.46	1.50
12	H	2116	CLA	CHC-C1C	2.29	1.43	1.38
12	H	2130	CLA	C3B-C4B	2.29	1.49	1.42
12	H	2133	CLA	CMD-C2D	-2.29	1.46	1.50
12	H	2140	CLA	C3B-C4B	2.29	1.49	1.42
12	F	204	CLA	CHC-C1C	2.29	1.43	1.38
12	H	2112	CLA	C3B-C4B	2.29	1.49	1.42
26	L	210	LMT	O2'-C2'	-2.29	1.37	1.43
12	H	2102	CLA	MG-NB	-2.29	2.01	2.05
12	B	2102	CLA	C1B-C2B	2.29	1.48	1.43
12	a	839	CLA	CMB-C2B	-2.29	1.46	1.50
12	f	203	CLA	C3B-C4B	2.29	1.49	1.42
12	b	2139	CLA	CHC-C1C	2.29	1.43	1.38
12	B	2124	CLA	CHC-C1C	2.29	1.43	1.38
12	H	2108	CLA	C3B-C4B	2.29	1.49	1.42
12	b	2114	CLA	CMC-C2C	-2.29	1.46	1.50
12	A	817	CLA	CMC-C2C	-2.29	1.46	1.50
12	a	820	CLA	C1B-C2B	2.29	1.48	1.43
12	a	831	CLA	C3B-C4B	2.29	1.49	1.42
12	b	2140	CLA	C3B-C4B	2.29	1.49	1.42
26	l	210	LMT	O2'-C2'	-2.29	1.37	1.43
12	b	2108	CLA	C3B-C4B	2.29	1.49	1.42
12	H	2101	CLA	CHC-C1C	2.29	1.43	1.38
12	F	201	CLA	CHC-C1C	2.29	1.43	1.38
12	G	821	CLA	CHC-C1C	2.29	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	2141	CLA	C3B-C4B	2.29	1.49	1.42
12	b	2135	CLA	CHC-C1C	2.29	1.43	1.38
12	A	805	CLA	C3B-C4B	2.29	1.49	1.42
12	B	2130	CLA	C3B-C4B	2.29	1.49	1.42
12	Q	201	CLA	CHC-C1C	2.29	1.43	1.38
12	f	204	CLA	CHC-C1C	2.29	1.43	1.38
12	G	805	CLA	C3B-C4B	2.29	1.49	1.42
12	H	2130	CLA	MG-NB	-2.29	2.01	2.05
12	B	2110	CLA	C3B-C4B	2.29	1.49	1.42
12	b	2141	CLA	CHC-C1C	2.29	1.43	1.38
12	A	811	CLA	CHC-C1C	2.29	1.43	1.38
12	H	2141	CLA	CHC-C1C	2.29	1.43	1.38
24	m	102	SQD	O9-S	2.29	1.51	1.45
12	b	2123	CLA	CHC-C1C	2.29	1.43	1.38
12	b	2102	CLA	MG-NB	-2.29	2.01	2.05
12	H	2129	CLA	C1B-C2B	2.29	1.48	1.43
12	G	839	CLA	CMB-C2B	-2.28	1.46	1.50
12	Q	203	CLA	C3B-C4B	2.28	1.49	1.42
12	A	825	CLA	C1B-C2B	2.28	1.48	1.43
12	a	805	CLA	C3B-C4B	2.28	1.49	1.42
12	a	814	CLA	C3B-C4B	2.28	1.49	1.42
12	a	819	CLA	C3B-C4B	2.28	1.49	1.42
12	b	2101	CLA	C1B-C2B	2.28	1.48	1.43
12	b	2119	CLA	MG-NB	-2.28	2.01	2.05
12	b	2133	CLA	CMD-C2D	-2.28	1.46	1.50
25	L	209	DGD	C4D-C3D	2.28	1.58	1.52
16	V	103	LHG	O7-C5	-2.28	1.41	1.46
12	a	825	CLA	CMD-C2D	-2.28	1.46	1.50
12	A	801	CLA	CMD-C2D	-2.28	1.46	1.50
12	G	811	CLA	CHC-C1C	2.28	1.43	1.38
12	Q	204	CLA	CHC-C1C	2.28	1.43	1.38
12	b	2101	CLA	CHC-C1C	2.28	1.43	1.38
12	B	2126	CLA	C3B-C4B	2.28	1.49	1.42
12	G	819	CLA	C3B-C4B	2.28	1.49	1.42
12	F	203	CLA	C3B-C4B	2.28	1.49	1.42
12	b	2139	CLA	CMB-C2B	-2.28	1.46	1.50
12	A	814	CLA	C3B-C4B	2.28	1.49	1.42
12	G	825	CLA	C1B-C2B	2.28	1.48	1.43
12	l	201	CLA	C3B-C4B	2.28	1.49	1.42
12	B	2134	CLA	CMD-C2D	-2.28	1.46	1.50
12	G	809	CLA	CHC-C1C	2.28	1.43	1.38
12	H	2139	CLA	CMD-C2D	-2.28	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	2103	CLA	MG-NB	-2.28	2.01	2.05
25	L	209	DGD	C4D-C5D	2.28	1.57	1.53
12	H	2109	CLA	C3B-C4B	2.28	1.49	1.42
24	M	101	SQD	O9-S	2.28	1.51	1.45
12	B	2141	CLA	CMB-C2B	-2.28	1.46	1.50
12	B	2142	CLA	CHC-C1C	2.28	1.43	1.38
12	b	2140	CLA	CMB-C2B	-2.28	1.46	1.50
12	a	825	CLA	C1B-C2B	2.28	1.48	1.43
12	G	823	CLA	C3B-C4B	2.28	1.49	1.42
12	G	820	CLA	C1B-C2B	2.28	1.48	1.43
24	V	102	SQD	O9-S	2.28	1.51	1.45
24	l	208	SQD	O9-S	2.28	1.51	1.45
12	Q	201	CLA	CMD-C2D	-2.27	1.46	1.50
12	H	2120	CLA	C3B-C4B	2.27	1.49	1.42
12	H	2126	CLA	CMB-C2B	-2.27	1.46	1.50
12	H	2123	CLA	CHC-C1C	2.27	1.43	1.38
12	A	819	CLA	C3B-C4B	2.27	1.49	1.42
12	H	2130	CLA	CMB-C2B	-2.27	1.46	1.50
12	B	2131	CLA	MG-NB	-2.27	2.01	2.05
12	B	2140	CLA	CHC-C1C	2.27	1.43	1.38
12	b	2109	CLA	C3B-C4B	2.27	1.49	1.42
12	L	201	CLA	C3B-C4B	2.27	1.49	1.42
12	b	2115	CLA	CHC-C1C	2.27	1.43	1.38
12	G	801	CLA	CMD-C2D	-2.27	1.46	1.50
12	B	2102	CLA	CHC-C1C	2.27	1.43	1.38
12	H	2125	CLA	C3B-C4B	2.27	1.49	1.42
12	A	810	CLA	C3B-C4B	2.27	1.49	1.42
12	b	2130	CLA	MG-NB	-2.27	2.01	2.05
15	k	4001	BCR	C30-C25	-2.27	1.50	1.53
12	a	835	CLA	MG-NB	-2.27	2.01	2.05
12	a	809	CLA	CHC-C1C	2.27	1.43	1.38
12	H	2140	CLA	CMB-C2B	-2.27	1.46	1.50
12	H	2135	CLA	CHC-C1C	2.27	1.43	1.38
16	m	103	LHG	O7-C5	-2.27	1.41	1.46
25	U	209	DGD	C4D-C3D	2.27	1.58	1.52
12	G	827	CLA	CHC-C1C	2.27	1.43	1.38
12	f	201	CLA	CHC-C1C	2.27	1.43	1.38
12	B	2117	CLA	CHC-C1C	2.27	1.43	1.38
25	l	209	DGD	C4D-C3D	2.27	1.58	1.52
12	A	825	CLA	CMD-C2D	-2.27	1.46	1.50
24	L	208	SQD	O9-S	2.26	1.51	1.45
12	G	810	CLA	C3B-C4B	2.26	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	806	CLA	CHC-C1C	2.26	1.43	1.38
12	H	2101	CLA	C3B-C4B	2.26	1.49	1.42
12	b	2125	CLA	C3B-C4B	2.26	1.49	1.42
12	B	2121	CLA	C3B-C4B	2.26	1.49	1.42
12	B	2136	CLA	CHC-C1C	2.26	1.43	1.38
12	b	2101	CLA	C3B-C4B	2.26	1.49	1.42
16	M	102	LHG	O7-C5	-2.26	1.41	1.46
12	b	2121	CLA	CHC-C1C	2.26	1.43	1.38
12	G	804	CLA	CMD-C2D	-2.26	1.46	1.50
25	l	209	DGD	C4D-C5D	2.26	1.57	1.53
12	a	822	CLA	CMD-C2D	-2.26	1.46	1.50
12	b	2130	CLA	CMB-C2B	-2.26	1.46	1.50
12	F	201	CLA	CMD-C2D	-2.26	1.46	1.50
12	H	2139	CLA	CHC-C1C	2.26	1.43	1.38
12	B	2102	CLA	C3B-C4B	2.26	1.49	1.42
12	b	2120	CLA	C3B-C4B	2.26	1.49	1.42
12	B	2119	CLA	CMB-C2B	-2.26	1.46	1.50
12	B	2140	CLA	CMB-C2B	-2.26	1.46	1.50
12	A	835	CLA	MG-NB	-2.26	2.01	2.05
26	U	210	LMT	O2'-C2'	-2.26	1.37	1.43
12	B	2116	CLA	CHC-C1C	2.26	1.43	1.38
12	G	850	CLA	CMB-C2B	-2.26	1.46	1.50
12	a	810	CLA	C3B-C4B	2.26	1.49	1.42
12	b	2116	CLA	CHC-C1C	2.26	1.43	1.38
15	b	2144	BCR	C30-C25	-2.26	1.50	1.53
12	G	813	CLA	CHC-C1C	2.26	1.43	1.38
12	G	814	CLA	C3B-C4B	2.25	1.49	1.42
12	f	201	CLA	CMD-C2D	-2.25	1.46	1.50
12	H	2115	CLA	CHC-C1C	2.25	1.43	1.38
24	l	208	SQD	O7-S	2.25	1.51	1.45
12	a	804	CLA	CMC-C2C	-2.25	1.46	1.50
12	G	825	CLA	CMD-C2D	-2.25	1.46	1.50
12	b	2126	CLA	CMB-C2B	-2.25	1.46	1.50
12	A	850	CLA	CMB-C2B	-2.25	1.46	1.50
12	a	827	CLA	CHC-C1C	2.25	1.43	1.38
17	a	849	LMG	O7-C8	-2.25	1.41	1.46
12	G	835	CLA	MG-NB	-2.25	2.01	2.05
24	L	208	SQD	O7-S	2.25	1.51	1.45
12	a	806	CLA	CHC-C1C	2.25	1.43	1.38
12	a	850	CLA	CMB-C2B	-2.25	1.46	1.50
12	B	2131	CLA	CMB-C2B	-2.25	1.46	1.50
12	a	810	CLA	CMD-C2D	-2.25	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	2127	CLA	CMB-C2B	-2.25	1.46	1.50
12	B	2120	CLA	C3B-C4B	2.25	1.49	1.42
12	G	806	CLA	CHC-C1C	2.25	1.43	1.38
17	G	847	LMG	C1-C2	2.25	1.59	1.52
12	G	832	CLA	CMD-C2D	-2.25	1.46	1.50
12	G	802	CLA	C3B-C4B	2.25	1.49	1.42
12	J	103	CLA	C3B-C4B	2.25	1.49	1.42
12	a	820	CLA	MG-NB	-2.25	2.01	2.05
17	A	847	LMG	C1-C2	2.25	1.59	1.52
17	G	849	LMG	O7-C8	-2.25	1.41	1.46
12	B	2122	CLA	CHC-C1C	2.25	1.43	1.38
12	G	820	CLA	MG-NB	-2.25	2.01	2.05
12	B	2140	CLA	CMD-C2D	-2.24	1.46	1.50
17	A	849	LMG	O7-C8	-2.24	1.41	1.46
12	H	2133	CLA	C3B-C4B	2.24	1.49	1.42
12	b	2138	CLA	CMD-C2D	-2.24	1.46	1.50
12	U	201	CLA	C3B-C4B	2.24	1.49	1.42
24	U	208	SQD	O9-S	2.24	1.51	1.45
12	L	203	CLA	CHC-C1C	2.24	1.43	1.38
12	H	2121	CLA	CHC-C1C	2.24	1.43	1.38
12	S	103	CLA	C3B-C4B	2.24	1.49	1.42
12	B	2120	CLA	MG-NB	-2.24	2.01	2.05
24	U	208	SQD	O7-S	2.24	1.51	1.45
12	T	4002	CLA	CHC-C1C	2.24	1.43	1.38
12	b	2137	CLA	MG-NB	-2.24	2.01	2.05
12	b	2119	CLA	C3B-C4B	2.24	1.49	1.42
12	H	2139	CLA	CMB-C2B	-2.24	1.46	1.50
12	A	813	CLA	CHC-C1C	2.24	1.43	1.38
12	H	2136	CLA	MG-NB	-2.24	2.01	2.05
12	A	820	CLA	MG-NB	-2.24	2.01	2.05
12	b	2118	CLA	CMB-C2B	-2.24	1.46	1.50
23	Q	205	ZEX	C20-C13	2.24	1.55	1.50
12	j	103	CLA	C3B-C4B	2.24	1.49	1.42
17	a	847	LMG	C1-C2	2.24	1.59	1.52
12	H	2118	CLA	CMB-C2B	-2.24	1.46	1.50
12	G	805	CLA	CHC-C1C	2.24	1.43	1.38
12	H	2126	CLA	C3B-C4B	2.23	1.49	1.42
12	b	2126	CLA	C3B-C4B	2.23	1.49	1.42
12	a	813	CLA	CHC-C1C	2.23	1.43	1.38
12	b	2139	CLA	CMD-C2D	-2.23	1.46	1.50
12	B	2137	CLA	MG-NB	-2.23	2.01	2.05
12	l	204	CLA	CMD-C2D	-2.23	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	K	4002	CLA	CHC-C1C	2.23	1.43	1.38
24	V	102	SQD	O7-S	2.23	1.51	1.45
12	S	103	CLA	CHC-C1C	2.23	1.43	1.38
12	a	854	CLA	C3B-C4B	2.23	1.49	1.42
12	b	2124	CLA	CHC-C1C	2.23	1.43	1.38
12	A	809	CLA	CHC-C1C	2.23	1.43	1.38
12	H	2135	CLA	CMB-C2B	-2.23	1.46	1.50
12	a	851	CLA	CMD-C2D	-2.23	1.46	1.50
12	H	2119	CLA	C3B-C4B	2.23	1.49	1.42
12	a	805	CLA	CHC-C1C	2.23	1.42	1.38
12	A	805	CLA	CHC-C1C	2.23	1.42	1.38
12	A	802	CLA	C3B-C4B	2.23	1.49	1.42
12	l	203	CLA	CHC-C1C	2.23	1.42	1.38
12	a	850	CLA	C1B-C2B	2.23	1.48	1.43
12	a	804	CLA	CMD-C2D	-2.23	1.46	1.50
12	G	816	CLA	CHC-C1C	2.23	1.42	1.38
12	A	810	CLA	CMD-C2D	-2.23	1.46	1.50
12	a	816	CLA	CHC-C1C	2.22	1.42	1.38
12	G	804	CLA	CMC-C2C	-2.22	1.46	1.50
12	l	204	CLA	C3B-C4B	2.22	1.49	1.42
12	U	204	CLA	CMD-C2D	-2.22	1.46	1.50
12	L	204	CLA	MG-NB	-2.22	2.01	2.05
12	G	810	CLA	CMD-C2D	-2.22	1.46	1.50
12	a	802	CLA	C3B-C4B	2.22	1.49	1.42
12	A	854	CLA	C3B-C4B	2.22	1.49	1.42
12	G	818	CLA	MG-NB	-2.22	2.01	2.05
12	b	2136	CLA	MG-NB	-2.22	2.01	2.05
12	A	822	CLA	CMD-C2D	-2.22	1.46	1.50
12	B	2134	CLA	C3B-C4B	2.22	1.49	1.42
12	a	832	CLA	CMD-C2D	-2.22	1.46	1.50
12	A	804	CLA	CMC-C2C	-2.22	1.46	1.50
12	L	204	CLA	CMD-C2D	-2.22	1.46	1.50
12	A	816	CLA	CHC-C1C	2.22	1.42	1.38
12	A	812	CLA	C3B-C4B	2.22	1.49	1.42
12	G	833	CLA	CMB-C2B	-2.22	1.46	1.50
12	A	804	CLA	CMD-C2D	-2.22	1.46	1.50
12	B	2127	CLA	C3B-C4B	2.22	1.49	1.42
12	G	837	CLA	CMD-C2D	-2.22	1.46	1.50
12	U	203	CLA	CHC-C1C	2.22	1.42	1.38
12	H	2139	CLA	C1B-C2B	2.22	1.48	1.43
12	a	829	CLA	C3B-C4B	2.22	1.49	1.42
15	B	2145	BCR	C30-C25	-2.22	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	812	CLA	C3B-C4B	2.22	1.49	1.42
12	G	820	CLA	CMB-C2B	-2.22	1.46	1.50
12	b	2128	CLA	CHC-C1C	2.22	1.42	1.38
12	B	2140	CLA	C1B-C2B	2.21	1.48	1.43
12	a	836	CLA	CMB-C2B	-2.21	1.46	1.50
12	A	818	CLA	MG-NB	-2.21	2.01	2.05
12	A	850	CLA	C1B-C2B	2.21	1.48	1.43
24	m	102	SQD	O7-S	2.21	1.51	1.45
12	A	830	CLA	CMB-C2B	-2.21	1.46	1.50
12	A	832	CLA	CMD-C2D	-2.21	1.46	1.50
12	b	2137	CLA	CHC-C1C	2.21	1.42	1.38
12	A	824	CLA	CHC-C1C	2.21	1.42	1.38
12	b	2133	CLA	C3B-C4B	2.21	1.49	1.42
12	H	2119	CLA	MG-NB	-2.21	2.01	2.05
12	a	831	CLA	CHC-C1C	2.21	1.42	1.38
12	B	2118	CLA	CHC-C1C	2.21	1.42	1.38
12	B	2125	CLA	CHC-C1C	2.21	1.42	1.38
12	G	829	CLA	C3B-C4B	2.21	1.49	1.42
12	G	830	CLA	CMB-C2B	-2.21	1.46	1.50
12	b	2102	CLA	CHC-C1C	2.21	1.42	1.38
12	G	854	CLA	C3B-C4B	2.21	1.49	1.42
12	B	2103	CLA	CHC-C1C	2.21	1.42	1.38
12	A	818	CLA	CMB-C2B	-2.21	1.46	1.50
12	B	2139	CLA	CMD-C2D	-2.21	1.46	1.50
12	G	817	CLA	CMD-C2D	-2.21	1.46	1.50
12	a	812	CLA	C3B-C4B	2.21	1.49	1.42
12	A	829	CLA	C3B-C4B	2.21	1.49	1.42
12	k	4002	CLA	CHC-C1C	2.21	1.42	1.38
12	a	830	CLA	CMB-C2B	-2.21	1.46	1.50
12	H	2124	CLA	CHC-C1C	2.21	1.42	1.38
12	J	102	CLA	CHC-C1C	2.21	1.42	1.38
12	b	2110	CLA	CMD-C2D	-2.21	1.46	1.50
12	B	2138	CLA	CHC-C1C	2.21	1.42	1.38
12	G	836	CLA	CMB-C2B	-2.21	1.46	1.50
12	B	2129	CLA	CMB-C2B	-2.21	1.46	1.50
12	H	2139	CLA	MG-NB	-2.21	2.01	2.05
12	B	2140	CLA	MG-NB	-2.21	2.01	2.05
12	B	2111	CLA	CMD-C2D	-2.21	1.46	1.50
12	A	837	CLA	CMD-C2D	-2.21	1.46	1.50
12	a	833	CLA	CMB-C2B	-2.21	1.46	1.50
12	B	2136	CLA	CMB-C2B	-2.21	1.46	1.50
12	G	819	CLA	CMD-C2D	-2.20	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	j	102	CLA	CHC-C1C	2.20	1.42	1.38
12	A	836	CLA	CMB-C2B	-2.20	1.46	1.50
12	F	201	CLA	C3B-C4B	2.20	1.49	1.42
12	H	2137	CLA	MG-NB	-2.20	2.01	2.05
12	b	2135	CLA	CMB-C2B	-2.20	1.46	1.50
12	G	850	CLA	C1B-C2B	2.20	1.48	1.43
12	J	103	CLA	CHC-C1C	2.20	1.42	1.38
12	b	2139	CLA	C1B-C2B	2.20	1.48	1.43
12	A	831	CLA	CHC-C1C	2.20	1.42	1.38
12	A	833	CLA	CMB-C2B	-2.20	1.46	1.50
12	l	203	CLA	MG-NB	-2.20	2.01	2.05
12	H	2120	CLA	CHC-C1C	2.20	1.42	1.38
12	a	819	CLA	CHC-C1C	2.20	1.42	1.38
12	G	822	CLA	CMD-C2D	-2.20	1.46	1.50
12	B	2108	CLA	C3B-C4B	2.20	1.49	1.42
12	G	825	CLA	MG-NB	-2.20	2.01	2.05
12	a	820	CLA	CMB-C2B	-2.20	1.46	1.50
12	B	2103	CLA	CMB-C2B	-2.20	1.46	1.50
12	a	837	CLA	CMD-C2D	-2.20	1.46	1.50
12	G	829	CLA	CMD-C2D	-2.20	1.46	1.50
12	H	2125	CLA	CMB-C2B	-2.20	1.46	1.50
12	G	854	CLA	MG-NB	-2.20	2.01	2.05
12	a	854	CLA	MG-NB	-2.20	2.01	2.05
12	Q	201	CLA	C3B-C4B	2.20	1.49	1.42
23	F	205	ZEX	C20-C13	2.20	1.55	1.50
12	A	820	CLA	CMB-C2B	-2.20	1.46	1.50
12	A	829	CLA	CMD-C2D	-2.20	1.46	1.50
12	H	2137	CLA	C3B-C4B	2.20	1.49	1.42
12	f	201	CLA	C3B-C4B	2.20	1.49	1.42
12	G	824	CLA	CHC-C1C	2.20	1.42	1.38
23	f	205	ZEX	C20-C13	2.20	1.55	1.50
12	H	2110	CLA	CMD-C2D	-2.19	1.46	1.50
12	H	2122	CLA	CHC-C1C	2.19	1.42	1.38
12	B	2101	CLA	CHC-C1C	2.19	1.42	1.38
12	A	851	CLA	CMD-C2D	-2.19	1.46	1.50
12	H	2114	CLA	C3B-C4B	2.19	1.49	1.42
12	a	804	CLA	C3B-C4B	2.19	1.49	1.42
12	A	819	CLA	CMD-C2D	-2.19	1.46	1.50
12	a	829	CLA	CMD-C2D	-2.19	1.46	1.50
12	G	831	CLA	CHC-C1C	2.19	1.42	1.38
12	B	2138	CLA	MG-NB	-2.19	2.01	2.05
24	M	101	SQD	O7-S	2.19	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	818	CLA	CMB-C2B	-2.19	1.46	1.50
12	b	2107	CLA	C3B-C4B	2.19	1.49	1.42
12	A	817	CLA	CMD-C2D	-2.19	1.46	1.50
13	a	840	A1AGD	C53-C6	-2.19	1.46	1.50
12	b	2117	CLA	CHC-C1C	2.19	1.42	1.38
12	H	2117	CLA	CHC-C1C	2.19	1.42	1.38
12	H	2137	CLA	CHC-C1C	2.19	1.42	1.38
12	L	204	CLA	C3B-C4B	2.19	1.49	1.42
12	H	2128	CLA	CMB-C2B	-2.19	1.46	1.50
12	b	2152	CLA	CHC-C1C	2.19	1.42	1.38
12	a	818	CLA	MG-NB	-2.19	2.01	2.05
23	f	205	ZEX	C18-C5	2.19	1.54	1.50
12	G	815	CLA	CMB-C2B	-2.19	1.46	1.50
12	b	2107	CLA	MG-NB	-2.19	2.01	2.05
13	G	840	A1AGD	C53-C6	-2.19	1.46	1.50
12	b	2114	CLA	C3B-C4B	2.19	1.49	1.42
12	B	2123	CLA	CHC-C1C	2.19	1.42	1.38
12	G	809	CLA	CMC-C2C	-2.19	1.46	1.50
12	a	828	CLA	MG-NB	-2.19	2.01	2.05
12	A	825	CLA	MG-NB	-2.19	2.01	2.05
12	A	809	CLA	CMC-C2C	-2.19	1.46	1.50
12	A	804	CLA	C3B-C4B	2.19	1.49	1.42
12	b	2133	CLA	CHC-C1C	2.19	1.42	1.38
12	A	819	CLA	CHC-C1C	2.19	1.42	1.38
12	U	203	CLA	MG-NB	-2.19	2.01	2.05
12	A	854	CLA	MG-NB	-2.19	2.01	2.05
12	H	2114	CLA	CMB-C2B	-2.19	1.46	1.50
12	H	2107	CLA	C3B-C4B	2.19	1.49	1.42
12	B	2115	CLA	C3B-C4B	2.19	1.49	1.42
12	H	2138	CLA	CMD-C2D	-2.19	1.46	1.50
12	b	2125	CLA	CMB-C2B	-2.19	1.46	1.50
12	B	2126	CLA	CMB-C2B	-2.18	1.46	1.50
12	b	2137	CLA	C3B-C4B	2.18	1.49	1.42
12	B	2115	CLA	CMB-C2B	-2.18	1.46	1.50
12	U	204	CLA	MG-NB	-2.18	2.01	2.05
12	l	204	CLA	MG-NB	-2.18	2.01	2.05
12	G	819	CLA	CHC-C1C	2.18	1.42	1.38
12	H	2152	CLA	CHC-C1C	2.18	1.42	1.38
12	H	2107	CLA	MG-NB	-2.18	2.01	2.05
12	b	2138	CLA	CHC-C1C	2.18	1.42	1.38
12	G	836	CLA	CHC-C1C	2.18	1.42	1.38
12	B	2125	CLA	CMD-C2D	-2.18	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	2138	CLA	C3B-C4B	2.18	1.49	1.42
12	b	2122	CLA	CHC-C1C	2.18	1.42	1.38
12	H	2111	CLA	CMB-C2B	-2.18	1.46	1.50
12	b	2124	CLA	CMD-C2D	-2.18	1.46	1.50
23	F	205	ZEX	C18-C5	2.18	1.54	1.50
12	a	829	CLA	CMC-C2C	-2.18	1.46	1.50
12	b	2114	CLA	CMB-C2B	-2.18	1.46	1.50
12	b	2128	CLA	CMB-C2B	-2.18	1.46	1.50
12	a	836	CLA	CHC-C1C	2.18	1.42	1.38
12	A	829	CLA	CMC-C2C	-2.18	1.46	1.50
12	G	829	CLA	CMC-C2C	-2.18	1.46	1.50
12	a	815	CLA	CMB-C2B	-2.18	1.46	1.50
12	A	836	CLA	CHC-C1C	2.18	1.42	1.38
12	B	2129	CLA	CHC-C1C	2.18	1.42	1.38
12	A	815	CLA	CMB-C2B	-2.18	1.46	1.50
12	G	820	CLA	CMC-C2C	-2.18	1.46	1.50
12	A	828	CLA	CMD-C2D	-2.18	1.46	1.50
12	b	2102	CLA	CMB-C2B	-2.18	1.46	1.50
12	B	2139	CLA	CHC-C1C	2.18	1.42	1.38
12	G	804	CLA	C3B-C4B	2.18	1.49	1.42
12	a	824	CLA	CHC-C1C	2.18	1.42	1.38
12	U	204	CLA	C3B-C4B	2.18	1.49	1.42
12	b	2139	CLA	MG-NB	-2.18	2.01	2.05
12	a	826	CLA	CMD-C2D	-2.18	1.46	1.50
12	H	2102	CLA	CHC-C1C	2.18	1.42	1.38
12	a	817	CLA	MG-NB	-2.18	2.01	2.05
12	B	2108	CLA	MG-NB	-2.18	2.01	2.05
15	H	2144	BCR	C30-C25	-2.17	1.51	1.53
12	A	817	CLA	MG-NB	-2.17	2.01	2.05
12	H	2122	CLA	CMD-C2D	-2.17	1.46	1.50
12	G	823	CLA	CHC-C1C	2.17	1.42	1.38
12	b	2108	CLA	CMD-C2D	-2.17	1.46	1.50
12	A	816	CLA	CMC-C2C	-2.17	1.46	1.50
12	a	809	CLA	CMC-C2C	-2.17	1.46	1.50
12	S	102	CLA	CHC-C1C	2.17	1.42	1.38
12	b	2108	CLA	MG-NB	-2.17	2.01	2.05
12	a	823	CLA	CHC-C1C	2.17	1.42	1.38
23	Q	205	ZEX	C18-C5	2.17	1.54	1.50
12	G	816	CLA	CMC-C2C	-2.17	1.46	1.50
12	a	816	CLA	CMC-C2C	-2.17	1.46	1.50
12	b	2115	CLA	CMD-C2D	-2.17	1.46	1.50
12	G	851	CLA	CMD-C2D	-2.17	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	819	CLA	CMD-C2D	-2.17	1.46	1.50
12	A	802	CLA	CMB-C2B	-2.17	1.46	1.50
12	L	203	CLA	MG-NB	-2.17	2.01	2.05
12	H	2138	CLA	CHC-C1C	2.17	1.42	1.38
12	b	2120	CLA	CHC-C1C	2.17	1.42	1.38
12	b	2118	CLA	C3B-C4B	2.17	1.49	1.42
12	j	103	CLA	CHC-C1C	2.17	1.42	1.38
12	l	204	CLA	CHC-C1C	2.17	1.42	1.38
12	A	826	CLA	CMD-C2D	-2.17	1.46	1.50
12	A	834	CLA	CMB-C2B	-2.17	1.46	1.50
12	B	2140	CLA	C3B-C4B	2.17	1.49	1.42
13	A	840	A1AGD	C53-C6	-2.17	1.46	1.50
12	G	818	CLA	CMB-C2B	-2.17	1.46	1.50
12	H	2119	CLA	CMB-C2B	-2.17	1.46	1.50
12	a	828	CLA	CMD-C2D	-2.17	1.46	1.50
12	B	2119	CLA	C3B-C4B	2.17	1.49	1.42
12	a	825	CLA	MG-NB	-2.17	2.01	2.05
12	H	2133	CLA	CHC-C1C	2.17	1.42	1.38
12	b	2139	CLA	C3B-C4B	2.16	1.49	1.42
12	G	808	CLA	CMD-C2D	-2.16	1.46	1.50
12	U	203	CLA	CMD-C2D	-2.16	1.46	1.50
12	B	2134	CLA	CHC-C1C	2.16	1.42	1.38
12	L	204	CLA	CHC-C1C	2.16	1.42	1.38
12	G	839	CLA	MG-NB	-2.16	2.01	2.05
12	H	2111	CLA	CHC-C1C	2.16	1.42	1.38
12	H	2108	CLA	CMD-C2D	-2.16	1.46	1.50
12	b	2119	CLA	CMB-C2B	-2.16	1.46	1.50
12	B	2109	CLA	MG-NB	-2.16	2.01	2.05
12	H	2113	CLA	CHC-C1C	2.16	1.42	1.38
12	A	823	CLA	CHC-C1C	2.16	1.42	1.38
12	G	801	CLA	CMC-C2C	-2.16	1.46	1.50
12	G	817	CLA	MG-NB	-2.16	2.01	2.05
12	B	2121	CLA	CHC-C1C	2.16	1.42	1.38
12	a	802	CLA	CMB-C2B	-2.16	1.46	1.50
12	a	808	CLA	CMD-C2D	-2.16	1.46	1.50
12	H	2139	CLA	C3B-C4B	2.16	1.49	1.42
12	A	828	CLA	MG-NB	-2.16	2.01	2.05
12	G	828	CLA	CMD-C2D	-2.16	1.46	1.50
12	G	834	CLA	CMB-C2B	-2.16	1.46	1.50
12	G	802	CLA	CMB-C2B	-2.16	1.46	1.50
12	A	850	CLA	CMD-C2D	-2.16	1.46	1.50
12	a	817	CLA	CMD-C2D	-2.16	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	2104	CLA	CMD-C2D	-2.16	1.46	1.50
12	B	2108	CLA	CHC-C1C	2.16	1.42	1.38
12	G	826	CLA	CMD-C2D	-2.16	1.46	1.50
12	H	2102	CLA	CMB-C2B	-2.16	1.46	1.50
12	b	2123	CLA	CMC-C2C	-2.16	1.46	1.50
12	H	2128	CLA	CHC-C1C	2.16	1.42	1.38
12	B	2123	CLA	CMD-C2D	-2.16	1.46	1.50
12	H	2107	CLA	CHC-C1C	2.16	1.42	1.38
12	A	839	CLA	MG-NB	-2.16	2.01	2.05
12	A	820	CLA	CMC-C2C	-2.16	1.46	1.50
12	a	839	CLA	MG-NB	-2.16	2.01	2.05
12	a	815	CLA	CHC-C1C	2.16	1.42	1.38
12	b	2111	CLA	CHC-C1C	2.16	1.42	1.38
12	f	201	CLA	MG-NB	-2.15	2.01	2.05
12	B	2112	CLA	CHC-C1C	2.15	1.42	1.38
12	A	816	CLA	CMD-C2D	-2.15	1.46	1.50
26	U	210	LMT	O3B-C3B	-2.15	1.37	1.43
23	b	2151	ZEX	C20-C13	2.15	1.55	1.50
12	U	201	CLA	CHC-C1C	2.15	1.42	1.38
12	G	828	CLA	MG-NB	-2.15	2.01	2.05
12	A	812	CLA	MG-NB	-2.15	2.01	2.05
12	a	830	CLA	C3B-C4B	2.15	1.49	1.42
12	H	2112	CLA	CHC-C1C	2.15	1.42	1.38
12	H	2123	CLA	CMC-C2C	-2.15	1.46	1.50
12	B	2124	CLA	CMC-C2C	-2.15	1.46	1.50
12	B	2113	CLA	CHC-C1C	2.15	1.42	1.38
12	H	2118	CLA	C3B-C4B	2.15	1.49	1.42
12	B	2114	CLA	CHC-C1C	2.15	1.42	1.38
12	b	2112	CLA	CHC-C1C	2.15	1.42	1.38
12	H	2112	CLA	CMB-C2B	-2.15	1.46	1.50
12	H	2111	CLA	CMD-C2D	-2.15	1.46	1.50
23	B	2152	ZEX	C20-C13	2.15	1.55	1.50
12	A	801	CLA	CMC-C2C	-2.15	1.46	1.50
12	L	203	CLA	CMD-C2D	-2.15	1.46	1.50
12	b	2107	CLA	CHC-C1C	2.15	1.42	1.38
12	A	801	CLA	C3B-C4B	2.15	1.49	1.42
12	G	801	CLA	C3B-C4B	2.15	1.49	1.42
12	G	808	CLA	CMC-C2C	-2.15	1.46	1.50
12	U	204	CLA	CHC-C1C	2.15	1.42	1.38
12	A	815	CLA	CHC-C1C	2.15	1.42	1.38
12	B	2126	CLA	CHC-C1C	2.15	1.42	1.38
12	A	810	CLA	CMB-C2B	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	2127	CLA	C3B-C4B	2.15	1.49	1.42
12	H	2108	CLA	MG-NB	-2.15	2.01	2.05
12	a	820	CLA	CMC-C2C	-2.15	1.46	1.50
12	a	834	CLA	CMB-C2B	-2.15	1.46	1.50
12	l	203	CLA	CMD-C2D	-2.15	1.46	1.50
12	H	2102	CLA	CMD-C2D	-2.14	1.46	1.50
12	B	2120	CLA	CMB-C2B	-2.14	1.46	1.50
12	b	2111	CLA	CMD-C2D	-2.14	1.46	1.50
12	b	2112	CLA	CMB-C2B	-2.14	1.46	1.50
12	B	2105	CLA	CMD-C2D	-2.14	1.46	1.50
12	b	2102	CLA	CMD-C2D	-2.14	1.46	1.50
12	b	2113	CLA	CHC-C1C	2.14	1.42	1.38
12	b	2125	CLA	CHC-C1C	2.14	1.42	1.38
12	B	2128	CLA	C3B-C4B	2.14	1.49	1.42
12	G	838	CLA	CHC-C1C	2.14	1.42	1.38
12	b	2125	CLA	CMD-C2D	-2.14	1.46	1.50
12	a	812	CLA	MG-NB	-2.14	2.01	2.05
12	f	201	CLA	CMB-C2B	-2.14	1.46	1.50
12	G	837	CLA	CMB-C2B	-2.14	1.46	1.50
12	G	830	CLA	C3B-C4B	2.14	1.49	1.42
12	G	835	CLA	C3B-C4B	2.14	1.49	1.42
12	H	2125	CLA	CHC-C1C	2.14	1.42	1.38
12	A	835	CLA	C3B-C4B	2.14	1.49	1.42
12	H	2124	CLA	CMD-C2D	-2.14	1.46	1.50
12	F	201	CLA	MG-NB	-2.14	2.01	2.05
12	b	2105	CLA	CMD-C2D	-2.14	1.46	1.50
12	b	2122	CLA	CMD-C2D	-2.14	1.46	1.50
12	a	825	CLA	CMB-C2B	-2.14	1.46	1.50
12	A	837	CLA	CHC-C1C	2.14	1.42	1.38
12	a	810	CLA	CMB-C2B	-2.14	1.46	1.50
12	a	835	CLA	C3B-C4B	2.14	1.49	1.42
12	A	831	CLA	MG-NB	-2.14	2.01	2.05
12	A	830	CLA	C3B-C4B	2.14	1.49	1.42
12	B	2112	CLA	CMB-C2B	-2.14	1.46	1.50
12	a	837	CLA	CHC-C1C	2.14	1.42	1.38
12	G	825	CLA	CMB-C2B	-2.14	1.46	1.50
12	B	2112	CLA	CMD-C2D	-2.14	1.46	1.50
12	B	2113	CLA	CMB-C2B	-2.14	1.46	1.50
12	A	808	CLA	CMD-C2D	-2.13	1.46	1.50
12	G	815	CLA	CHC-C1C	2.13	1.42	1.38
12	A	838	CLA	CHC-C1C	2.13	1.42	1.38
12	F	201	CLA	CMB-C2B	-2.13	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	2109	CLA	CMD-C2D	-2.13	1.46	1.50
12	B	2116	CLA	CMD-C2D	-2.13	1.46	1.50
12	G	827	CLA	CMD-C2D	-2.13	1.46	1.50
12	G	807	CLA	CMC-C2C	-2.13	1.46	1.50
12	G	816	CLA	CMD-C2D	-2.13	1.46	1.50
17	a	847	LMG	C3-C2	2.13	1.57	1.52
12	G	831	CLA	MG-NB	-2.13	2.01	2.05
12	a	801	CLA	CMC-C2C	-2.13	1.46	1.50
12	B	2128	CLA	CHC-C1C	2.13	1.42	1.38
12	G	807	CLA	CMD-C2D	-2.13	1.46	1.50
12	a	850	CLA	CMD-C2D	-2.13	1.46	1.50
12	A	807	CLA	CMD-C2D	-2.13	1.46	1.50
12	H	2127	CLA	CHC-C1C	2.13	1.42	1.38
12	L	201	CLA	CHC-C1C	2.13	1.42	1.38
12	b	2125	CLA	MG-NB	-2.13	2.01	2.05
12	B	2126	CLA	MG-NB	-2.13	2.01	2.05
12	A	814	CLA	CMD-C2D	-2.13	1.46	1.50
12	G	812	CLA	MG-NB	-2.13	2.01	2.05
12	G	850	CLA	CMD-C2D	-2.13	1.46	1.50
12	a	808	CLA	CMC-C2C	-2.13	1.46	1.50
12	a	801	CLA	C3B-C4B	2.13	1.48	1.42
12	H	2125	CLA	CMD-C2D	-2.13	1.46	1.50
12	B	2131	CLA	CHC-C1C	2.13	1.42	1.38
12	A	833	CLA	C3B-C4B	2.13	1.48	1.42
12	B	2103	CLA	CMD-C2D	-2.13	1.46	1.50
12	H	2136	CLA	CMD-C2D	-2.13	1.46	1.50
12	Q	201	CLA	MG-NB	-2.13	2.01	2.05
12	a	831	CLA	MG-NB	-2.13	2.01	2.05
12	a	816	CLA	CMD-C2D	-2.13	1.46	1.50
17	G	847	LMG	C3-C2	2.13	1.57	1.52
12	G	837	CLA	CHC-C1C	2.13	1.42	1.38
12	b	2127	CLA	C3B-C4B	2.12	1.48	1.42
12	A	808	CLA	CMC-C2C	-2.12	1.46	1.50
12	a	838	CLA	CHC-C1C	2.12	1.42	1.38
12	Q	201	CLA	CMB-C2B	-2.12	1.46	1.50
17	A	847	LMG	C3-C2	2.12	1.57	1.52
12	H	2104	CLA	CMD-C2D	-2.12	1.46	1.50
12	B	2106	CLA	CMD-C2D	-2.12	1.46	1.50
12	a	833	CLA	C3B-C4B	2.12	1.48	1.42
12	G	823	CLA	CMC-C2C	-2.12	1.46	1.50
12	a	814	CLA	CMC-C2C	-2.12	1.46	1.50
26	L	210	LMT	O3B-C3B	-2.12	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	2125	CLA	MG-NB	-2.12	2.01	2.05
12	b	2127	CLA	CHC-C1C	2.12	1.42	1.38
12	B	2126	CLA	CMD-C2D	-2.12	1.46	1.50
12	A	833	CLA	MG-NB	-2.12	2.01	2.05
12	H	2107	CLA	CMD-C2D	-2.12	1.46	1.50
12	H	2130	CLA	CHC-C1C	2.12	1.42	1.38
12	b	2111	CLA	CMB-C2B	-2.12	1.46	1.50
12	l	201	CLA	CHC-C1C	2.12	1.42	1.38
12	U	205	CLA	MG-NB	-2.12	2.01	2.05
12	a	821	CLA	MG-NB	-2.12	2.01	2.05
12	b	2107	CLA	CMD-C2D	-2.12	1.46	1.50
12	B	2121	CLA	MG-NB	-2.12	2.01	2.05
12	B	2120	CLA	CHC-C1C	2.12	1.42	1.38
12	H	2115	CLA	CMD-C2D	-2.12	1.46	1.50
12	G	833	CLA	C3B-C4B	2.12	1.48	1.42
12	B	2108	CLA	CMD-C2D	-2.12	1.46	1.50
12	B	2109	CLA	CMB-C2B	-2.12	1.46	1.50
12	A	827	CLA	CMD-C2D	-2.11	1.46	1.50
12	A	825	CLA	CMB-C2B	-2.11	1.46	1.50
13	H	2153	A1AGD	C7-C3	-2.11	1.48	1.51
12	G	814	CLA	CHC-C1C	2.11	1.42	1.38
12	b	2119	CLA	CHC-C1C	2.11	1.42	1.38
12	A	823	CLA	CMC-C2C	-2.11	1.46	1.50
12	a	810	CLA	CHC-C1C	2.11	1.42	1.38
12	a	837	CLA	CMB-C2B	-2.11	1.46	1.50
12	B	2110	CLA	CMB-C2B	-2.11	1.46	1.50
12	B	2128	CLA	CMD-C2D	-2.11	1.46	1.50
12	b	2119	CLA	CMD-C2D	-2.11	1.46	1.50
12	H	2127	CLA	CMD-C2D	-2.11	1.46	1.50
12	H	2108	CLA	CMB-C2B	-2.11	1.46	1.50
12	A	807	CLA	CMC-C2C	-2.11	1.46	1.50
12	a	807	CLA	CMD-C2D	-2.11	1.46	1.50
26	l	210	LMT	O3B-C3B	-2.11	1.37	1.43
12	a	833	CLA	MG-NB	-2.11	2.01	2.05
12	B	2130	CLA	CHC-C1C	2.11	1.42	1.38
12	U	201	CLA	CMC-C2C	-2.11	1.46	1.50
12	U	204	CLA	CMB-C2B	-2.11	1.46	1.50
12	b	2104	CLA	MG-NB	-2.11	2.01	2.05
12	b	2129	CLA	CHC-C1C	2.11	1.42	1.38
23	H	2151	ZEX	C20-C13	2.11	1.55	1.50
12	a	827	CLA	CMD-C2D	-2.11	1.46	1.50
12	F	203	CLA	CMD-C2D	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	833	CLA	MG-NB	-2.11	2.01	2.05
12	A	819	CLA	MG-NB	-2.11	2.01	2.05
12	a	807	CLA	CMC-C2C	-2.11	1.46	1.50
12	H	2129	CLA	CHC-C1C	2.11	1.42	1.38
12	G	810	CLA	CMB-C2B	-2.11	1.46	1.50
12	b	2101	CLA	CMD-C2D	-2.10	1.46	1.50
12	b	2109	CLA	CMB-C2B	-2.10	1.46	1.50
12	a	806	CLA	CMB-C2B	-2.10	1.46	1.50
12	Q	203	CLA	CMD-C2D	-2.10	1.46	1.50
12	b	2120	CLA	MG-NB	-2.10	2.01	2.05
12	H	2120	CLA	MG-NB	-2.10	2.01	2.05
12	a	804	CLA	MG-NB	-2.10	2.01	2.05
12	a	823	CLA	CMC-C2C	-2.10	1.46	1.50
12	A	814	CLA	CMC-C2C	-2.10	1.46	1.50
12	G	802	CLA	CHC-C1C	2.10	1.42	1.38
12	B	2104	CLA	CMB-C2B	-2.10	1.46	1.50
12	G	818	CLA	CMD-C2D	-2.10	1.46	1.50
12	B	2127	CLA	CMC-C2C	-2.10	1.46	1.50
12	a	804	CLA	CMB-C2B	-2.10	1.46	1.50
12	f	203	CLA	CMD-C2D	-2.10	1.46	1.50
12	l	205	CLA	MG-NB	-2.10	2.01	2.05
12	H	2119	CLA	CHC-C1C	2.10	1.42	1.38
12	L	205	CLA	MG-NB	-2.10	2.01	2.05
12	H	2105	CLA	CMD-C2D	-2.10	1.46	1.50
13	B	2153	A1AGD	C7-C3	-2.10	1.48	1.51
12	B	2120	CLA	CMD-C2D	-2.10	1.46	1.50
12	A	837	CLA	CMB-C2B	-2.09	1.46	1.50
12	L	204	CLA	CMB-C2B	-2.09	1.46	1.50
12	H	2103	CLA	CMB-C2B	-2.09	1.46	1.50
12	F	203	CLA	CMB-C2B	-2.09	1.46	1.50
12	A	804	CLA	CMB-C2B	-2.09	1.46	1.50
12	G	814	CLA	CMD-C2D	-2.09	1.46	1.50
16	G	846	LHG	P-O6	2.09	1.67	1.59
12	b	2127	CLA	CMD-C2D	-2.09	1.46	1.50
12	f	203	CLA	CMB-C2B	-2.09	1.46	1.50
12	A	802	CLA	CHC-C1C	2.09	1.42	1.38
12	A	808	CLA	MG-NB	-2.09	2.01	2.05
12	F	203	CLA	MG-NB	-2.09	2.01	2.05
12	G	814	CLA	CMC-C2C	-2.09	1.46	1.50
12	A	806	CLA	CMB-C2B	-2.09	1.46	1.50
12	B	2121	CLA	CMD-C2D	-2.09	1.46	1.50
12	L	201	CLA	CMC-C2C	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	l	204	CLA	CMB-C2B	-2.09	1.46	1.50
12	G	819	CLA	MG-NB	-2.09	2.01	2.05
12	G	806	CLA	CMB-C2B	-2.09	1.46	1.50
12	b	2103	CLA	CMB-C2B	-2.09	1.46	1.50
12	A	821	CLA	CMD-C2D	-2.09	1.46	1.50
12	A	810	CLA	CHC-C1C	2.09	1.42	1.38
12	Q	203	CLA	CMB-C2B	-2.09	1.46	1.50
12	b	2136	CLA	CMD-C2D	-2.09	1.46	1.50
12	a	802	CLA	CHC-C1C	2.09	1.42	1.38
12	b	2126	CLA	CMD-C2D	-2.09	1.46	1.50
12	b	2130	CLA	CHC-C1C	2.09	1.42	1.38
12	U	205	CLA	CMD-C2D	-2.09	1.46	1.50
12	b	2113	CLA	CMD-C2D	-2.09	1.46	1.50
12	b	2123	CLA	CMD-C2D	-2.09	1.46	1.50
12	b	2118	CLA	CHC-C1C	2.09	1.42	1.38
12	G	804	CLA	CMB-C2B	-2.09	1.46	1.50
12	b	2108	CLA	CMB-C2B	-2.09	1.46	1.50
12	H	2137	CLA	CMD-C2D	-2.09	1.46	1.50
12	G	804	CLA	MG-NB	-2.09	2.01	2.05
12	B	2123	CLA	MG-NB	-2.09	2.01	2.05
12	G	834	CLA	CMD-C2D	-2.09	1.46	1.50
12	B	2134	CLA	CMB-C2B	-2.09	1.46	1.50
12	B	2137	CLA	CMD-C2D	-2.09	1.46	1.50
12	G	821	CLA	CMD-C2D	-2.09	1.46	1.50
12	H	2126	CLA	CMC-C2C	-2.09	1.46	1.50
12	f	203	CLA	MG-NB	-2.09	2.01	2.05
12	A	804	CLA	MG-NB	-2.09	2.01	2.05
12	H	2113	CLA	CMD-C2D	-2.09	1.46	1.50
12	b	2121	CLA	CMD-C2D	-2.09	1.46	1.50
12	b	2134	CLA	CMD-C2D	-2.09	1.46	1.50
12	b	2126	CLA	CMC-C2C	-2.08	1.46	1.50
12	a	814	CLA	CMD-C2D	-2.08	1.46	1.50
12	B	2105	CLA	MG-NB	-2.08	2.01	2.05
12	H	2133	CLA	CMB-C2B	-2.08	1.46	1.50
12	A	838	CLA	MG-NB	-2.08	2.01	2.05
12	A	814	CLA	CHC-C1C	2.08	1.42	1.38
12	H	2122	CLA	MG-NB	-2.08	2.01	2.05
12	a	836	CLA	MG-NB	-2.08	2.01	2.05
12	A	802	CLA	MG-NB	-2.08	2.01	2.05
12	H	2120	CLA	CMD-C2D	-2.08	1.46	1.50
12	b	2121	CLA	MG-NB	-2.08	2.01	2.05
12	H	2104	CLA	MG-NB	-2.08	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	2122	CLA	MG-NB	-2.08	2.01	2.05
12	H	2138	CLA	MG-NB	-2.08	2.01	2.05
13	b	2153	A1AGD	C7-C3	-2.08	1.48	1.51
12	G	810	CLA	CHC-C1C	2.08	1.42	1.38
12	B	2127	CLA	CHC-C1C	2.08	1.42	1.38
12	k	4002	CLA	CMD-C2D	-2.08	1.46	1.50
12	B	2119	CLA	CMD-C2D	-2.08	1.46	1.50
12	Q	203	CLA	MG-NB	-2.08	2.01	2.05
12	A	836	CLA	MG-NB	-2.08	2.01	2.05
12	G	809	CLA	CMD-C2D	-2.08	1.46	1.50
16	A	846	LHG	P-O6	2.08	1.67	1.59
12	l	201	CLA	CMC-C2C	-2.08	1.46	1.50
12	B	2122	CLA	MG-NB	-2.08	2.01	2.05
12	G	802	CLA	MG-NB	-2.08	2.01	2.05
12	b	2116	CLA	MG-NB	-2.08	2.01	2.05
12	G	821	CLA	CMB-C2B	-2.07	1.46	1.50
12	H	2119	CLA	CMD-C2D	-2.07	1.46	1.50
12	H	2126	CLA	CMD-C2D	-2.07	1.46	1.50
12	L	205	CLA	CMD-C2D	-2.07	1.46	1.50
12	G	808	CLA	MG-NB	-2.07	2.01	2.05
12	G	854	CLA	CMD-C2D	-2.07	1.46	1.50
12	b	2152	CLA	CMC-C2C	-2.07	1.46	1.50
12	S	103	CLA	CMD-C2D	-2.07	1.46	1.50
12	A	821	CLA	MG-NB	-2.07	2.01	2.05
12	B	2138	CLA	CMD-C2D	-2.07	1.46	1.50
12	G	854	CLA	CHC-C1C	2.07	1.42	1.38
12	a	807	CLA	MG-NB	-2.07	2.01	2.05
12	H	2135	CLA	CMD-C2D	-2.07	1.46	1.50
12	A	818	CLA	CMD-C2D	-2.07	1.46	1.50
12	H	2134	CLA	CMD-C2D	-2.07	1.46	1.50
12	H	2138	CLA	CMB-C2B	-2.07	1.46	1.50
12	A	801	CLA	CMB-C2B	-2.07	1.46	1.50
23	Q	205	ZEX	C39-C29	2.07	1.55	1.50
12	H	2109	CLA	CMB-C2B	-2.07	1.46	1.50
12	a	809	CLA	CMD-C2D	-2.07	1.46	1.50
12	G	812	CLA	CHC-C1C	2.07	1.42	1.38
12	A	807	CLA	MG-NB	-2.07	2.01	2.05
12	a	834	CLA	CMD-C2D	-2.07	1.46	1.50
12	a	818	CLA	CMD-C2D	-2.07	1.46	1.50
12	B	2131	CLA	CMD-C2D	-2.07	1.46	1.50
12	a	808	CLA	MG-NB	-2.07	2.01	2.05
12	a	819	CLA	MG-NB	-2.07	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	a	846	LHG	P-O6	2.07	1.67	1.59
12	G	801	CLA	CMB-C2B	-2.07	1.46	1.50
12	H	2114	CLA	MG-NB	-2.07	2.01	2.05
12	B	2101	CLA	CMC-C2C	-2.07	1.46	1.50
12	H	2118	CLA	MG-NB	-2.07	2.01	2.05
12	B	2124	CLA	CMD-C2D	-2.07	1.46	1.50
12	a	838	CLA	MG-NB	-2.07	2.01	2.05
12	B	2139	CLA	CMB-C2B	-2.07	1.46	1.50
12	A	854	CLA	CHC-C1C	2.07	1.42	1.38
23	F	205	ZEX	C39-C29	2.07	1.55	1.50
12	H	2103	CLA	CMC-C2C	-2.07	1.46	1.50
12	a	801	CLA	CMB-C2B	-2.07	1.46	1.50
12	A	805	CLA	CMD-C2D	-2.07	1.46	1.50
12	G	838	CLA	MG-NB	-2.07	2.01	2.05
22	b	2150	EQ3	C28-C27	2.07	1.53	1.50
12	a	814	CLA	CHC-C1C	2.07	1.42	1.38
12	a	821	CLA	CMD-C2D	-2.07	1.46	1.50
12	A	805	CLA	CMC-C2C	-2.07	1.46	1.50
12	G	839	CLA	CMD-C2D	-2.07	1.46	1.50
12	b	2133	CLA	CMB-C2B	-2.07	1.46	1.50
12	b	2103	CLA	MG-NB	-2.07	2.01	2.05
12	a	826	CLA	MG-NB	-2.06	2.01	2.05
12	a	838	CLA	CMD-C2D	-2.06	1.46	1.50
12	a	805	CLA	CMC-C2C	-2.06	1.46	1.50
12	a	821	CLA	CMB-C2B	-2.06	1.46	1.50
12	B	2122	CLA	CMD-C2D	-2.06	1.46	1.50
12	a	835	CLA	CMC-C2C	-2.06	1.46	1.50
12	B	2115	CLA	MG-NB	-2.06	2.01	2.05
12	G	838	CLA	CMC-C2C	-2.06	1.46	1.50
12	B	2127	CLA	CMD-C2D	-2.06	1.46	1.50
12	A	826	CLA	MG-NB	-2.06	2.01	2.05
12	G	807	CLA	MG-NB	-2.06	2.01	2.05
12	G	821	CLA	MG-NB	-2.06	2.01	2.05
12	G	836	CLA	MG-NB	-2.06	2.01	2.05
12	a	811	CLA	CMB-C2B	-2.06	1.46	1.50
12	l	203	CLA	CMC-C2C	-2.06	1.46	1.50
12	A	809	CLA	CMD-C2D	-2.06	1.46	1.50
12	B	2114	CLA	CMD-C2D	-2.06	1.46	1.50
12	G	835	CLA	CMC-C2C	-2.06	1.46	1.50
12	a	839	CLA	CMD-C2D	-2.06	1.46	1.50
12	l	205	CLA	CMD-C2D	-2.06	1.46	1.50
12	b	2118	CLA	CMD-C2D	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	K	4002	CLA	CMB-C2B	-2.06	1.46	1.50
12	A	821	CLA	CMB-C2B	-2.06	1.46	1.50
12	b	2138	CLA	MG-NB	-2.06	2.01	2.05
12	B	2117	CLA	MG-NB	-2.06	2.01	2.05
12	H	2123	CLA	CMD-C2D	-2.06	1.46	1.50
12	B	2102	CLA	CMD-C2D	-2.06	1.46	1.50
12	H	2101	CLA	CMD-C2D	-2.06	1.46	1.50
12	H	2115	CLA	CMB-C2B	-2.06	1.46	1.50
12	G	811	CLA	CMD-C2D	-2.06	1.46	1.50
12	a	802	CLA	CMD-C2D	-2.06	1.46	1.50
12	b	2120	CLA	CMD-C2D	-2.06	1.46	1.50
12	A	835	CLA	CMC-C2C	-2.06	1.46	1.50
12	a	812	CLA	CHC-C1C	2.06	1.42	1.38
12	A	811	CLA	CMD-C2D	-2.06	1.46	1.50
12	A	836	CLA	CMD-C2D	-2.06	1.46	1.50
12	B	2139	CLA	MG-NB	-2.06	2.01	2.05
12	H	2126	CLA	CHC-C1C	2.06	1.42	1.38
12	G	805	CLA	CMD-C2D	-2.05	1.46	1.50
12	G	826	CLA	MG-NB	-2.05	2.01	2.05
12	H	2121	CLA	MG-NB	-2.05	2.01	2.05
12	H	2121	CLA	CMD-C2D	-2.05	1.46	1.50
12	j	103	CLA	CMD-C2D	-2.05	1.46	1.50
12	G	851	CLA	CMC-C2C	-2.05	1.46	1.50
12	U	201	CLA	CMD-C2D	-2.05	1.46	1.50
12	a	831	CLA	CMB-C2B	-2.05	1.46	1.50
12	a	835	CLA	CMB-C2B	-2.05	1.46	1.50
12	J	103	CLA	CMD-C2D	-2.05	1.46	1.50
12	b	2110	CLA	C1B-NB	-2.05	1.35	1.37
12	A	854	CLA	CMD-C2D	-2.05	1.46	1.50
12	B	2119	CLA	CHC-C1C	2.05	1.42	1.38
12	a	802	CLA	MG-NB	-2.05	2.01	2.05
12	b	2118	CLA	MG-NB	-2.05	2.01	2.05
12	H	2118	CLA	CMD-C2D	-2.05	1.46	1.50
12	B	2119	CLA	MG-NB	-2.05	2.01	2.05
12	a	817	CLA	CMB-C2B	-2.05	1.46	1.50
12	b	2137	CLA	CMD-C2D	-2.05	1.46	1.50
12	H	2118	CLA	CHC-C1C	2.05	1.42	1.38
12	G	805	CLA	CMC-C2C	-2.05	1.46	1.50
12	G	806	CLA	CMD-C2D	-2.05	1.46	1.50
12	b	2138	CLA	CMB-C2B	-2.05	1.46	1.50
12	A	806	CLA	CMD-C2D	-2.05	1.46	1.50
12	B	2116	CLA	CMB-C2B	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	801	CLA	CHC-C1C	2.05	1.42	1.38
12	G	831	CLA	CMB-C2B	-2.05	1.46	1.50
12	L	203	CLA	CMC-C2C	-2.05	1.46	1.50
12	b	2103	CLA	CMC-C2C	-2.05	1.46	1.50
12	B	2125	CLA	MG-NB	-2.05	2.01	2.05
12	B	2111	CLA	C1B-NB	-2.05	1.35	1.37
12	T	4002	CLA	CMB-C2B	-2.05	1.46	1.50
12	A	802	CLA	CMD-C2D	-2.05	1.46	1.50
12	a	838	CLA	CMC-C2C	-2.05	1.46	1.50
12	k	4002	CLA	CMB-C2B	-2.05	1.46	1.50
12	A	835	CLA	CMB-C2B	-2.05	1.46	1.50
12	b	2127	CLA	MG-NB	-2.05	2.01	2.05
12	G	833	CLA	CHC-C1C	2.05	1.42	1.38
12	Q	204	CLA	CMD-C2D	-2.05	1.46	1.50
12	b	2114	CLA	CHC-C1C	2.05	1.42	1.38
23	f	205	ZEX	C39-C29	2.05	1.55	1.50
12	a	806	CLA	CMD-C2D	-2.05	1.46	1.50
12	B	2132	CLA	CMC-C2C	-2.05	1.46	1.50
12	B	2135	CLA	CMD-C2D	-2.05	1.46	1.50
12	H	2116	CLA	MG-NB	-2.05	2.01	2.05
12	b	2129	CLA	MG-ND	-2.05	2.01	2.05
12	b	2107	CLA	CMB-C2B	-2.05	1.46	1.50
12	B	2136	CLA	MG-NB	-2.05	2.01	2.05
12	H	2107	CLA	CMB-C2B	-2.05	1.46	1.50
12	a	811	CLA	CMD-C2D	-2.05	1.46	1.50
12	b	2115	CLA	CMB-C2B	-2.05	1.46	1.50
12	b	2109	CLA	CHC-C1C	2.05	1.42	1.38
12	H	2103	CLA	MG-NB	-2.05	2.01	2.05
12	a	827	CLA	CMC-C2C	-2.05	1.46	1.50
12	A	827	CLA	CMC-C2C	-2.05	1.46	1.50
12	B	2108	CLA	CMB-C2B	-2.05	1.46	1.50
12	H	2131	CLA	CMC-C2C	-2.05	1.46	1.50
12	A	839	CLA	CMD-C2D	-2.05	1.46	1.50
12	G	801	CLA	CHC-C1C	2.05	1.42	1.38
12	a	836	CLA	CMD-C2D	-2.05	1.46	1.50
12	H	2114	CLA	CHC-C1C	2.05	1.42	1.38
12	B	2110	CLA	CHC-C1C	2.05	1.42	1.38
12	A	812	CLA	CHC-C1C	2.04	1.42	1.38
12	A	838	CLA	CMC-C2C	-2.04	1.46	1.50
12	b	2136	CLA	CMB-C2B	-2.04	1.46	1.50
15	j	104	BCR	C33-C5	-2.04	1.47	1.50
12	a	835	CLA	CHC-C1C	2.04	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	838	CLA	CMD-C2D	-2.04	1.46	1.50
12	G	836	CLA	CMD-C2D	-2.04	1.46	1.50
12	a	805	CLA	CMD-C2D	-2.04	1.46	1.50
12	A	801	CLA	CHC-C1C	2.04	1.42	1.38
12	G	816	CLA	MG-NB	-2.04	2.01	2.05
12	H	2130	CLA	CMD-C2D	-2.04	1.46	1.50
12	B	2136	CLA	CMD-C2D	-2.04	1.46	1.50
12	A	850	CLA	MG-ND	-2.04	2.01	2.05
22	H	2150	EQ3	C28-C27	2.04	1.53	1.50
12	b	2130	CLA	CMD-C2D	-2.04	1.46	1.50
12	B	2137	CLA	CMB-C2B	-2.04	1.46	1.50
12	B	2104	CLA	CMC-C2C	-2.04	1.46	1.50
12	A	835	CLA	CHC-C1C	2.04	1.42	1.38
12	A	816	CLA	MG-NB	-2.04	2.01	2.05
12	A	817	CLA	CMB-C2B	-2.04	1.46	1.50
12	A	838	CLA	CMD-C2D	-2.04	1.46	1.50
12	a	850	CLA	CHC-C1C	2.04	1.42	1.38
12	b	2126	CLA	CHC-C1C	2.04	1.42	1.38
12	a	823	CLA	MG-NB	-2.04	2.01	2.05
12	b	2124	CLA	MG-NB	-2.04	2.01	2.05
12	B	2132	CLA	MG-NB	-2.04	2.01	2.05
12	F	204	CLA	CMD-C2D	-2.04	1.46	1.50
12	A	805	CLA	MG-NB	-2.04	2.01	2.05
12	H	2152	CLA	CMC-C2C	-2.04	1.46	1.50
12	a	809	CLA	CMB-C2B	-2.04	1.46	1.50
12	a	854	CLA	CHC-C1C	2.04	1.42	1.38
12	A	834	CLA	CMD-C2D	-2.04	1.46	1.50
12	a	833	CLA	CHC-C1C	2.04	1.42	1.38
12	b	2141	CLA	CMD-C2D	-2.04	1.46	1.50
12	G	829	CLA	MG-NB	-2.04	2.01	2.05
12	G	823	CLA	CMD-C2D	-2.04	1.46	1.50
12	G	823	CLA	MG-NB	-2.04	2.01	2.05
12	B	2115	CLA	CHC-C1C	2.04	1.42	1.38
12	G	817	CLA	CMB-C2B	-2.04	1.46	1.50
12	L	201	CLA	CMD-C2D	-2.04	1.46	1.50
12	H	2135	CLA	MG-NB	-2.04	2.01	2.05
12	A	823	CLA	MG-NB	-2.04	2.01	2.05
12	A	824	CLA	MG-NB	-2.04	2.01	2.05
12	G	835	CLA	CHC-C1C	2.04	1.42	1.38
12	A	811	CLA	CMB-C2B	-2.03	1.46	1.50
12	A	823	CLA	CMD-C2D	-2.03	1.46	1.50
12	H	2105	CLA	CMC-C2C	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	851	CLA	CMC-C2C	-2.03	1.46	1.50
12	H	2136	CLA	CMB-C2B	-2.03	1.46	1.50
12	G	810	CLA	MG-NB	-2.03	2.01	2.05
12	b	2131	CLA	MG-NB	-2.03	2.01	2.05
12	G	833	CLA	CMD-C2D	-2.03	1.46	1.50
12	a	833	CLA	CMD-C2D	-2.03	1.46	1.50
12	B	2141	CLA	CMD-C2D	-2.03	1.46	1.50
12	b	2135	CLA	MG-NB	-2.03	2.01	2.05
12	G	854	CLA	CMC-C2C	-2.03	1.46	1.50
12	b	2135	CLA	CMD-C2D	-2.03	1.46	1.50
12	A	833	CLA	CHC-C1C	2.03	1.42	1.38
12	B	2104	CLA	MG-NB	-2.03	2.01	2.05
12	A	829	CLA	MG-NB	-2.03	2.01	2.05
12	A	831	CLA	CMB-C2B	-2.03	1.46	1.50
12	H	2124	CLA	MG-NB	-2.03	2.01	2.05
12	B	2130	CLA	MG-ND	-2.03	2.01	2.05
12	b	2140	CLA	CMD-C2D	-2.03	1.46	1.50
12	H	2140	CLA	CMD-C2D	-2.03	1.46	1.50
12	a	810	CLA	MG-NB	-2.03	2.01	2.05
12	H	2109	CLA	CHC-C1C	2.03	1.42	1.38
12	A	850	CLA	CHC-C1C	2.03	1.42	1.38
12	b	2114	CLA	MG-NB	-2.03	2.01	2.05
12	G	830	CLA	CHC-C1C	2.03	1.42	1.38
12	H	2114	CLA	CMD-C2D	-2.03	1.46	1.50
12	B	2115	CLA	CMD-C2D	-2.03	1.46	1.50
15	J	104	BCR	C33-C5	-2.03	1.47	1.50
12	H	2107	CLA	CMC-C2C	-2.03	1.46	1.50
12	a	854	CLA	CMD-C2D	-2.03	1.46	1.50
22	B	2151	EQ3	C28-C27	2.03	1.53	1.50
12	G	823	CLA	CMB-C2B	-2.02	1.46	1.50
12	b	2114	CLA	CMD-C2D	-2.02	1.46	1.50
12	G	850	CLA	MG-ND	-2.02	2.01	2.05
12	H	2127	CLA	MG-NB	-2.02	2.01	2.05
12	G	850	CLA	C3B-C4B	2.02	1.48	1.42
12	b	2129	CLA	C1B-NB	-2.02	1.35	1.37
12	H	2128	CLA	CMC-C2C	-2.02	1.46	1.50
12	A	832	CLA	CMB-C2B	-2.02	1.46	1.50
12	G	805	CLA	MG-NB	-2.02	2.01	2.05
12	a	816	CLA	MG-NB	-2.02	2.01	2.05
12	H	2129	CLA	CMC-C2C	-2.02	1.46	1.50
23	b	2151	ZEX	C39-C29	2.02	1.54	1.50
12	f	204	CLA	CMD-C2D	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	833	CLA	CMD-C2D	-2.02	1.46	1.50
12	H	2129	CLA	C1B-NB	-2.02	1.35	1.37
12	H	2131	CLA	CMD-C2D	-2.02	1.46	1.50
12	a	836	CLA	CMC-C2C	-2.02	1.46	1.50
12	G	818	CLA	CMC-C2C	-2.02	1.46	1.50
12	a	823	CLA	CMD-C2D	-2.02	1.46	1.50
12	b	2131	CLA	CMD-C2D	-2.02	1.46	1.50
12	B	2129	CLA	CMC-C2C	-2.02	1.46	1.50
12	B	2128	CLA	MG-NB	-2.02	2.01	2.05
12	G	822	CLA	MG-NB	-2.02	2.01	2.05
12	U	203	CLA	CMC-C2C	-2.02	1.46	1.50
12	B	2130	CLA	CMC-C2C	-2.02	1.46	1.50
12	B	2106	CLA	CMC-C2C	-2.02	1.46	1.50
15	T	4001	BCR	C33-C5	-2.02	1.47	1.50
12	a	805	CLA	MG-NB	-2.02	2.01	2.05
12	A	830	CLA	CHC-C1C	2.02	1.42	1.38
12	G	802	CLA	CMD-C2D	-2.02	1.46	1.50
12	l	201	CLA	CMD-C2D	-2.02	1.46	1.50
12	A	831	CLA	CMD-C2D	-2.02	1.46	1.50
12	S	102	CLA	CMB-C2B	-2.02	1.46	1.50
12	a	805	CLA	CMB-C2B	-2.02	1.46	1.50
12	T	4002	CLA	MG-NB	-2.02	2.01	2.05
12	a	822	CLA	MG-NB	-2.02	2.01	2.05
12	H	2152	CLA	MG-NB	-2.02	2.01	2.05
12	G	827	CLA	CMC-C2C	-2.02	1.46	1.50
12	l	204	CLA	CMC-C2C	-2.02	1.46	1.50
12	B	2113	CLA	CMD-C2D	-2.02	1.46	1.50
12	B	2102	CLA	MG-ND	-2.02	2.01	2.05
12	a	813	CLA	CMB-C2B	-2.02	1.46	1.50
12	b	2128	CLA	CMC-C2C	-2.02	1.46	1.50
12	H	2131	CLA	MG-NB	-2.01	2.01	2.05
12	K	4002	CLA	CMD-C2D	-2.01	1.46	1.50
12	a	850	CLA	MG-ND	-2.01	2.01	2.05
12	a	832	CLA	CMB-C2B	-2.01	1.46	1.50
12	B	2117	CLA	CMD-C2D	-2.01	1.46	1.50
12	A	815	CLA	MG-NB	-2.01	2.01	2.05
12	B	2132	CLA	CMD-C2D	-2.01	1.46	1.50
12	b	2105	CLA	CMC-C2C	-2.01	1.46	1.50
12	H	2116	CLA	CMD-C2D	-2.01	1.46	1.50
12	a	801	CLA	C3D-C4D	2.01	1.48	1.44
12	H	2112	CLA	CMD-C2D	-2.01	1.46	1.50
12	b	2104	CLA	CMB-C2B	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	810	CLA	MG-NB	-2.01	2.01	2.05
12	B	2101	CLA	CMD-C2D	-2.01	1.46	1.50
12	G	824	CLA	MG-NB	-2.01	2.01	2.05
12	G	831	CLA	CMD-C2D	-2.01	1.46	1.50
12	A	803	CLA	CMD-C2D	-2.01	1.46	1.50
22	H	2150	EQ3	O27-C27	-2.01	1.19	1.23
22	b	2150	EQ3	O27-C27	-2.01	1.19	1.23
12	B	2108	CLA	CMC-C2C	-2.01	1.46	1.50
12	B	2116	CLA	CMC-C2C	-2.01	1.46	1.50
12	G	850	CLA	CHC-C1C	2.01	1.42	1.38
23	H	2151	ZEX	C39-C29	2.01	1.54	1.50
12	G	813	CLA	MG-NB	-2.01	2.01	2.05
12	b	2101	CLA	MG-ND	-2.01	2.01	2.05
12	H	2141	CLA	CMD-C2D	-2.01	1.46	1.50
23	B	2152	ZEX	C39-C29	2.01	1.54	1.50
12	b	2152	CLA	MG-NB	-2.01	2.01	2.05
12	G	835	CLA	CMB-C2B	-2.01	1.46	1.50
26	L	210	LMT	O4'-C4B	-2.01	1.38	1.43
12	b	2129	CLA	CMC-C2C	-2.01	1.46	1.50
12	H	2124	CLA	CMC-C2C	-2.01	1.46	1.50
26	U	210	LMT	O4'-C4B	-2.01	1.38	1.43
12	B	2138	CLA	CMB-C2B	-2.01	1.46	1.50
12	A	822	CLA	MG-NB	-2.01	2.01	2.05
12	G	836	CLA	CMC-C2C	-2.01	1.46	1.50
12	a	851	CLA	CMC-C2C	-2.01	1.46	1.50
12	b	2107	CLA	CMC-C2C	-2.01	1.46	1.50
12	B	2130	CLA	C1B-NB	-2.01	1.35	1.37
12	b	2112	CLA	CMD-C2D	-2.01	1.46	1.50
12	J	102	CLA	CMD-C2D	-2.01	1.46	1.50
12	H	2101	CLA	MG-ND	-2.01	2.01	2.05
12	H	2112	CLA	MG-NB	-2.01	2.01	2.05
12	a	830	CLA	CHC-C1C	2.01	1.42	1.38
12	B	2142	CLA	CMD-C2D	-2.00	1.46	1.50
12	a	850	CLA	C3B-C4B	2.00	1.48	1.42
12	b	2133	CLA	CMC-C2C	-2.00	1.46	1.50
12	a	803	CLA	CMD-C2D	-2.00	1.46	1.50
12	b	2116	CLA	CMD-C2D	-2.00	1.46	1.50
12	B	2123	CLA	CMB-C2B	-2.00	1.46	1.50
26	l	210	LMT	O4'-C4B	-2.00	1.38	1.43
12	b	2152	CLA	CMD-C2D	-2.00	1.46	1.50
12	T	4002	CLA	CMD-C2D	-2.00	1.46	1.50
12	b	2131	CLA	CMC-C2C	-2.00	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	831	CLA	CMD-C2D	-2.00	1.46	1.50
12	j	102	CLA	CMD-C2D	-2.00	1.46	1.50
12	a	824	CLA	MG-NB	-2.00	2.01	2.05
12	b	2136	CLA	CMC-C2C	-2.00	1.46	1.50

All (2630) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Q	205	ZEX	C39-C29-C28	-32.45	68.51	118.09
23	F	205	ZEX	C39-C29-C28	-32.45	68.52	118.09
23	f	205	ZEX	C39-C29-C28	-32.44	68.54	118.09
23	b	2151	ZEX	C39-C29-C28	-32.08	69.09	118.09
23	B	2152	ZEX	C39-C29-C28	-32.07	69.10	118.09
23	H	2151	ZEX	C39-C29-C28	-32.06	69.11	118.09
23	f	205	ZEX	C32-C33-C34	30.42	166.86	119.01
23	Q	205	ZEX	C32-C33-C34	30.41	166.84	119.01
23	F	205	ZEX	C32-C33-C34	30.40	166.83	119.01
23	B	2152	ZEX	C32-C33-C34	30.14	166.42	119.01
23	b	2151	ZEX	C32-C33-C34	30.14	166.41	119.01
23	H	2151	ZEX	C32-C33-C34	30.14	166.41	119.01
23	F	205	ZEX	C40-C33-C32	-23.23	82.60	118.09
23	f	205	ZEX	C40-C33-C32	-23.22	82.62	118.09
23	Q	205	ZEX	C40-C33-C32	-23.22	82.62	118.09
23	b	2151	ZEX	C40-C33-C32	-22.54	83.65	118.09
23	B	2152	ZEX	C40-C33-C32	-22.54	83.66	118.09
23	H	2151	ZEX	C40-C33-C32	-22.52	83.69	118.09
23	F	205	ZEX	C39-C29-C30	20.76	156.46	122.82
23	f	205	ZEX	C39-C29-C30	20.75	156.43	122.82
23	Q	205	ZEX	C39-C29-C30	20.74	156.41	122.82
23	H	2151	ZEX	C39-C29-C30	20.59	156.17	122.82
23	b	2151	ZEX	C39-C29-C30	20.57	156.13	122.82
23	B	2152	ZEX	C39-C29-C30	20.56	156.12	122.82
23	B	2152	ZEX	C28-C29-C30	-20.33	87.03	119.01
23	b	2151	ZEX	C28-C29-C30	-20.32	87.05	119.01
23	H	2151	ZEX	C28-C29-C30	-20.31	87.06	119.01
23	f	205	ZEX	C28-C29-C30	-19.77	87.92	119.01
23	Q	205	ZEX	C28-C29-C30	-19.76	87.93	119.01
23	F	205	ZEX	C28-C29-C30	-19.74	87.97	119.01
23	b	2151	ZEX	C15-C35-C34	-17.62	87.47	123.52
23	B	2152	ZEX	C15-C35-C34	-17.62	87.47	123.52
23	H	2151	ZEX	C15-C35-C34	-17.61	87.48	123.52
23	f	205	ZEX	C15-C35-C34	-17.43	87.85	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	F	205	ZEX	C15-C35-C34	-17.43	87.86	123.52
23	Q	205	ZEX	C15-C35-C34	-17.41	87.89	123.52
23	Q	205	ZEX	C7-C8-C9	16.21	150.21	126.23
23	f	205	ZEX	C7-C8-C9	16.19	150.19	126.23
23	F	205	ZEX	C7-C8-C9	16.19	150.18	126.23
23	Q	205	ZEX	C19-C9-C8	-15.93	93.75	118.09
23	f	205	ZEX	C19-C9-C8	-15.92	93.78	118.09
23	F	205	ZEX	C19-C9-C8	-15.90	93.79	118.09
23	f	205	ZEX	C20-C13-C12	-15.86	93.86	118.09
23	F	205	ZEX	C20-C13-C12	-15.84	93.89	118.09
23	Q	205	ZEX	C20-C13-C12	-15.84	93.89	118.09
23	H	2151	ZEX	C19-C9-C8	-15.51	94.39	118.09
23	B	2152	ZEX	C19-C9-C8	-15.50	94.40	118.09
23	b	2151	ZEX	C19-C9-C8	-15.48	94.45	118.09
23	B	2152	ZEX	C20-C13-C12	-15.17	94.91	118.09
23	b	2151	ZEX	C20-C13-C12	-15.16	94.93	118.09
23	H	2151	ZEX	C20-C13-C12	-15.15	94.95	118.09
23	B	2152	ZEX	C7-C8-C9	15.01	148.43	126.23
23	H	2151	ZEX	C7-C8-C9	14.98	148.40	126.23
23	b	2151	ZEX	C7-C8-C9	14.97	148.38	126.23
22	H	2150	EQ3	C11-C12-C13	-14.38	86.95	126.36
22	B	2151	EQ3	C11-C12-C13	-14.37	86.95	126.36
22	b	2150	EQ3	C11-C12-C13	-14.37	86.96	126.36
22	B	2151	EQ3	C35-C13-C12	-14.03	96.65	118.09
22	b	2150	EQ3	C35-C13-C12	-14.01	96.69	118.09
22	H	2150	EQ3	C35-C13-C12	-14.00	96.71	118.09
22	b	2150	EQ3	C21-C20-C19	-13.69	83.52	123.20
22	B	2151	EQ3	C21-C20-C19	-13.69	83.54	123.20
22	H	2150	EQ3	C21-C20-C19	-13.69	83.55	123.20
23	Q	205	ZEX	C11-C10-C9	-13.25	108.70	127.28
23	f	205	ZEX	C11-C10-C9	-13.24	108.71	127.28
23	F	205	ZEX	C11-C10-C9	-13.22	108.74	127.28
23	b	2151	ZEX	C11-C10-C9	-12.35	109.96	127.28
23	B	2152	ZEX	C11-C10-C9	-12.33	109.98	127.28
23	H	2151	ZEX	C11-C10-C9	-12.33	109.99	127.28
22	H	2150	EQ3	C15-C16-C17	12.28	148.65	123.52
22	B	2151	EQ3	C15-C16-C17	12.28	148.64	123.52
22	b	2150	EQ3	C15-C16-C17	12.28	148.64	123.52
22	H	2150	EQ3	C34-C9-C8	-12.03	99.72	118.09
22	B	2151	EQ3	C34-C9-C8	-12.00	99.76	118.09
22	b	2150	EQ3	C34-C9-C8	-11.98	99.79	118.09
22	b	2150	EQ3	C15-C14-C13	-11.52	111.12	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	2151	EQ3	C15-C14-C13	-11.52	111.13	127.28
22	H	2150	EQ3	C15-C14-C13	-11.49	111.17	127.28
23	B	2152	ZEX	C15-C14-C13	-11.33	111.39	127.28
23	H	2151	ZEX	C15-C14-C13	-11.32	111.40	127.28
23	b	2151	ZEX	C15-C14-C13	-11.31	111.42	127.28
23	Q	205	ZEX	C30-C31-C32	-11.27	90.54	123.20
23	F	205	ZEX	C30-C31-C32	-11.26	90.56	123.20
23	f	205	ZEX	C30-C31-C32	-11.26	90.57	123.20
23	b	2151	ZEX	C30-C31-C32	-11.01	91.31	123.20
23	B	2152	ZEX	C30-C31-C32	-11.00	91.32	123.20
23	H	2151	ZEX	C30-C31-C32	-10.99	91.35	123.20
23	Q	205	ZEX	C12-C13-C14	10.69	135.83	119.01
23	f	205	ZEX	C12-C13-C14	10.68	135.81	119.01
23	F	205	ZEX	C12-C13-C14	10.66	135.78	119.01
23	f	205	ZEX	C21-C26-C25	-10.36	114.83	122.84
23	F	205	ZEX	C21-C26-C25	-10.36	114.83	122.84
23	Q	205	ZEX	C21-C26-C25	-10.32	114.86	122.84
23	B	2152	ZEX	C31-C30-C29	-10.32	112.81	127.28
23	b	2151	ZEX	C31-C30-C29	-10.31	112.82	127.28
23	H	2151	ZEX	C31-C30-C29	-10.29	112.85	127.28
23	Q	205	ZEX	C31-C30-C29	-10.24	112.91	127.28
23	f	205	ZEX	C31-C30-C29	-10.23	112.93	127.28
23	F	205	ZEX	C31-C30-C29	-10.22	112.94	127.28
22	H	2150	EQ3	C8-C9-C10	10.06	134.84	119.01
22	B	2151	EQ3	C8-C9-C10	10.03	134.78	119.01
22	b	2150	EQ3	C8-C9-C10	10.01	134.76	119.01
23	f	205	ZEX	C8-C9-C10	9.80	134.42	119.01
23	F	205	ZEX	C8-C9-C10	9.79	134.42	119.01
23	Q	205	ZEX	C8-C9-C10	9.79	134.41	119.01
23	B	2152	ZEX	C8-C9-C10	9.52	133.99	119.01
23	H	2151	ZEX	C8-C9-C10	9.51	133.96	119.01
23	b	2151	ZEX	C8-C9-C10	9.49	133.94	119.01
23	b	2151	ZEX	C12-C13-C14	8.97	133.12	119.01
23	B	2152	ZEX	C12-C13-C14	8.95	133.09	119.01
23	H	2151	ZEX	C12-C13-C14	8.95	133.08	119.01
23	B	2152	ZEX	C21-C26-C25	-8.94	115.93	122.84
23	b	2151	ZEX	C21-C26-C25	-8.92	115.95	122.84
23	B	2152	ZEX	C11-C12-C13	8.92	150.82	126.36
23	H	2151	ZEX	C11-C12-C13	8.91	150.80	126.36
23	b	2151	ZEX	C11-C12-C13	8.91	150.79	126.36
23	H	2151	ZEX	C21-C26-C25	-8.89	115.97	122.84
12	b	2109	CLA	C4A-NA-C1A	8.37	110.50	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	a	829	CLA	C4A-NA-C1A	8.32	110.47	106.68
12	H	2109	CLA	C4A-NA-C1A	8.30	110.47	106.68
12	B	2110	CLA	C4A-NA-C1A	8.30	110.47	106.68
12	G	829	CLA	C4A-NA-C1A	8.23	110.43	106.68
12	A	829	CLA	C4A-NA-C1A	8.21	110.42	106.68
23	F	205	ZEX	C15-C14-C13	-8.16	115.83	127.28
23	f	205	ZEX	C15-C14-C13	-8.16	115.83	127.28
23	Q	205	ZEX	C15-C14-C13	-8.16	115.84	127.28
22	B	2151	EQ3	C12-C13-C14	8.09	131.73	119.01
22	H	2150	EQ3	C12-C13-C14	8.09	131.73	119.01
22	b	2150	EQ3	C12-C13-C14	8.06	131.68	119.01
12	H	2104	CLA	C4A-NA-C1A	8.06	110.35	106.68
22	H	2150	EQ3	C23-C24-C25	8.03	148.44	127.00
22	B	2151	EQ3	C23-C24-C25	8.01	148.41	127.00
23	H	2151	ZEX	C40-C33-C34	-8.01	109.84	122.82
12	B	2105	CLA	C4A-NA-C1A	8.01	110.33	106.68
22	b	2150	EQ3	C23-C24-C25	8.01	148.38	127.00
23	B	2152	ZEX	C40-C33-C34	-8.00	109.86	122.82
23	b	2151	ZEX	C40-C33-C34	-7.99	109.88	122.82
12	b	2104	CLA	C4A-NA-C1A	7.98	110.32	106.68
23	f	205	ZEX	C11-C12-C13	7.97	148.22	126.36
12	b	2140	CLA	C4A-NA-C1A	7.97	110.31	106.68
23	Q	205	ZEX	C11-C12-C13	7.96	148.19	126.36
23	F	205	ZEX	C11-C12-C13	7.96	148.18	126.36
12	B	2141	CLA	C4A-NA-C1A	7.92	110.29	106.68
12	G	804	CLA	C4A-NA-C1A	7.85	110.26	106.68
12	a	816	CLA	C4A-NA-C1A	7.84	110.25	106.68
12	H	2140	CLA	C4A-NA-C1A	7.84	110.25	106.68
12	A	804	CLA	C4A-NA-C1A	7.81	110.24	106.68
12	G	816	CLA	C4A-NA-C1A	7.79	110.23	106.68
12	A	816	CLA	C4A-NA-C1A	7.78	110.23	106.68
12	a	804	CLA	C4A-NA-C1A	7.76	110.22	106.68
23	b	2151	ZEX	C18-C5-C6	-7.68	116.10	124.48
23	H	2151	ZEX	C18-C5-C6	-7.68	116.10	124.48
23	B	2152	ZEX	C18-C5-C6	-7.68	116.11	124.48
12	U	204	CLA	C4A-NA-C1A	7.64	110.16	106.68
12	b	2108	CLA	C4A-NA-C1A	7.63	110.16	106.68
12	B	2101	CLA	C4A-NA-C1A	7.60	110.15	106.68
12	H	2111	CLA	C4A-NA-C1A	7.60	110.15	106.68
12	b	2111	CLA	C4A-NA-C1A	7.59	110.14	106.68
12	H	2152	CLA	C4A-NA-C1A	7.59	110.14	106.68
23	f	205	ZEX	C40-C33-C34	-7.59	110.52	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	b	2152	CLA	C4A-NA-C1A	7.58	110.14	106.68
23	Q	205	ZEX	C40-C33-C34	-7.58	110.53	122.82
12	G	823	CLA	C4A-NA-C1A	7.58	110.14	106.68
12	B	2109	CLA	C4A-NA-C1A	7.57	110.13	106.68
12	a	823	CLA	C4A-NA-C1A	7.57	110.13	106.68
12	a	838	CLA	C4A-NA-C1A	7.57	110.13	106.68
12	A	823	CLA	C4A-NA-C1A	7.56	110.13	106.68
23	F	205	ZEX	C40-C33-C34	-7.56	110.57	122.82
12	L	204	CLA	C4A-NA-C1A	7.55	110.12	106.68
12	l	204	CLA	C4A-NA-C1A	7.53	110.11	106.68
12	B	2112	CLA	C4A-NA-C1A	7.53	110.11	106.68
12	b	2103	CLA	C4A-NA-C1A	7.52	110.11	106.68
12	H	2108	CLA	C4A-NA-C1A	7.51	110.11	106.68
12	A	806	CLA	C4A-NA-C1A	7.51	110.10	106.68
12	H	2102	CLA	C4A-NA-C1A	7.50	110.10	106.68
12	a	806	CLA	C4A-NA-C1A	7.50	110.10	106.68
12	B	2104	CLA	C4A-NA-C1A	7.50	110.10	106.68
12	A	838	CLA	C4A-NA-C1A	7.48	110.09	106.68
12	H	2103	CLA	C4A-NA-C1A	7.47	110.09	106.68
12	B	2103	CLA	C4A-NA-C1A	7.47	110.09	106.68
12	G	838	CLA	C4A-NA-C1A	7.46	110.08	106.68
12	G	806	CLA	C4A-NA-C1A	7.45	110.08	106.68
12	b	2102	CLA	C4A-NA-C1A	7.44	110.07	106.68
12	a	805	CLA	C4A-NA-C1A	7.42	110.06	106.68
12	U	203	CLA	C4A-NA-C1A	7.41	110.06	106.68
12	H	2117	CLA	C4A-NA-C1A	7.38	110.05	106.68
12	A	805	CLA	C4A-NA-C1A	7.36	110.04	106.68
12	L	203	CLA	C4A-NA-C1A	7.36	110.04	106.68
12	G	805	CLA	C4A-NA-C1A	7.34	110.03	106.68
12	A	819	CLA	C4A-NA-C1A	7.32	110.02	106.68
12	G	814	CLA	C4A-NA-C1A	7.32	110.02	106.68
12	H	2120	CLA	C4A-NA-C1A	7.32	110.02	106.68
12	b	2133	CLA	C4A-NA-C1A	7.32	110.02	106.68
12	b	2120	CLA	C4A-NA-C1A	7.31	110.02	106.68
12	B	2121	CLA	C4A-NA-C1A	7.31	110.02	106.68
12	B	2134	CLA	C4A-NA-C1A	7.31	110.02	106.68
12	B	2118	CLA	C4A-NA-C1A	7.30	110.01	106.68
12	a	819	CLA	C4A-NA-C1A	7.30	110.01	106.68
12	A	814	CLA	C4A-NA-C1A	7.30	110.01	106.68
12	G	824	CLA	C4A-NA-C1A	7.27	110.00	106.68
12	l	203	CLA	C4A-NA-C1A	7.26	109.99	106.68
12	H	2133	CLA	C4A-NA-C1A	7.26	109.99	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	a	814	CLA	C4A-NA-C1A	7.26	109.99	106.68
12	a	807	CLA	C4A-NA-C1A	7.24	109.98	106.68
12	G	819	CLA	C4A-NA-C1A	7.23	109.98	106.68
12	A	824	CLA	C4A-NA-C1A	7.22	109.97	106.68
12	b	2117	CLA	C4A-NA-C1A	7.22	109.97	106.68
12	G	837	CLA	C4A-NA-C1A	7.19	109.96	106.68
12	b	2115	CLA	C4A-NA-C1A	7.18	109.95	106.68
12	A	837	CLA	C4A-NA-C1A	7.15	109.94	106.68
12	J	102	CLA	C4A-NA-C1A	7.15	109.94	106.68
12	H	2115	CLA	C4A-NA-C1A	7.15	109.94	106.68
12	a	824	CLA	C4A-NA-C1A	7.14	109.94	106.68
12	B	2116	CLA	C4A-NA-C1A	7.13	109.93	106.68
12	B	2119	CLA	C4A-NA-C1A	7.13	109.93	106.68
12	b	2132	CLA	C4A-NA-C1A	7.12	109.93	106.68
12	a	810	CLA	C4A-NA-C1A	7.11	109.92	106.68
12	A	807	CLA	C4A-NA-C1A	7.11	109.92	106.68
12	H	2118	CLA	C4A-NA-C1A	7.11	109.92	106.68
12	b	2123	CLA	C4A-NA-C1A	7.11	109.92	106.68
12	A	834	CLA	C4A-NA-C1A	7.10	109.92	106.68
12	b	2134	CLA	C4A-NA-C1A	7.10	109.92	106.68
12	G	807	CLA	C4A-NA-C1A	7.10	109.92	106.68
12	H	2132	CLA	C4A-NA-C1A	7.10	109.92	106.68
12	B	2135	CLA	C4A-NA-C1A	7.10	109.92	106.68
12	B	2133	CLA	C4A-NA-C1A	7.09	109.92	106.68
12	B	2124	CLA	C4A-NA-C1A	7.09	109.91	106.68
12	a	834	CLA	C4A-NA-C1A	7.08	109.91	106.68
12	A	810	CLA	C4A-NA-C1A	7.08	109.91	106.68
12	j	102	CLA	C4A-NA-C1A	7.08	109.91	106.68
12	S	102	CLA	C4A-NA-C1A	7.07	109.91	106.68
12	B	2107	CLA	C4A-NA-C1A	7.07	109.90	106.68
13	B	2153	A1AGD	C2-C1-C6	7.07	127.39	119.00
12	a	837	CLA	C4A-NA-C1A	7.06	109.90	106.68
13	H	2153	A1AGD	C2-C1-C6	7.06	127.39	119.00
12	G	810	CLA	C4A-NA-C1A	7.06	109.90	106.68
13	b	2153	A1AGD	C2-C1-C6	7.05	127.37	119.00
12	G	834	CLA	C4A-NA-C1A	7.04	109.89	106.68
12	H	2116	CLA	C4A-NA-C1A	7.03	109.89	106.68
12	k	4002	CLA	C4A-NA-C1A	7.03	109.89	106.68
12	H	2123	CLA	C4A-NA-C1A	7.03	109.89	106.68
12	H	2134	CLA	C4A-NA-C1A	7.02	109.88	106.68
12	b	2106	CLA	C4A-NA-C1A	7.00	109.87	106.68
12	b	2118	CLA	C4A-NA-C1A	7.00	109.87	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	b	2116	CLA	C4A-NA-C1A	6.99	109.87	106.68
12	H	2106	CLA	C4A-NA-C1A	6.98	109.86	106.68
12	B	2125	CLA	C4A-NA-C1A	6.98	109.86	106.68
12	B	2117	CLA	C4A-NA-C1A	6.97	109.86	106.68
12	K	4002	CLA	C4A-NA-C1A	6.97	109.86	106.68
23	f	205	ZEX	C35-C15-C14	-6.94	109.31	123.52
12	T	4002	CLA	C4A-NA-C1A	6.94	109.84	106.68
12	b	2124	CLA	C4A-NA-C1A	6.94	109.84	106.68
23	F	205	ZEX	C35-C15-C14	-6.94	109.32	123.52
23	Q	205	ZEX	C35-C15-C14	-6.93	109.35	123.52
12	G	808	CLA	C4A-NA-C1A	6.92	109.84	106.68
12	A	808	CLA	C4A-NA-C1A	6.92	109.84	106.68
12	b	2138	CLA	C4A-NA-C1A	6.92	109.83	106.68
12	B	2106	CLA	C4A-NA-C1A	6.92	109.83	106.68
12	B	2142	CLA	C4A-NA-C1A	6.91	109.83	106.68
12	H	2138	CLA	C4A-NA-C1A	6.91	109.83	106.68
12	B	2139	CLA	C4A-NA-C1A	6.91	109.83	106.68
12	H	2124	CLA	C4A-NA-C1A	6.91	109.83	106.68
12	H	2105	CLA	C4A-NA-C1A	6.90	109.83	106.68
12	A	833	CLA	C4A-NA-C1A	6.90	109.83	106.68
12	G	833	CLA	C4A-NA-C1A	6.90	109.83	106.68
12	a	808	CLA	C4A-NA-C1A	6.90	109.83	106.68
12	H	2127	CLA	C4A-NA-C1A	6.89	109.82	106.68
12	b	2141	CLA	C4A-NA-C1A	6.88	109.82	106.68
12	a	831	CLA	C4A-NA-C1A	6.88	109.82	106.68
12	a	833	CLA	C4A-NA-C1A	6.87	109.81	106.68
12	B	2128	CLA	C4A-NA-C1A	6.87	109.81	106.68
12	b	2105	CLA	C4A-NA-C1A	6.87	109.81	106.68
12	A	803	CLA	C4A-NA-C1A	6.86	109.81	106.68
12	a	827	CLA	C4A-NA-C1A	6.86	109.81	106.68
12	A	831	CLA	C4A-NA-C1A	6.85	109.80	106.68
12	B	2127	CLA	C4A-NA-C1A	6.84	109.80	106.68
12	G	803	CLA	C4A-NA-C1A	6.83	109.79	106.68
12	H	2126	CLA	C4A-NA-C1A	6.82	109.79	106.68
12	A	827	CLA	C4A-NA-C1A	6.82	109.79	106.68
12	a	803	CLA	C4A-NA-C1A	6.81	109.79	106.68
12	b	2127	CLA	C4A-NA-C1A	6.81	109.78	106.68
12	G	827	CLA	C4A-NA-C1A	6.80	109.78	106.68
12	a	851	CLA	C4A-NA-C1A	6.80	109.78	106.68
12	H	2141	CLA	C4A-NA-C1A	6.80	109.78	106.68
12	A	851	CLA	C4A-NA-C1A	6.80	109.78	106.68
12	a	820	CLA	C4A-NA-C1A	6.79	109.78	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	b	2126	CLA	C4A-NA-C1A	6.78	109.77	106.68
12	G	815	CLA	C4A-NA-C1A	6.78	109.77	106.68
12	A	820	CLA	C4A-NA-C1A	6.76	109.77	106.68
12	b	2107	CLA	C4A-NA-C1A	6.76	109.76	106.68
12	H	2107	CLA	C4A-NA-C1A	6.75	109.76	106.68
12	G	851	CLA	C4A-NA-C1A	6.75	109.76	106.68
12	a	815	CLA	C4A-NA-C1A	6.75	109.76	106.68
12	b	2129	CLA	C4A-NA-C1A	6.74	109.75	106.68
12	B	2108	CLA	C4A-NA-C1A	6.74	109.75	106.68
12	A	815	CLA	C4A-NA-C1A	6.73	109.75	106.68
12	G	831	CLA	C4A-NA-C1A	6.72	109.75	106.68
12	a	809	CLA	C4A-NA-C1A	6.72	109.75	106.68
13	H	2153	A1AGD	C13-C12-C11	-6.71	95.37	113.26
12	A	809	CLA	C4A-NA-C1A	6.71	109.74	106.68
12	B	2132	CLA	C4A-NA-C1A	6.71	109.74	106.68
13	b	2153	A1AGD	C13-C12-C11	-6.71	95.38	113.26
12	H	2131	CLA	C4A-NA-C1A	6.71	109.74	106.68
13	B	2153	A1AGD	C13-C12-C11	-6.71	95.39	113.26
12	b	2137	CLA	C4A-NA-C1A	6.70	109.74	106.68
12	B	2130	CLA	C4A-NA-C1A	6.70	109.73	106.68
12	G	809	CLA	C4A-NA-C1A	6.69	109.73	106.68
12	b	2112	CLA	C4A-NA-C1A	6.69	109.73	106.68
12	G	820	CLA	C4A-NA-C1A	6.69	109.73	106.68
12	G	818	CLA	C4A-NA-C1A	6.67	109.72	106.68
12	B	2138	CLA	C4A-NA-C1A	6.67	109.72	106.68
12	a	801	CLA	C4A-NA-C1A	6.67	109.72	106.68
12	A	801	CLA	C4A-NA-C1A	6.65	109.71	106.68
12	B	2113	CLA	C4A-NA-C1A	6.65	109.71	106.68
12	G	811	CLA	C4A-NA-C1A	6.64	109.71	106.68
12	S	103	CLA	C4A-NA-C1A	6.64	109.71	106.68
12	H	2129	CLA	C4A-NA-C1A	6.63	109.71	106.68
12	A	811	CLA	C4A-NA-C1A	6.63	109.71	106.68
12	H	2137	CLA	C4A-NA-C1A	6.63	109.70	106.68
12	b	2131	CLA	C4A-NA-C1A	6.63	109.70	106.68
12	A	812	CLA	C4A-NA-C1A	6.63	109.70	106.68
12	B	2114	CLA	C4A-NA-C1A	6.63	109.70	106.68
12	A	821	CLA	C4A-NA-C1A	6.62	109.70	106.68
12	G	812	CLA	C4A-NA-C1A	6.62	109.70	106.68
12	a	818	CLA	C4A-NA-C1A	6.62	109.70	106.68
12	b	2113	CLA	C4A-NA-C1A	6.62	109.70	106.68
12	j	103	CLA	C4A-NA-C1A	6.61	109.70	106.68
12	a	813	CLA	C4A-NA-C1A	6.61	109.69	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	a	821	CLA	C4A-NA-C1A	6.61	109.69	106.68
12	H	2125	CLA	C4A-NA-C1A	6.61	109.69	106.68
12	H	2113	CLA	C4A-NA-C1A	6.61	109.69	106.68
12	f	204	CLA	C4A-NA-C1A	6.61	109.69	106.68
12	F	204	CLA	C4A-NA-C1A	6.60	109.69	106.68
12	a	811	CLA	C4A-NA-C1A	6.60	109.69	106.68
12	a	812	CLA	C4A-NA-C1A	6.60	109.69	106.68
12	G	801	CLA	C4A-NA-C1A	6.58	109.68	106.68
12	H	2139	CLA	C4A-NA-C1A	6.58	109.68	106.68
12	b	2125	CLA	C4A-NA-C1A	6.58	109.68	106.68
12	J	103	CLA	C4A-NA-C1A	6.58	109.68	106.68
12	G	821	CLA	C4A-NA-C1A	6.58	109.68	106.68
12	H	2112	CLA	C4A-NA-C1A	6.58	109.68	106.68
12	G	813	CLA	C4A-NA-C1A	6.57	109.68	106.68
12	b	2139	CLA	C4A-NA-C1A	6.57	109.68	106.68
12	B	2140	CLA	C4A-NA-C1A	6.57	109.67	106.68
12	A	818	CLA	C4A-NA-C1A	6.56	109.67	106.68
12	A	813	CLA	C4A-NA-C1A	6.56	109.67	106.68
12	Q	204	CLA	C4A-NA-C1A	6.55	109.67	106.68
12	B	2126	CLA	C4A-NA-C1A	6.53	109.66	106.68
12	f	201	CLA	C4A-NA-C1A	6.51	109.65	106.68
12	F	201	CLA	C4A-NA-C1A	6.50	109.65	106.68
12	B	2115	CLA	C4A-NA-C1A	6.47	109.63	106.68
12	B	2131	CLA	C4A-NA-C1A	6.46	109.63	106.68
12	G	822	CLA	C4A-NA-C1A	6.44	109.62	106.68
12	b	2114	CLA	C4A-NA-C1A	6.44	109.62	106.68
12	b	2130	CLA	C4A-NA-C1A	6.44	109.62	106.68
12	H	2130	CLA	C4A-NA-C1A	6.43	109.61	106.68
12	Q	201	CLA	C4A-NA-C1A	6.42	109.61	106.68
12	H	2121	CLA	C4A-NA-C1A	6.39	109.59	106.68
12	a	836	CLA	C4A-NA-C1A	6.39	109.59	106.68
22	B	2151	EQ3	C24-C23-C22	-6.37	116.81	126.23
12	H	2114	CLA	C4A-NA-C1A	6.37	109.59	106.68
12	A	802	CLA	C4A-NA-C1A	6.37	109.58	106.68
22	b	2150	EQ3	C24-C23-C22	-6.36	116.82	126.23
12	A	822	CLA	C4A-NA-C1A	6.36	109.58	106.68
22	H	2150	EQ3	C24-C23-C22	-6.35	116.84	126.23
12	a	822	CLA	C4A-NA-C1A	6.35	109.58	106.68
12	b	2121	CLA	C4A-NA-C1A	6.35	109.57	106.68
12	A	836	CLA	C4A-NA-C1A	6.34	109.57	106.68
12	B	2122	CLA	C4A-NA-C1A	6.33	109.57	106.68
12	a	854	CLA	C4A-NA-C1A	6.32	109.56	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	G	836	CLA	C4A-NA-C1A	6.31	109.56	106.68
12	I	201	CLA	C4A-NA-C1A	6.30	109.56	106.68
12	A	854	CLA	C4A-NA-C1A	6.28	109.55	106.68
12	A	839	CLA	C4A-NA-C1A	6.28	109.54	106.68
12	G	854	CLA	C4A-NA-C1A	6.28	109.54	106.68
12	G	802	CLA	C4A-NA-C1A	6.27	109.54	106.68
12	U	201	CLA	C4A-NA-C1A	6.27	109.54	106.68
12	a	802	CLA	C4A-NA-C1A	6.27	109.54	106.68
12	b	2136	CLA	C4A-NA-C1A	6.26	109.53	106.68
12	G	839	CLA	C4A-NA-C1A	6.25	109.53	106.68
12	G	835	CLA	C4A-NA-C1A	6.25	109.53	106.68
12	B	2137	CLA	C4A-NA-C1A	6.25	109.53	106.68
12	L	201	CLA	C4A-NA-C1A	6.22	109.52	106.68
12	B	2136	CLA	C4A-NA-C1A	6.21	109.51	106.68
12	b	2135	CLA	C4A-NA-C1A	6.21	109.51	106.68
12	a	839	CLA	C4A-NA-C1A	6.21	109.51	106.68
12	A	835	CLA	C4A-NA-C1A	6.20	109.51	106.68
12	a	835	CLA	C4A-NA-C1A	6.19	109.50	106.68
12	H	2136	CLA	C4A-NA-C1A	6.15	109.49	106.68
12	H	2135	CLA	C4A-NA-C1A	6.15	109.48	106.68
12	G	832	CLA	C4A-NA-C1A	6.14	109.48	106.68
12	A	832	CLA	C4A-NA-C1A	6.12	109.47	106.68
12	b	2128	CLA	C4A-NA-C1A	6.12	109.47	106.68
12	b	2110	CLA	C4A-NA-C1A	6.11	109.47	106.68
12	b	2119	CLA	C4A-NA-C1A	6.10	109.46	106.68
13	H	2153	A1AGD	C7-C8-C9	-6.09	116.34	126.83
12	B	2129	CLA	C4A-NA-C1A	6.09	109.46	106.68
13	B	2153	A1AGD	C7-C8-C9	-6.08	116.35	126.83
13	b	2153	A1AGD	C7-C8-C9	-6.05	116.41	126.83
12	H	2110	CLA	C4A-NA-C1A	6.04	109.44	106.68
12	L	205	CLA	C4A-NA-C1A	6.03	109.43	106.68
12	I	205	CLA	C4A-NA-C1A	6.03	109.43	106.68
12	A	817	CLA	C4A-NA-C1A	6.03	109.43	106.68
12	B	2111	CLA	C4A-NA-C1A	6.03	109.43	106.68
12	B	2120	CLA	C4A-NA-C1A	6.02	109.42	106.68
12	G	817	CLA	C4A-NA-C1A	6.01	109.42	106.68
12	H	2119	CLA	C4A-NA-C1A	6.00	109.42	106.68
12	a	826	CLA	C4A-NA-C1A	6.00	109.42	106.68
12	b	2122	CLA	C4A-NA-C1A	6.00	109.42	106.68
12	G	825	CLA	C4A-NA-C1A	6.00	109.42	106.68
12	H	2128	CLA	C4A-NA-C1A	5.99	109.41	106.68
12	a	832	CLA	C4A-NA-C1A	5.99	109.41	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	2153	A1AGD	C3-C2-C1	-5.99	112.50	122.59
13	B	2153	A1AGD	C3-C2-C1	-5.98	112.51	122.59
13	H	2153	A1AGD	C3-C2-C1	-5.97	112.53	122.59
12	B	2123	CLA	C4A-NA-C1A	5.97	109.40	106.68
12	A	825	CLA	C4A-NA-C1A	5.95	109.39	106.68
12	H	2122	CLA	C4A-NA-C1A	5.94	109.39	106.68
12	A	826	CLA	C4A-NA-C1A	5.94	109.39	106.68
12	U	205	CLA	C4A-NA-C1A	5.94	109.39	106.68
12	G	826	CLA	C4A-NA-C1A	5.93	109.39	106.68
12	a	817	CLA	C4A-NA-C1A	5.93	109.39	106.68
12	a	825	CLA	C4A-NA-C1A	5.91	109.38	106.68
23	b	2151	ZEX	C31-C32-C33	-5.87	110.26	126.36
23	B	2152	ZEX	C31-C32-C33	-5.87	110.27	126.36
23	H	2151	ZEX	C31-C32-C33	-5.85	110.32	126.36
12	G	850	CLA	C4A-NA-C1A	5.84	109.34	106.68
23	H	2151	ZEX	C35-C15-C14	-5.84	111.58	123.52
23	B	2152	ZEX	C35-C15-C14	-5.82	111.61	123.52
23	b	2151	ZEX	C35-C15-C14	-5.82	111.61	123.52
12	a	830	CLA	C4A-NA-C1A	5.81	109.33	106.68
12	G	830	CLA	C4A-NA-C1A	5.79	109.32	106.68
12	A	830	CLA	C4A-NA-C1A	5.77	109.31	106.68
12	a	850	CLA	C4A-NA-C1A	5.75	109.30	106.68
12	A	850	CLA	C4A-NA-C1A	5.74	109.30	106.68
12	F	203	CLA	C4A-NA-C1A	5.68	109.27	106.68
12	f	203	CLA	C4A-NA-C1A	5.68	109.27	106.68
23	B	2152	ZEX	C20-C13-C14	5.67	131.99	122.82
23	H	2151	ZEX	C20-C13-C14	5.65	131.97	122.82
12	H	2101	CLA	C4A-NA-C1A	5.64	109.25	106.68
23	b	2151	ZEX	C20-C13-C14	5.63	131.94	122.82
12	Q	203	CLA	C4A-NA-C1A	5.62	109.24	106.68
12	b	2101	CLA	C4A-NA-C1A	5.62	109.24	106.68
12	B	2102	CLA	C4A-NA-C1A	5.62	109.24	106.68
23	Q	205	ZEX	C19-C9-C10	5.57	131.84	122.82
23	f	205	ZEX	C19-C9-C10	5.55	131.81	122.82
23	F	205	ZEX	C19-C9-C10	5.54	131.79	122.82
13	G	840	A1AGD	C7-C3-C4	5.52	121.46	116.91
13	A	840	A1AGD	C7-C3-C4	5.50	121.44	116.91
13	a	840	A1AGD	C7-C3-C4	5.48	121.43	116.91
12	a	828	CLA	C4A-NA-C1A	5.47	109.17	106.68
23	H	2151	ZEX	C19-C9-C10	5.45	131.64	122.82
23	Q	205	ZEX	C31-C32-C33	-5.44	111.44	126.36
12	A	828	CLA	C4A-NA-C1A	5.44	109.16	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	F	205	ZEX	C31-C32-C33	-5.44	111.45	126.36
22	b	2150	EQ3	C35-C13-C14	5.43	131.62	122.82
23	b	2151	ZEX	C19-C9-C10	5.43	131.62	122.82
23	f	205	ZEX	C31-C32-C33	-5.43	111.47	126.36
22	B	2151	EQ3	C35-C13-C14	5.43	131.61	122.82
23	B	2152	ZEX	C19-C9-C10	5.43	131.61	122.82
22	H	2150	EQ3	C35-C13-C14	5.40	131.56	122.82
12	G	828	CLA	C4A-NA-C1A	5.38	109.13	106.68
13	b	2153	A1AGD	O2-C1-C2	-5.10	110.22	121.83
23	b	2151	ZEX	C28-C27-C26	-5.10	118.73	126.94
13	B	2153	A1AGD	O2-C1-C2	-5.10	110.22	121.83
23	H	2151	ZEX	C28-C27-C26	-5.10	118.73	126.94
13	H	2153	A1AGD	O2-C1-C2	-5.09	110.24	121.83
23	B	2152	ZEX	C28-C27-C26	-5.08	118.77	126.94
20	b	2143	ECH	C16-C17-C18	-4.75	120.62	127.28
20	B	2144	ECH	C16-C17-C18	-4.75	120.62	127.28
20	H	2143	ECH	C16-C17-C18	-4.74	120.63	127.28
23	f	205	ZEX	C20-C13-C14	4.64	130.33	122.82
23	F	205	ZEX	C20-C13-C14	4.64	130.33	122.82
23	Q	205	ZEX	C20-C13-C14	4.61	130.28	122.82
24	U	208	SQD	O9-S-C6	4.57	113.58	106.76
24	L	208	SQD	O9-S-C6	4.57	113.58	106.76
24	l	208	SQD	O9-S-C6	4.56	113.57	106.76
16	H	2148	LHG	O4-P-O5	4.52	133.47	112.44
16	B	2149	LHG	O4-P-O5	4.52	133.46	112.44
16	b	2148	LHG	O4-P-O5	4.51	133.43	112.44
23	F	205	ZEX	C35-C34-C33	-4.42	121.07	127.28
20	H	2143	ECH	C15-C14-C13	4.41	133.47	127.28
16	V	103	LHG	O4-P-O5	4.41	132.96	112.44
16	m	103	LHG	O4-P-O5	4.41	132.96	112.44
16	M	102	LHG	O4-P-O5	4.40	132.93	112.44
23	f	205	ZEX	C35-C34-C33	-4.40	121.11	127.28
20	B	2144	ECH	C15-C14-C13	4.40	133.44	127.28
23	Q	205	ZEX	C35-C34-C33	-4.40	121.11	127.28
16	G	846	LHG	O4-P-O5	4.39	132.88	112.44
16	a	846	LHG	O4-P-O5	4.39	132.85	112.44
16	A	846	LHG	O4-P-O5	4.39	132.85	112.44
20	b	2143	ECH	C15-C14-C13	4.38	133.43	127.28
12	b	2129	CLA	CMB-C2B-C1B	-4.36	118.79	125.42
12	H	2129	CLA	CMB-C2B-C1B	-4.34	118.81	125.42
22	H	2150	EQ3	C20-C19-C18	-4.34	114.47	126.36
16	a	848	LHG	O4-P-O5	4.33	132.61	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	848	LHG	O4-P-O5	4.33	132.57	112.44
16	G	848	LHG	O4-P-O5	4.32	132.56	112.44
12	B	2130	CLA	CMB-C2B-C1B	-4.32	118.83	125.42
22	B	2151	EQ3	C20-C19-C18	-4.32	114.51	126.36
22	b	2150	EQ3	C20-C19-C18	-4.32	114.52	126.36
23	f	205	ZEX	C8-C7-C6	-4.31	115.49	127.00
23	F	205	ZEX	C8-C7-C6	-4.30	115.52	127.00
23	Q	205	ZEX	C8-C7-C6	-4.28	115.56	127.00
23	f	205	ZEX	C28-C27-C26	-4.26	120.08	126.94
22	H	2150	EQ3	C1-C6-C5	-4.26	116.82	122.64
23	Q	205	ZEX	C28-C27-C26	-4.25	120.11	126.94
23	F	205	ZEX	C28-C27-C26	-4.23	120.13	126.94
22	b	2150	EQ3	C1-C6-C5	-4.23	116.85	122.64
22	B	2151	EQ3	C1-C6-C5	-4.22	116.87	122.64
20	H	2143	ECH	C16-C15-C14	-4.19	114.95	123.52
20	B	2144	ECH	C16-C15-C14	-4.18	114.96	123.52
20	b	2143	ECH	C16-C15-C14	-4.18	114.97	123.52
13	G	840	A1AGD	C7-C3-C2	-4.16	118.49	123.39
13	a	840	A1AGD	C7-C3-C2	-4.15	118.50	123.39
23	b	2151	ZEX	C35-C34-C33	-4.15	121.46	127.28
12	a	826	CLA	C3B-C4B-NB	-4.13	106.84	110.53
23	B	2152	ZEX	C35-C34-C33	-4.13	121.49	127.28
15	a	842	BCR	C2-C1-C6	4.13	116.43	110.44
13	A	840	A1AGD	C7-C3-C2	-4.13	118.53	123.39
24	l	208	SQD	O47-C7-C8	4.12	120.40	111.48
24	L	208	SQD	O47-C7-C8	4.12	120.40	111.48
24	U	208	SQD	O47-C7-C8	4.11	120.38	111.48
15	A	842	BCR	C2-C1-C6	4.11	116.41	110.44
12	G	826	CLA	C3B-C4B-NB	-4.10	106.87	110.53
15	G	842	BCR	C2-C1-C6	4.10	116.40	110.44
23	H	2151	ZEX	C35-C34-C33	-4.10	121.53	127.28
12	A	826	CLA	C3B-C4B-NB	-4.10	106.87	110.53
25	l	209	DGD	O3G-C3G-C2G	-4.08	100.90	110.82
25	L	209	DGD	O3G-C3G-C2G	-4.07	100.91	110.82
25	U	209	DGD	O3G-C3G-C2G	-4.06	100.94	110.82
15	T	4001	BCR	C2-C1-C6	4.04	116.30	110.44
15	k	4001	BCR	C2-C1-C6	4.03	116.30	110.44
15	K	4001	BCR	C2-C1-C6	4.03	116.30	110.44
23	b	2151	ZEX	C1-C6-C5	-4.02	117.14	122.64
15	H	2146	BCR	C2-C1-C6	4.02	116.28	110.44
23	B	2152	ZEX	C1-C6-C5	-4.02	117.15	122.64
15	b	2146	BCR	C2-C1-C6	4.01	116.27	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	H	2151	ZEX	C1-C6-C5	-3.99	117.18	122.64
15	B	2147	BCR	C2-C1-C6	3.99	116.24	110.44
24	L	208	SQD	O9-S-O7	-3.98	100.88	113.82
12	H	2104	CLA	CAC-C3C-C4C	3.98	129.96	124.79
12	a	820	CLA	CMB-C2B-C1B	-3.97	119.37	125.42
24	l	208	SQD	O9-S-O7	-3.97	100.91	113.82
12	A	820	CLA	CMB-C2B-C1B	-3.97	119.38	125.42
24	U	208	SQD	O9-S-O7	-3.97	100.92	113.82
12	b	2104	CLA	CAC-C3C-C4C	3.95	129.92	124.79
12	G	820	CLA	CMB-C2B-C1B	-3.94	119.41	125.42
12	B	2105	CLA	CAC-C3C-C4C	3.94	129.92	124.79
24	l	208	SQD	O5-C5-C4	3.90	116.73	109.70
12	H	2132	CLA	CAC-C3C-C4C	3.90	129.86	124.79
24	L	208	SQD	O5-C5-C4	3.90	116.72	109.70
12	B	2133	CLA	CAC-C3C-C4C	3.89	129.86	124.79
13	H	2153	A1AGD	C15-C14-C16	-3.87	97.47	111.27
24	U	208	SQD	O5-C5-C4	3.87	116.67	109.70
13	b	2153	A1AGD	C15-C14-C16	-3.87	97.48	111.27
12	b	2132	CLA	CAC-C3C-C4C	3.87	129.82	124.79
12	H	2111	CLA	CBC-CAC-C3C	3.87	122.90	112.42
12	b	2111	CLA	CBC-CAC-C3C	3.86	122.89	112.42
12	B	2112	CLA	CBC-CAC-C3C	3.86	122.88	112.42
13	B	2153	A1AGD	C15-C14-C16	-3.86	97.52	111.27
13	B	2153	A1AGD	C3-C4-C5	3.83	123.35	118.57
13	b	2153	A1AGD	C3-C4-C5	3.82	123.34	118.57
13	H	2153	A1AGD	C3-C4-C5	3.82	123.34	118.57
15	i	101	BCR	C2-C1-C6	3.81	115.97	110.44
24	m	102	SQD	O9-S-O7	-3.80	101.45	113.82
24	V	102	SQD	O9-S-O7	-3.80	101.46	113.82
24	M	101	SQD	O9-S-O7	-3.80	101.47	113.82
22	B	2151	EQ3	C16-C15-C14	-3.79	115.77	123.52
15	b	2144	BCR	C2-C1-C6	3.78	115.93	110.44
22	H	2150	EQ3	C16-C15-C14	-3.78	115.79	123.52
22	b	2150	EQ3	C16-C15-C14	-3.78	115.79	123.52
15	I	101	BCR	C2-C1-C6	3.77	115.92	110.44
12	U	201	CLA	O2D-CGD-O1D	-3.77	116.51	123.85
15	R	101	BCR	C2-C1-C6	3.76	115.89	110.44
15	B	2145	BCR	C2-C1-C6	3.76	115.89	110.44
15	H	2144	BCR	C2-C1-C6	3.75	115.88	110.44
12	L	201	CLA	O2D-CGD-O1D	-3.74	116.56	123.85
12	l	201	CLA	O2D-CGD-O1D	-3.73	116.59	123.85
22	b	2150	EQ3	C20-C21-C22	-3.73	122.05	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	H	2104	CLA	C3B-C4B-NB	-3.72	107.21	110.53
22	H	2150	EQ3	C20-C21-C22	-3.70	122.08	127.28
22	B	2151	EQ3	C20-C21-C22	-3.70	122.08	127.28
12	B	2105	CLA	C3B-C4B-NB	-3.69	107.23	110.53
24	M	101	SQD	O47-C7-C8	3.67	119.42	111.48
15	G	844	BCR	C2-C1-C6	3.66	115.76	110.44
24	V	102	SQD	O47-C7-C8	3.66	119.40	111.48
12	b	2104	CLA	C3B-C4B-NB	-3.66	107.27	110.53
24	m	102	SQD	O47-C7-C8	3.65	119.38	111.48
15	A	844	BCR	C2-C1-C6	3.65	115.73	110.44
15	a	844	BCR	C2-C1-C6	3.64	115.73	110.44
12	H	2136	CLA	CMB-C2B-C1B	-3.63	119.90	125.42
12	B	2137	CLA	CMB-C2B-C1B	-3.61	119.92	125.42
12	b	2136	CLA	CMB-C2B-C1B	-3.60	119.94	125.42
12	b	2102	CLA	CMB-C2B-C1B	-3.57	119.98	125.42
12	H	2102	CLA	CMB-C2B-C1B	-3.56	120.00	125.42
15	j	101	BCR	C2-C1-C6	3.56	115.60	110.44
12	B	2103	CLA	CMB-C2B-C1B	-3.55	120.01	125.42
12	G	808	CLA	CMB-C2B-C1B	-3.54	120.03	125.42
12	a	808	CLA	CMB-C2B-C1B	-3.53	120.04	125.42
13	b	2153	A1AGD	C2-C3-C4	3.53	123.52	118.78
15	J	101	BCR	C2-C1-C6	3.53	115.56	110.44
12	A	808	CLA	CMB-C2B-C1B	-3.52	120.06	125.42
12	S	103	CLA	O2D-CGD-O1D	-3.52	117.00	123.85
13	B	2153	A1AGD	C2-C3-C4	3.51	123.50	118.78
12	J	103	CLA	O2D-CGD-O1D	-3.50	117.03	123.85
15	S	101	BCR	C2-C1-C6	3.50	115.53	110.44
13	H	2153	A1AGD	C2-C3-C4	3.50	123.49	118.78
12	j	103	CLA	O2D-CGD-O1D	-3.49	117.05	123.85
15	a	845	BCR	C24-C23-C22	-3.47	121.10	126.23
15	R	101	BCR	C3-C4-C5	-3.45	107.89	114.06
12	G	801	CLA	C1D-ND-C4D	-3.45	103.89	106.31
15	G	845	BCR	C24-C23-C22	-3.45	121.13	126.23
15	I	101	BCR	C3-C4-C5	-3.45	107.91	114.06
15	A	845	BCR	C24-C23-C22	-3.45	121.14	126.23
12	A	801	CLA	C1D-ND-C4D	-3.44	103.90	106.31
15	i	101	BCR	C3-C4-C5	-3.44	107.92	114.06
12	B	2112	CLA	CAC-C3C-C2C	3.43	133.87	127.56
12	b	2111	CLA	CAC-C3C-C2C	3.42	133.84	127.56
12	a	801	CLA	C1D-ND-C4D	-3.42	103.91	106.31
12	B	2142	CLA	O2D-CGD-O1D	-3.42	117.19	123.85
12	H	2111	CLA	CAC-C3C-C2C	3.42	133.84	127.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	b	2139	CLA	C3B-C4B-NB	-3.41	107.48	110.53
12	b	2141	CLA	O2D-CGD-O1D	-3.41	117.22	123.85
12	H	2141	CLA	O2D-CGD-O1D	-3.40	117.23	123.85
12	H	2139	CLA	C3B-C4B-NB	-3.37	107.52	110.53
12	B	2140	CLA	C3B-C4B-NB	-3.36	107.53	110.53
15	B	2147	BCR	C15-C16-C17	-3.34	116.68	123.52
12	H	2130	CLA	C3B-C4B-NB	-3.34	107.55	110.53
15	b	2146	BCR	C15-C16-C17	-3.34	116.69	123.52
12	B	2131	CLA	C3B-C4B-NB	-3.34	107.55	110.53
12	H	2101	CLA	CMB-C2B-C1B	-3.34	120.34	125.42
15	H	2146	BCR	C24-C23-C22	-3.33	121.30	126.23
12	B	2102	CLA	CMB-C2B-C1B	-3.32	120.36	125.42
15	H	2146	BCR	C15-C16-C17	-3.32	116.73	123.52
12	b	2101	CLA	CMB-C2B-C1B	-3.32	120.37	125.42
23	H	2151	ZEX	C8-C7-C6	-3.31	118.15	127.00
15	b	2146	BCR	C24-C23-C22	-3.31	121.34	126.23
15	B	2147	BCR	C24-C23-C22	-3.31	121.34	126.23
23	b	2151	ZEX	C8-C7-C6	-3.31	118.17	127.00
12	j	102	CLA	O2D-CGD-O1D	-3.31	117.41	123.85
23	B	2152	ZEX	C8-C7-C6	-3.31	118.17	127.00
12	b	2130	CLA	C3B-C4B-NB	-3.30	107.58	110.53
13	A	840	A1AGD	C17-C18-C19	3.30	126.94	115.97
12	a	836	CLA	C3B-C4B-NB	-3.30	107.58	110.53
12	J	102	CLA	O2D-CGD-O1D	-3.30	117.43	123.85
12	H	2132	CLA	CMB-C2B-C1B	-3.29	120.40	125.42
13	G	840	A1AGD	C17-C18-C19	3.29	126.91	115.97
12	B	2133	CLA	CMB-C2B-C1B	-3.29	120.41	125.42
12	A	836	CLA	C3B-C4B-NB	-3.29	107.59	110.53
13	a	840	A1AGD	C17-C18-C19	3.29	126.89	115.97
23	f	205	ZEX	C18-C5-C6	-3.28	120.91	124.48
23	F	205	ZEX	C18-C5-C6	-3.28	120.91	124.48
12	b	2132	CLA	CMB-C2B-C1B	-3.27	120.44	125.42
12	S	102	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
24	m	102	SQD	O9-S-C6	3.25	111.61	106.76
12	A	839	CLA	C3B-C4B-NB	-3.25	107.63	110.53
24	V	102	SQD	O9-S-C6	3.25	111.61	106.76
12	b	2111	CLA	CAC-C3C-C4C	-3.25	120.56	124.79
23	Q	205	ZEX	C18-C5-C6	-3.24	120.95	124.48
12	G	830	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
12	B	2112	CLA	CAC-C3C-C4C	-3.24	120.58	124.79
24	M	101	SQD	O9-S-C6	3.23	111.58	106.76
12	G	836	CLA	C3B-C4B-NB	-3.23	107.64	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	G	839	CLA	C3B-C4B-NB	-3.23	107.65	110.53
12	a	810	CLA	O2D-CGD-O1D	-3.23	117.57	123.85
12	A	830	CLA	O2D-CGD-O1D	-3.22	117.57	123.85
12	a	830	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
12	H	2111	CLA	CAC-C3C-C4C	-3.22	120.60	124.79
12	H	2111	CLA	CMC-C2C-C1C	-3.22	120.01	125.03
12	a	825	CLA	C3B-C4B-NB	-3.21	107.66	110.53
12	b	2113	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
12	a	839	CLA	C3B-C4B-NB	-3.21	107.66	110.53
12	B	2112	CLA	CMC-C2C-C1C	-3.21	120.02	125.03
12	A	810	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
12	a	811	CLA	C3B-C4B-NB	-3.20	107.67	110.53
12	G	810	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
12	a	854	CLA	CAA-C2A-C3A	-3.20	104.36	113.00
12	B	2114	CLA	O2D-CGD-O1D	-3.20	117.63	123.85
12	b	2111	CLA	CMC-C2C-C1C	-3.19	120.04	125.03
15	S	104	BCR	C15-C16-C17	-3.19	116.98	123.52
15	l	207	BCR	C28-C27-C26	-3.19	108.36	114.06
12	G	825	CLA	C3B-C4B-NB	-3.19	107.68	110.53
12	G	804	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
12	H	2113	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
12	A	854	CLA	CAA-C2A-C3A	-3.19	104.39	113.00
15	U	207	BCR	C28-C27-C26	-3.18	108.38	114.06
12	G	854	CLA	CAA-C2A-C3A	-3.18	104.40	113.00
15	L	207	BCR	C28-C27-C26	-3.18	108.38	114.06
12	A	825	CLA	C3B-C4B-NB	-3.18	107.69	110.53
15	j	104	BCR	C15-C16-C17	-3.18	117.02	123.52
13	H	2153	A1AGD	C15-C14-C13	3.18	122.59	111.27
12	A	811	CLA	C3B-C4B-NB	-3.17	107.70	110.53
15	J	104	BCR	C15-C16-C17	-3.17	117.03	123.52
13	B	2153	A1AGD	C15-C14-C13	3.17	122.58	111.27
12	G	811	CLA	C3B-C4B-NB	-3.17	107.70	110.53
13	b	2153	A1AGD	C15-C14-C13	3.17	122.56	111.27
12	H	2103	CLA	O2D-CGD-O1D	-3.17	117.69	123.85
15	j	101	BCR	C3-C4-C5	-3.16	108.42	114.06
12	b	2103	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
12	B	2104	CLA	O2D-CGD-O1D	-3.16	117.71	123.85
12	A	804	CLA	O2D-CGD-O1D	-3.15	117.71	123.85
12	Q	201	CLA	C3B-C4B-NB	-3.15	107.72	110.53
12	A	817	CLA	C3B-C4B-NB	-3.14	107.72	110.53
15	S	101	BCR	C3-C4-C5	-3.14	108.46	114.06
15	J	101	BCR	C3-C4-C5	-3.14	108.46	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	V	102	SQD	O7-S-C6	3.14	111.44	106.76
24	M	101	SQD	O7-S-C6	3.14	111.44	106.76
24	m	102	SQD	O7-S-C6	3.14	111.44	106.76
20	b	2143	ECH	C15-C16-C17	3.13	129.93	123.52
12	G	817	CLA	C3B-C4B-NB	-3.13	107.73	110.53
12	B	2102	CLA	CMB-C2B-C3B	3.13	133.91	126.55
12	a	817	CLA	C3B-C4B-NB	-3.13	107.74	110.53
12	H	2101	CLA	CMB-C2B-C3B	3.13	133.91	126.55
12	a	804	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
12	b	2101	CLA	CMB-C2B-C3B	3.12	133.89	126.55
12	a	825	CLA	CAA-C2A-C1A	-3.12	101.75	111.97
12	F	201	CLA	C3B-C4B-NB	-3.11	107.75	110.53
12	G	825	CLA	CAA-C2A-C1A	-3.11	101.77	111.97
20	B	2144	ECH	C15-C16-C17	3.11	129.89	123.52
13	H	2153	A1AGD	O1-C4-C3	-3.11	117.45	120.73
12	G	808	CLA	CAA-C2A-C3A	-3.11	104.59	113.00
12	a	806	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
12	A	828	CLA	CMB-C2B-C1B	-3.11	120.68	125.42
12	A	825	CLA	CAA-C2A-C1A	-3.11	101.78	111.97
12	U	205	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
20	H	2143	ECH	C15-C16-C17	3.11	129.88	123.52
12	A	806	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
12	A	808	CLA	CAA-C2A-C3A	-3.10	104.61	113.00
12	a	808	CLA	CAA-C2A-C3A	-3.10	104.62	113.00
22	B	2151	EQ3	C29-C30-C25	3.10	114.94	110.44
12	b	2105	CLA	C3B-C4B-NB	-3.10	107.76	110.53
22	H	2150	EQ3	C29-C30-C25	3.10	114.94	110.44
12	G	806	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
12	a	828	CLA	CMB-C2B-C1B	-3.09	120.71	125.42
20	b	2143	ECH	C40-C30-C25	3.09	115.09	110.24
13	B	2153	A1AGD	O1-C4-C3	-3.09	117.47	120.73
22	b	2150	EQ3	C29-C30-C25	3.09	114.93	110.44
13	b	2153	A1AGD	O1-C4-C3	-3.09	117.47	120.73
12	G	828	CLA	CMB-C2B-C1B	-3.09	120.72	125.42
12	L	205	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
12	l	205	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
12	A	850	CLA	CMB-C2B-C1B	-3.08	120.72	125.42
12	H	2139	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
12	B	2142	CLA	O2D-CGD-CBD	3.08	116.62	111.23
12	B	2106	CLA	C3B-C4B-NB	-3.08	107.78	110.53
15	U	207	BCR	C15-C16-C17	-3.08	117.22	123.52
12	H	2105	CLA	C3B-C4B-NB	-3.08	107.78	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	f	201	CLA	C3B-C4B-NB	-3.07	107.78	110.53
12	H	2141	CLA	O2D-CGD-CBD	3.07	116.61	111.23
12	a	850	CLA	CMB-C2B-C1B	-3.07	120.74	125.42
15	L	207	BCR	C15-C16-C17	-3.07	117.24	123.52
20	B	2144	ECH	C40-C30-C25	3.07	115.06	110.24
22	b	2150	EQ3	C38-C26-C25	-3.07	119.17	124.11
12	G	850	CLA	CMB-C2B-C1B	-3.07	120.75	125.42
12	b	2141	CLA	O2D-CGD-CBD	3.07	116.59	111.23
22	B	2151	EQ3	C38-C26-C25	-3.06	119.18	124.11
24	U	208	SQD	O7-S-C6	3.06	111.33	106.76
22	H	2150	EQ3	C11-C10-C9	-3.06	122.99	127.28
24	L	208	SQD	O7-S-C6	3.06	111.32	106.76
12	B	2140	CLA	O2D-CGD-O1D	-3.05	117.90	123.85
12	b	2139	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
24	l	208	SQD	O7-S-C6	3.05	111.31	106.76
20	H	2143	ECH	C40-C30-C25	3.05	115.02	110.24
22	H	2150	EQ3	C38-C26-C25	-3.04	119.22	124.11
15	l	207	BCR	C15-C16-C17	-3.04	117.30	123.52
12	G	804	CLA	CHB-C4A-NA	3.04	128.78	124.40
12	A	816	CLA	CMB-C2B-C1B	-3.03	120.80	125.42
22	B	2151	EQ3	C11-C10-C9	-3.03	123.02	127.28
12	a	830	CLA	C3B-C4B-NB	-3.03	107.82	110.53
12	a	816	CLA	CMB-C2B-C1B	-3.03	120.81	125.42
12	G	830	CLA	C3B-C4B-NB	-3.03	107.83	110.53
12	A	830	CLA	C3B-C4B-NB	-3.02	107.83	110.53
12	a	804	CLA	CHB-C4A-NA	3.02	128.76	124.40
12	G	816	CLA	CMB-C2B-C1B	-3.02	120.82	125.42
12	a	820	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
12	a	813	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
12	G	817	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
20	b	2143	ECH	C11-C10-C9	-3.01	123.05	127.28
15	a	843	BCR	C15-C16-C17	-3.01	117.35	123.52
20	B	2144	ECH	C11-C10-C9	-3.01	123.05	127.28
23	b	2151	ZEX	C10-C11-C12	-3.01	114.48	123.20
12	A	820	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
12	A	817	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
20	H	2143	ECH	C11-C10-C9	-3.01	123.06	127.28
12	a	812	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
22	b	2150	EQ3	C11-C10-C9	-3.01	123.06	127.28
12	A	804	CLA	CHB-C4A-NA	3.01	128.74	124.40
12	a	817	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
12	G	811	CLA	O2D-CGD-O1D	-3.00	118.00	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	a	829	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
12	A	811	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
12	G	820	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
23	B	2152	ZEX	C10-C11-C12	-3.00	114.50	123.20
12	a	814	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
13	a	840	A1AGD	C15-C14-C13	3.00	121.96	111.27
12	A	813	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
12	A	820	CLA	CMB-C2B-C3B	3.00	133.60	126.55
12	G	812	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
13	G	840	A1AGD	C15-C14-C13	3.00	121.95	111.27
13	A	840	A1AGD	C15-C14-C13	3.00	121.95	111.27
12	G	838	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
12	a	811	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
12	A	838	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
12	b	2102	CLA	C1-C2-C3	2.99	131.10	126.20
12	G	814	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
12	a	820	CLA	CMB-C2B-C3B	2.99	133.59	126.55
12	H	2109	CLA	O2A-CGA-O1A	-2.99	116.14	123.63
12	B	2110	CLA	O2A-CGA-O1A	-2.99	116.14	123.63
23	H	2151	ZEX	C10-C11-C12	-2.99	114.53	123.20
12	A	814	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
12	H	2118	CLA	C1-C2-C3	-2.99	121.92	126.76
12	G	813	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
12	A	829	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
12	S	103	CLA	O2D-CGD-CBD	2.99	116.45	111.23
12	G	824	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
12	b	2109	CLA	O2A-CGA-O1A	-2.99	116.16	123.63
12	b	2133	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
12	b	2124	CLA	CHB-C4A-NA	2.99	128.71	124.40
15	A	843	BCR	C15-C16-C17	-2.98	117.42	123.52
12	A	824	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
12	A	812	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
12	G	820	CLA	CMB-C2B-C3B	2.98	133.56	126.55
12	b	2136	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
12	B	2125	CLA	CHB-C4A-NA	2.98	128.70	124.40
12	a	824	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
12	a	834	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
15	G	843	BCR	C15-C16-C17	-2.98	117.43	123.52
12	H	2109	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
12	B	2119	CLA	C1-C2-C3	-2.97	121.95	126.76
15	H	2144	BCR	C15-C16-C17	-2.97	117.44	123.52
15	B	2145	BCR	C15-C16-C17	-2.97	117.44	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	G	829	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
12	A	834	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
12	j	103	CLA	O2D-CGD-CBD	2.97	116.42	111.23
12	G	835	CLA	CMB-C2B-C1B	-2.97	120.90	125.42
12	a	838	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
12	J	103	CLA	O2D-CGD-CBD	2.97	116.42	111.23
12	B	2134	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
12	B	2103	CLA	C1-C2-C3	2.97	131.06	126.20
12	B	2137	CLA	O2D-CGD-O1D	-2.97	118.08	123.85
12	a	805	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
12	T	4002	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
12	B	2110	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
23	B	2152	ZEX	C7-C6-C5	-2.96	114.73	121.56
12	b	2118	CLA	C1-C2-C3	-2.96	121.97	126.76
15	b	2144	BCR	C15-C16-C17	-2.96	117.46	123.52
12	B	2116	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
12	G	805	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
12	H	2136	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
23	H	2151	ZEX	C7-C6-C5	-2.96	114.74	121.56
12	H	2115	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
12	A	805	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
12	b	2109	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
15	H	2144	BCR	C15-C14-C13	-2.96	123.13	127.28
12	G	834	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
23	b	2151	ZEX	C7-C6-C5	-2.95	114.75	121.56
12	H	2124	CLA	CHB-C4A-NA	2.95	128.66	124.40
15	L	206	BCR	C29-C30-C25	2.95	114.72	110.44
12	A	835	CLA	CMB-C2B-C1B	-2.95	120.93	125.42
12	H	2133	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
15	U	206	BCR	C29-C30-C25	2.95	114.72	110.44
12	b	2115	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
12	a	835	CLA	CMB-C2B-C1B	-2.94	120.94	125.42
12	A	833	CLA	C3B-C4B-NB	-2.94	107.90	110.53
12	B	2112	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
12	a	833	CLA	C3B-C4B-NB	-2.94	107.90	110.53
12	k	4002	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
12	G	833	CLA	C3B-C4B-NB	-2.94	107.91	110.53
12	k	4002	CLA	CHB-C4A-NA	2.94	128.64	124.40
12	H	2132	CLA	CHB-C4A-NA	2.94	128.64	124.40
12	U	203	CLA	CHB-C4A-NA	2.94	128.64	124.40
12	b	2109	CLA	CHB-C4A-NA	2.94	128.64	124.40
12	B	2110	CLA	CHB-C4A-NA	2.93	128.63	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	2150	EQ3	C28-C29-C30	2.93	117.51	113.21
12	K	4002	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
12	a	816	CLA	CHB-C4A-NA	2.93	128.63	124.40
12	A	854	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
12	B	2133	CLA	CHB-C4A-NA	2.93	128.63	124.40
12	H	2102	CLA	C1-C2-C3	2.93	131.00	126.20
12	b	2132	CLA	CHB-C4A-NA	2.93	128.63	124.40
12	a	818	CLA	C3B-C4B-NB	-2.93	107.92	110.53
15	l	206	BCR	C29-C30-C25	2.93	114.69	110.44
12	H	2114	CLA	CAC-C3C-C4C	2.93	128.60	124.79
12	H	2117	CLA	CHB-C4A-NA	2.93	128.63	124.40
12	b	2111	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
12	H	2111	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
13	b	2153	A1AGD	C7-C3-C2	-2.93	119.94	123.39
12	G	854	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
12	b	2152	CLA	CHB-C4A-NA	2.93	128.62	124.40
12	L	203	CLA	CHB-C4A-NA	2.93	128.62	124.40
12	B	2115	CLA	CAC-C3C-C4C	2.92	128.59	124.79
12	G	816	CLA	CHB-C4A-NA	2.92	128.62	124.40
12	b	2108	CLA	CHB-C4A-NA	2.92	128.61	124.40
15	B	2145	BCR	C15-C14-C13	-2.92	123.19	127.28
13	B	2153	A1AGD	C7-C3-C2	-2.92	119.95	123.39
12	H	2152	CLA	CHB-C4A-NA	2.92	128.61	124.40
22	B	2151	EQ3	C28-C29-C30	2.92	117.48	113.21
12	B	2116	CLA	CHB-C4A-NA	2.92	128.61	124.40
12	a	854	CLA	O2D-CGD-O1D	-2.91	118.17	123.85
12	B	2103	CLA	C3B-C4B-NB	-2.91	107.93	110.53
22	H	2150	EQ3	C28-C29-C30	2.91	117.48	113.21
12	K	4002	CLA	CHB-C4A-NA	2.91	128.60	124.40
12	G	819	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
12	H	2115	CLA	CHB-C4A-NA	2.91	128.60	124.40
12	a	808	CLA	CMB-C2B-C3B	2.91	133.40	126.55
12	B	2109	CLA	CHB-C4A-NA	2.91	128.60	124.40
12	T	4002	CLA	CHB-C4A-NA	2.91	128.60	124.40
15	b	2144	BCR	C15-C14-C13	-2.91	123.20	127.28
12	B	2101	CLA	CHB-C4A-NA	2.91	128.60	124.40
12	a	819	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
12	H	2102	CLA	C3B-C4B-NB	-2.91	107.94	110.53
12	b	2114	CLA	CAC-C3C-C4C	2.91	128.57	124.79
12	H	2109	CLA	CHB-C4A-NA	2.91	128.59	124.40
12	a	818	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
12	H	2108	CLA	CHB-C4A-NA	2.90	128.59	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	G	808	CLA	CMB-C2B-C3B	2.90	133.38	126.55
12	G	833	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
12	l	203	CLA	CHB-C4A-NA	2.90	128.59	124.40
13	H	2153	A1AGD	C7-C3-C2	-2.90	119.97	123.39
12	b	2134	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
12	B	2118	CLA	CHB-C4A-NA	2.90	128.58	124.40
12	G	833	CLA	CHB-C4A-NA	2.90	128.58	124.40
12	b	2117	CLA	CHB-C4A-NA	2.90	128.58	124.40
12	A	819	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
12	A	816	CLA	CHB-C4A-NA	2.90	128.58	124.40
12	A	833	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
12	H	2127	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
12	A	818	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
12	b	2115	CLA	CHB-C4A-NA	2.89	128.57	124.40
12	A	808	CLA	CMB-C2B-C3B	2.89	133.35	126.55
12	B	2128	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
12	G	803	CLA	CHB-C4A-NA	2.89	128.57	124.40
12	A	803	CLA	CHB-C4A-NA	2.89	128.57	124.40
12	B	2137	CLA	CMB-C2B-C3B	2.89	133.34	126.55
15	S	104	BCR	C24-C23-C22	-2.89	121.97	126.23
12	G	818	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
12	H	2136	CLA	CMB-C2B-C3B	2.89	133.34	126.55
12	b	2136	CLA	CMB-C2B-C3B	2.89	133.34	126.55
12	j	102	CLA	O2D-CGD-CBD	2.88	116.27	111.23
12	A	818	CLA	C3B-C4B-NB	-2.88	107.95	110.53
12	J	102	CLA	O2D-CGD-CBD	2.88	116.27	111.23
12	G	804	CLA	CMB-C2B-C1B	-2.88	121.03	125.42
12	b	2123	CLA	CHB-C4A-NA	2.88	128.56	124.40
12	A	833	CLA	CHB-C4A-NA	2.88	128.56	124.40
12	a	839	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
12	a	833	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
12	G	802	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
12	H	2139	CLA	CHB-C4A-NA	2.88	128.55	124.40
12	B	2118	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
12	G	815	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
12	H	2132	CLA	CBC-CAC-C3C	2.88	120.21	112.42
12	H	2131	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
12	A	802	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
12	B	2135	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
12	b	2117	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
12	a	834	CLA	C3B-C4B-NB	-2.87	107.97	110.53
12	S	102	CLA	O2D-CGD-CBD	2.87	116.25	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	a	802	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
12	H	2117	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
12	A	806	CLA	CHB-C4A-NA	2.87	128.54	124.40
12	a	803	CLA	CHB-C4A-NA	2.87	128.54	124.40
12	b	2127	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
12	b	2132	CLA	CBC-CAC-C3C	2.87	120.20	112.42
12	a	806	CLA	CHB-C4A-NA	2.87	128.54	124.40
15	A	843	BCR	C27-C26-C25	2.87	126.58	122.70
12	b	2131	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
12	H	2123	CLA	CHB-C4A-NA	2.87	128.54	124.40
12	A	839	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
15	a	843	BCR	C27-C26-C25	2.87	126.58	122.70
12	a	833	CLA	CHB-C4A-NA	2.87	128.54	124.40
12	b	2102	CLA	C3B-C4B-NB	-2.87	107.97	110.53
12	H	2134	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
12	B	2133	CLA	CBC-CAC-C3C	2.86	120.18	112.42
12	G	818	CLA	C3B-C4B-NB	-2.86	107.97	110.53
12	G	821	CLA	C3B-C4B-NB	-2.86	107.97	110.53
12	L	201	CLA	O2D-CGD-CBD	2.86	116.23	111.23
12	b	2106	CLA	CHB-C4A-NA	2.86	128.53	124.40
15	b	2144	BCR	C27-C26-C25	2.86	126.57	122.70
12	B	2132	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
15	j	104	BCR	C24-C23-C22	-2.86	122.00	126.23
12	G	839	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
12	B	2124	CLA	CHB-C4A-NA	2.86	128.53	124.40
12	B	2119	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
15	J	104	BCR	C24-C23-C22	-2.86	122.01	126.23
12	A	821	CLA	C3B-C4B-NB	-2.86	107.98	110.53
12	l	201	CLA	O2D-CGD-CBD	2.86	116.22	111.23
12	A	804	CLA	CMB-C2B-C1B	-2.85	121.07	125.42
12	U	201	CLA	O2D-CGD-CBD	2.85	116.22	111.23
12	b	2118	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
12	A	815	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
22	B	2151	EQ3	C28-C27-C26	2.85	121.20	118.64
12	a	804	CLA	CMB-C2B-C1B	-2.85	121.08	125.42
12	a	815	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
12	B	2107	CLA	CHB-C4A-NA	2.85	128.51	124.40
12	H	2118	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
12	U	204	CLA	C3B-C4B-NB	-2.85	107.99	110.53
12	H	2111	CLA	C3B-C4B-NB	-2.85	107.99	110.53
12	B	2140	CLA	CHB-C4A-NA	2.84	128.50	124.40
12	G	827	CLA	CMB-C2B-C1B	-2.84	121.09	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	2138	CLA	C3B-C4B-NB	-2.84	107.99	110.53
12	b	2152	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
12	B	2136	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
12	a	832	CLA	C3B-C4B-NB	-2.84	107.99	110.53
12	L	205	CLA	C3B-C4B-NB	-2.84	107.99	110.53
22	b	2150	EQ3	C28-C27-C26	2.84	121.19	118.64
12	H	2124	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
12	G	831	CLA	CMB-C2B-C1B	-2.84	121.10	125.42
12	G	806	CLA	CHB-C4A-NA	2.84	128.50	124.40
12	H	2135	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
12	H	2109	CLA	CBA-CAA-C2A	2.84	122.23	113.79
12	B	2133	CLA	CMB-C2B-C3B	2.84	133.22	126.55
12	B	2112	CLA	C3B-C4B-NB	-2.84	108.00	110.53
15	H	2144	BCR	C27-C26-C25	2.84	126.54	122.70
12	A	807	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
12	a	807	CLA	CHB-C4A-NA	2.83	128.49	124.40
12	a	827	CLA	CMB-C2B-C1B	-2.83	121.10	125.42
12	G	825	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
16	B	2149	LHG	O8-C23-C24	2.83	120.48	111.83
12	A	827	CLA	CMB-C2B-C1B	-2.83	121.10	125.42
12	a	822	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
12	B	2110	CLA	CBA-CAA-C2A	2.83	122.22	113.79
12	A	831	CLA	CMB-C2B-C1B	-2.83	121.11	125.42
12	G	807	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
12	G	822	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
12	H	2152	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
12	G	811	CLA	CHB-C4A-NA	2.83	128.48	124.40
12	B	2115	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
12	b	2109	CLA	CBA-CAA-C2A	2.83	122.21	113.79
12	H	2114	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
12	B	2106	CLA	CHB-C4A-NA	2.83	128.48	124.40
15	B	2145	BCR	C27-C26-C25	2.83	126.53	122.70
12	H	2132	CLA	CMB-C2B-C3B	2.83	133.20	126.55
12	G	834	CLA	C3B-C4B-NB	-2.83	108.00	110.53
12	H	2137	CLA	C3B-C4B-NB	-2.83	108.00	110.53
12	l	205	CLA	C3B-C4B-NB	-2.83	108.00	110.53
15	G	843	BCR	C27-C26-C25	2.83	126.53	122.70
12	b	2139	CLA	CHB-C4A-NA	2.83	128.48	124.40
12	b	2120	CLA	C3B-C4B-NB	-2.83	108.01	110.53
12	l	204	CLA	C3B-C4B-NB	-2.83	108.01	110.53
12	a	807	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
12	a	831	CLA	CMB-C2B-C1B	-2.83	121.12	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	2101	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
12	B	2122	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
12	a	825	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
16	b	2148	LHG	O8-C23-C24	2.82	120.44	111.83
15	A	843	BCR	C15-C14-C13	-2.82	123.32	127.28
12	A	825	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
12	b	2135	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
12	a	814	CLA	CMB-C2B-C1B	-2.82	121.12	125.42
12	l	203	CLA	CMB-C2B-C1B	-2.82	121.12	125.42
12	b	2132	CLA	CMB-C2B-C3B	2.82	133.19	126.55
12	G	837	CLA	C3B-C4B-NB	-2.82	108.01	110.53
12	A	834	CLA	C3B-C4B-NB	-2.82	108.01	110.53
15	G	843	BCR	C15-C14-C13	-2.82	123.32	127.28
12	b	2121	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
12	b	2111	CLA	C3B-C4B-NB	-2.82	108.01	110.53
12	A	837	CLA	C3B-C4B-NB	-2.82	108.01	110.53
22	H	2150	EQ3	C28-C27-C26	2.82	121.18	118.64
12	b	2105	CLA	CHB-C4A-NA	2.82	128.47	124.40
12	A	810	CLA	CHB-C4A-NA	2.82	128.47	124.40
12	a	827	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
12	B	2125	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
12	A	811	CLA	CHB-C4A-NA	2.82	128.47	124.40
12	U	205	CLA	C3B-C4B-NB	-2.82	108.02	110.53
16	H	2148	LHG	O8-C23-C24	2.82	120.42	111.83
12	A	822	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
12	b	2123	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
12	H	2105	CLA	CHB-C4A-NA	2.82	128.46	124.40
12	b	2114	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
15	a	843	BCR	C15-C14-C13	-2.81	123.33	127.28
12	a	801	CLA	C2A-C1A-CHA	2.81	128.75	123.87
12	a	821	CLA	C3B-C4B-NB	-2.81	108.02	110.53
12	H	2106	CLA	CHB-C4A-NA	2.81	128.46	124.40
12	a	806	CLA	C3B-C4B-NB	-2.81	108.02	110.53
12	A	827	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
12	a	810	CLA	CHB-C4A-NA	2.81	128.46	124.40
12	H	2121	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
22	B	2151	EQ3	C38-C26-C27	2.81	119.74	115.49
22	b	2150	EQ3	C38-C26-C27	2.81	119.74	115.49
12	a	811	CLA	CHB-C4A-NA	2.81	128.45	124.40
12	b	2137	CLA	C3B-C4B-NB	-2.81	108.03	110.53
12	G	827	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
12	H	2132	CLA	O2D-CGD-O1D	-2.80	118.39	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	b	2132	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
12	L	204	CLA	C3B-C4B-NB	-2.80	108.03	110.53
12	H	2123	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
12	A	832	CLA	C3B-C4B-NB	-2.80	108.03	110.53
22	H	2150	EQ3	C38-C26-C27	2.80	119.73	115.49
12	B	2121	CLA	C3B-C4B-NB	-2.80	108.03	110.53
12	b	2124	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
12	B	2124	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
12	G	809	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
12	H	2112	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
12	L	203	CLA	CMB-C2B-C1B	-2.80	121.16	125.42
12	G	807	CLA	CHB-C4A-NA	2.80	128.44	124.40
12	U	204	CLA	CHB-C4A-NA	2.80	128.44	124.40
12	A	801	CLA	C2A-C1A-CHA	2.80	128.72	123.87
12	G	814	CLA	CMB-C2B-C1B	-2.80	121.16	125.42
12	A	809	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
12	B	2113	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
12	b	2120	CLA	CHB-C4A-NA	2.80	128.44	124.40
12	A	814	CLA	CMB-C2B-C1B	-2.80	121.16	125.42
12	a	809	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
12	b	2102	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
12	A	807	CLA	CHB-C4A-NA	2.79	128.43	124.40
12	b	2112	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
12	G	806	CLA	C3B-C4B-NB	-2.79	108.04	110.53
12	A	834	CLA	CHB-C4A-NA	2.79	128.43	124.40
12	H	2103	CLA	C3B-C4B-NB	-2.79	108.04	110.53
12	A	837	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
12	b	2129	CLA	CMB-C2B-C3B	2.79	133.11	126.55
15	A	845	BCR	C27-C26-C25	2.79	126.47	122.70
12	H	2128	CLA	C3B-C4B-NB	-2.79	108.04	110.53
12	J	102	CLA	CHB-C4A-NA	2.79	128.43	124.40
12	B	2103	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
12	B	2133	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
12	H	2120	CLA	CHB-C4A-NA	2.79	128.42	124.40
12	a	823	CLA	CHB-C4A-NA	2.78	128.42	124.40
12	B	2121	CLA	CHB-C4A-NA	2.78	128.42	124.40
12	G	837	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
12	B	2129	CLA	C3B-C4B-NB	-2.78	108.05	110.53
12	A	826	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
12	L	204	CLA	CHB-C4A-NA	2.78	128.42	124.40
12	b	2111	CLA	CMC-C2C-C3C	2.78	133.68	126.15
12	H	2111	CLA	CMC-C2C-C3C	2.78	133.68	126.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	G	810	CLA	CHB-C4A-NA	2.78	128.42	124.40
12	G	832	CLA	C3B-C4B-NB	-2.78	108.05	110.53
12	H	2120	CLA	C3B-C4B-NB	-2.78	108.05	110.53
12	a	834	CLA	CHB-C4A-NA	2.78	128.41	124.40
12	j	102	CLA	CHB-C4A-NA	2.78	128.41	124.40
16	V	103	LHG	O8-C23-C24	2.78	120.32	111.83
12	B	2121	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
12	a	837	CLA	C3B-C4B-NB	-2.78	108.05	110.53
12	G	834	CLA	CHB-C4A-NA	2.78	128.41	124.40
12	H	2122	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
12	U	203	CLA	CMB-C2B-C1B	-2.78	121.19	125.42
12	b	2128	CLA	C3B-C4B-NB	-2.78	108.05	110.53
12	G	801	CLA	C2A-C1A-CHA	2.78	128.69	123.87
12	B	2108	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
12	B	2123	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
12	G	814	CLA	CHB-C4A-NA	2.78	128.41	124.40
12	G	823	CLA	CHB-C4A-NA	2.78	128.41	124.40
12	a	828	CLA	C3B-C4B-NB	-2.78	108.05	110.53
12	B	2112	CLA	CMC-C2C-C3C	2.78	133.66	126.15
24	U	208	SQD	O48-C23-C24	2.78	120.30	111.83
12	A	814	CLA	CHB-C4A-NA	2.77	128.40	124.40
12	A	823	CLA	CHB-C4A-NA	2.77	128.40	124.40
12	A	806	CLA	C3B-C4B-NB	-2.77	108.05	110.53
12	b	2108	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
15	a	845	BCR	C27-C26-C25	2.77	126.45	122.70
12	b	2120	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
13	a	840	A1AGD	C13-C12-C11	-2.77	105.88	113.26
12	H	2108	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
12	A	828	CLA	CMB-C2B-C3B	2.77	133.07	126.55
12	a	803	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
16	m	103	LHG	O8-C23-C24	2.77	120.28	111.83
24	l	208	SQD	O48-C23-C24	2.77	120.28	111.83
12	B	2130	CLA	CMB-C2B-C3B	2.77	133.06	126.55
12	H	2129	CLA	CMB-C2B-C3B	2.77	133.06	126.55
12	b	2122	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
24	L	208	SQD	O48-C23-C24	2.77	120.28	111.83
12	b	2107	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
16	M	102	LHG	O8-C23-C24	2.77	120.27	111.83
12	G	803	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
12	a	837	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
12	H	2102	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
15	f	202	BCR	C27-C26-C25	2.77	126.44	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	F	202	BCR	C27-C26-C25	2.77	126.44	122.70
12	H	2120	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
13	A	840	A1AGD	C13-C12-C11	-2.76	105.89	113.26
12	I	204	CLA	CHB-C4A-NA	2.76	128.39	124.40
12	B	2104	CLA	C3B-C4B-NB	-2.76	108.06	110.53
12	G	828	CLA	CMB-C2B-C3B	2.76	133.05	126.55
12	B	2139	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
12	S	102	CLA	CHB-C4A-NA	2.76	128.39	124.40
15	H	2142	BCR	C27-C26-C25	2.76	126.44	122.70
12	a	826	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
12	B	2109	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
13	G	840	A1AGD	C13-C12-C11	-2.76	105.91	113.26
12	G	826	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
12	b	2138	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
12	H	2138	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
12	A	803	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
12	B	2112	CLA	C2A-C1A-CHA	2.76	128.65	123.87
12	b	2102	CLA	CMB-C2B-C3B	2.76	133.03	126.55
15	G	845	BCR	C27-C26-C25	2.75	126.43	122.70
15	B	2143	BCR	C27-C26-C25	2.75	126.42	122.70
12	H	2102	CLA	CMB-C2B-C3B	2.75	133.02	126.55
12	G	805	CLA	CHB-C4A-NA	2.75	128.37	124.40
12	B	2103	CLA	CMB-C2B-C3B	2.75	133.02	126.55
12	a	828	CLA	CMB-C2B-C3B	2.75	133.02	126.55
12	H	2126	CLA	C3B-C4B-NB	-2.75	108.08	110.53
12	H	2109	CLA	C3B-C4B-NB	-2.75	108.08	110.53
15	j	104	BCR	C27-C26-C25	2.75	126.42	122.70
12	b	2111	CLA	C2A-C1A-CHA	2.75	128.63	123.87
12	A	823	CLA	C3B-C4B-NB	-2.74	108.08	110.53
12	a	814	CLA	CHB-C4A-NA	2.74	128.36	124.40
12	B	2132	CLA	CHB-C4A-NA	2.74	128.36	124.40
15	b	2142	BCR	C27-C26-C25	2.74	126.41	122.70
12	H	2107	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
12	A	850	CLA	CMB-C2B-C3B	2.74	133.00	126.55
12	a	850	CLA	CMB-C2B-C3B	2.74	133.00	126.55
12	I	203	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
22	b	2150	EQ3	C10-C11-C12	-2.74	115.26	123.20
12	b	2103	CLA	C3B-C4B-NB	-2.74	108.08	110.53
12	b	2116	CLA	C3B-C4B-NB	-2.74	108.08	110.53
12	A	828	CLA	C3B-C4B-NB	-2.74	108.08	110.53
15	b	2145	BCR	C27-C26-C25	2.74	126.41	122.70
15	B	2146	BCR	C27-C26-C25	2.74	126.41	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	H	2101	CLA	C3B-C4B-NB	-2.74	108.09	110.53
22	B	2151	EQ3	C10-C11-C12	-2.74	115.27	123.20
12	B	2102	CLA	C3B-C4B-NB	-2.74	108.09	110.53
12	G	823	CLA	C3B-C4B-NB	-2.74	108.09	110.53
12	G	821	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
12	U	203	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
12	f	203	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
12	L	203	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
15	f	202	BCR	C24-C23-C22	-2.73	122.19	126.23
22	H	2150	EQ3	C10-C11-C12	-2.73	115.28	123.20
15	Q	202	BCR	C27-C26-C25	2.73	126.40	122.70
12	H	2141	CLA	C3B-C4B-NB	-2.73	108.09	110.53
12	a	823	CLA	C3B-C4B-NB	-2.73	108.09	110.53
12	A	821	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
15	H	2145	BCR	C27-C26-C25	2.73	126.39	122.70
12	H	2111	CLA	C2A-C1A-CHA	2.73	128.61	123.87
12	G	824	CLA	CHB-C4A-NA	2.73	128.34	124.40
12	H	2131	CLA	CHB-C4A-NA	2.73	128.34	124.40
12	G	850	CLA	CMB-C2B-C3B	2.73	132.97	126.55
17	b	2147	LMG	O6-C1-O1	-2.73	103.60	110.04
15	S	104	BCR	C27-C26-C25	2.73	126.39	122.70
12	H	2134	CLA	CHB-C4A-NA	2.73	128.34	124.40
12	A	805	CLA	CHB-C4A-NA	2.73	128.34	124.40
25	l	209	DGD	C3G-C2G-C1G	-2.73	105.43	111.78
12	B	2141	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
12	F	203	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
15	b	2146	BCR	C27-C26-C25	2.72	126.39	122.70
15	a	844	BCR	C15-C16-C17	-2.72	117.94	123.52
12	b	2131	CLA	CHB-C4A-NA	2.72	128.33	124.40
12	b	2107	CLA	C3B-C4B-NB	-2.72	108.10	110.53
25	L	209	DGD	C3G-C2G-C1G	-2.72	105.43	111.78
12	B	2135	CLA	CHB-C4A-NA	2.72	128.33	124.40
12	a	805	CLA	CHB-C4A-NA	2.72	128.33	124.40
15	J	104	BCR	C27-C26-C25	2.72	126.38	122.70
12	b	2101	CLA	C3B-C4B-NB	-2.72	108.10	110.53
12	H	2140	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
12	a	821	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
12	G	828	CLA	C3B-C4B-NB	-2.72	108.10	110.53
12	S	102	CLA	C3B-C4B-NB	-2.72	108.10	110.53
12	Q	203	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
12	b	2140	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
12	H	2116	CLA	C3B-C4B-NB	-2.72	108.11	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	2110	CLA	C3B-C4B-NB	-2.72	108.11	110.53
12	a	838	CLA	CHB-C4A-NA	2.72	128.32	124.40
12	A	824	CLA	CHB-C4A-NA	2.72	128.32	124.40
12	b	2116	CLA	CHB-C4A-NA	2.71	128.32	124.40
15	F	202	BCR	C24-C23-C22	-2.71	122.22	126.23
12	b	2109	CLA	C3B-C4B-NB	-2.71	108.11	110.53
12	H	2116	CLA	CHB-C4A-NA	2.71	128.32	124.40
12	a	818	CLA	CHB-C4A-NA	2.71	128.32	124.40
17	B	2148	LMG	O6-C1-O1	-2.71	103.63	110.04
12	H	2110	CLA	O2A-CGA-O1A	-2.71	116.84	123.63
25	U	209	DGD	C3G-C2G-C1G	-2.71	105.46	111.78
12	a	824	CLA	CHB-C4A-NA	2.71	128.31	124.40
12	b	2126	CLA	C3B-C4B-NB	-2.71	108.11	110.53
12	B	2138	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
15	A	844	BCR	C15-C16-C17	-2.71	117.97	123.52
15	B	2147	BCR	C27-C26-C25	2.71	126.36	122.70
15	G	844	BCR	C15-C16-C17	-2.71	117.98	123.52
15	b	2142	BCR	C15-C16-C17	-2.71	117.98	123.52
12	b	2110	CLA	O2A-CGA-O1A	-2.71	116.85	123.63
12	b	2141	CLA	C3B-C4B-NB	-2.71	108.11	110.53
12	b	2134	CLA	CHB-C4A-NA	2.71	128.31	124.40
15	A	842	BCR	C27-C26-C25	2.71	126.36	122.70
15	B	2143	BCR	C15-C16-C17	-2.71	117.98	123.52
12	G	818	CLA	CHB-C4A-NA	2.71	128.31	124.40
12	a	813	CLA	CHB-C4A-NA	2.71	128.31	124.40
15	Q	202	BCR	C24-C23-C22	-2.71	122.23	126.23
12	B	2127	CLA	C3B-C4B-NB	-2.71	108.11	110.53
12	b	2137	CLA	O2D-CGD-O1D	-2.70	118.58	123.85
12	a	809	CLA	C3B-C4B-NB	-2.70	108.12	110.53
12	J	102	CLA	C3B-C4B-NB	-2.70	108.12	110.53
12	U	204	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
12	A	813	CLA	CHB-C4A-NA	2.70	128.30	124.40
12	B	2111	CLA	O2A-CGA-O1A	-2.70	116.87	123.63
15	G	842	BCR	C27-C26-C25	2.70	126.35	122.70
12	H	2137	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
12	A	818	CLA	CHB-C4A-NA	2.70	128.29	124.40
12	B	2117	CLA	CHB-C4A-NA	2.70	128.29	124.40
12	H	2107	CLA	C3B-C4B-NB	-2.70	108.12	110.53
12	B	2108	CLA	C3B-C4B-NB	-2.70	108.12	110.53
15	H	2142	BCR	C15-C16-C17	-2.70	118.00	123.52
12	f	201	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
12	Q	201	CLA	O2D-CGD-O1D	-2.70	118.60	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	H	2147	LMG	O6-C1-O1	-2.70	103.67	110.04
12	G	819	CLA	C3B-C4B-NB	-2.70	108.12	110.53
12	b	2126	CLA	O2D-CGD-O1D	-2.69	118.60	123.85
12	l	204	CLA	O2D-CGD-O1D	-2.69	118.60	123.85
12	B	2127	CLA	O2D-CGD-O1D	-2.69	118.60	123.85
12	H	2130	CLA	CHB-C4A-NA	2.69	128.29	124.40
12	B	2111	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
12	a	803	CLA	C3B-C4B-NB	-2.69	108.13	110.53
12	A	809	CLA	C3B-C4B-NB	-2.69	108.13	110.53
12	b	2110	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
15	B	2143	BCR	C15-C14-C13	-2.69	123.50	127.28
15	A	844	BCR	C27-C26-C25	2.69	126.34	122.70
12	b	2119	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
12	G	803	CLA	C3B-C4B-NB	-2.69	108.13	110.53
12	L	204	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
12	A	838	CLA	CHB-C4A-NA	2.69	128.28	124.40
15	H	2146	BCR	C27-C26-C25	2.69	126.34	122.70
12	H	2135	CLA	C3B-C4B-NB	-2.69	108.13	110.53
12	A	803	CLA	C3B-C4B-NB	-2.69	108.13	110.53
12	B	2117	CLA	C3B-C4B-NB	-2.69	108.13	110.53
15	H	2142	BCR	C15-C14-C13	-2.69	123.51	127.28
15	a	842	BCR	C27-C26-C25	2.69	126.34	122.70
12	B	2131	CLA	CHB-C4A-NA	2.69	128.28	124.40
12	G	812	CLA	CHB-C4A-NA	2.68	128.27	124.40
12	b	2130	CLA	CHB-C4A-NA	2.68	128.27	124.40
15	a	844	BCR	C27-C26-C25	2.68	126.33	122.70
12	G	838	CLA	CHB-C4A-NA	2.68	128.27	124.40
12	B	2142	CLA	C3B-C4B-NB	-2.68	108.14	110.53
12	B	2109	CLA	C3B-C4B-NB	-2.68	108.14	110.53
12	H	2110	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
12	H	2126	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
12	H	2129	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
12	B	2113	CLA	CHB-C4A-NA	2.68	128.26	124.40
15	J	101	BCR	C27-C26-C25	2.68	126.32	122.70
12	b	2122	CLA	C3B-C4B-NB	-2.68	108.14	110.53
12	a	801	CLA	C3B-C4B-NB	-2.68	108.14	110.53
12	F	201	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
12	G	807	CLA	C3B-C4B-NB	-2.68	108.14	110.53
12	a	819	CLA	CHB-C4A-NA	2.67	128.26	124.40
12	A	830	CLA	CMB-C2B-C1B	-2.67	121.35	125.42
12	a	830	CLA	CMB-C2B-C1B	-2.67	121.35	125.42
12	a	807	CLA	C3B-C4B-NB	-2.67	108.14	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	j	102	CLA	C3B-C4B-NB	-2.67	108.14	110.53
12	G	813	CLA	CHB-C4A-NA	2.67	128.26	124.40
12	A	819	CLA	CHB-C4A-NA	2.67	128.26	124.40
12	A	807	CLA	C3B-C4B-NB	-2.67	108.14	110.53
15	G	844	BCR	C27-C26-C25	2.67	126.31	122.70
15	b	2142	BCR	C15-C14-C13	-2.67	123.53	127.28
15	A	845	BCR	C15-C16-C17	-2.67	118.06	123.52
12	a	808	CLA	CHB-C4A-NA	2.67	128.25	124.40
12	B	2120	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
12	A	801	CLA	C3B-C4B-NB	-2.67	108.15	110.53
15	G	844	BCR	C3-C4-C5	-2.67	109.30	114.06
12	a	819	CLA	C3B-C4B-NB	-2.67	108.15	110.53
12	b	2106	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
12	b	2112	CLA	CHB-C4A-NA	2.67	128.25	124.40
15	j	101	BCR	C27-C26-C25	2.66	126.31	122.70
12	F	203	CLA	C3B-C4B-NB	-2.66	108.15	110.53
15	S	101	BCR	C27-C26-C25	2.66	126.30	122.70
12	B	2107	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
12	A	808	CLA	CHB-C4A-NA	2.66	128.24	124.40
12	G	808	CLA	CHB-C4A-NA	2.66	128.24	124.40
12	b	2137	CLA	CHB-C4A-NA	2.66	128.24	124.40
12	f	203	CLA	C3B-C4B-NB	-2.66	108.16	110.53
12	B	2130	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
12	G	801	CLA	C3B-C4B-NB	-2.66	108.16	110.53
12	H	2112	CLA	CHB-C4A-NA	2.66	128.24	124.40
12	b	2141	CLA	CHB-C4A-NA	2.66	128.24	124.40
12	a	815	CLA	C3B-C4B-NB	-2.66	108.16	110.53
12	B	2142	CLA	CHB-C4A-NA	2.66	128.24	124.40
12	H	2122	CLA	C3B-C4B-NB	-2.66	108.16	110.53
12	H	2130	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
12	B	2105	CLA	CMB-C2B-C1B	-2.66	121.38	125.42
12	B	2131	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
12	U	203	CLA	C3B-C4B-NB	-2.65	108.16	110.53
12	A	819	CLA	C3B-C4B-NB	-2.65	108.16	110.53
12	A	829	CLA	CMB-C2B-C1B	-2.65	121.38	125.42
12	H	2109	CLA	O2D-CGD-CBD	2.65	115.87	111.23
12	H	2119	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
12	b	2130	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
12	B	2138	CLA	CHB-C4A-NA	2.65	128.23	124.40
12	G	809	CLA	C3B-C4B-NB	-2.65	108.16	110.53
12	f	204	CLA	C3B-C4B-NB	-2.65	108.16	110.53
12	A	812	CLA	CHB-C4A-NA	2.65	128.22	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	840	A1AGD	O2-C1-C6	2.65	124.69	120.48
12	b	2104	CLA	CMB-C2B-C1B	-2.65	121.39	125.42
12	H	2108	CLA	C3B-C4B-NB	-2.65	108.17	110.53
12	Q	203	CLA	C3B-C4B-NB	-2.65	108.17	110.53
12	B	2136	CLA	C3B-C4B-NB	-2.65	108.17	110.53
12	A	816	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
15	a	845	BCR	C15-C16-C17	-2.65	118.10	123.52
24	M	101	SQD	O48-C23-C24	2.65	119.91	111.83
12	B	2123	CLA	C3B-C4B-NB	-2.65	108.17	110.53
15	G	845	BCR	C15-C16-C17	-2.65	118.10	123.52
12	G	819	CLA	CHB-C4A-NA	2.65	128.22	124.40
15	A	844	BCR	C3-C4-C5	-2.64	109.34	114.06
12	b	2129	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
15	a	843	BCR	C30-C25-C26	-2.64	119.02	122.64
12	a	812	CLA	CHB-C4A-NA	2.64	128.22	124.40
12	H	2107	CLA	CHB-C4A-NA	2.64	128.21	124.40
12	a	816	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
13	G	840	A1AGD	O2-C1-C6	2.64	124.68	120.48
12	H	2137	CLA	O2A-CGA-O1A	-2.64	117.02	123.63
25	L	209	DGD	O6D-C1D-O3G	-2.64	103.81	110.04
12	A	825	CLA	CAA-C2A-C3A	-2.64	105.87	113.00
12	G	837	CLA	CHB-C4A-NA	2.64	128.21	124.40
15	S	104	BCR	C15-C14-C13	-2.64	123.58	127.28
12	H	2141	CLA	CHB-C4A-NA	2.64	128.21	124.40
12	b	2107	CLA	CHB-C4A-NA	2.64	128.21	124.40
12	F	204	CLA	C3B-C4B-NB	-2.64	108.18	110.53
15	A	843	BCR	C30-C25-C26	-2.64	119.03	122.64
12	H	2106	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
12	b	2109	CLA	O2D-CGD-CBD	2.64	115.84	111.23
17	G	847	LMG	O1-C1-C2	2.64	112.28	108.27
24	V	102	SQD	O48-C23-C24	2.63	119.87	111.83
23	B	2152	ZEX	C21-C26-C27	2.63	122.80	115.65
12	b	2133	CLA	CHB-C4A-NA	2.63	128.20	124.40
12	G	830	CLA	CMB-C2B-C1B	-2.63	121.41	125.42
12	G	829	CLA	CMB-C2B-C1B	-2.63	121.41	125.42
12	a	825	CLA	CAA-C2A-C3A	-2.63	105.89	113.00
12	H	2111	CLA	CHB-C4A-NA	2.63	128.20	124.40
23	b	2151	ZEX	C21-C26-C27	2.63	122.79	115.65
12	a	813	CLA	C3B-C4B-NB	-2.63	108.18	110.53
24	m	102	SQD	O48-C23-C24	2.63	119.86	111.83
12	H	2104	CLA	CMB-C2B-C1B	-2.63	121.41	125.42
12	a	829	CLA	CMB-C2B-C1B	-2.63	121.41	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	l	209	DGD	O6D-C1D-O3G	-2.63	103.83	110.04
12	G	825	CLA	CAA-C2A-C3A	-2.63	105.89	113.00
12	b	2135	CLA	C3B-C4B-NB	-2.63	108.18	110.53
12	B	2138	CLA	O2A-CGA-O1A	-2.63	117.05	123.63
12	L	203	CLA	C3B-C4B-NB	-2.63	108.18	110.53
12	G	816	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
12	A	837	CLA	CHB-C4A-NA	2.63	128.19	124.40
12	a	820	CLA	C3B-C4B-NB	-2.63	108.19	110.53
12	A	831	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
12	G	830	CLA	O2D-CGD-CBD	2.63	115.82	111.23
13	a	840	A1AGD	O2-C1-C6	2.63	124.66	120.48
12	l	201	CLA	C3B-C4B-NB	-2.63	108.19	110.53
23	F	205	ZEX	C1-C6-C5	-2.63	119.05	122.64
15	j	104	BCR	C15-C14-C13	-2.63	123.60	127.28
12	G	831	CLA	O2D-CGD-O1D	-2.63	118.74	123.85
12	f	204	CLA	CHB-C4A-NA	2.62	128.19	124.40
12	a	851	CLA	C3B-C4B-NB	-2.62	108.19	110.53
12	B	2108	CLA	CHB-C4A-NA	2.62	128.19	124.40
25	U	209	DGD	O6D-C1D-O3G	-2.62	103.84	110.04
16	G	846	LHG	O8-C23-C24	2.62	119.83	111.83
17	A	847	LMG	O1-C1-C2	2.62	112.26	108.27
15	J	104	BCR	C15-C14-C13	-2.62	123.60	127.28
16	a	846	LHG	O8-C23-C24	2.62	119.83	111.83
17	a	847	LMG	O1-C1-C2	2.62	112.25	108.27
12	H	2133	CLA	CHB-C4A-NA	2.62	128.18	124.40
22	B	2151	EQ3	C33-C5-C4	2.62	119.24	114.42
12	a	831	CLA	CHB-C4A-NA	2.62	128.18	124.40
12	B	2110	CLA	O2D-CGD-CBD	2.62	115.81	111.23
12	A	851	CLA	C3B-C4B-NB	-2.62	108.19	110.53
22	H	2150	EQ3	C33-C5-C4	2.62	119.24	114.42
15	T	4001	BCR	C24-C23-C22	-2.62	122.36	126.23
12	b	2108	CLA	C3B-C4B-NB	-2.62	108.19	110.53
12	B	2134	CLA	CHB-C4A-NA	2.62	128.18	124.40
15	a	844	BCR	C3-C4-C5	-2.62	109.39	114.06
12	G	851	CLA	C3B-C4B-NB	-2.62	108.19	110.53
15	G	843	BCR	C30-C25-C26	-2.62	119.06	122.64
12	G	836	CLA	O2D-CGD-O1D	-2.62	118.76	123.85
12	b	2111	CLA	CHB-C4A-NA	2.62	128.17	124.40
12	a	830	CLA	O2D-CGD-CBD	2.61	115.80	111.23
16	A	846	LHG	O8-C23-C24	2.61	119.81	111.83
12	B	2112	CLA	CHB-C4A-NA	2.61	128.17	124.40
12	H	2137	CLA	CHB-C4A-NA	2.61	128.17	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	2150	EQ3	C33-C5-C4	2.61	119.22	114.42
15	k	4001	BCR	C24-C23-C22	-2.61	122.37	126.23
23	H	2151	ZEX	C21-C26-C27	2.61	122.73	115.65
12	G	813	CLA	C3B-C4B-NB	-2.61	108.20	110.53
12	A	813	CLA	C3B-C4B-NB	-2.61	108.20	110.53
12	A	836	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
12	F	204	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
12	A	827	CLA	CMB-C2B-C3B	2.61	132.69	126.55
12	f	204	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
12	Q	204	CLA	C3B-C4B-NB	-2.61	108.20	110.53
12	G	816	CLA	CMB-C2B-C3B	2.61	132.69	126.55
12	B	2141	CLA	CHB-C4A-NA	2.61	128.16	124.40
12	B	2115	CLA	CHB-C4A-NA	2.61	128.16	124.40
12	G	827	CLA	CMB-C2B-C3B	2.61	132.68	126.55
12	G	831	CLA	C3B-C4B-NB	-2.61	108.20	110.53
12	b	2137	CLA	O2A-CGA-O1A	-2.61	117.11	123.63
12	G	832	CLA	CHB-C4A-NA	2.61	128.16	124.40
12	Q	204	CLA	CHB-C4A-NA	2.61	128.16	124.40
12	Q	204	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
12	b	2106	CLA	CMB-C2B-C1B	-2.61	121.45	125.42
23	f	205	ZEX	C1-C6-C5	-2.61	119.08	122.64
12	a	831	CLA	C3B-C4B-NB	-2.61	108.20	110.53
12	A	815	CLA	C3B-C4B-NB	-2.61	108.20	110.53
12	A	830	CLA	O2D-CGD-CBD	2.60	115.78	111.23
12	H	2102	CLA	CHB-C4A-NA	2.60	128.16	124.40
12	T	4002	CLA	C3B-C4B-NB	-2.60	108.20	110.53
12	F	204	CLA	CHB-C4A-NA	2.60	128.16	124.40
12	A	816	CLA	CMB-C2B-C3B	2.60	132.67	126.55
12	a	831	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
12	b	2102	CLA	CHB-C4A-NA	2.60	128.16	124.40
12	b	2140	CLA	CHB-C4A-NA	2.60	128.15	124.40
12	K	4002	CLA	C3B-C4B-NB	-2.60	108.21	110.53
12	B	2107	CLA	CMB-C2B-C1B	-2.60	121.46	125.42
12	a	837	CLA	CHB-C4A-NA	2.60	128.15	124.40
12	A	831	CLA	CHB-C4A-NA	2.60	128.15	124.40
12	a	836	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
15	b	2144	BCR	C40-C30-C25	2.60	114.32	110.24
15	K	4001	BCR	C24-C23-C22	-2.60	122.39	126.23
12	G	851	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
12	b	2140	CLA	O2A-CGA-O1A	-2.60	117.13	123.63
12	H	2140	CLA	O2A-CGA-O1A	-2.59	117.14	123.63
15	U	207	BCR	C15-C14-C13	-2.59	123.64	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Q	205	ZEX	C1-C6-C5	-2.59	119.09	122.64
12	A	820	CLA	C3B-C4B-NB	-2.59	108.22	110.53
12	B	2103	CLA	CHB-C4A-NA	2.59	128.14	124.40
12	B	2141	CLA	O2A-CGA-O1A	-2.59	117.15	123.63
12	a	827	CLA	CMB-C2B-C3B	2.59	132.64	126.55
15	H	2144	BCR	C40-C30-C25	2.59	114.30	110.24
12	a	816	CLA	CMB-C2B-C3B	2.59	132.64	126.55
12	A	835	CLA	C3B-C4B-NB	-2.59	108.22	110.53
12	H	2104	CLA	CBC-CAC-C3C	2.59	119.44	112.42
12	a	835	CLA	C3B-C4B-NB	-2.59	108.22	110.53
16	G	848	LHG	O8-C23-C24	2.58	119.72	111.83
12	l	203	CLA	C3B-C4B-NB	-2.58	108.22	110.53
12	B	2136	CLA	CHB-C4A-NA	2.58	128.13	124.40
12	H	2106	CLA	CMB-C2B-C1B	-2.58	121.48	125.42
12	b	2104	CLA	CBC-CAC-C3C	2.58	119.42	112.42
12	B	2105	CLA	CBC-CAC-C3C	2.58	119.42	112.42
12	a	802	CLA	C3B-C4B-NB	-2.58	108.22	110.53
15	A	843	BCR	C40-C30-C25	2.58	114.29	110.24
12	G	815	CLA	C3B-C4B-NB	-2.58	108.23	110.53
12	L	201	CLA	C3B-C4B-NB	-2.58	108.23	110.53
15	B	2145	BCR	C40-C30-C25	2.58	114.29	110.24
12	G	820	CLA	C3B-C4B-NB	-2.58	108.23	110.53
12	H	2140	CLA	CHB-C4A-NA	2.58	128.12	124.40
16	a	848	LHG	O8-C23-C24	2.58	119.70	111.83
12	G	815	CLA	CHB-C4A-NA	2.58	128.12	124.40
12	k	4002	CLA	C3B-C4B-NB	-2.58	108.23	110.53
12	a	808	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
12	U	204	CLA	O2D-CGD-CBD	2.58	115.73	111.23
24	M	101	SQD	O6-C1-C2	2.58	112.18	108.27
15	a	843	BCR	C40-C30-C25	2.57	114.28	110.24
12	B	2127	CLA	CHB-C4A-NA	2.57	128.12	124.40
16	A	848	LHG	O8-C23-C24	2.57	119.68	111.83
15	i	101	BCR	C27-C26-C25	2.57	126.18	122.70
12	A	832	CLA	CHB-C4A-NA	2.57	128.11	124.40
15	I	101	BCR	C27-C26-C25	2.57	126.18	122.70
12	G	835	CLA	C3B-C4B-NB	-2.57	108.23	110.53
12	G	831	CLA	CHB-C4A-NA	2.57	128.11	124.40
12	a	829	CLA	CHB-C4A-NA	2.57	128.11	124.40
12	H	2135	CLA	CHB-C4A-NA	2.57	128.11	124.40
12	a	815	CLA	CHB-C4A-NA	2.57	128.11	124.40
12	b	2114	CLA	CHB-C4A-NA	2.57	128.11	124.40
12	H	2114	CLA	CHB-C4A-NA	2.57	128.11	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	L	207	BCR	C15-C14-C13	-2.57	123.68	127.28
12	A	831	CLA	C3B-C4B-NB	-2.57	108.24	110.53
12	A	808	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
12	A	815	CLA	CHB-C4A-NA	2.57	128.10	124.40
12	A	851	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
15	l	207	BCR	C24-C23-C22	-2.57	122.44	126.23
12	B	2102	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
12	a	824	CLA	CMB-C2B-C1B	-2.56	121.51	125.42
12	H	2126	CLA	CHB-C4A-NA	2.56	128.10	124.40
12	L	204	CLA	O2D-CGD-CBD	2.56	115.71	111.23
13	A	840	A1AGD	C20-C19-C18	2.56	120.41	111.27
12	A	802	CLA	C3B-C4B-NB	-2.56	108.24	110.53
15	G	843	BCR	C40-C30-C25	2.56	114.26	110.24
12	H	2101	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
12	G	824	CLA	CMB-C2B-C1B	-2.56	121.52	125.42
12	A	824	CLA	CMB-C2B-C1B	-2.56	121.52	125.42
13	a	840	A1AGD	C20-C19-C18	2.56	120.40	111.27
12	A	822	CLA	C3B-C4B-NB	-2.56	108.24	110.53
13	G	840	A1AGD	C20-C19-C18	2.56	120.40	111.27
12	b	2101	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
12	b	2135	CLA	CHB-C4A-NA	2.56	128.09	124.40
12	l	204	CLA	O2D-CGD-CBD	2.56	115.70	111.23
12	G	808	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
12	G	822	CLA	C3B-C4B-NB	-2.56	108.25	110.53
12	b	2126	CLA	CHB-C4A-NA	2.55	128.09	124.40
12	a	851	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
15	T	4001	BCR	C27-C26-C25	2.55	126.15	122.70
12	S	103	CLA	CHB-C4A-NA	2.55	128.08	124.40
12	b	2112	CLA	C3B-C4B-NB	-2.55	108.26	110.53
12	a	832	CLA	CHB-C4A-NA	2.55	128.07	124.40
12	G	802	CLA	C3B-C4B-NB	-2.54	108.26	110.53
12	U	201	CLA	C3B-C4B-NB	-2.54	108.26	110.53
12	A	831	CLA	C1-C2-C3	-2.54	122.03	126.20
12	A	809	CLA	CHB-C4A-NA	2.54	128.07	124.40
12	a	822	CLA	C3B-C4B-NB	-2.54	108.26	110.53
24	m	102	SQD	O6-C1-C2	2.54	112.13	108.27
15	R	101	BCR	C27-C26-C25	2.54	126.14	122.70
12	B	2101	CLA	C3B-C4B-NB	-2.54	108.26	110.53
15	S	104	BCR	C11-C10-C9	-2.54	123.72	127.28
15	L	207	BCR	C24-C23-C22	-2.54	122.48	126.23
12	J	103	CLA	CHB-C4A-NA	2.54	128.06	124.40
12	a	821	CLA	CHB-C4A-NA	2.54	128.06	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	a	822	CLA	CHB-C4A-NA	2.54	128.06	124.40
12	G	838	CLA	C3B-C4B-NB	-2.54	108.27	110.53
15	l	207	BCR	C15-C14-C13	-2.54	123.72	127.28
12	G	822	CLA	CHB-C4A-NA	2.54	128.06	124.40
12	G	818	CLA	CMB-C2B-C1B	-2.54	121.56	125.42
12	A	829	CLA	CHB-C4A-NA	2.54	128.06	124.40
12	H	2119	CLA	C4-C3-C5	2.53	119.63	115.23
12	G	809	CLA	CHB-C4A-NA	2.53	128.06	124.40
12	A	821	CLA	CHB-C4A-NA	2.53	128.06	124.40
12	b	2119	CLA	C4-C3-C5	2.53	119.62	115.23
15	U	207	BCR	C24-C23-C22	-2.53	122.49	126.23
15	K	4001	BCR	C27-C26-C25	2.53	126.13	122.70
12	B	2113	CLA	C3B-C4B-NB	-2.53	108.27	110.53
15	H	2144	BCR	C3-C4-C5	-2.53	109.54	114.06
12	A	838	CLA	C3B-C4B-NB	-2.53	108.27	110.53
12	G	829	CLA	CHB-C4A-NA	2.53	128.05	124.40
15	J	104	BCR	C11-C10-C9	-2.53	123.73	127.28
15	b	2144	BCR	C3-C4-C5	-2.53	109.55	114.06
12	A	854	CLA	C3B-C4B-NB	-2.53	108.27	110.53
12	b	2125	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
15	j	101	BCR	C15-C16-C17	-2.53	118.35	123.52
12	a	809	CLA	CHB-C4A-NA	2.53	128.04	124.40
12	H	2152	CLA	C3B-C4B-NB	-2.52	108.28	110.53
12	B	2115	CLA	C3B-C4B-NB	-2.52	108.28	110.53
12	A	822	CLA	CHB-C4A-NA	2.52	128.04	124.40
12	b	2114	CLA	C3B-C4B-NB	-2.52	108.28	110.53
15	B	2145	BCR	C3-C4-C5	-2.52	109.56	114.06
12	B	2126	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
12	B	2120	CLA	C4-C3-C5	2.52	119.61	115.23
12	a	836	CLA	CHB-C4A-NA	2.52	128.04	124.40
12	a	854	CLA	C3B-C4B-NB	-2.52	108.28	110.53
12	j	103	CLA	CHB-C4A-NA	2.52	128.04	124.40
12	a	831	CLA	C1-C2-C3	-2.52	122.07	126.20
12	G	831	CLA	C1-C2-C3	-2.52	122.07	126.20
12	H	2116	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
12	U	203	CLA	CMB-C2B-C3B	2.52	132.47	126.55
24	V	102	SQD	O6-C1-C2	2.52	112.10	108.27
15	k	4001	BCR	C27-C26-C25	2.52	126.11	122.70
12	a	803	CLA	CMB-C2B-C1B	-2.52	121.59	125.42
15	j	104	BCR	C11-C10-C9	-2.51	123.75	127.28
12	B	2117	CLA	O2D-CGD-O1D	-2.51	118.95	123.85
12	G	807	CLA	CMB-C2B-C1B	-2.51	121.59	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	H	2153	A1AGD	C11-C9-C8	-2.51	115.53	121.17
12	b	2117	CLA	C3B-C4B-NB	-2.51	108.29	110.53
12	b	2104	CLA	CHB-C4A-NA	2.51	128.03	124.40
15	J	101	BCR	C15-C16-C17	-2.51	118.38	123.52
12	a	818	CLA	CMB-C2B-C1B	-2.51	121.59	125.42
12	G	821	CLA	CHB-C4A-NA	2.51	128.03	124.40
12	b	2116	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
12	A	802	CLA	O2D-CGD-CBD	2.51	115.62	111.23
12	l	203	CLA	CMB-C2B-C3B	2.51	132.45	126.55
12	L	203	CLA	CMB-C2B-C3B	2.51	132.45	126.55
12	H	2104	CLA	CHB-C4A-NA	2.51	128.02	124.40
12	G	802	CLA	O2D-CGD-CBD	2.51	115.62	111.23
12	G	854	CLA	C3B-C4B-NB	-2.51	108.29	110.53
12	b	2105	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
12	a	838	CLA	C3B-C4B-NB	-2.51	108.29	110.53
12	H	2125	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
15	S	101	BCR	C15-C16-C17	-2.51	118.39	123.52
12	a	802	CLA	O2D-CGD-CBD	2.51	115.61	111.23
12	b	2152	CLA	C3B-C4B-NB	-2.50	108.29	110.53
12	B	2105	CLA	CHB-C4A-NA	2.50	128.01	124.40
12	a	839	CLA	CHB-C4A-NA	2.50	128.01	124.40
12	A	803	CLA	CMB-C2B-C1B	-2.50	121.61	125.42
12	H	2114	CLA	C3B-C4B-NB	-2.50	108.30	110.53
12	B	2139	CLA	C3B-C4B-NB	-2.50	108.30	110.53
12	a	828	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
12	G	803	CLA	CMB-C2B-C1B	-2.50	121.61	125.42
12	A	818	CLA	CMB-C2B-C1B	-2.50	121.61	125.42
12	B	2119	CLA	CHB-C4A-NA	2.50	128.01	124.40
12	a	805	CLA	C1-C2-C3	-2.50	122.10	126.20
13	B	2153	A1AGD	C11-C9-C8	-2.50	115.56	121.17
12	H	2118	CLA	CHB-C4A-NA	2.50	128.00	124.40
12	a	830	CLA	CHB-C4A-NA	2.50	128.00	124.40
12	A	839	CLA	CHB-C4A-NA	2.50	128.00	124.40
12	B	2106	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
13	b	2153	A1AGD	C11-C9-C8	-2.50	115.56	121.17
12	G	828	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
12	G	839	CLA	CHB-C4A-NA	2.50	128.00	124.40
12	G	836	CLA	CHB-C4A-NA	2.49	128.00	124.40
12	H	2117	CLA	C3B-C4B-NB	-2.49	108.30	110.53
12	a	807	CLA	CMB-C2B-C1B	-2.49	121.62	125.42
12	b	2138	CLA	C3B-C4B-NB	-2.49	108.31	110.53
12	A	828	CLA	O2D-CGD-O1D	-2.49	119.00	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	a	846	LHG	C11-C10-C9	-2.49	101.77	114.37
15	Q	202	BCR	C1-C6-C5	-2.49	119.23	122.64
12	H	2124	CLA	CMB-C2B-C1B	-2.49	121.63	125.42
12	a	804	CLA	CAC-C3C-C4C	2.49	128.03	124.79
12	B	2118	CLA	C3B-C4B-NB	-2.49	108.31	110.53
12	a	820	CLA	CHB-C4A-NA	2.49	127.99	124.40
15	F	202	BCR	C1-C6-C5	-2.49	119.23	122.64
16	G	846	LHG	C11-C10-C9	-2.49	101.79	114.37
12	A	836	CLA	CHB-C4A-NA	2.49	127.99	124.40
12	G	805	CLA	CMB-C2B-C1B	-2.49	121.63	125.42
12	A	807	CLA	CMB-C2B-C1B	-2.49	121.63	125.42
16	A	846	LHG	C11-C10-C9	-2.49	101.80	114.37
12	A	817	CLA	CHB-C4A-NA	2.48	127.99	124.40
12	A	805	CLA	C1-C2-C3	-2.48	122.13	126.20
12	b	2118	CLA	CHB-C4A-NA	2.48	127.98	124.40
12	a	817	CLA	CHB-C4A-NA	2.48	127.98	124.40
12	H	2112	CLA	C3B-C4B-NB	-2.48	108.31	110.53
12	H	2138	CLA	C3B-C4B-NB	-2.48	108.32	110.53
15	f	202	BCR	C1-C6-C5	-2.48	119.25	122.64
12	b	2124	CLA	CMB-C2B-C1B	-2.48	121.65	125.42
12	G	817	CLA	CHB-C4A-NA	2.48	127.97	124.40
12	A	804	CLA	CAC-C3C-C4C	2.47	128.01	124.79
12	B	2103	CLA	O2A-CGA-O1A	-2.47	117.44	123.63
12	L	205	CLA	CHB-C4A-NA	2.47	127.97	124.40
12	H	2105	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
12	A	820	CLA	CHB-C4A-NA	2.47	127.97	124.40
12	b	2102	CLA	O2A-CGA-O1A	-2.47	117.45	123.63
12	a	854	CLA	CHB-C4A-NA	2.47	127.97	124.40
12	A	802	CLA	CHB-C4A-NA	2.47	127.97	124.40
22	b	2150	EQ3	C7-C8-C9	-2.47	122.58	126.23
12	l	201	CLA	CHB-C4A-NA	2.47	127.96	124.40
12	a	805	CLA	CMB-C2B-C1B	-2.47	121.66	125.42
12	G	830	CLA	CHB-C4A-NA	2.47	127.96	124.40
12	A	805	CLA	CMB-C2B-C1B	-2.47	121.66	125.42
12	a	807	CLA	O2A-CGA-O1A	-2.47	117.45	123.63
15	S	101	BCR	C7-C8-C9	-2.47	122.58	126.23
12	l	205	CLA	CHB-C4A-NA	2.47	127.96	124.40
12	B	2125	CLA	CMB-C2B-C1B	-2.47	121.66	125.42
22	B	2151	EQ3	C7-C8-C9	-2.47	122.59	126.23
12	U	201	CLA	CHB-C4A-NA	2.47	127.96	124.40
12	A	807	CLA	O2A-CGA-O1A	-2.47	117.46	123.63
12	G	804	CLA	CAC-C3C-C4C	2.47	128.00	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	G	807	CLA	O2A-CGA-O1A	-2.47	117.46	123.63
15	j	101	BCR	C11-C10-C9	-2.46	123.82	127.28
12	A	830	CLA	CHB-C4A-NA	2.46	127.95	124.40
15	A	845	BCR	C15-C14-C13	-2.46	123.83	127.28
12	a	827	CLA	CHB-C4A-NA	2.46	127.95	124.40
12	A	835	CLA	CMB-C2B-C3B	2.46	132.34	126.55
12	a	808	CLA	C3B-C4B-NB	-2.46	108.33	110.53
12	H	2121	CLA	CHB-C4A-NA	2.46	127.95	124.40
12	B	2135	CLA	C3B-C4B-NB	-2.46	108.33	110.53
15	J	101	BCR	C11-C10-C9	-2.46	123.83	127.28
12	G	805	CLA	C1-C2-C3	-2.46	122.17	126.20
12	H	2102	CLA	O2A-CGA-O1A	-2.46	117.48	123.63
15	G	845	BCR	C15-C14-C13	-2.46	123.83	127.28
12	G	835	CLA	CMB-C2B-C3B	2.46	132.33	126.55
12	G	820	CLA	CHB-C4A-NA	2.46	127.94	124.40
12	b	2111	CLA	O2D-CGD-CBD	2.45	115.52	111.23
12	A	827	CLA	CHB-C4A-NA	2.45	127.94	124.40
12	a	835	CLA	CMB-C2B-C3B	2.45	132.32	126.55
12	A	854	CLA	CHB-C4A-NA	2.45	127.94	124.40
12	L	201	CLA	CHB-C4A-NA	2.45	127.94	124.40
12	G	827	CLA	CHB-C4A-NA	2.45	127.94	124.40
12	G	814	CLA	CMB-C2B-C3B	2.45	132.31	126.55
22	H	2150	EQ3	C7-C8-C9	-2.45	122.61	126.23
12	a	814	CLA	CMB-C2B-C3B	2.45	132.31	126.55
12	A	814	CLA	CMB-C2B-C3B	2.45	132.31	126.55
12	B	2112	CLA	O2D-CGD-CBD	2.45	115.51	111.23
12	a	802	CLA	CHB-C4A-NA	2.45	127.93	124.40
12	H	2127	CLA	CHB-C4A-NA	2.44	127.93	124.40
15	b	2146	BCR	C3-C4-C5	-2.44	109.70	114.06
15	H	2146	BCR	C3-C4-C5	-2.44	109.70	114.06
12	B	2114	CLA	CHB-C4A-NA	2.44	127.93	124.40
12	U	205	CLA	CHB-C4A-NA	2.44	127.92	124.40
12	H	2134	CLA	CMB-C2B-C1B	-2.44	121.70	125.42
15	J	101	BCR	C7-C8-C9	-2.44	122.62	126.23
12	G	802	CLA	CHB-C4A-NA	2.44	127.92	124.40
12	b	2134	CLA	CMB-C2B-C1B	-2.44	121.70	125.42
12	B	2135	CLA	CMB-C2B-C1B	-2.44	121.70	125.42
16	A	848	LHG	C11-C10-C9	-2.44	102.03	114.37
12	B	2128	CLA	CHB-C4A-NA	2.44	127.92	124.40
12	H	2131	CLA	C3B-C4B-NB	-2.44	108.35	110.53
16	G	848	LHG	C11-C10-C9	-2.44	102.04	114.37
12	b	2113	CLA	CHB-C4A-NA	2.44	127.92	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	2132	CLA	C3B-C4B-NB	-2.44	108.35	110.53
12	b	2114	CLA	C1-C2-C3	-2.44	122.20	126.20
12	b	2121	CLA	CHB-C4A-NA	2.44	127.92	124.40
16	a	848	LHG	C11-C10-C9	-2.44	102.05	114.37
12	H	2123	CLA	C3B-C4B-NB	-2.44	108.36	110.53
12	G	854	CLA	CHB-C4A-NA	2.43	127.91	124.40
12	B	2122	CLA	CHB-C4A-NA	2.43	127.91	124.40
12	b	2131	CLA	C3B-C4B-NB	-2.43	108.36	110.53
15	H	2146	BCR	C15-C14-C13	-2.43	123.87	127.28
15	a	845	BCR	C15-C14-C13	-2.43	123.87	127.28
12	B	2115	CLA	C1-C2-C3	-2.43	122.22	126.20
15	j	101	BCR	C7-C8-C9	-2.43	122.64	126.23
15	B	2147	BCR	C15-C14-C13	-2.43	123.87	127.28
12	a	832	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
15	S	101	BCR	C11-C10-C9	-2.43	123.87	127.28
12	H	2111	CLA	O2D-CGD-CBD	2.43	115.47	111.23
12	G	832	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
12	b	2123	CLA	C3B-C4B-NB	-2.43	108.36	110.53
12	A	835	CLA	O2D-CGD-O1D	-2.43	119.13	123.85
12	a	854	CLA	CMB-C2B-C1B	-2.43	121.73	125.42
12	B	2139	CLA	CHB-C4A-NA	2.43	127.90	124.40
12	b	2131	CLA	CMB-C2B-C1B	-2.42	121.73	125.42
12	B	2124	CLA	C3B-C4B-NB	-2.42	108.37	110.53
12	a	835	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
12	G	851	CLA	CHB-C4A-NA	2.42	127.89	124.40
12	b	2136	CLA	C3B-C4B-NB	-2.42	108.37	110.53
12	H	2138	CLA	CHB-C4A-NA	2.42	127.89	124.40
12	H	2134	CLA	C3B-C4B-NB	-2.42	108.37	110.53
12	A	851	CLA	CHB-C4A-NA	2.42	127.89	124.40
12	A	854	CLA	CMB-C2B-C1B	-2.42	121.74	125.42
12	a	830	CLA	CBC-CAC-C3C	2.42	118.97	112.42
12	A	830	CLA	CBC-CAC-C3C	2.42	118.97	112.42
15	B	2147	BCR	C3-C4-C5	-2.42	109.75	114.06
12	H	2114	CLA	C1-C2-C3	-2.42	122.24	126.20
12	G	810	CLA	C3B-C4B-NB	-2.42	108.37	110.53
12	G	854	CLA	CMB-C2B-C1B	-2.41	121.74	125.42
13	G	840	A1AGD	O2-C1-C2	-2.41	116.34	121.83
12	a	826	CLA	CHB-C4A-NA	2.41	127.88	124.40
12	A	808	CLA	C3B-C4B-NB	-2.41	108.38	110.53
12	H	2113	CLA	CHB-C4A-NA	2.41	127.88	124.40
12	b	2134	CLA	C3B-C4B-NB	-2.41	108.38	110.53
12	a	851	CLA	CHB-C4A-NA	2.41	127.88	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	b	2127	CLA	CHB-C4A-NA	2.41	127.88	124.40
16	M	102	LHG	C11-C10-C9	-2.41	102.18	114.37
12	H	2127	CLA	C3B-C4B-NB	-2.41	108.38	110.53
12	H	2123	CLA	CMB-C2B-C1B	-2.41	121.75	125.42
13	A	840	A1AGD	C7-C8-C9	-2.41	122.68	126.83
12	b	2138	CLA	CHB-C4A-NA	2.41	127.88	124.40
13	A	840	A1AGD	O2-C1-C2	-2.41	116.36	121.83
13	a	840	A1AGD	O2-C1-C2	-2.41	116.36	121.83
12	G	808	CLA	C3B-C4B-NB	-2.41	108.38	110.53
16	m	103	LHG	C11-C10-C9	-2.41	102.21	114.37
12	G	830	CLA	CBC-CAC-C3C	2.41	118.94	112.42
12	B	2132	CLA	CMB-C2B-C1B	-2.41	121.76	125.42
12	A	832	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
12	B	2137	CLA	C3B-C4B-NB	-2.40	108.39	110.53
12	a	825	CLA	CMB-C2B-C1B	-2.40	121.76	125.42
12	A	810	CLA	C3B-C4B-NB	-2.40	108.39	110.53
16	V	103	LHG	C11-C10-C9	-2.40	102.23	114.37
12	G	835	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
13	G	840	A1AGD	C7-C8-C9	-2.40	122.70	126.83
15	b	2146	BCR	C15-C14-C13	-2.40	123.92	127.28
15	S	101	BCR	C15-C14-C13	-2.40	123.92	127.28
12	A	825	CLA	CMB-C2B-C1B	-2.39	121.77	125.42
12	a	831	CLA	CMB-C2B-C3B	2.39	132.18	126.55
13	a	840	A1AGD	C7-C8-C9	-2.39	122.71	126.83
15	k	4001	BCR	C3-C4-C5	-2.39	109.79	114.06
12	A	826	CLA	CHB-C4A-NA	2.39	127.85	124.40
12	G	831	CLA	CMB-C2B-C3B	2.39	132.17	126.55
12	a	807	CLA	CAA-C2A-C1A	-2.39	104.15	111.97
12	b	2115	CLA	C3B-C4B-NB	-2.39	108.40	110.53
12	b	2119	CLA	C3B-C4B-NB	-2.39	108.40	110.53
12	B	2124	CLA	CMB-C2B-C1B	-2.39	121.78	125.42
12	U	205	CLA	CMB-C2B-C1B	-2.39	121.78	125.42
12	A	831	CLA	CMB-C2B-C3B	2.39	132.16	126.55
12	A	807	CLA	CAA-C2A-C1A	-2.39	104.16	111.97
12	H	2131	CLA	CMB-C2B-C1B	-2.39	121.79	125.42
12	b	2127	CLA	C3B-C4B-NB	-2.38	108.40	110.53
13	A	840	A1AGD	C20-C19-C21	2.38	119.77	111.27
12	A	830	CLA	CMB-C2B-C3B	2.38	132.16	126.55
12	G	825	CLA	CHB-C4A-NA	2.38	127.84	124.40
13	G	840	A1AGD	C20-C19-C21	2.38	119.77	111.27
15	j	101	BCR	C15-C14-C13	-2.38	123.94	127.28
12	G	807	CLA	CAA-C2A-C1A	-2.38	104.17	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	2120	CLA	C3B-C4B-NB	-2.38	108.41	110.53
15	K	4001	BCR	C3-C4-C5	-2.38	109.81	114.06
22	H	2150	EQ3	C33-C5-C6	-2.38	121.89	124.48
12	G	825	CLA	CMB-C2B-C1B	-2.38	121.80	125.42
15	J	101	BCR	C15-C14-C13	-2.38	123.94	127.28
12	B	2128	CLA	C3B-C4B-NB	-2.38	108.41	110.53
13	a	840	A1AGD	C20-C19-C21	2.38	119.74	111.27
12	a	830	CLA	CMB-C2B-C3B	2.38	132.14	126.55
12	U	205	CLA	O2D-CGD-CBD	2.38	115.38	111.23
12	G	830	CLA	CMB-C2B-C3B	2.37	132.13	126.55
12	H	2136	CLA	C3B-C4B-NB	-2.37	108.41	110.53
12	b	2127	CLA	CMB-C2B-C1B	-2.37	121.81	125.42
15	T	4001	BCR	C3-C4-C5	-2.37	109.83	114.06
12	A	809	CLA	CAA-C2A-C3A	-2.37	106.60	113.00
12	L	205	CLA	CMB-C2B-C1B	-2.37	121.81	125.42
12	b	2123	CLA	CMB-C2B-C1B	-2.37	121.81	125.42
12	H	2133	CLA	C3B-C4B-NB	-2.37	108.42	110.53
12	G	809	CLA	CAA-C2A-C3A	-2.37	106.60	113.00
12	l	205	CLA	O2D-CGD-CBD	2.37	115.37	111.23
17	A	847	LMG	C38-C37-C36	-2.37	102.41	114.37
22	B	2151	EQ3	C33-C5-C6	-2.37	121.90	124.48
12	a	809	CLA	CAA-C2A-C3A	-2.36	106.61	113.00
17	a	847	LMG	C38-C37-C36	-2.36	102.42	114.37
12	H	2124	CLA	C3B-C4B-NB	-2.36	108.42	110.53
12	H	2115	CLA	C3B-C4B-NB	-2.36	108.42	110.53
17	G	847	LMG	C38-C37-C36	-2.36	102.43	114.37
12	a	825	CLA	CHB-C4A-NA	2.36	127.81	124.40
12	B	2128	CLA	CMB-C2B-C1B	-2.36	121.83	125.42
12	L	205	CLA	O2D-CGD-CBD	2.36	115.35	111.23
12	G	826	CLA	CHB-C4A-NA	2.35	127.80	124.40
16	b	2148	LHG	C11-C10-C9	-2.35	102.47	114.37
12	l	205	CLA	CMB-C2B-C1B	-2.35	121.83	125.42
15	B	2145	BCR	C11-C10-C9	-2.35	123.98	127.28
12	B	2105	CLA	O1D-CGD-CBD	2.35	129.16	124.52
16	B	2149	LHG	C11-C10-C9	-2.35	102.48	114.37
12	B	2116	CLA	C3B-C4B-NB	-2.35	108.43	110.53
12	B	2126	CLA	C3B-C4B-NB	-2.35	108.43	110.53
12	a	824	CLA	C2A-C1A-CHA	2.35	127.95	123.87
12	b	2125	CLA	CHB-C4A-NA	2.35	127.79	124.40
12	A	825	CLA	CHB-C4A-NA	2.35	127.79	124.40
12	B	2126	CLA	CHB-C4A-NA	2.35	127.79	124.40
12	b	2104	CLA	O1D-CGD-CBD	2.35	129.15	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	824	CLA	C2A-C1A-CHA	2.35	127.94	123.87
12	H	2119	CLA	C3B-C4B-NB	-2.35	108.43	110.53
12	H	2125	CLA	CHB-C4A-NA	2.35	127.79	124.40
16	H	2148	LHG	C11-C10-C9	-2.35	102.51	114.37
12	a	810	CLA	C3B-C4B-NB	-2.34	108.44	110.53
12	H	2133	CLA	O2D-CGD-CBD	2.34	115.33	111.23
22	b	2150	EQ3	C33-C5-C6	-2.34	121.93	124.48
15	R	101	BCR	C16-C15-C14	-2.34	118.72	123.52
12	a	812	CLA	C3B-C4B-NB	-2.34	108.44	110.53
12	A	850	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
17	B	2148	LMG	C40-C39-C38	-2.34	102.54	114.37
12	H	2125	CLA	C3B-C4B-NB	-2.34	108.44	110.53
12	H	2104	CLA	O1D-CGD-CBD	2.34	129.13	124.52
17	b	2147	LMG	C40-C39-C38	-2.34	102.55	114.37
15	I	101	BCR	C16-C15-C14	-2.34	118.74	123.52
12	a	807	CLA	CMB-C2B-C3B	2.34	132.05	126.55
12	G	824	CLA	C2A-C1A-CHA	2.34	127.92	123.87
22	H	2150	EQ3	C29-C28-C27	2.34	116.98	112.71
12	b	2136	CLA	CHB-C4A-NA	2.34	127.77	124.40
12	a	850	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
17	H	2147	LMG	C40-C39-C38	-2.33	102.57	114.37
15	H	2144	BCR	C11-C10-C9	-2.33	124.00	127.28
17	G	849	LMG	O6-C1-O1	-2.33	104.53	110.04
12	G	850	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
16	a	846	LHG	C20-C19-C18	-2.33	102.59	114.37
16	G	846	LHG	C20-C19-C18	-2.33	102.59	114.37
15	i	101	BCR	C16-C15-C14	-2.33	118.75	123.52
17	A	849	LMG	O6-C1-O1	-2.33	104.54	110.04
15	b	2144	BCR	C11-C10-C9	-2.33	124.01	127.28
16	A	846	LHG	C20-C19-C18	-2.33	102.60	114.37
12	G	804	CLA	CMB-C2B-C3B	2.33	132.03	126.55
22	B	2151	EQ3	C29-C28-C27	2.33	116.97	112.71
12	H	2121	CLA	CMB-C2B-C1B	-2.33	121.88	125.42
12	G	803	CLA	CMB-C2B-C3B	2.33	132.02	126.55
12	H	2127	CLA	CMB-C2B-C1B	-2.32	121.88	125.42
12	B	2136	CLA	CMB-C2B-C1B	-2.32	121.88	125.42
12	H	2136	CLA	CHB-C4A-NA	2.32	127.75	124.40
12	a	803	CLA	CMB-C2B-C3B	2.32	132.02	126.55
22	b	2150	EQ3	C29-C28-C27	2.32	116.96	112.71
12	B	2137	CLA	CHB-C4A-NA	2.32	127.75	124.40
12	G	807	CLA	CMB-C2B-C3B	2.32	132.01	126.55
12	B	2134	CLA	O2D-CGD-CBD	2.32	115.29	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	G	812	CLA	C3B-C4B-NB	-2.32	108.46	110.53
17	a	849	LMG	O6-C1-O1	-2.32	104.56	110.04
12	b	2117	CLA	C2A-C1A-CHA	2.32	127.90	123.87
12	H	2106	CLA	CMB-C2B-C3B	2.32	132.01	126.55
12	A	803	CLA	CMB-C2B-C3B	2.32	132.01	126.55
12	A	807	CLA	CMB-C2B-C3B	2.32	132.01	126.55
12	B	2134	CLA	C3B-C4B-NB	-2.32	108.46	110.53
12	A	812	CLA	C3B-C4B-NB	-2.32	108.46	110.53
12	H	2135	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
12	G	830	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
12	B	2125	CLA	C3B-C4B-NB	-2.32	108.46	110.53
12	a	804	CLA	CMB-C2B-C3B	2.31	132.00	126.55
12	b	2133	CLA	O2D-CGD-CBD	2.31	115.28	111.23
12	b	2106	CLA	CMB-C2B-C3B	2.31	131.99	126.55
12	B	2107	CLA	CMB-C2B-C3B	2.31	131.98	126.55
12	a	817	CLA	CMB-C2B-C1B	-2.31	121.90	125.42
12	b	2135	CLA	CMB-C2B-C1B	-2.31	121.90	125.42
12	A	804	CLA	CMB-C2B-C3B	2.31	131.98	126.55
12	A	830	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
12	b	2113	CLA	O2D-CGD-CBD	2.31	115.26	111.23
15	H	2142	BCR	C30-C25-C26	-2.31	119.48	122.64
12	b	2133	CLA	C3B-C4B-NB	-2.31	108.47	110.53
12	b	2121	CLA	CMB-C2B-C1B	-2.31	121.91	125.42
12	G	834	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
12	A	834	CLA	O2A-CGA-O1A	-2.30	117.86	123.63
12	B	2111	CLA	CMB-C2B-C1B	-2.30	121.91	125.42
12	B	2118	CLA	C2A-C1A-CHA	2.30	127.86	123.87
12	H	2105	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
16	G	848	LHG	C20-C19-C18	-2.30	102.74	114.37
12	B	2105	CLA	CMB-C2B-C3B	2.30	131.96	126.55
12	B	2122	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
12	H	2106	CLA	C3B-C4B-NB	-2.30	108.48	110.53
12	H	2125	CLA	CAA-C2A-C1A	-2.30	104.44	111.97
16	A	848	LHG	C20-C19-C18	-2.30	102.75	114.37
17	A	847	LMG	C40-C39-C38	-2.30	102.75	114.37
12	b	2125	CLA	C3B-C4B-NB	-2.30	108.48	110.53
17	a	847	LMG	C40-C39-C38	-2.30	102.75	114.37
12	F	201	CLA	CHB-C4A-NA	2.30	127.72	124.40
16	a	848	LHG	C20-C19-C18	-2.30	102.75	114.37
12	a	830	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
12	H	2110	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
24	V	102	SQD	C4-C3-C2	2.30	114.86	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	b	2104	CLA	CMB-C2B-C3B	2.30	131.95	126.55
17	b	2147	LMG	C38-C37-C36	-2.30	102.76	114.37
12	A	817	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
17	G	847	LMG	C40-C39-C38	-2.30	102.77	114.37
17	B	2148	LMG	C38-C37-C36	-2.30	102.77	114.37
12	a	805	CLA	CAA-CBA-CGA	-2.29	106.69	113.21
12	a	834	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
15	B	2143	BCR	C30-C25-C26	-2.29	119.50	122.64
12	A	805	CLA	CAA-CBA-CGA	-2.29	106.70	113.21
12	B	2126	CLA	CAA-C2A-C1A	-2.29	104.47	111.97
17	H	2147	LMG	C38-C37-C36	-2.29	102.79	114.37
12	B	2114	CLA	O2D-CGD-CBD	2.29	115.23	111.23
12	B	2106	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
12	G	805	CLA	CAA-CBA-CGA	-2.29	106.71	113.21
12	b	2105	CLA	CMB-C2B-C1B	-2.29	121.94	125.42
12	b	2110	CLA	CMB-C2B-C1B	-2.29	121.94	125.42
12	H	2117	CLA	C2A-C1A-CHA	2.28	127.83	123.87
12	b	2125	CLA	CAA-C2A-C1A	-2.28	104.49	111.97
12	H	2104	CLA	CMB-C2B-C3B	2.28	131.92	126.55
15	S	104	BCR	C33-C5-C6	-2.28	121.99	124.48
12	B	2130	CLA	CHB-C4A-NA	2.28	127.69	124.40
12	G	805	CLA	C3B-C4B-NB	-2.28	108.49	110.53
12	b	2124	CLA	C3B-C4B-NB	-2.28	108.49	110.53
12	A	805	CLA	C3B-C4B-NB	-2.28	108.49	110.53
12	H	2129	CLA	CHB-C4A-NA	2.28	127.69	124.40
12	A	801	CLA	CED-O2D-CGD	-2.28	110.75	115.92
12	Q	201	CLA	CHB-C4A-NA	2.28	127.69	124.40
15	j	104	BCR	C33-C5-C6	-2.28	122.00	124.48
12	f	203	CLA	CHB-C4A-NA	2.28	127.69	124.40
12	G	801	CLA	CED-O2D-CGD	-2.28	110.75	115.92
15	b	2142	BCR	C30-C25-C26	-2.28	119.53	122.64
12	B	2120	CLA	CMB-C2B-C1B	-2.27	121.95	125.42
16	a	848	LHG	C18-C17-C16	-2.27	102.88	114.37
12	A	828	CLA	CHB-C4A-NA	2.27	127.68	124.40
12	a	809	CLA	CBA-CAA-C2A	2.27	120.55	113.79
16	m	103	LHG	C27-C26-C25	-2.27	102.89	114.37
12	a	824	CLA	C3B-C4B-NB	-2.27	108.50	110.53
16	V	103	LHG	C27-C26-C25	-2.27	102.89	114.37
12	F	203	CLA	CHB-C4A-NA	2.27	127.68	124.40
16	A	848	LHG	C18-C17-C16	-2.27	102.89	114.37
16	M	102	LHG	C27-C26-C25	-2.27	102.89	114.37
24	m	102	SQD	C4-C3-C2	2.27	114.81	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	a	801	CLA	CED-O2D-CGD	-2.27	110.77	115.92
12	b	2129	CLA	CHB-C4A-NA	2.27	127.67	124.40
12	G	817	CLA	CMB-C2B-C1B	-2.27	121.97	125.42
12	b	2119	CLA	CMB-C2B-C1B	-2.27	121.97	125.42
12	H	2113	CLA	O2D-CGD-CBD	2.27	115.19	111.23
12	H	2139	CLA	CAA-C2A-C3A	-2.27	106.88	113.00
12	b	2128	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
12	A	809	CLA	CBA-CAA-C2A	2.27	120.53	113.79
24	M	101	SQD	C4-C3-C2	2.26	114.81	110.83
12	a	828	CLA	CHB-C4A-NA	2.26	127.67	124.40
16	G	848	LHG	C18-C17-C16	-2.26	102.92	114.37
12	f	201	CLA	CHB-C4A-NA	2.26	127.67	124.40
12	b	2106	CLA	C3B-C4B-NB	-2.26	108.51	110.53
15	j	101	BCR	C24-C23-C22	-2.26	122.89	126.23
12	B	2140	CLA	CAA-C2A-C3A	-2.26	106.89	113.00
15	J	104	BCR	C33-C5-C6	-2.26	122.02	124.48
12	a	805	CLA	C3B-C4B-NB	-2.26	108.52	110.53
12	A	824	CLA	C3B-C4B-NB	-2.26	108.52	110.53
17	b	2147	LMG	O3-C3-C2	-2.26	105.06	110.38
12	J	103	CLA	C3B-C4B-NB	-2.26	108.52	110.53
12	a	822	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
15	L	207	BCR	C33-C5-C6	-2.26	122.02	124.48
12	b	2139	CLA	CAA-C2A-C3A	-2.26	106.91	113.00
12	l	203	CLA	C3A-C2A-C1A	2.25	104.72	101.34
12	G	809	CLA	CBA-CAA-C2A	2.25	120.50	113.79
12	a	833	CLA	C4-C3-C5	2.25	119.14	115.23
12	H	2101	CLA	CHB-C4A-NA	2.25	127.65	124.40
12	G	824	CLA	C3B-C4B-NB	-2.25	108.52	110.53
12	S	103	CLA	C3B-C4B-NB	-2.25	108.52	110.53
12	H	2119	CLA	CMB-C2B-C1B	-2.25	121.99	125.42
15	l	207	BCR	C33-C5-C6	-2.25	122.03	124.48
15	G	842	BCR	C3-C4-C5	-2.25	110.04	114.06
24	U	208	SQD	C1-O5-C5	2.25	118.11	113.72
12	b	2133	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
12	H	2122	CLA	CHB-C4A-NA	2.25	127.64	124.40
12	H	2121	CLA	C3B-C4B-NB	-2.25	108.52	110.53
12	B	2122	CLA	C3B-C4B-NB	-2.25	108.52	110.53
15	H	2145	BCR	C16-C15-C14	-2.25	118.92	123.52
12	Q	203	CLA	CHB-C4A-NA	2.25	127.64	124.40
12	B	2123	CLA	CHB-C4A-NA	2.25	127.64	124.40
12	A	833	CLA	C4-C3-C5	2.25	119.13	115.23
12	A	814	CLA	C3B-C4B-NB	-2.25	108.52	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	2148	LMG	O3-C3-C2	-2.25	105.08	110.38
12	B	2134	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
12	G	809	CLA	CAA-C2A-C1A	2.25	119.33	111.97
12	H	2133	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
12	b	2121	CLA	C3B-C4B-NB	-2.24	108.53	110.53
12	a	806	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
12	L	201	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
12	B	2129	CLA	O2D-CGD-O1D	-2.24	119.48	123.85
17	H	2147	LMG	O3-C3-C2	-2.24	105.09	110.38
12	a	814	CLA	C3B-C4B-NB	-2.24	108.53	110.53
12	B	2107	CLA	C3B-C4B-NB	-2.24	108.53	110.53
12	A	822	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
12	j	103	CLA	C3B-C4B-NB	-2.24	108.53	110.53
12	G	828	CLA	CHB-C4A-NA	2.24	127.63	124.40
12	G	806	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
12	A	854	CLA	CMB-C2B-C3B	2.24	131.81	126.55
15	A	842	BCR	C3-C4-C5	-2.24	110.07	114.06
12	G	854	CLA	O2D-CGD-CBD	2.24	115.14	111.23
12	b	2122	CLA	CHB-C4A-NA	2.24	127.63	124.40
15	R	101	BCR	C15-C16-C17	-2.24	118.94	123.52
12	A	809	CLA	CAA-C2A-C1A	2.23	119.30	111.97
12	G	854	CLA	CMB-C2B-C3B	2.23	131.80	126.55
24	l	208	SQD	C1-O5-C5	2.23	118.08	113.72
12	G	833	CLA	C4-C3-C5	2.23	119.11	115.23
12	l	201	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
15	B	2146	BCR	C16-C15-C14	-2.23	118.95	123.52
12	b	2108	CLA	O2D-CGD-CBD	2.23	115.13	111.23
12	G	818	CLA	C1-C2-C3	-2.23	122.54	126.20
12	A	854	CLA	O2D-CGD-CBD	2.23	115.13	111.23
15	S	101	BCR	C24-C23-C22	-2.23	122.94	126.23
12	U	201	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
23	f	205	ZEX	C18-C5-C4	2.23	118.52	114.42
15	G	844	BCR	C11-C10-C9	-2.23	124.15	127.28
12	A	806	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
16	G	846	LHG	C18-C17-C16	-2.23	103.10	114.37
12	a	809	CLA	CAA-C2A-C1A	2.23	119.28	111.97
15	J	101	BCR	C24-C23-C22	-2.23	122.94	126.23
24	L	208	SQD	C1-O5-C5	2.23	118.07	113.72
12	a	854	CLA	O2D-CGD-CBD	2.23	115.13	111.23
12	a	854	CLA	CMB-C2B-C3B	2.23	131.79	126.55
12	b	2101	CLA	CHB-C4A-NA	2.23	127.61	124.40
12	b	2124	CLA	CMB-C2B-C3B	2.23	131.78	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	G	822	CLA	O2A-CGA-O1A	-2.22	118.06	123.63
15	U	207	BCR	C33-C5-C6	-2.22	122.06	124.48
17	A	847	LMG	C42-C41-C40	-2.22	103.13	114.37
12	H	2124	CLA	CMB-C2B-C3B	2.22	131.78	126.55
16	A	846	LHG	C18-C17-C16	-2.22	103.13	114.37
15	a	842	BCR	C3-C4-C5	-2.22	110.09	114.06
12	B	2125	CLA	CMB-C2B-C3B	2.22	131.78	126.55
17	G	847	LMG	C42-C41-C40	-2.22	103.13	114.37
15	I	101	BCR	C15-C16-C17	-2.22	118.97	123.52
23	F	205	ZEX	C18-C5-C4	2.22	118.51	114.42
15	a	842	BCR	C24-C23-C22	-2.22	122.95	126.23
12	B	2102	CLA	CHB-C4A-NA	2.22	127.61	124.40
16	a	846	LHG	C18-C17-C16	-2.22	103.14	114.37
17	a	847	LMG	C42-C41-C40	-2.22	103.14	114.37
12	a	851	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
12	H	2128	CLA	O2D-CGD-O1D	-2.22	119.53	123.85
12	H	2108	CLA	O2D-CGD-CBD	2.22	115.11	111.23
15	b	2144	BCR	C30-C25-C26	-2.22	119.60	122.64
12	B	2109	CLA	O2D-CGD-CBD	2.22	115.11	111.23
12	b	2125	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
15	i	101	BCR	C15-C16-C17	-2.22	118.98	123.52
12	U	203	CLA	C3A-C2A-C1A	2.22	104.66	101.34
12	L	203	CLA	C3A-C2A-C1A	2.22	104.66	101.34
15	a	844	BCR	C24-C23-C22	-2.22	122.96	126.23
12	a	818	CLA	C1-C2-C3	-2.21	122.57	126.20
12	A	818	CLA	C1-C2-C3	-2.21	122.57	126.20
15	A	844	BCR	C24-C23-C22	-2.21	122.96	126.23
12	G	824	CLA	CAC-C3C-C4C	2.21	127.67	124.79
15	b	2145	BCR	C16-C15-C14	-2.21	118.99	123.52
16	a	848	LHG	C27-C26-C25	-2.21	103.19	114.37
15	B	2146	BCR	C10-C11-C12	-2.21	116.79	123.20
12	H	2134	CLA	CMB-C2B-C3B	2.21	131.75	126.55
12	B	2135	CLA	CMB-C2B-C3B	2.21	131.75	126.55
12	A	824	CLA	CAC-C3C-C4C	2.21	127.67	124.79
12	H	2139	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
12	b	2124	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
12	B	2140	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
15	U	207	BCR	C29-C30-C25	2.21	113.65	110.44
12	a	835	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
15	H	2144	BCR	C30-C25-C26	-2.21	119.62	122.64
12	A	851	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
15	B	2145	BCR	C30-C25-C26	-2.21	119.62	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	G	851	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
12	a	805	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
12	b	2134	CLA	CMB-C2B-C3B	2.21	131.74	126.55
16	A	848	LHG	C27-C26-C25	-2.21	103.22	114.37
15	b	2145	BCR	C10-C11-C12	-2.21	116.81	123.20
12	a	824	CLA	CAC-C3C-C4C	2.21	127.66	124.79
12	b	2131	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
12	G	817	CLA	C1-C2-C3	-2.20	122.58	126.20
12	G	801	CLA	CHA-C1A-NA	-2.20	121.40	126.39
12	H	2124	CLA	O2A-CGA-O1A	-2.20	118.11	123.63
12	B	2126	CLA	O2A-CGA-O1A	-2.20	118.11	123.63
15	G	844	BCR	C24-C23-C22	-2.20	122.97	126.23
12	A	817	CLA	C1-C2-C3	-2.20	122.59	126.20
12	a	817	CLA	C1-C2-C3	-2.20	122.59	126.20
15	A	844	BCR	C11-C10-C9	-2.20	124.19	127.28
12	A	835	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
12	G	850	CLA	C3B-C4B-NB	-2.20	108.56	110.53
12	b	2139	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
12	B	2132	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
15	G	842	BCR	C24-C23-C22	-2.20	122.98	126.23
17	b	2147	LMG	O2-C2-C1	-2.20	104.83	110.08
12	G	805	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
16	G	848	LHG	C27-C26-C25	-2.20	103.25	114.37
15	H	2145	BCR	C10-C11-C12	-2.20	116.83	123.20
15	G	844	BCR	C15-C14-C13	-2.20	124.19	127.28
12	B	2139	CLA	O2D-CGD-CBD	2.20	115.08	111.23
23	Q	205	ZEX	C18-C5-C4	2.20	118.47	114.42
15	U	206	BCR	C15-C14-C13	-2.20	124.19	127.28
12	a	801	CLA	CHA-C1A-NA	-2.20	121.41	126.39
12	B	2125	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
15	A	842	BCR	C24-C23-C22	-2.20	122.98	126.23
12	H	2123	CLA	CMB-C2B-C3B	2.20	131.72	126.55
12	a	818	CLA	CMB-C2B-C3B	2.19	131.71	126.55
12	G	835	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
12	A	801	CLA	CHA-C1A-NA	-2.19	121.42	126.39
15	l	207	BCR	C29-C30-C25	2.19	113.62	110.44
15	L	207	BCR	C29-C30-C25	2.19	113.62	110.44
12	A	805	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
12	H	2138	CLA	O2D-CGD-CBD	2.19	115.06	111.23
12	G	814	CLA	C3B-C4B-NB	-2.19	108.57	110.53
12	A	826	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
12	a	805	CLA	CMB-C2B-C3B	2.19	131.70	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	a	844	BCR	C11-C10-C9	-2.19	124.20	127.28
17	B	2148	LMG	O2-C2-C1	-2.19	104.86	110.08
12	H	2125	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
12	G	826	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
12	H	2131	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
12	b	2141	CLA	CBC-CAC-C3C	2.19	118.35	112.42
17	A	847	LMG	O2-C2-C1	-2.19	104.87	110.08
15	A	844	BCR	C15-C14-C13	-2.19	124.21	127.28
12	G	802	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
12	A	817	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
17	H	2147	LMG	O2-C2-C1	-2.19	104.87	110.08
12	B	2112	CLA	O2A-CGA-O1A	-2.18	118.16	123.63
12	G	810	CLA	O1D-CGD-CBD	2.18	128.83	124.52
12	A	837	CLA	O2D-CGD-CBD	2.18	115.05	111.23
12	a	826	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
12	A	805	CLA	CMB-C2B-C3B	2.18	131.69	126.55
17	a	847	LMG	O2-C2-C1	-2.18	104.87	110.08
12	A	818	CLA	CMB-C2B-C3B	2.18	131.68	126.55
17	G	847	LMG	O2-C2-C1	-2.18	104.88	110.08
17	a	849	LMG	O2-C2-C1	-2.18	104.88	110.08
13	G	840	A1AGD	C12-C13-C14	2.18	123.22	115.97
12	a	817	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
15	L	206	BCR	C15-C14-C13	-2.18	124.22	127.28
12	a	810	CLA	O1D-CGD-CBD	2.18	128.82	124.52
12	B	2142	CLA	CBC-CAC-C3C	2.18	118.33	112.42
12	G	805	CLA	CMB-C2B-C3B	2.18	131.68	126.55
13	A	840	A1AGD	C12-C13-C14	2.18	123.22	115.97
12	b	2138	CLA	O2D-CGD-CBD	2.18	115.04	111.23
12	a	802	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
12	A	850	CLA	C3B-C4B-NB	-2.18	108.58	110.53
17	H	2147	LMG	C42-C41-C40	-2.18	103.35	114.37
12	G	818	CLA	CMB-C2B-C3B	2.18	131.68	126.55
12	G	817	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
12	B	2124	CLA	CMB-C2B-C3B	2.18	131.68	126.55
17	b	2147	LMG	C42-C41-C40	-2.18	103.35	114.37
12	A	802	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
12	G	839	CLA	CMB-C2B-C1B	-2.18	122.10	125.42
12	A	810	CLA	O1D-CGD-CBD	2.18	128.81	124.52
12	a	820	CLA	CHB-C1B-NB	2.18	127.32	124.05
20	H	2143	ECH	C8-C9-C10	-2.18	115.58	119.01
17	A	849	LMG	O2-C2-C1	-2.18	104.89	110.08
15	a	844	BCR	C15-C14-C13	-2.18	124.22	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	H	2141	CLA	CBC-CAC-C3C	2.18	118.32	112.42
12	a	850	CLA	C3B-C4B-NB	-2.18	108.59	110.53
12	a	809	CLA	C1-C2-C3	-2.18	123.24	126.76
17	B	2148	LMG	C42-C41-C40	-2.18	103.37	114.37
16	A	846	LHG	C27-C26-C25	-2.17	103.38	114.37
12	U	205	CLA	CMB-C2B-C3B	2.17	131.66	126.55
16	G	846	LHG	C27-C26-C25	-2.17	103.39	114.37
16	a	846	LHG	C27-C26-C25	-2.17	103.39	114.37
12	b	2123	CLA	CMB-C2B-C3B	2.17	131.66	126.55
12	G	813	CLA	C2A-C1A-CHA	2.17	127.64	123.87
12	G	837	CLA	O2D-CGD-CBD	2.17	115.03	111.23
15	L	207	BCR	C11-C10-C9	-2.17	124.23	127.28
20	B	2144	ECH	C8-C9-C10	-2.17	115.59	119.01
13	a	840	A1AGD	C12-C13-C14	2.17	123.18	115.97
15	l	206	BCR	C15-C14-C13	-2.17	124.23	127.28
15	l	207	BCR	C20-C21-C22	-2.17	124.23	127.28
20	b	2143	ECH	C8-C9-C10	-2.17	115.60	119.01
12	L	205	CLA	CMB-C2B-C3B	2.17	131.65	126.55
12	a	839	CLA	CMB-C2B-C1B	-2.17	122.12	125.42
12	H	2141	CLA	CMB-C2B-C1B	-2.17	122.12	125.42
12	b	2141	CLA	CMB-C2B-C1B	-2.17	122.12	125.42
15	l	207	BCR	C11-C10-C9	-2.17	124.24	127.28
12	H	2111	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
12	a	837	CLA	O2D-CGD-CBD	2.17	115.02	111.23
17	G	849	LMG	O2-C2-C1	-2.17	104.92	110.08
12	a	816	CLA	C3B-C4B-NB	-2.17	108.60	110.53
12	a	806	CLA	C1-C2-C3	-2.17	123.26	126.76
15	L	207	BCR	C20-C21-C22	-2.16	124.24	127.28
12	A	835	CLA	CHB-C4A-NA	2.16	127.52	124.40
12	b	2111	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
12	U	204	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
12	H	2117	CLA	O2D-CGD-CBD	2.16	115.01	111.23
12	H	2137	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
12	A	809	CLA	C1-C2-C3	-2.16	123.27	126.76
12	B	2132	CLA	CMB-C2B-C3B	2.16	131.63	126.55
12	b	2137	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
12	A	813	CLA	C2A-C1A-CHA	2.16	127.61	123.87
12	B	2118	CLA	O2D-CGD-CBD	2.16	115.00	111.23
12	b	2131	CLA	CMB-C2B-C3B	2.16	131.62	126.55
12	B	2142	CLA	CMB-C2B-C1B	-2.16	122.14	125.42
12	a	824	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
12	B	2141	CLA	C3B-C4B-NB	-2.16	108.61	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	a	801	CLA	O2D-CGD-O1D	-2.16	119.65	123.85
15	B	2143	BCR	C33-C5-C6	-2.16	122.13	124.48
12	H	2131	CLA	CMB-C2B-C3B	2.16	131.62	126.55
17	G	849	LMG	O3-C3-C2	-2.16	105.30	110.38
12	b	2140	CLA	C3B-C4B-NB	-2.16	108.61	110.53
12	A	801	CLA	O2D-CGD-O1D	-2.16	119.65	123.85
12	G	835	CLA	CHB-C4A-NA	2.16	127.51	124.40
12	a	813	CLA	C2A-C1A-CHA	2.15	127.61	123.87
12	A	820	CLA	CHB-C1B-NB	2.15	127.28	124.05
12	H	2129	CLA	C2D-C1D-ND	-2.15	108.00	110.13
12	B	2106	CLA	CMB-C2B-C3B	2.15	131.61	126.55
12	b	2105	CLA	CMB-C2B-C3B	2.15	131.61	126.55
17	A	849	LMG	O3-C3-C2	-2.15	105.30	110.38
12	l	205	CLA	CMB-C2B-C3B	2.15	131.61	126.55
15	F	202	BCR	C2-C1-C6	2.15	113.56	110.44
12	G	820	CLA	CHB-C1B-NB	2.15	127.28	124.05
17	a	849	LMG	O3-C3-C2	-2.15	105.31	110.38
12	A	839	CLA	CMB-C2B-C1B	-2.15	122.15	125.42
12	B	2106	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
12	b	2105	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
12	G	854	CLA	CAA-CBA-CGA	-2.15	107.11	113.21
15	f	202	BCR	C2-C1-C6	2.15	113.56	110.44
12	G	801	CLA	O2D-CGD-O1D	-2.15	119.67	123.85
12	A	834	CLA	C2A-C1A-CHA	2.15	127.59	123.87
12	H	2105	CLA	CMB-C2B-C3B	2.15	131.60	126.55
12	A	854	CLA	CAA-CBA-CGA	-2.15	107.11	113.21
15	U	207	BCR	C11-C10-C9	-2.15	124.27	127.28
12	A	806	CLA	C1-C2-C3	-2.15	123.29	126.76
12	a	812	CLA	C2A-C1A-CHA	2.15	127.59	123.87
12	A	824	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
12	L	204	CLA	O2A-CGA-O1A	-2.14	118.26	123.63
12	a	834	CLA	CAA-C2A-C3A	-2.14	107.20	113.00
12	a	835	CLA	CHB-C4A-NA	2.14	127.49	124.40
12	A	834	CLA	CAA-C2A-C3A	-2.14	107.21	113.00
15	H	2142	BCR	C33-C5-C6	-2.14	122.14	124.48
15	b	2142	BCR	C33-C5-C6	-2.14	122.14	124.48
12	G	838	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
15	U	207	BCR	C20-C21-C22	-2.14	124.27	127.28
12	l	204	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
12	G	819	CLA	C2A-C1A-CHA	2.14	127.58	123.87
12	H	2140	CLA	C3B-C4B-NB	-2.14	108.62	110.53
12	l	203	CLA	C2A-C1A-CHA	2.14	127.58	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	a	834	CLA	C2A-C1A-CHA	2.14	127.58	123.87
12	G	819	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
12	B	2138	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
12	G	820	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
12	G	834	CLA	C2A-C1A-CHA	2.14	127.58	123.87
12	H	2105	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
15	Q	202	BCR	C16-C15-C14	-2.14	119.15	123.52
12	G	824	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
12	b	2117	CLA	O2D-CGD-CBD	2.14	114.97	111.23
15	S	104	BCR	C20-C21-C22	-2.14	124.28	127.28
12	G	809	CLA	C1-C2-C3	-2.14	123.31	126.76
12	a	854	CLA	CAA-CBA-CGA	-2.14	107.14	113.21
12	A	820	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
12	G	834	CLA	CAA-C2A-C3A	-2.13	107.23	113.00
12	H	2118	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
12	a	825	CLA	CMB-C2B-C3B	2.13	131.57	126.55
12	A	834	CLA	CBA-CAA-C2A	2.13	120.14	113.79
12	a	838	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
12	A	838	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
25	U	209	DGD	O5D-C6D-C5D	-2.13	104.07	111.33
16	B	2149	LHG	C27-C26-C25	-2.13	103.59	114.37
12	a	819	CLA	C2A-C1A-CHA	2.13	127.57	123.87
16	b	2148	LHG	C27-C26-C25	-2.13	103.59	114.37
12	G	823	CLA	C2A-C1A-CHA	2.13	127.56	123.87
16	H	2148	LHG	C27-C26-C25	-2.13	103.60	114.37
12	G	834	CLA	CBA-CAA-C2A	2.13	120.13	113.79
12	H	2152	CLA	CMB-C2B-C1B	-2.13	122.18	125.42
12	A	819	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
25	l	209	DGD	O5D-C6D-C5D	-2.13	104.09	111.33
15	A	843	BCR	C38-C26-C27	-2.13	109.06	113.60
12	H	2103	CLA	C4-C3-C5	2.13	118.92	115.23
15	G	843	BCR	C38-C26-C27	-2.13	109.06	113.60
12	G	823	CLA	O2D-CGD-O1D	-2.13	119.71	123.85
15	L	206	BCR	C11-C10-C9	-2.13	124.30	127.28
12	b	2128	CLA	CHB-C4A-NA	2.13	127.47	124.40
15	i	101	BCR	C38-C26-C27	-2.13	109.06	113.60
12	A	838	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
25	L	209	DGD	O5D-C6D-C5D	-2.12	104.10	111.33
15	U	206	BCR	C11-C10-C9	-2.12	124.30	127.28
12	G	838	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
12	a	824	CLA	CMB-C2B-C3B	2.12	131.54	126.55
15	Q	202	BCR	C2-C1-C6	2.12	113.52	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	a	843	BCR	C38-C26-C27	-2.12	109.07	113.60
12	B	2101	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
12	b	2103	CLA	C4-C3-C5	2.12	118.91	115.23
17	G	847	LMG	O3-C3-C2	-2.12	105.38	110.38
12	A	819	CLA	C2A-C1A-CHA	2.12	127.55	123.87
12	L	203	CLA	C2A-C1A-CHA	2.12	127.55	123.87
12	a	820	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
12	A	822	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
12	A	812	CLA	C2A-C1A-CHA	2.12	127.55	123.87
12	A	834	CLA	C1-C2-C3	-2.12	122.73	126.20
15	J	104	BCR	C20-C21-C22	-2.12	124.31	127.28
12	A	816	CLA	C3B-C4B-NB	-2.12	108.64	110.53
12	B	2130	CLA	C2D-C1D-ND	-2.12	108.03	110.13
17	a	847	LMG	O3-C3-C2	-2.12	105.38	110.38
15	F	202	BCR	C16-C15-C14	-2.12	119.19	123.52
12	U	203	CLA	C2A-C1A-CHA	2.12	127.54	123.87
12	B	2119	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
25	L	209	DGD	CAB-C9B-C8B	-2.12	103.67	114.37
17	A	847	LMG	O3-C3-C2	-2.12	105.39	110.38
12	G	834	CLA	C1-C2-C3	-2.12	122.73	126.20
12	G	806	CLA	C1-C2-C3	-2.12	123.34	126.76
12	a	819	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
12	A	823	CLA	O2D-CGD-O1D	-2.12	119.73	123.85
12	a	834	CLA	CMB-C2B-C1B	-2.12	122.20	125.42
12	A	825	CLA	CMB-C2B-C3B	2.12	131.53	126.55
15	G	843	BCR	C35-C13-C14	-2.12	119.39	122.82
15	R	101	BCR	C38-C26-C27	-2.12	109.09	113.60
25	U	209	DGD	CAB-C9B-C8B	-2.12	103.68	114.37
12	a	834	CLA	CBA-CAA-C2A	2.12	120.09	113.79
12	b	2123	CLA	C1-C2-C3	-2.11	122.73	126.20
12	G	812	CLA	C2A-C1A-CHA	2.11	127.54	123.87
12	a	830	CLA	CHB-C1B-NB	2.11	127.22	124.05
12	H	2120	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
15	j	104	BCR	C20-C21-C22	-2.11	124.31	127.28
12	b	2152	CLA	CMB-C2B-C1B	-2.11	122.20	125.42
12	G	824	CLA	CMB-C2B-C3B	2.11	131.52	126.55
12	G	825	CLA	CMB-C2B-C3B	2.11	131.52	126.55
12	A	824	CLA	CMB-C2B-C3B	2.11	131.52	126.55
12	b	2118	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
15	I	101	BCR	C38-C26-C27	-2.11	109.09	113.60
15	f	202	BCR	C16-C15-C14	-2.11	119.20	123.52
12	B	2129	CLA	CHB-C4A-NA	2.11	127.45	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	l	206	BCR	C11-C10-C9	-2.11	124.32	127.28
12	b	2129	CLA	C2D-C1D-ND	-2.11	108.04	110.13
16	a	846	LHG	O8-C23-O10	-2.11	118.35	123.63
12	G	822	CLA	CMB-C2B-C1B	-2.11	122.20	125.42
12	H	2139	CLA	O2D-CGD-CBD	2.11	114.92	111.23
12	a	827	CLA	C1-C2-C3	-2.11	122.74	126.20
12	a	834	CLA	C1-C2-C3	-2.11	122.74	126.20
12	B	2124	CLA	C1-C2-C3	-2.11	122.74	126.20
16	G	846	LHG	O8-C23-O10	-2.11	118.35	123.63
12	b	2127	CLA	CMB-C2B-C3B	2.11	131.51	126.55
25	l	209	DGD	CAB-C9B-C8B	-2.11	103.71	114.37
12	a	823	CLA	O2D-CGD-O1D	-2.11	119.75	123.85
12	H	2121	CLA	CMB-C2B-C3B	2.11	131.51	126.55
12	b	2116	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
12	b	2120	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
16	A	846	LHG	O8-C23-O10	-2.11	118.36	123.63
12	B	2130	CLA	CHB-C1B-NB	2.11	127.21	124.05
12	B	2140	CLA	O2D-CGD-CBD	2.11	114.91	111.23
17	b	2147	LMG	O1-C7-C8	-2.11	105.70	110.82
15	a	843	BCR	C7-C8-C9	-2.10	123.12	126.23
17	B	2148	LMG	O1-C7-C8	-2.10	105.70	110.82
12	A	823	CLA	C2A-C1A-CHA	2.10	127.52	123.87
12	b	2121	CLA	CMB-C2B-C3B	2.10	131.50	126.55
12	A	834	CLA	O2D-CGD-CBD	2.10	114.91	111.23
12	B	2138	CLA	CMB-C2B-C3B	2.10	131.50	126.55
12	a	822	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
17	H	2147	LMG	O1-C7-C8	-2.10	105.71	110.82
15	A	843	BCR	C35-C13-C14	-2.10	119.41	122.82
12	B	2121	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
12	b	2132	CLA	C3B-C4B-NB	-2.10	108.65	110.53
12	G	827	CLA	C1-C2-C3	-2.10	122.75	126.20
12	G	834	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
12	b	2139	CLA	O2D-CGD-CBD	2.10	114.90	111.23
12	A	827	CLA	C1-C2-C3	-2.10	122.76	126.20
15	a	843	BCR	C35-C13-C14	-2.10	119.41	122.82
12	B	2128	CLA	CMB-C2B-C3B	2.10	131.49	126.55
12	A	834	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
12	H	2137	CLA	CMB-C2B-C3B	2.10	131.49	126.55
12	a	834	CLA	O2D-CGD-CBD	2.10	114.90	111.23
12	B	2122	CLA	CMB-C2B-C3B	2.10	131.49	126.55
12	b	2129	CLA	CHB-C1B-NB	2.10	127.20	124.05
12	H	2123	CLA	C1-C2-C3	-2.10	122.76	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	2104	CLA	C4-C3-C5	2.10	118.87	115.23
24	m	102	SQD	O8-S-C6	2.10	110.02	105.97
24	M	101	SQD	O8-S-C6	2.10	110.02	105.97
12	a	823	CLA	C2A-C1A-CHA	2.10	127.50	123.87
15	l	206	BCR	C2-C1-C6	2.09	113.48	110.44
12	G	816	CLA	C3B-C4B-NB	-2.09	108.66	110.53
12	a	851	CLA	C4-C3-C5	2.09	118.86	115.23
12	A	851	CLA	C4-C3-C5	2.09	118.86	115.23
24	V	102	SQD	O8-S-C6	2.09	110.01	105.97
15	G	842	BCR	C15-C16-C17	-2.09	119.24	123.52
12	a	838	CLA	CMB-C2B-C1B	-2.09	122.23	125.42
12	b	2137	CLA	CMB-C2B-C3B	2.09	131.47	126.55
12	H	2128	CLA	CHB-C4A-NA	2.09	127.42	124.40
15	K	4001	BCR	C15-C14-C13	-2.09	124.35	127.28
12	B	2117	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
25	L	209	DGD	O2D-C2D-C1D	-2.09	105.09	110.08
12	H	2129	CLA	CHB-C1B-NB	2.09	127.18	124.05
25	l	209	DGD	O2D-C2D-C1D	-2.09	105.10	110.08
15	A	843	BCR	C7-C8-C9	-2.09	123.14	126.23
12	H	2102	CLA	CMD-C2D-C3D	2.09	132.48	127.69
25	U	209	DGD	O2D-C2D-C1D	-2.09	105.10	110.08
15	U	206	BCR	C2-C1-C6	2.09	113.47	110.44
12	H	2121	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
12	B	2103	CLA	CMD-C2D-C3D	2.09	132.47	127.69
15	k	4001	BCR	C15-C14-C13	-2.09	124.35	127.28
12	H	2116	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
23	Q	205	ZEX	C27-C28-C29	-2.09	123.15	126.23
17	H	2147	LMG	O7-C10-O9	-2.08	118.83	123.70
12	a	839	CLA	C16-C15-C13	-2.08	109.04	115.97
12	H	2127	CLA	CMB-C2B-C3B	2.08	131.45	126.55
15	G	843	BCR	C7-C8-C9	-2.08	123.15	126.23
12	A	839	CLA	C16-C15-C13	-2.08	109.04	115.97
12	B	2133	CLA	C3B-C4B-NB	-2.08	108.67	110.53
12	G	809	CLA	C2A-C1A-CHA	2.08	127.48	123.87
23	f	205	ZEX	C27-C28-C29	-2.08	123.16	126.23
12	b	2102	CLA	CMD-C2D-C3D	2.08	132.46	127.69
23	F	205	ZEX	C27-C28-C29	-2.08	123.16	126.23
12	G	830	CLA	CHB-C1B-NB	2.08	127.17	124.05
12	H	2132	CLA	C3B-C4B-NB	-2.08	108.67	110.53
12	G	837	CLA	C2A-C1A-CHA	2.08	127.47	123.87
12	G	834	CLA	O2D-CGD-CBD	2.08	114.86	111.23
12	G	851	CLA	C4-C3-C5	2.08	118.83	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	L	206	BCR	C15-C16-C17	-2.08	119.27	123.52
12	A	809	CLA	C2A-C1A-CHA	2.08	127.47	123.87
12	G	839	CLA	C16-C15-C13	-2.08	109.06	115.97
12	G	825	CLA	C3A-C2A-C1A	2.08	104.45	101.34
12	a	809	CLA	C2A-C1A-CHA	2.08	127.47	123.87
12	b	2121	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
15	U	206	BCR	C15-C16-C17	-2.08	119.27	123.52
15	A	842	BCR	C15-C16-C17	-2.08	119.27	123.52
12	a	803	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
12	a	812	CLA	CHA-C1A-NA	-2.07	121.69	126.39
15	l	206	BCR	C15-C16-C17	-2.07	119.28	123.52
12	A	830	CLA	CHB-C1B-NB	2.07	127.16	124.05
12	G	818	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
12	b	2103	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
15	L	206	BCR	C2-C1-C6	2.07	113.45	110.44
17	B	2148	LMG	O7-C10-O9	-2.07	118.87	123.70
12	a	817	CLA	CMB-C2B-C3B	2.07	131.41	126.55
12	B	2119	CLA	C3B-C4B-NB	-2.07	108.68	110.53
12	B	2104	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
12	B	2122	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
12	G	812	CLA	CHA-C1A-NA	-2.07	121.71	126.39
12	A	817	CLA	CMB-C2B-C3B	2.07	131.41	126.55
12	A	818	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
15	a	842	BCR	C15-C16-C17	-2.07	119.29	123.52
17	b	2147	LMG	O7-C10-O9	-2.07	118.88	123.70
25	l	209	DGD	C5B-C4B-C3B	-2.07	103.93	114.37
12	H	2114	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
12	a	825	CLA	C3A-C2A-C1A	2.07	104.43	101.34
23	Q	205	ZEX	C10-C11-C12	-2.06	117.22	123.20
12	A	825	CLA	C3A-C2A-C1A	2.06	104.43	101.34
12	F	203	CLA	O2A-CGA-O1A	-2.06	118.03	123.33
25	U	209	DGD	C5B-C4B-C3B	-2.06	103.94	114.37
12	b	2103	CLA	CHB-C4A-NA	2.06	127.38	124.40
25	L	209	DGD	C5B-C4B-C3B	-2.06	103.94	114.37
12	A	812	CLA	CHA-C1A-NA	-2.06	121.72	126.39
15	T	4001	BCR	C15-C14-C13	-2.06	124.39	127.28
12	A	835	CLA	CHA-C1A-NA	-2.06	121.72	126.39
12	a	835	CLA	CHA-C1A-NA	-2.06	121.72	126.39
12	a	837	CLA	C2A-C1A-CHA	2.06	127.44	123.87
12	A	837	CLA	C2A-C1A-CHA	2.06	127.44	123.87
12	A	829	CLA	O2D-CGD-CBD	2.06	114.83	111.23
12	B	2112	CLA	CHA-C1A-NA	-2.06	121.73	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	2104	CLA	CHB-C4A-NA	2.06	127.37	124.40
17	G	849	LMG	O7-C10-O9	-2.06	119.02	122.99
12	a	824	CLA	O2D-CGD-CBD	2.06	114.82	111.23
12	a	826	CLA	CHB-C1B-NB	2.06	127.13	124.05
12	f	203	CLA	O2A-CGA-O1A	-2.06	118.05	123.33
12	a	829	CLA	O2D-CGD-CBD	2.06	114.82	111.23
23	F	205	ZEX	C10-C11-C12	-2.05	117.25	123.20
12	A	803	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
23	f	205	ZEX	C10-C11-C12	-2.05	117.25	123.20
12	Q	203	CLA	O2A-CGA-O1A	-2.05	118.05	123.33
12	b	2114	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
12	b	2101	CLA	C2A-C1A-CHA	2.05	127.43	123.87
12	G	803	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
12	B	2115	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
22	b	2150	EQ3	C4-C5-C6	-2.05	116.54	120.76
12	A	816	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
12	j	102	CLA	C2A-C1A-CHA	2.05	127.43	123.87
12	G	835	CLA	CHA-C1A-NA	-2.05	121.75	126.39
12	H	2103	CLA	CHB-C4A-NA	2.05	127.36	124.40
12	H	2103	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
12	A	824	CLA	O2D-CGD-CBD	2.05	114.81	111.23
12	a	808	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
12	B	2107	CLA	CHD-C1D-ND	-2.05	121.92	124.80
17	A	849	LMG	O7-C10-O9	-2.05	119.04	122.99
12	H	2101	CLA	C2A-C1A-CHA	2.05	127.42	123.87
12	G	829	CLA	O2D-CGD-CBD	2.05	114.81	111.23
22	H	2150	EQ3	C4-C5-C6	-2.05	116.55	120.76
12	G	816	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
22	B	2151	EQ3	C4-C5-C6	-2.05	116.56	120.76
12	a	818	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
12	A	808	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
13	H	2153	A1AGD	C53-C6-C1	2.04	119.47	115.28
12	J	102	CLA	C2A-C1A-CHA	2.04	127.41	123.87
12	S	102	CLA	C2A-C1A-CHA	2.04	127.41	123.87
17	a	849	LMG	O7-C10-O9	-2.04	119.05	122.99
12	G	824	CLA	O2D-CGD-CBD	2.04	114.80	111.23
12	H	2110	CLA	C3B-C4B-NB	-2.04	108.71	110.53
12	a	812	CLA	O2D-CGD-CBD	2.04	114.79	111.23
12	B	2102	CLA	C2A-C1A-CHA	2.04	127.40	123.87
12	B	2111	CLA	C3B-C4B-NB	-2.04	108.71	110.53
12	l	201	CLA	CMB-C2B-C1B	-2.04	122.32	125.42
12	a	823	CLA	O2A-CGA-O1A	-2.04	118.53	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	H	2118	CLA	C3B-C4B-NB	-2.04	108.71	110.53
12	a	825	CLA	CAA-CBA-CGA	-2.03	107.43	113.21
12	G	808	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
12	a	816	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
12	A	825	CLA	CAA-CBA-CGA	-2.03	107.44	113.21
12	G	825	CLA	CAA-CBA-CGA	-2.03	107.44	113.21
12	G	817	CLA	CMB-C2B-C3B	2.03	131.33	126.55
12	b	2118	CLA	C3B-C4B-NB	-2.03	108.72	110.53
12	U	203	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
12	b	2128	CLA	O1D-CGD-CBD	2.03	128.52	124.52
12	H	2111	CLA	CHA-C1A-NA	-2.03	121.80	126.39
12	b	2106	CLA	CHD-C1D-ND	-2.03	121.95	124.80
13	G	840	A1AGD	C13-C14-C16	2.03	122.35	112.07
12	b	2111	CLA	CHA-C1A-NA	-2.03	121.80	126.39
12	H	2123	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
12	b	2123	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
12	b	2119	CLA	O2D-CGD-CBD	2.03	114.78	111.23
12	H	2106	CLA	CHD-C1D-ND	-2.03	121.95	124.80
13	B	2153	A1AGD	C53-C6-C1	2.03	119.43	115.28
13	a	840	A1AGD	C13-C14-C16	2.03	122.34	112.07
12	B	2126	CLA	O1D-CGD-CBD	2.03	128.51	124.52
12	B	2126	CLA	C1-C2-C3	-2.03	123.48	126.76
12	A	812	CLA	O2D-CGD-CBD	2.03	114.77	111.23
12	H	2119	CLA	CAA-CBA-CGA	-2.03	107.46	113.21
13	A	840	A1AGD	C13-C14-C16	2.03	122.33	112.07
12	b	2125	CLA	C1-C2-C3	-2.02	123.49	126.76
12	b	2119	CLA	CAA-CBA-CGA	-2.02	107.46	113.21
12	H	2124	CLA	C2A-C1A-CHA	2.02	127.38	123.87
12	G	812	CLA	O2D-CGD-CBD	2.02	114.77	111.23
12	H	2106	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
12	b	2125	CLA	O1D-CGD-CBD	2.02	128.50	124.52
12	A	823	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
13	b	2153	A1AGD	C53-C6-C1	2.02	119.42	115.28
12	f	201	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
12	B	2125	CLA	C2A-C1A-CHA	2.02	127.37	123.87
12	L	201	CLA	CMB-C2B-C1B	-2.02	122.35	125.42
12	G	838	CLA	C2A-C1A-CHA	2.02	127.37	123.87
12	F	201	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
12	B	2124	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
12	U	201	CLA	CMB-C2B-C1B	-2.01	122.35	125.42
12	B	2120	CLA	CAA-CBA-CGA	-2.01	107.49	113.21
12	b	2110	CLA	C3B-C4B-NB	-2.01	108.73	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	826	CLA	CHB-C1B-NB	2.01	127.07	124.05
12	B	2133	CLA	C2A-C1A-CHA	2.01	127.36	123.87
12	b	2102	CLA	O1D-CGD-CBD	2.01	128.49	124.52
12	G	823	CLA	C3A-C2A-C1A	2.01	104.35	101.34
12	G	832	CLA	O1D-CGD-CBD	2.01	128.49	124.52
12	a	810	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
12	H	2125	CLA	O1D-CGD-CBD	2.01	128.49	124.52
15	T	4001	BCR	C40-C30-C25	2.01	113.40	110.24
12	B	2129	CLA	O1D-CGD-CBD	2.01	128.48	124.52
12	B	2107	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
12	b	2124	CLA	C2A-C1A-CHA	2.01	127.35	123.87
12	B	2113	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
12	H	2128	CLA	O1D-CGD-CBD	2.01	128.48	124.52
12	G	826	CLA	CHB-C1B-NB	2.01	127.06	124.05
12	H	2107	CLA	C1-C2-C3	-2.01	122.91	126.20
12	G	813	CLA	CHA-C1A-NA	-2.01	121.85	126.39
12	b	2106	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
12	B	2120	CLA	O2D-CGD-CBD	2.01	114.74	111.23
12	a	803	CLA	O2D-CGD-CBD	2.00	114.73	111.23
12	l	201	CLA	CMB-C2B-C3B	2.00	131.26	126.55
12	G	810	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
12	b	2128	CLA	C2A-C1A-CHA	2.00	127.34	123.87
12	b	2119	CLA	CMB-C2B-C3B	2.00	131.26	126.55
12	L	203	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
12	a	823	CLA	C3A-C2A-C1A	2.00	104.34	101.34
12	G	823	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
12	a	832	CLA	O1D-CGD-CBD	2.00	128.47	124.52
12	B	2103	CLA	O1D-CGD-CBD	2.00	128.47	124.52
12	b	2112	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
12	B	2120	CLA	CMB-C2B-C3B	2.00	131.26	126.55
12	H	2127	CLA	C2A-C1A-CHA	2.00	127.34	123.87
12	G	803	CLA	O2D-CGD-CBD	2.00	114.73	111.23
12	A	810	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
12	b	2101	CLA	CHA-C1A-NA	-2.00	121.86	126.39

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	G	840	A1AGD	C14
13	G	840	A1AGD	C19
13	H	2153	A1AGD	C14
13	H	2153	A1AGD	C19

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Mol	Chain	Res	Type	Atom
13	a	840	A1AGD	C14
13	a	840	A1AGD	C19
13	b	2153	A1AGD	C14
13	b	2153	A1AGD	C19
13	A	840	A1AGD	C14
13	A	840	A1AGD	C19
13	B	2153	A1AGD	C14
13	B	2153	A1AGD	C19

All (4249) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	G	802	CLA	C1A-C2A-CAA-CBA
12	G	804	CLA	C1A-C2A-CAA-CBA
12	G	804	CLA	C3A-C2A-CAA-CBA
12	G	804	CLA	CAD-CBD-CGD-O1D
12	G	804	CLA	CAD-CBD-CGD-O2D
12	G	805	CLA	C1A-C2A-CAA-CBA
12	G	805	CLA	C3A-C2A-CAA-CBA
12	G	805	CLA	CBA-CGA-O2A-C1
12	G	806	CLA	C2B-C3B-CAB-CBB
12	G	806	CLA	C4B-C3B-CAB-CBB
12	G	807	CLA	C3A-C2A-CAA-CBA
12	G	807	CLA	CHA-CBD-CGD-O2D
12	G	808	CLA	C3A-C2A-CAA-CBA
12	G	809	CLA	C1A-C2A-CAA-CBA
12	G	810	CLA	C4-C3-C5-C6
12	G	811	CLA	C1A-C2A-CAA-CBA
12	G	812	CLA	C1A-C2A-CAA-CBA
12	G	812	CLA	C3A-C2A-CAA-CBA
12	G	815	CLA	CBD-CGD-O2D-CED
12	G	817	CLA	C3A-C2A-CAA-CBA
12	G	824	CLA	CHA-CBD-CGD-O1D
12	G	824	CLA	CHA-CBD-CGD-O2D
12	G	826	CLA	C1A-C2A-CAA-CBA
12	G	826	CLA	C3A-C2A-CAA-CBA
12	G	832	CLA	C2B-C3B-CAB-CBB
12	G	832	CLA	C4B-C3B-CAB-CBB
12	G	832	CLA	C6-C7-C8-C9
12	G	833	CLA	C1A-C2A-CAA-CBA
12	G	834	CLA	C1A-C2A-CAA-CBA
12	G	834	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	G	834	CLA	C4B-C3B-CAB-CBB
12	G	839	CLA	C2B-C3B-CAB-CBB
12	G	839	CLA	C4B-C3B-CAB-CBB
12	G	854	CLA	C1A-C2A-CAA-CBA
12	H	2103	CLA	CBD-CGD-O2D-CED
12	H	2106	CLA	C3A-C2A-CAA-CBA
12	H	2108	CLA	C2B-C3B-CAB-CBB
12	H	2108	CLA	C4B-C3B-CAB-CBB
12	H	2109	CLA	C4B-C3B-CAB-CBB
12	H	2109	CLA	CHA-CBD-CGD-O1D
12	H	2109	CLA	CHA-CBD-CGD-O2D
12	H	2113	CLA	C2B-C3B-CAB-CBB
12	H	2113	CLA	C4B-C3B-CAB-CBB
12	H	2113	CLA	CHA-CBD-CGD-O1D
12	H	2113	CLA	CHA-CBD-CGD-O2D
12	H	2116	CLA	C1A-C2A-CAA-CBA
12	H	2116	CLA	C3A-C2A-CAA-CBA
12	H	2116	CLA	CBD-CGD-O2D-CED
12	H	2119	CLA	C1A-C2A-CAA-CBA
12	H	2119	CLA	C3A-C2A-CAA-CBA
12	H	2120	CLA	C1A-C2A-CAA-CBA
12	H	2120	CLA	C3A-C2A-CAA-CBA
12	H	2120	CLA	C2B-C3B-CAB-CBB
12	H	2120	CLA	C4B-C3B-CAB-CBB
12	H	2121	CLA	CBD-CGD-O2D-CED
12	H	2122	CLA	C1A-C2A-CAA-CBA
12	H	2122	CLA	C4B-C3B-CAB-CBB
12	H	2124	CLA	CHA-CBD-CGD-O1D
12	H	2124	CLA	CHA-CBD-CGD-O2D
12	H	2127	CLA	C1A-C2A-CAA-CBA
12	H	2127	CLA	C3A-C2A-CAA-CBA
12	H	2128	CLA	C1A-C2A-CAA-CBA
12	H	2128	CLA	C3A-C2A-CAA-CBA
12	H	2130	CLA	C4B-C3B-CAB-CBB
12	H	2133	CLA	C3A-C2A-CAA-CBA
12	H	2133	CLA	CHA-CBD-CGD-O1D
12	H	2133	CLA	CHA-CBD-CGD-O2D
12	H	2134	CLA	CBD-CGD-O2D-CED
12	H	2135	CLA	C1A-C2A-CAA-CBA
12	H	2135	CLA	C3A-C2A-CAA-CBA
12	H	2136	CLA	C1A-C2A-CAA-CBA
12	H	2138	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
12	H	2139	CLA	C2B-C3B-CAB-CBB
12	H	2139	CLA	C4B-C3B-CAB-CBB
12	H	2141	CLA	C1A-C2A-CAA-CBA
12	H	2141	CLA	CHA-CBD-CGD-O1D
12	H	2141	CLA	CHA-CBD-CGD-O2D
12	Q	201	CLA	C1A-C2A-CAA-CBA
12	Q	201	CLA	C2B-C3B-CAB-CBB
12	Q	201	CLA	C4B-C3B-CAB-CBB
12	Q	201	CLA	CBD-CGD-O2D-CED
12	S	102	CLA	C4B-C3B-CAB-CBB
12	S	102	CLA	CHA-CBD-CGD-O1D
12	S	102	CLA	CHA-CBD-CGD-O2D
12	S	103	CLA	CHA-CBD-CGD-O1D
12	S	103	CLA	CHA-CBD-CGD-O2D
12	T	4002	CLA	C1A-C2A-CAA-CBA
12	T	4002	CLA	CAD-CBD-CGD-O2D
12	T	4002	CLA	CBD-CGD-O2D-CED
12	U	201	CLA	CHA-CBD-CGD-O2D
12	U	203	CLA	C1A-C2A-CAA-CBA
12	U	203	CLA	C3A-C2A-CAA-CBA
12	U	204	CLA	C1A-C2A-CAA-CBA
12	a	802	CLA	C1A-C2A-CAA-CBA
12	a	804	CLA	C1A-C2A-CAA-CBA
12	a	804	CLA	C3A-C2A-CAA-CBA
12	a	804	CLA	CAD-CBD-CGD-O1D
12	a	804	CLA	CAD-CBD-CGD-O2D
12	a	805	CLA	C1A-C2A-CAA-CBA
12	a	805	CLA	C3A-C2A-CAA-CBA
12	a	805	CLA	CBA-CGA-O2A-C1
12	a	806	CLA	C2B-C3B-CAB-CBB
12	a	806	CLA	C4B-C3B-CAB-CBB
12	a	807	CLA	C3A-C2A-CAA-CBA
12	a	807	CLA	CHA-CBD-CGD-O2D
12	a	808	CLA	C3A-C2A-CAA-CBA
12	a	809	CLA	C1A-C2A-CAA-CBA
12	a	810	CLA	C4-C3-C5-C6
12	a	811	CLA	C1A-C2A-CAA-CBA
12	a	812	CLA	C1A-C2A-CAA-CBA
12	a	812	CLA	C3A-C2A-CAA-CBA
12	a	815	CLA	CBD-CGD-O2D-CED
12	a	817	CLA	C3A-C2A-CAA-CBA
12	a	824	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
12	a	824	CLA	CHA-CBD-CGD-O2D
12	a	826	CLA	C1A-C2A-CAA-CBA
12	a	826	CLA	C3A-C2A-CAA-CBA
12	a	832	CLA	C2B-C3B-CAB-CBB
12	a	832	CLA	C4B-C3B-CAB-CBB
12	a	832	CLA	C6-C7-C8-C9
12	a	833	CLA	C1A-C2A-CAA-CBA
12	a	834	CLA	C1A-C2A-CAA-CBA
12	a	834	CLA	C3A-C2A-CAA-CBA
12	a	834	CLA	C4B-C3B-CAB-CBB
12	a	839	CLA	C2B-C3B-CAB-CBB
12	a	839	CLA	C4B-C3B-CAB-CBB
12	a	854	CLA	C1A-C2A-CAA-CBA
12	b	2103	CLA	CBD-CGD-O2D-CED
12	b	2106	CLA	C3A-C2A-CAA-CBA
12	b	2108	CLA	C2B-C3B-CAB-CBB
12	b	2108	CLA	C4B-C3B-CAB-CBB
12	b	2109	CLA	C4B-C3B-CAB-CBB
12	b	2109	CLA	CHA-CBD-CGD-O1D
12	b	2109	CLA	CHA-CBD-CGD-O2D
12	b	2113	CLA	C2B-C3B-CAB-CBB
12	b	2113	CLA	C4B-C3B-CAB-CBB
12	b	2113	CLA	CHA-CBD-CGD-O1D
12	b	2113	CLA	CHA-CBD-CGD-O2D
12	b	2116	CLA	C1A-C2A-CAA-CBA
12	b	2116	CLA	C3A-C2A-CAA-CBA
12	b	2116	CLA	CBD-CGD-O2D-CED
12	b	2119	CLA	C1A-C2A-CAA-CBA
12	b	2119	CLA	C3A-C2A-CAA-CBA
12	b	2120	CLA	C1A-C2A-CAA-CBA
12	b	2120	CLA	C3A-C2A-CAA-CBA
12	b	2120	CLA	C2B-C3B-CAB-CBB
12	b	2120	CLA	C4B-C3B-CAB-CBB
12	b	2121	CLA	CBD-CGD-O2D-CED
12	b	2122	CLA	C1A-C2A-CAA-CBA
12	b	2122	CLA	C4B-C3B-CAB-CBB
12	b	2124	CLA	CHA-CBD-CGD-O1D
12	b	2124	CLA	CHA-CBD-CGD-O2D
12	b	2127	CLA	C1A-C2A-CAA-CBA
12	b	2127	CLA	C3A-C2A-CAA-CBA
12	b	2128	CLA	C1A-C2A-CAA-CBA
12	b	2128	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	b	2130	CLA	C4B-C3B-CAB-CBB
12	b	2133	CLA	C3A-C2A-CAA-CBA
12	b	2133	CLA	CHA-CBD-CGD-O1D
12	b	2133	CLA	CHA-CBD-CGD-O2D
12	b	2134	CLA	CBD-CGD-O2D-CED
12	b	2135	CLA	C1A-C2A-CAA-CBA
12	b	2135	CLA	C3A-C2A-CAA-CBA
12	b	2136	CLA	C1A-C2A-CAA-CBA
12	b	2138	CLA	C4B-C3B-CAB-CBB
12	b	2139	CLA	C2B-C3B-CAB-CBB
12	b	2139	CLA	C4B-C3B-CAB-CBB
12	b	2141	CLA	C1A-C2A-CAA-CBA
12	b	2141	CLA	CHA-CBD-CGD-O1D
12	b	2141	CLA	CHA-CBD-CGD-O2D
12	f	201	CLA	C1A-C2A-CAA-CBA
12	f	201	CLA	C2B-C3B-CAB-CBB
12	f	201	CLA	C4B-C3B-CAB-CBB
12	f	201	CLA	CBD-CGD-O2D-CED
12	j	102	CLA	C4B-C3B-CAB-CBB
12	j	102	CLA	CHA-CBD-CGD-O1D
12	j	102	CLA	CHA-CBD-CGD-O2D
12	j	103	CLA	CHA-CBD-CGD-O1D
12	j	103	CLA	CHA-CBD-CGD-O2D
12	k	4002	CLA	C1A-C2A-CAA-CBA
12	k	4002	CLA	CAD-CBD-CGD-O2D
12	k	4002	CLA	CBD-CGD-O2D-CED
12	l	201	CLA	CHA-CBD-CGD-O2D
12	l	203	CLA	C1A-C2A-CAA-CBA
12	l	203	CLA	C3A-C2A-CAA-CBA
12	l	204	CLA	C1A-C2A-CAA-CBA
12	A	802	CLA	C1A-C2A-CAA-CBA
12	A	804	CLA	C1A-C2A-CAA-CBA
12	A	804	CLA	C3A-C2A-CAA-CBA
12	A	804	CLA	CAD-CBD-CGD-O1D
12	A	804	CLA	CAD-CBD-CGD-O2D
12	A	805	CLA	C1A-C2A-CAA-CBA
12	A	805	CLA	C3A-C2A-CAA-CBA
12	A	805	CLA	CBA-CGA-O2A-C1
12	A	806	CLA	C2B-C3B-CAB-CBB
12	A	806	CLA	C4B-C3B-CAB-CBB
12	A	807	CLA	C3A-C2A-CAA-CBA
12	A	807	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
12	A	808	CLA	C3A-C2A-CAA-CBA
12	A	809	CLA	C1A-C2A-CAA-CBA
12	A	810	CLA	C4-C3-C5-C6
12	A	811	CLA	C1A-C2A-CAA-CBA
12	A	812	CLA	C1A-C2A-CAA-CBA
12	A	812	CLA	C3A-C2A-CAA-CBA
12	A	815	CLA	CBD-CGD-O2D-CED
12	A	817	CLA	C3A-C2A-CAA-CBA
12	A	824	CLA	CHA-CBD-CGD-O1D
12	A	824	CLA	CHA-CBD-CGD-O2D
12	A	826	CLA	C1A-C2A-CAA-CBA
12	A	826	CLA	C3A-C2A-CAA-CBA
12	A	832	CLA	C2B-C3B-CAB-CBB
12	A	832	CLA	C4B-C3B-CAB-CBB
12	A	832	CLA	C6-C7-C8-C9
12	A	833	CLA	C1A-C2A-CAA-CBA
12	A	834	CLA	C1A-C2A-CAA-CBA
12	A	834	CLA	C3A-C2A-CAA-CBA
12	A	834	CLA	C4B-C3B-CAB-CBB
12	A	839	CLA	C2B-C3B-CAB-CBB
12	A	839	CLA	C4B-C3B-CAB-CBB
12	A	854	CLA	C1A-C2A-CAA-CBA
12	B	2104	CLA	CBD-CGD-O2D-CED
12	B	2107	CLA	C3A-C2A-CAA-CBA
12	B	2109	CLA	C2B-C3B-CAB-CBB
12	B	2109	CLA	C4B-C3B-CAB-CBB
12	B	2110	CLA	C4B-C3B-CAB-CBB
12	B	2110	CLA	CHA-CBD-CGD-O1D
12	B	2110	CLA	CHA-CBD-CGD-O2D
12	B	2114	CLA	C2B-C3B-CAB-CBB
12	B	2114	CLA	C4B-C3B-CAB-CBB
12	B	2114	CLA	CHA-CBD-CGD-O1D
12	B	2114	CLA	CHA-CBD-CGD-O2D
12	B	2117	CLA	C1A-C2A-CAA-CBA
12	B	2117	CLA	C3A-C2A-CAA-CBA
12	B	2117	CLA	CBD-CGD-O2D-CED
12	B	2120	CLA	C1A-C2A-CAA-CBA
12	B	2120	CLA	C3A-C2A-CAA-CBA
12	B	2121	CLA	C1A-C2A-CAA-CBA
12	B	2121	CLA	C3A-C2A-CAA-CBA
12	B	2121	CLA	C2B-C3B-CAB-CBB
12	B	2121	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
12	B	2122	CLA	CBD-CGD-O2D-CED
12	B	2123	CLA	C1A-C2A-CAA-CBA
12	B	2123	CLA	C4B-C3B-CAB-CBB
12	B	2125	CLA	CHA-CBD-CGD-O1D
12	B	2125	CLA	CHA-CBD-CGD-O2D
12	B	2128	CLA	C1A-C2A-CAA-CBA
12	B	2128	CLA	C3A-C2A-CAA-CBA
12	B	2129	CLA	C1A-C2A-CAA-CBA
12	B	2129	CLA	C3A-C2A-CAA-CBA
12	B	2131	CLA	C4B-C3B-CAB-CBB
12	B	2134	CLA	C3A-C2A-CAA-CBA
12	B	2134	CLA	CHA-CBD-CGD-O1D
12	B	2134	CLA	CHA-CBD-CGD-O2D
12	B	2135	CLA	CBD-CGD-O2D-CED
12	B	2136	CLA	C1A-C2A-CAA-CBA
12	B	2136	CLA	C3A-C2A-CAA-CBA
12	B	2137	CLA	C1A-C2A-CAA-CBA
12	B	2139	CLA	C4B-C3B-CAB-CBB
12	B	2140	CLA	C2B-C3B-CAB-CBB
12	B	2140	CLA	C4B-C3B-CAB-CBB
12	B	2142	CLA	C1A-C2A-CAA-CBA
12	B	2142	CLA	CHA-CBD-CGD-O1D
12	B	2142	CLA	CHA-CBD-CGD-O2D
12	F	201	CLA	C1A-C2A-CAA-CBA
12	F	201	CLA	C2B-C3B-CAB-CBB
12	F	201	CLA	C4B-C3B-CAB-CBB
12	F	201	CLA	CBD-CGD-O2D-CED
12	J	102	CLA	C4B-C3B-CAB-CBB
12	J	102	CLA	CHA-CBD-CGD-O1D
12	J	102	CLA	CHA-CBD-CGD-O2D
12	J	103	CLA	CHA-CBD-CGD-O1D
12	J	103	CLA	CHA-CBD-CGD-O2D
12	K	4002	CLA	C1A-C2A-CAA-CBA
12	K	4002	CLA	CAD-CBD-CGD-O2D
12	K	4002	CLA	CBD-CGD-O2D-CED
12	L	201	CLA	CHA-CBD-CGD-O2D
12	L	203	CLA	C1A-C2A-CAA-CBA
12	L	203	CLA	C3A-C2A-CAA-CBA
12	L	204	CLA	C1A-C2A-CAA-CBA
13	G	840	A1AGD	C20-C19-C21-C22
13	a	840	A1AGD	C20-C19-C21-C22
13	A	840	A1AGD	C20-C19-C21-C22

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Mol	Chain	Res	Type	Atoms
15	G	842	BCR	C16-C17-C18-C36
15	G	842	BCR	C18-C19-C20-C21
15	G	842	BCR	C20-C21-C22-C37
15	G	842	BCR	C37-C22-C23-C24
15	G	843	BCR	C11-C10-C9-C8
15	G	843	BCR	C11-C10-C9-C34
15	G	843	BCR	C10-C11-C12-C13
15	G	843	BCR	C11-C12-C13-C14
15	G	843	BCR	C37-C22-C23-C24
15	G	844	BCR	C7-C8-C9-C34
15	G	844	BCR	C21-C22-C23-C24
15	G	845	BCR	C21-C22-C23-C24
15	H	2142	BCR	C21-C22-C23-C24
15	H	2146	BCR	C11-C10-C9-C8
15	H	2146	BCR	C10-C11-C12-C13
15	H	2146	BCR	C11-C12-C13-C14
15	H	2146	BCR	C11-C12-C13-C35
15	H	2146	BCR	C16-C17-C18-C19
15	H	2146	BCR	C16-C17-C18-C36
15	Q	202	BCR	C7-C8-C9-C10
15	Q	202	BCR	C7-C8-C9-C34
15	Q	202	BCR	C35-C13-C14-C15
15	Q	202	BCR	C20-C21-C22-C37
15	Q	202	BCR	C21-C22-C23-C24
15	R	101	BCR	C20-C21-C22-C23
15	R	101	BCR	C21-C22-C23-C24
15	S	101	BCR	C21-C22-C23-C24
15	S	101	BCR	C37-C22-C23-C24
15	S	104	BCR	C7-C8-C9-C10
15	S	104	BCR	C7-C8-C9-C34
15	T	4001	BCR	C21-C22-C23-C24
15	U	206	BCR	C23-C24-C25-C26
15	U	207	BCR	C22-C23-C24-C25
15	a	842	BCR	C16-C17-C18-C36
15	a	842	BCR	C18-C19-C20-C21
15	a	842	BCR	C20-C21-C22-C37
15	a	842	BCR	C37-C22-C23-C24
15	a	843	BCR	C11-C10-C9-C8
15	a	843	BCR	C11-C10-C9-C34
15	a	843	BCR	C10-C11-C12-C13
15	a	843	BCR	C11-C12-C13-C14
15	a	843	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
15	a	844	BCR	C7-C8-C9-C34
15	a	844	BCR	C21-C22-C23-C24
15	a	845	BCR	C21-C22-C23-C24
15	b	2142	BCR	C21-C22-C23-C24
15	b	2146	BCR	C11-C10-C9-C8
15	b	2146	BCR	C10-C11-C12-C13
15	b	2146	BCR	C11-C12-C13-C14
15	b	2146	BCR	C11-C12-C13-C35
15	b	2146	BCR	C16-C17-C18-C19
15	b	2146	BCR	C16-C17-C18-C36
15	f	202	BCR	C7-C8-C9-C10
15	f	202	BCR	C7-C8-C9-C34
15	f	202	BCR	C35-C13-C14-C15
15	f	202	BCR	C20-C21-C22-C37
15	f	202	BCR	C21-C22-C23-C24
15	i	101	BCR	C20-C21-C22-C23
15	i	101	BCR	C21-C22-C23-C24
15	j	101	BCR	C21-C22-C23-C24
15	j	101	BCR	C37-C22-C23-C24
15	j	104	BCR	C7-C8-C9-C10
15	j	104	BCR	C7-C8-C9-C34
15	k	4001	BCR	C21-C22-C23-C24
15	l	206	BCR	C23-C24-C25-C26
15	l	207	BCR	C22-C23-C24-C25
15	A	842	BCR	C16-C17-C18-C36
15	A	842	BCR	C18-C19-C20-C21
15	A	842	BCR	C20-C21-C22-C37
15	A	842	BCR	C37-C22-C23-C24
15	A	843	BCR	C11-C10-C9-C8
15	A	843	BCR	C11-C10-C9-C34
15	A	843	BCR	C10-C11-C12-C13
15	A	843	BCR	C11-C12-C13-C14
15	A	843	BCR	C37-C22-C23-C24
15	A	844	BCR	C7-C8-C9-C34
15	A	844	BCR	C21-C22-C23-C24
15	A	845	BCR	C21-C22-C23-C24
15	B	2143	BCR	C21-C22-C23-C24
15	B	2147	BCR	C11-C10-C9-C8
15	B	2147	BCR	C10-C11-C12-C13
15	B	2147	BCR	C11-C12-C13-C14
15	B	2147	BCR	C11-C12-C13-C35
15	B	2147	BCR	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
15	B	2147	BCR	C16-C17-C18-C36
15	F	202	BCR	C7-C8-C9-C10
15	F	202	BCR	C7-C8-C9-C34
15	F	202	BCR	C35-C13-C14-C15
15	F	202	BCR	C20-C21-C22-C37
15	F	202	BCR	C21-C22-C23-C24
15	I	101	BCR	C20-C21-C22-C23
15	I	101	BCR	C21-C22-C23-C24
15	J	101	BCR	C21-C22-C23-C24
15	J	101	BCR	C37-C22-C23-C24
15	J	104	BCR	C7-C8-C9-C10
15	J	104	BCR	C7-C8-C9-C34
15	K	4001	BCR	C21-C22-C23-C24
15	L	206	BCR	C23-C24-C25-C26
15	L	207	BCR	C22-C23-C24-C25
16	G	846	LHG	O7-C5-C6-O8
16	G	848	LHG	C4-O6-P-O3
16	H	2148	LHG	C3-O3-P-O4
16	H	2148	LHG	C3-O3-P-O5
16	H	2148	LHG	C3-O3-P-O6
16	H	2148	LHG	C4-O6-P-O3
16	H	2148	LHG	C4-O6-P-O4
16	V	103	LHG	O1-C1-C2-C3
16	V	103	LHG	C3-O3-P-O5
16	V	103	LHG	C8-C7-O7-C5
16	a	846	LHG	O7-C5-C6-O8
16	a	848	LHG	C4-O6-P-O3
16	b	2148	LHG	C3-O3-P-O4
16	b	2148	LHG	C3-O3-P-O5
16	b	2148	LHG	C3-O3-P-O6
16	b	2148	LHG	C4-O6-P-O3
16	b	2148	LHG	C4-O6-P-O4
16	m	103	LHG	O1-C1-C2-C3
16	m	103	LHG	C3-O3-P-O5
16	m	103	LHG	C8-C7-O7-C5
16	A	846	LHG	O7-C5-C6-O8
16	A	848	LHG	C4-O6-P-O3
16	B	2149	LHG	C3-O3-P-O4
16	B	2149	LHG	C3-O3-P-O5
16	B	2149	LHG	C3-O3-P-O6
16	B	2149	LHG	C4-O6-P-O3
16	B	2149	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
16	M	102	LHG	O1-C1-C2-C3
16	M	102	LHG	C3-O3-P-O5
16	M	102	LHG	C8-C7-O7-C5
17	G	847	LMG	C2-C1-O1-C7
17	G	847	LMG	C11-C10-O7-C8
17	a	847	LMG	C2-C1-O1-C7
17	a	847	LMG	C11-C10-O7-C8
17	A	847	LMG	C2-C1-O1-C7
17	A	847	LMG	C11-C10-O7-C8
18	G	852	45D	C15-C07-C19-C23
18	G	852	45D	C19-C23-C25-C29
18	a	852	45D	C15-C07-C19-C23
18	a	852	45D	C19-C23-C25-C29
18	A	852	45D	C15-C07-C19-C23
18	A	852	45D	C19-C23-C25-C29
20	H	2143	ECH	C7-C8-C9-C10
20	H	2143	ECH	C17-C18-C19-C20
20	V	101	ECH	C17-C18-C19-C20
20	V	101	ECH	C23-C24-C25-C26
20	V	101	ECH	C23-C24-C25-C30
20	b	2143	ECH	C7-C8-C9-C10
20	b	2143	ECH	C17-C18-C19-C20
20	m	101	ECH	C17-C18-C19-C20
20	m	101	ECH	C23-C24-C25-C26
20	m	101	ECH	C23-C24-C25-C30
20	B	2144	ECH	C7-C8-C9-C10
20	B	2144	ECH	C17-C18-C19-C20
20	M	103	ECH	C17-C18-C19-C20
20	M	103	ECH	C23-C24-C25-C26
20	M	103	ECH	C23-C24-C25-C30
22	H	2150	EQ3	C7-C8-C9-C34
22	H	2150	EQ3	C7-C8-C9-C10
22	H	2150	EQ3	C11-C12-C13-C35
22	H	2150	EQ3	C11-C12-C13-C14
22	H	2150	EQ3	C21-C22-C23-C24
22	b	2150	EQ3	C7-C8-C9-C34
22	b	2150	EQ3	C7-C8-C9-C10
22	b	2150	EQ3	C11-C12-C13-C35
22	b	2150	EQ3	C11-C12-C13-C14
22	b	2150	EQ3	C21-C22-C23-C24
22	B	2151	EQ3	C7-C8-C9-C34
22	B	2151	EQ3	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
22	B	2151	EQ3	C11-C12-C13-C35
22	B	2151	EQ3	C11-C12-C13-C14
22	B	2151	EQ3	C21-C22-C23-C24
23	H	2151	ZEX	C5-C6-C7-C8
23	H	2151	ZEX	C25-C26-C27-C28
23	H	2151	ZEX	C7-C8-C9-C10
23	H	2151	ZEX	C31-C32-C33-C34
23	H	2151	ZEX	C31-C32-C33-C40
23	H	2151	ZEX	C27-C28-C29-C30
23	H	2151	ZEX	C27-C28-C29-C39
23	Q	205	ZEX	C21-C26-C27-C28
23	Q	205	ZEX	C7-C8-C9-C10
23	Q	205	ZEX	C31-C32-C33-C34
23	Q	205	ZEX	C31-C32-C33-C40
23	Q	205	ZEX	C29-C30-C31-C32
23	Q	205	ZEX	C27-C28-C29-C30
23	Q	205	ZEX	C27-C28-C29-C39
23	b	2151	ZEX	C5-C6-C7-C8
23	b	2151	ZEX	C25-C26-C27-C28
23	b	2151	ZEX	C7-C8-C9-C10
23	b	2151	ZEX	C31-C32-C33-C34
23	b	2151	ZEX	C31-C32-C33-C40
23	b	2151	ZEX	C27-C28-C29-C30
23	b	2151	ZEX	C27-C28-C29-C39
23	f	205	ZEX	C21-C26-C27-C28
23	f	205	ZEX	C7-C8-C9-C10
23	f	205	ZEX	C31-C32-C33-C34
23	f	205	ZEX	C31-C32-C33-C40
23	f	205	ZEX	C29-C30-C31-C32
23	f	205	ZEX	C27-C28-C29-C30
23	f	205	ZEX	C27-C28-C29-C39
23	B	2152	ZEX	C5-C6-C7-C8
23	B	2152	ZEX	C25-C26-C27-C28
23	B	2152	ZEX	C7-C8-C9-C10
23	B	2152	ZEX	C31-C32-C33-C34
23	B	2152	ZEX	C31-C32-C33-C40
23	B	2152	ZEX	C27-C28-C29-C30
23	B	2152	ZEX	C27-C28-C29-C39
23	F	205	ZEX	C21-C26-C27-C28
23	F	205	ZEX	C7-C8-C9-C10
23	F	205	ZEX	C31-C32-C33-C34
23	F	205	ZEX	C31-C32-C33-C40

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Mol	Chain	Res	Type	Atoms
23	F	205	ZEX	C29-C30-C31-C32
23	F	205	ZEX	C27-C28-C29-C30
23	F	205	ZEX	C27-C28-C29-C39
24	U	208	SQD	O47-C45-C46-O48
24	U	208	SQD	O5-C5-C6-S
24	U	208	SQD	C5-C6-S-O9
24	V	102	SQD	O5-C1-O6-C44
24	l	208	SQD	O47-C45-C46-O48
24	l	208	SQD	O5-C5-C6-S
24	l	208	SQD	C5-C6-S-O9
24	m	102	SQD	O5-C1-O6-C44
24	L	208	SQD	O47-C45-C46-O48
24	L	208	SQD	O5-C5-C6-S
24	L	208	SQD	C5-C6-S-O9
24	M	101	SQD	O5-C1-O6-C44
25	U	209	DGD	C2B-C1B-O2G-C2G
25	l	209	DGD	C2B-C1B-O2G-C2G
25	L	209	DGD	C2B-C1B-O2G-C2G
26	U	210	LMT	C2'-C1'-O1'-C1
26	U	210	LMT	O5'-C1'-O1'-C1
26	U	210	LMT	C2-C1-O1'-C1'
26	l	210	LMT	C2'-C1'-O1'-C1
26	l	210	LMT	O5'-C1'-O1'-C1
26	l	210	LMT	C2-C1-O1'-C1'
26	L	210	LMT	C2'-C1'-O1'-C1
26	L	210	LMT	O5'-C1'-O1'-C1
26	L	210	LMT	C2-C1-O1'-C1'
12	H	2111	CLA	C4C-C3C-CAC-CBC
12	b	2111	CLA	C4C-C3C-CAC-CBC
12	B	2112	CLA	C4C-C3C-CAC-CBC
12	G	805	CLA	O1D-CGD-O2D-CED
12	G	809	CLA	O1D-CGD-O2D-CED
12	G	819	CLA	O1D-CGD-O2D-CED
12	H	2122	CLA	O1D-CGD-O2D-CED
12	H	2123	CLA	O1D-CGD-O2D-CED
12	T	4002	CLA	O1D-CGD-O2D-CED
12	a	805	CLA	O1D-CGD-O2D-CED
12	a	809	CLA	O1D-CGD-O2D-CED
12	a	819	CLA	O1D-CGD-O2D-CED
12	b	2122	CLA	O1D-CGD-O2D-CED
12	b	2123	CLA	O1D-CGD-O2D-CED
12	k	4002	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	A	805	CLA	O1D-CGD-O2D-CED
12	A	809	CLA	O1D-CGD-O2D-CED
12	A	819	CLA	O1D-CGD-O2D-CED
12	B	2123	CLA	O1D-CGD-O2D-CED
12	B	2124	CLA	O1D-CGD-O2D-CED
12	K	4002	CLA	O1D-CGD-O2D-CED
12	H	2134	CLA	O1D-CGD-O2D-CED
12	H	2135	CLA	O1D-CGD-O2D-CED
12	b	2134	CLA	O1D-CGD-O2D-CED
12	b	2135	CLA	O1D-CGD-O2D-CED
12	B	2135	CLA	O1D-CGD-O2D-CED
12	B	2136	CLA	O1D-CGD-O2D-CED
17	G	849	LMG	C11-C10-O7-C8
17	a	849	LMG	C11-C10-O7-C8
17	A	849	LMG	C11-C10-O7-C8
12	G	805	CLA	CBD-CGD-O2D-CED
12	G	806	CLA	CBD-CGD-O2D-CED
12	G	809	CLA	CBD-CGD-O2D-CED
12	G	810	CLA	CBD-CGD-O2D-CED
12	G	811	CLA	CBD-CGD-O2D-CED
12	G	814	CLA	CBD-CGD-O2D-CED
12	G	819	CLA	CBD-CGD-O2D-CED
12	G	822	CLA	CBD-CGD-O2D-CED
12	G	838	CLA	CBD-CGD-O2D-CED
12	H	2110	CLA	CBD-CGD-O2D-CED
12	H	2122	CLA	CBD-CGD-O2D-CED
12	H	2123	CLA	CBD-CGD-O2D-CED
12	H	2127	CLA	CBD-CGD-O2D-CED
12	H	2132	CLA	CBD-CGD-O2D-CED
12	H	2135	CLA	CBD-CGD-O2D-CED
12	H	2152	CLA	CBD-CGD-O2D-CED
12	U	201	CLA	CBD-CGD-O2D-CED
12	a	805	CLA	CBD-CGD-O2D-CED
12	a	806	CLA	CBD-CGD-O2D-CED
12	a	809	CLA	CBD-CGD-O2D-CED
12	a	810	CLA	CBD-CGD-O2D-CED
12	a	811	CLA	CBD-CGD-O2D-CED
12	a	814	CLA	CBD-CGD-O2D-CED
12	a	819	CLA	CBD-CGD-O2D-CED
12	a	822	CLA	CBD-CGD-O2D-CED
12	a	838	CLA	CBD-CGD-O2D-CED
12	b	2110	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	b	2122	CLA	CBD-CGD-O2D-CED
12	b	2123	CLA	CBD-CGD-O2D-CED
12	b	2127	CLA	CBD-CGD-O2D-CED
12	b	2132	CLA	CBD-CGD-O2D-CED
12	b	2135	CLA	CBD-CGD-O2D-CED
12	b	2152	CLA	CBD-CGD-O2D-CED
12	l	201	CLA	CBD-CGD-O2D-CED
12	A	805	CLA	CBD-CGD-O2D-CED
12	A	806	CLA	CBD-CGD-O2D-CED
12	A	809	CLA	CBD-CGD-O2D-CED
12	A	810	CLA	CBD-CGD-O2D-CED
12	A	811	CLA	CBD-CGD-O2D-CED
12	A	814	CLA	CBD-CGD-O2D-CED
12	A	819	CLA	CBD-CGD-O2D-CED
12	A	822	CLA	CBD-CGD-O2D-CED
12	A	838	CLA	CBD-CGD-O2D-CED
12	B	2101	CLA	CBD-CGD-O2D-CED
12	B	2111	CLA	CBD-CGD-O2D-CED
12	B	2123	CLA	CBD-CGD-O2D-CED
12	B	2124	CLA	CBD-CGD-O2D-CED
12	B	2128	CLA	CBD-CGD-O2D-CED
12	B	2133	CLA	CBD-CGD-O2D-CED
12	B	2136	CLA	CBD-CGD-O2D-CED
12	L	201	CLA	CBD-CGD-O2D-CED
12	G	805	CLA	O1A-CGA-O2A-C1
12	H	2102	CLA	O1A-CGA-O2A-C1
12	H	2110	CLA	O1A-CGA-O2A-C1
12	H	2131	CLA	O1A-CGA-O2A-C1
12	H	2137	CLA	O1A-CGA-O2A-C1
12	H	2140	CLA	O1A-CGA-O2A-C1
12	Q	201	CLA	O1A-CGA-O2A-C1
12	a	805	CLA	O1A-CGA-O2A-C1
12	b	2102	CLA	O1A-CGA-O2A-C1
12	b	2110	CLA	O1A-CGA-O2A-C1
12	b	2131	CLA	O1A-CGA-O2A-C1
12	b	2137	CLA	O1A-CGA-O2A-C1
12	b	2140	CLA	O1A-CGA-O2A-C1
12	f	201	CLA	O1A-CGA-O2A-C1
12	A	805	CLA	O1A-CGA-O2A-C1
12	B	2103	CLA	O1A-CGA-O2A-C1
12	B	2111	CLA	O1A-CGA-O2A-C1
12	B	2132	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	B	2138	CLA	O1A-CGA-O2A-C1
12	B	2141	CLA	O1A-CGA-O2A-C1
12	F	201	CLA	O1A-CGA-O2A-C1
12	H	2111	CLA	C2C-C3C-CAC-CBC
12	b	2111	CLA	C2C-C3C-CAC-CBC
12	B	2112	CLA	C2C-C3C-CAC-CBC
12	H	2102	CLA	CBA-CGA-O2A-C1
12	H	2110	CLA	CBA-CGA-O2A-C1
12	H	2131	CLA	CBA-CGA-O2A-C1
12	H	2137	CLA	CBA-CGA-O2A-C1
12	b	2102	CLA	CBA-CGA-O2A-C1
12	b	2110	CLA	CBA-CGA-O2A-C1
12	b	2131	CLA	CBA-CGA-O2A-C1
12	b	2137	CLA	CBA-CGA-O2A-C1
12	B	2103	CLA	CBA-CGA-O2A-C1
12	B	2111	CLA	CBA-CGA-O2A-C1
12	B	2132	CLA	CBA-CGA-O2A-C1
12	B	2138	CLA	CBA-CGA-O2A-C1
12	S	103	CLA	CBD-CGD-O2D-CED
12	j	103	CLA	CBD-CGD-O2D-CED
12	J	103	CLA	CBD-CGD-O2D-CED
12	G	809	CLA	O1A-CGA-O2A-C1
12	G	822	CLA	O1A-CGA-O2A-C1
12	G	831	CLA	O1A-CGA-O2A-C1
12	H	2120	CLA	O1A-CGA-O2A-C1
12	H	2121	CLA	O1A-CGA-O2A-C1
12	H	2133	CLA	O1A-CGA-O2A-C1
12	H	2152	CLA	O1A-CGA-O2A-C1
12	U	203	CLA	O1A-CGA-O2A-C1
12	a	809	CLA	O1A-CGA-O2A-C1
12	a	822	CLA	O1A-CGA-O2A-C1
12	a	831	CLA	O1A-CGA-O2A-C1
12	b	2120	CLA	O1A-CGA-O2A-C1
12	b	2121	CLA	O1A-CGA-O2A-C1
12	b	2133	CLA	O1A-CGA-O2A-C1
12	b	2152	CLA	O1A-CGA-O2A-C1
12	l	203	CLA	O1A-CGA-O2A-C1
12	A	809	CLA	O1A-CGA-O2A-C1
12	A	822	CLA	O1A-CGA-O2A-C1
12	A	831	CLA	O1A-CGA-O2A-C1
12	B	2101	CLA	O1A-CGA-O2A-C1
12	B	2121	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	B	2122	CLA	O1A-CGA-O2A-C1
12	B	2134	CLA	O1A-CGA-O2A-C1
12	L	203	CLA	O1A-CGA-O2A-C1
17	G	847	LMG	O10-C28-O8-C9
17	G	849	LMG	O10-C28-O8-C9
17	a	847	LMG	O10-C28-O8-C9
17	a	849	LMG	O10-C28-O8-C9
17	A	847	LMG	O10-C28-O8-C9
17	A	849	LMG	O10-C28-O8-C9
12	H	2121	CLA	O1D-CGD-O2D-CED
12	b	2121	CLA	O1D-CGD-O2D-CED
12	B	2122	CLA	O1D-CGD-O2D-CED
12	H	2103	CLA	O1D-CGD-O2D-CED
12	H	2116	CLA	O1D-CGD-O2D-CED
12	b	2103	CLA	O1D-CGD-O2D-CED
12	b	2116	CLA	O1D-CGD-O2D-CED
12	B	2104	CLA	O1D-CGD-O2D-CED
12	B	2117	CLA	O1D-CGD-O2D-CED
17	G	849	LMG	O6-C5-C6-O5
17	a	849	LMG	O6-C5-C6-O5
17	A	849	LMG	O6-C5-C6-O5
12	H	2115	CLA	CBD-CGD-O2D-CED
12	b	2115	CLA	CBD-CGD-O2D-CED
12	B	2116	CLA	CBD-CGD-O2D-CED
16	V	103	LHG	O9-C7-O7-C5
16	m	103	LHG	O9-C7-O7-C5
16	M	102	LHG	O9-C7-O7-C5
17	G	847	LMG	O9-C10-O7-C8
17	a	847	LMG	O9-C10-O7-C8
17	A	847	LMG	O9-C10-O7-C8
25	U	209	DGD	O1B-C1B-O2G-C2G
25	l	209	DGD	O1B-C1B-O2G-C2G
25	L	209	DGD	O1B-C1B-O2G-C2G
12	G	807	CLA	C3-C5-C6-C7
12	G	816	CLA	C3-C5-C6-C7
12	G	817	CLA	C3-C5-C6-C7
12	G	837	CLA	C3-C5-C6-C7
12	H	2101	CLA	C3-C5-C6-C7
12	H	2107	CLA	C3-C5-C6-C7
12	H	2109	CLA	C3-C5-C6-C7
12	H	2112	CLA	C3-C5-C6-C7
12	H	2123	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
12	a	807	CLA	C3-C5-C6-C7
12	a	816	CLA	C3-C5-C6-C7
12	a	817	CLA	C3-C5-C6-C7
12	a	837	CLA	C3-C5-C6-C7
12	b	2101	CLA	C3-C5-C6-C7
12	b	2107	CLA	C3-C5-C6-C7
12	b	2109	CLA	C3-C5-C6-C7
12	b	2112	CLA	C3-C5-C6-C7
12	b	2123	CLA	C3-C5-C6-C7
12	A	807	CLA	C3-C5-C6-C7
12	A	816	CLA	C3-C5-C6-C7
12	A	817	CLA	C3-C5-C6-C7
12	A	837	CLA	C3-C5-C6-C7
12	B	2102	CLA	C3-C5-C6-C7
12	B	2108	CLA	C3-C5-C6-C7
12	B	2110	CLA	C3-C5-C6-C7
12	B	2113	CLA	C3-C5-C6-C7
12	B	2124	CLA	C3-C5-C6-C7
12	G	809	CLA	CBA-CGA-O2A-C1
12	G	822	CLA	CBA-CGA-O2A-C1
12	G	831	CLA	CBA-CGA-O2A-C1
12	G	851	CLA	CBA-CGA-O2A-C1
12	H	2121	CLA	CBA-CGA-O2A-C1
12	H	2140	CLA	CBA-CGA-O2A-C1
12	Q	201	CLA	CBA-CGA-O2A-C1
12	a	809	CLA	CBA-CGA-O2A-C1
12	a	822	CLA	CBA-CGA-O2A-C1
12	a	831	CLA	CBA-CGA-O2A-C1
12	a	851	CLA	CBA-CGA-O2A-C1
12	b	2121	CLA	CBA-CGA-O2A-C1
12	b	2140	CLA	CBA-CGA-O2A-C1
12	f	201	CLA	CBA-CGA-O2A-C1
12	A	809	CLA	CBA-CGA-O2A-C1
12	A	822	CLA	CBA-CGA-O2A-C1
12	A	831	CLA	CBA-CGA-O2A-C1
12	A	851	CLA	CBA-CGA-O2A-C1
12	B	2122	CLA	CBA-CGA-O2A-C1
12	B	2141	CLA	CBA-CGA-O2A-C1
12	F	201	CLA	CBA-CGA-O2A-C1
17	G	847	LMG	C29-C28-O8-C9
17	a	847	LMG	C29-C28-O8-C9
17	A	847	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
12	G	820	CLA	CBD-CGD-O2D-CED
12	H	2114	CLA	CBD-CGD-O2D-CED
12	H	2118	CLA	CBD-CGD-O2D-CED
12	H	2131	CLA	CBD-CGD-O2D-CED
12	H	2139	CLA	CBD-CGD-O2D-CED
12	H	2140	CLA	CBD-CGD-O2D-CED
12	H	2141	CLA	CBD-CGD-O2D-CED
12	Q	203	CLA	CBD-CGD-O2D-CED
12	a	820	CLA	CBD-CGD-O2D-CED
12	b	2114	CLA	CBD-CGD-O2D-CED
12	b	2118	CLA	CBD-CGD-O2D-CED
12	b	2131	CLA	CBD-CGD-O2D-CED
12	b	2139	CLA	CBD-CGD-O2D-CED
12	b	2140	CLA	CBD-CGD-O2D-CED
12	b	2141	CLA	CBD-CGD-O2D-CED
12	f	203	CLA	CBD-CGD-O2D-CED
12	A	820	CLA	CBD-CGD-O2D-CED
12	B	2115	CLA	CBD-CGD-O2D-CED
12	B	2119	CLA	CBD-CGD-O2D-CED
12	B	2132	CLA	CBD-CGD-O2D-CED
12	B	2140	CLA	CBD-CGD-O2D-CED
12	B	2141	CLA	CBD-CGD-O2D-CED
12	B	2142	CLA	CBD-CGD-O2D-CED
12	F	203	CLA	CBD-CGD-O2D-CED
12	G	815	CLA	O1D-CGD-O2D-CED
12	H	2110	CLA	O1D-CGD-O2D-CED
12	H	2132	CLA	O1D-CGD-O2D-CED
12	a	815	CLA	O1D-CGD-O2D-CED
12	b	2110	CLA	O1D-CGD-O2D-CED
12	b	2132	CLA	O1D-CGD-O2D-CED
12	A	815	CLA	O1D-CGD-O2D-CED
12	B	2111	CLA	O1D-CGD-O2D-CED
12	B	2133	CLA	O1D-CGD-O2D-CED
12	Q	201	CLA	O1D-CGD-O2D-CED
12	f	201	CLA	O1D-CGD-O2D-CED
12	F	201	CLA	O1D-CGD-O2D-CED
12	G	805	CLA	C4-C3-C5-C6
12	G	827	CLA	C4-C3-C5-C6
12	H	2103	CLA	C4-C3-C5-C6
12	Q	201	CLA	C4-C3-C5-C6
12	a	805	CLA	C4-C3-C5-C6
12	a	827	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
12	b	2103	CLA	C4-C3-C5-C6
12	f	201	CLA	C4-C3-C5-C6
12	A	805	CLA	C4-C3-C5-C6
12	A	827	CLA	C4-C3-C5-C6
12	B	2104	CLA	C4-C3-C5-C6
12	F	201	CLA	C4-C3-C5-C6
12	G	805	CLA	C2-C3-C5-C6
12	G	810	CLA	C2-C3-C5-C6
12	a	805	CLA	C2-C3-C5-C6
12	a	810	CLA	C2-C3-C5-C6
12	A	805	CLA	C2-C3-C5-C6
12	A	810	CLA	C2-C3-C5-C6
12	G	829	CLA	CBD-CGD-O2D-CED
12	H	2133	CLA	CBD-CGD-O2D-CED
12	a	829	CLA	CBD-CGD-O2D-CED
12	b	2133	CLA	CBD-CGD-O2D-CED
12	A	829	CLA	CBD-CGD-O2D-CED
12	B	2134	CLA	CBD-CGD-O2D-CED
26	U	210	LMT	O5B-C5B-C6B-O6B
26	l	210	LMT	O5B-C5B-C6B-O6B
26	L	210	LMT	O5B-C5B-C6B-O6B
12	G	830	CLA	C2A-CAA-CBA-CGA
12	a	830	CLA	C2A-CAA-CBA-CGA
12	A	830	CLA	C2A-CAA-CBA-CGA
12	G	823	CLA	C3-C5-C6-C7
12	H	2114	CLA	C3-C5-C6-C7
12	H	2121	CLA	C3-C5-C6-C7
12	a	823	CLA	C3-C5-C6-C7
12	b	2114	CLA	C3-C5-C6-C7
12	b	2121	CLA	C3-C5-C6-C7
12	A	823	CLA	C3-C5-C6-C7
12	B	2115	CLA	C3-C5-C6-C7
12	B	2122	CLA	C3-C5-C6-C7
12	G	802	CLA	CBA-CGA-O2A-C1
12	H	2120	CLA	CBA-CGA-O2A-C1
12	H	2133	CLA	CBA-CGA-O2A-C1
12	H	2152	CLA	CBA-CGA-O2A-C1
12	U	203	CLA	CBA-CGA-O2A-C1
12	a	802	CLA	CBA-CGA-O2A-C1
12	b	2120	CLA	CBA-CGA-O2A-C1
12	b	2133	CLA	CBA-CGA-O2A-C1
12	b	2152	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	l	203	CLA	CBA-CGA-O2A-C1
12	A	802	CLA	CBA-CGA-O2A-C1
12	B	2101	CLA	CBA-CGA-O2A-C1
12	B	2121	CLA	CBA-CGA-O2A-C1
12	B	2134	CLA	CBA-CGA-O2A-C1
12	L	203	CLA	CBA-CGA-O2A-C1
16	V	103	LHG	C24-C23-O8-C6
16	m	103	LHG	C24-C23-O8-C6
16	M	102	LHG	C24-C23-O8-C6
17	G	849	LMG	C29-C28-O8-C9
17	a	849	LMG	C29-C28-O8-C9
17	A	849	LMG	C29-C28-O8-C9
23	H	2151	ZEX	C29-C30-C31-C32
23	b	2151	ZEX	C29-C30-C31-C32
23	B	2152	ZEX	C29-C30-C31-C32
12	G	810	CLA	O1A-CGA-O2A-C1
12	G	816	CLA	O1A-CGA-O2A-C1
12	G	851	CLA	O1A-CGA-O2A-C1
12	a	810	CLA	O1A-CGA-O2A-C1
12	a	816	CLA	O1A-CGA-O2A-C1
12	a	851	CLA	O1A-CGA-O2A-C1
12	A	810	CLA	O1A-CGA-O2A-C1
12	A	816	CLA	O1A-CGA-O2A-C1
12	A	851	CLA	O1A-CGA-O2A-C1
16	V	103	LHG	O10-C23-O8-C6
16	m	103	LHG	O10-C23-O8-C6
16	M	102	LHG	O10-C23-O8-C6
12	G	806	CLA	O1D-CGD-O2D-CED
12	G	811	CLA	O1D-CGD-O2D-CED
12	a	806	CLA	O1D-CGD-O2D-CED
12	a	811	CLA	O1D-CGD-O2D-CED
12	A	806	CLA	O1D-CGD-O2D-CED
12	A	811	CLA	O1D-CGD-O2D-CED
12	G	830	CLA	C3-C5-C6-C7
12	G	833	CLA	C3-C5-C6-C7
12	G	839	CLA	C3-C5-C6-C7
12	a	830	CLA	C3-C5-C6-C7
12	a	833	CLA	C3-C5-C6-C7
12	a	839	CLA	C3-C5-C6-C7
12	A	830	CLA	C3-C5-C6-C7
12	A	833	CLA	C3-C5-C6-C7
12	A	839	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
12	G	810	CLA	O1D-CGD-O2D-CED
12	a	810	CLA	O1D-CGD-O2D-CED
12	A	810	CLA	O1D-CGD-O2D-CED
12	G	807	CLA	CBA-CGA-O2A-C1
12	G	810	CLA	CBA-CGA-O2A-C1
12	G	823	CLA	CBA-CGA-O2A-C1
12	G	833	CLA	CBA-CGA-O2A-C1
12	H	2103	CLA	CBA-CGA-O2A-C1
12	H	2118	CLA	CBA-CGA-O2A-C1
12	a	807	CLA	CBA-CGA-O2A-C1
12	a	810	CLA	CBA-CGA-O2A-C1
12	a	823	CLA	CBA-CGA-O2A-C1
12	a	833	CLA	CBA-CGA-O2A-C1
12	b	2103	CLA	CBA-CGA-O2A-C1
12	b	2118	CLA	CBA-CGA-O2A-C1
12	A	807	CLA	CBA-CGA-O2A-C1
12	A	810	CLA	CBA-CGA-O2A-C1
12	A	823	CLA	CBA-CGA-O2A-C1
12	A	833	CLA	CBA-CGA-O2A-C1
12	B	2104	CLA	CBA-CGA-O2A-C1
12	B	2119	CLA	CBA-CGA-O2A-C1
16	G	846	LHG	O10-C23-O8-C6
16	a	846	LHG	O10-C23-O8-C6
16	A	846	LHG	O10-C23-O8-C6
12	G	817	CLA	CBD-CGD-O2D-CED
12	a	817	CLA	CBD-CGD-O2D-CED
12	A	817	CLA	CBD-CGD-O2D-CED
12	G	822	CLA	O1D-CGD-O2D-CED
12	U	201	CLA	O1D-CGD-O2D-CED
12	a	822	CLA	O1D-CGD-O2D-CED
12	l	201	CLA	O1D-CGD-O2D-CED
12	A	822	CLA	O1D-CGD-O2D-CED
12	L	201	CLA	O1D-CGD-O2D-CED
12	G	832	CLA	CBD-CGD-O2D-CED
12	H	2107	CLA	CBD-CGD-O2D-CED
12	a	832	CLA	CBD-CGD-O2D-CED
12	b	2107	CLA	CBD-CGD-O2D-CED
12	A	832	CLA	CBD-CGD-O2D-CED
12	B	2108	CLA	CBD-CGD-O2D-CED
12	G	838	CLA	O1D-CGD-O2D-CED
12	H	2152	CLA	O1D-CGD-O2D-CED
12	a	838	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	b	2152	CLA	O1D-CGD-O2D-CED
12	A	838	CLA	O1D-CGD-O2D-CED
12	B	2101	CLA	O1D-CGD-O2D-CED
12	G	816	CLA	CBA-CGA-O2A-C1
12	a	816	CLA	CBA-CGA-O2A-C1
12	A	816	CLA	CBA-CGA-O2A-C1
12	H	2119	CLA	C4-C3-C5-C6
12	b	2119	CLA	C4-C3-C5-C6
12	B	2120	CLA	C4-C3-C5-C6
12	H	2103	CLA	C2-C3-C5-C6
12	H	2119	CLA	C2-C3-C5-C6
12	Q	201	CLA	C2-C3-C5-C6
12	b	2103	CLA	C2-C3-C5-C6
12	b	2119	CLA	C2-C3-C5-C6
12	f	201	CLA	C2-C3-C5-C6
12	B	2104	CLA	C2-C3-C5-C6
12	B	2120	CLA	C2-C3-C5-C6
12	F	201	CLA	C2-C3-C5-C6
12	G	802	CLA	O1A-CGA-O2A-C1
12	G	807	CLA	O1A-CGA-O2A-C1
12	a	802	CLA	O1A-CGA-O2A-C1
12	a	807	CLA	O1A-CGA-O2A-C1
12	A	802	CLA	O1A-CGA-O2A-C1
12	A	807	CLA	O1A-CGA-O2A-C1
26	U	210	LMT	C4B-C5B-C6B-O6B
26	l	210	LMT	C4B-C5B-C6B-O6B
26	L	210	LMT	C4B-C5B-C6B-O6B
12	G	801	CLA	CBD-CGD-O2D-CED
12	a	801	CLA	CBD-CGD-O2D-CED
12	A	801	CLA	CBD-CGD-O2D-CED
17	G	849	LMG	C4-C5-C6-O5
17	a	849	LMG	C4-C5-C6-O5
17	A	849	LMG	C4-C5-C6-O5
12	H	2105	CLA	C2A-CAA-CBA-CGA
12	U	204	CLA	C2A-CAA-CBA-CGA
12	b	2105	CLA	C2A-CAA-CBA-CGA
12	l	204	CLA	C2A-CAA-CBA-CGA
12	B	2106	CLA	C2A-CAA-CBA-CGA
12	L	204	CLA	C2A-CAA-CBA-CGA
12	H	2132	CLA	C2C-C3C-CAC-CBC
12	b	2132	CLA	C2C-C3C-CAC-CBC
12	G	814	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	S	103	CLA	O1D-CGD-O2D-CED
12	a	814	CLA	O1D-CGD-O2D-CED
12	j	103	CLA	O1D-CGD-O2D-CED
12	A	814	CLA	O1D-CGD-O2D-CED
12	J	103	CLA	O1D-CGD-O2D-CED
12	G	823	CLA	O1A-CGA-O2A-C1
12	G	833	CLA	O1A-CGA-O2A-C1
12	H	2103	CLA	O1A-CGA-O2A-C1
12	a	823	CLA	O1A-CGA-O2A-C1
12	a	833	CLA	O1A-CGA-O2A-C1
12	b	2103	CLA	O1A-CGA-O2A-C1
12	A	823	CLA	O1A-CGA-O2A-C1
12	A	833	CLA	O1A-CGA-O2A-C1
12	B	2104	CLA	O1A-CGA-O2A-C1
12	B	2133	CLA	C2C-C3C-CAC-CBC
12	G	830	CLA	CBA-CGA-O2A-C1
12	G	835	CLA	CBA-CGA-O2A-C1
12	a	830	CLA	CBA-CGA-O2A-C1
12	a	835	CLA	CBA-CGA-O2A-C1
12	A	830	CLA	CBA-CGA-O2A-C1
12	A	835	CLA	CBA-CGA-O2A-C1
12	G	813	CLA	CBD-CGD-O2D-CED
12	G	837	CLA	CBD-CGD-O2D-CED
12	H	2104	CLA	CBD-CGD-O2D-CED
12	H	2106	CLA	CBD-CGD-O2D-CED
12	H	2117	CLA	CBD-CGD-O2D-CED
12	H	2136	CLA	CBD-CGD-O2D-CED
12	S	102	CLA	CBD-CGD-O2D-CED
12	a	813	CLA	CBD-CGD-O2D-CED
12	a	837	CLA	CBD-CGD-O2D-CED
12	b	2104	CLA	CBD-CGD-O2D-CED
12	b	2106	CLA	CBD-CGD-O2D-CED
12	b	2117	CLA	CBD-CGD-O2D-CED
12	b	2136	CLA	CBD-CGD-O2D-CED
12	j	102	CLA	CBD-CGD-O2D-CED
12	A	813	CLA	CBD-CGD-O2D-CED
12	A	837	CLA	CBD-CGD-O2D-CED
12	B	2105	CLA	CBD-CGD-O2D-CED
12	B	2107	CLA	CBD-CGD-O2D-CED
12	B	2118	CLA	CBD-CGD-O2D-CED
12	B	2137	CLA	CBD-CGD-O2D-CED
12	J	102	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	H	2118	CLA	O1A-CGA-O2A-C1
12	b	2118	CLA	O1A-CGA-O2A-C1
12	B	2119	CLA	O1A-CGA-O2A-C1
12	G	834	CLA	CBD-CGD-O2D-CED
12	G	839	CLA	CBD-CGD-O2D-CED
12	a	834	CLA	CBD-CGD-O2D-CED
12	a	839	CLA	CBD-CGD-O2D-CED
12	A	834	CLA	CBD-CGD-O2D-CED
12	A	839	CLA	CBD-CGD-O2D-CED
12	G	819	CLA	CBA-CGA-O2A-C1
12	G	826	CLA	CBA-CGA-O2A-C1
12	G	854	CLA	CBA-CGA-O2A-C1
12	H	2132	CLA	CBA-CGA-O2A-C1
12	a	819	CLA	CBA-CGA-O2A-C1
12	a	826	CLA	CBA-CGA-O2A-C1
12	a	854	CLA	CBA-CGA-O2A-C1
12	b	2132	CLA	CBA-CGA-O2A-C1
12	A	819	CLA	CBA-CGA-O2A-C1
12	A	826	CLA	CBA-CGA-O2A-C1
12	A	854	CLA	CBA-CGA-O2A-C1
12	B	2133	CLA	CBA-CGA-O2A-C1
16	G	846	LHG	C24-C23-O8-C6
16	a	846	LHG	C24-C23-O8-C6
16	A	846	LHG	C24-C23-O8-C6
12	H	2115	CLA	O1D-CGD-O2D-CED
12	H	2127	CLA	O1D-CGD-O2D-CED
12	b	2115	CLA	O1D-CGD-O2D-CED
12	b	2127	CLA	O1D-CGD-O2D-CED
12	B	2116	CLA	O1D-CGD-O2D-CED
12	B	2128	CLA	O1D-CGD-O2D-CED
12	G	830	CLA	O1A-CGA-O2A-C1
12	a	830	CLA	O1A-CGA-O2A-C1
12	A	830	CLA	O1A-CGA-O2A-C1
12	G	833	CLA	C4-C3-C5-C6
12	G	851	CLA	C4-C3-C5-C6
12	a	833	CLA	C4-C3-C5-C6
12	a	851	CLA	C4-C3-C5-C6
12	A	833	CLA	C4-C3-C5-C6
12	A	851	CLA	C4-C3-C5-C6
12	G	827	CLA	C2-C3-C5-C6
12	G	833	CLA	C2-C3-C5-C6
12	G	851	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
12	a	827	CLA	C2-C3-C5-C6
12	a	833	CLA	C2-C3-C5-C6
12	a	851	CLA	C2-C3-C5-C6
12	A	827	CLA	C2-C3-C5-C6
12	A	833	CLA	C2-C3-C5-C6
12	A	851	CLA	C2-C3-C5-C6
12	H	2108	CLA	C3-C5-C6-C7
12	Q	201	CLA	C3-C5-C6-C7
12	f	201	CLA	C3-C5-C6-C7
12	F	201	CLA	C3-C5-C6-C7
12	H	2101	CLA	C11-C12-C13-C14
12	H	2110	CLA	C14-C13-C15-C16
12	Q	201	CLA	C11-C10-C8-C9
12	b	2101	CLA	C11-C12-C13-C14
12	b	2110	CLA	C14-C13-C15-C16
12	f	201	CLA	C11-C10-C8-C9
12	B	2102	CLA	C11-C12-C13-C14
12	B	2111	CLA	C14-C13-C15-C16
12	F	201	CLA	C11-C10-C8-C9
13	G	840	A1AGD	C12-C13-C14-C15
13	a	840	A1AGD	C12-C13-C14-C15
13	A	840	A1AGD	C12-C13-C14-C15
16	V	103	LHG	O2-C2-C3-O3
16	m	103	LHG	O2-C2-C3-O3
16	M	102	LHG	O2-C2-C3-O3
15	G	842	BCR	C36-C18-C19-C20
15	G	843	BCR	C11-C12-C13-C35
15	G	845	BCR	C37-C22-C23-C24
15	H	2142	BCR	C37-C22-C23-C24
15	H	2144	BCR	C7-C8-C9-C34
15	H	2145	BCR	C7-C8-C9-C34
15	R	101	BCR	C7-C8-C9-C34
15	R	101	BCR	C37-C22-C23-C24
15	S	101	BCR	C7-C8-C9-C34
15	S	101	BCR	C36-C18-C19-C20
15	U	206	BCR	C37-C22-C23-C24
15	a	842	BCR	C36-C18-C19-C20
15	a	843	BCR	C11-C12-C13-C35
15	a	845	BCR	C37-C22-C23-C24
15	b	2142	BCR	C37-C22-C23-C24
15	b	2144	BCR	C7-C8-C9-C34
15	b	2145	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
15	i	101	BCR	C7-C8-C9-C34
15	i	101	BCR	C37-C22-C23-C24
15	j	101	BCR	C7-C8-C9-C34
15	j	101	BCR	C36-C18-C19-C20
15	l	206	BCR	C37-C22-C23-C24
15	A	842	BCR	C36-C18-C19-C20
15	A	843	BCR	C11-C12-C13-C35
15	A	845	BCR	C37-C22-C23-C24
15	B	2143	BCR	C37-C22-C23-C24
15	B	2145	BCR	C7-C8-C9-C34
15	B	2146	BCR	C7-C8-C9-C34
15	I	101	BCR	C7-C8-C9-C34
15	I	101	BCR	C37-C22-C23-C24
15	J	101	BCR	C7-C8-C9-C34
15	J	101	BCR	C36-C18-C19-C20
15	L	206	BCR	C37-C22-C23-C24
18	G	852	45D	C19-C23-C25-C27
18	a	852	45D	C19-C23-C25-C27
18	A	852	45D	C19-C23-C25-C27
20	H	2143	ECH	C7-C8-C9-C34
20	H	2143	ECH	C36-C18-C19-C20
20	H	2143	ECH	C37-C22-C23-C24
20	V	101	ECH	C36-C18-C19-C20
20	b	2143	ECH	C7-C8-C9-C34
20	b	2143	ECH	C36-C18-C19-C20
20	b	2143	ECH	C37-C22-C23-C24
20	m	101	ECH	C36-C18-C19-C20
20	B	2144	ECH	C7-C8-C9-C34
20	B	2144	ECH	C36-C18-C19-C20
20	B	2144	ECH	C37-C22-C23-C24
20	M	103	ECH	C36-C18-C19-C20
22	H	2150	EQ3	C37-C22-C23-C24
22	b	2150	EQ3	C37-C22-C23-C24
22	B	2151	EQ3	C37-C22-C23-C24
23	H	2151	ZEX	C7-C8-C9-C19
23	Q	205	ZEX	C7-C8-C9-C19
23	b	2151	ZEX	C7-C8-C9-C19
23	f	205	ZEX	C7-C8-C9-C19
23	B	2152	ZEX	C7-C8-C9-C19
23	F	205	ZEX	C7-C8-C9-C19
15	G	842	BCR	C21-C22-C23-C24
15	U	206	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
15	U	206	BCR	C21-C22-C23-C24
15	a	842	BCR	C21-C22-C23-C24
15	l	206	BCR	C7-C8-C9-C10
15	l	206	BCR	C21-C22-C23-C24
15	A	842	BCR	C21-C22-C23-C24
15	L	206	BCR	C7-C8-C9-C10
15	L	206	BCR	C21-C22-C23-C24
20	H	2143	ECH	C21-C22-C23-C24
20	b	2143	ECH	C21-C22-C23-C24
20	B	2144	ECH	C21-C22-C23-C24
12	G	851	CLA	C2A-CAA-CBA-CGA
12	H	2131	CLA	C2A-CAA-CBA-CGA
12	H	2135	CLA	C2A-CAA-CBA-CGA
12	a	851	CLA	C2A-CAA-CBA-CGA
12	b	2131	CLA	C2A-CAA-CBA-CGA
12	b	2135	CLA	C2A-CAA-CBA-CGA
12	A	851	CLA	C2A-CAA-CBA-CGA
12	B	2132	CLA	C2A-CAA-CBA-CGA
12	B	2136	CLA	C2A-CAA-CBA-CGA
12	b	2108	CLA	C3-C5-C6-C7
12	B	2109	CLA	C3-C5-C6-C7
12	G	835	CLA	C5-C6-C7-C8
12	a	835	CLA	C5-C6-C7-C8
12	b	2109	CLA	C8-C10-C11-C12
12	A	835	CLA	C5-C6-C7-C8
12	G	812	CLA	CBD-CGD-O2D-CED
12	a	812	CLA	CBD-CGD-O2D-CED
12	A	812	CLA	CBD-CGD-O2D-CED
12	H	2109	CLA	C8-C10-C11-C12
12	B	2110	CLA	C8-C10-C11-C12
12	H	2140	CLA	C2-C1-O2A-CGA
12	b	2140	CLA	C2-C1-O2A-CGA
12	B	2141	CLA	C2-C1-O2A-CGA
12	G	839	CLA	C10-C11-C12-C13
12	a	839	CLA	C10-C11-C12-C13
12	A	839	CLA	C10-C11-C12-C13
17	a	849	LMG	O9-C10-O7-C8
17	A	849	LMG	O9-C10-O7-C8
16	V	103	LHG	O1-C1-C2-O2
16	m	103	LHG	O1-C1-C2-O2
16	M	102	LHG	O1-C1-C2-O2
12	H	2139	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	Q	203	CLA	O1D-CGD-O2D-CED
12	b	2139	CLA	O1D-CGD-O2D-CED
12	f	203	CLA	O1D-CGD-O2D-CED
12	B	2140	CLA	O1D-CGD-O2D-CED
12	F	203	CLA	O1D-CGD-O2D-CED
17	G	849	LMG	O9-C10-O7-C8
12	G	804	CLA	CBD-CGD-O2D-CED
12	a	804	CLA	CBD-CGD-O2D-CED
12	A	804	CLA	CBD-CGD-O2D-CED
12	G	819	CLA	C6-C7-C8-C10
12	a	819	CLA	C6-C7-C8-C10
12	A	819	CLA	C6-C7-C8-C10
13	G	840	A1AGD	C17-C18-C19-C21
13	a	840	A1AGD	C17-C18-C19-C21
13	A	840	A1AGD	C17-C18-C19-C21
12	G	820	CLA	C15-C16-C17-C18
12	G	836	CLA	C8-C10-C11-C12
12	a	836	CLA	C8-C10-C11-C12
12	A	820	CLA	C15-C16-C17-C18
12	A	836	CLA	C8-C10-C11-C12
16	H	2148	LHG	C7-C8-C9-C10
16	b	2148	LHG	C7-C8-C9-C10
16	B	2149	LHG	C7-C8-C9-C10
22	H	2150	EQ3	C9-C10-C11-C12
22	H	2150	EQ3	C13-C14-C15-C16
22	b	2150	EQ3	C9-C10-C11-C12
22	b	2150	EQ3	C13-C14-C15-C16
22	B	2151	EQ3	C9-C10-C11-C12
22	B	2151	EQ3	C13-C14-C15-C16
26	U	210	LMT	C3'-C4'-O1B-C1B
26	l	210	LMT	C3'-C4'-O1B-C1B
26	L	210	LMT	C3'-C4'-O1B-C1B
12	H	2118	CLA	O1D-CGD-O2D-CED
12	b	2118	CLA	O1D-CGD-O2D-CED
12	B	2119	CLA	O1D-CGD-O2D-CED
12	G	805	CLA	C10-C11-C12-C13
12	G	832	CLA	C8-C10-C11-C12
12	H	2107	CLA	C10-C11-C12-C13
12	a	820	CLA	C15-C16-C17-C18
12	a	832	CLA	C8-C10-C11-C12
12	b	2107	CLA	C10-C11-C12-C13
12	A	805	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
12	A	832	CLA	C8-C10-C11-C12
12	B	2108	CLA	C10-C11-C12-C13
16	H	2148	LHG	C23-C24-C25-C26
16	b	2148	LHG	C23-C24-C25-C26
16	B	2149	LHG	C23-C24-C25-C26
25	U	209	DGD	C1A-C2A-C3A-C4A
25	l	209	DGD	C1A-C2A-C3A-C4A
25	L	209	DGD	C1A-C2A-C3A-C4A
12	G	802	CLA	C15-C16-C17-C18
12	G	817	CLA	C5-C6-C7-C8
12	G	835	CLA	C13-C15-C16-C17
12	H	2112	CLA	C13-C15-C16-C17
12	H	2132	CLA	C13-C15-C16-C17
12	Q	201	CLA	C10-C11-C12-C13
12	a	802	CLA	C15-C16-C17-C18
12	a	805	CLA	C10-C11-C12-C13
12	a	817	CLA	C5-C6-C7-C8
12	a	835	CLA	C13-C15-C16-C17
12	b	2112	CLA	C13-C15-C16-C17
12	b	2132	CLA	C13-C15-C16-C17
12	f	201	CLA	C10-C11-C12-C13
12	A	802	CLA	C15-C16-C17-C18
12	A	817	CLA	C5-C6-C7-C8
12	A	835	CLA	C13-C15-C16-C17
12	B	2113	CLA	C13-C15-C16-C17
12	B	2133	CLA	C13-C15-C16-C17
12	F	201	CLA	C10-C11-C12-C13
12	G	826	CLA	C2A-CAA-CBA-CGA
12	H	2132	CLA	C2A-CAA-CBA-CGA
12	H	2139	CLA	C2A-CAA-CBA-CGA
12	Q	201	CLA	C2A-CAA-CBA-CGA
12	a	826	CLA	C2A-CAA-CBA-CGA
12	b	2132	CLA	C2A-CAA-CBA-CGA
12	b	2139	CLA	C2A-CAA-CBA-CGA
12	f	201	CLA	C2A-CAA-CBA-CGA
12	A	826	CLA	C2A-CAA-CBA-CGA
12	B	2133	CLA	C2A-CAA-CBA-CGA
12	B	2140	CLA	C2A-CAA-CBA-CGA
12	F	201	CLA	C2A-CAA-CBA-CGA
12	H	2133	CLA	O1D-CGD-O2D-CED
12	H	2141	CLA	O1D-CGD-O2D-CED
12	b	2131	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	b	2133	CLA	O1D-CGD-O2D-CED
12	b	2141	CLA	O1D-CGD-O2D-CED
12	B	2134	CLA	O1D-CGD-O2D-CED
12	B	2142	CLA	O1D-CGD-O2D-CED
15	T	4001	BCR	C18-C19-C20-C21
15	k	4001	BCR	C18-C19-C20-C21
15	K	4001	BCR	C18-C19-C20-C21
12	G	832	CLA	C10-C11-C12-C13
12	U	203	CLA	C13-C15-C16-C17
12	a	832	CLA	C10-C11-C12-C13
12	l	203	CLA	C13-C15-C16-C17
12	A	832	CLA	C10-C11-C12-C13
12	L	203	CLA	C13-C15-C16-C17
13	G	840	A1AGD	C16-C17-C18-C19
13	a	840	A1AGD	C16-C17-C18-C19
13	A	840	A1AGD	C16-C17-C18-C19
16	G	846	LHG	C23-C24-C25-C26
16	a	846	LHG	C23-C24-C25-C26
16	A	846	LHG	C23-C24-C25-C26
12	H	2114	CLA	O1D-CGD-O2D-CED
12	H	2131	CLA	O1D-CGD-O2D-CED
12	b	2114	CLA	O1D-CGD-O2D-CED
12	B	2115	CLA	O1D-CGD-O2D-CED
12	B	2132	CLA	O1D-CGD-O2D-CED
12	G	819	CLA	O1A-CGA-O2A-C1
12	G	826	CLA	O1A-CGA-O2A-C1
12	G	854	CLA	O1A-CGA-O2A-C1
12	H	2132	CLA	O1A-CGA-O2A-C1
12	a	819	CLA	O1A-CGA-O2A-C1
12	a	826	CLA	O1A-CGA-O2A-C1
12	a	854	CLA	O1A-CGA-O2A-C1
12	b	2132	CLA	O1A-CGA-O2A-C1
12	A	819	CLA	O1A-CGA-O2A-C1
12	A	826	CLA	O1A-CGA-O2A-C1
12	A	854	CLA	O1A-CGA-O2A-C1
12	B	2133	CLA	O1A-CGA-O2A-C1
15	S	101	BCR	C22-C23-C24-C25
15	j	101	BCR	C22-C23-C24-C25
15	J	101	BCR	C22-C23-C24-C25
12	G	824	CLA	C13-C15-C16-C17
12	G	828	CLA	C5-C6-C7-C8
12	G	837	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
12	H	2102	CLA	C13-C15-C16-C17
12	H	2107	CLA	C13-C15-C16-C17
12	H	2109	CLA	C5-C6-C7-C8
12	H	2128	CLA	C15-C16-C17-C18
12	a	824	CLA	C13-C15-C16-C17
12	a	828	CLA	C5-C6-C7-C8
12	a	837	CLA	C8-C10-C11-C12
12	b	2102	CLA	C13-C15-C16-C17
12	b	2107	CLA	C13-C15-C16-C17
12	b	2109	CLA	C5-C6-C7-C8
12	b	2128	CLA	C15-C16-C17-C18
12	A	824	CLA	C13-C15-C16-C17
12	A	828	CLA	C5-C6-C7-C8
12	A	837	CLA	C8-C10-C11-C12
12	B	2103	CLA	C13-C15-C16-C17
12	B	2108	CLA	C13-C15-C16-C17
12	B	2110	CLA	C5-C6-C7-C8
12	B	2129	CLA	C15-C16-C17-C18
16	G	848	LHG	O2-C2-C3-O3
16	a	848	LHG	O2-C2-C3-O3
16	A	848	LHG	O2-C2-C3-O3
12	H	2124	CLA	CBA-CGA-O2A-C1
12	b	2124	CLA	CBA-CGA-O2A-C1
12	B	2125	CLA	CBA-CGA-O2A-C1
12	H	2129	CLA	CBD-CGD-O2D-CED
12	b	2129	CLA	CBD-CGD-O2D-CED
12	B	2130	CLA	CBD-CGD-O2D-CED
12	G	835	CLA	O1A-CGA-O2A-C1
12	a	835	CLA	O1A-CGA-O2A-C1
12	A	835	CLA	O1A-CGA-O2A-C1
12	G	807	CLA	C10-C11-C12-C13
12	G	828	CLA	C15-C16-C17-C18
12	H	2101	CLA	C8-C10-C11-C12
12	H	2126	CLA	C13-C15-C16-C17
12	H	2127	CLA	C5-C6-C7-C8
12	a	807	CLA	C10-C11-C12-C13
12	a	828	CLA	C15-C16-C17-C18
12	b	2101	CLA	C8-C10-C11-C12
12	b	2126	CLA	C13-C15-C16-C17
12	b	2127	CLA	C5-C6-C7-C8
12	A	807	CLA	C10-C11-C12-C13
12	A	828	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
12	B	2102	CLA	C8-C10-C11-C12
12	B	2127	CLA	C13-C15-C16-C17
12	B	2128	CLA	C5-C6-C7-C8
12	G	820	CLA	O1D-CGD-O2D-CED
12	G	829	CLA	O1D-CGD-O2D-CED
12	H	2140	CLA	O1D-CGD-O2D-CED
12	a	820	CLA	O1D-CGD-O2D-CED
12	a	829	CLA	O1D-CGD-O2D-CED
12	b	2140	CLA	O1D-CGD-O2D-CED
12	A	820	CLA	O1D-CGD-O2D-CED
12	A	829	CLA	O1D-CGD-O2D-CED
12	B	2141	CLA	O1D-CGD-O2D-CED
12	G	819	CLA	C15-C16-C17-C18
12	H	2132	CLA	C10-C11-C12-C13
12	a	819	CLA	C15-C16-C17-C18
12	b	2132	CLA	C10-C11-C12-C13
12	A	819	CLA	C15-C16-C17-C18
12	B	2133	CLA	C10-C11-C12-C13
12	G	804	CLA	C13-C15-C16-C17
12	G	823	CLA	C8-C10-C11-C12
12	G	826	CLA	C8-C10-C11-C12
12	G	826	CLA	C15-C16-C17-C18
12	H	2101	CLA	C10-C11-C12-C13
12	H	2106	CLA	C13-C15-C16-C17
12	H	2119	CLA	C8-C10-C11-C12
12	U	205	CLA	C15-C16-C17-C18
12	a	804	CLA	C13-C15-C16-C17
12	a	823	CLA	C8-C10-C11-C12
12	a	826	CLA	C8-C10-C11-C12
12	a	826	CLA	C15-C16-C17-C18
12	b	2101	CLA	C10-C11-C12-C13
12	b	2106	CLA	C13-C15-C16-C17
12	b	2119	CLA	C8-C10-C11-C12
12	l	205	CLA	C15-C16-C17-C18
12	A	804	CLA	C13-C15-C16-C17
12	A	823	CLA	C8-C10-C11-C12
12	A	826	CLA	C8-C10-C11-C12
12	A	826	CLA	C15-C16-C17-C18
12	B	2102	CLA	C10-C11-C12-C13
12	B	2107	CLA	C13-C15-C16-C17
12	B	2120	CLA	C8-C10-C11-C12
12	L	205	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
12	G	803	CLA	CBA-CGA-O2A-C1
12	H	2106	CLA	CBA-CGA-O2A-C1
12	H	2119	CLA	CBA-CGA-O2A-C1
12	a	803	CLA	CBA-CGA-O2A-C1
12	b	2106	CLA	CBA-CGA-O2A-C1
12	b	2119	CLA	CBA-CGA-O2A-C1
12	A	803	CLA	CBA-CGA-O2A-C1
12	B	2107	CLA	CBA-CGA-O2A-C1
12	B	2120	CLA	CBA-CGA-O2A-C1
24	V	102	SQD	C8-C7-O47-C45
24	m	102	SQD	C8-C7-O47-C45
24	M	101	SQD	C8-C7-O47-C45
12	G	821	CLA	C3-C5-C6-C7
12	a	821	CLA	C3-C5-C6-C7
12	A	821	CLA	C3-C5-C6-C7
12	G	819	CLA	C10-C11-C12-C13
12	G	850	CLA	C15-C16-C17-C18
12	a	836	CLA	C13-C15-C16-C17
12	A	836	CLA	C13-C15-C16-C17
24	V	102	SQD	O49-C7-O47-C45
24	m	102	SQD	O49-C7-O47-C45
24	M	101	SQD	O49-C7-O47-C45
12	H	2118	CLA	C2A-CAA-CBA-CGA
12	b	2118	CLA	C2A-CAA-CBA-CGA
12	B	2119	CLA	C2A-CAA-CBA-CGA
12	U	205	CLA	CBA-CGA-O2A-C1
12	l	205	CLA	CBA-CGA-O2A-C1
12	L	205	CLA	CBA-CGA-O2A-C1
12	G	802	CLA	C8-C10-C11-C12
12	G	810	CLA	C10-C11-C12-C13
12	G	818	CLA	C15-C16-C17-C18
12	G	824	CLA	C10-C11-C12-C13
12	G	836	CLA	C13-C15-C16-C17
12	a	802	CLA	C8-C10-C11-C12
12	a	810	CLA	C10-C11-C12-C13
12	a	818	CLA	C15-C16-C17-C18
12	a	819	CLA	C10-C11-C12-C13
12	a	824	CLA	C10-C11-C12-C13
12	a	850	CLA	C15-C16-C17-C18
12	A	802	CLA	C8-C10-C11-C12
12	A	810	CLA	C10-C11-C12-C13
12	A	818	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
12	A	819	CLA	C10-C11-C12-C13
12	A	824	CLA	C10-C11-C12-C13
12	A	850	CLA	C15-C16-C17-C18
12	G	817	CLA	O1D-CGD-O2D-CED
12	H	2138	CLA	CBD-CGD-O2D-CED
12	b	2138	CLA	CBD-CGD-O2D-CED
12	B	2139	CLA	CBD-CGD-O2D-CED
12	a	817	CLA	O1D-CGD-O2D-CED
12	A	817	CLA	O1D-CGD-O2D-CED
12	G	804	CLA	C15-C16-C17-C18
12	H	2124	CLA	C13-C15-C16-C17
12	H	2126	CLA	C10-C11-C12-C13
12	H	2129	CLA	C5-C6-C7-C8
12	U	203	CLA	C10-C11-C12-C13
12	a	804	CLA	C15-C16-C17-C18
12	b	2124	CLA	C13-C15-C16-C17
12	b	2126	CLA	C10-C11-C12-C13
12	b	2129	CLA	C5-C6-C7-C8
12	A	804	CLA	C15-C16-C17-C18
12	B	2125	CLA	C13-C15-C16-C17
12	B	2127	CLA	C10-C11-C12-C13
12	B	2130	CLA	C5-C6-C7-C8
12	L	203	CLA	C10-C11-C12-C13
12	G	807	CLA	C13-C15-C16-C17
12	G	813	CLA	C5-C6-C7-C8
12	H	2111	CLA	C13-C15-C16-C17
12	H	2132	CLA	C15-C16-C17-C18
12	a	807	CLA	C13-C15-C16-C17
12	a	813	CLA	C5-C6-C7-C8
12	b	2103	CLA	C5-C6-C7-C8
12	b	2111	CLA	C13-C15-C16-C17
12	b	2132	CLA	C15-C16-C17-C18
12	l	203	CLA	C10-C11-C12-C13
12	A	807	CLA	C13-C15-C16-C17
12	A	813	CLA	C5-C6-C7-C8
12	B	2104	CLA	C5-C6-C7-C8
12	B	2112	CLA	C13-C15-C16-C17
12	B	2133	CLA	C15-C16-C17-C18
13	G	840	A1AGD	C14-C16-C17-C18
13	a	840	A1AGD	C14-C16-C17-C18
13	A	840	A1AGD	C14-C16-C17-C18
12	G	837	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	a	837	CLA	CBA-CGA-O2A-C1
12	A	837	CLA	CBA-CGA-O2A-C1
12	G	837	CLA	C15-C16-C17-C18
12	H	2103	CLA	C5-C6-C7-C8
12	a	837	CLA	C15-C16-C17-C18
12	A	837	CLA	C15-C16-C17-C18
12	H	2119	CLA	C3-C5-C6-C7
12	b	2119	CLA	C3-C5-C6-C7
12	B	2120	CLA	C3-C5-C6-C7
26	l	210	LMT	C5'-C4'-O1B-C1B
26	L	210	LMT	C5'-C4'-O1B-C1B
13	H	2153	A1AGD	C7-C8-C9-C10
13	b	2153	A1AGD	C7-C8-C9-C10
13	B	2153	A1AGD	C7-C8-C9-C10
26	U	210	LMT	C5'-C4'-O1B-C1B
12	G	824	CLA	C16-C17-C18-C20
12	a	824	CLA	C16-C17-C18-C20
12	A	824	CLA	C16-C17-C18-C20
15	H	2146	BCR	C11-C10-C9-C34
15	H	2146	BCR	C20-C21-C22-C37
15	S	101	BCR	C20-C21-C22-C37
15	S	104	BCR	C20-C21-C22-C37
15	b	2146	BCR	C11-C10-C9-C34
15	b	2146	BCR	C20-C21-C22-C37
15	j	101	BCR	C20-C21-C22-C37
15	j	104	BCR	C20-C21-C22-C37
15	B	2147	BCR	C11-C10-C9-C34
15	B	2147	BCR	C20-C21-C22-C37
15	J	101	BCR	C20-C21-C22-C37
15	J	104	BCR	C20-C21-C22-C37
12	G	829	CLA	C3-C5-C6-C7
12	a	829	CLA	C3-C5-C6-C7
12	A	829	CLA	C3-C5-C6-C7
12	G	805	CLA	C15-C16-C17-C18
12	A	805	CLA	C15-C16-C17-C18
12	B	2140	CLA	C13-C15-C16-C17
15	Q	202	BCR	C37-C22-C23-C24
15	U	206	BCR	C7-C8-C9-C34
15	f	202	BCR	C37-C22-C23-C24
15	l	206	BCR	C7-C8-C9-C34
15	F	202	BCR	C37-C22-C23-C24
15	L	206	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
20	V	101	ECH	C11-C12-C13-C35
20	m	101	ECH	C11-C12-C13-C35
20	M	103	ECH	C11-C12-C13-C35
15	H	2146	BCR	C21-C22-C23-C24
15	b	2146	BCR	C21-C22-C23-C24
15	B	2147	BCR	C21-C22-C23-C24
12	H	2106	CLA	O1A-CGA-O2A-C1
12	b	2106	CLA	O1A-CGA-O2A-C1
12	B	2107	CLA	O1A-CGA-O2A-C1
25	U	209	DGD	O1A-C1A-O1G-C1G
25	l	209	DGD	O1A-C1A-O1G-C1G
25	L	209	DGD	O1A-C1A-O1G-C1G
12	G	828	CLA	C2A-CAA-CBA-CGA
12	H	2101	CLA	C2A-CAA-CBA-CGA
12	H	2152	CLA	C2A-CAA-CBA-CGA
12	a	828	CLA	C2A-CAA-CBA-CGA
12	b	2101	CLA	C2A-CAA-CBA-CGA
12	b	2152	CLA	C2A-CAA-CBA-CGA
12	A	828	CLA	C2A-CAA-CBA-CGA
12	B	2101	CLA	C2A-CAA-CBA-CGA
12	B	2102	CLA	C2A-CAA-CBA-CGA
12	H	2110	CLA	C15-C16-C17-C18
12	H	2133	CLA	C10-C11-C12-C13
12	H	2139	CLA	C13-C15-C16-C17
12	a	805	CLA	C15-C16-C17-C18
12	b	2110	CLA	C15-C16-C17-C18
12	b	2133	CLA	C10-C11-C12-C13
12	b	2139	CLA	C13-C15-C16-C17
12	B	2111	CLA	C15-C16-C17-C18
12	B	2134	CLA	C10-C11-C12-C13
16	G	846	LHG	O1-C1-C2-C3
16	a	846	LHG	O1-C1-C2-C3
16	A	846	LHG	O1-C1-C2-C3
12	B	2108	CLA	O1D-CGD-O2D-CED
12	G	831	CLA	C11-C12-C13-C15
12	G	834	CLA	C6-C7-C8-C10
12	a	834	CLA	C6-C7-C8-C10
12	A	831	CLA	C11-C12-C13-C15
12	A	834	CLA	C6-C7-C8-C10
12	G	801	CLA	O1D-CGD-O2D-CED
12	G	832	CLA	O1D-CGD-O2D-CED
12	H	2107	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	a	801	CLA	O1D-CGD-O2D-CED
12	a	832	CLA	O1D-CGD-O2D-CED
12	b	2107	CLA	O1D-CGD-O2D-CED
12	A	801	CLA	O1D-CGD-O2D-CED
12	A	832	CLA	O1D-CGD-O2D-CED
12	H	2124	CLA	O1A-CGA-O2A-C1
12	b	2124	CLA	O1A-CGA-O2A-C1
12	B	2125	CLA	O1A-CGA-O2A-C1
12	H	2110	CLA	C3-C5-C6-C7
12	H	2129	CLA	C3-C5-C6-C7
12	b	2110	CLA	C3-C5-C6-C7
12	b	2129	CLA	C3-C5-C6-C7
12	B	2111	CLA	C3-C5-C6-C7
12	B	2130	CLA	C3-C5-C6-C7
15	G	842	BCR	C16-C17-C18-C19
15	Q	202	BCR	C12-C13-C14-C15
15	Q	202	BCR	C20-C21-C22-C23
15	S	104	BCR	C20-C21-C22-C23
15	U	206	BCR	C20-C21-C22-C23
15	a	842	BCR	C16-C17-C18-C19
15	f	202	BCR	C12-C13-C14-C15
15	f	202	BCR	C20-C21-C22-C23
15	j	104	BCR	C20-C21-C22-C23
15	l	206	BCR	C20-C21-C22-C23
15	A	842	BCR	C16-C17-C18-C19
15	F	202	BCR	C12-C13-C14-C15
15	F	202	BCR	C20-C21-C22-C23
15	J	104	BCR	C20-C21-C22-C23
15	L	206	BCR	C20-C21-C22-C23
16	G	846	LHG	C7-C8-C9-C10
16	a	846	LHG	C7-C8-C9-C10
16	A	846	LHG	C7-C8-C9-C10
12	H	2121	CLA	C2-C1-O2A-CGA
12	H	2131	CLA	C2-C1-O2A-CGA
12	b	2121	CLA	C2-C1-O2A-CGA
12	b	2131	CLA	C2-C1-O2A-CGA
12	B	2122	CLA	C2-C1-O2A-CGA
12	B	2132	CLA	C2-C1-O2A-CGA
12	G	831	CLA	C11-C12-C13-C14
12	G	834	CLA	C6-C7-C8-C9
12	G	835	CLA	C16-C17-C18-C19
12	H	2133	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
12	H	2139	CLA	C16-C17-C18-C19
12	H	2139	CLA	C16-C17-C18-C20
12	a	831	CLA	C11-C12-C13-C14
12	a	831	CLA	C11-C12-C13-C15
12	a	834	CLA	C6-C7-C8-C9
12	a	835	CLA	C16-C17-C18-C19
12	b	2107	CLA	C16-C17-C18-C20
12	b	2133	CLA	C16-C17-C18-C19
12	b	2139	CLA	C16-C17-C18-C19
12	b	2139	CLA	C16-C17-C18-C20
12	A	831	CLA	C11-C12-C13-C14
12	A	834	CLA	C6-C7-C8-C9
12	A	835	CLA	C16-C17-C18-C19
12	B	2108	CLA	C16-C17-C18-C20
12	B	2134	CLA	C16-C17-C18-C19
12	B	2140	CLA	C16-C17-C18-C20
16	b	2148	LHG	C24-C25-C26-C27
17	a	847	LMG	C31-C32-C33-C34
17	A	847	LMG	C31-C32-C33-C34
15	S	104	BCR	C14-C15-C16-C17
15	j	104	BCR	C14-C15-C16-C17
15	J	104	BCR	C14-C15-C16-C17
16	H	2148	LHG	C24-C25-C26-C27
16	B	2149	LHG	C24-C25-C26-C27
17	G	847	LMG	C17-C18-C19-C20
17	G	847	LMG	C31-C32-C33-C34
17	a	847	LMG	C17-C18-C19-C20
17	a	849	LMG	C33-C34-C35-C36
17	A	847	LMG	C17-C18-C19-C20
26	U	210	LMT	C11-C10-C9-C8
26	l	210	LMT	C11-C10-C9-C8
26	L	210	LMT	C11-C10-C9-C8
17	G	849	LMG	C32-C33-C34-C35
17	G	849	LMG	C33-C34-C35-C36
17	H	2147	LMG	C18-C19-C20-C21
17	a	849	LMG	C32-C33-C34-C35
17	A	849	LMG	C32-C33-C34-C35
17	A	849	LMG	C33-C34-C35-C36
17	B	2148	LMG	C18-C19-C20-C21
24	V	102	SQD	C24-C25-C26-C27
24	m	102	SQD	C24-C25-C26-C27
24	M	101	SQD	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
17	b	2147	LMG	C18-C19-C20-C21
12	G	837	CLA	O1D-CGD-O2D-CED
12	a	837	CLA	O1D-CGD-O2D-CED
12	j	102	CLA	O1D-CGD-O2D-CED
12	A	837	CLA	O1D-CGD-O2D-CED
12	G	815	CLA	C4B-C3B-CAB-CBB
12	G	826	CLA	C4B-C3B-CAB-CBB
12	G	833	CLA	C4B-C3B-CAB-CBB
12	H	2103	CLA	C4B-C3B-CAB-CBB
12	H	2114	CLA	C4B-C3B-CAB-CBB
12	H	2128	CLA	C4B-C3B-CAB-CBB
12	H	2133	CLA	C4B-C3B-CAB-CBB
12	Q	203	CLA	C4B-C3B-CAB-CBB
12	S	103	CLA	C4B-C3B-CAB-CBB
12	T	4002	CLA	C4B-C3B-CAB-CBB
12	a	815	CLA	C4B-C3B-CAB-CBB
12	a	826	CLA	C4B-C3B-CAB-CBB
12	a	833	CLA	C4B-C3B-CAB-CBB
12	b	2103	CLA	C4B-C3B-CAB-CBB
12	b	2114	CLA	C4B-C3B-CAB-CBB
12	b	2128	CLA	C4B-C3B-CAB-CBB
12	b	2133	CLA	C4B-C3B-CAB-CBB
12	f	203	CLA	C4B-C3B-CAB-CBB
12	j	103	CLA	C4B-C3B-CAB-CBB
12	k	4002	CLA	C4B-C3B-CAB-CBB
12	A	815	CLA	C4B-C3B-CAB-CBB
12	A	826	CLA	C4B-C3B-CAB-CBB
12	A	833	CLA	C4B-C3B-CAB-CBB
12	B	2104	CLA	C4B-C3B-CAB-CBB
12	B	2115	CLA	C4B-C3B-CAB-CBB
12	B	2129	CLA	C4B-C3B-CAB-CBB
12	B	2134	CLA	C4B-C3B-CAB-CBB
12	F	203	CLA	C4B-C3B-CAB-CBB
12	J	103	CLA	C4B-C3B-CAB-CBB
12	K	4002	CLA	C4B-C3B-CAB-CBB
12	G	828	CLA	C16-C17-C18-C19
12	G	828	CLA	C16-C17-C18-C20
12	G	835	CLA	C16-C17-C18-C20
12	H	2107	CLA	C16-C17-C18-C20
12	H	2133	CLA	C16-C17-C18-C20
12	a	828	CLA	C16-C17-C18-C19
12	a	828	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
12	a	835	CLA	C16-C17-C18-C20
12	b	2128	CLA	C16-C17-C18-C19
12	b	2133	CLA	C16-C17-C18-C20
12	A	828	CLA	C16-C17-C18-C19
12	A	828	CLA	C16-C17-C18-C20
12	A	835	CLA	C16-C17-C18-C20
12	B	2129	CLA	C16-C17-C18-C19
12	B	2134	CLA	C16-C17-C18-C20
12	B	2140	CLA	C16-C17-C18-C19
13	G	840	A1AGD	C22-C23-C24-C26
13	a	840	A1AGD	C22-C23-C24-C26
13	A	840	A1AGD	C22-C23-C24-C26
12	S	102	CLA	O1D-CGD-O2D-CED
12	J	102	CLA	O1D-CGD-O2D-CED
12	a	803	CLA	O1A-CGA-O2A-C1
12	G	810	CLA	C2A-CAA-CBA-CGA
12	H	2121	CLA	C2A-CAA-CBA-CGA
12	a	810	CLA	C2A-CAA-CBA-CGA
12	b	2121	CLA	C2A-CAA-CBA-CGA
12	A	810	CLA	C2A-CAA-CBA-CGA
12	B	2122	CLA	C2A-CAA-CBA-CGA
12	G	810	CLA	C8-C10-C11-C12
12	a	810	CLA	C8-C10-C11-C12
12	A	810	CLA	C8-C10-C11-C12
16	G	846	LHG	C8-C7-O7-C5
16	a	846	LHG	C8-C7-O7-C5
16	A	846	LHG	C8-C7-O7-C5
12	G	812	CLA	C12-C13-C15-C16
12	G	813	CLA	C11-C10-C8-C7
12	G	824	CLA	C11-C10-C8-C7
12	H	2107	CLA	C11-C10-C8-C7
12	a	812	CLA	C12-C13-C15-C16
12	a	813	CLA	C11-C10-C8-C7
12	b	2107	CLA	C11-C10-C8-C7
12	A	812	CLA	C12-C13-C15-C16
12	A	813	CLA	C11-C10-C8-C7
12	A	824	CLA	C11-C10-C8-C7
12	B	2108	CLA	C11-C10-C8-C7
12	H	2119	CLA	C15-C16-C17-C18
12	b	2119	CLA	C15-C16-C17-C18
12	B	2120	CLA	C15-C16-C17-C18
25	U	209	DGD	CEA-CFA-CGA-CHA

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Mol	Chain	Res	Type	Atoms
25	l	209	DGD	CEA-CFA-CGA-CHA
25	L	209	DGD	CEA-CFA-CGA-CHA
12	G	803	CLA	O1A-CGA-O2A-C1
12	a	837	CLA	O1A-CGA-O2A-C1
12	A	803	CLA	O1A-CGA-O2A-C1
12	A	837	CLA	O1A-CGA-O2A-C1
12	G	802	CLA	C3A-C2A-CAA-CBA
12	G	809	CLA	C3A-C2A-CAA-CBA
12	G	811	CLA	C3A-C2A-CAA-CBA
12	G	824	CLA	C3A-C2A-CAA-CBA
12	G	835	CLA	C3A-C2A-CAA-CBA
12	H	2122	CLA	C3A-C2A-CAA-CBA
12	H	2136	CLA	C3A-C2A-CAA-CBA
12	H	2141	CLA	C3A-C2A-CAA-CBA
12	Q	201	CLA	C3A-C2A-CAA-CBA
12	Q	204	CLA	C3A-C2A-CAA-CBA
12	U	204	CLA	C3A-C2A-CAA-CBA
12	a	802	CLA	C3A-C2A-CAA-CBA
12	a	809	CLA	C3A-C2A-CAA-CBA
12	a	811	CLA	C3A-C2A-CAA-CBA
12	a	824	CLA	C3A-C2A-CAA-CBA
12	a	835	CLA	C3A-C2A-CAA-CBA
12	b	2122	CLA	C3A-C2A-CAA-CBA
12	b	2136	CLA	C3A-C2A-CAA-CBA
12	b	2141	CLA	C3A-C2A-CAA-CBA
12	f	201	CLA	C3A-C2A-CAA-CBA
12	f	204	CLA	C3A-C2A-CAA-CBA
12	l	204	CLA	C3A-C2A-CAA-CBA
12	A	802	CLA	C3A-C2A-CAA-CBA
12	A	809	CLA	C3A-C2A-CAA-CBA
12	A	811	CLA	C3A-C2A-CAA-CBA
12	A	824	CLA	C3A-C2A-CAA-CBA
12	A	835	CLA	C3A-C2A-CAA-CBA
12	B	2123	CLA	C3A-C2A-CAA-CBA
12	B	2137	CLA	C3A-C2A-CAA-CBA
12	B	2142	CLA	C3A-C2A-CAA-CBA
12	F	201	CLA	C3A-C2A-CAA-CBA
12	F	204	CLA	C3A-C2A-CAA-CBA
12	L	204	CLA	C3A-C2A-CAA-CBA
12	H	2106	CLA	O1D-CGD-O2D-CED
12	b	2106	CLA	O1D-CGD-O2D-CED
12	B	2107	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	U	209	DGD	C5B-C6B-C7B-C8B
25	l	209	DGD	C5B-C6B-C7B-C8B
25	L	209	DGD	C5B-C6B-C7B-C8B
12	G	826	CLA	C5-C6-C7-C8
12	G	827	CLA	C10-C11-C12-C13
12	H	2119	CLA	C10-C11-C12-C13
12	H	2129	CLA	C8-C10-C11-C12
12	H	2131	CLA	C5-C6-C7-C8
12	a	826	CLA	C5-C6-C7-C8
12	a	827	CLA	C10-C11-C12-C13
12	b	2119	CLA	C10-C11-C12-C13
12	b	2129	CLA	C8-C10-C11-C12
12	b	2131	CLA	C5-C6-C7-C8
12	A	826	CLA	C5-C6-C7-C8
12	A	827	CLA	C10-C11-C12-C13
12	B	2120	CLA	C10-C11-C12-C13
12	B	2130	CLA	C8-C10-C11-C12
12	B	2132	CLA	C5-C6-C7-C8
16	G	848	LHG	C7-C8-C9-C10
16	a	848	LHG	C7-C8-C9-C10
16	A	848	LHG	C7-C8-C9-C10
12	H	2107	CLA	C16-C17-C18-C19
12	H	2128	CLA	C16-C17-C18-C19
12	b	2107	CLA	C16-C17-C18-C19
12	B	2108	CLA	C16-C17-C18-C19
12	G	837	CLA	O1A-CGA-O2A-C1
12	H	2119	CLA	O1A-CGA-O2A-C1
12	U	205	CLA	O1A-CGA-O2A-C1
12	b	2119	CLA	O1A-CGA-O2A-C1
12	l	205	CLA	O1A-CGA-O2A-C1
12	B	2120	CLA	O1A-CGA-O2A-C1
12	L	205	CLA	O1A-CGA-O2A-C1
12	H	2107	CLA	C5-C6-C7-C8
12	b	2107	CLA	C5-C6-C7-C8
24	M	101	SQD	C9-C10-C11-C12
12	H	2136	CLA	O1D-CGD-O2D-CED
12	B	2137	CLA	O1D-CGD-O2D-CED
16	H	2148	LHG	C9-C10-C11-C12
16	b	2148	LHG	C9-C10-C11-C12
16	B	2149	LHG	C9-C10-C11-C12
24	V	102	SQD	C9-C10-C11-C12
24	m	102	SQD	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
26	U	210	LMT	C7-C8-C9-C10
26	l	210	LMT	C7-C8-C9-C10
26	L	210	LMT	C7-C8-C9-C10
16	G	848	LHG	C23-C24-C25-C26
16	a	848	LHG	C23-C24-C25-C26
16	A	848	LHG	C23-C24-C25-C26
12	G	829	CLA	C10-C11-C12-C13
12	a	829	CLA	C10-C11-C12-C13
12	A	829	CLA	C10-C11-C12-C13
12	B	2108	CLA	C5-C6-C7-C8
12	H	2104	CLA	O1D-CGD-O2D-CED
12	b	2136	CLA	O1D-CGD-O2D-CED
12	B	2105	CLA	O1D-CGD-O2D-CED
24	V	102	SQD	C27-C28-C29-C30
24	m	102	SQD	C27-C28-C29-C30
24	m	102	SQD	C31-C32-C33-C34
24	M	101	SQD	C27-C28-C29-C30
17	G	847	LMG	C36-C37-C38-C39
17	G	849	LMG	C34-C35-C36-C37
17	a	847	LMG	C36-C37-C38-C39
17	a	849	LMG	C34-C35-C36-C37
17	A	847	LMG	C36-C37-C38-C39
17	A	849	LMG	C34-C35-C36-C37
24	V	102	SQD	C31-C32-C33-C34
24	m	102	SQD	C26-C27-C28-C29
24	M	101	SQD	C26-C27-C28-C29
24	M	101	SQD	C31-C32-C33-C34
12	b	2104	CLA	O1D-CGD-O2D-CED
16	G	846	LHG	C15-C16-C17-C18
16	a	846	LHG	C15-C16-C17-C18
16	A	846	LHG	C15-C16-C17-C18
16	H	2148	LHG	C27-C28-C29-C30
16	b	2148	LHG	C27-C28-C29-C30
16	B	2149	LHG	C27-C28-C29-C30
24	V	102	SQD	C26-C27-C28-C29
16	V	103	LHG	C7-C8-C9-C10
16	m	103	LHG	C7-C8-C9-C10
16	M	102	LHG	C7-C8-C9-C10
12	G	815	CLA	C2B-C3B-CAB-CBB
12	G	834	CLA	C2B-C3B-CAB-CBB
12	H	2109	CLA	C2B-C3B-CAB-CBB
12	H	2122	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
12	H	2128	CLA	C2B-C3B-CAB-CBB
12	H	2130	CLA	C2B-C3B-CAB-CBB
12	H	2138	CLA	C2B-C3B-CAB-CBB
12	S	102	CLA	C2B-C3B-CAB-CBB
12	a	815	CLA	C2B-C3B-CAB-CBB
12	a	834	CLA	C2B-C3B-CAB-CBB
12	b	2109	CLA	C2B-C3B-CAB-CBB
12	b	2122	CLA	C2B-C3B-CAB-CBB
12	b	2128	CLA	C2B-C3B-CAB-CBB
12	b	2130	CLA	C2B-C3B-CAB-CBB
12	b	2138	CLA	C2B-C3B-CAB-CBB
12	j	102	CLA	C2B-C3B-CAB-CBB
12	A	815	CLA	C2B-C3B-CAB-CBB
12	A	834	CLA	C2B-C3B-CAB-CBB
12	B	2110	CLA	C2B-C3B-CAB-CBB
12	B	2123	CLA	C2B-C3B-CAB-CBB
12	B	2129	CLA	C2B-C3B-CAB-CBB
12	B	2131	CLA	C2B-C3B-CAB-CBB
12	B	2139	CLA	C2B-C3B-CAB-CBB
12	J	102	CLA	C2B-C3B-CAB-CBB
15	G	845	BCR	C23-C24-C25-C26
15	G	845	BCR	C23-C24-C25-C30
15	H	2142	BCR	C1-C6-C7-C8
15	H	2142	BCR	C5-C6-C7-C8
15	S	104	BCR	C1-C6-C7-C8
15	S	104	BCR	C5-C6-C7-C8
15	U	206	BCR	C23-C24-C25-C30
15	U	207	BCR	C1-C6-C7-C8
15	U	207	BCR	C5-C6-C7-C8
15	U	207	BCR	C23-C24-C25-C26
15	U	207	BCR	C23-C24-C25-C30
15	a	845	BCR	C23-C24-C25-C26
15	a	845	BCR	C23-C24-C25-C30
15	b	2142	BCR	C1-C6-C7-C8
15	b	2142	BCR	C5-C6-C7-C8
15	j	104	BCR	C1-C6-C7-C8
15	j	104	BCR	C5-C6-C7-C8
15	l	206	BCR	C23-C24-C25-C30
15	l	207	BCR	C1-C6-C7-C8
15	l	207	BCR	C5-C6-C7-C8
15	l	207	BCR	C23-C24-C25-C26
15	l	207	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
15	A	845	BCR	C23-C24-C25-C26
15	A	845	BCR	C23-C24-C25-C30
15	B	2143	BCR	C1-C6-C7-C8
15	B	2143	BCR	C5-C6-C7-C8
15	J	104	BCR	C5-C6-C7-C8
15	L	206	BCR	C23-C24-C25-C30
15	L	207	BCR	C1-C6-C7-C8
15	L	207	BCR	C5-C6-C7-C8
15	L	207	BCR	C23-C24-C25-C26
15	L	207	BCR	C23-C24-C25-C30
18	G	852	45D	C03-C07-C19-C23
18	a	852	45D	C03-C07-C19-C23
18	A	852	45D	C03-C07-C19-C23
20	H	2143	ECH	C23-C24-C25-C26
20	V	101	ECH	C5-C6-C7-C8
20	b	2143	ECH	C23-C24-C25-C26
20	m	101	ECH	C5-C6-C7-C8
20	B	2144	ECH	C23-C24-C25-C26
20	M	103	ECH	C5-C6-C7-C8
12	H	2101	CLA	CBD-CGD-O2D-CED
12	H	2113	CLA	CBD-CGD-O2D-CED
12	b	2101	CLA	CBD-CGD-O2D-CED
12	b	2113	CLA	CBD-CGD-O2D-CED
12	B	2102	CLA	CBD-CGD-O2D-CED
12	B	2114	CLA	CBD-CGD-O2D-CED
24	U	208	SQD	C10-C11-C12-C13
24	V	102	SQD	C14-C15-C16-C17
24	l	208	SQD	C10-C11-C12-C13
24	m	102	SQD	C14-C15-C16-C17
24	L	208	SQD	C10-C11-C12-C13
24	M	101	SQD	C14-C15-C16-C17
12	G	850	CLA	C2A-CAA-CBA-CGA
12	H	2102	CLA	C2A-CAA-CBA-CGA
12	H	2113	CLA	C2A-CAA-CBA-CGA
12	a	850	CLA	C2A-CAA-CBA-CGA
12	b	2102	CLA	C2A-CAA-CBA-CGA
12	b	2113	CLA	C2A-CAA-CBA-CGA
12	A	850	CLA	C2A-CAA-CBA-CGA
12	B	2103	CLA	C2A-CAA-CBA-CGA
12	B	2114	CLA	C2A-CAA-CBA-CGA
12	a	810	CLA	C15-C16-C17-C18
12	a	831	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
12	b	2108	CLA	C5-C6-C7-C8
12	A	831	CLA	C5-C6-C7-C8
12	B	2109	CLA	C5-C6-C7-C8
17	G	847	LMG	C18-C19-C20-C21
17	a	847	LMG	C18-C19-C20-C21
17	A	847	LMG	C18-C19-C20-C21
15	H	2145	BCR	C10-C11-C12-C13
15	H	2146	BCR	C18-C19-C20-C21
15	U	206	BCR	C18-C19-C20-C21
15	U	207	BCR	C10-C11-C12-C13
15	b	2145	BCR	C10-C11-C12-C13
15	b	2146	BCR	C18-C19-C20-C21
15	l	206	BCR	C18-C19-C20-C21
15	l	207	BCR	C10-C11-C12-C13
15	B	2146	BCR	C10-C11-C12-C13
15	B	2147	BCR	C18-C19-C20-C21
15	L	206	BCR	C18-C19-C20-C21
15	L	207	BCR	C10-C11-C12-C13
12	G	810	CLA	C15-C16-C17-C18
12	G	831	CLA	C5-C6-C7-C8
12	H	2108	CLA	C5-C6-C7-C8
12	A	810	CLA	C15-C16-C17-C18
25	U	209	DGD	C6A-C7A-C8A-C9A
25	l	209	DGD	C6A-C7A-C8A-C9A
25	L	209	DGD	C6A-C7A-C8A-C9A
12	H	2117	CLA	O1D-CGD-O2D-CED
12	b	2117	CLA	O1D-CGD-O2D-CED
12	G	839	CLA	C11-C12-C13-C14
12	H	2129	CLA	C11-C12-C13-C14
12	a	839	CLA	C11-C12-C13-C14
12	b	2129	CLA	C11-C12-C13-C14
12	A	839	CLA	C11-C12-C13-C14
12	B	2130	CLA	C11-C12-C13-C14
12	G	836	CLA	C15-C16-C17-C18
12	U	203	CLA	C5-C6-C7-C8
12	a	836	CLA	C15-C16-C17-C18
12	l	203	CLA	C5-C6-C7-C8
12	A	836	CLA	C15-C16-C17-C18
12	L	203	CLA	C5-C6-C7-C8
12	B	2118	CLA	O1D-CGD-O2D-CED
15	T	4001	BCR	C6-C7-C8-C9
15	k	4001	BCR	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
15	K	4001	BCR	C6-C7-C8-C9
12	H	2103	CLA	C13-C15-C16-C17
12	U	205	CLA	C10-C11-C12-C13
12	b	2103	CLA	C13-C15-C16-C17
12	l	205	CLA	C10-C11-C12-C13
12	B	2104	CLA	C13-C15-C16-C17
12	L	205	CLA	C10-C11-C12-C13
12	H	2106	CLA	C15-C16-C17-C18
12	b	2106	CLA	C15-C16-C17-C18
12	B	2107	CLA	C15-C16-C17-C18
12	a	831	CLA	C3-C5-C6-C7
20	V	101	ECH	C9-C10-C11-C12
20	m	101	ECH	C9-C10-C11-C12
20	M	103	ECH	C9-C10-C11-C12
12	H	2112	CLA	C16-C17-C18-C20
12	b	2112	CLA	C16-C17-C18-C20
12	B	2113	CLA	C16-C17-C18-C20
17	H	2147	LMG	C28-C29-C30-C31
17	b	2147	LMG	C28-C29-C30-C31
17	B	2148	LMG	C28-C29-C30-C31
12	H	2112	CLA	C5-C6-C7-C8
12	b	2112	CLA	C5-C6-C7-C8
12	B	2113	CLA	C5-C6-C7-C8
16	G	846	LHG	C30-C31-C32-C33
16	a	846	LHG	C30-C31-C32-C33
16	A	846	LHG	C30-C31-C32-C33
17	b	2147	LMG	C4-C5-C6-O5
12	H	2119	CLA	C5-C6-C7-C8
12	H	2126	CLA	C5-C6-C7-C8
12	H	2128	CLA	C13-C15-C16-C17
12	b	2119	CLA	C5-C6-C7-C8
12	b	2128	CLA	C13-C15-C16-C17
12	B	2120	CLA	C5-C6-C7-C8
12	B	2127	CLA	C5-C6-C7-C8
12	B	2129	CLA	C13-C15-C16-C17
17	H	2147	LMG	C4-C5-C6-O5
17	B	2148	LMG	C4-C5-C6-O5
12	G	831	CLA	C3-C5-C6-C7
12	A	831	CLA	C3-C5-C6-C7
12	G	813	CLA	CBA-CGA-O2A-C1
12	G	806	CLA	C2A-CAA-CBA-CGA
12	H	2123	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
12	a	806	CLA	C2A-CAA-CBA-CGA
12	b	2123	CLA	C2A-CAA-CBA-CGA
12	A	806	CLA	C2A-CAA-CBA-CGA
12	B	2124	CLA	C2A-CAA-CBA-CGA
12	G	824	CLA	C16-C17-C18-C19
17	G	847	LMG	C37-C38-C39-C40
17	a	847	LMG	C37-C38-C39-C40
17	A	847	LMG	C37-C38-C39-C40
12	H	2110	CLA	C5-C6-C7-C8
12	b	2110	CLA	C5-C6-C7-C8
12	b	2126	CLA	C5-C6-C7-C8
12	B	2111	CLA	C5-C6-C7-C8
24	m	102	SQD	C16-C17-C18-C19
12	G	805	CLA	C3-C5-C6-C7
12	a	805	CLA	C3-C5-C6-C7
12	A	805	CLA	C3-C5-C6-C7
12	H	2102	CLA	C5-C6-C7-C8
12	H	2129	CLA	C13-C15-C16-C17
12	b	2129	CLA	C13-C15-C16-C17
12	B	2103	CLA	C5-C6-C7-C8
12	B	2130	CLA	C13-C15-C16-C17
24	V	102	SQD	C16-C17-C18-C19
24	M	101	SQD	C16-C17-C18-C19
12	G	828	CLA	CBA-CGA-O2A-C1
12	a	813	CLA	CBA-CGA-O2A-C1
12	a	828	CLA	CBA-CGA-O2A-C1
12	A	813	CLA	CBA-CGA-O2A-C1
12	A	828	CLA	CBA-CGA-O2A-C1
16	H	2148	LHG	C11-C10-C9-C8
16	b	2148	LHG	C11-C10-C9-C8
16	B	2149	LHG	C11-C10-C9-C8
16	m	103	LHG	C27-C28-C29-C30
16	M	102	LHG	C27-C28-C29-C30
24	V	102	SQD	C11-C10-C9-C8
24	M	101	SQD	C11-C10-C9-C8
16	H	2148	LHG	C8-C7-O7-C5
16	b	2148	LHG	C8-C7-O7-C5
16	B	2149	LHG	C8-C7-O7-C5
12	A	824	CLA	C16-C17-C18-C19
16	V	103	LHG	C27-C28-C29-C30
24	m	102	SQD	C11-C10-C9-C8
12	H	2104	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
12	H	2109	CLA	C13-C15-C16-C17
12	b	2102	CLA	C5-C6-C7-C8
12	b	2104	CLA	C10-C11-C12-C13
12	b	2109	CLA	C13-C15-C16-C17
12	B	2105	CLA	C10-C11-C12-C13
12	B	2110	CLA	C13-C15-C16-C17
13	H	2153	A1AGD	C11-C12-C13-C14
13	b	2153	A1AGD	C11-C12-C13-C14
13	B	2153	A1AGD	C11-C12-C13-C14
12	a	813	CLA	O1D-CGD-O2D-CED
12	a	839	CLA	O1D-CGD-O2D-CED
12	A	813	CLA	O1D-CGD-O2D-CED
12	A	834	CLA	O1D-CGD-O2D-CED
25	l	209	DGD	C3B-C4B-C5B-C6B
25	L	209	DGD	C3B-C4B-C5B-C6B
25	U	209	DGD	C3B-C4B-C5B-C6B
12	G	813	CLA	O1D-CGD-O2D-CED
12	G	834	CLA	O1D-CGD-O2D-CED
12	G	839	CLA	O1D-CGD-O2D-CED
12	a	834	CLA	O1D-CGD-O2D-CED
12	A	839	CLA	O1D-CGD-O2D-CED
24	U	208	SQD	C24-C23-O48-C46
24	l	208	SQD	C24-C23-O48-C46
24	L	208	SQD	C24-C23-O48-C46
12	a	854	CLA	C5-C6-C7-C8
24	V	102	SQD	C10-C11-C12-C13
24	m	102	SQD	C10-C11-C12-C13
12	a	824	CLA	C16-C17-C18-C19
12	G	854	CLA	C5-C6-C7-C8
12	A	854	CLA	C5-C6-C7-C8
24	M	101	SQD	C10-C11-C12-C13
16	G	848	LHG	C12-C13-C14-C15
16	a	848	LHG	C12-C13-C14-C15
16	A	848	LHG	C12-C13-C14-C15
16	G	848	LHG	C1-C2-C3-O3
16	a	848	LHG	C1-C2-C3-O3
16	A	848	LHG	C1-C2-C3-O3
16	G	846	LHG	C25-C26-C27-C28
16	a	846	LHG	C25-C26-C27-C28
25	U	209	DGD	C3A-C4A-C5A-C6A
25	l	209	DGD	C3A-C4A-C5A-C6A
25	L	209	DGD	C3A-C4A-C5A-C6A

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Mol	Chain	Res	Type	Atoms
12	G	807	CLA	C2A-CAA-CBA-CGA
12	G	816	CLA	C2A-CAA-CBA-CGA
12	H	2127	CLA	C2A-CAA-CBA-CGA
12	a	807	CLA	C2A-CAA-CBA-CGA
12	a	816	CLA	C2A-CAA-CBA-CGA
12	b	2127	CLA	C2A-CAA-CBA-CGA
12	A	807	CLA	C2A-CAA-CBA-CGA
12	A	816	CLA	C2A-CAA-CBA-CGA
12	B	2128	CLA	C2A-CAA-CBA-CGA
16	G	846	LHG	C9-C10-C11-C12
16	H	2148	LHG	C33-C34-C35-C36
16	V	103	LHG	C33-C34-C35-C36
16	a	846	LHG	C9-C10-C11-C12
16	b	2148	LHG	C33-C34-C35-C36
16	m	103	LHG	C33-C34-C35-C36
16	A	846	LHG	C9-C10-C11-C12
16	A	846	LHG	C25-C26-C27-C28
16	B	2149	LHG	C33-C34-C35-C36
16	M	102	LHG	C33-C34-C35-C36
12	H	2114	CLA	C10-C11-C12-C13
12	b	2114	CLA	C10-C11-C12-C13
12	B	2115	CLA	C10-C11-C12-C13
12	b	2106	CLA	C16-C17-C18-C19
12	G	807	CLA	C1A-C2A-CAA-CBA
12	G	808	CLA	C1A-C2A-CAA-CBA
12	G	817	CLA	C1A-C2A-CAA-CBA
12	G	821	CLA	C1A-C2A-CAA-CBA
12	G	822	CLA	C1A-C2A-CAA-CBA
12	G	823	CLA	C1A-C2A-CAA-CBA
12	G	824	CLA	C1A-C2A-CAA-CBA
12	G	835	CLA	C1A-C2A-CAA-CBA
12	G	839	CLA	C1A-C2A-CAA-CBA
12	H	2106	CLA	C1A-C2A-CAA-CBA
12	H	2117	CLA	C1A-C2A-CAA-CBA
12	H	2123	CLA	C1A-C2A-CAA-CBA
12	H	2133	CLA	C1A-C2A-CAA-CBA
12	Q	204	CLA	C1A-C2A-CAA-CBA
12	S	103	CLA	C1A-C2A-CAA-CBA
12	a	807	CLA	C1A-C2A-CAA-CBA
12	a	808	CLA	C1A-C2A-CAA-CBA
12	a	817	CLA	C1A-C2A-CAA-CBA
12	a	821	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	a	822	CLA	C1A-C2A-CAA-CBA
12	a	823	CLA	C1A-C2A-CAA-CBA
12	a	824	CLA	C1A-C2A-CAA-CBA
12	a	835	CLA	C1A-C2A-CAA-CBA
12	a	839	CLA	C1A-C2A-CAA-CBA
12	a	851	CLA	C1A-C2A-CAA-CBA
12	b	2106	CLA	C1A-C2A-CAA-CBA
12	b	2117	CLA	C1A-C2A-CAA-CBA
12	b	2123	CLA	C1A-C2A-CAA-CBA
12	b	2133	CLA	C1A-C2A-CAA-CBA
12	f	204	CLA	C1A-C2A-CAA-CBA
12	j	103	CLA	C1A-C2A-CAA-CBA
12	A	807	CLA	C1A-C2A-CAA-CBA
12	A	808	CLA	C1A-C2A-CAA-CBA
12	A	817	CLA	C1A-C2A-CAA-CBA
12	A	821	CLA	C1A-C2A-CAA-CBA
12	A	822	CLA	C1A-C2A-CAA-CBA
12	A	823	CLA	C1A-C2A-CAA-CBA
12	A	824	CLA	C1A-C2A-CAA-CBA
12	A	835	CLA	C1A-C2A-CAA-CBA
12	A	839	CLA	C1A-C2A-CAA-CBA
12	A	851	CLA	C1A-C2A-CAA-CBA
12	B	2107	CLA	C1A-C2A-CAA-CBA
12	B	2118	CLA	C1A-C2A-CAA-CBA
12	B	2124	CLA	C1A-C2A-CAA-CBA
12	B	2134	CLA	C1A-C2A-CAA-CBA
12	F	204	CLA	C1A-C2A-CAA-CBA
12	J	103	CLA	C1A-C2A-CAA-CBA
12	H	2101	CLA	C5-C6-C7-C8
12	b	2101	CLA	C5-C6-C7-C8
12	B	2102	CLA	C5-C6-C7-C8
12	G	804	CLA	C11-C12-C13-C15
12	G	819	CLA	C11-C10-C8-C7
12	G	826	CLA	C6-C7-C8-C10
12	G	828	CLA	C12-C13-C15-C16
12	G	832	CLA	C6-C7-C8-C10
12	G	832	CLA	C11-C12-C13-C15
12	H	2104	CLA	C11-C10-C8-C7
12	H	2107	CLA	C6-C7-C8-C10
12	H	2126	CLA	C6-C7-C8-C10
12	H	2126	CLA	C11-C12-C13-C15
12	H	2127	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
12	H	2133	CLA	C6-C7-C8-C10
12	a	804	CLA	C11-C12-C13-C15
12	a	819	CLA	C11-C10-C8-C7
12	a	824	CLA	C11-C10-C8-C7
12	a	826	CLA	C6-C7-C8-C10
12	a	828	CLA	C12-C13-C15-C16
12	a	832	CLA	C6-C7-C8-C10
12	a	832	CLA	C11-C12-C13-C15
12	b	2104	CLA	C11-C10-C8-C7
12	b	2107	CLA	C6-C7-C8-C10
12	b	2126	CLA	C6-C7-C8-C10
12	b	2126	CLA	C11-C12-C13-C15
12	b	2127	CLA	C6-C7-C8-C10
12	b	2133	CLA	C6-C7-C8-C10
12	A	804	CLA	C11-C12-C13-C15
12	A	819	CLA	C11-C10-C8-C7
12	A	826	CLA	C6-C7-C8-C10
12	A	828	CLA	C12-C13-C15-C16
12	A	832	CLA	C6-C7-C8-C10
12	A	832	CLA	C11-C12-C13-C15
12	B	2105	CLA	C11-C10-C8-C7
12	B	2108	CLA	C6-C7-C8-C10
12	B	2127	CLA	C6-C7-C8-C10
12	B	2127	CLA	C11-C12-C13-C15
12	B	2128	CLA	C6-C7-C8-C10
12	B	2134	CLA	C6-C7-C8-C10
13	G	840	A1AGD	C13-C14-C16-C17
13	a	840	A1AGD	C13-C14-C16-C17
13	A	840	A1AGD	C13-C14-C16-C17
12	G	804	CLA	C16-C17-C18-C19
12	H	2106	CLA	C16-C17-C18-C19
12	H	2106	CLA	C16-C17-C18-C20
12	a	804	CLA	C16-C17-C18-C19
12	b	2106	CLA	C16-C17-C18-C20
12	A	804	CLA	C16-C17-C18-C19
12	B	2107	CLA	C16-C17-C18-C19
12	B	2107	CLA	C16-C17-C18-C20
12	H	2123	CLA	C5-C6-C7-C8
12	b	2123	CLA	C5-C6-C7-C8
12	B	2124	CLA	C5-C6-C7-C8
17	G	849	LMG	C28-C29-C30-C31
17	a	849	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
17	A	849	LMG	C28-C29-C30-C31
17	G	847	LMG	C30-C31-C32-C33
17	a	847	LMG	C30-C31-C32-C33
17	A	847	LMG	C30-C31-C32-C33
25	l	209	DGD	C4A-C5A-C6A-C7A
25	L	209	DGD	C4A-C5A-C6A-C7A
12	G	812	CLA	C13-C15-C16-C17
12	a	812	CLA	C13-C15-C16-C17
12	A	812	CLA	C13-C15-C16-C17
12	G	817	CLA	C2A-CAA-CBA-CGA
12	G	823	CLA	C2A-CAA-CBA-CGA
12	H	2128	CLA	C2A-CAA-CBA-CGA
12	H	2141	CLA	C2A-CAA-CBA-CGA
12	Q	204	CLA	C2A-CAA-CBA-CGA
12	a	817	CLA	C2A-CAA-CBA-CGA
12	a	823	CLA	C2A-CAA-CBA-CGA
12	b	2128	CLA	C2A-CAA-CBA-CGA
12	b	2141	CLA	C2A-CAA-CBA-CGA
12	f	204	CLA	C2A-CAA-CBA-CGA
12	A	817	CLA	C2A-CAA-CBA-CGA
12	A	823	CLA	C2A-CAA-CBA-CGA
12	B	2129	CLA	C2A-CAA-CBA-CGA
12	B	2142	CLA	C2A-CAA-CBA-CGA
12	F	204	CLA	C2A-CAA-CBA-CGA
12	G	819	CLA	C14-C13-C15-C16
12	G	825	CLA	C11-C10-C8-C9
12	G	826	CLA	C6-C7-C8-C9
12	G	828	CLA	C14-C13-C15-C16
12	G	829	CLA	C6-C7-C8-C9
12	G	833	CLA	C14-C13-C15-C16
12	G	851	CLA	C6-C7-C8-C9
12	H	2104	CLA	C11-C10-C8-C9
12	H	2105	CLA	C6-C7-C8-C9
12	H	2107	CLA	C6-C7-C8-C9
12	H	2108	CLA	C11-C10-C8-C9
12	H	2111	CLA	C11-C10-C8-C9
12	H	2126	CLA	C6-C7-C8-C9
12	H	2127	CLA	C6-C7-C8-C9
12	H	2127	CLA	C11-C12-C13-C14
12	H	2132	CLA	C6-C7-C8-C9
12	U	203	CLA	C14-C13-C15-C16
12	a	819	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
12	a	825	CLA	C11-C10-C8-C9
12	a	826	CLA	C6-C7-C8-C9
12	a	828	CLA	C14-C13-C15-C16
12	a	829	CLA	C6-C7-C8-C9
12	a	832	CLA	C11-C12-C13-C14
12	a	833	CLA	C14-C13-C15-C16
12	a	851	CLA	C6-C7-C8-C9
12	b	2104	CLA	C11-C10-C8-C9
12	b	2105	CLA	C6-C7-C8-C9
12	b	2107	CLA	C6-C7-C8-C9
12	b	2108	CLA	C11-C10-C8-C9
12	b	2111	CLA	C11-C10-C8-C9
12	b	2126	CLA	C6-C7-C8-C9
12	b	2127	CLA	C6-C7-C8-C9
12	b	2127	CLA	C11-C12-C13-C14
12	b	2132	CLA	C6-C7-C8-C9
12	l	203	CLA	C14-C13-C15-C16
12	A	819	CLA	C14-C13-C15-C16
12	A	825	CLA	C11-C10-C8-C9
12	A	826	CLA	C6-C7-C8-C9
12	A	828	CLA	C14-C13-C15-C16
12	A	829	CLA	C6-C7-C8-C9
12	A	832	CLA	C11-C12-C13-C14
12	A	833	CLA	C14-C13-C15-C16
12	A	851	CLA	C6-C7-C8-C9
12	B	2105	CLA	C11-C10-C8-C9
12	B	2106	CLA	C6-C7-C8-C9
12	B	2108	CLA	C6-C7-C8-C9
12	B	2109	CLA	C11-C10-C8-C9
12	B	2112	CLA	C11-C10-C8-C9
12	B	2127	CLA	C6-C7-C8-C9
12	B	2128	CLA	C6-C7-C8-C9
12	B	2128	CLA	C11-C12-C13-C14
12	B	2133	CLA	C6-C7-C8-C9
12	L	203	CLA	C14-C13-C15-C16
16	G	846	LHG	C14-C15-C16-C17
16	V	103	LHG	C28-C29-C30-C31
16	a	846	LHG	C14-C15-C16-C17
16	A	846	LHG	C14-C15-C16-C17
16	M	102	LHG	C28-C29-C30-C31
25	U	209	DGD	C4A-C5A-C6A-C7A
12	H	2112	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
12	b	2112	CLA	C16-C17-C18-C19
12	B	2113	CLA	C16-C17-C18-C19
16	m	103	LHG	C28-C29-C30-C31
12	G	833	CLA	CBD-CGD-O2D-CED
12	a	833	CLA	CBD-CGD-O2D-CED
24	U	208	SQD	C44-C45-C46-O48
24	l	208	SQD	C44-C45-C46-O48
24	L	208	SQD	C44-C45-C46-O48
25	U	209	DGD	O1G-C1G-C2G-C3G
25	l	209	DGD	O1G-C1G-C2G-C3G
25	L	209	DGD	O1G-C1G-C2G-C3G
12	G	828	CLA	O1A-CGA-O2A-C1
12	A	833	CLA	CBD-CGD-O2D-CED
16	G	848	LHG	C24-C23-O8-C6
16	a	848	LHG	C24-C23-O8-C6
16	A	848	LHG	C24-C23-O8-C6
12	G	817	CLA	C11-C12-C13-C15
12	G	818	CLA	C16-C17-C18-C20
12	a	817	CLA	C11-C12-C13-C15
12	a	818	CLA	C16-C17-C18-C20
12	A	817	CLA	C11-C12-C13-C15
12	A	818	CLA	C16-C17-C18-C20
12	a	828	CLA	O1A-CGA-O2A-C1
12	A	828	CLA	O1A-CGA-O2A-C1
15	a	843	BCR	C16-C17-C18-C36
15	A	843	BCR	C16-C17-C18-C36
17	a	847	LMG	C28-C29-C30-C31
12	G	813	CLA	O1A-CGA-O2A-C1
12	a	813	CLA	O1A-CGA-O2A-C1
12	A	813	CLA	O1A-CGA-O2A-C1
24	U	208	SQD	O10-C23-O48-C46
24	l	208	SQD	O10-C23-O48-C46
24	L	208	SQD	O10-C23-O48-C46
15	H	2146	BCR	C37-C22-C23-C24
15	b	2146	BCR	C37-C22-C23-C24
15	k	4001	BCR	C37-C22-C23-C24
15	B	2147	BCR	C37-C22-C23-C24
15	K	4001	BCR	C37-C22-C23-C24
12	G	812	CLA	O1D-CGD-O2D-CED
17	A	847	LMG	C28-C29-C30-C31
20	m	101	ECH	C11-C12-C13-C14
12	G	808	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
12	a	808	CLA	C2A-CAA-CBA-CGA
12	A	808	CLA	C2A-CAA-CBA-CGA
12	G	819	CLA	C5-C6-C7-C8
12	a	819	CLA	C5-C6-C7-C8
12	b	2114	CLA	C15-C16-C17-C18
12	A	819	CLA	C5-C6-C7-C8
12	B	2115	CLA	C15-C16-C17-C18
25	U	209	DGD	CBA-CCA-CDA-CEA
25	l	209	DGD	CBA-CCA-CDA-CEA
25	L	209	DGD	CBA-CCA-CDA-CEA
17	G	847	LMG	C28-C29-C30-C31
12	G	804	CLA	O1D-CGD-O2D-CED
12	a	804	CLA	O1D-CGD-O2D-CED
12	a	812	CLA	O1D-CGD-O2D-CED
12	A	804	CLA	O1D-CGD-O2D-CED
12	A	812	CLA	O1D-CGD-O2D-CED
12	G	824	CLA	CBA-CGA-O2A-C1
12	G	834	CLA	CBA-CGA-O2A-C1
12	a	824	CLA	CBA-CGA-O2A-C1
12	a	834	CLA	CBA-CGA-O2A-C1
12	A	824	CLA	CBA-CGA-O2A-C1
12	A	834	CLA	CBA-CGA-O2A-C1
12	H	2102	CLA	O2A-C1-C2-C3
12	b	2102	CLA	O2A-C1-C2-C3
12	B	2103	CLA	O2A-C1-C2-C3
16	A	846	LHG	C27-C28-C29-C30
12	H	2114	CLA	C15-C16-C17-C18
16	G	846	LHG	C27-C28-C29-C30
16	a	846	LHG	C27-C28-C29-C30
24	U	208	SQD	C29-C30-C31-C32
24	l	208	SQD	C29-C30-C31-C32
24	L	208	SQD	C29-C30-C31-C32
26	U	210	LMT	C4-C5-C6-C7
26	L	210	LMT	C4-C5-C6-C7
15	H	2146	BCR	C9-C10-C11-C12
15	b	2146	BCR	C9-C10-C11-C12
15	B	2147	BCR	C9-C10-C11-C12
12	H	2104	CLA	C2C-C3C-CAC-CBC
26	l	210	LMT	C4-C5-C6-C7
12	G	825	CLA	C3-C5-C6-C7
12	a	825	CLA	C3-C5-C6-C7
12	A	825	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
12	A	839	CLA	C13-C15-C16-C17
15	R	101	BCR	C11-C10-C9-C8
15	i	101	BCR	C11-C10-C9-C8
15	I	101	BCR	C11-C10-C9-C8
12	b	2104	CLA	C2C-C3C-CAC-CBC
12	B	2105	CLA	C2C-C3C-CAC-CBC
15	G	845	BCR	C22-C23-C24-C25
15	H	2144	BCR	C6-C7-C8-C9
15	a	845	BCR	C22-C23-C24-C25
15	b	2144	BCR	C6-C7-C8-C9
15	A	845	BCR	C22-C23-C24-C25
15	B	2145	BCR	C6-C7-C8-C9
16	G	848	LHG	C30-C31-C32-C33
16	a	848	LHG	C30-C31-C32-C33
16	A	848	LHG	C30-C31-C32-C33
25	U	209	DGD	C8B-C9B-CAB-CBB
25	l	209	DGD	C8B-C9B-CAB-CBB
12	H	2111	CLA	C2-C3-C5-C6
12	b	2111	CLA	C2-C3-C5-C6
12	B	2112	CLA	C2-C3-C5-C6
16	G	848	LHG	C25-C26-C27-C28
16	a	846	LHG	C12-C13-C14-C15
16	a	848	LHG	C25-C26-C27-C28
16	A	848	LHG	C25-C26-C27-C28
25	L	209	DGD	C8B-C9B-CAB-CBB
12	H	2103	CLA	C16-C17-C18-C19
12	b	2103	CLA	C16-C17-C18-C19
12	B	2104	CLA	C16-C17-C18-C19
16	A	846	LHG	C12-C13-C14-C15
12	G	839	CLA	C13-C15-C16-C17
16	G	846	LHG	C12-C13-C14-C15
12	G	835	CLA	C2A-CAA-CBA-CGA
12	U	201	CLA	C2A-CAA-CBA-CGA
12	a	835	CLA	C2A-CAA-CBA-CGA
12	l	201	CLA	C2A-CAA-CBA-CGA
12	A	835	CLA	C2A-CAA-CBA-CGA
12	L	201	CLA	C2A-CAA-CBA-CGA
12	a	839	CLA	C13-C15-C16-C17
12	H	2103	CLA	C16-C17-C18-C20
12	b	2103	CLA	C16-C17-C18-C20
12	B	2104	CLA	C16-C17-C18-C20
17	b	2147	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
17	H	2147	LMG	C38-C39-C40-C41
17	B	2148	LMG	C38-C39-C40-C41
12	G	806	CLA	CBA-CGA-O2A-C1
12	H	2139	CLA	CBA-CGA-O2A-C1
12	a	806	CLA	CBA-CGA-O2A-C1
12	A	806	CLA	CBA-CGA-O2A-C1
12	B	2140	CLA	CBA-CGA-O2A-C1
25	U	209	DGD	C2A-C1A-O1G-C1G
25	l	209	DGD	C2A-C1A-O1G-C1G
25	L	209	DGD	C2A-C1A-O1G-C1G
26	U	210	LMT	C9-C10-C11-C12
26	l	210	LMT	C9-C10-C11-C12
26	L	210	LMT	C9-C10-C11-C12
17	a	847	LMG	C16-C17-C18-C19
12	G	812	CLA	C3-C5-C6-C7
17	G	847	LMG	C16-C17-C18-C19
12	H	2138	CLA	O1D-CGD-O2D-CED
12	b	2129	CLA	O1D-CGD-O2D-CED
17	A	847	LMG	C16-C17-C18-C19
12	G	832	CLA	C15-C16-C17-C18
12	a	832	CLA	C15-C16-C17-C18
12	A	832	CLA	C15-C16-C17-C18
12	H	2129	CLA	O1D-CGD-O2D-CED
12	b	2138	CLA	O1D-CGD-O2D-CED
12	B	2130	CLA	O1D-CGD-O2D-CED
12	B	2139	CLA	O1D-CGD-O2D-CED
12	G	829	CLA	C16-C17-C18-C20
12	a	829	CLA	C16-C17-C18-C20
12	A	829	CLA	C16-C17-C18-C20
12	G	817	CLA	C4-C3-C5-C6
12	G	836	CLA	C4-C3-C5-C6
12	H	2121	CLA	C4-C3-C5-C6
12	H	2123	CLA	C4-C3-C5-C6
12	a	817	CLA	C4-C3-C5-C6
12	a	836	CLA	C4-C3-C5-C6
12	b	2121	CLA	C4-C3-C5-C6
12	b	2123	CLA	C4-C3-C5-C6
12	A	817	CLA	C4-C3-C5-C6
12	A	836	CLA	C4-C3-C5-C6
12	B	2122	CLA	C4-C3-C5-C6
12	B	2124	CLA	C4-C3-C5-C6
17	H	2147	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
12	H	2128	CLA	CBA-CGA-O2A-C1
12	b	2128	CLA	CBA-CGA-O2A-C1
12	b	2139	CLA	CBA-CGA-O2A-C1
12	B	2129	CLA	CBA-CGA-O2A-C1
12	G	833	CLA	C10-C11-C12-C13
12	H	2110	CLA	C13-C15-C16-C17
12	a	833	CLA	C10-C11-C12-C13
12	b	2110	CLA	C13-C15-C16-C17
12	A	833	CLA	C10-C11-C12-C13
12	B	2111	CLA	C13-C15-C16-C17
17	b	2147	LMG	C31-C32-C33-C34
17	B	2148	LMG	C31-C32-C33-C34
24	V	102	SQD	C12-C13-C14-C15
24	m	102	SQD	C12-C13-C14-C15
24	M	101	SQD	C12-C13-C14-C15
16	G	846	LHG	O1-C1-C2-O2
16	a	846	LHG	O1-C1-C2-O2
16	A	846	LHG	O1-C1-C2-O2
12	a	812	CLA	C3-C5-C6-C7
12	A	812	CLA	C3-C5-C6-C7
12	G	804	CLA	C11-C12-C13-C14
12	G	813	CLA	C11-C10-C8-C9
12	G	819	CLA	C11-C10-C8-C9
12	G	824	CLA	C11-C10-C8-C9
12	G	832	CLA	C11-C12-C13-C14
12	H	2101	CLA	C11-C10-C8-C9
12	H	2114	CLA	C14-C13-C15-C16
12	H	2126	CLA	C11-C12-C13-C14
12	H	2133	CLA	C6-C7-C8-C9
12	H	2140	CLA	C6-C7-C8-C9
12	U	201	CLA	C14-C13-C15-C16
12	a	804	CLA	C11-C12-C13-C14
12	a	813	CLA	C11-C10-C8-C9
12	a	819	CLA	C11-C10-C8-C9
12	a	824	CLA	C11-C10-C8-C9
12	b	2101	CLA	C11-C10-C8-C9
12	b	2114	CLA	C14-C13-C15-C16
12	b	2126	CLA	C11-C12-C13-C14
12	b	2133	CLA	C6-C7-C8-C9
12	b	2140	CLA	C6-C7-C8-C9
12	l	201	CLA	C14-C13-C15-C16
12	A	804	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
12	A	813	CLA	C11-C10-C8-C9
12	A	819	CLA	C11-C10-C8-C9
12	A	824	CLA	C11-C10-C8-C9
12	B	2102	CLA	C11-C10-C8-C9
12	B	2115	CLA	C14-C13-C15-C16
12	B	2127	CLA	C11-C12-C13-C14
12	B	2134	CLA	C6-C7-C8-C9
12	B	2141	CLA	C6-C7-C8-C9
12	L	201	CLA	C14-C13-C15-C16
24	m	102	SQD	C30-C31-C32-C33
12	G	804	CLA	C10-C11-C12-C13
12	A	835	CLA	C15-C16-C17-C18
12	G	802	CLA	C4B-C3B-CAB-CBB
12	G	809	CLA	C4B-C3B-CAB-CBB
12	G	810	CLA	C4B-C3B-CAB-CBB
12	G	812	CLA	C4B-C3B-CAB-CBB
12	G	813	CLA	C4B-C3B-CAB-CBB
12	G	817	CLA	C4B-C3B-CAB-CBB
12	G	819	CLA	C4B-C3B-CAB-CBB
12	G	821	CLA	C4B-C3B-CAB-CBB
12	G	823	CLA	C4B-C3B-CAB-CBB
12	G	825	CLA	C4B-C3B-CAB-CBB
12	G	836	CLA	C4B-C3B-CAB-CBB
12	G	851	CLA	C4B-C3B-CAB-CBB
12	H	2110	CLA	C4B-C3B-CAB-CBB
12	H	2115	CLA	C4B-C3B-CAB-CBB
12	H	2118	CLA	C4B-C3B-CAB-CBB
12	H	2125	CLA	C4B-C3B-CAB-CBB
12	H	2126	CLA	C4B-C3B-CAB-CBB
12	H	2135	CLA	C4B-C3B-CAB-CBB
12	H	2140	CLA	C4B-C3B-CAB-CBB
12	Q	204	CLA	C4B-C3B-CAB-CBB
12	U	204	CLA	C4B-C3B-CAB-CBB
12	a	802	CLA	C4B-C3B-CAB-CBB
12	a	809	CLA	C4B-C3B-CAB-CBB
12	a	810	CLA	C4B-C3B-CAB-CBB
12	a	812	CLA	C4B-C3B-CAB-CBB
12	a	813	CLA	C4B-C3B-CAB-CBB
12	a	817	CLA	C4B-C3B-CAB-CBB
12	a	819	CLA	C4B-C3B-CAB-CBB
12	a	821	CLA	C4B-C3B-CAB-CBB
12	a	823	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
12	a	825	CLA	C4B-C3B-CAB-CBB
12	a	836	CLA	C4B-C3B-CAB-CBB
12	a	851	CLA	C4B-C3B-CAB-CBB
12	b	2110	CLA	C4B-C3B-CAB-CBB
12	b	2115	CLA	C4B-C3B-CAB-CBB
12	b	2118	CLA	C4B-C3B-CAB-CBB
12	b	2125	CLA	C4B-C3B-CAB-CBB
12	b	2126	CLA	C4B-C3B-CAB-CBB
12	b	2135	CLA	C4B-C3B-CAB-CBB
12	b	2140	CLA	C4B-C3B-CAB-CBB
12	f	204	CLA	C4B-C3B-CAB-CBB
12	l	204	CLA	C4B-C3B-CAB-CBB
12	A	802	CLA	C4B-C3B-CAB-CBB
12	A	809	CLA	C4B-C3B-CAB-CBB
12	A	810	CLA	C4B-C3B-CAB-CBB
12	A	812	CLA	C4B-C3B-CAB-CBB
12	A	813	CLA	C4B-C3B-CAB-CBB
12	A	817	CLA	C4B-C3B-CAB-CBB
12	A	819	CLA	C4B-C3B-CAB-CBB
12	A	821	CLA	C4B-C3B-CAB-CBB
12	A	823	CLA	C4B-C3B-CAB-CBB
12	A	825	CLA	C4B-C3B-CAB-CBB
12	A	836	CLA	C4B-C3B-CAB-CBB
12	A	851	CLA	C4B-C3B-CAB-CBB
12	B	2111	CLA	C4B-C3B-CAB-CBB
12	B	2116	CLA	C4B-C3B-CAB-CBB
12	B	2119	CLA	C4B-C3B-CAB-CBB
12	B	2126	CLA	C4B-C3B-CAB-CBB
12	B	2127	CLA	C4B-C3B-CAB-CBB
12	B	2136	CLA	C4B-C3B-CAB-CBB
12	B	2141	CLA	C4B-C3B-CAB-CBB
12	F	204	CLA	C4B-C3B-CAB-CBB
12	L	204	CLA	C4B-C3B-CAB-CBB
24	V	102	SQD	C30-C31-C32-C33
24	M	101	SQD	C30-C31-C32-C33
12	G	835	CLA	C15-C16-C17-C18
12	a	804	CLA	C10-C11-C12-C13
12	a	835	CLA	C15-C16-C17-C18
12	A	804	CLA	C10-C11-C12-C13
12	G	818	CLA	C16-C17-C18-C19
12	a	818	CLA	C16-C17-C18-C19
12	A	818	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
16	V	103	LHG	C14-C15-C16-C17
12	H	2104	CLA	C2A-CAA-CBA-CGA
12	U	205	CLA	C2A-CAA-CBA-CGA
12	b	2104	CLA	C2A-CAA-CBA-CGA
12	l	205	CLA	C2A-CAA-CBA-CGA
12	B	2105	CLA	C2A-CAA-CBA-CGA
12	L	205	CLA	C2A-CAA-CBA-CGA
25	U	209	DGD	C2D-C1D-O3G-C3G
25	l	209	DGD	C2D-C1D-O3G-C3G
25	L	209	DGD	C2D-C1D-O3G-C3G
12	H	2105	CLA	C10-C11-C12-C13
12	H	2121	CLA	C5-C6-C7-C8
12	b	2105	CLA	C10-C11-C12-C13
12	b	2121	CLA	C5-C6-C7-C8
12	B	2106	CLA	C10-C11-C12-C13
12	B	2122	CLA	C5-C6-C7-C8
16	m	103	LHG	C14-C15-C16-C17
16	M	102	LHG	C14-C15-C16-C17
12	G	810	CLA	C11-C12-C13-C15
12	G	813	CLA	C11-C12-C13-C15
12	G	818	CLA	C12-C13-C15-C16
12	G	819	CLA	C12-C13-C15-C16
12	G	825	CLA	C11-C10-C8-C7
12	G	829	CLA	C6-C7-C8-C10
12	G	833	CLA	C12-C13-C15-C16
12	G	851	CLA	C6-C7-C8-C10
12	H	2105	CLA	C6-C7-C8-C10
12	H	2108	CLA	C11-C10-C8-C7
12	H	2114	CLA	C12-C13-C15-C16
12	H	2127	CLA	C11-C12-C13-C15
12	H	2129	CLA	C11-C10-C8-C7
12	H	2132	CLA	C6-C7-C8-C10
12	H	2137	CLA	C12-C13-C15-C16
12	H	2140	CLA	C6-C7-C8-C10
12	U	201	CLA	C12-C13-C15-C16
12	U	203	CLA	C12-C13-C15-C16
12	a	810	CLA	C11-C12-C13-C15
12	a	813	CLA	C11-C12-C13-C15
12	a	818	CLA	C12-C13-C15-C16
12	a	819	CLA	C12-C13-C15-C16
12	a	825	CLA	C11-C10-C8-C7
12	a	829	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
12	a	833	CLA	C12-C13-C15-C16
12	a	851	CLA	C6-C7-C8-C10
12	b	2105	CLA	C6-C7-C8-C10
12	b	2108	CLA	C11-C10-C8-C7
12	b	2114	CLA	C12-C13-C15-C16
12	b	2127	CLA	C11-C12-C13-C15
12	b	2129	CLA	C11-C10-C8-C7
12	b	2132	CLA	C6-C7-C8-C10
12	b	2137	CLA	C12-C13-C15-C16
12	b	2140	CLA	C6-C7-C8-C10
12	l	201	CLA	C12-C13-C15-C16
12	l	203	CLA	C12-C13-C15-C16
12	A	810	CLA	C11-C12-C13-C15
12	A	813	CLA	C11-C12-C13-C15
12	A	818	CLA	C12-C13-C15-C16
12	A	819	CLA	C12-C13-C15-C16
12	A	825	CLA	C11-C10-C8-C7
12	A	829	CLA	C6-C7-C8-C10
12	A	833	CLA	C12-C13-C15-C16
12	A	851	CLA	C6-C7-C8-C10
12	B	2106	CLA	C6-C7-C8-C10
12	B	2109	CLA	C11-C10-C8-C7
12	B	2115	CLA	C12-C13-C15-C16
12	B	2128	CLA	C11-C12-C13-C15
12	B	2130	CLA	C11-C10-C8-C7
12	B	2133	CLA	C6-C7-C8-C10
12	B	2138	CLA	C12-C13-C15-C16
12	B	2141	CLA	C6-C7-C8-C10
12	L	201	CLA	C12-C13-C15-C16
12	L	203	CLA	C12-C13-C15-C16
12	G	819	CLA	C8-C10-C11-C12
12	a	819	CLA	C8-C10-C11-C12
12	f	201	CLA	C8-C10-C11-C12
12	F	201	CLA	C8-C10-C11-C12
12	Q	201	CLA	C8-C10-C11-C12
12	A	819	CLA	C8-C10-C11-C12
12	G	833	CLA	C3A-C2A-CAA-CBA
12	G	854	CLA	C3A-C2A-CAA-CBA
12	H	2106	CLA	C4-C3-C5-C6
12	H	2111	CLA	C4-C3-C5-C6
12	T	4002	CLA	C3A-C2A-CAA-CBA
12	a	833	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	a	854	CLA	C3A-C2A-CAA-CBA
12	b	2106	CLA	C4-C3-C5-C6
12	b	2111	CLA	C4-C3-C5-C6
12	k	4002	CLA	C3A-C2A-CAA-CBA
12	A	833	CLA	C3A-C2A-CAA-CBA
12	A	854	CLA	C3A-C2A-CAA-CBA
12	B	2107	CLA	C4-C3-C5-C6
12	B	2112	CLA	C4-C3-C5-C6
12	K	4002	CLA	C3A-C2A-CAA-CBA
12	H	2106	CLA	C2-C3-C5-C6
12	b	2106	CLA	C2-C3-C5-C6
12	B	2107	CLA	C2-C3-C5-C6
24	V	102	SQD	C33-C34-C35-C36
24	M	101	SQD	C33-C34-C35-C36
12	G	807	CLA	C15-C16-C17-C18
12	H	2103	CLA	C15-C16-C17-C18
12	a	807	CLA	C15-C16-C17-C18
12	A	807	CLA	C15-C16-C17-C18
12	H	2132	CLA	C4C-C3C-CAC-CBC
24	m	102	SQD	C33-C34-C35-C36
15	G	842	BCR	C19-C20-C21-C22
15	G	843	BCR	C9-C10-C11-C12
15	H	2146	BCR	C15-C16-C17-C18
15	a	842	BCR	C19-C20-C21-C22
15	a	843	BCR	C9-C10-C11-C12
15	b	2146	BCR	C15-C16-C17-C18
15	A	842	BCR	C19-C20-C21-C22
15	A	843	BCR	C9-C10-C11-C12
15	B	2147	BCR	C15-C16-C17-C18
22	H	2150	EQ3	C15-C16-C17-C18
22	b	2150	EQ3	C15-C16-C17-C18
22	B	2151	EQ3	C15-C16-C17-C18
13	G	840	A1AGD	C22-C23-C24-C25
13	a	840	A1AGD	C22-C23-C24-C25
13	A	840	A1AGD	C22-C23-C24-C25
12	b	2103	CLA	C15-C16-C17-C18
12	B	2104	CLA	C15-C16-C17-C18
15	T	4001	BCR	C37-C22-C23-C24
17	H	2147	LMG	O6-C5-C6-O5
17	b	2147	LMG	O6-C5-C6-O5
17	B	2148	LMG	O6-C5-C6-O5
12	G	824	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	a	824	CLA	O1A-CGA-O2A-C1
12	A	824	CLA	O1A-CGA-O2A-C1
24	U	208	SQD	C9-C10-C11-C12
24	l	208	SQD	C9-C10-C11-C12
24	L	208	SQD	C9-C10-C11-C12
12	G	829	CLA	C13-C15-C16-C17
12	a	829	CLA	C13-C15-C16-C17
12	A	829	CLA	C13-C15-C16-C17
15	G	843	BCR	C7-C8-C9-C10
15	a	843	BCR	C7-C8-C9-C10
15	A	843	BCR	C7-C8-C9-C10
20	V	101	ECH	C11-C12-C13-C14
20	M	103	ECH	C11-C12-C13-C14
12	B	2133	CLA	C4C-C3C-CAC-CBC
12	G	820	CLA	C2A-CAA-CBA-CGA
12	H	2140	CLA	C2A-CAA-CBA-CGA
12	a	820	CLA	C2A-CAA-CBA-CGA
12	b	2140	CLA	C2A-CAA-CBA-CGA
12	A	820	CLA	C2A-CAA-CBA-CGA
12	B	2141	CLA	C2A-CAA-CBA-CGA
12	b	2132	CLA	C4C-C3C-CAC-CBC
16	G	846	LHG	C4-C5-C6-O8
16	a	846	LHG	C4-C5-C6-O8
16	A	846	LHG	C4-C5-C6-O8
12	G	817	CLA	C11-C12-C13-C14
12	H	2128	CLA	C16-C17-C18-C20
12	a	817	CLA	C11-C12-C13-C14
12	b	2128	CLA	C16-C17-C18-C20
12	A	817	CLA	C11-C12-C13-C14
12	B	2129	CLA	C16-C17-C18-C20
12	G	839	CLA	C5-C6-C7-C8
12	H	2124	CLA	C10-C11-C12-C13
12	H	2132	CLA	C8-C10-C11-C12
12	a	839	CLA	C5-C6-C7-C8
12	b	2124	CLA	C10-C11-C12-C13
12	b	2132	CLA	C8-C10-C11-C12
12	A	839	CLA	C5-C6-C7-C8
12	B	2125	CLA	C10-C11-C12-C13
12	B	2133	CLA	C8-C10-C11-C12
24	U	208	SQD	C30-C31-C32-C33
24	l	208	SQD	C30-C31-C32-C33
24	L	208	SQD	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
16	G	846	LHG	O6-C4-C5-O7
16	a	846	LHG	O6-C4-C5-O7
16	A	846	LHG	O6-C4-C5-O7
16	G	846	LHG	C26-C27-C28-C29
16	G	848	LHG	C10-C11-C12-C13
16	A	846	LHG	C33-C34-C35-C36
16	A	848	LHG	C10-C11-C12-C13
12	G	836	CLA	C2B-C3B-CAB-CBB
12	H	2140	CLA	C2B-C3B-CAB-CBB
12	a	836	CLA	C2B-C3B-CAB-CBB
12	b	2140	CLA	C2B-C3B-CAB-CBB
12	A	836	CLA	C2B-C3B-CAB-CBB
12	B	2141	CLA	C2B-C3B-CAB-CBB
15	G	843	BCR	C1-C6-C7-C8
15	G	845	BCR	C1-C6-C7-C8
15	H	2145	BCR	C1-C6-C7-C8
15	H	2146	BCR	C23-C24-C25-C30
15	S	101	BCR	C1-C6-C7-C8
15	S	101	BCR	C23-C24-C25-C30
15	S	104	BCR	C23-C24-C25-C30
15	U	206	BCR	C1-C6-C7-C8
15	a	843	BCR	C1-C6-C7-C8
15	a	845	BCR	C1-C6-C7-C8
15	b	2145	BCR	C1-C6-C7-C8
15	b	2146	BCR	C23-C24-C25-C30
15	j	101	BCR	C1-C6-C7-C8
15	j	101	BCR	C23-C24-C25-C30
15	j	104	BCR	C23-C24-C25-C30
15	l	206	BCR	C1-C6-C7-C8
15	A	843	BCR	C1-C6-C7-C8
15	A	845	BCR	C1-C6-C7-C8
15	B	2146	BCR	C1-C6-C7-C8
15	B	2147	BCR	C23-C24-C25-C30
15	J	101	BCR	C1-C6-C7-C8
15	J	101	BCR	C23-C24-C25-C30
15	J	104	BCR	C1-C6-C7-C8
15	J	104	BCR	C23-C24-C25-C30
15	L	206	BCR	C1-C6-C7-C8
20	H	2143	ECH	C23-C24-C25-C30
20	b	2143	ECH	C23-C24-C25-C30
20	B	2144	ECH	C23-C24-C25-C30
22	H	2150	EQ3	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
22	b	2150	EQ3	C23-C24-C25-C30
22	B	2151	EQ3	C23-C24-C25-C30
16	a	846	LHG	C26-C27-C28-C29
16	a	846	LHG	C33-C34-C35-C36
16	a	848	LHG	C10-C11-C12-C13
16	A	846	LHG	C26-C27-C28-C29
16	G	846	LHG	C33-C34-C35-C36
12	G	804	CLA	C16-C17-C18-C20
12	G	829	CLA	C16-C17-C18-C19
12	a	804	CLA	C16-C17-C18-C20
12	A	804	CLA	C16-C17-C18-C20
12	U	201	CLA	C13-C15-C16-C17
12	l	201	CLA	C13-C15-C16-C17
12	L	201	CLA	C13-C15-C16-C17
25	U	209	DGD	O1G-C1G-C2G-O2G
25	l	209	DGD	O1G-C1G-C2G-O2G
25	L	209	DGD	O1G-C1G-C2G-O2G
16	G	848	LHG	C24-C25-C26-C27
16	a	848	LHG	C24-C25-C26-C27
16	A	848	LHG	C24-C25-C26-C27
12	a	813	CLA	C10-C11-C12-C13
12	H	2121	CLA	C2-C3-C5-C6
12	b	2121	CLA	C2-C3-C5-C6
12	B	2122	CLA	C2-C3-C5-C6
16	H	2148	LHG	C28-C29-C30-C31
16	b	2148	LHG	C28-C29-C30-C31
16	B	2149	LHG	C28-C29-C30-C31
12	H	2102	CLA	C16-C17-C18-C20
12	a	829	CLA	C16-C17-C18-C19
12	A	829	CLA	C16-C17-C18-C19
12	B	2103	CLA	C16-C17-C18-C20
16	H	2148	LHG	C34-C35-C36-C37
16	b	2148	LHG	C34-C35-C36-C37
16	B	2149	LHG	C34-C35-C36-C37
12	G	813	CLA	C10-C11-C12-C13
12	A	813	CLA	C10-C11-C12-C13
12	H	2137	CLA	C11-C10-C8-C9
12	U	204	CLA	C14-C13-C15-C16
12	b	2137	CLA	C11-C10-C8-C9
12	l	204	CLA	C14-C13-C15-C16
12	B	2138	CLA	C11-C10-C8-C9
12	L	204	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
17	G	847	LMG	C39-C40-C41-C42
17	a	847	LMG	C39-C40-C41-C42
17	A	847	LMG	C39-C40-C41-C42
12	b	2113	CLA	O1D-CGD-O2D-CED
12	H	2113	CLA	O1D-CGD-O2D-CED
12	B	2114	CLA	O1D-CGD-O2D-CED
16	G	846	LHG	C11-C12-C13-C14
16	a	846	LHG	C11-C12-C13-C14
16	A	846	LHG	C11-C12-C13-C14
12	b	2102	CLA	C16-C17-C18-C20
24	V	102	SQD	C19-C20-C21-C22
24	m	102	SQD	C19-C20-C21-C22
24	M	101	SQD	C19-C20-C21-C22
12	b	2127	CLA	C10-C11-C12-C13
12	B	2128	CLA	C10-C11-C12-C13
23	H	2151	ZEX	C9-C10-C11-C12
23	b	2151	ZEX	C9-C10-C11-C12
23	B	2152	ZEX	C9-C10-C11-C12
12	G	836	CLA	C2-C3-C5-C6
12	H	2123	CLA	C2-C3-C5-C6
12	a	836	CLA	C2-C3-C5-C6
12	b	2123	CLA	C2-C3-C5-C6
12	A	836	CLA	C2-C3-C5-C6
12	B	2124	CLA	C2-C3-C5-C6
12	H	2101	CLA	O1D-CGD-O2D-CED
12	H	2127	CLA	C10-C11-C12-C13
12	B	2102	CLA	O1D-CGD-O2D-CED
16	G	846	LHG	O9-C7-O7-C5
16	a	846	LHG	O9-C7-O7-C5
16	A	846	LHG	O9-C7-O7-C5
15	G	843	BCR	C16-C17-C18-C36
15	H	2144	BCR	C20-C21-C22-C37
15	H	2145	BCR	C35-C13-C14-C15
15	b	2144	BCR	C20-C21-C22-C37
15	b	2145	BCR	C35-C13-C14-C15
15	B	2145	BCR	C20-C21-C22-C37
15	B	2146	BCR	C35-C13-C14-C15
12	b	2125	CLA	CBA-CGA-O2A-C1
16	V	103	LHG	O6-C4-C5-C6
16	m	103	LHG	O6-C4-C5-C6
16	M	102	LHG	O6-C4-C5-C6
12	G	805	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
12	G	820	CLA	C6-C7-C8-C10
12	G	836	CLA	C11-C12-C13-C15
12	G	836	CLA	C12-C13-C15-C16
12	H	2101	CLA	C11-C12-C13-C15
12	H	2109	CLA	C11-C10-C8-C7
12	H	2137	CLA	C11-C10-C8-C7
12	U	204	CLA	C12-C13-C15-C16
12	a	805	CLA	C12-C13-C15-C16
12	a	820	CLA	C6-C7-C8-C10
12	a	836	CLA	C11-C12-C13-C15
12	a	836	CLA	C12-C13-C15-C16
12	b	2101	CLA	C11-C12-C13-C15
12	b	2109	CLA	C11-C10-C8-C7
12	b	2137	CLA	C11-C10-C8-C7
12	l	204	CLA	C12-C13-C15-C16
12	A	805	CLA	C12-C13-C15-C16
12	A	820	CLA	C6-C7-C8-C10
12	A	836	CLA	C11-C12-C13-C15
12	A	836	CLA	C12-C13-C15-C16
12	B	2102	CLA	C11-C12-C13-C15
12	B	2110	CLA	C11-C10-C8-C7
12	B	2138	CLA	C11-C10-C8-C7
12	L	204	CLA	C12-C13-C15-C16
13	H	2153	A1AGD	C13-C14-C16-C17
13	b	2153	A1AGD	C13-C14-C16-C17
13	B	2153	A1AGD	C13-C14-C16-C17
15	G	844	BCR	C7-C8-C9-C10
15	a	844	BCR	C7-C8-C9-C10
15	A	844	BCR	C7-C8-C9-C10
12	b	2101	CLA	O1D-CGD-O2D-CED
12	H	2125	CLA	CBA-CGA-O2A-C1
12	B	2126	CLA	CBA-CGA-O2A-C1
12	G	834	CLA	O1A-CGA-O2A-C1
12	H	2128	CLA	O1A-CGA-O2A-C1
12	a	834	CLA	O1A-CGA-O2A-C1
12	b	2128	CLA	O1A-CGA-O2A-C1
12	A	834	CLA	O1A-CGA-O2A-C1
12	B	2129	CLA	O1A-CGA-O2A-C1
12	H	2122	CLA	C2A-CAA-CBA-CGA
12	b	2122	CLA	C2A-CAA-CBA-CGA
12	B	2123	CLA	C2A-CAA-CBA-CGA
12	G	824	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	H	2139	CLA	O1A-CGA-O2A-C1
12	G	831	CLA	C10-C11-C12-C13
12	a	831	CLA	C10-C11-C12-C13
12	A	831	CLA	C10-C11-C12-C13
12	a	824	CLA	CBD-CGD-O2D-CED
12	A	824	CLA	CBD-CGD-O2D-CED
12	G	826	CLA	C10-C11-C12-C13
12	a	826	CLA	C10-C11-C12-C13
12	A	826	CLA	C10-C11-C12-C13
12	b	2139	CLA	O1A-CGA-O2A-C1
12	B	2140	CLA	O1A-CGA-O2A-C1
17	b	2147	LMG	C32-C33-C34-C35
17	H	2147	LMG	C32-C33-C34-C35
17	B	2148	LMG	C32-C33-C34-C35
15	S	101	BCR	C11-C10-C9-C8
15	j	101	BCR	C11-C10-C9-C8
15	J	101	BCR	C11-C10-C9-C8
17	G	849	LMG	O1-C7-C8-C9
17	a	849	LMG	O1-C7-C8-C9
17	A	849	LMG	O1-C7-C8-C9
12	G	806	CLA	O1A-CGA-O2A-C1
12	G	824	CLA	C14-C13-C15-C16
12	H	2137	CLA	C14-C13-C15-C16
12	a	824	CLA	C14-C13-C15-C16
12	b	2137	CLA	C14-C13-C15-C16
12	A	824	CLA	C14-C13-C15-C16
12	B	2138	CLA	C14-C13-C15-C16
24	U	208	SQD	C25-C26-C27-C28
25	U	209	DGD	C4B-C5B-C6B-C7B
25	l	209	DGD	C4B-C5B-C6B-C7B
25	L	209	DGD	C4B-C5B-C6B-C7B
12	H	2125	CLA	O1A-CGA-O2A-C1
12	a	806	CLA	O1A-CGA-O2A-C1
12	b	2125	CLA	O1A-CGA-O2A-C1
12	A	806	CLA	O1A-CGA-O2A-C1
12	B	2126	CLA	O1A-CGA-O2A-C1
24	l	208	SQD	C25-C26-C27-C28
24	L	208	SQD	C25-C26-C27-C28
12	B	2141	CLA	C13-C15-C16-C17
12	H	2140	CLA	C13-C15-C16-C17
12	Q	201	CLA	C5-C6-C7-C8
12	b	2140	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
12	f	201	CLA	C5-C6-C7-C8
12	F	201	CLA	C5-C6-C7-C8
13	b	2153	A1AGD	C9-C11-C12-C13
23	Q	205	ZEX	C25-C26-C27-C28
23	f	205	ZEX	C25-C26-C27-C28
23	F	205	ZEX	C25-C26-C27-C28
12	H	2132	CLA	C3-C5-C6-C7
12	B	2133	CLA	C3-C5-C6-C7
13	H	2153	A1AGD	C9-C11-C12-C13
13	B	2153	A1AGD	C9-C11-C12-C13
12	H	2104	CLA	C13-C15-C16-C17
12	b	2104	CLA	C13-C15-C16-C17
12	B	2105	CLA	C13-C15-C16-C17
12	a	837	CLA	C2A-CAA-CBA-CGA
12	A	837	CLA	C2A-CAA-CBA-CGA
12	G	817	CLA	CBA-CGA-O2A-C1
12	a	817	CLA	CBA-CGA-O2A-C1
12	A	817	CLA	CBA-CGA-O2A-C1
12	G	830	CLA	C4C-C3C-CAC-CBC
12	A	830	CLA	C4C-C3C-CAC-CBC
12	H	2127	CLA	C16-C17-C18-C20
12	b	2127	CLA	C16-C17-C18-C20
12	B	2128	CLA	C16-C17-C18-C20
12	b	2132	CLA	C3-C5-C6-C7
17	H	2147	LMG	C33-C34-C35-C36
17	b	2147	LMG	C33-C34-C35-C36
17	B	2148	LMG	C33-C34-C35-C36
12	H	2102	CLA	C16-C17-C18-C19
12	b	2102	CLA	C16-C17-C18-C19
12	B	2103	CLA	C16-C17-C18-C19
12	a	830	CLA	C4C-C3C-CAC-CBC
17	G	847	LMG	C19-C20-C21-C22
17	a	847	LMG	C19-C20-C21-C22
17	A	847	LMG	C19-C20-C21-C22
12	G	811	CLA	C4B-C3B-CAB-CBB
12	G	815	CLA	C1A-C2A-CAA-CBA
12	G	829	CLA	C1A-C2A-CAA-CBA
12	G	851	CLA	C1A-C2A-CAA-CBA
12	H	2111	CLA	C4B-C3B-CAB-CBB
12	U	201	CLA	C1A-C2A-CAA-CBA
12	a	811	CLA	C4B-C3B-CAB-CBB
12	a	815	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	a	829	CLA	C1A-C2A-CAA-CBA
12	b	2111	CLA	C4B-C3B-CAB-CBB
12	l	201	CLA	C1A-C2A-CAA-CBA
12	A	811	CLA	C4B-C3B-CAB-CBB
12	A	815	CLA	C1A-C2A-CAA-CBA
12	A	829	CLA	C1A-C2A-CAA-CBA
12	B	2112	CLA	C4B-C3B-CAB-CBB
12	L	201	CLA	C1A-C2A-CAA-CBA
15	S	101	BCR	C6-C7-C8-C9
15	j	101	BCR	C6-C7-C8-C9
15	J	101	BCR	C6-C7-C8-C9
12	G	837	CLA	C2A-CAA-CBA-CGA
12	b	2116	CLA	C2A-CAA-CBA-CGA
12	B	2117	CLA	C2A-CAA-CBA-CGA
16	G	846	LHG	C32-C33-C34-C35
16	A	846	LHG	C32-C33-C34-C35
16	G	846	LHG	O6-C4-C5-C6
16	a	846	LHG	O6-C4-C5-C6
16	A	846	LHG	O6-C4-C5-C6
16	a	846	LHG	C32-C33-C34-C35
24	V	102	SQD	C5-C6-S-O7
24	m	102	SQD	C5-C6-S-O7
24	M	101	SQD	C5-C6-S-O7
12	G	831	CLA	C6-C7-C8-C10
12	G	835	CLA	C11-C10-C8-C7
12	G	838	CLA	C11-C10-C8-C7
12	H	2102	CLA	C6-C7-C8-C10
12	H	2103	CLA	C11-C10-C8-C7
12	H	2106	CLA	C11-C10-C8-C7
12	H	2111	CLA	C11-C10-C8-C7
12	H	2129	CLA	C6-C7-C8-C10
12	a	831	CLA	C6-C7-C8-C10
12	a	835	CLA	C11-C10-C8-C7
12	a	838	CLA	C11-C10-C8-C7
12	b	2102	CLA	C6-C7-C8-C10
12	b	2103	CLA	C11-C10-C8-C7
12	b	2106	CLA	C11-C10-C8-C7
12	b	2111	CLA	C11-C10-C8-C7
12	b	2129	CLA	C6-C7-C8-C10
12	A	831	CLA	C6-C7-C8-C10
12	A	835	CLA	C11-C10-C8-C7
12	A	838	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
12	B	2103	CLA	C6-C7-C8-C10
12	B	2104	CLA	C11-C10-C8-C7
12	B	2107	CLA	C11-C10-C8-C7
12	B	2112	CLA	C11-C10-C8-C7
12	B	2130	CLA	C6-C7-C8-C10
12	G	827	CLA	CBD-CGD-O2D-CED
12	A	827	CLA	CBD-CGD-O2D-CED
24	V	102	SQD	O48-C23-C24-C25
24	m	102	SQD	O48-C23-C24-C25
24	M	101	SQD	O48-C23-C24-C25
16	V	103	LHG	O6-C4-C5-O7
16	m	103	LHG	O6-C4-C5-O7
16	M	102	LHG	O6-C4-C5-O7
12	a	827	CLA	CBD-CGD-O2D-CED
12	G	833	CLA	O1D-CGD-O2D-CED
12	H	2116	CLA	C2A-CAA-CBA-CGA
12	G	810	CLA	C11-C12-C13-C14
12	G	813	CLA	C11-C12-C13-C14
12	G	818	CLA	C14-C13-C15-C16
12	G	819	CLA	C6-C7-C8-C9
12	G	820	CLA	C6-C7-C8-C9
12	G	836	CLA	C11-C12-C13-C14
12	G	836	CLA	C14-C13-C15-C16
12	a	810	CLA	C11-C12-C13-C14
12	a	813	CLA	C11-C12-C13-C14
12	a	818	CLA	C14-C13-C15-C16
12	a	819	CLA	C6-C7-C8-C9
12	a	820	CLA	C6-C7-C8-C9
12	a	836	CLA	C11-C12-C13-C14
12	a	836	CLA	C14-C13-C15-C16
12	A	810	CLA	C11-C12-C13-C14
12	A	813	CLA	C11-C12-C13-C14
12	A	818	CLA	C14-C13-C15-C16
12	A	819	CLA	C6-C7-C8-C9
12	A	820	CLA	C6-C7-C8-C9
12	A	836	CLA	C11-C12-C13-C14
12	A	836	CLA	C14-C13-C15-C16
13	H	2153	A1AGD	C15-C14-C16-C17
13	b	2153	A1AGD	C15-C14-C16-C17
13	B	2153	A1AGD	C15-C14-C16-C17
12	a	833	CLA	O1D-CGD-O2D-CED
24	V	102	SQD	O5-C5-C6-S

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Mol	Chain	Res	Type	Atoms
24	m	102	SQD	O5-C5-C6-S
24	M	101	SQD	O5-C5-C6-S
12	A	833	CLA	O1D-CGD-O2D-CED
12	G	817	CLA	O1A-CGA-O2A-C1
12	a	817	CLA	O1A-CGA-O2A-C1
12	A	817	CLA	O1A-CGA-O2A-C1
17	G	849	LMG	O1-C7-C8-O7
17	a	849	LMG	O1-C7-C8-O7
17	A	849	LMG	O1-C7-C8-O7
25	U	209	DGD	O2G-C2G-C3G-O3G
25	l	209	DGD	O2G-C2G-C3G-O3G
25	L	209	DGD	O2G-C2G-C3G-O3G
24	V	102	SQD	C44-C45-C46-O48
24	m	102	SQD	C44-C45-C46-O48
24	M	101	SQD	C44-C45-C46-O48
25	U	209	DGD	C1G-C2G-C3G-O3G
25	l	209	DGD	C1G-C2G-C3G-O3G
25	L	209	DGD	C1G-C2G-C3G-O3G
12	G	834	CLA	C5-C6-C7-C8
16	m	103	LHG	C32-C33-C34-C35
12	H	2101	CLA	CAD-CBD-CGD-O2D
12	H	2106	CLA	CAD-CBD-CGD-O2D
12	H	2114	CLA	CAD-CBD-CGD-O2D
12	H	2123	CLA	CAD-CBD-CGD-O2D
12	H	2129	CLA	CAD-CBD-CGD-O2D
12	H	2136	CLA	CAD-CBD-CGD-O2D
12	b	2101	CLA	CAD-CBD-CGD-O2D
12	b	2106	CLA	CAD-CBD-CGD-O2D
12	b	2114	CLA	CAD-CBD-CGD-O2D
12	b	2123	CLA	CAD-CBD-CGD-O2D
12	b	2129	CLA	CAD-CBD-CGD-O2D
12	b	2136	CLA	CAD-CBD-CGD-O2D
12	B	2102	CLA	CAD-CBD-CGD-O2D
12	B	2107	CLA	CAD-CBD-CGD-O2D
12	B	2115	CLA	CAD-CBD-CGD-O2D
12	B	2124	CLA	CAD-CBD-CGD-O2D
12	B	2130	CLA	CAD-CBD-CGD-O2D
12	B	2137	CLA	CAD-CBD-CGD-O2D
12	a	834	CLA	C5-C6-C7-C8
12	A	834	CLA	C5-C6-C7-C8
16	V	103	LHG	C32-C33-C34-C35
16	M	102	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
24	V	102	SQD	O10-C23-O48-C46
24	V	102	SQD	C24-C23-O48-C46
24	m	102	SQD	C24-C23-O48-C46
24	M	101	SQD	C24-C23-O48-C46
12	G	837	CLA	C10-C11-C12-C13
12	a	837	CLA	C10-C11-C12-C13
12	A	837	CLA	C10-C11-C12-C13
12	G	826	CLA	C16-C17-C18-C20
12	a	826	CLA	C16-C17-C18-C20
12	A	826	CLA	C16-C17-C18-C20
24	m	102	SQD	O10-C23-O48-C46
24	M	101	SQD	O10-C23-O48-C46
12	G	807	CLA	CHA-CBD-CGD-O1D
12	H	2101	CLA	CAD-CBD-CGD-O1D
12	H	2106	CLA	CAD-CBD-CGD-O1D
12	H	2114	CLA	CAD-CBD-CGD-O1D
12	H	2117	CLA	CHA-CBD-CGD-O1D
12	H	2117	CLA	CHA-CBD-CGD-O2D
12	H	2123	CLA	CAD-CBD-CGD-O1D
12	H	2129	CLA	CAD-CBD-CGD-O1D
12	H	2136	CLA	CAD-CBD-CGD-O1D
12	T	4002	CLA	CAD-CBD-CGD-O1D
12	U	201	CLA	CHA-CBD-CGD-O1D
12	a	807	CLA	CHA-CBD-CGD-O1D
12	b	2101	CLA	CAD-CBD-CGD-O1D
12	b	2106	CLA	CAD-CBD-CGD-O1D
12	b	2114	CLA	CAD-CBD-CGD-O1D
12	b	2117	CLA	CHA-CBD-CGD-O1D
12	b	2117	CLA	CHA-CBD-CGD-O2D
12	b	2123	CLA	CAD-CBD-CGD-O1D
12	b	2129	CLA	CAD-CBD-CGD-O1D
12	b	2136	CLA	CAD-CBD-CGD-O1D
12	k	4002	CLA	CAD-CBD-CGD-O1D
12	l	201	CLA	CHA-CBD-CGD-O1D
12	A	807	CLA	CHA-CBD-CGD-O1D
12	B	2102	CLA	CAD-CBD-CGD-O1D
12	B	2107	CLA	CAD-CBD-CGD-O1D
12	B	2115	CLA	CAD-CBD-CGD-O1D
12	B	2118	CLA	CHA-CBD-CGD-O1D
12	B	2118	CLA	CHA-CBD-CGD-O2D
12	B	2124	CLA	CAD-CBD-CGD-O1D
12	B	2130	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
12	B	2137	CLA	CAD-CBD-CGD-O1D
12	K	4002	CLA	CAD-CBD-CGD-O1D
12	L	201	CLA	CHA-CBD-CGD-O1D
16	G	846	LHG	C3-O3-P-O5
16	G	848	LHG	C3-O3-P-O5
16	G	848	LHG	C4-O6-P-O5
16	a	846	LHG	C3-O3-P-O5
16	a	848	LHG	C3-O3-P-O5
16	a	848	LHG	C4-O6-P-O5
16	A	846	LHG	C3-O3-P-O5
16	A	848	LHG	C3-O3-P-O5
16	A	848	LHG	C4-O6-P-O5
23	Q	205	ZEX	C13-C14-C15-C35
23	f	205	ZEX	C13-C14-C15-C35
23	F	205	ZEX	C13-C14-C15-C35
12	H	2127	CLA	C4-C3-C5-C6
12	H	2132	CLA	C4-C3-C5-C6
12	b	2127	CLA	C4-C3-C5-C6
12	B	2128	CLA	C4-C3-C5-C6
12	G	810	CLA	C2B-C3B-CAB-CBB
12	G	826	CLA	C2B-C3B-CAB-CBB
12	G	833	CLA	C2B-C3B-CAB-CBB
12	G	851	CLA	C2B-C3B-CAB-CBB
12	H	2111	CLA	C2B-C3B-CAB-CBB
12	H	2114	CLA	C2B-C3B-CAB-CBB
12	H	2118	CLA	C2B-C3B-CAB-CBB
12	H	2126	CLA	C2B-C3B-CAB-CBB
12	H	2133	CLA	C2B-C3B-CAB-CBB
12	Q	203	CLA	C2B-C3B-CAB-CBB
12	S	103	CLA	C2B-C3B-CAB-CBB
12	T	4002	CLA	C2B-C3B-CAB-CBB
12	a	810	CLA	C2B-C3B-CAB-CBB
12	a	826	CLA	C2B-C3B-CAB-CBB
12	a	851	CLA	C2B-C3B-CAB-CBB
12	b	2111	CLA	C2B-C3B-CAB-CBB
12	b	2114	CLA	C2B-C3B-CAB-CBB
12	b	2118	CLA	C2B-C3B-CAB-CBB
12	b	2126	CLA	C2B-C3B-CAB-CBB
12	b	2133	CLA	C2B-C3B-CAB-CBB
12	f	203	CLA	C2B-C3B-CAB-CBB
12	j	103	CLA	C2B-C3B-CAB-CBB
12	k	4002	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
12	A	810	CLA	C2B-C3B-CAB-CBB
12	A	826	CLA	C2B-C3B-CAB-CBB
12	A	833	CLA	C2B-C3B-CAB-CBB
12	A	851	CLA	C2B-C3B-CAB-CBB
12	B	2112	CLA	C2B-C3B-CAB-CBB
12	B	2115	CLA	C2B-C3B-CAB-CBB
12	B	2119	CLA	C2B-C3B-CAB-CBB
12	B	2127	CLA	C2B-C3B-CAB-CBB
12	B	2134	CLA	C2B-C3B-CAB-CBB
12	F	203	CLA	C2B-C3B-CAB-CBB
12	J	103	CLA	C2B-C3B-CAB-CBB
12	K	4002	CLA	C2B-C3B-CAB-CBB
15	G	844	BCR	C1-C6-C7-C8
15	H	2146	BCR	C1-C6-C7-C8
15	Q	202	BCR	C23-C24-C25-C30
15	a	844	BCR	C1-C6-C7-C8
15	b	2146	BCR	C1-C6-C7-C8
15	f	202	BCR	C23-C24-C25-C30
15	A	844	BCR	C1-C6-C7-C8
15	A	844	BCR	C23-C24-C25-C30
15	B	2147	BCR	C1-C6-C7-C8
15	F	202	BCR	C23-C24-C25-C30
17	b	2147	LMG	C35-C36-C37-C38
17	B	2148	LMG	C35-C36-C37-C38
24	m	102	SQD	C11-C12-C13-C14
17	H	2147	LMG	C35-C36-C37-C38
15	G	844	BCR	C37-C22-C23-C24
15	a	844	BCR	C37-C22-C23-C24
15	A	844	BCR	C37-C22-C23-C24
16	H	2148	LHG	C5-C4-O6-P
16	V	103	LHG	C2-C3-O3-P
16	b	2148	LHG	C5-C4-O6-P
16	m	103	LHG	C2-C3-O3-P
16	B	2149	LHG	C5-C4-O6-P
16	M	102	LHG	C2-C3-O3-P
24	V	102	SQD	C11-C12-C13-C14
24	M	101	SQD	C11-C12-C13-C14
17	G	847	LMG	C14-C15-C16-C17
17	a	847	LMG	C14-C15-C16-C17
17	A	847	LMG	C14-C15-C16-C17
12	a	837	CLA	C16-C17-C18-C20
12	A	837	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
12	A	830	CLA	C2C-C3C-CAC-CBC
12	b	2132	CLA	C4-C3-C5-C6
12	B	2133	CLA	C4-C3-C5-C6
12	U	205	CLA	C13-C15-C16-C17
12	l	205	CLA	C13-C15-C16-C17
12	L	205	CLA	C13-C15-C16-C17
12	G	830	CLA	C2C-C3C-CAC-CBC
12	G	837	CLA	C16-C17-C18-C20
12	H	2109	CLA	C16-C17-C18-C20
12	a	830	CLA	C2C-C3C-CAC-CBC
12	G	805	CLA	C14-C13-C15-C16
12	G	818	CLA	C11-C12-C13-C14
12	G	831	CLA	C6-C7-C8-C9
12	G	838	CLA	C11-C10-C8-C9
12	H	2108	CLA	C11-C12-C13-C14
12	H	2129	CLA	C11-C10-C8-C9
12	a	805	CLA	C14-C13-C15-C16
12	a	818	CLA	C11-C12-C13-C14
12	a	831	CLA	C6-C7-C8-C9
12	a	838	CLA	C11-C10-C8-C9
12	b	2108	CLA	C11-C12-C13-C14
12	b	2129	CLA	C11-C10-C8-C9
12	A	805	CLA	C14-C13-C15-C16
12	A	818	CLA	C11-C12-C13-C14
12	A	831	CLA	C6-C7-C8-C9
12	B	2109	CLA	C11-C12-C13-C14
12	B	2130	CLA	C11-C10-C8-C9
12	G	818	CLA	C11-C12-C13-C15
12	a	818	CLA	C11-C12-C13-C15
12	A	818	CLA	C11-C12-C13-C15
17	b	2147	LMG	C15-C16-C17-C18
15	G	843	BCR	C16-C17-C18-C19
15	a	843	BCR	C16-C17-C18-C19
15	A	843	BCR	C16-C17-C18-C19
17	H	2147	LMG	C15-C16-C17-C18
17	B	2148	LMG	C15-C16-C17-C18
12	H	2127	CLA	C16-C17-C18-C19
12	b	2127	CLA	C16-C17-C18-C19
12	B	2128	CLA	C16-C17-C18-C19
12	G	835	CLA	C3-C5-C6-C7
12	a	835	CLA	C3-C5-C6-C7
12	A	835	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
12	G	823	CLA	C4-C3-C5-C6
12	G	817	CLA	C2-C3-C5-C6
12	A	817	CLA	C2-C3-C5-C6
12	G	837	CLA	C16-C17-C18-C19
12	a	837	CLA	C16-C17-C18-C19
12	b	2109	CLA	C16-C17-C18-C20
12	A	837	CLA	C16-C17-C18-C19
12	B	2110	CLA	C16-C17-C18-C20
16	A	848	LHG	C27-C28-C29-C30
16	G	848	LHG	C27-C28-C29-C30
16	a	848	LHG	C27-C28-C29-C30
24	V	102	SQD	O47-C45-C46-O48
24	m	102	SQD	O47-C45-C46-O48
24	M	101	SQD	O47-C45-C46-O48
12	G	822	CLA	C2A-CAA-CBA-CGA
12	a	822	CLA	C2A-CAA-CBA-CGA
12	A	822	CLA	C2A-CAA-CBA-CGA
12	a	823	CLA	C4-C3-C5-C6
12	A	823	CLA	C4-C3-C5-C6
12	a	817	CLA	C2-C3-C5-C6
15	T	4001	BCR	C7-C8-C9-C34
15	k	4001	BCR	C7-C8-C9-C34
15	K	4001	BCR	C7-C8-C9-C34
12	G	810	CLA	C16-C17-C18-C20
12	a	810	CLA	C16-C17-C18-C20
12	A	810	CLA	C16-C17-C18-C20
12	G	804	CLA	CBA-CGA-O2A-C1
12	A	804	CLA	CBA-CGA-O2A-C1
12	b	2132	CLA	C2-C3-C5-C6
12	B	2133	CLA	C2-C3-C5-C6
12	a	804	CLA	CBA-CGA-O2A-C1
12	H	2119	CLA	C14-C13-C15-C16
12	Q	201	CLA	C14-C13-C15-C16
12	b	2119	CLA	C14-C13-C15-C16
12	f	201	CLA	C14-C13-C15-C16
12	A	838	CLA	C11-C10-C8-C9
12	B	2120	CLA	C14-C13-C15-C16
12	F	201	CLA	C14-C13-C15-C16
12	G	821	CLA	CBA-CGA-O2A-C1
12	H	2105	CLA	CBA-CGA-O2A-C1
12	a	821	CLA	CBA-CGA-O2A-C1
12	A	821	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	B	2106	CLA	CBA-CGA-O2A-C1
12	H	2107	CLA	C4B-C3B-CAB-CBB
12	H	2112	CLA	C4B-C3B-CAB-CBB
12	H	2117	CLA	C4B-C3B-CAB-CBB
12	U	201	CLA	C4B-C3B-CAB-CBB
12	a	830	CLA	C4B-C3B-CAB-CBB
12	b	2107	CLA	C4B-C3B-CAB-CBB
12	b	2112	CLA	C4B-C3B-CAB-CBB
12	b	2117	CLA	C4B-C3B-CAB-CBB
12	l	201	CLA	C4B-C3B-CAB-CBB
12	A	830	CLA	C4B-C3B-CAB-CBB
12	B	2108	CLA	C4B-C3B-CAB-CBB
12	B	2113	CLA	C4B-C3B-CAB-CBB
12	B	2118	CLA	C4B-C3B-CAB-CBB
12	L	201	CLA	C4B-C3B-CAB-CBB
12	A	812	CLA	C10-C11-C12-C13
12	H	2116	CLA	CAA-CBA-CGA-O2A
12	B	2117	CLA	CAA-CBA-CGA-O2A
12	a	812	CLA	C10-C11-C12-C13
12	G	804	CLA	O1A-CGA-O2A-C1
12	a	804	CLA	O1A-CGA-O2A-C1
12	A	804	CLA	O1A-CGA-O2A-C1
12	H	2102	CLA	C4-C3-C5-C6
12	b	2102	CLA	C4-C3-C5-C6
12	B	2103	CLA	C4-C3-C5-C6
12	H	2132	CLA	C2-C3-C5-C6
12	G	812	CLA	C10-C11-C12-C13
16	G	848	LHG	C28-C29-C30-C31
16	a	848	LHG	C28-C29-C30-C31
16	A	848	LHG	C28-C29-C30-C31
12	b	2105	CLA	CBA-CGA-O2A-C1
12	G	826	CLA	C16-C17-C18-C19
12	a	826	CLA	C16-C17-C18-C19
12	A	826	CLA	C16-C17-C18-C19
12	G	805	CLA	C11-C10-C8-C7
12	G	820	CLA	C11-C12-C13-C15
12	H	2140	CLA	C11-C12-C13-C15
12	a	805	CLA	C11-C10-C8-C7
12	a	820	CLA	C11-C12-C13-C15
12	b	2140	CLA	C11-C12-C13-C15
12	A	805	CLA	C11-C10-C8-C7
12	A	820	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
12	B	2141	CLA	C11-C12-C13-C15
12	G	821	CLA	O1A-CGA-O2A-C1
12	a	821	CLA	O1A-CGA-O2A-C1
12	A	821	CLA	O1A-CGA-O2A-C1
12	b	2116	CLA	CAA-CBA-CGA-O2A
12	G	836	CLA	C5-C6-C7-C8
12	a	836	CLA	C5-C6-C7-C8
12	A	836	CLA	C5-C6-C7-C8
12	H	2133	CLA	C4-C3-C5-C6
12	b	2133	CLA	C4-C3-C5-C6
12	B	2134	CLA	C4-C3-C5-C6
18	G	852	45D	C28-C26-C30-C32
18	G	852	45D	C39-C35-C37-C41
18	a	852	45D	C28-C26-C30-C32
18	a	852	45D	C39-C35-C37-C41
18	A	852	45D	C28-C26-C30-C32
18	A	852	45D	C39-C35-C37-C41
20	H	2143	ECH	C11-C10-C9-C34
20	H	2143	ECH	C35-C13-C14-C15
20	V	101	ECH	C11-C10-C9-C34
20	b	2143	ECH	C11-C10-C9-C34
20	b	2143	ECH	C35-C13-C14-C15
20	m	101	ECH	C11-C10-C9-C34
20	B	2144	ECH	C11-C10-C9-C34
20	B	2144	ECH	C35-C13-C14-C15
20	M	103	ECH	C11-C10-C9-C34
22	H	2150	EQ3	C11-C10-C9-C34
22	b	2150	EQ3	C11-C10-C9-C34
22	B	2151	EQ3	C11-C10-C9-C34
23	H	2151	ZEX	C39-C29-C30-C31
23	Q	205	ZEX	C20-C13-C14-C15
23	Q	205	ZEX	C39-C29-C30-C31
23	b	2151	ZEX	C39-C29-C30-C31
23	f	205	ZEX	C20-C13-C14-C15
23	f	205	ZEX	C39-C29-C30-C31
23	B	2152	ZEX	C39-C29-C30-C31
23	F	205	ZEX	C20-C13-C14-C15
23	F	205	ZEX	C39-C29-C30-C31
12	H	2105	CLA	O1A-CGA-O2A-C1
12	B	2117	CLA	CAA-CBA-CGA-O1A
12	a	829	CLA	C5-C6-C7-C8
12	A	829	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
16	a	848	LHG	C11-C12-C13-C14
16	A	848	LHG	C11-C12-C13-C14
16	G	848	LHG	C11-C12-C13-C14
15	Q	202	BCR	C19-C20-C21-C22
15	f	202	BCR	C19-C20-C21-C22
15	F	202	BCR	C19-C20-C21-C22
25	L	209	DGD	CDA-CEA-CFA-CGA
12	G	829	CLA	C5-C6-C7-C8
16	H	2148	LHG	C2-C3-O3-P
16	b	2148	LHG	C2-C3-O3-P
16	B	2149	LHG	C2-C3-O3-P
12	H	2116	CLA	CAA-CBA-CGA-O1A
12	b	2116	CLA	CAA-CBA-CGA-O1A
17	G	847	LMG	C15-C16-C17-C18
25	U	209	DGD	CDA-CEA-CFA-CGA
25	l	209	DGD	CDA-CEA-CFA-CGA
17	a	847	LMG	C15-C16-C17-C18
17	A	847	LMG	C15-C16-C17-C18
13	H	2153	A1AGD	C16-C17-C18-C19
13	b	2153	A1AGD	C16-C17-C18-C19
13	B	2153	A1AGD	C16-C17-C18-C19
15	S	101	BCR	C17-C18-C19-C20
15	j	101	BCR	C17-C18-C19-C20
15	J	101	BCR	C17-C18-C19-C20
12	H	2127	CLA	C2-C3-C5-C6
12	b	2127	CLA	C2-C3-C5-C6
12	B	2128	CLA	C2-C3-C5-C6
12	a	812	CLA	C8-C10-C11-C12
12	A	812	CLA	C8-C10-C11-C12
16	M	102	LHG	C13-C14-C15-C16
24	V	102	SQD	C18-C19-C20-C21
12	b	2108	CLA	C2A-CAA-CBA-CGA
12	B	2109	CLA	C2A-CAA-CBA-CGA
16	m	103	LHG	C13-C14-C15-C16
24	m	102	SQD	C18-C19-C20-C21
24	M	101	SQD	C18-C19-C20-C21
12	G	812	CLA	C8-C10-C11-C12
16	V	103	LHG	C13-C14-C15-C16
24	V	102	SQD	C17-C18-C19-C20
24	m	102	SQD	C17-C18-C19-C20
24	M	101	SQD	C17-C18-C19-C20
12	B	2106	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	G	812	CLA	C14-C13-C15-C16
12	G	817	CLA	C6-C7-C8-C9
12	H	2102	CLA	C6-C7-C8-C9
12	H	2119	CLA	C6-C7-C8-C9
12	H	2129	CLA	C6-C7-C8-C9
12	H	2132	CLA	C11-C10-C8-C9
12	H	2140	CLA	C11-C12-C13-C14
12	a	812	CLA	C14-C13-C15-C16
12	a	817	CLA	C6-C7-C8-C9
12	b	2102	CLA	C6-C7-C8-C9
12	b	2119	CLA	C6-C7-C8-C9
12	b	2129	CLA	C6-C7-C8-C9
12	b	2140	CLA	C11-C12-C13-C14
12	A	812	CLA	C14-C13-C15-C16
12	A	817	CLA	C6-C7-C8-C9
12	B	2103	CLA	C6-C7-C8-C9
12	B	2120	CLA	C6-C7-C8-C9
12	B	2130	CLA	C6-C7-C8-C9
12	B	2141	CLA	C11-C12-C13-C14
12	b	2101	CLA	C16-C17-C18-C20
12	H	2119	CLA	C13-C15-C16-C17
12	b	2119	CLA	C13-C15-C16-C17
12	B	2120	CLA	C13-C15-C16-C17
17	H	2147	LMG	C42-C43-C44-C45
17	b	2147	LMG	C42-C43-C44-C45
17	B	2148	LMG	C42-C43-C44-C45
12	H	2117	CLA	CAA-CBA-CGA-O1A
12	H	2127	CLA	CAA-CBA-CGA-O2A
12	b	2127	CLA	CAA-CBA-CGA-O2A
12	b	2114	CLA	C5-C6-C7-C8
12	H	2117	CLA	CAA-CBA-CGA-O2A
12	b	2117	CLA	CAA-CBA-CGA-O1A
12	B	2118	CLA	CAA-CBA-CGA-O1A
12	B	2118	CLA	CAA-CBA-CGA-O2A
12	H	2101	CLA	C16-C17-C18-C20
12	B	2102	CLA	C16-C17-C18-C20
12	B	2128	CLA	CAA-CBA-CGA-O2A
12	b	2105	CLA	O1A-CGA-O2A-C1
12	a	801	CLA	C3-C5-C6-C7
12	b	2103	CLA	C3-C5-C6-C7
12	A	801	CLA	C3-C5-C6-C7
12	B	2104	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
12	b	2117	CLA	CAA-CBA-CGA-O2A
12	H	2108	CLA	C2A-CAA-CBA-CGA
12	G	850	CLA	C1A-C2A-CAA-CBA
12	H	2113	CLA	C1A-C2A-CAA-CBA
12	H	2114	CLA	C1A-C2A-CAA-CBA
12	a	850	CLA	C1A-C2A-CAA-CBA
12	b	2113	CLA	C1A-C2A-CAA-CBA
12	b	2114	CLA	C1A-C2A-CAA-CBA
12	A	850	CLA	C1A-C2A-CAA-CBA
12	B	2114	CLA	C1A-C2A-CAA-CBA
12	B	2115	CLA	C1A-C2A-CAA-CBA
18	G	852	45D	C24-C26-C30-C32
18	G	852	45D	C33-C35-C37-C41
18	a	852	45D	C24-C26-C30-C32
18	a	852	45D	C33-C35-C37-C41
18	A	852	45D	C24-C26-C30-C32
18	A	852	45D	C33-C35-C37-C41
20	H	2143	ECH	C11-C10-C9-C8
20	H	2143	ECH	C12-C13-C14-C15
20	V	101	ECH	C11-C10-C9-C8
20	b	2143	ECH	C11-C10-C9-C8
20	b	2143	ECH	C12-C13-C14-C15
20	m	101	ECH	C11-C10-C9-C8
20	B	2144	ECH	C11-C10-C9-C8
20	B	2144	ECH	C12-C13-C14-C15
20	M	103	ECH	C11-C10-C9-C8
22	H	2150	EQ3	C11-C10-C9-C8
22	b	2150	EQ3	C11-C10-C9-C8
22	B	2151	EQ3	C11-C10-C9-C8
23	Q	205	ZEX	C12-C13-C14-C15
23	f	205	ZEX	C12-C13-C14-C15
23	F	205	ZEX	C12-C13-C14-C15
12	H	2109	CLA	C16-C17-C18-C19
12	b	2109	CLA	C16-C17-C18-C19
12	B	2110	CLA	C16-C17-C18-C19
12	H	2114	CLA	C5-C6-C7-C8
12	B	2115	CLA	C5-C6-C7-C8
12	H	2103	CLA	C3-C5-C6-C7
12	G	802	CLA	C2B-C3B-CAB-CBB
12	G	809	CLA	C2B-C3B-CAB-CBB
12	G	811	CLA	C2B-C3B-CAB-CBB
12	G	812	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
12	G	817	CLA	C2B-C3B-CAB-CBB
12	G	821	CLA	C2B-C3B-CAB-CBB
12	G	823	CLA	C2B-C3B-CAB-CBB
12	G	825	CLA	C2B-C3B-CAB-CBB
12	H	2103	CLA	C2B-C3B-CAB-CBB
12	H	2110	CLA	C2B-C3B-CAB-CBB
12	H	2112	CLA	C2B-C3B-CAB-CBB
12	H	2117	CLA	C2B-C3B-CAB-CBB
12	H	2125	CLA	C2B-C3B-CAB-CBB
12	Q	204	CLA	C2B-C3B-CAB-CBB
12	U	201	CLA	C2B-C3B-CAB-CBB
12	a	802	CLA	C2B-C3B-CAB-CBB
12	a	809	CLA	C2B-C3B-CAB-CBB
12	a	811	CLA	C2B-C3B-CAB-CBB
12	a	812	CLA	C2B-C3B-CAB-CBB
12	a	817	CLA	C2B-C3B-CAB-CBB
12	a	821	CLA	C2B-C3B-CAB-CBB
12	a	823	CLA	C2B-C3B-CAB-CBB
12	a	825	CLA	C2B-C3B-CAB-CBB
12	a	833	CLA	C2B-C3B-CAB-CBB
12	b	2103	CLA	C2B-C3B-CAB-CBB
12	b	2110	CLA	C2B-C3B-CAB-CBB
12	b	2112	CLA	C2B-C3B-CAB-CBB
12	b	2117	CLA	C2B-C3B-CAB-CBB
12	b	2125	CLA	C2B-C3B-CAB-CBB
12	f	204	CLA	C2B-C3B-CAB-CBB
12	l	201	CLA	C2B-C3B-CAB-CBB
12	A	802	CLA	C2B-C3B-CAB-CBB
12	A	809	CLA	C2B-C3B-CAB-CBB
12	A	811	CLA	C2B-C3B-CAB-CBB
12	A	812	CLA	C2B-C3B-CAB-CBB
12	A	817	CLA	C2B-C3B-CAB-CBB
12	A	821	CLA	C2B-C3B-CAB-CBB
12	A	823	CLA	C2B-C3B-CAB-CBB
12	A	825	CLA	C2B-C3B-CAB-CBB
12	B	2104	CLA	C2B-C3B-CAB-CBB
12	B	2111	CLA	C2B-C3B-CAB-CBB
12	B	2113	CLA	C2B-C3B-CAB-CBB
12	B	2118	CLA	C2B-C3B-CAB-CBB
12	B	2126	CLA	C2B-C3B-CAB-CBB
12	F	204	CLA	C2B-C3B-CAB-CBB
12	L	201	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
15	G	842	BCR	C1-C6-C7-C8
15	G	842	BCR	C23-C24-C25-C30
15	G	843	BCR	C5-C6-C7-C8
15	G	844	BCR	C23-C24-C25-C26
15	G	844	BCR	C23-C24-C25-C30
15	G	845	BCR	C5-C6-C7-C8
15	H	2142	BCR	C23-C24-C25-C30
15	H	2144	BCR	C1-C6-C7-C8
15	H	2144	BCR	C23-C24-C25-C30
15	H	2145	BCR	C5-C6-C7-C8
15	H	2145	BCR	C23-C24-C25-C30
15	H	2146	BCR	C5-C6-C7-C8
15	H	2146	BCR	C23-C24-C25-C26
15	Q	202	BCR	C23-C24-C25-C26
15	R	101	BCR	C1-C6-C7-C8
15	S	101	BCR	C5-C6-C7-C8
15	S	101	BCR	C23-C24-C25-C26
15	S	104	BCR	C23-C24-C25-C26
15	T	4001	BCR	C1-C6-C7-C8
15	U	206	BCR	C5-C6-C7-C8
15	a	842	BCR	C1-C6-C7-C8
15	a	842	BCR	C23-C24-C25-C30
15	a	843	BCR	C5-C6-C7-C8
15	a	844	BCR	C23-C24-C25-C30
15	a	845	BCR	C5-C6-C7-C8
15	b	2142	BCR	C23-C24-C25-C30
15	b	2144	BCR	C1-C6-C7-C8
15	b	2144	BCR	C23-C24-C25-C30
15	b	2145	BCR	C5-C6-C7-C8
15	b	2145	BCR	C23-C24-C25-C30
15	b	2146	BCR	C5-C6-C7-C8
15	b	2146	BCR	C23-C24-C25-C26
15	f	202	BCR	C23-C24-C25-C26
15	i	101	BCR	C1-C6-C7-C8
15	j	101	BCR	C5-C6-C7-C8
15	j	101	BCR	C23-C24-C25-C26
15	j	104	BCR	C23-C24-C25-C26
15	k	4001	BCR	C1-C6-C7-C8
15	l	206	BCR	C5-C6-C7-C8
15	A	842	BCR	C1-C6-C7-C8
15	A	842	BCR	C23-C24-C25-C30
15	A	843	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
15	A	845	BCR	C5-C6-C7-C8
15	B	2143	BCR	C23-C24-C25-C30
15	B	2145	BCR	C1-C6-C7-C8
15	B	2145	BCR	C23-C24-C25-C30
15	B	2146	BCR	C5-C6-C7-C8
15	B	2146	BCR	C23-C24-C25-C30
15	B	2147	BCR	C5-C6-C7-C8
15	B	2147	BCR	C23-C24-C25-C26
15	F	202	BCR	C23-C24-C25-C26
15	I	101	BCR	C1-C6-C7-C8
15	J	101	BCR	C5-C6-C7-C8
15	J	101	BCR	C23-C24-C25-C26
15	J	104	BCR	C23-C24-C25-C26
15	K	4001	BCR	C1-C6-C7-C8
15	L	206	BCR	C5-C6-C7-C8
23	Q	205	ZEX	C5-C6-C7-C8
23	f	205	ZEX	C5-C6-C7-C8
23	F	205	ZEX	C5-C6-C7-C8
17	G	847	LMG	C10-C11-C12-C13
17	a	847	LMG	C10-C11-C12-C13
17	A	847	LMG	C10-C11-C12-C13
12	H	2134	CLA	CAA-CBA-CGA-O1A
12	G	801	CLA	C3-C5-C6-C7
12	H	2108	CLA	C4-C3-C5-C6
12	b	2108	CLA	C4-C3-C5-C6
12	B	2109	CLA	C4-C3-C5-C6
12	b	2134	CLA	CAA-CBA-CGA-O1A
12	B	2135	CLA	CAA-CBA-CGA-O1A
12	G	819	CLA	C11-C12-C13-C15
12	H	2110	CLA	C12-C13-C15-C16
12	H	2119	CLA	C12-C13-C15-C16
12	H	2132	CLA	C11-C10-C8-C7
12	Q	201	CLA	C12-C13-C15-C16
12	a	819	CLA	C11-C12-C13-C15
12	b	2110	CLA	C12-C13-C15-C16
12	b	2119	CLA	C12-C13-C15-C16
12	b	2126	CLA	C12-C13-C15-C16
12	b	2132	CLA	C11-C10-C8-C7
12	f	201	CLA	C12-C13-C15-C16
12	A	819	CLA	C11-C12-C13-C15
12	B	2111	CLA	C12-C13-C15-C16
12	B	2120	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
12	B	2127	CLA	C12-C13-C15-C16
12	B	2133	CLA	C11-C10-C8-C7
12	F	201	CLA	C12-C13-C15-C16
12	G	827	CLA	C2A-CAA-CBA-CGA
12	a	827	CLA	C2A-CAA-CBA-CGA
12	A	827	CLA	C2A-CAA-CBA-CGA
12	H	2103	CLA	CAA-CBA-CGA-O2A
12	B	2104	CLA	CAA-CBA-CGA-O2A
17	B	2148	LMG	C39-C40-C41-C42
12	H	2128	CLA	CBD-CGD-O2D-CED
17	H	2147	LMG	C39-C40-C41-C42
17	b	2147	LMG	C39-C40-C41-C42
15	G	845	BCR	C11-C12-C13-C35
15	a	845	BCR	C11-C12-C13-C35
15	A	845	BCR	C11-C12-C13-C35
22	H	2150	EQ3	C36-C18-C19-C20
22	b	2150	EQ3	C36-C18-C19-C20
22	B	2151	EQ3	C36-C18-C19-C20
12	H	2134	CLA	CAA-CBA-CGA-O2A
12	a	824	CLA	O1D-CGD-O2D-CED
12	A	824	CLA	O1D-CGD-O2D-CED
12	G	801	CLA	CAA-CBA-CGA-O2A
12	G	817	CLA	CAA-CBA-CGA-O2A
12	a	801	CLA	CAA-CBA-CGA-O2A
12	a	817	CLA	CAA-CBA-CGA-O2A
12	b	2103	CLA	CAA-CBA-CGA-O2A
12	A	801	CLA	CAA-CBA-CGA-O2A
12	A	817	CLA	CAA-CBA-CGA-O2A
12	H	2102	CLA	C2-C3-C5-C6
12	b	2102	CLA	C2-C3-C5-C6
12	B	2103	CLA	C2-C3-C5-C6
12	H	2123	CLA	C2-C1-O2A-CGA
12	b	2123	CLA	C2-C1-O2A-CGA
12	B	2124	CLA	C2-C1-O2A-CGA
12	G	832	CLA	C13-C15-C16-C17
12	a	832	CLA	C13-C15-C16-C17
12	A	832	CLA	C13-C15-C16-C17
12	G	824	CLA	O1D-CGD-O2D-CED
12	b	2134	CLA	CAA-CBA-CGA-O2A
12	B	2135	CLA	CAA-CBA-CGA-O2A
12	G	813	CLA	C6-C7-C8-C9
12	U	203	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
12	a	813	CLA	C6-C7-C8-C9
12	b	2132	CLA	C11-C10-C8-C9
12	l	203	CLA	C11-C12-C13-C14
12	A	813	CLA	C6-C7-C8-C9
12	B	2133	CLA	C11-C10-C8-C9
12	L	203	CLA	C11-C12-C13-C14
12	b	2128	CLA	CBD-CGD-O2D-CED
12	B	2129	CLA	CBD-CGD-O2D-CED
15	G	843	BCR	C13-C14-C15-C16
15	a	843	BCR	C13-C14-C15-C16
15	A	843	BCR	C13-C14-C15-C16
15	Q	202	BCR	C6-C7-C8-C9
15	f	202	BCR	C6-C7-C8-C9
15	F	202	BCR	C6-C7-C8-C9
12	G	850	CLA	C4-C3-C5-C6
12	a	850	CLA	C4-C3-C5-C6
12	A	850	CLA	C4-C3-C5-C6
12	H	2135	CLA	CAA-CBA-CGA-O2A
12	b	2135	CLA	CAA-CBA-CGA-O2A
12	B	2136	CLA	CAA-CBA-CGA-O2A
12	H	2113	CLA	CAA-CBA-CGA-O2A
12	Q	203	CLA	CAA-CBA-CGA-O2A
12	f	203	CLA	CAA-CBA-CGA-O2A
12	B	2114	CLA	CAA-CBA-CGA-O2A
12	F	203	CLA	CAA-CBA-CGA-O2A
12	G	830	CLA	C4B-C3B-CAB-CBB
12	H	2105	CLA	C4B-C3B-CAB-CBB
12	H	2116	CLA	C4B-C3B-CAB-CBB
12	b	2105	CLA	C4B-C3B-CAB-CBB
12	b	2116	CLA	C4B-C3B-CAB-CBB
12	B	2106	CLA	C4B-C3B-CAB-CBB
12	B	2117	CLA	C4B-C3B-CAB-CBB
12	b	2113	CLA	CAA-CBA-CGA-O2A
12	a	828	CLA	C13-C15-C16-C17
12	G	811	CLA	CAA-CBA-CGA-O2A
12	a	811	CLA	CAA-CBA-CGA-O2A
12	A	811	CLA	CAA-CBA-CGA-O2A
12	H	2101	CLA	C16-C17-C18-C19
12	H	2108	CLA	C16-C17-C18-C20
12	b	2101	CLA	C16-C17-C18-C19
12	b	2108	CLA	C16-C17-C18-C20
12	B	2102	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
12	B	2109	CLA	C16-C17-C18-C20
16	V	103	LHG	C1-C2-C3-O3
16	m	103	LHG	C1-C2-C3-O3
16	M	102	LHG	C1-C2-C3-O3
16	G	848	LHG	C29-C30-C31-C32
16	a	848	LHG	C29-C30-C31-C32
15	G	843	BCR	C35-C13-C14-C15
15	a	843	BCR	C35-C13-C14-C15
15	A	843	BCR	C35-C13-C14-C15
12	G	828	CLA	C13-C15-C16-C17
12	A	828	CLA	C13-C15-C16-C17
16	V	103	LHG	C30-C31-C32-C33
16	m	103	LHG	C30-C31-C32-C33
16	A	848	LHG	C29-C30-C31-C32
16	M	102	LHG	C30-C31-C32-C33
16	H	2148	LHG	C29-C30-C31-C32
12	Q	201	CLA	C13-C15-C16-C17
12	f	201	CLA	C13-C15-C16-C17
12	F	201	CLA	C13-C15-C16-C17
12	H	2126	CLA	C12-C13-C15-C16
12	H	2135	CLA	CAA-CBA-CGA-O1A
16	b	2148	LHG	C29-C30-C31-C32
16	B	2149	LHG	C29-C30-C31-C32
12	b	2135	CLA	CAA-CBA-CGA-O1A
12	B	2136	CLA	CAA-CBA-CGA-O1A
12	G	821	CLA	C11-C10-C8-C9
12	G	828	CLA	C11-C12-C13-C14
12	G	835	CLA	C11-C10-C8-C9
12	H	2103	CLA	C11-C10-C8-C9
12	Q	201	CLA	C6-C7-C8-C9
12	a	821	CLA	C11-C10-C8-C9
12	a	828	CLA	C11-C12-C13-C14
12	a	835	CLA	C11-C10-C8-C9
12	b	2103	CLA	C11-C10-C8-C9
12	f	201	CLA	C6-C7-C8-C9
12	A	821	CLA	C11-C10-C8-C9
12	A	828	CLA	C11-C12-C13-C14
12	A	835	CLA	C11-C10-C8-C9
12	B	2104	CLA	C11-C10-C8-C9
12	F	201	CLA	C6-C7-C8-C9
12	a	851	CLA	C13-C15-C16-C17
24	U	208	SQD	C5-C6-S-O8

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Mol	Chain	Res	Type	Atoms
24	l	208	SQD	C5-C6-S-O8
24	L	208	SQD	C5-C6-S-O8
12	G	851	CLA	C13-C15-C16-C17
12	A	851	CLA	C13-C15-C16-C17
12	G	818	CLA	C2A-CAA-CBA-CGA
12	a	818	CLA	C2A-CAA-CBA-CGA
12	A	818	CLA	C2A-CAA-CBA-CGA
12	H	2105	CLA	C3-C5-C6-C7
12	b	2105	CLA	C3-C5-C6-C7
12	B	2106	CLA	C3-C5-C6-C7
12	G	850	CLA	C3A-C2A-CAA-CBA
12	H	2114	CLA	C3A-C2A-CAA-CBA
12	H	2117	CLA	C3A-C2A-CAA-CBA
12	S	102	CLA	C3A-C2A-CAA-CBA
12	a	850	CLA	C3A-C2A-CAA-CBA
12	b	2114	CLA	C3A-C2A-CAA-CBA
12	b	2117	CLA	C3A-C2A-CAA-CBA
12	j	102	CLA	C3A-C2A-CAA-CBA
12	A	850	CLA	C3A-C2A-CAA-CBA
12	B	2115	CLA	C3A-C2A-CAA-CBA
12	B	2118	CLA	C3A-C2A-CAA-CBA
12	J	102	CLA	C3A-C2A-CAA-CBA
12	G	823	CLA	C2-C3-C5-C6
12	a	823	CLA	C2-C3-C5-C6
12	A	823	CLA	C2-C3-C5-C6
12	H	2110	CLA	O2A-C1-C2-C3
12	b	2110	CLA	O2A-C1-C2-C3
12	B	2111	CLA	O2A-C1-C2-C3
15	b	2144	BCR	C14-C15-C16-C17
12	A	827	CLA	O1D-CGD-O2D-CED
12	H	2113	CLA	CAA-CBA-CGA-O1A
12	b	2113	CLA	CAA-CBA-CGA-O1A
12	B	2114	CLA	CAA-CBA-CGA-O1A
12	G	811	CLA	CAA-CBA-CGA-O1A
12	Q	203	CLA	CAA-CBA-CGA-O1A
12	a	811	CLA	CAA-CBA-CGA-O1A
12	f	203	CLA	CAA-CBA-CGA-O1A
12	A	811	CLA	CAA-CBA-CGA-O1A
12	F	203	CLA	CAA-CBA-CGA-O1A
12	G	827	CLA	O1D-CGD-O2D-CED
15	Q	202	BCR	C22-C23-C24-C25
15	f	202	BCR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
15	F	202	BCR	C22-C23-C24-C25
12	a	825	CLA	O1A-CGA-O2A-C1
12	l	201	CLA	O1A-CGA-O2A-C1
12	A	825	CLA	O1A-CGA-O2A-C1
16	G	848	LHG	C16-C17-C18-C19
16	a	848	LHG	C16-C17-C18-C19
16	A	848	LHG	C16-C17-C18-C19
12	a	827	CLA	O1D-CGD-O2D-CED
16	G	846	LHG	C34-C35-C36-C37
16	A	846	LHG	C34-C35-C36-C37
12	U	201	CLA	O1A-CGA-O2A-C1
12	L	201	CLA	O1A-CGA-O2A-C1
16	a	846	LHG	C34-C35-C36-C37
12	H	2138	CLA	CAA-CBA-CGA-O1A
12	B	2139	CLA	CAA-CBA-CGA-O1A
12	G	819	CLA	C13-C15-C16-C17
12	A	819	CLA	C13-C15-C16-C17
12	b	2138	CLA	CAA-CBA-CGA-O1A
12	G	825	CLA	O1A-CGA-O2A-C1
12	b	2120	CLA	CAA-CBA-CGA-O2A
12	a	819	CLA	C13-C15-C16-C17
15	H	2144	BCR	C14-C15-C16-C17
15	B	2145	BCR	C14-C15-C16-C17
12	H	2106	CLA	C11-C10-C8-C9
12	H	2109	CLA	C11-C10-C8-C9
12	b	2106	CLA	C11-C10-C8-C9
12	b	2109	CLA	C11-C10-C8-C9
12	B	2107	CLA	C11-C10-C8-C9
12	B	2110	CLA	C11-C10-C8-C9
13	H	2153	A1AGD	C12-C13-C14-C15
13	b	2153	A1AGD	C12-C13-C14-C15
13	B	2153	A1AGD	C12-C13-C14-C15
12	H	2120	CLA	CAA-CBA-CGA-O2A
12	B	2121	CLA	CAA-CBA-CGA-O2A
17	H	2147	LMG	O7-C10-C11-C12
17	b	2147	LMG	O7-C10-C11-C12
17	B	2148	LMG	O7-C10-C11-C12
12	G	824	CLA	C4-C3-C5-C6
12	a	824	CLA	C4-C3-C5-C6
12	A	824	CLA	C4-C3-C5-C6
24	U	208	SQD	C12-C13-C14-C15
24	l	208	SQD	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
24	L	208	SQD	C12-C13-C14-C15
24	U	208	SQD	O47-C7-C8-C9
12	H	2138	CLA	CAA-CBA-CGA-O2A
12	b	2138	CLA	CAA-CBA-CGA-O2A
12	B	2139	CLA	CAA-CBA-CGA-O2A
12	G	813	CLA	C6-C7-C8-C10
12	G	821	CLA	C11-C10-C8-C7
12	G	828	CLA	C11-C12-C13-C15
12	G	833	CLA	C6-C7-C8-C10
12	G	836	CLA	C6-C7-C8-C10
12	Q	201	CLA	C11-C10-C8-C7
12	U	203	CLA	C6-C7-C8-C10
12	U	203	CLA	C11-C12-C13-C15
12	a	813	CLA	C6-C7-C8-C10
12	a	821	CLA	C11-C10-C8-C7
12	a	828	CLA	C11-C12-C13-C15
12	a	833	CLA	C6-C7-C8-C10
12	a	836	CLA	C6-C7-C8-C10
12	f	201	CLA	C11-C10-C8-C7
12	l	203	CLA	C6-C7-C8-C10
12	l	203	CLA	C11-C12-C13-C15
12	A	813	CLA	C6-C7-C8-C10
12	A	821	CLA	C11-C10-C8-C7
12	A	828	CLA	C11-C12-C13-C15
12	A	833	CLA	C6-C7-C8-C10
12	A	836	CLA	C6-C7-C8-C10
12	F	201	CLA	C11-C10-C8-C7
12	L	203	CLA	C6-C7-C8-C10
12	L	203	CLA	C11-C12-C13-C15
13	H	2153	A1AGD	C12-C13-C14-C16
13	b	2153	A1AGD	C12-C13-C14-C16
13	B	2153	A1AGD	C12-C13-C14-C16
12	G	813	CLA	C2B-C3B-CAB-CBB
12	G	819	CLA	C2B-C3B-CAB-CBB
12	G	830	CLA	C2B-C3B-CAB-CBB
12	G	838	CLA	C2B-C3B-CAB-CBB
12	H	2105	CLA	C2B-C3B-CAB-CBB
12	H	2107	CLA	C2B-C3B-CAB-CBB
12	H	2115	CLA	C2B-C3B-CAB-CBB
12	H	2116	CLA	C2B-C3B-CAB-CBB
12	H	2135	CLA	C2B-C3B-CAB-CBB
12	H	2136	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
12	U	204	CLA	C2B-C3B-CAB-CBB
12	a	813	CLA	C2B-C3B-CAB-CBB
12	a	819	CLA	C2B-C3B-CAB-CBB
12	a	830	CLA	C2B-C3B-CAB-CBB
12	a	838	CLA	C2B-C3B-CAB-CBB
12	b	2105	CLA	C2B-C3B-CAB-CBB
12	b	2107	CLA	C2B-C3B-CAB-CBB
12	b	2115	CLA	C2B-C3B-CAB-CBB
12	b	2116	CLA	C2B-C3B-CAB-CBB
12	b	2135	CLA	C2B-C3B-CAB-CBB
12	b	2136	CLA	C2B-C3B-CAB-CBB
12	l	204	CLA	C2B-C3B-CAB-CBB
12	A	813	CLA	C2B-C3B-CAB-CBB
12	A	819	CLA	C2B-C3B-CAB-CBB
12	A	830	CLA	C2B-C3B-CAB-CBB
12	A	838	CLA	C2B-C3B-CAB-CBB
12	B	2106	CLA	C2B-C3B-CAB-CBB
12	B	2108	CLA	C2B-C3B-CAB-CBB
12	B	2116	CLA	C2B-C3B-CAB-CBB
12	B	2117	CLA	C2B-C3B-CAB-CBB
12	B	2136	CLA	C2B-C3B-CAB-CBB
12	B	2137	CLA	C2B-C3B-CAB-CBB
12	L	204	CLA	C2B-C3B-CAB-CBB
15	G	842	BCR	C5-C6-C7-C8
15	G	842	BCR	C23-C24-C25-C26
15	G	844	BCR	C5-C6-C7-C8
15	H	2142	BCR	C23-C24-C25-C26
15	H	2144	BCR	C5-C6-C7-C8
15	H	2144	BCR	C23-C24-C25-C26
15	H	2145	BCR	C23-C24-C25-C26
15	R	101	BCR	C5-C6-C7-C8
15	T	4001	BCR	C5-C6-C7-C8
15	T	4001	BCR	C23-C24-C25-C26
15	a	842	BCR	C23-C24-C25-C26
15	a	844	BCR	C5-C6-C7-C8
15	a	844	BCR	C23-C24-C25-C26
15	b	2142	BCR	C23-C24-C25-C26
15	b	2144	BCR	C5-C6-C7-C8
15	b	2144	BCR	C23-C24-C25-C26
15	b	2145	BCR	C23-C24-C25-C26
15	i	101	BCR	C5-C6-C7-C8
15	k	4001	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
15	k	4001	BCR	C23-C24-C25-C26
15	A	842	BCR	C5-C6-C7-C8
15	A	842	BCR	C23-C24-C25-C26
15	A	844	BCR	C5-C6-C7-C8
15	A	844	BCR	C23-C24-C25-C26
15	B	2143	BCR	C23-C24-C25-C26
15	B	2145	BCR	C5-C6-C7-C8
15	B	2145	BCR	C23-C24-C25-C26
15	B	2146	BCR	C23-C24-C25-C26
15	I	101	BCR	C5-C6-C7-C8
15	K	4001	BCR	C5-C6-C7-C8
15	K	4001	BCR	C23-C24-C25-C26
16	V	103	LHG	C9-C10-C11-C12
16	m	103	LHG	C9-C10-C11-C12
16	M	102	LHG	C9-C10-C11-C12
12	G	824	CLA	C2-C1-O2A-CGA
12	H	2110	CLA	C2-C1-O2A-CGA
12	H	2137	CLA	C2-C1-O2A-CGA
12	a	824	CLA	C2-C1-O2A-CGA
12	b	2110	CLA	C2-C1-O2A-CGA
12	b	2137	CLA	C2-C1-O2A-CGA
12	A	824	CLA	C2-C1-O2A-CGA
12	B	2111	CLA	C2-C1-O2A-CGA
12	B	2138	CLA	C2-C1-O2A-CGA
12	l	201	CLA	CBA-CGA-O2A-C1
16	a	846	LHG	C13-C14-C15-C16
16	A	846	LHG	C13-C14-C15-C16
12	G	854	CLA	CAA-CBA-CGA-O2A
12	a	854	CLA	CAA-CBA-CGA-O2A
12	A	854	CLA	CAA-CBA-CGA-O2A
24	l	208	SQD	O47-C7-C8-C9
24	L	208	SQD	O47-C7-C8-C9
16	G	846	LHG	C13-C14-C15-C16
12	U	201	CLA	CBA-CGA-O2A-C1
12	L	201	CLA	CBA-CGA-O2A-C1
12	H	2140	CLA	C3-C5-C6-C7
12	B	2141	CLA	C3-C5-C6-C7
12	a	824	CLA	C2-C3-C5-C6
12	A	824	CLA	C2-C3-C5-C6
12	G	829	CLA	C2A-CAA-CBA-CGA
12	a	829	CLA	C2A-CAA-CBA-CGA
12	A	829	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
12	G	825	CLA	CBA-CGA-O2A-C1
12	a	825	CLA	CBA-CGA-O2A-C1
12	A	825	CLA	CBA-CGA-O2A-C1
12	b	2140	CLA	C3-C5-C6-C7
12	G	850	CLA	C13-C15-C16-C17
12	a	850	CLA	C13-C15-C16-C17
12	A	850	CLA	C13-C15-C16-C17
12	G	809	CLA	CAA-CBA-CGA-O2A
12	a	809	CLA	CAA-CBA-CGA-O2A
12	A	809	CLA	CAA-CBA-CGA-O2A
16	G	846	LHG	O8-C23-C24-C25
16	a	846	LHG	O8-C23-C24-C25
16	A	846	LHG	O8-C23-C24-C25
26	U	210	LMT	C4'-C5'-C6'-O6'
12	G	818	CLA	C2-C3-C5-C6
12	G	824	CLA	C2-C3-C5-C6
12	H	2133	CLA	C2-C3-C5-C6
12	a	818	CLA	C2-C3-C5-C6
12	b	2133	CLA	C2-C3-C5-C6
12	A	818	CLA	C2-C3-C5-C6
12	B	2134	CLA	C2-C3-C5-C6
26	L	210	LMT	C4'-C5'-C6'-O6'
12	S	102	CLA	C2A-CAA-CBA-CGA
12	j	102	CLA	C2A-CAA-CBA-CGA
26	l	210	LMT	C4'-C5'-C6'-O6'
12	S	103	CLA	CAA-CBA-CGA-O1A
12	J	103	CLA	CAA-CBA-CGA-O1A
12	J	103	CLA	CAA-CBA-CGA-O2A
12	G	807	CLA	C11-C12-C13-C14
12	H	2111	CLA	C6-C7-C8-C9
12	b	2111	CLA	C6-C7-C8-C9
12	b	2126	CLA	C14-C13-C15-C16
12	B	2112	CLA	C6-C7-C8-C9
12	B	2127	CLA	C14-C13-C15-C16
12	H	2140	CLA	CAA-CBA-CGA-O2A
12	b	2140	CLA	CAA-CBA-CGA-O2A
12	B	2115	CLA	CAA-CBA-CGA-O2A
12	B	2141	CLA	CAA-CBA-CGA-O2A
24	V	102	SQD	O6-C44-C45-C46
24	m	102	SQD	O6-C44-C45-C46
24	M	101	SQD	O6-C44-C45-C46
12	G	818	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
12	H	2111	CLA	C1A-C2A-CAA-CBA
12	S	102	CLA	C1A-C2A-CAA-CBA
12	a	818	CLA	C4B-C3B-CAB-CBB
12	b	2111	CLA	C1A-C2A-CAA-CBA
12	j	102	CLA	C1A-C2A-CAA-CBA
12	A	818	CLA	C4B-C3B-CAB-CBB
12	B	2112	CLA	C1A-C2A-CAA-CBA
12	J	102	CLA	C1A-C2A-CAA-CBA
12	S	103	CLA	CAA-CBA-CGA-O2A
12	j	103	CLA	CAA-CBA-CGA-O2A
12	U	204	CLA	C4-C3-C5-C6
12	l	204	CLA	C4-C3-C5-C6
12	L	204	CLA	C4-C3-C5-C6
15	G	843	BCR	C22-C23-C24-C25
15	a	843	BCR	C22-C23-C24-C25
15	A	843	BCR	C22-C23-C24-C25
12	G	807	CLA	CAA-CBA-CGA-O2A
12	H	2107	CLA	CAA-CBA-CGA-O2A
12	H	2114	CLA	CAA-CBA-CGA-O2A
12	b	2107	CLA	CAA-CBA-CGA-O2A
12	b	2114	CLA	CAA-CBA-CGA-O2A
12	A	807	CLA	CAA-CBA-CGA-O2A
12	B	2108	CLA	CAA-CBA-CGA-O2A
12	H	2108	CLA	C2-C3-C5-C6
12	b	2108	CLA	C2-C3-C5-C6
12	B	2109	CLA	C2-C3-C5-C6
12	j	103	CLA	CAA-CBA-CGA-O1A
22	H	2150	EQ3	C17-C18-C19-C20
22	b	2150	EQ3	C17-C18-C19-C20
22	B	2151	EQ3	C17-C18-C19-C20
17	G	847	LMG	C33-C34-C35-C36
17	A	847	LMG	C33-C34-C35-C36
12	H	2109	CLA	CBA-CGA-O2A-C1
12	b	2109	CLA	CBA-CGA-O2A-C1
12	B	2110	CLA	CBA-CGA-O2A-C1
12	a	807	CLA	CAA-CBA-CGA-O2A
12	a	851	CLA	CAA-CBA-CGA-O2A
12	A	851	CLA	CAA-CBA-CGA-O2A
12	J	102	CLA	C2A-CAA-CBA-CGA
17	a	847	LMG	C33-C34-C35-C36
17	H	2147	LMG	C37-C38-C39-C40
17	b	2147	LMG	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
12	G	851	CLA	CAA-CBA-CGA-O2A
16	m	103	LHG	O7-C7-C8-C9
16	M	102	LHG	O7-C7-C8-C9
17	B	2148	LMG	C37-C38-C39-C40
12	G	830	CLA	C2-C1-O2A-CGA
12	G	834	CLA	C2-C1-O2A-CGA
12	U	201	CLA	C2-C1-O2A-CGA
12	a	830	CLA	C2-C1-O2A-CGA
12	a	834	CLA	C2-C1-O2A-CGA
12	A	830	CLA	C2-C1-O2A-CGA
12	A	834	CLA	C2-C1-O2A-CGA
12	L	201	CLA	C2-C1-O2A-CGA
16	V	103	LHG	O7-C7-C8-C9
12	G	824	CLA	C8-C10-C11-C12
12	a	824	CLA	C8-C10-C11-C12
12	A	824	CLA	C8-C10-C11-C12
12	G	836	CLA	C2A-CAA-CBA-CGA
12	H	2114	CLA	C2A-CAA-CBA-CGA
12	a	814	CLA	C2A-CAA-CBA-CGA
12	a	836	CLA	C2A-CAA-CBA-CGA
12	b	2114	CLA	C2A-CAA-CBA-CGA
12	A	814	CLA	C2A-CAA-CBA-CGA
12	A	836	CLA	C2A-CAA-CBA-CGA
12	B	2115	CLA	C2A-CAA-CBA-CGA
12	a	802	CLA	C10-C11-C12-C13
12	S	103	CLA	C3A-C2A-CAA-CBA
12	j	103	CLA	C3A-C2A-CAA-CBA
12	J	103	CLA	C3A-C2A-CAA-CBA
12	G	802	CLA	C10-C11-C12-C13
12	A	802	CLA	C10-C11-C12-C13
16	m	103	LHG	C10-C11-C12-C13
16	M	102	LHG	C10-C11-C12-C13
16	V	103	LHG	C10-C11-C12-C13
24	l	208	SQD	C13-C14-C15-C16
24	L	208	SQD	C13-C14-C15-C16
12	G	814	CLA	C2A-CAA-CBA-CGA
12	H	2111	CLA	C14-C13-C15-C16
12	H	2114	CLA	C11-C10-C8-C9
12	H	2126	CLA	C14-C13-C15-C16
12	a	807	CLA	C11-C12-C13-C14
12	b	2111	CLA	C14-C13-C15-C16
12	b	2114	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
12	A	807	CLA	C11-C12-C13-C14
12	B	2112	CLA	C14-C13-C15-C16
12	B	2115	CLA	C11-C10-C8-C9
12	G	822	CLA	CAA-CBA-CGA-O2A
12	a	822	CLA	CAA-CBA-CGA-O2A
12	A	822	CLA	CAA-CBA-CGA-O2A
12	G	809	CLA	CAA-CBA-CGA-O1A
12	H	2120	CLA	CAA-CBA-CGA-O1A
12	b	2120	CLA	CAA-CBA-CGA-O1A
12	B	2121	CLA	CAA-CBA-CGA-O1A
24	U	208	SQD	C13-C14-C15-C16
12	G	818	CLA	C4-C3-C5-C6
12	a	818	CLA	C4-C3-C5-C6
12	A	818	CLA	C4-C3-C5-C6
12	a	809	CLA	CAA-CBA-CGA-O1A
12	b	2107	CLA	CAA-CBA-CGA-O1A
12	b	2114	CLA	CAA-CBA-CGA-O1A
12	A	809	CLA	CAA-CBA-CGA-O1A
12	A	854	CLA	CAA-CBA-CGA-O1A
12	B	2108	CLA	CAA-CBA-CGA-O1A
12	B	2115	CLA	CAA-CBA-CGA-O1A
12	U	201	CLA	C5-C6-C7-C8
12	l	201	CLA	C5-C6-C7-C8
12	H	2107	CLA	CAA-CBA-CGA-O1A
12	H	2114	CLA	CAA-CBA-CGA-O1A
12	a	807	CLA	CAA-CBA-CGA-O1A
25	U	209	DGD	O1G-C1A-C2A-C3A
25	l	209	DGD	O1G-C1A-C2A-C3A
25	L	209	DGD	O1G-C1A-C2A-C3A
12	L	201	CLA	C5-C6-C7-C8
12	G	807	CLA	CAA-CBA-CGA-O1A
12	G	854	CLA	CAA-CBA-CGA-O1A
12	H	2140	CLA	CAA-CBA-CGA-O1A
12	a	854	CLA	CAA-CBA-CGA-O1A
12	A	807	CLA	CAA-CBA-CGA-O1A
12	B	2141	CLA	CAA-CBA-CGA-O1A
16	V	103	LHG	C23-C24-C25-C26
16	m	103	LHG	C23-C24-C25-C26
17	G	849	LMG	C8-C7-O1-C1
17	a	849	LMG	C8-C7-O1-C1
17	A	849	LMG	C8-C7-O1-C1
12	k	4002	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
12	K	4002	CLA	CAA-CBA-CGA-O2A
12	b	2140	CLA	CAA-CBA-CGA-O1A
12	T	4002	CLA	CAA-CBA-CGA-O2A
12	G	804	CLA	CAA-CBA-CGA-O2A
12	a	804	CLA	CAA-CBA-CGA-O2A
12	A	804	CLA	CAA-CBA-CGA-O2A
17	A	847	LMG	O10-C28-C29-C30
16	M	102	LHG	C23-C24-C25-C26
12	G	801	CLA	CAD-CBD-CGD-O2D
12	G	812	CLA	CAD-CBD-CGD-O2D
12	G	814	CLA	CAD-CBD-CGD-O2D
12	H	2107	CLA	CAD-CBD-CGD-O2D
12	H	2112	CLA	CAD-CBD-CGD-O2D
12	H	2119	CLA	CAD-CBD-CGD-O2D
12	a	801	CLA	CAD-CBD-CGD-O2D
12	a	812	CLA	CAD-CBD-CGD-O2D
12	a	814	CLA	CAD-CBD-CGD-O2D
12	b	2107	CLA	CAD-CBD-CGD-O2D
12	b	2112	CLA	CAD-CBD-CGD-O2D
12	b	2119	CLA	CAD-CBD-CGD-O2D
12	f	201	CLA	CAD-CBD-CGD-O2D
12	A	801	CLA	CAD-CBD-CGD-O2D
12	A	812	CLA	CAD-CBD-CGD-O2D
12	A	814	CLA	CAD-CBD-CGD-O2D
12	B	2108	CLA	CAD-CBD-CGD-O2D
12	B	2113	CLA	CAD-CBD-CGD-O2D
12	B	2120	CLA	CAD-CBD-CGD-O2D
12	F	201	CLA	CAD-CBD-CGD-O2D
17	G	847	LMG	O10-C28-C29-C30
17	a	847	LMG	O10-C28-C29-C30
12	l	201	CLA	C2-C1-O2A-CGA
17	G	849	LMG	O10-C28-C29-C30
12	H	2111	CLA	CAA-CBA-CGA-O2A
12	b	2111	CLA	CAA-CBA-CGA-O2A
12	B	2112	CLA	CAA-CBA-CGA-O2A
24	V	102	SQD	O47-C7-C8-C9
24	m	102	SQD	O47-C7-C8-C9
12	a	822	CLA	CAA-CBA-CGA-O1A
12	A	822	CLA	CAA-CBA-CGA-O1A
17	a	849	LMG	O10-C28-C29-C30
12	H	2111	CLA	C5-C6-C7-C8
12	b	2111	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
12	B	2112	CLA	C5-C6-C7-C8
12	H	2133	CLA	CAA-CBA-CGA-O2A
12	b	2133	CLA	CAA-CBA-CGA-O2A
12	B	2134	CLA	CAA-CBA-CGA-O2A
24	M	101	SQD	O47-C7-C8-C9
12	G	821	CLA	C10-C11-C12-C13
12	G	822	CLA	CAA-CBA-CGA-O1A
17	A	849	LMG	O10-C28-C29-C30
12	a	821	CLA	C10-C11-C12-C13
12	A	821	CLA	C10-C11-C12-C13
12	H	2123	CLA	CAA-CBA-CGA-O2A
12	b	2123	CLA	CAA-CBA-CGA-O2A
12	B	2124	CLA	CAA-CBA-CGA-O2A
16	G	846	LHG	C28-C29-C30-C31
12	G	851	CLA	CAA-CBA-CGA-O1A
12	a	851	CLA	CAA-CBA-CGA-O1A
12	A	851	CLA	CAA-CBA-CGA-O1A
16	a	848	LHG	C13-C14-C15-C16
16	A	848	LHG	C13-C14-C15-C16

There are no ring outliers.

344 monomers are involved in 685 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	a	819	CLA	3	0
12	Q	204	CLA	2	0
12	a	810	CLA	5	0
12	b	2124	CLA	3	0
12	G	805	CLA	4	0
12	b	2110	CLA	1	0
12	A	801	CLA	1	0
12	H	2133	CLA	1	0
12	B	2132	CLA	6	0
15	j	104	BCR	6	0
12	b	2135	CLA	1	0
12	H	2141	CLA	4	0
12	b	2140	CLA	3	0
12	H	2129	CLA	2	0
24	L	208	SQD	4	0
12	G	804	CLA	2	0
12	H	2139	CLA	3	0
24	l	208	SQD	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	H	2124	CLA	3	0
24	m	102	SQD	8	0
12	B	2131	CLA	3	0
12	b	2112	CLA	1	0
12	G	836	CLA	2	0
12	b	2125	CLA	2	0
12	B	2106	CLA	2	0
15	B	2143	BCR	5	0
15	A	843	BCR	2	0
12	G	829	CLA	3	0
12	H	2126	CLA	4	0
12	G	810	CLA	3	0
13	a	840	A1AGD	1	0
12	A	806	CLA	1	0
12	G	851	CLA	4	0
12	G	832	CLA	1	0
12	a	805	CLA	3	0
12	A	808	CLA	1	0
15	i	101	BCR	1	0
15	H	2146	BCR	2	0
12	H	2127	CLA	3	0
12	G	808	CLA	1	0
12	S	102	CLA	1	0
16	B	2149	LHG	4	0
12	a	836	CLA	1	0
12	H	2130	CLA	3	0
12	F	204	CLA	1	0
12	a	812	CLA	6	0
20	B	2144	ECH	7	0
12	a	829	CLA	2	0
12	G	831	CLA	1	0
12	B	2135	CLA	3	0
12	l	201	CLA	2	0
12	H	2106	CLA	2	0
12	H	2152	CLA	1	0
12	A	837	CLA	1	0
25	l	209	DGD	3	0
16	m	103	LHG	2	0
12	b	2115	CLA	1	0
12	b	2106	CLA	2	0
12	A	805	CLA	3	0
15	J	104	BCR	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	U	209	DGD	3	0
12	H	2108	CLA	4	0
12	A	804	CLA	2	0
12	a	802	CLA	2	0
12	A	829	CLA	3	0
23	B	2152	ZEX	2	0
12	B	2120	CLA	4	0
12	b	2136	CLA	2	0
12	b	2132	CLA	2	0
12	H	2114	CLA	2	0
12	H	2134	CLA	3	0
12	J	102	CLA	1	0
15	A	842	BCR	1	0
16	G	846	LHG	2	0
12	A	819	CLA	3	0
12	Q	201	CLA	3	0
17	A	849	LMG	1	0
12	B	2142	CLA	4	0
12	B	2133	CLA	2	0
15	j	101	BCR	4	0
12	G	816	CLA	1	0
12	A	831	CLA	1	0
12	B	2121	CLA	3	0
12	b	2123	CLA	1	0
12	B	2114	CLA	1	0
12	A	824	CLA	2	0
12	H	2137	CLA	3	0
12	b	2127	CLA	3	0
12	G	833	CLA	4	0
16	a	846	LHG	2	0
12	H	2118	CLA	3	0
12	B	2116	CLA	1	0
12	L	201	CLA	2	0
12	l	204	CLA	1	0
12	B	2138	CLA	3	0
15	G	843	BCR	3	0
12	a	818	CLA	5	0
12	A	816	CLA	2	0
20	m	101	ECH	1	0
15	S	101	BCR	3	0
12	H	2104	CLA	3	0
12	b	2120	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	H	2131	CLA	5	0
15	I	207	BCR	4	0
12	B	2140	CLA	3	0
12	b	2134	CLA	3	0
12	G	801	CLA	1	0
15	U	206	BCR	2	0
12	H	2109	CLA	1	0
12	H	2138	CLA	5	0
15	b	2145	BCR	3	0
15	F	202	BCR	2	0
12	H	2102	CLA	1	0
12	B	2137	CLA	2	0
23	F	205	ZEX	2	0
17	a	847	LMG	5	0
16	A	848	LHG	6	0
17	G	847	LMG	5	0
12	G	854	CLA	3	0
12	F	203	CLA	1	0
12	b	2128	CLA	6	0
12	A	821	CLA	1	0
12	A	803	CLA	3	0
12	a	834	CLA	2	0
15	G	845	BCR	4	0
12	G	837	CLA	1	0
15	T	4001	BCR	2	0
12	H	2116	CLA	2	0
12	B	2102	CLA	2	0
15	H	2145	BCR	4	0
12	A	836	CLA	1	0
12	B	2129	CLA	7	0
13	H	2153	A1AGD	2	0
12	B	2105	CLA	3	0
12	b	2141	CLA	4	0
12	a	801	CLA	1	0
12	H	2140	CLA	2	0
12	b	2107	CLA	3	0
12	B	2108	CLA	3	0
12	B	2126	CLA	1	0
12	G	817	CLA	4	0
12	G	835	CLA	3	0
15	K	4001	BCR	2	0
12	G	825	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	2134	CLA	2	0
12	A	832	CLA	1	0
12	G	812	CLA	5	0
12	A	839	CLA	4	0
23	f	205	ZEX	2	0
15	R	101	BCR	2	0
15	k	4001	BCR	2	0
12	a	803	CLA	4	0
17	A	847	LMG	5	0
15	B	2147	BCR	2	0
12	B	2136	CLA	2	0
12	B	2141	CLA	2	0
23	b	2151	ZEX	2	0
16	b	2148	LHG	4	0
15	f	202	BCR	2	0
15	a	842	BCR	2	0
12	H	2105	CLA	2	0
12	a	839	CLA	3	0
24	U	208	SQD	4	0
12	G	826	CLA	3	0
16	M	102	LHG	2	0
12	b	2108	CLA	4	0
12	B	2111	CLA	1	0
16	V	103	LHG	3	0
12	G	820	CLA	5	0
12	B	2107	CLA	2	0
12	H	2115	CLA	1	0
12	B	2123	CLA	1	0
12	B	2113	CLA	1	0
12	A	812	CLA	6	0
13	B	2153	A1AGD	2	0
12	A	811	CLA	3	0
12	G	834	CLA	2	0
12	G	828	CLA	2	0
12	A	807	CLA	8	0
12	B	2139	CLA	5	0
12	H	2136	CLA	2	0
16	a	848	LHG	6	0
15	I	101	BCR	2	0
15	b	2144	BCR	1	0
12	G	830	CLA	3	0
12	B	2124	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	U	204	CLA	1	0
15	G	842	BCR	1	0
24	V	102	SQD	8	0
18	a	852	45D	1	0
12	B	2119	CLA	2	0
12	A	818	CLA	5	0
12	a	820	CLA	4	0
15	a	845	BCR	3	0
16	A	846	LHG	2	0
12	G	807	CLA	8	0
25	L	209	DGD	3	0
12	G	818	CLA	3	0
12	b	2111	CLA	2	0
12	a	808	CLA	1	0
12	l	203	CLA	3	0
12	H	2107	CLA	3	0
15	B	2146	BCR	3	0
12	a	828	CLA	2	0
12	G	823	CLA	5	0
12	H	2123	CLA	2	0
12	A	828	CLA	2	0
12	b	2119	CLA	5	0
12	B	2112	CLA	2	0
20	M	103	ECH	1	0
12	b	2113	CLA	1	0
12	B	2125	CLA	3	0
12	b	2137	CLA	3	0
12	f	204	CLA	1	0
12	a	830	CLA	3	0
12	L	205	CLA	5	0
12	b	2129	CLA	2	0
12	a	826	CLA	3	0
12	a	854	CLA	3	0
12	U	205	CLA	6	0
18	A	852	45D	1	0
12	b	2139	CLA	4	0
15	H	2142	BCR	4	0
12	b	2105	CLA	2	0
12	b	2101	CLA	2	0
12	H	2119	CLA	4	0
12	G	839	CLA	4	0
12	a	824	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	a	821	CLA	2	0
12	a	811	CLA	4	0
12	G	824	CLA	2	0
12	A	825	CLA	3	0
12	H	2120	CLA	3	0
15	A	844	BCR	2	0
12	a	817	CLA	4	0
12	a	807	CLA	7	0
12	B	2127	CLA	4	0
15	G	844	BCR	3	0
12	H	2113	CLA	1	0
17	G	849	LMG	2	0
12	G	806	CLA	1	0
12	b	2126	CLA	4	0
23	H	2151	ZEX	3	0
12	A	834	CLA	2	0
12	a	825	CLA	3	0
13	b	2153	A1AGD	2	0
15	b	2146	BCR	1	0
12	H	2112	CLA	2	0
16	G	848	LHG	6	0
20	V	101	ECH	2	0
12	b	2117	CLA	2	0
12	A	851	CLA	3	0
12	G	811	CLA	4	0
12	G	819	CLA	3	0
12	G	803	CLA	4	0
12	L	203	CLA	4	0
12	A	810	CLA	2	0
12	B	2103	CLA	1	0
15	S	104	BCR	6	0
12	U	201	CLA	2	0
12	b	2133	CLA	1	0
12	a	833	CLA	4	0
15	H	2144	BCR	1	0
12	b	2102	CLA	1	0
12	H	2125	CLA	2	0
15	b	2142	BCR	3	0
12	f	203	CLA	1	0
12	A	838	CLA	2	0
12	H	2117	CLA	2	0
12	B	2110	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	G	802	CLA	2	0
20	H	2143	ECH	6	0
12	B	2128	CLA	3	0
12	b	2114	CLA	2	0
15	Q	202	BCR	2	0
15	a	843	BCR	3	0
12	B	2101	CLA	1	0
12	B	2115	CLA	2	0
12	a	823	CLA	4	0
12	a	806	CLA	1	0
12	U	203	CLA	3	0
12	b	2116	CLA	2	0
12	H	2135	CLA	2	0
12	G	838	CLA	1	0
15	L	206	BCR	2	0
15	U	207	BCR	3	0
12	L	204	CLA	1	0
12	A	833	CLA	4	0
12	A	802	CLA	2	0
12	A	830	CLA	3	0
12	B	2117	CLA	1	0
12	a	837	CLA	2	0
26	L	210	LMT	3	0
12	B	2118	CLA	2	0
12	H	2122	CLA	1	0
12	b	2131	CLA	5	0
15	l	206	BCR	3	0
12	H	2128	CLA	7	0
12	a	816	CLA	1	0
18	G	852	45D	1	0
12	Q	203	CLA	1	0
12	H	2101	CLA	2	0
15	A	845	BCR	3	0
15	J	101	BCR	3	0
12	B	2109	CLA	3	0
24	M	101	SQD	9	0
12	a	804	CLA	4	0
12	f	201	CLA	3	0
12	H	2132	CLA	2	0
12	G	827	CLA	2	0
16	H	2148	LHG	4	0
12	l	205	CLA	6	0

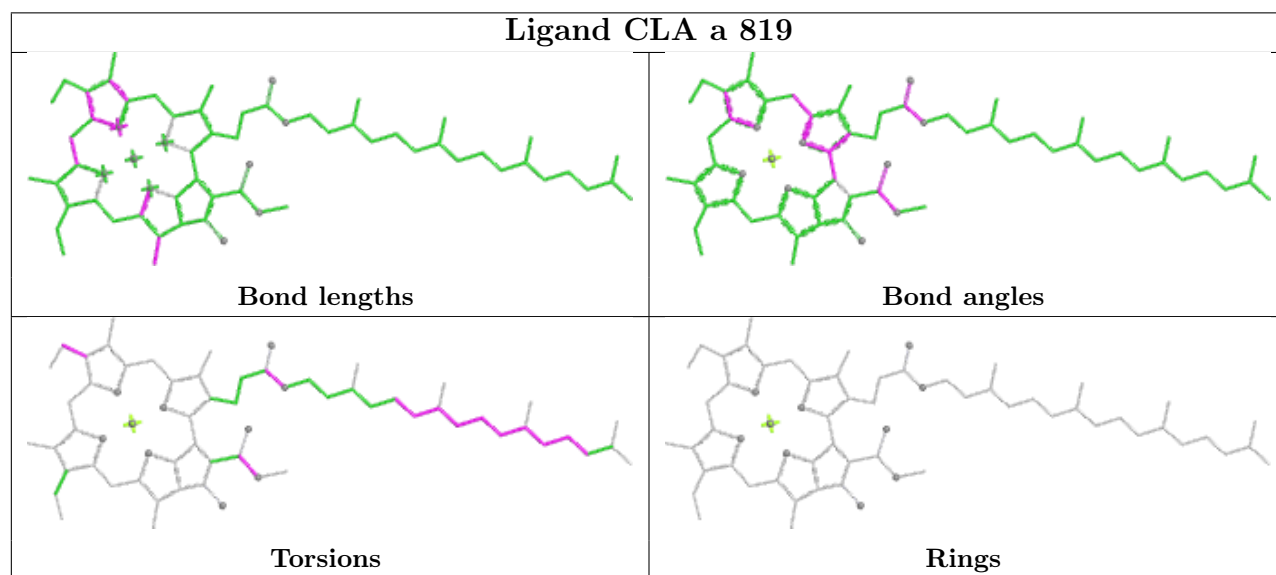
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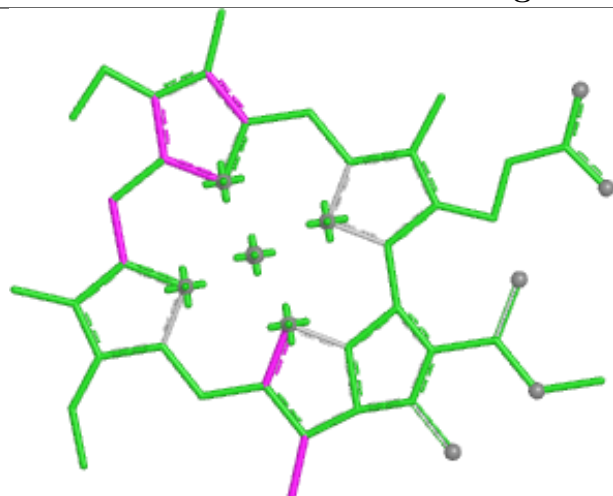
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	a	838	CLA	2	0
12	A	820	CLA	5	0
12	b	2118	CLA	3	0
12	B	2130	CLA	1	0
20	b	2143	ECH	7	0
12	b	2130	CLA	3	0
26	l	210	LMT	3	0
17	a	849	LMG	1	0
12	A	826	CLA	3	0
12	A	854	CLA	3	0
12	F	201	CLA	3	0
23	Q	205	ZEX	2	0
12	b	2104	CLA	3	0
15	a	844	BCR	3	0
12	a	851	CLA	3	0
12	G	821	CLA	2	0
12	b	2122	CLA	1	0
12	H	2111	CLA	2	0
12	a	835	CLA	3	0
15	L	207	BCR	5	0
12	b	2152	CLA	1	0
12	a	827	CLA	3	0
13	A	840	A1AGD	1	0
12	A	823	CLA	5	0
12	A	817	CLA	4	0
13	G	840	A1AGD	1	0
12	j	102	CLA	1	0
12	b	2109	CLA	1	0
12	b	2138	CLA	5	0
12	A	835	CLA	3	0
12	A	827	CLA	3	0
26	U	210	LMT	3	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.

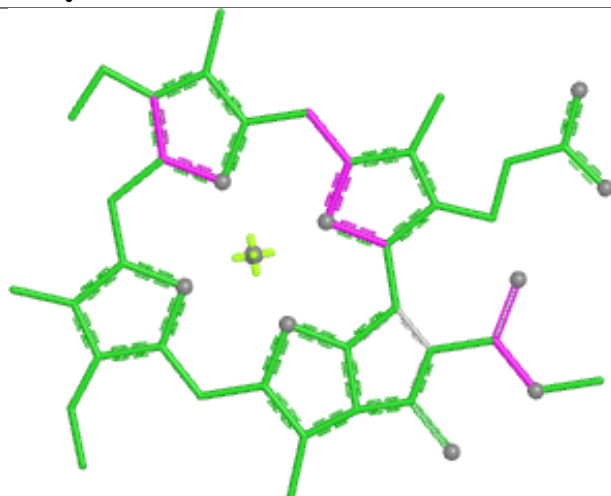
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



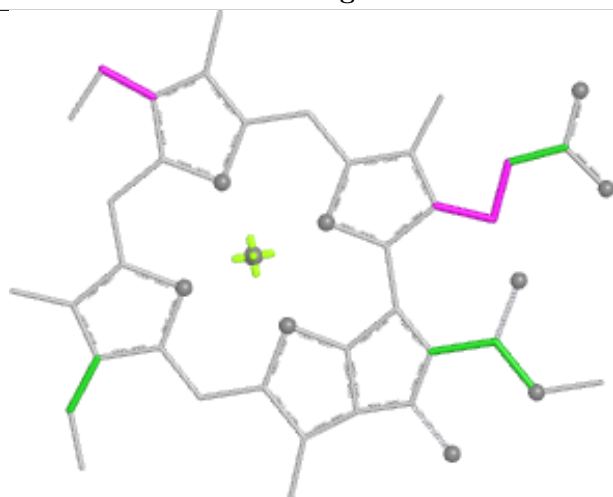
Ligand CLA Q 204



Bond lengths



Bond angles

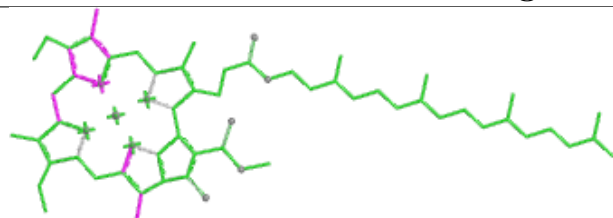


Torsions

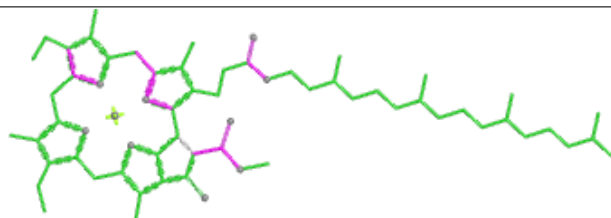


Rings

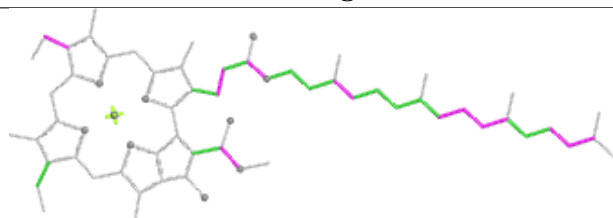
Ligand CLA a 810



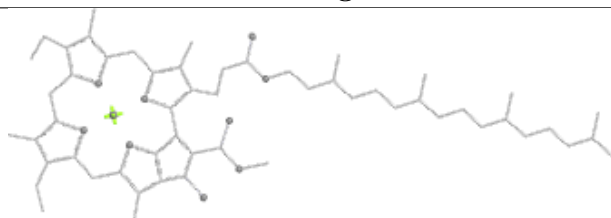
Bond lengths



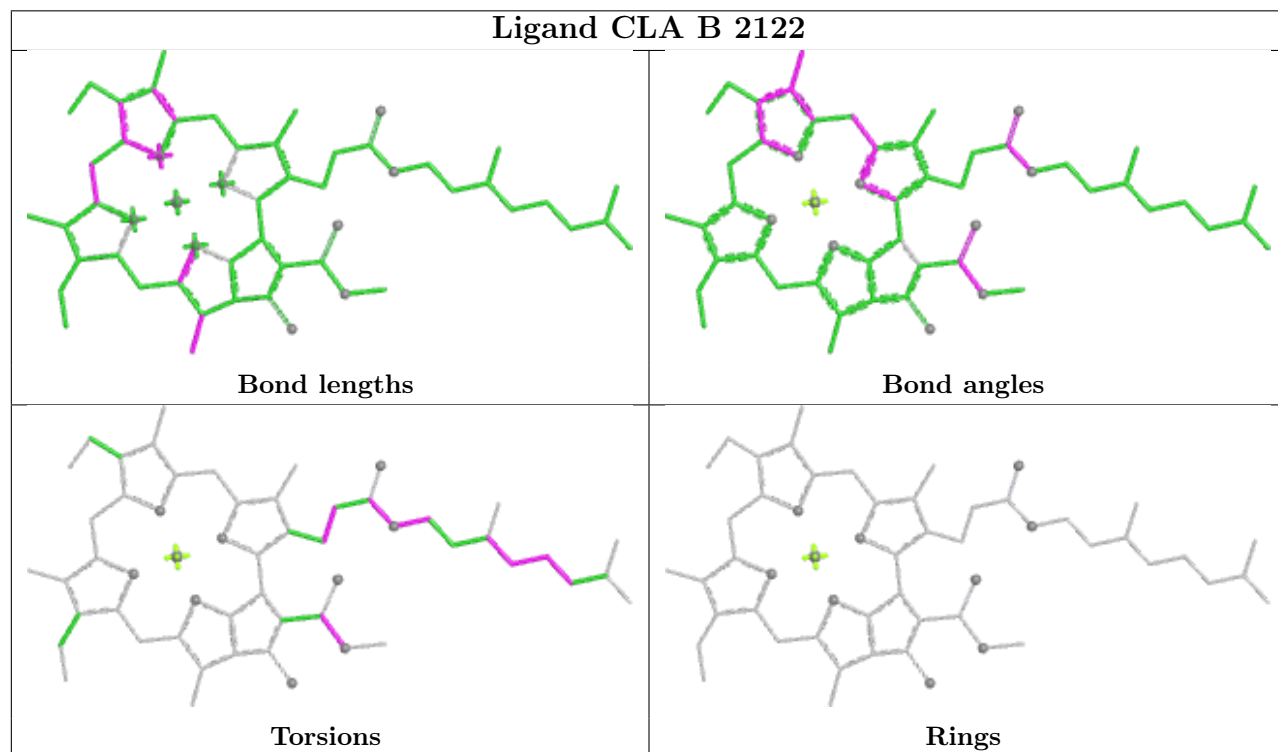
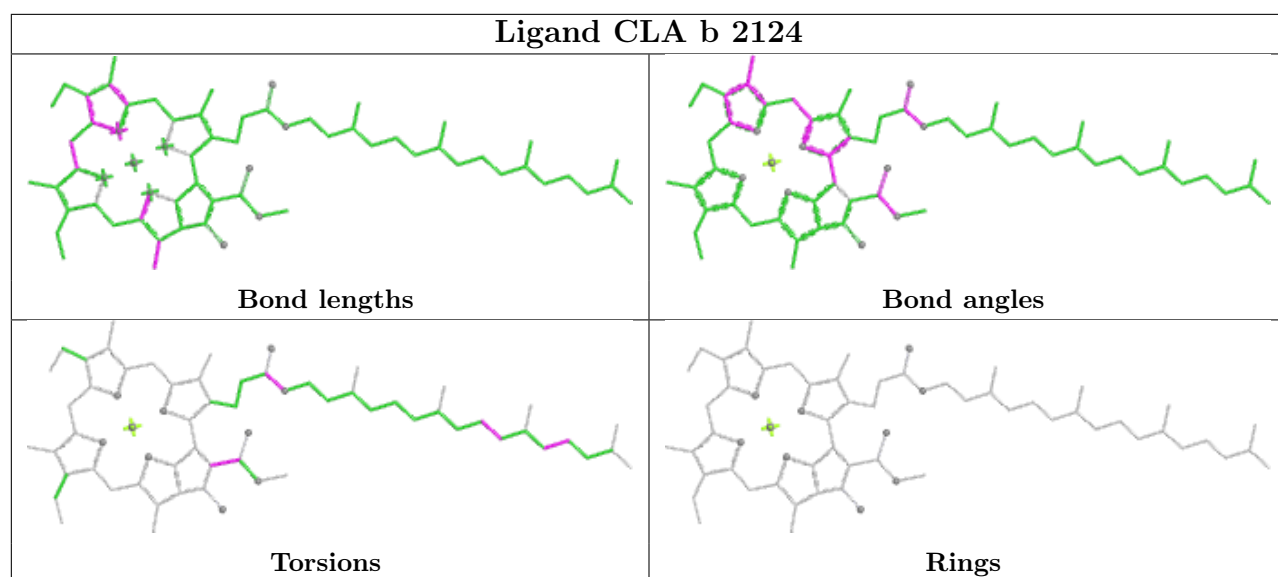
Bond angles

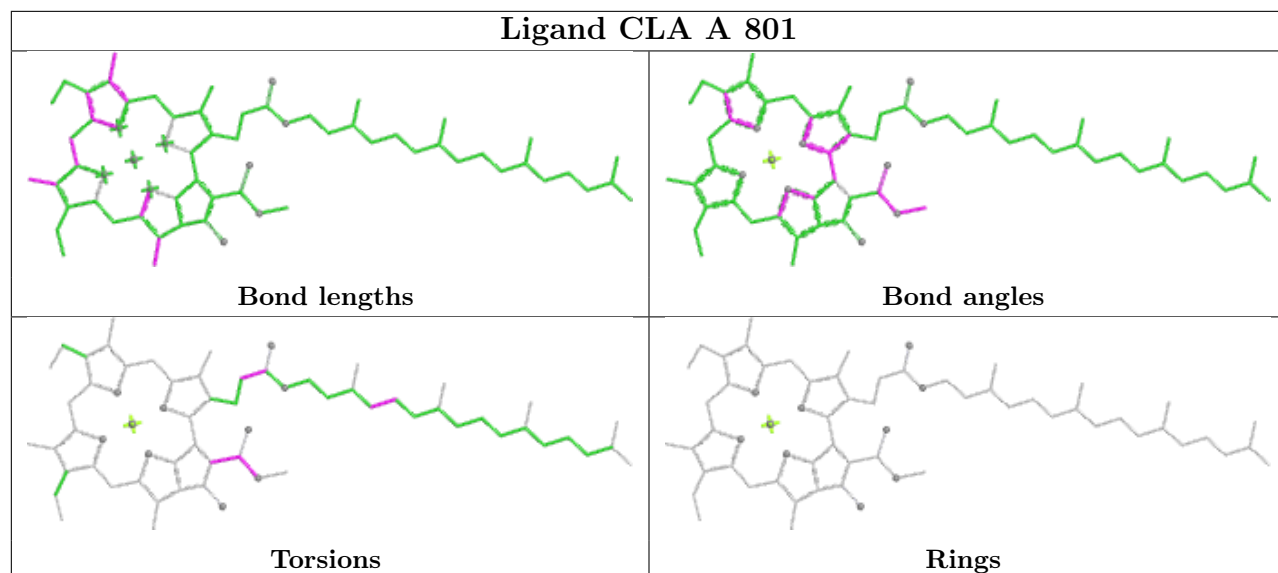
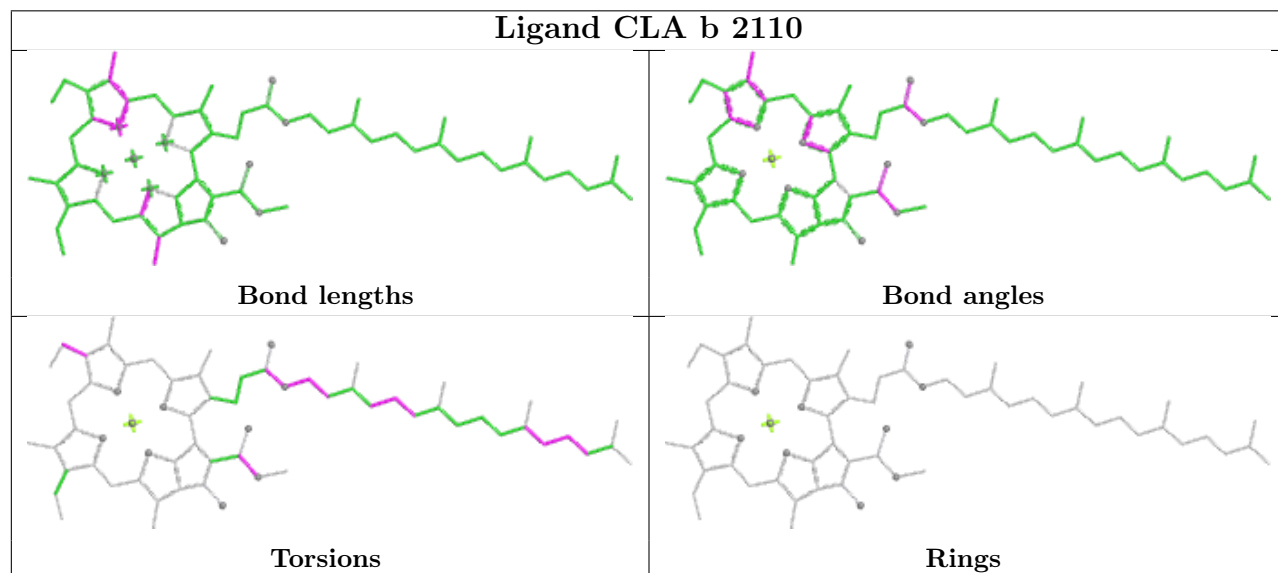
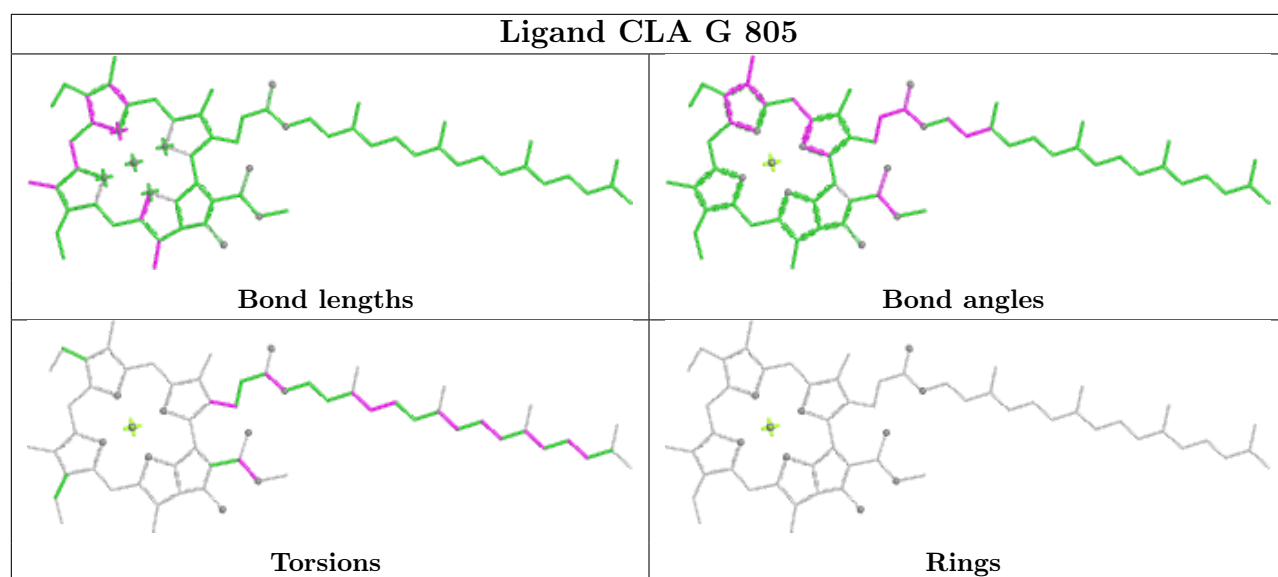


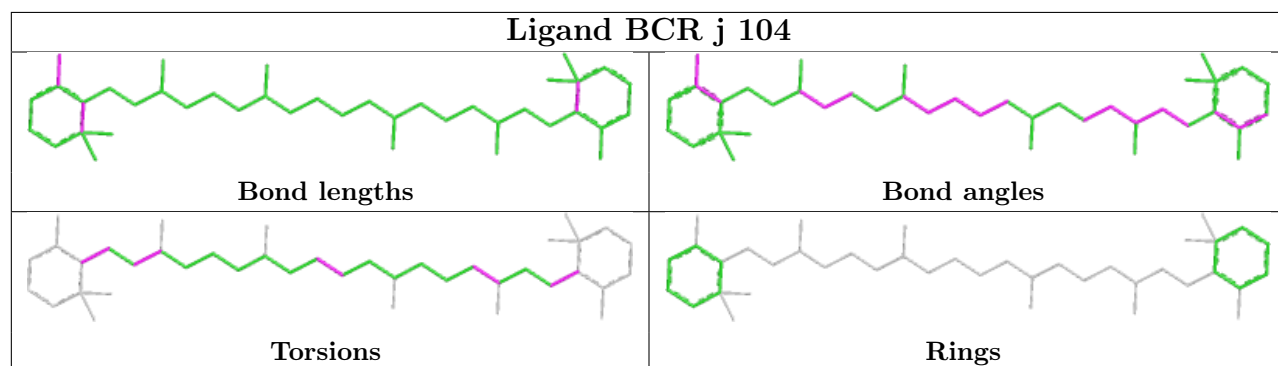
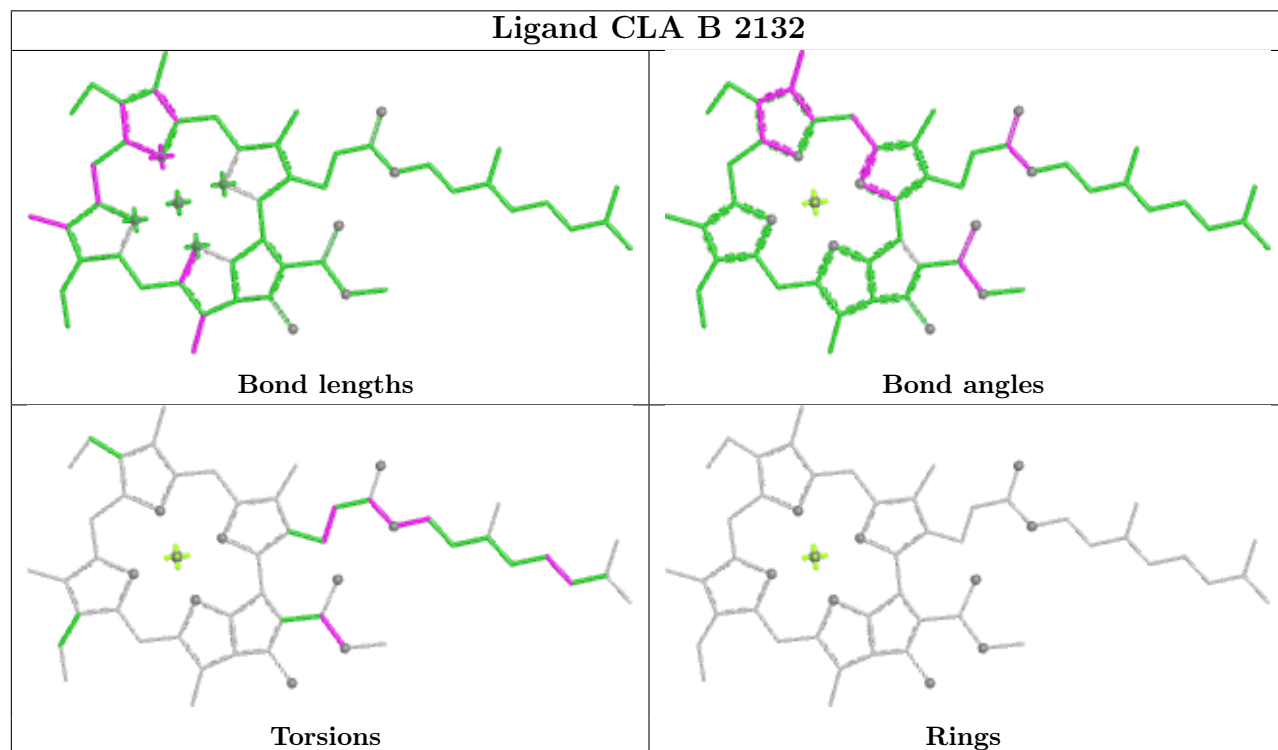
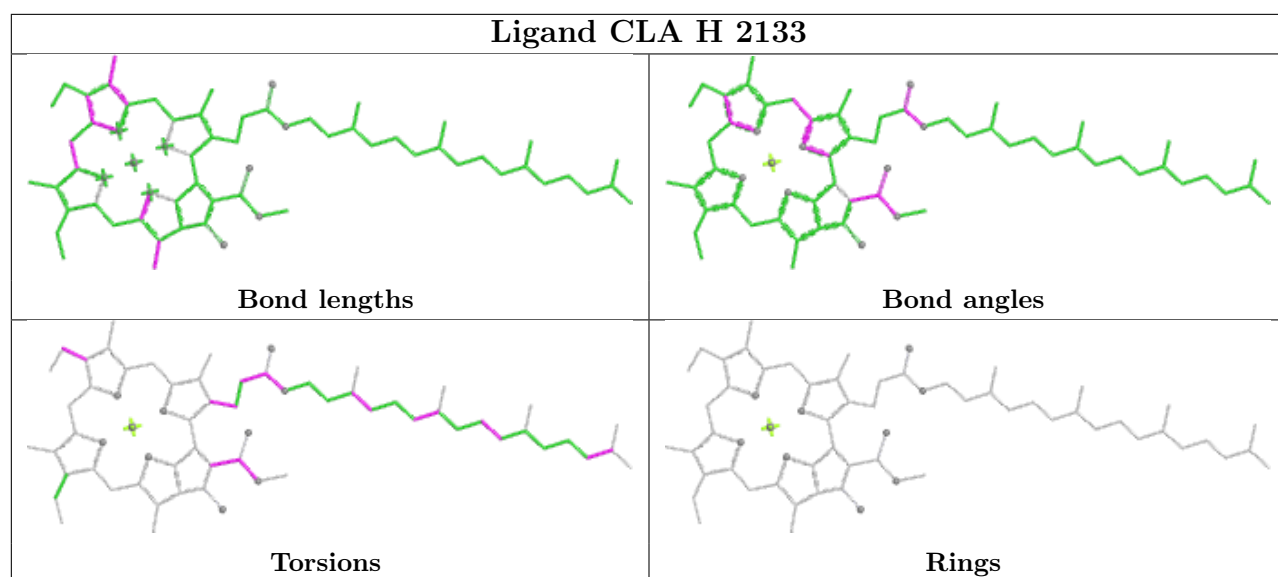
Torsions

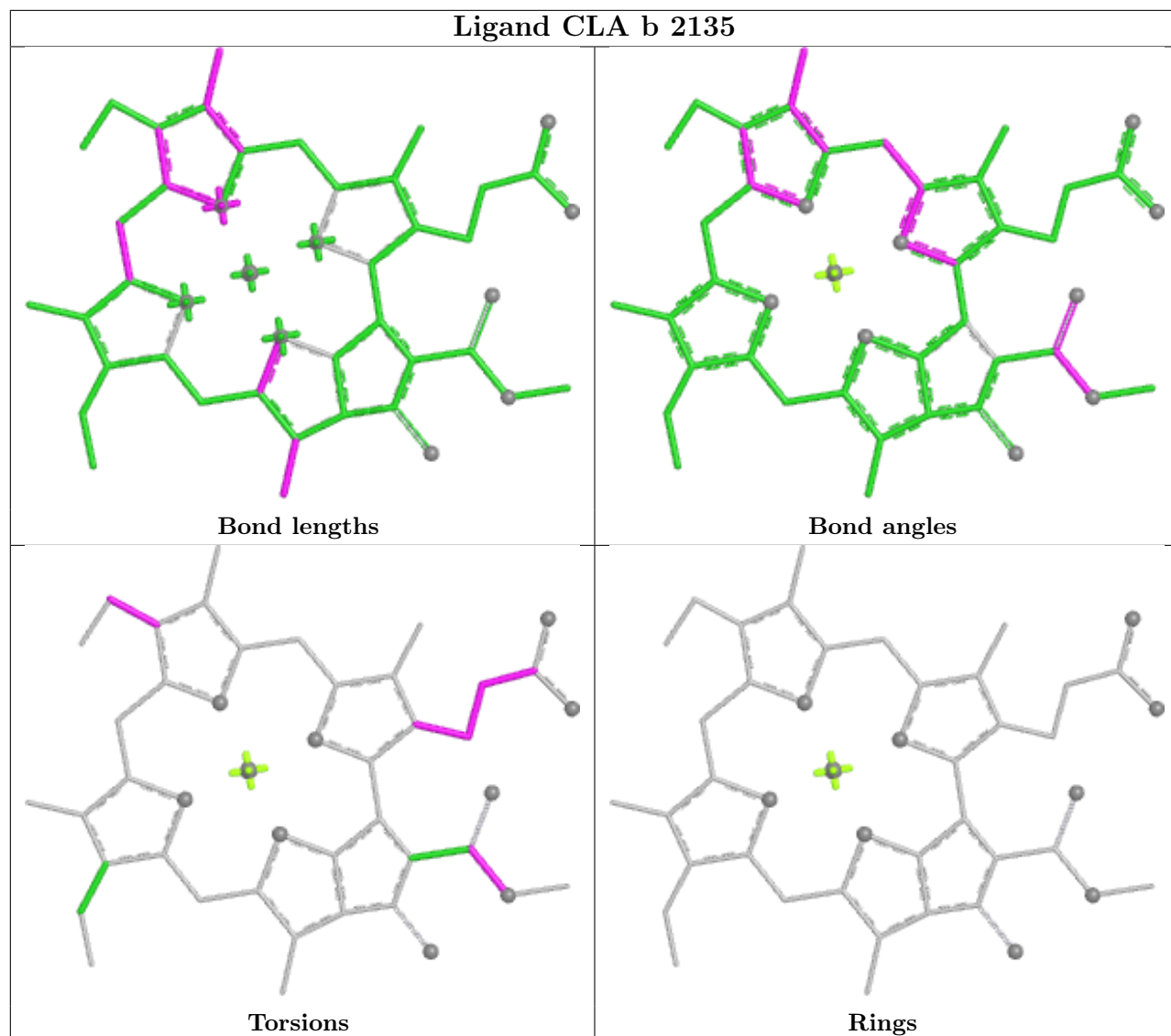


Rings

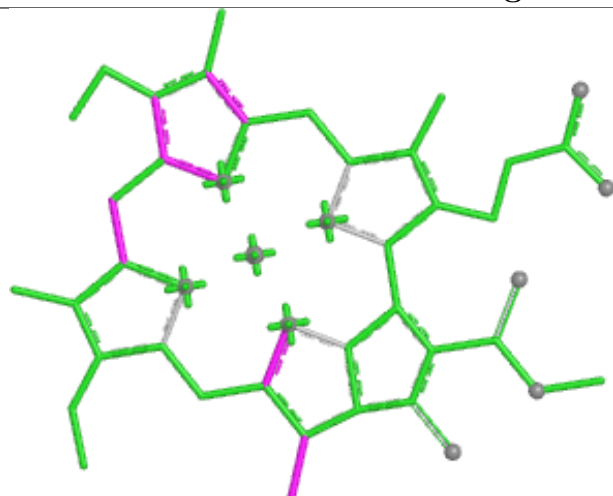




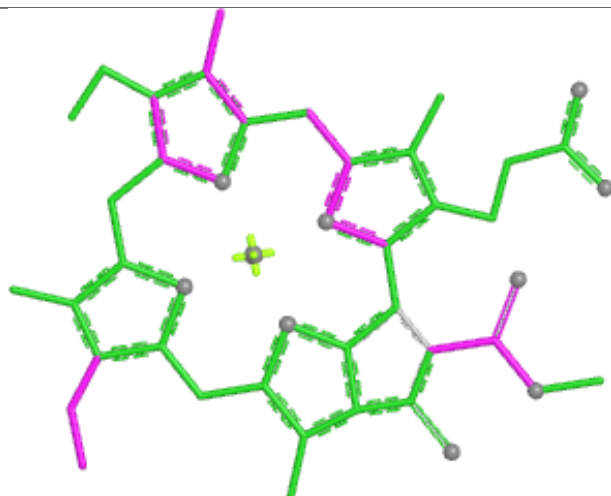




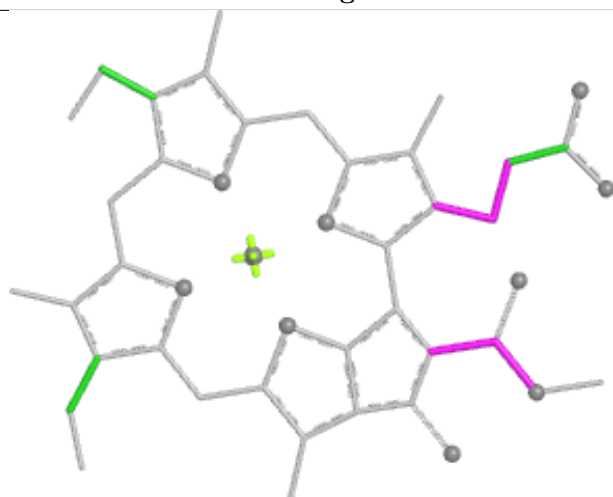
Ligand CLA H 2141



Bond lengths



Bond angles

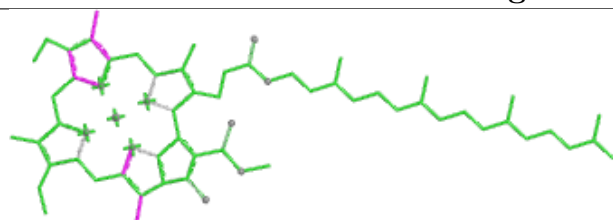


Torsions

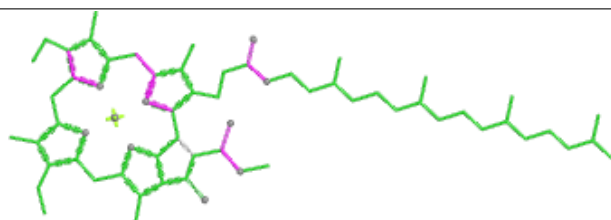


Rings

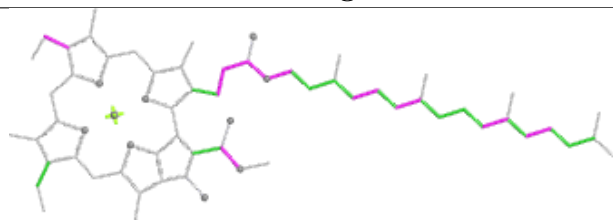
Ligand CLA b 2140



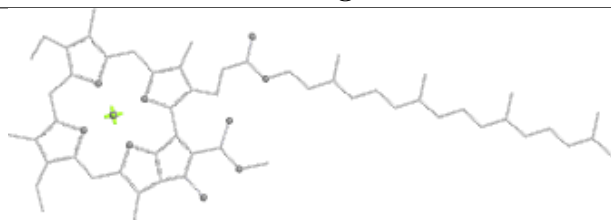
Bond lengths



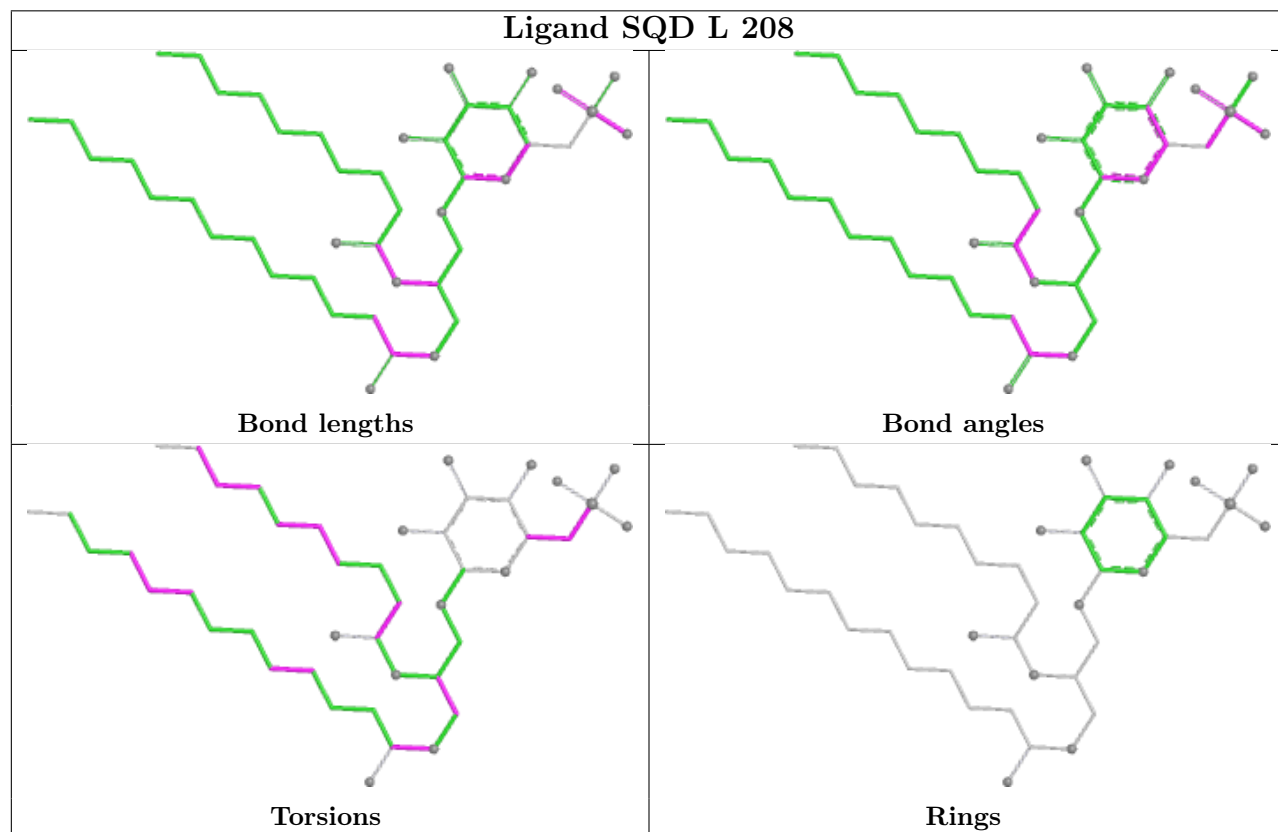
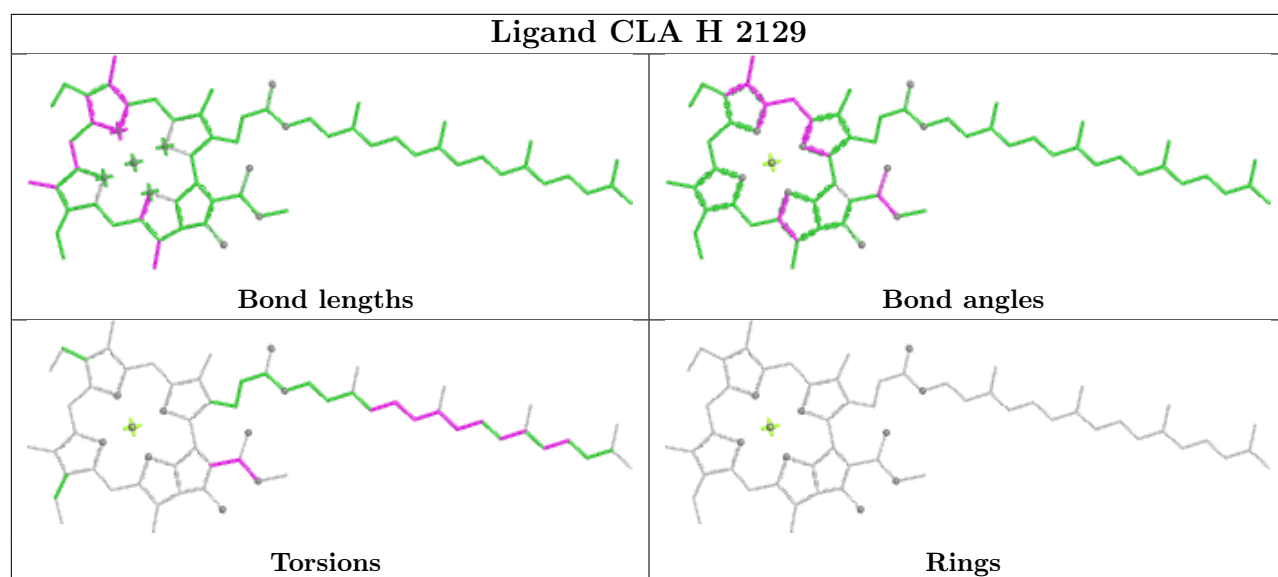
Bond angles

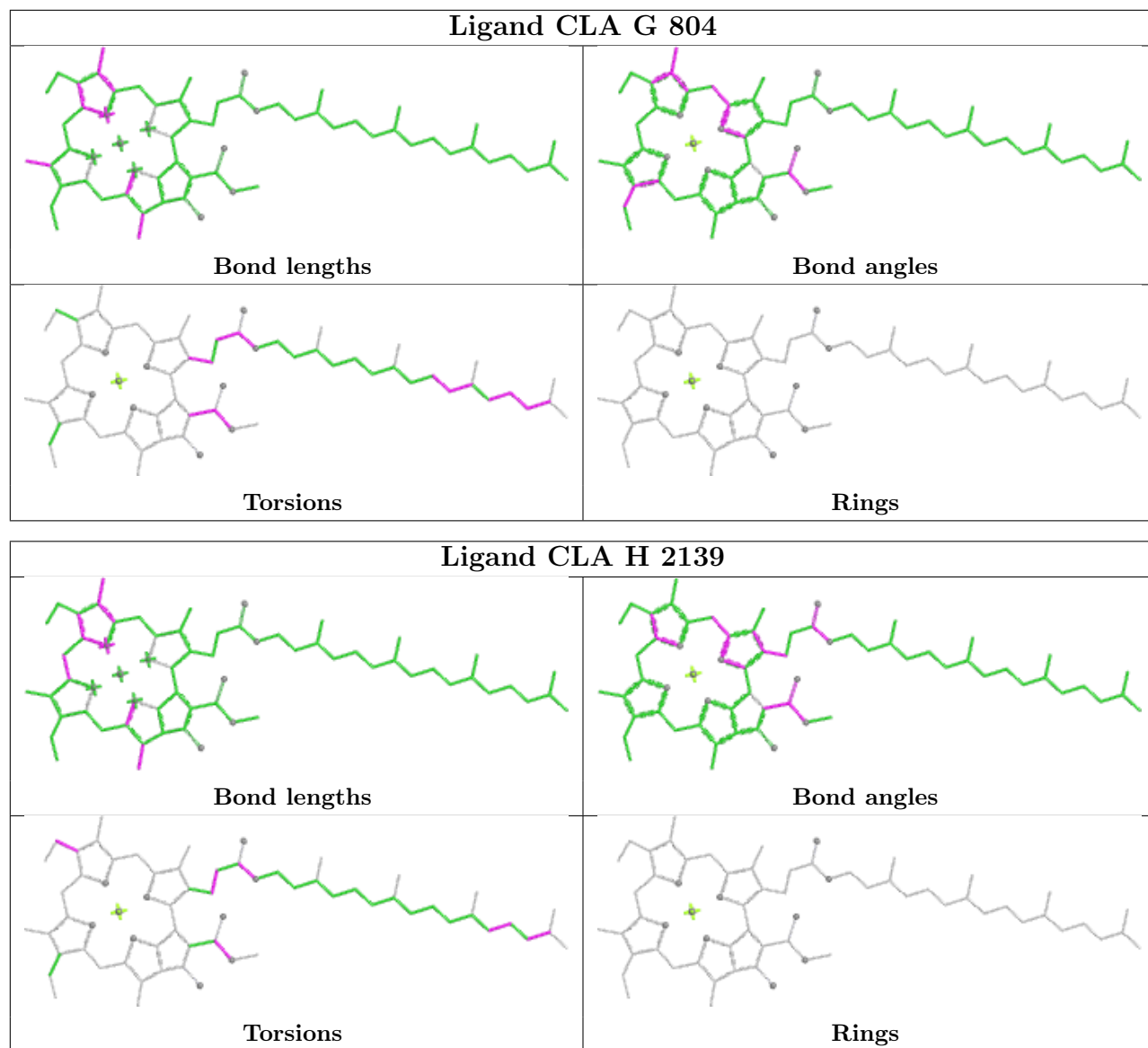


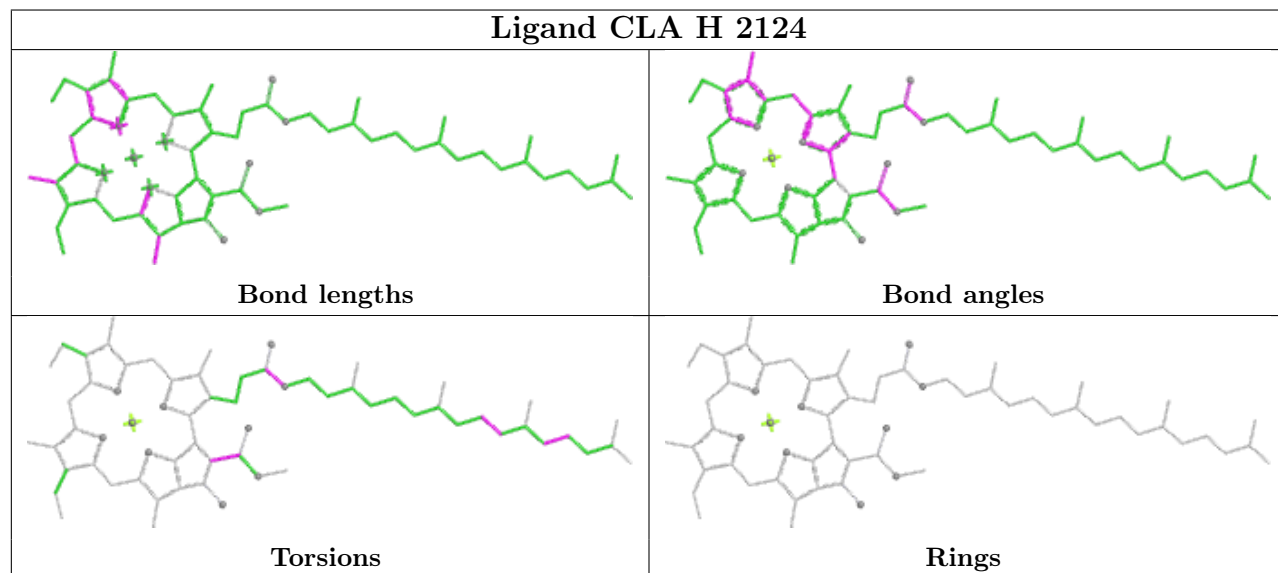
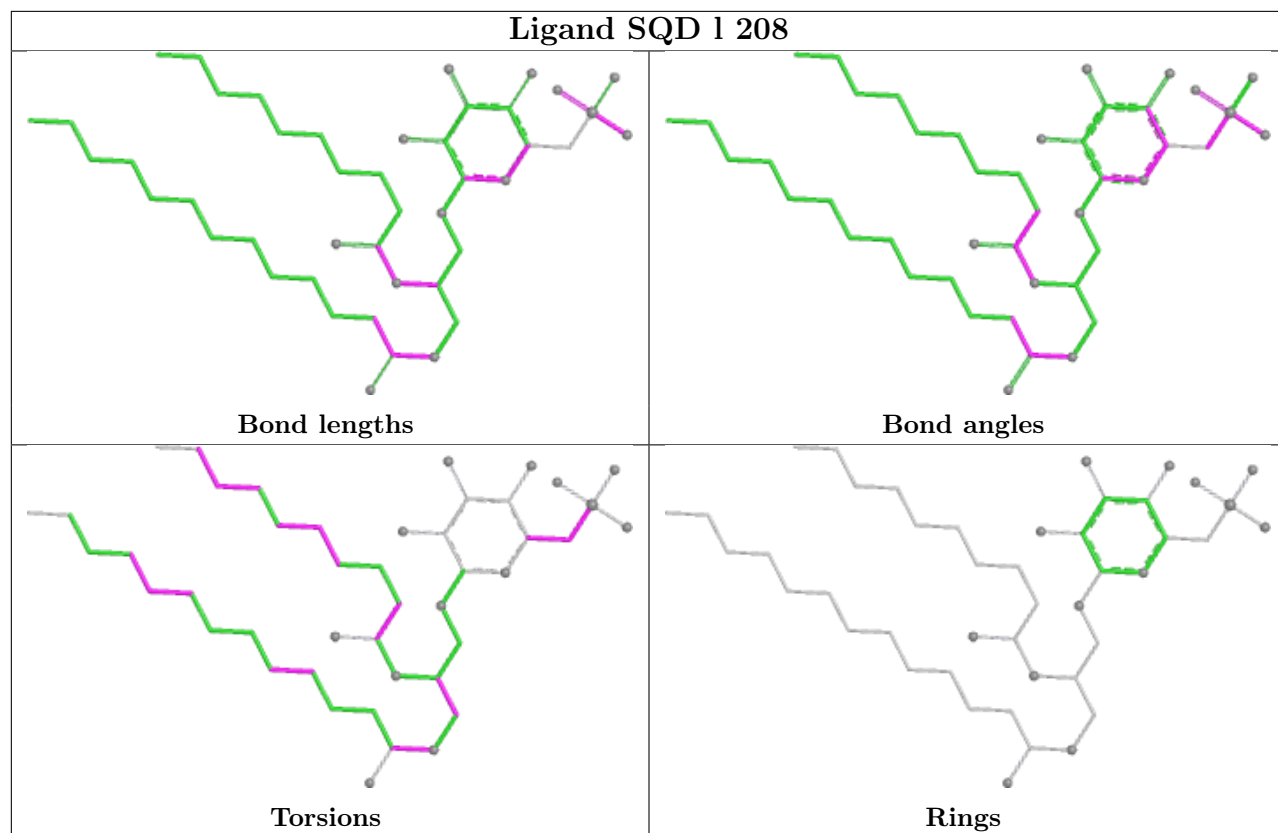
Torsions

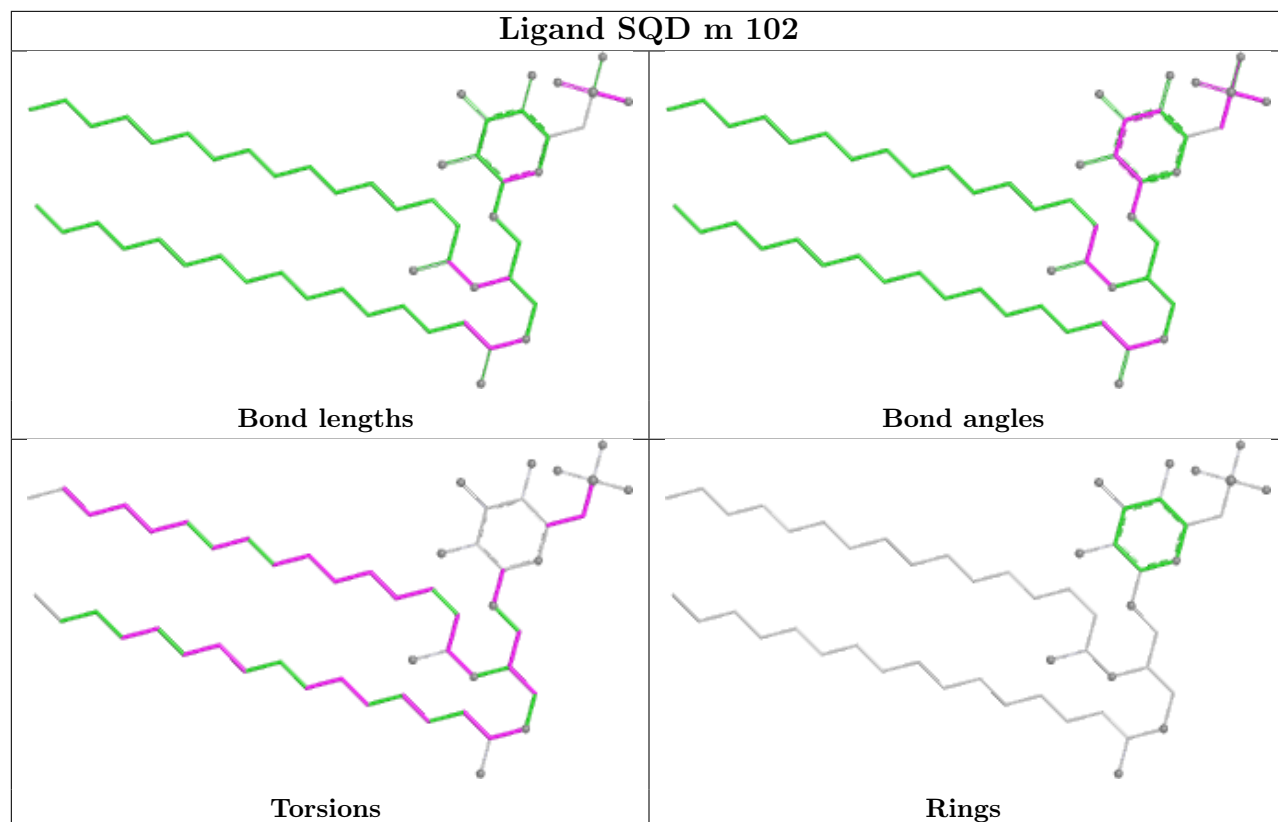


Rings

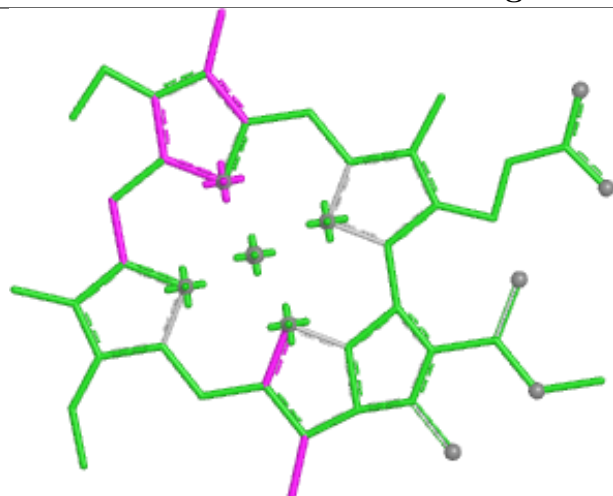




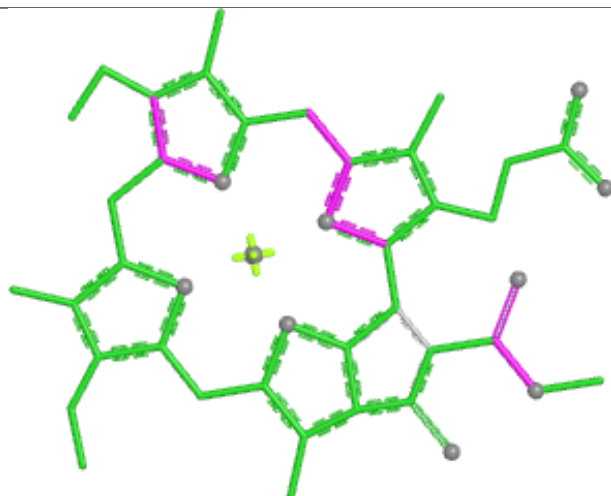




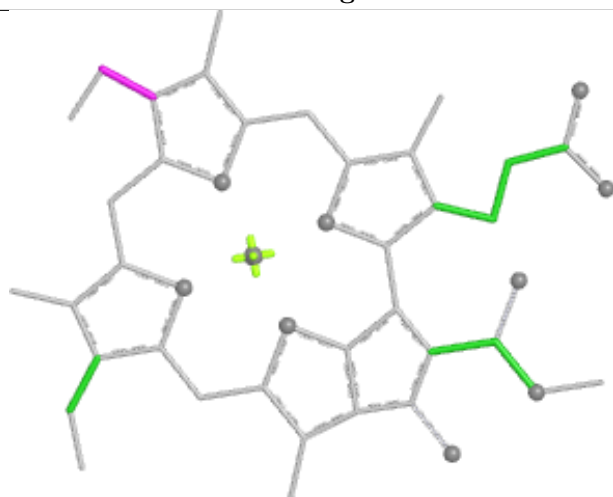
Ligand CLA B 2131



Bond lengths



Bond angles

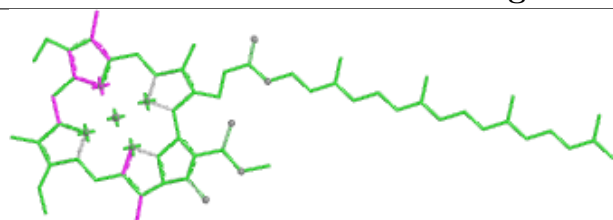


Torsions

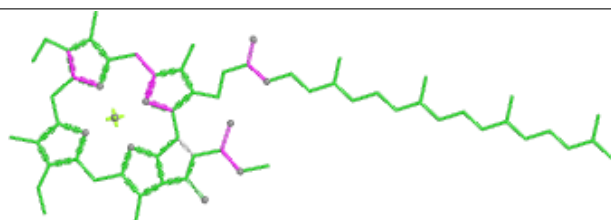


Rings

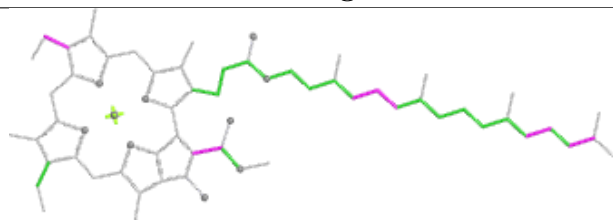
Ligand CLA b 2112



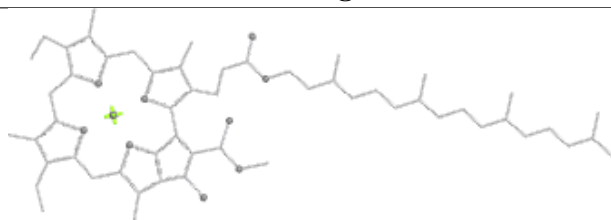
Bond lengths



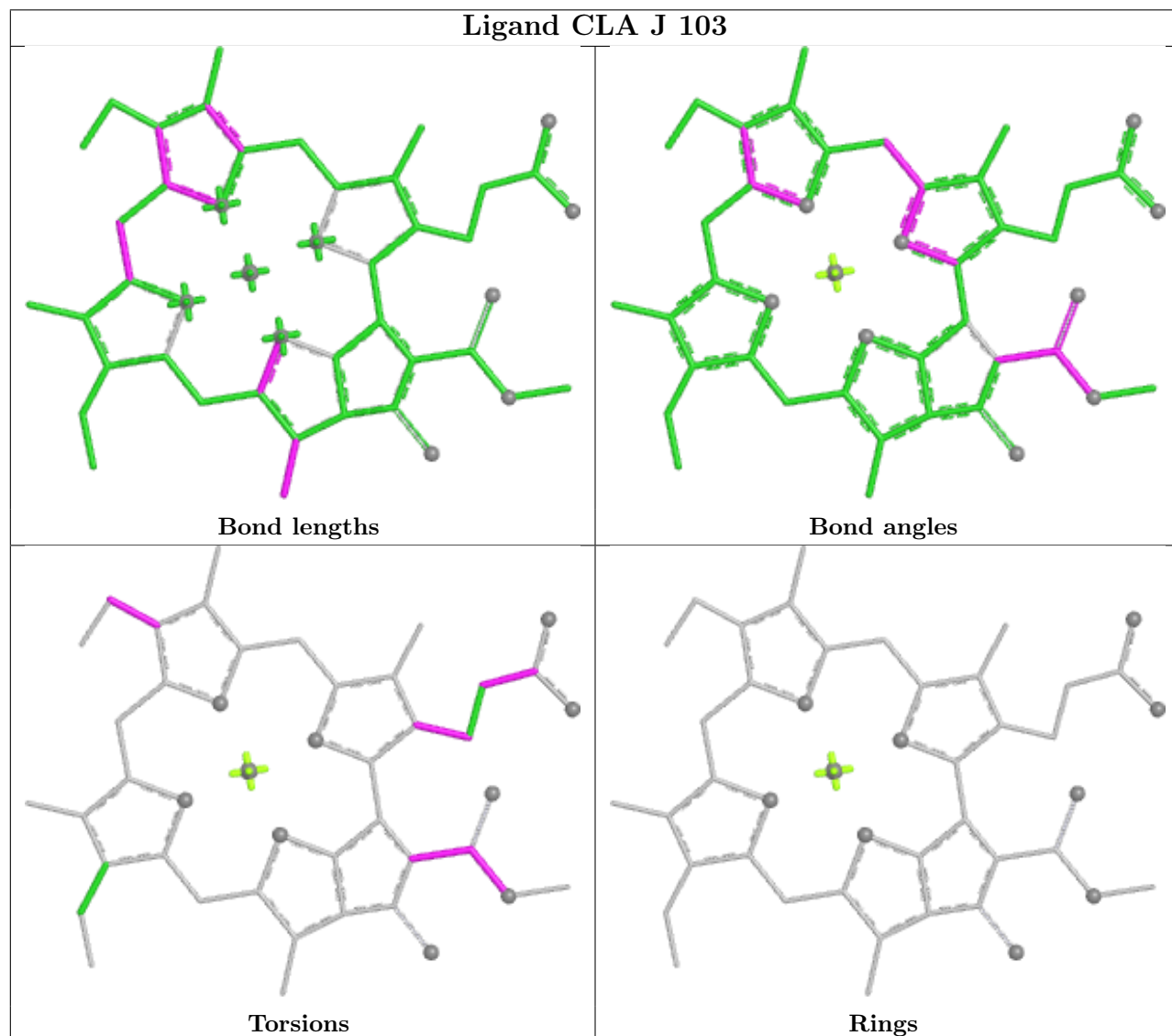
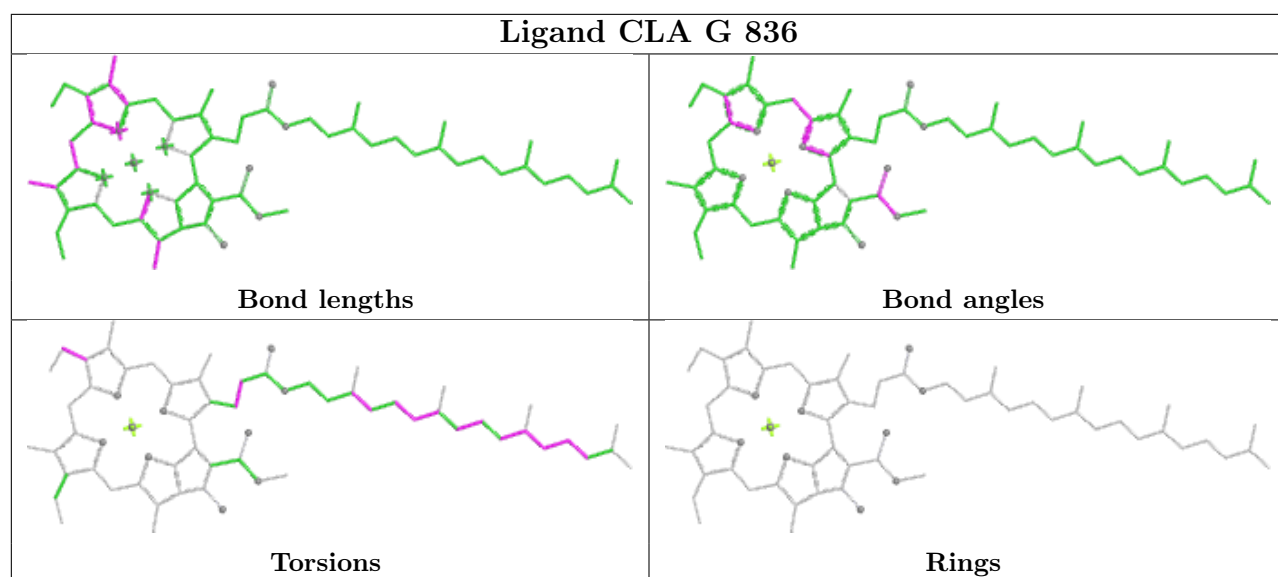
Bond angles

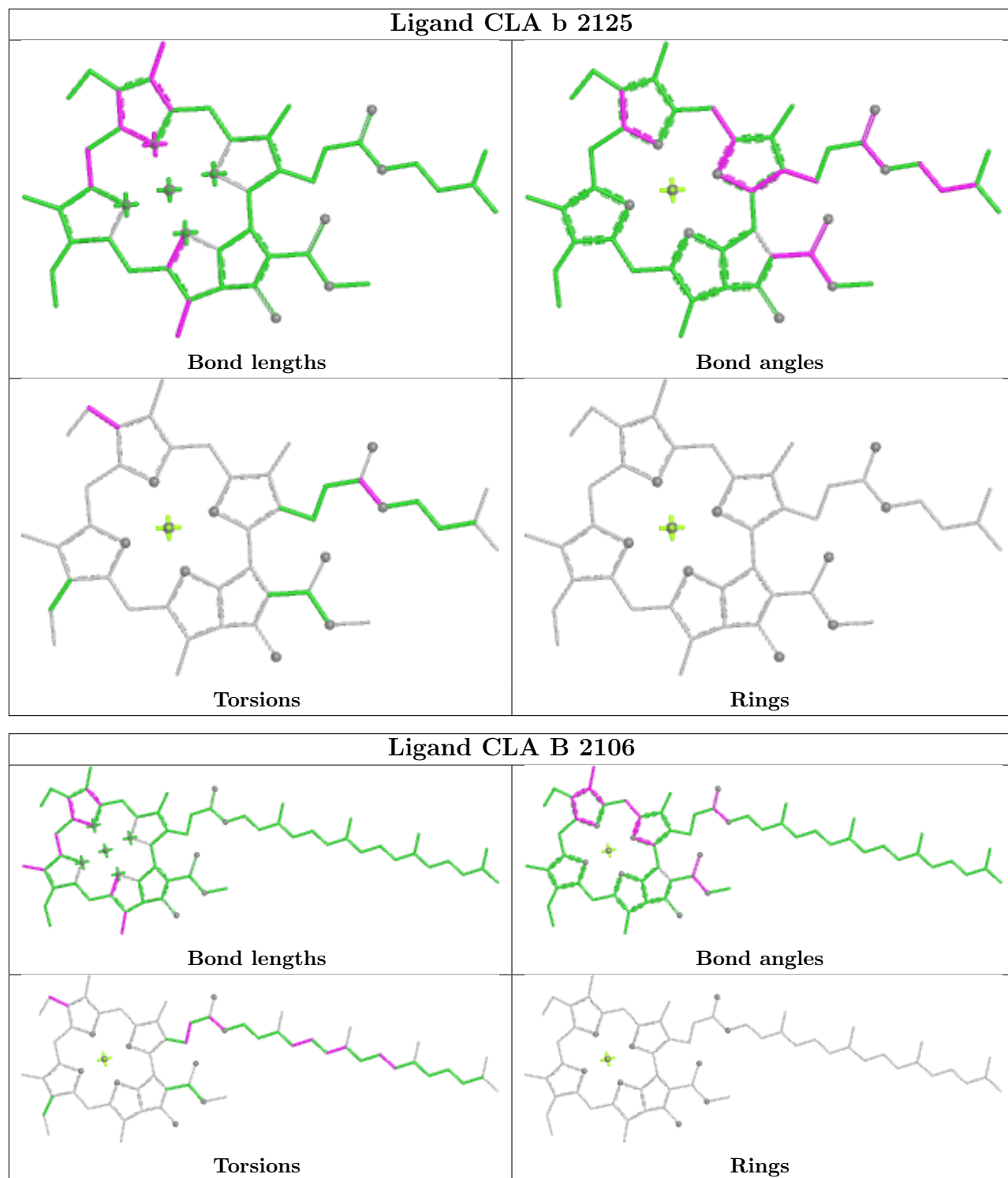


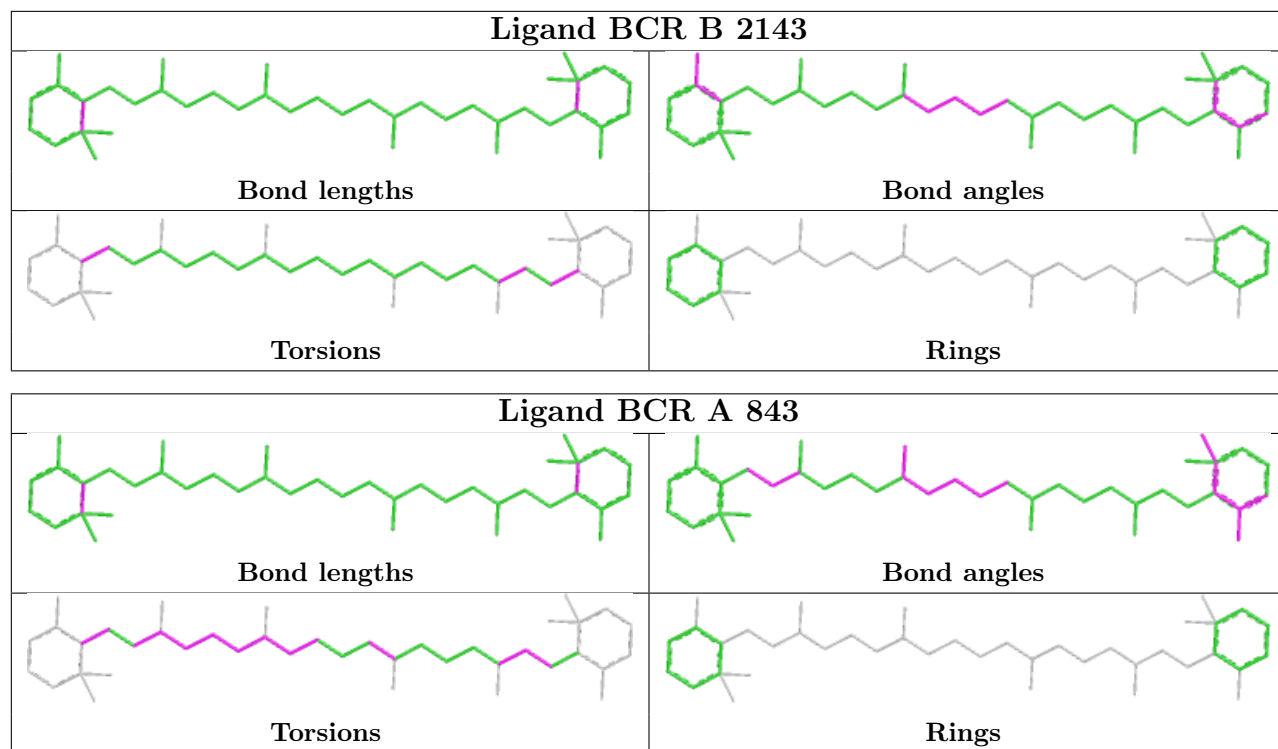
Torsions

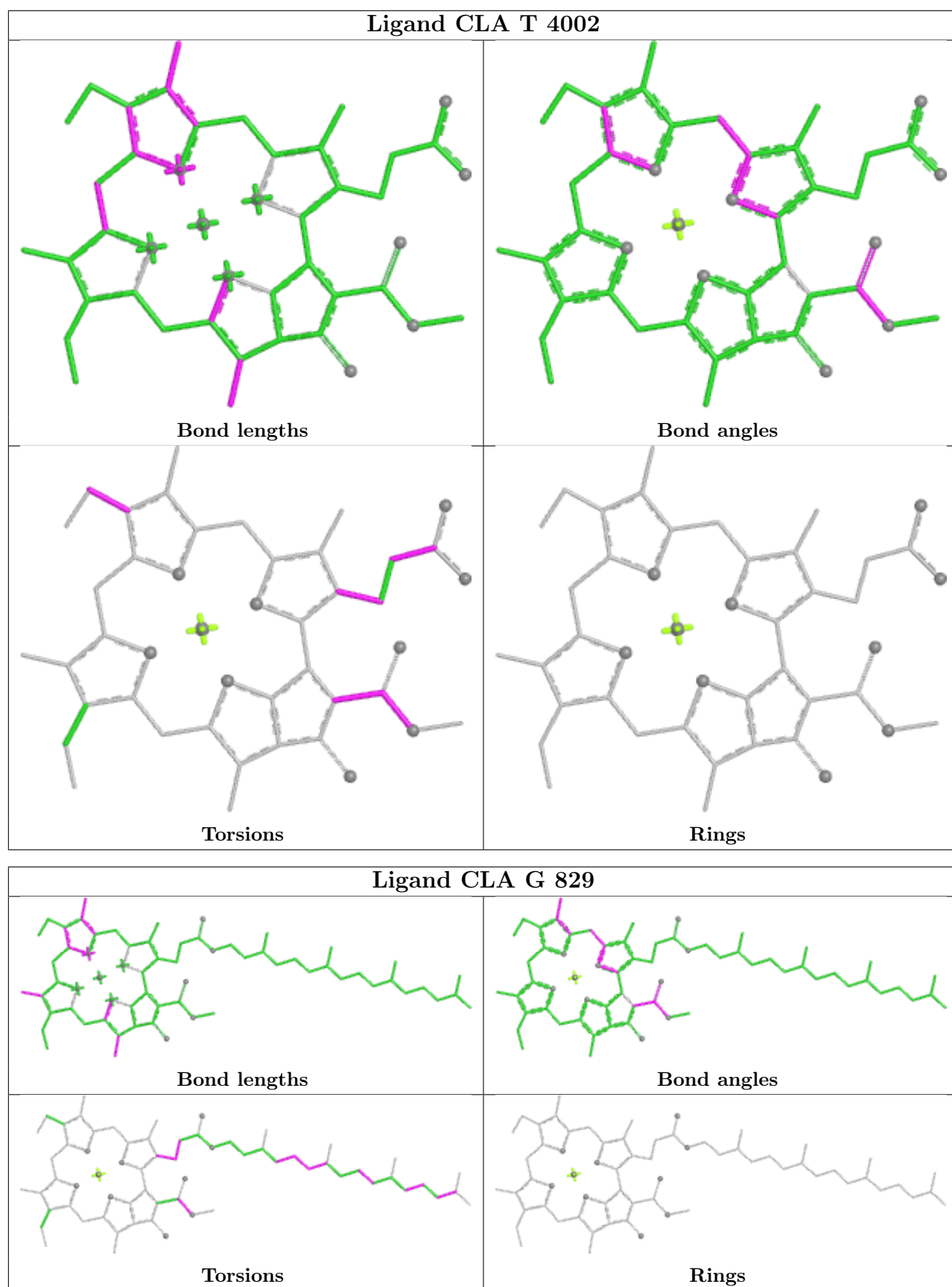


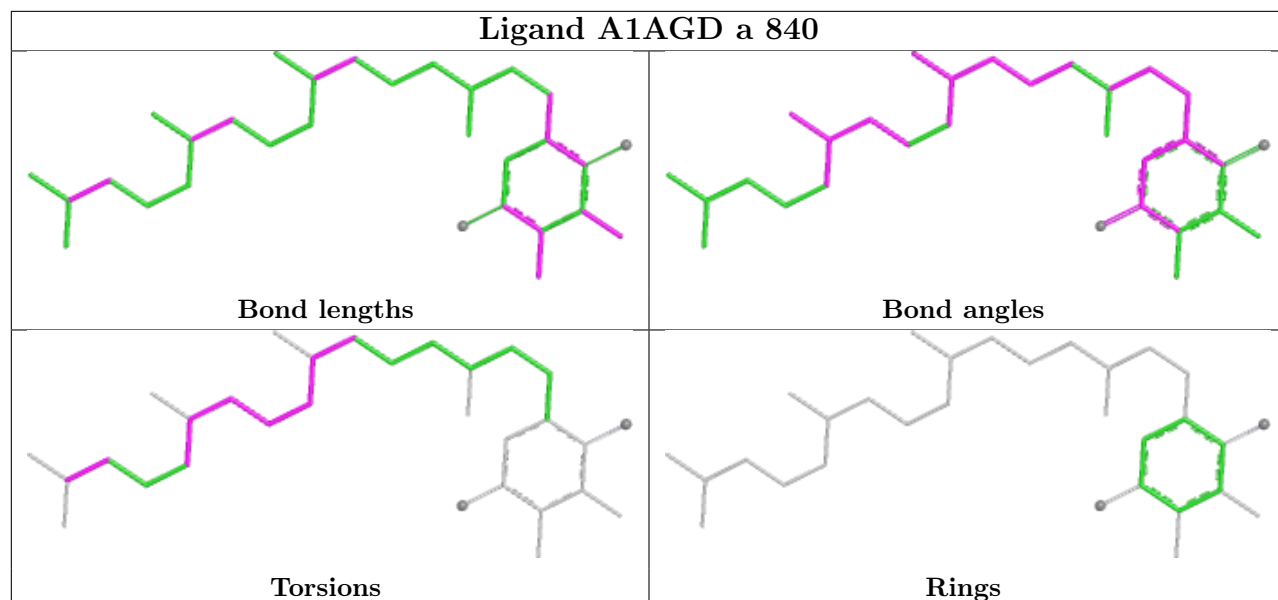
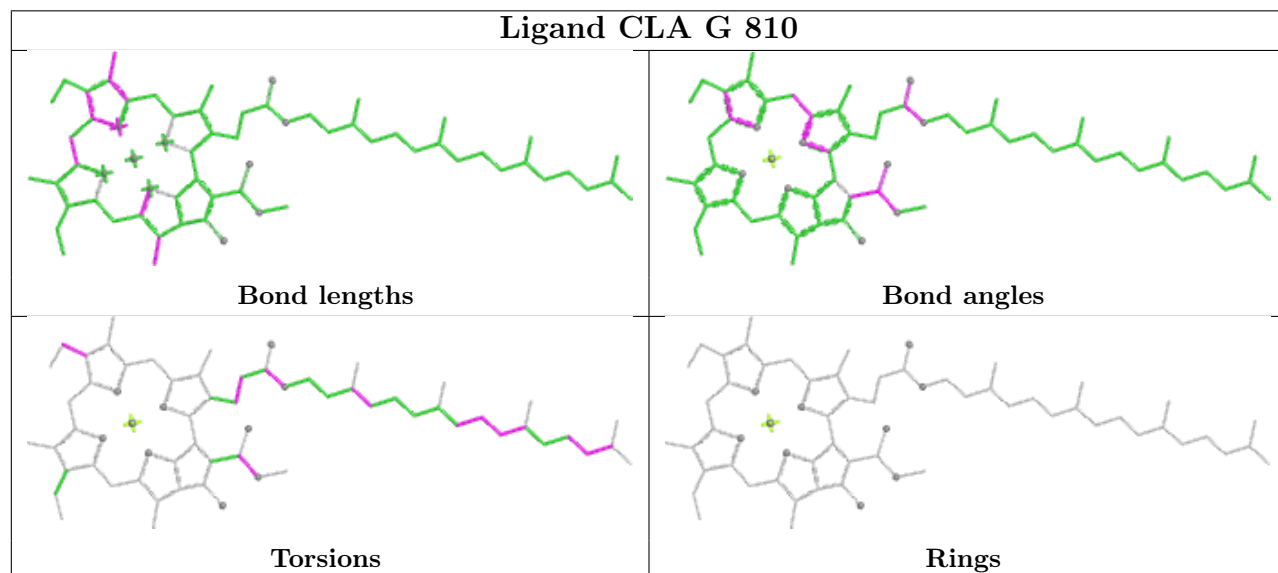
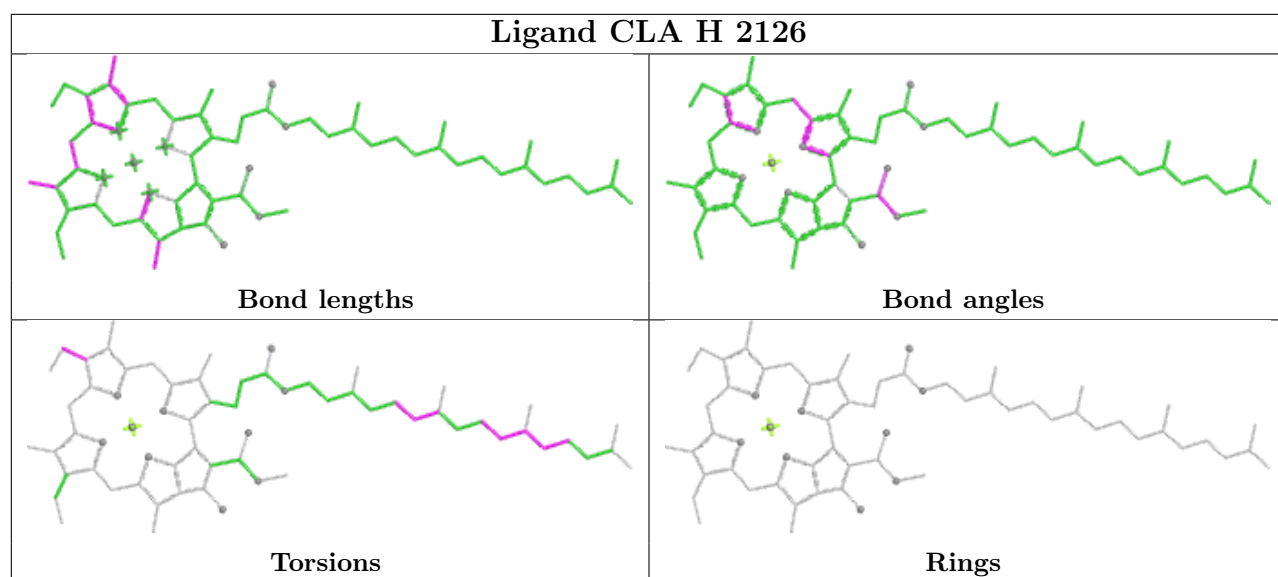
Rings



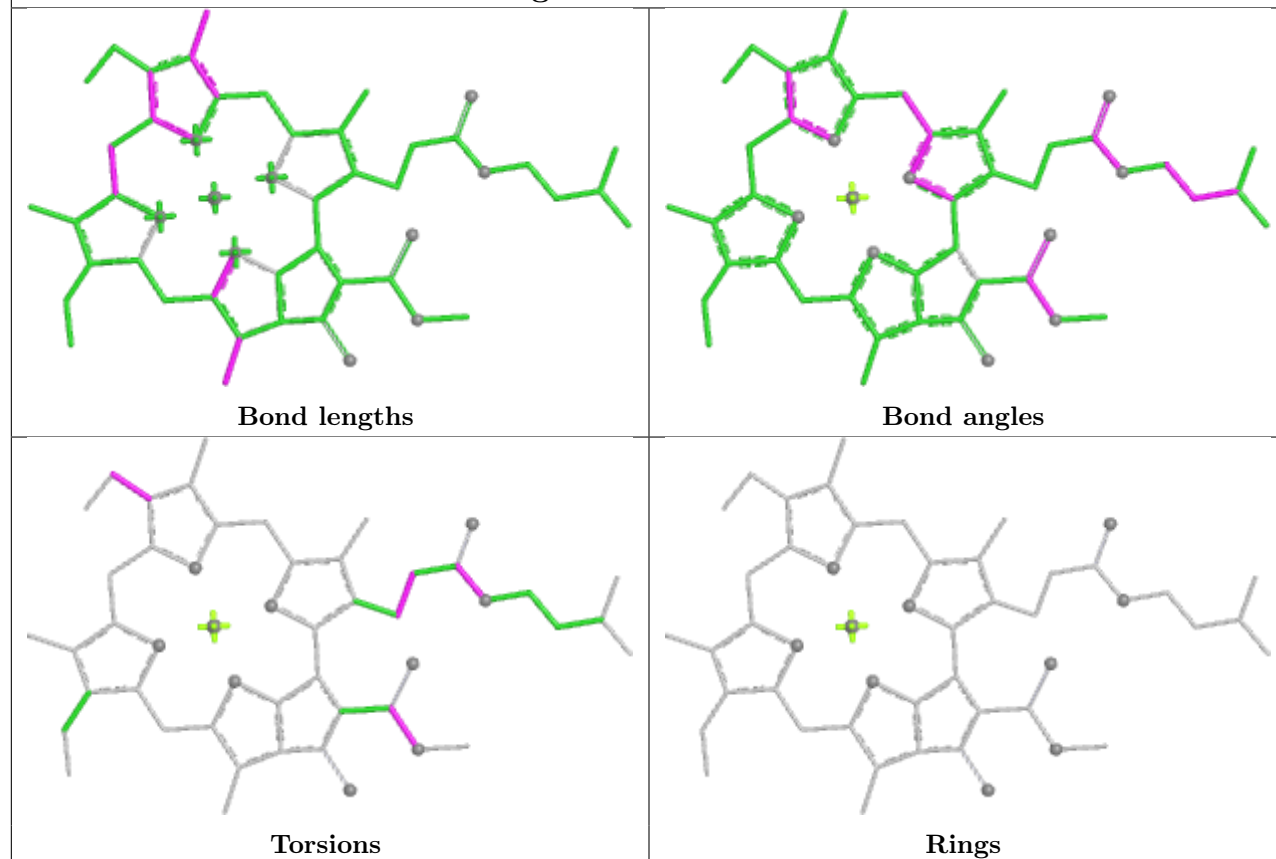




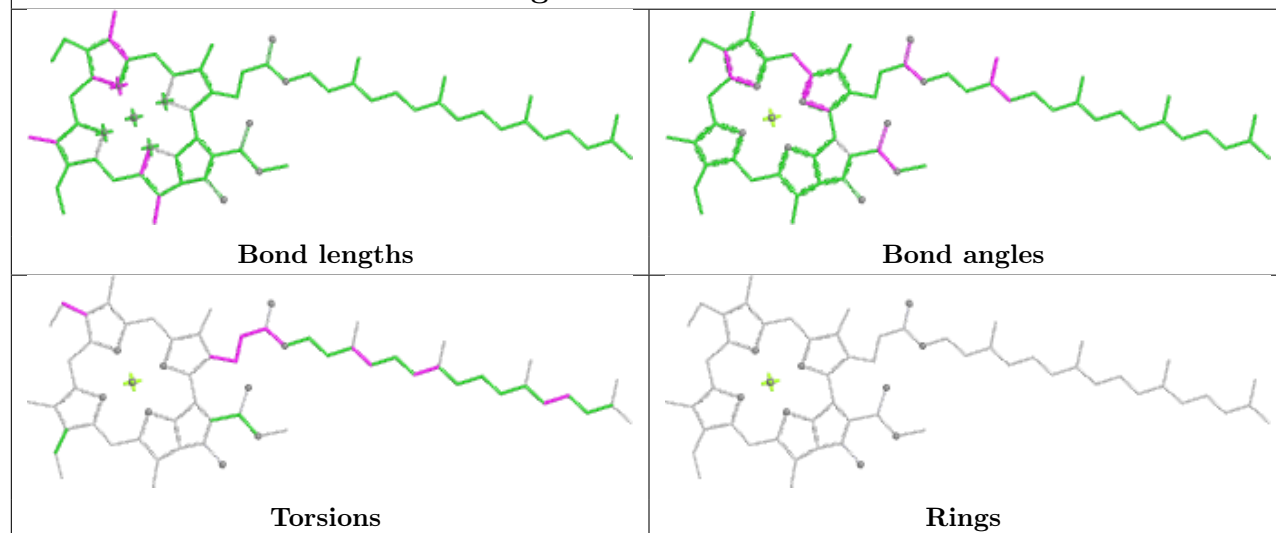


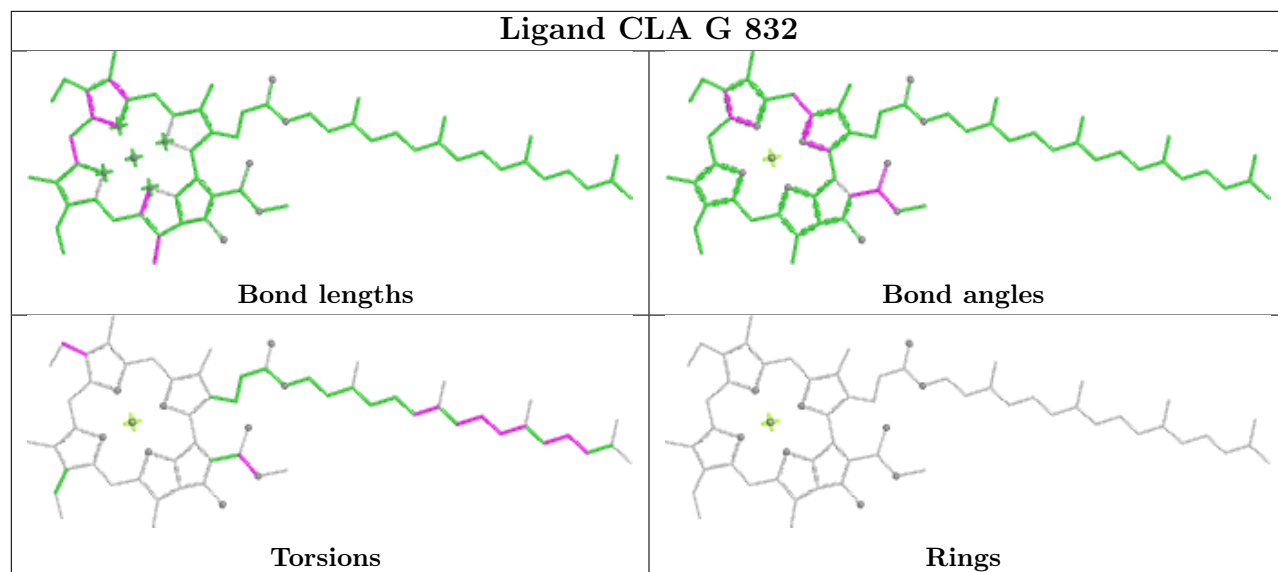
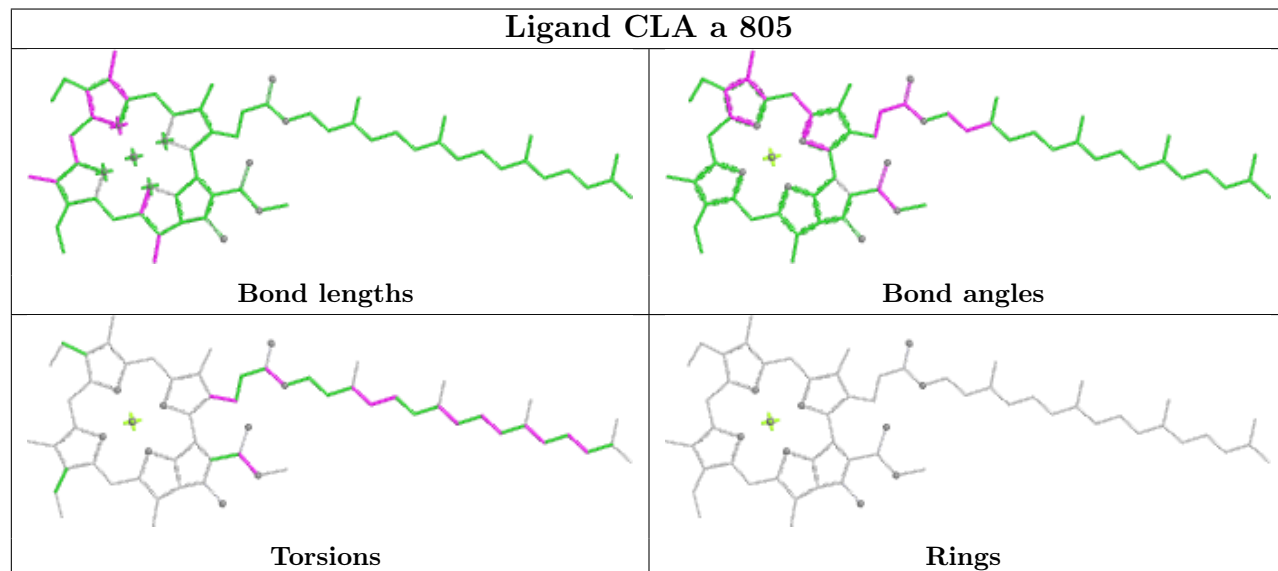


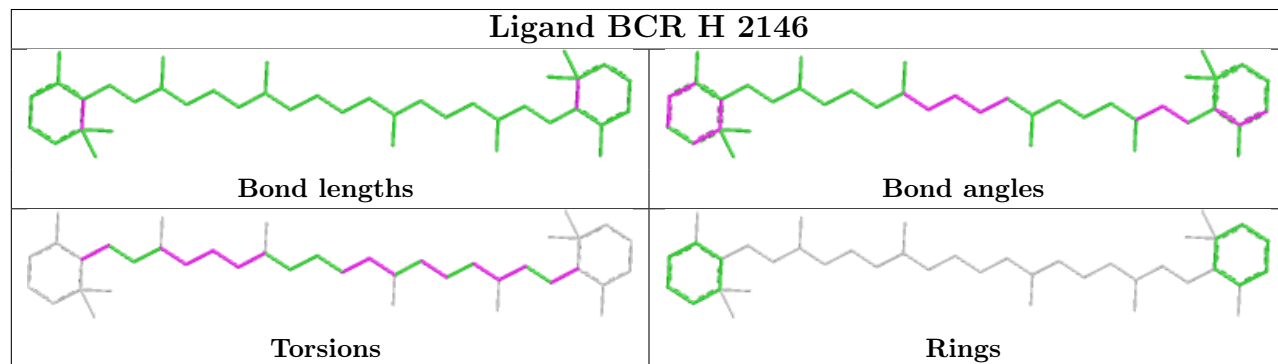
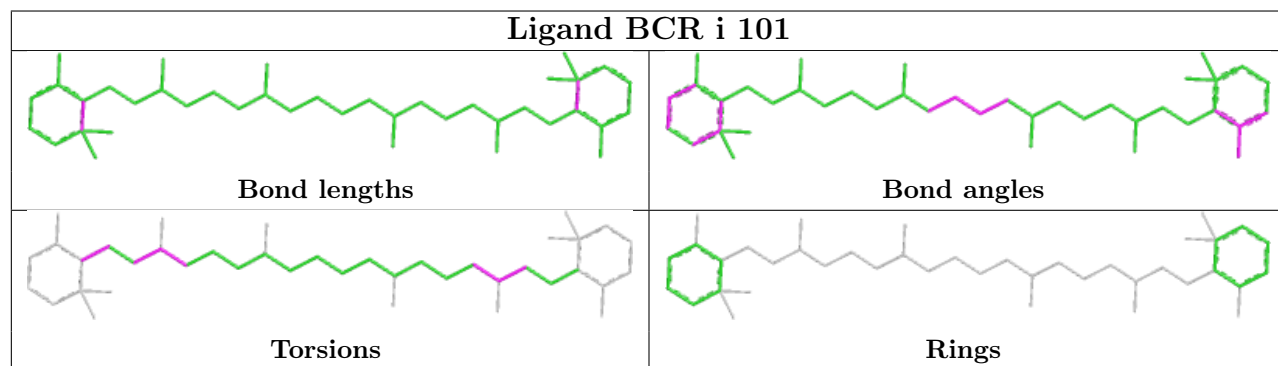
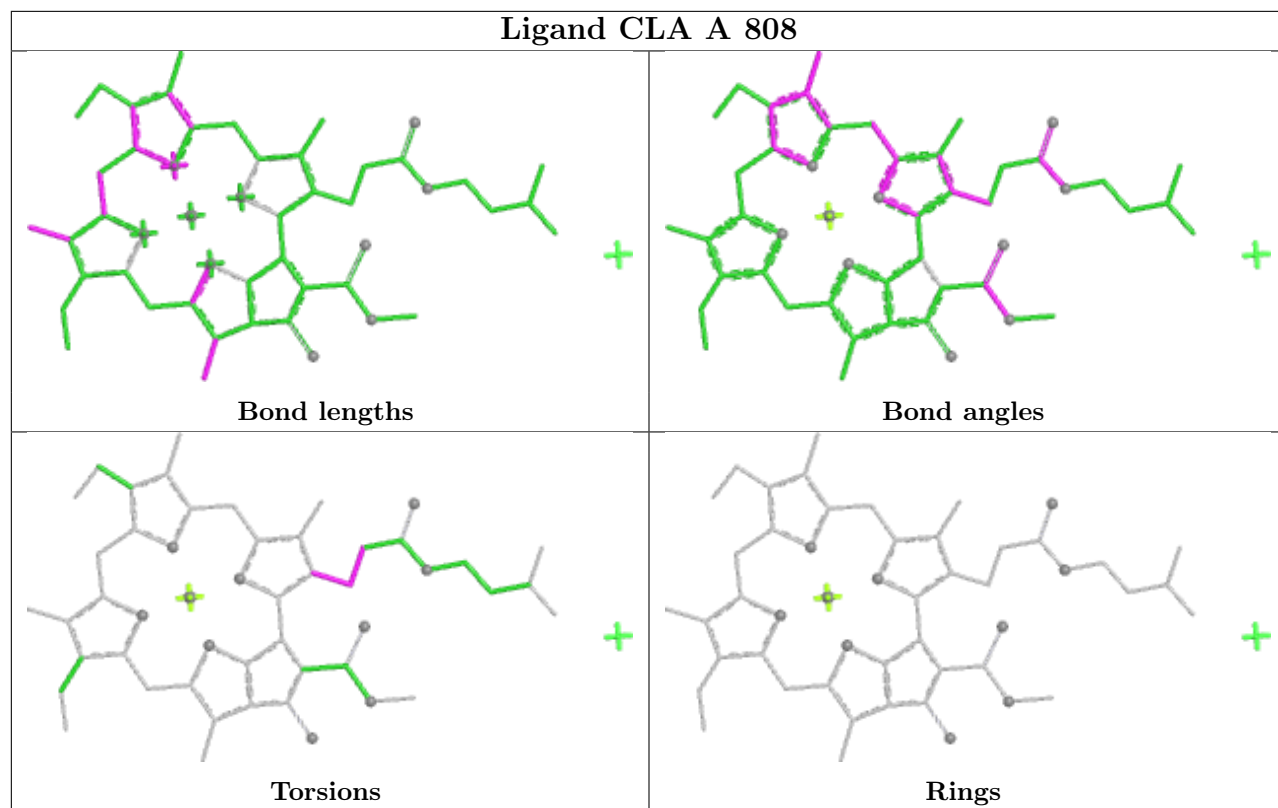
Ligand CLA A 806

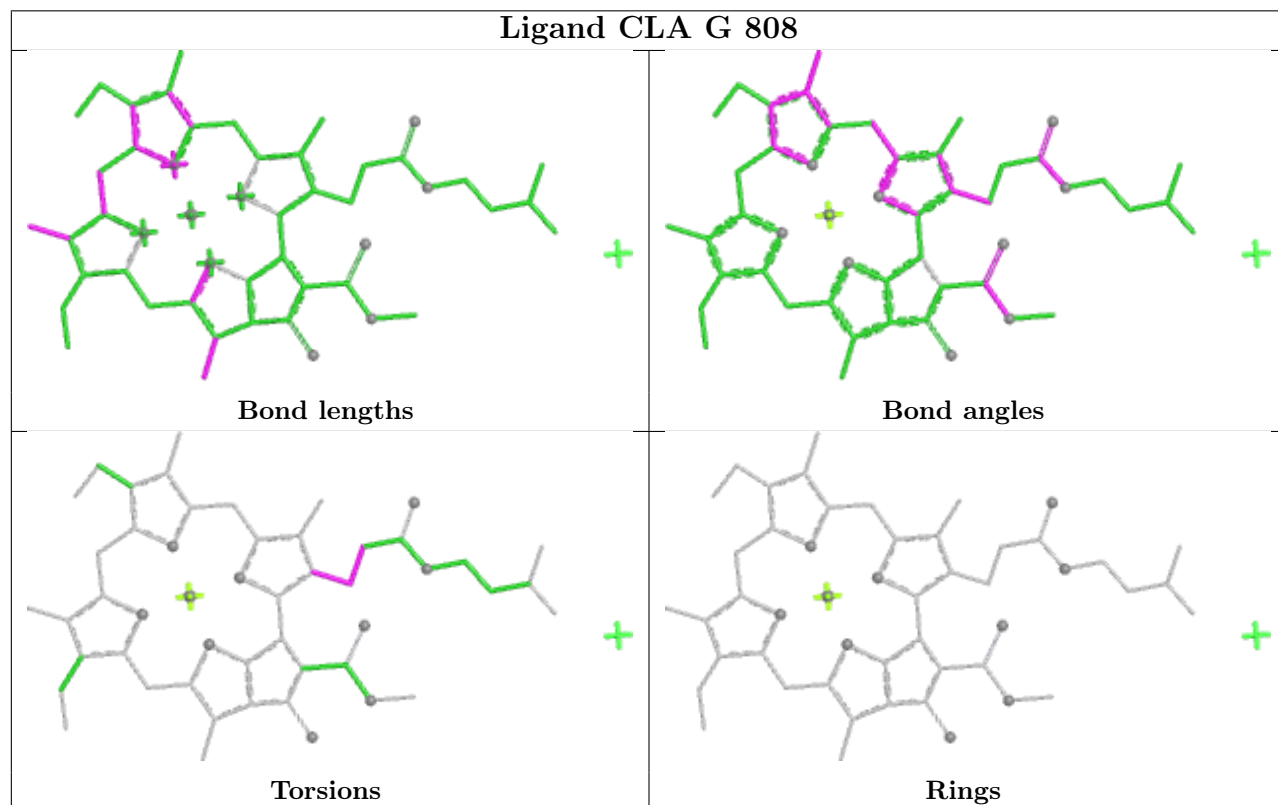
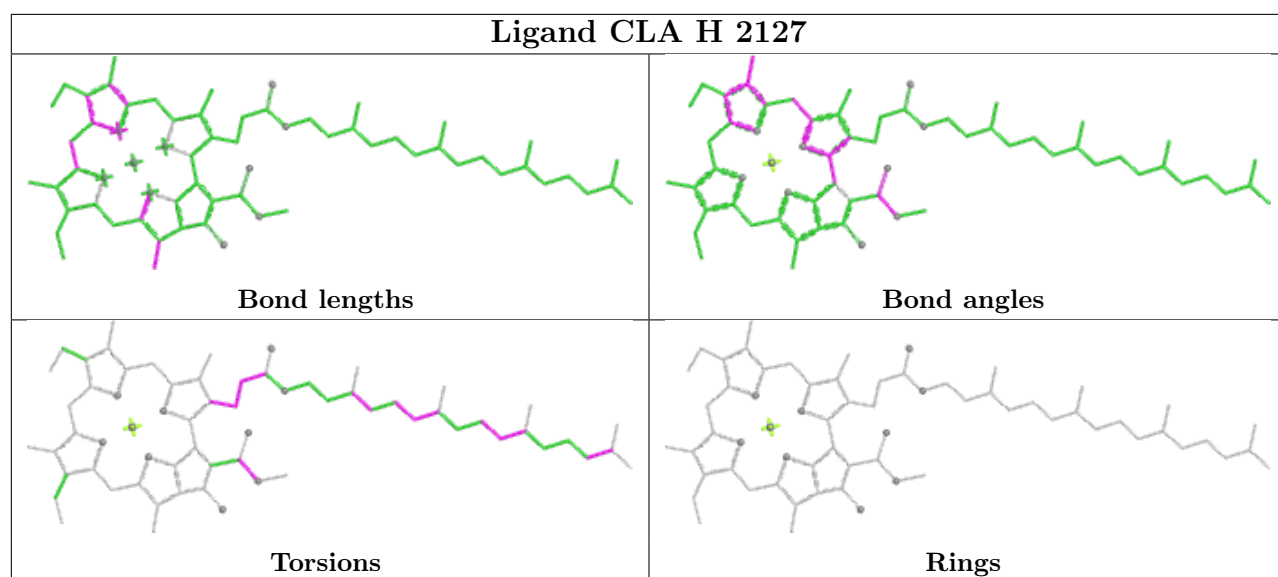


Ligand CLA G 851

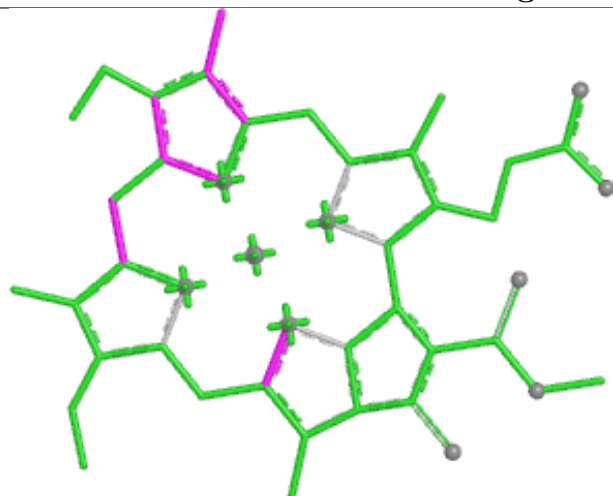


Ligand CLA G 832**Ligand CLA a 805**

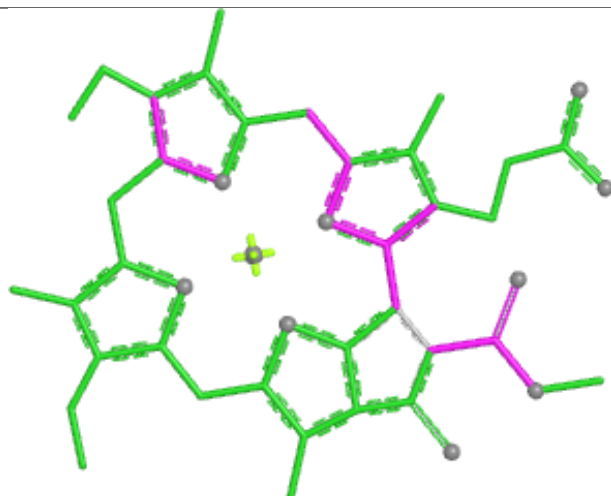




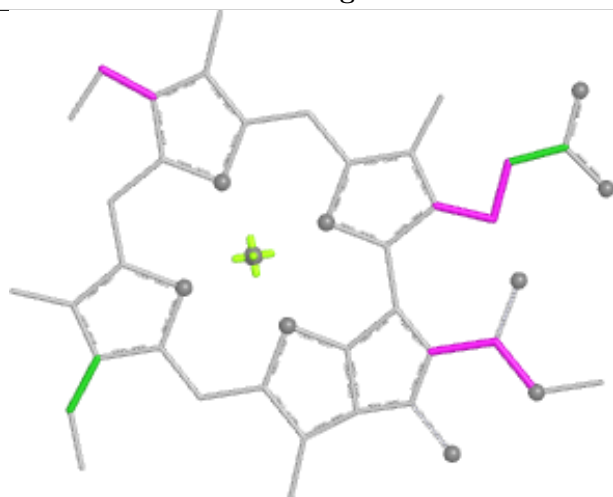
Ligand CLA S 102



Bond lengths



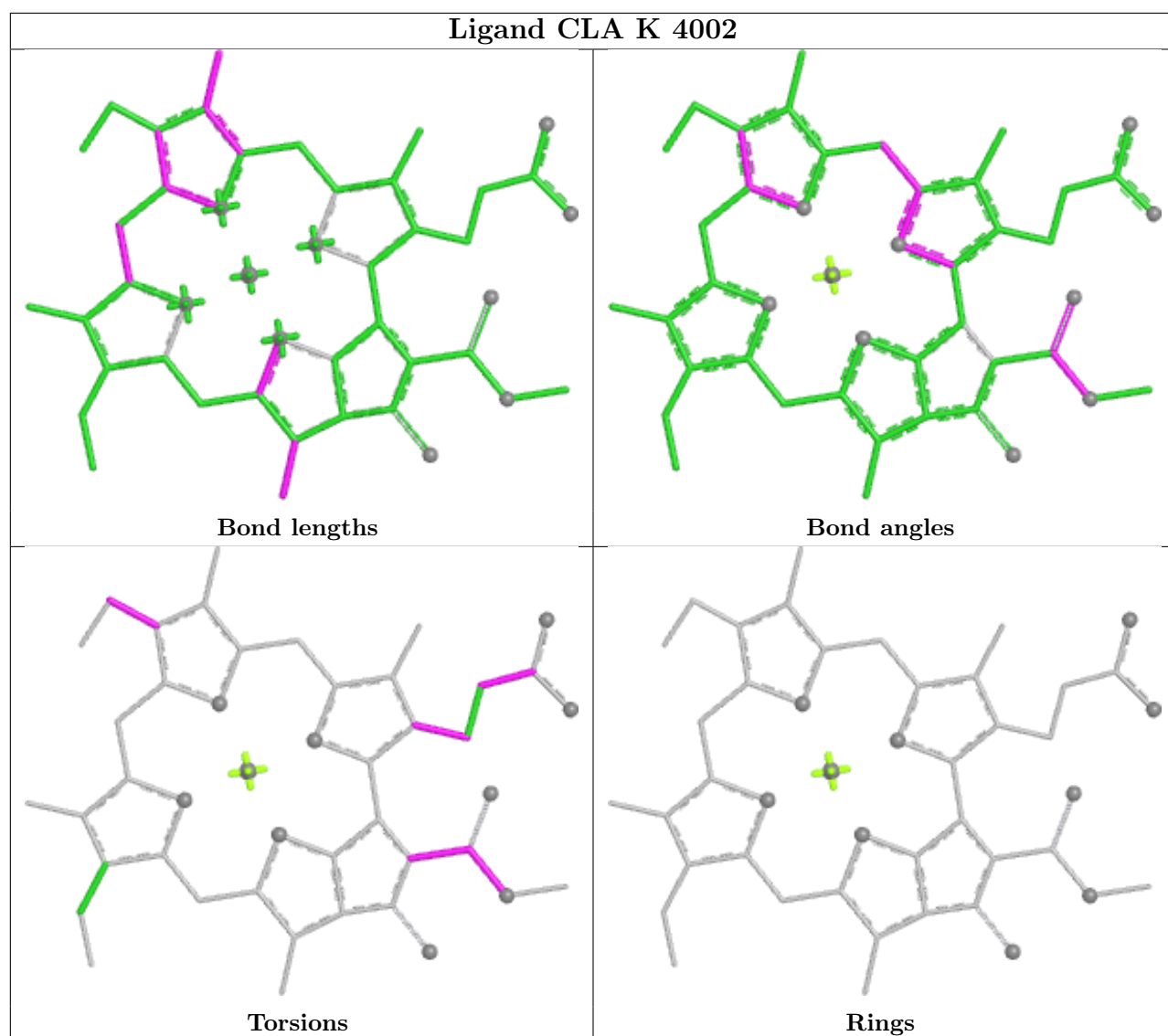
Bond angles



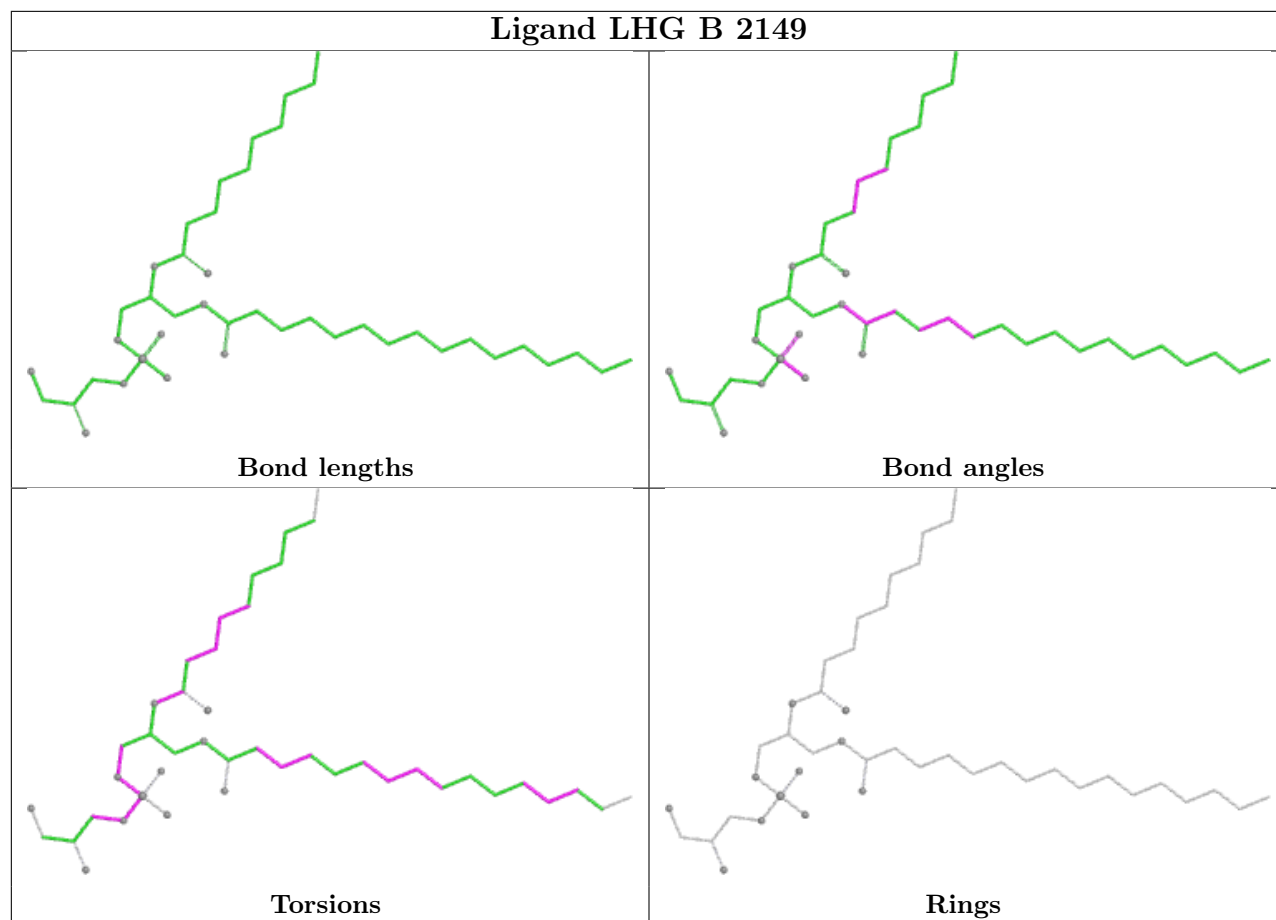
Torsions



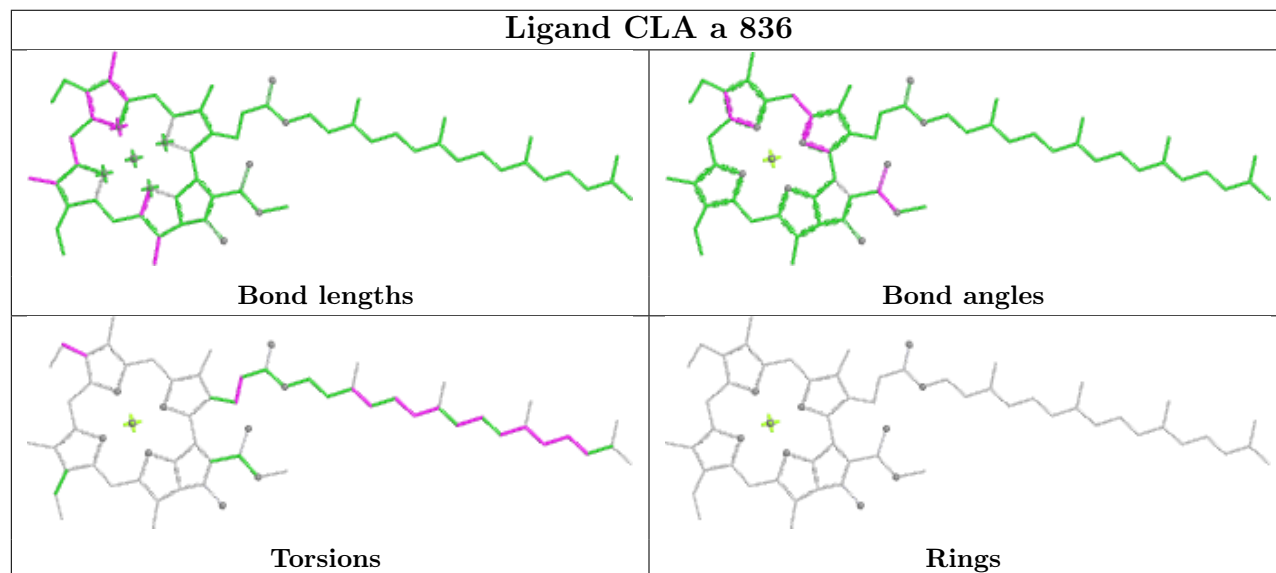
Rings

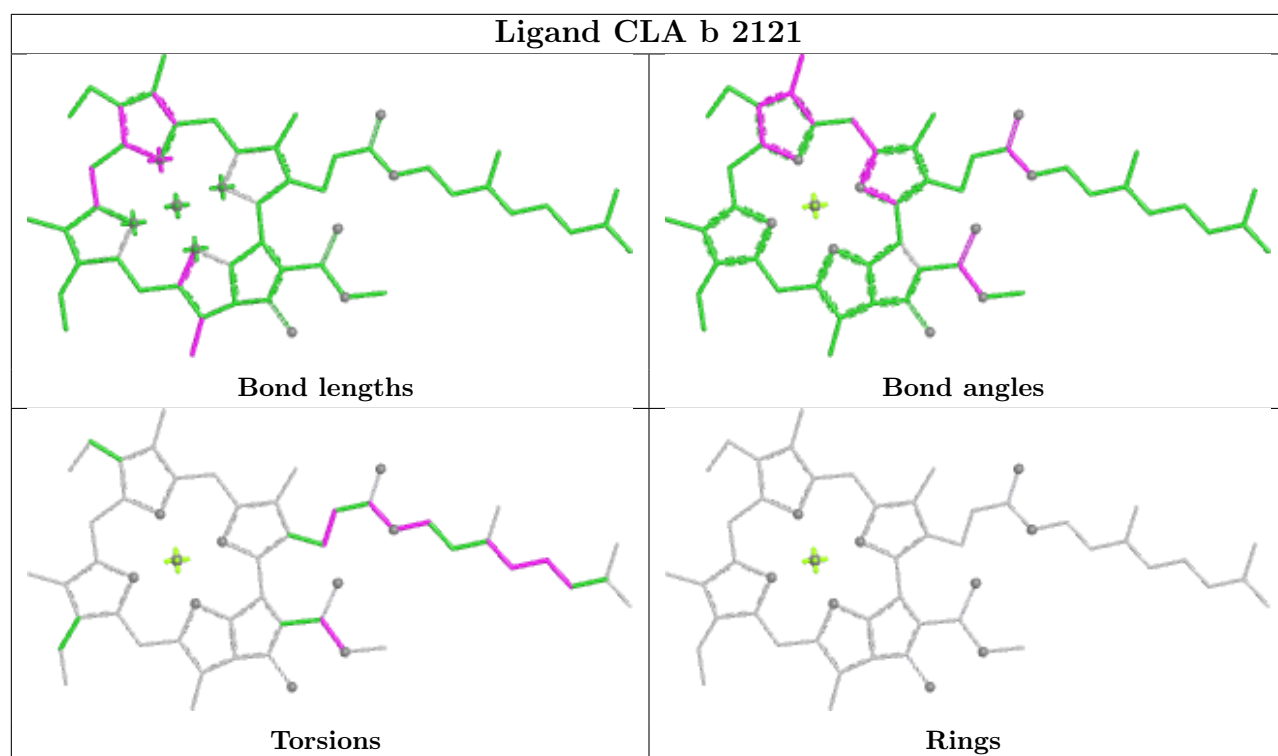


Ligand LHG B 2149

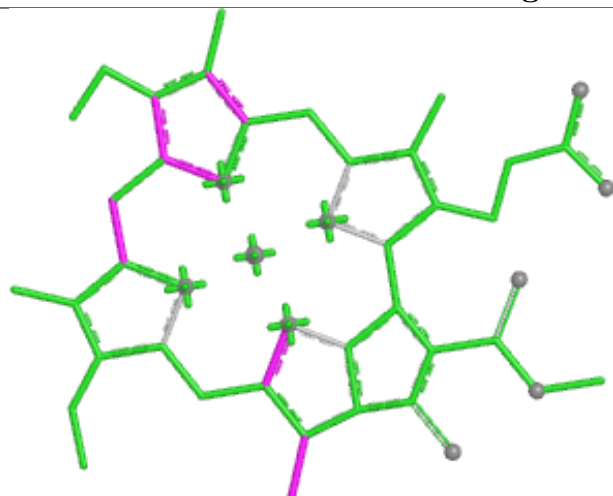


Ligand CLA a 836

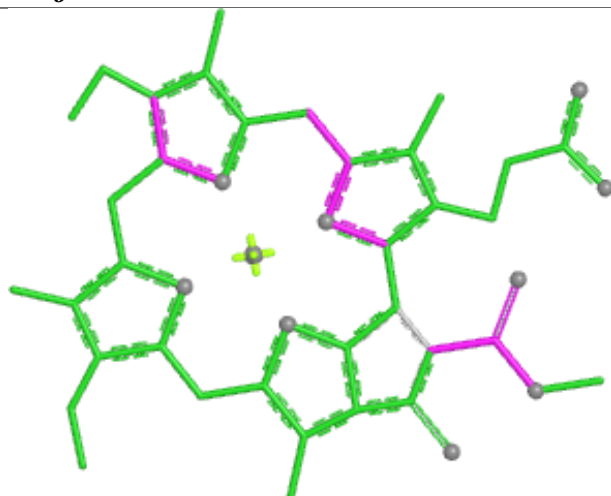




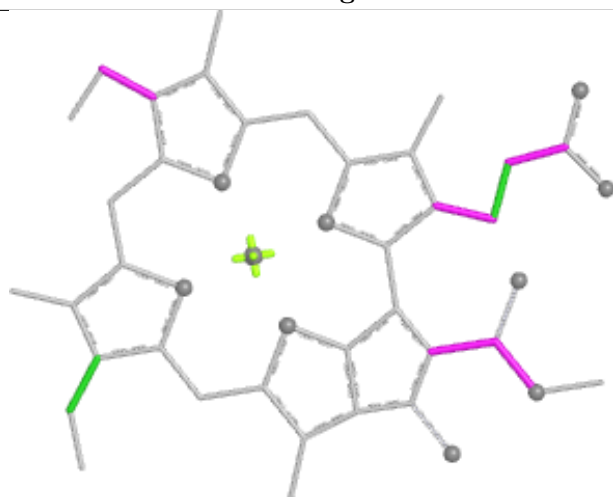
Ligand CLA j 103



Bond lengths



Bond angles

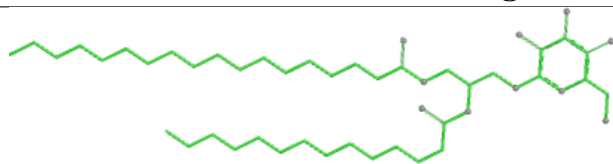


Torsions

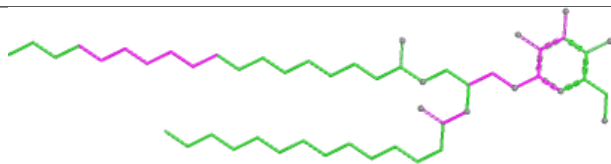


Rings

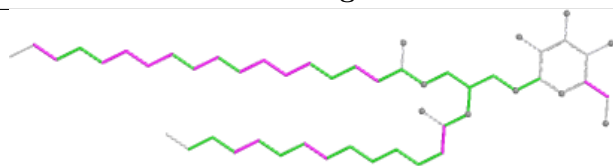
Ligand LMG B 2148



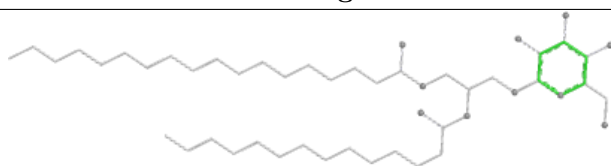
Bond lengths



Bond angles

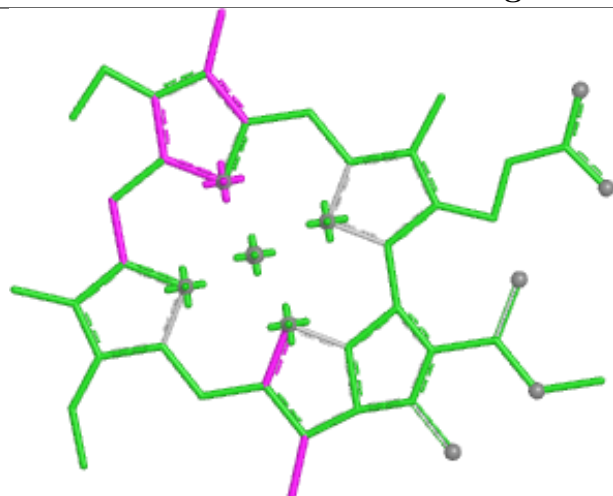


Torsions

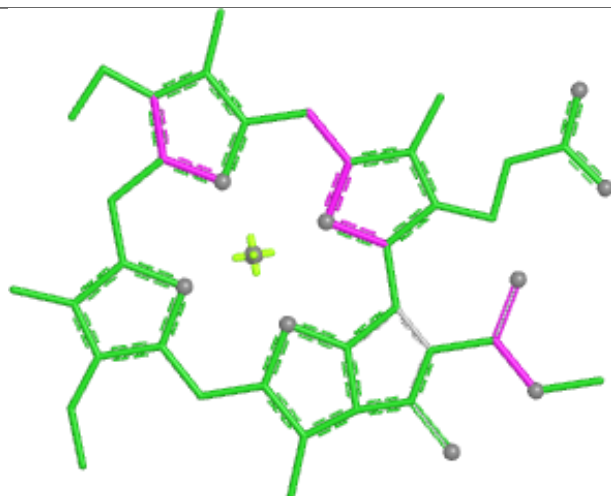


Rings

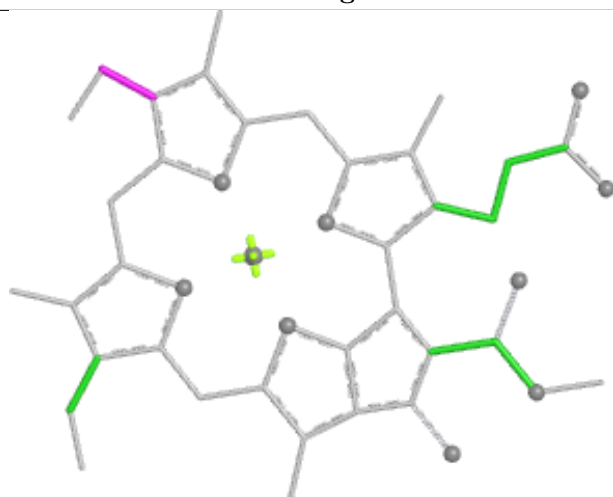
Ligand CLA H 2130



Bond lengths



Bond angles

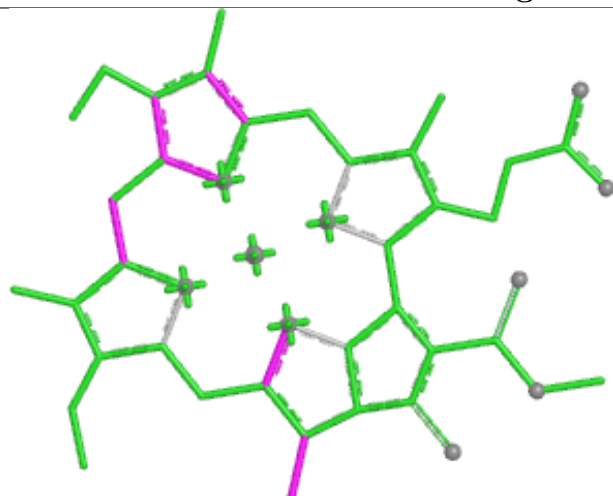


Torsions

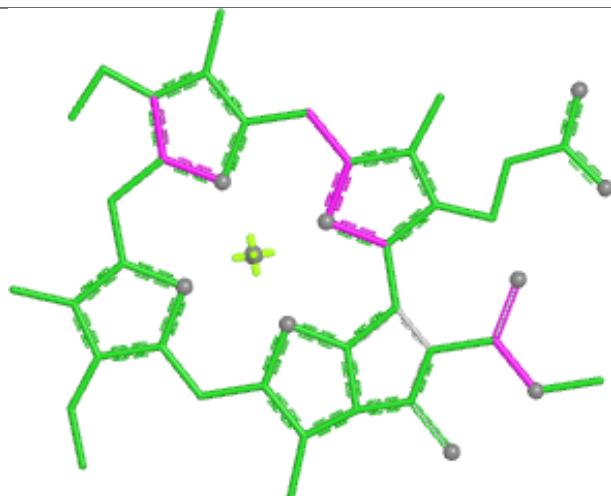


Rings

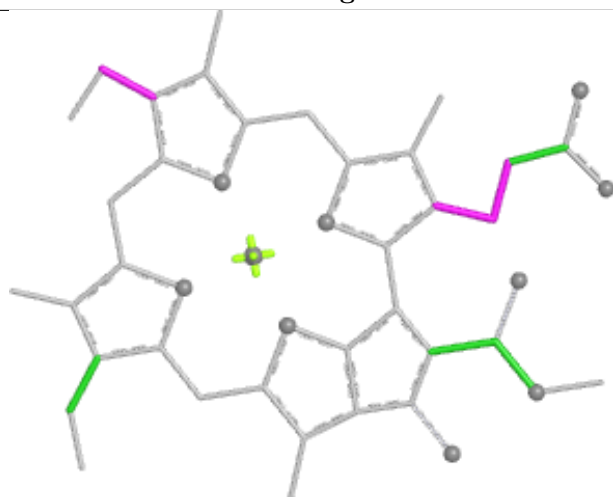
Ligand CLA F 204



Bond lengths



Bond angles

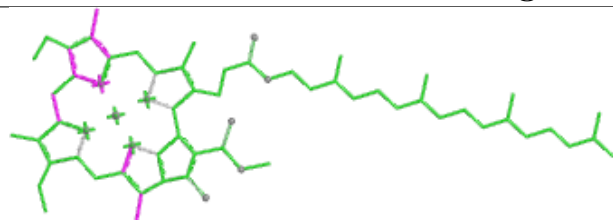


Torsions

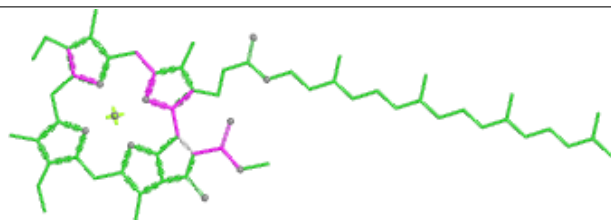


Rings

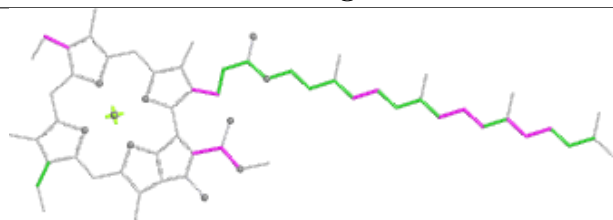
Ligand CLA a 812



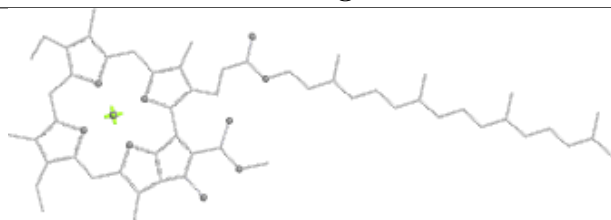
Bond lengths



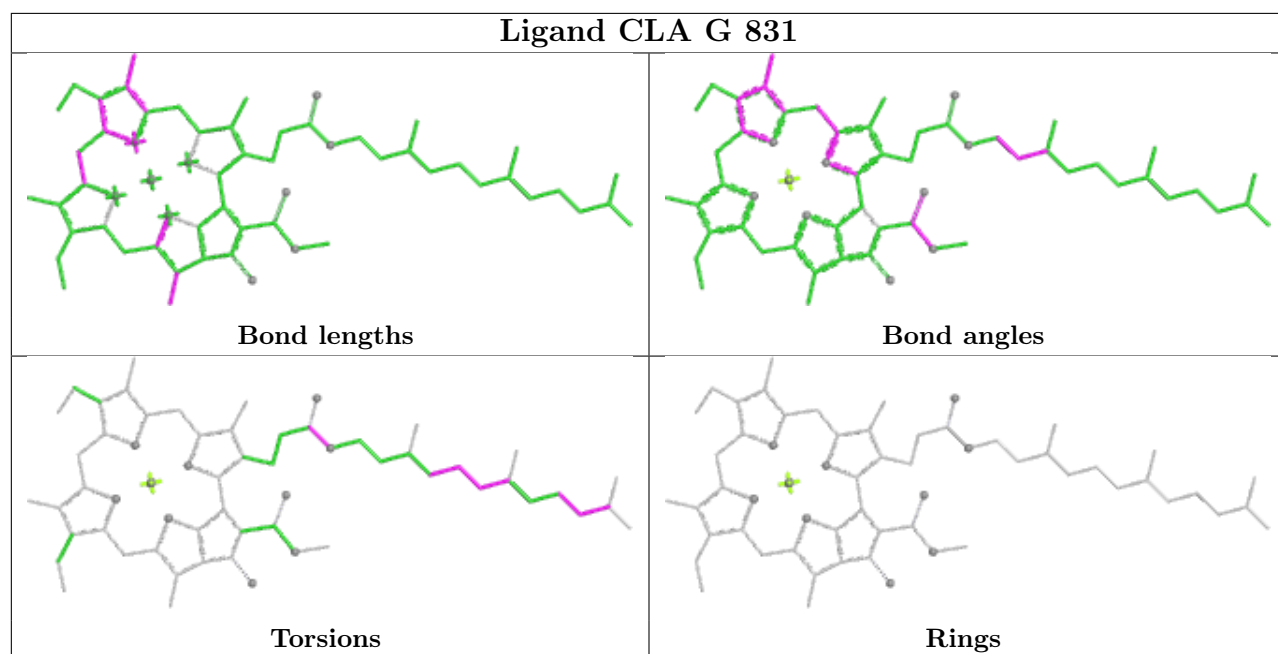
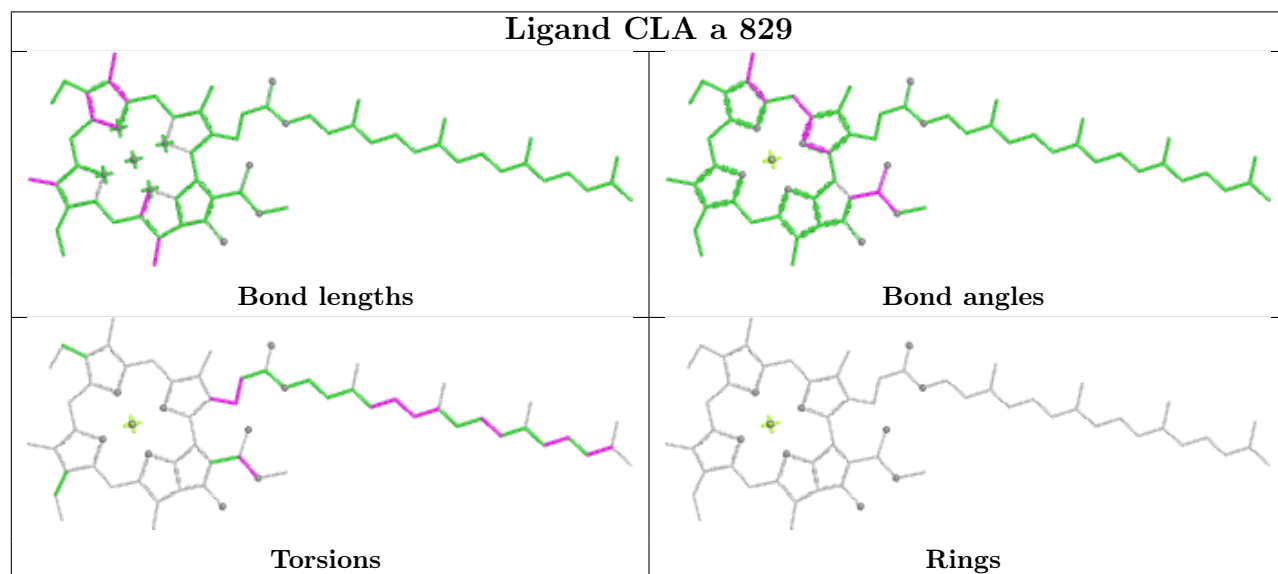
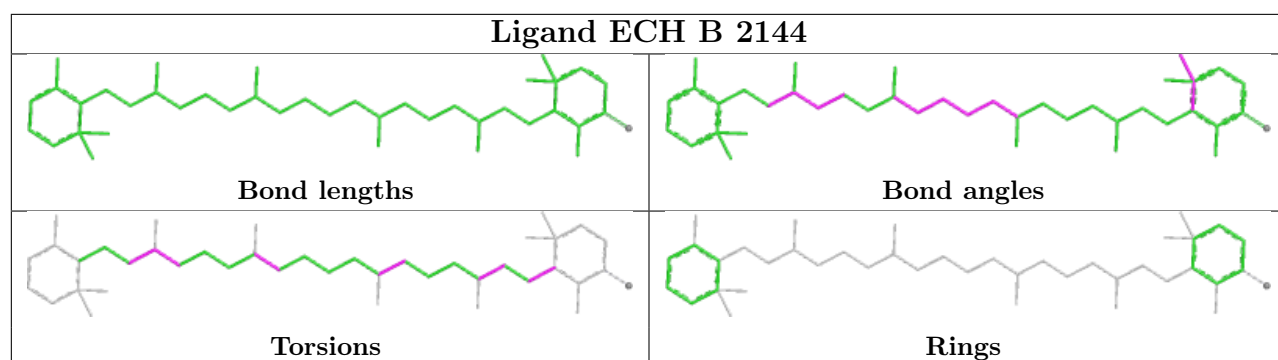
Bond angles



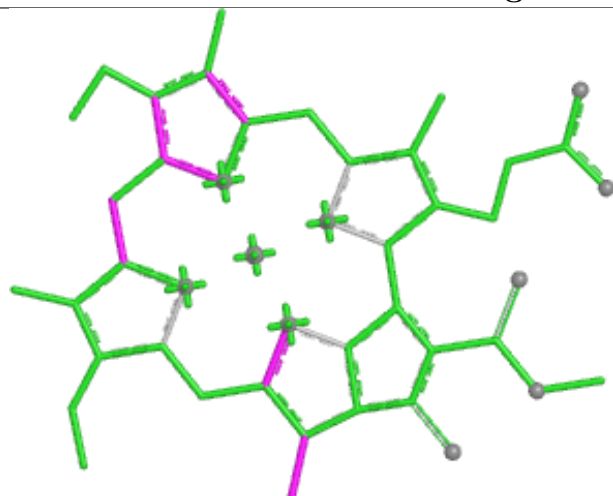
Torsions



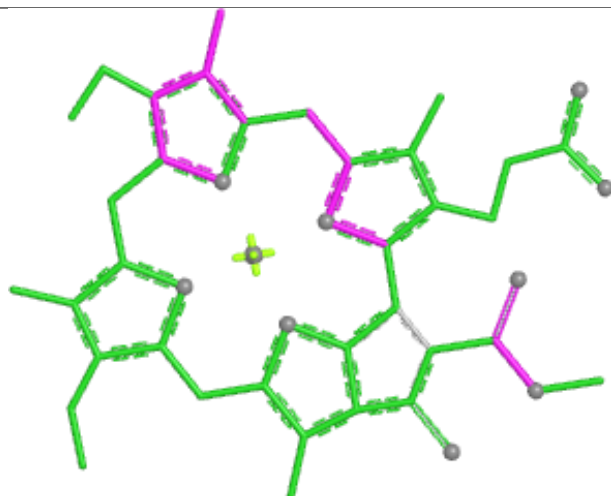
Rings



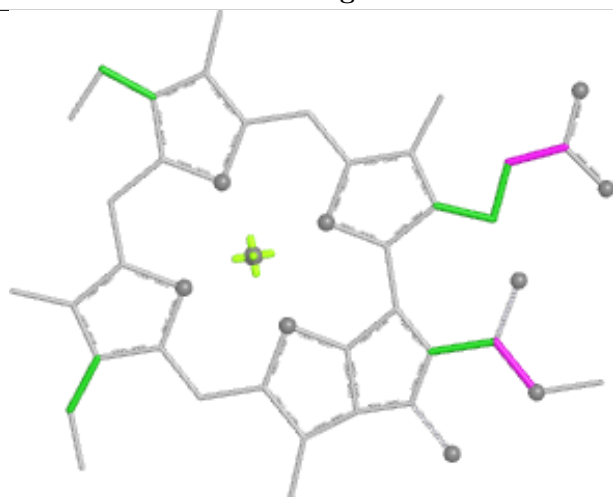
Ligand CLA B 2135



Bond lengths



Bond angles

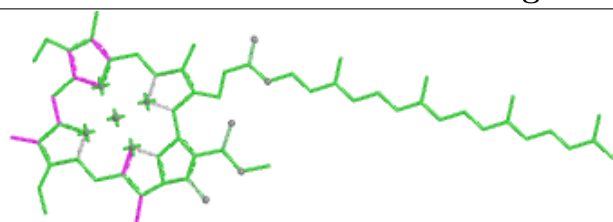


Torsions

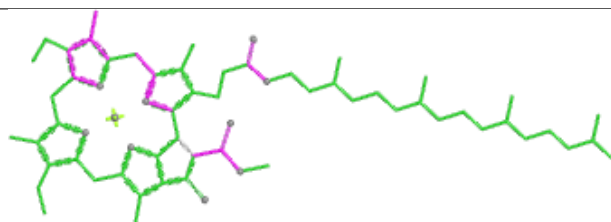


Rings

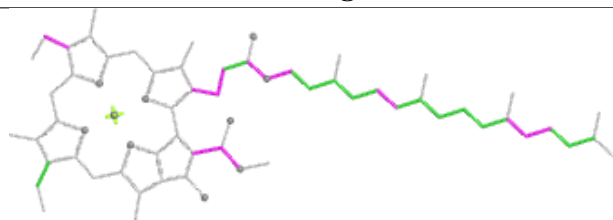
Ligand CLA I 201



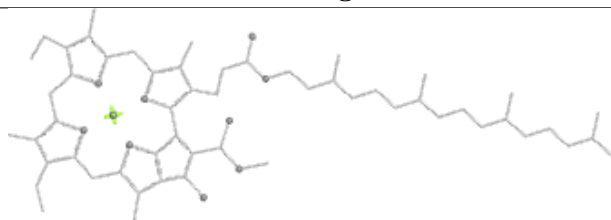
Bond lengths



Bond angles

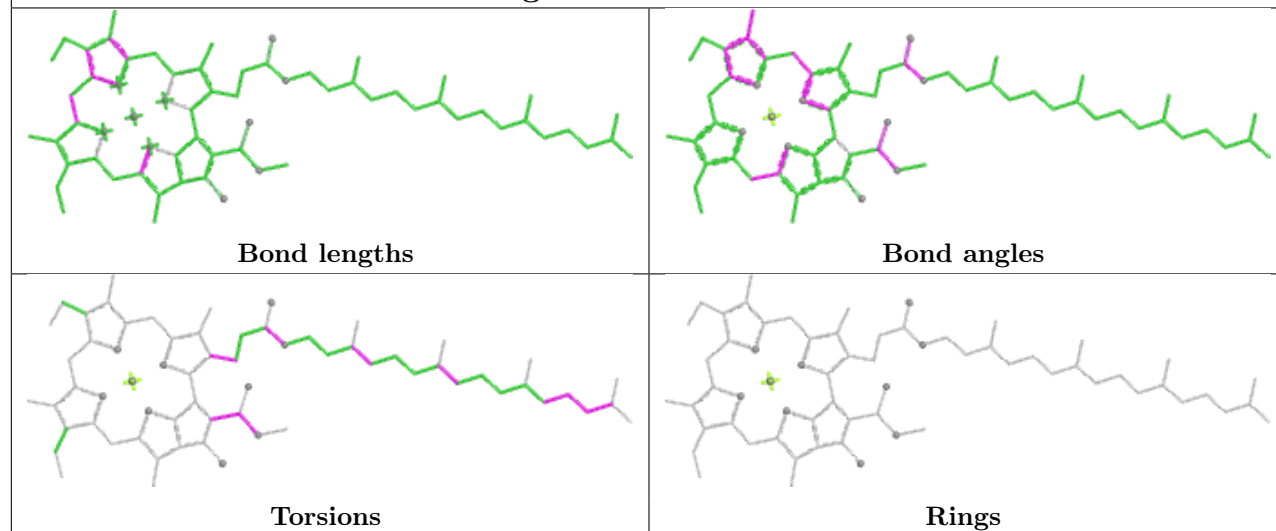


Torsions

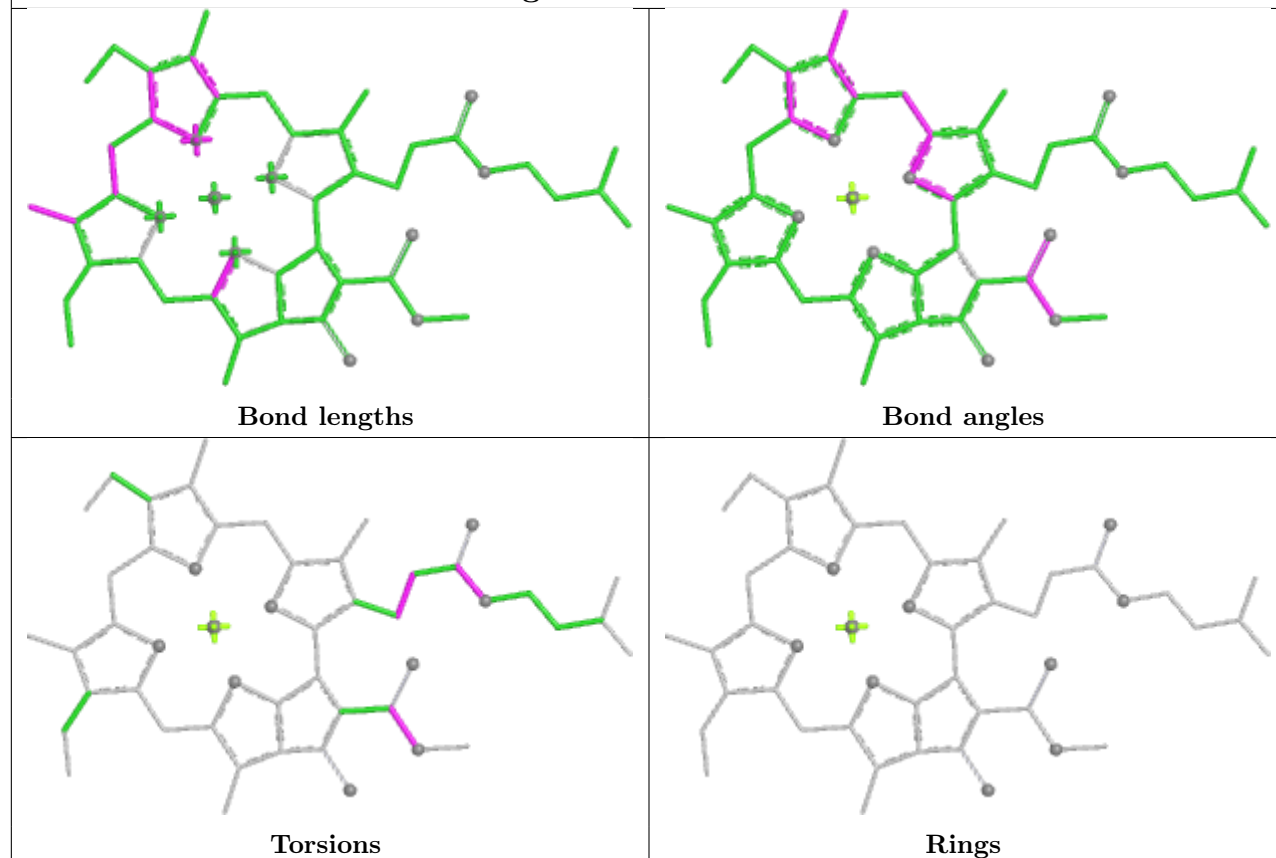


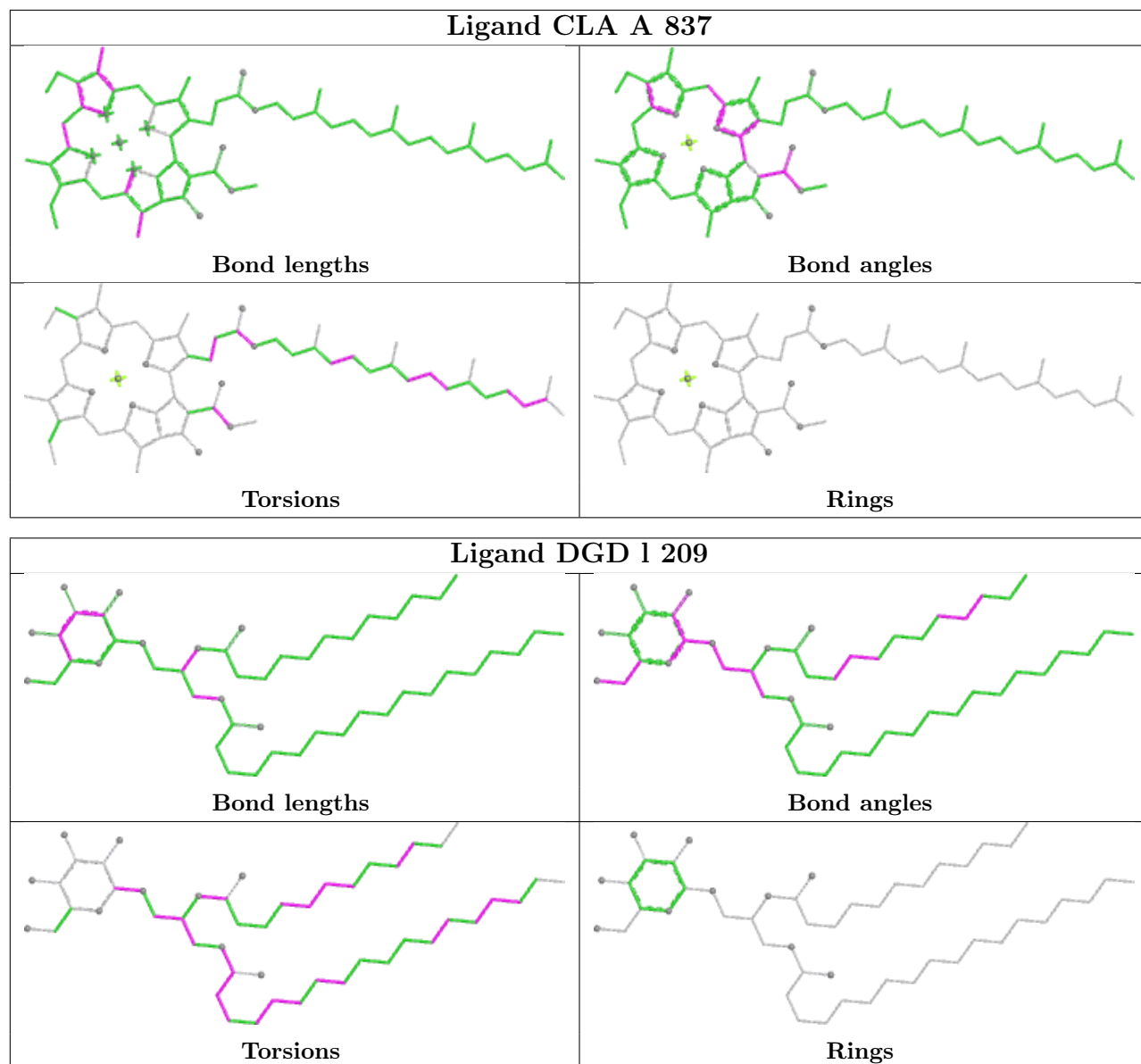
Rings

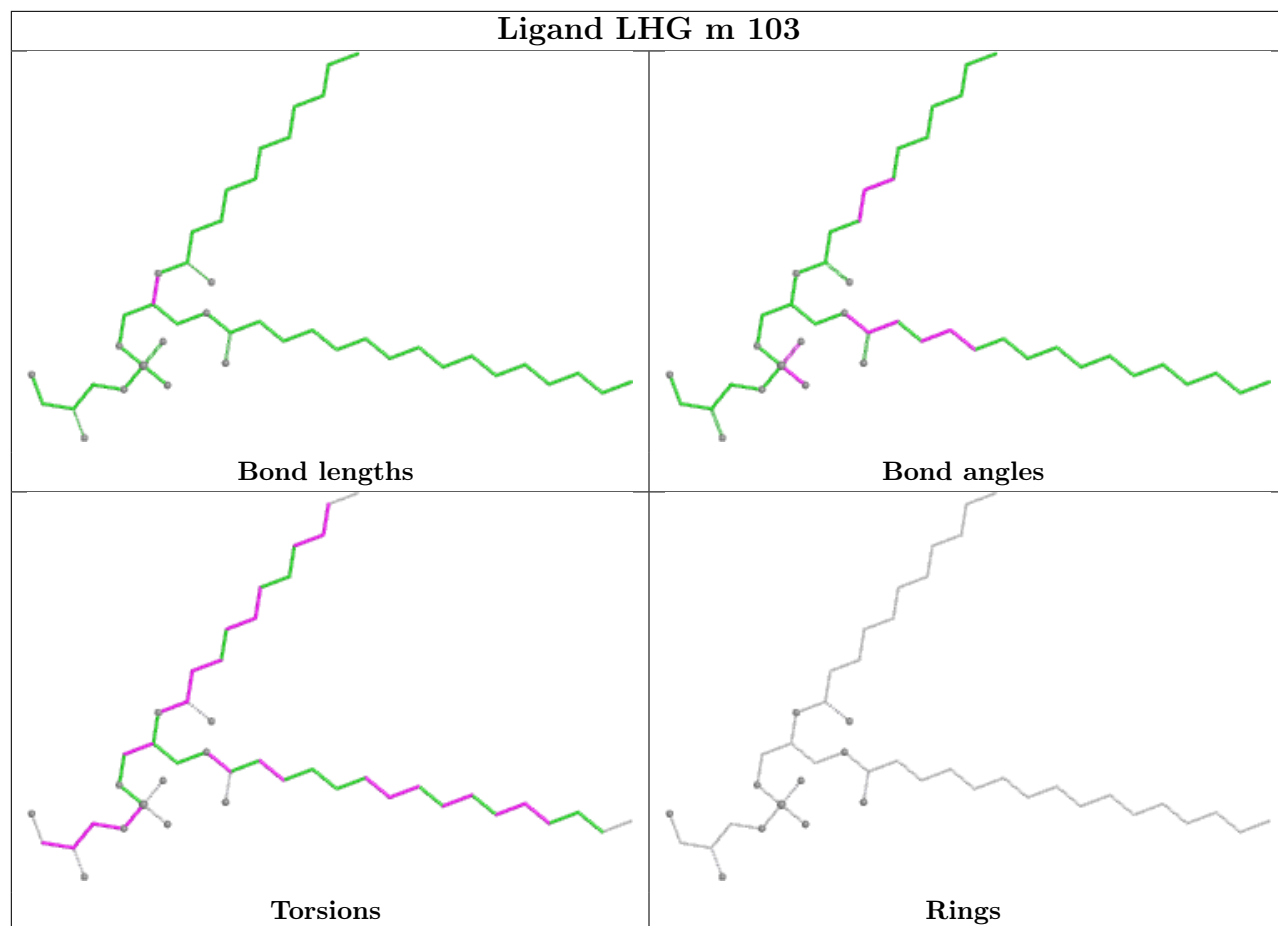
Ligand CLA H 2106

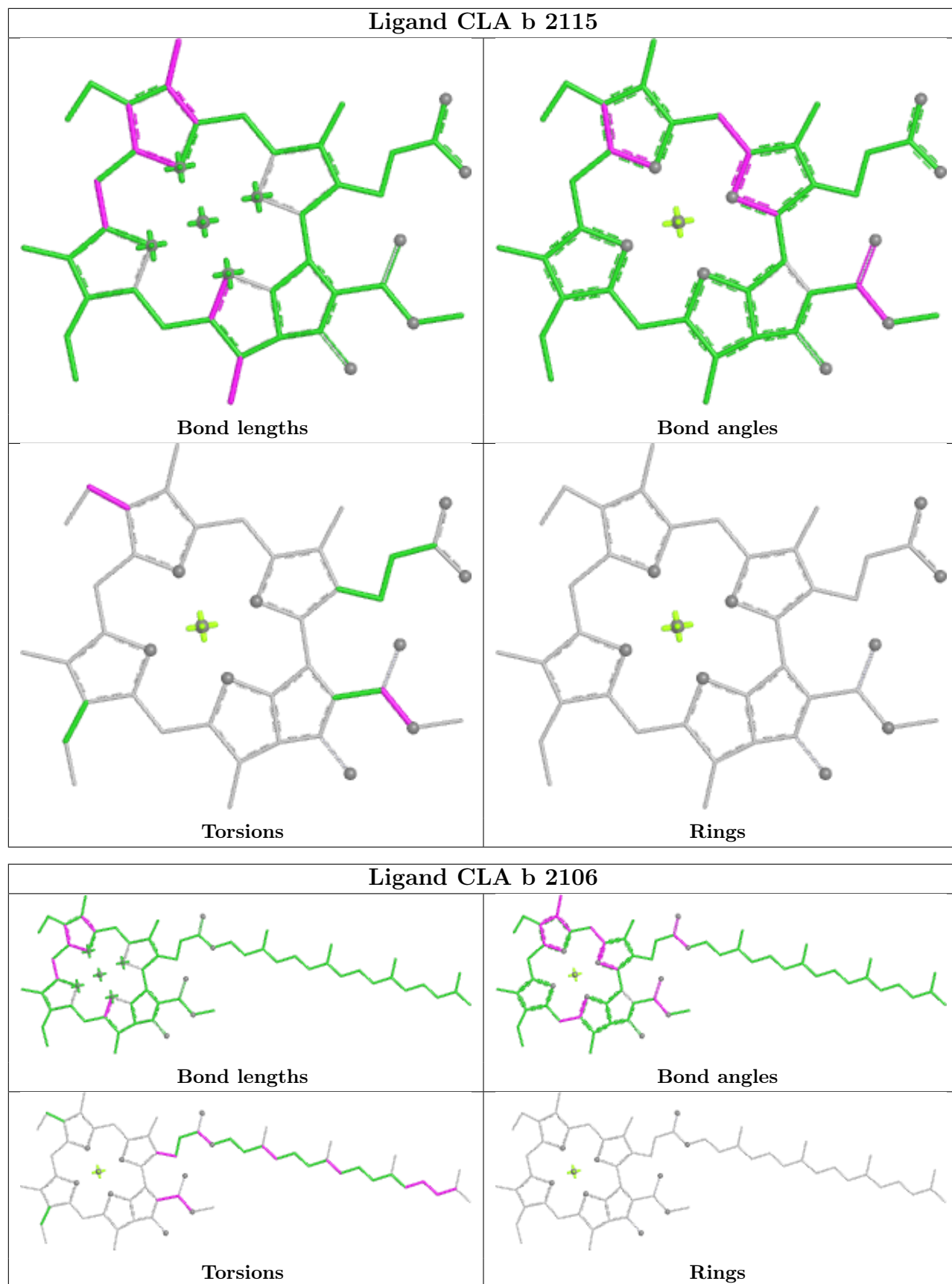


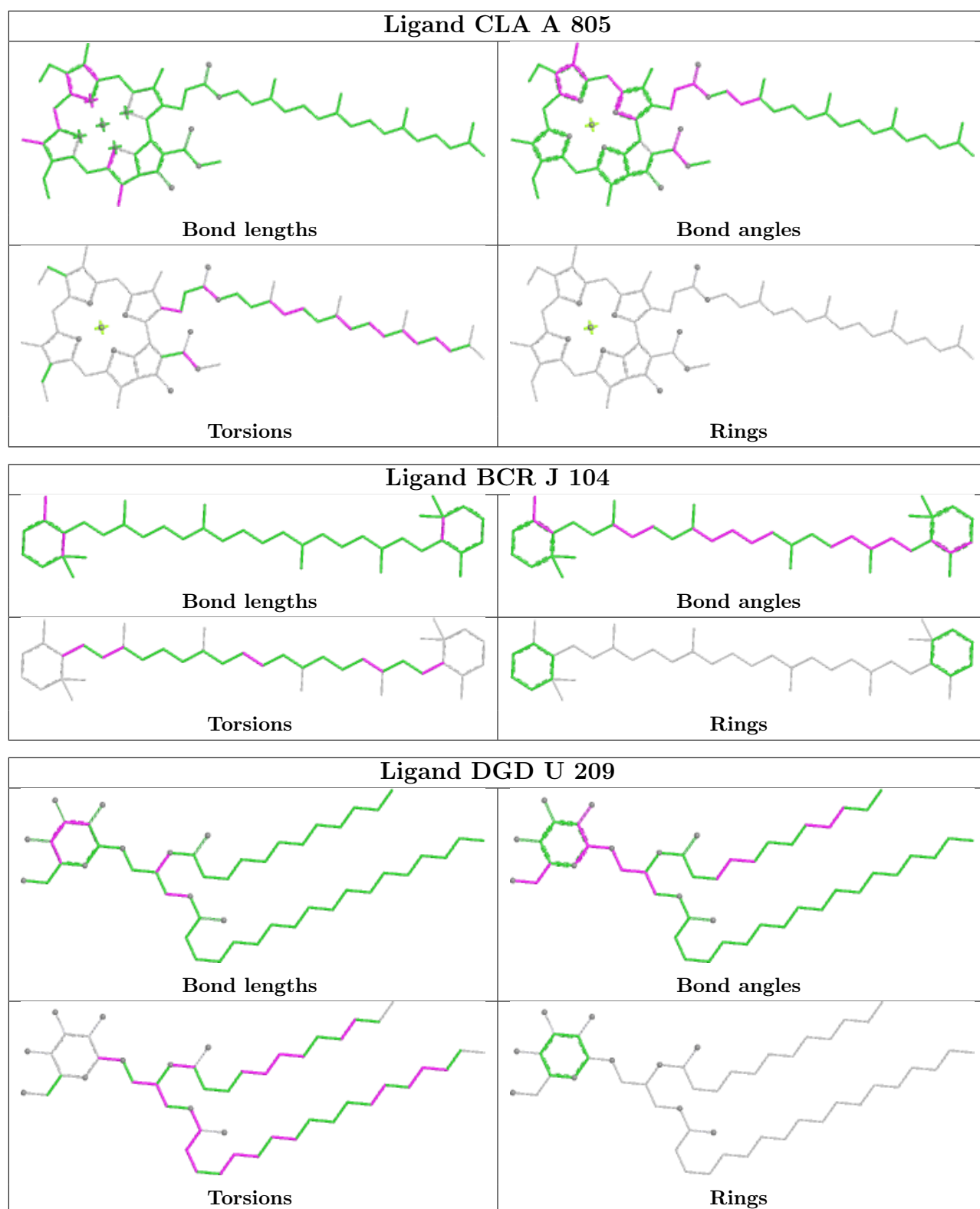
Ligand CLA H 2152

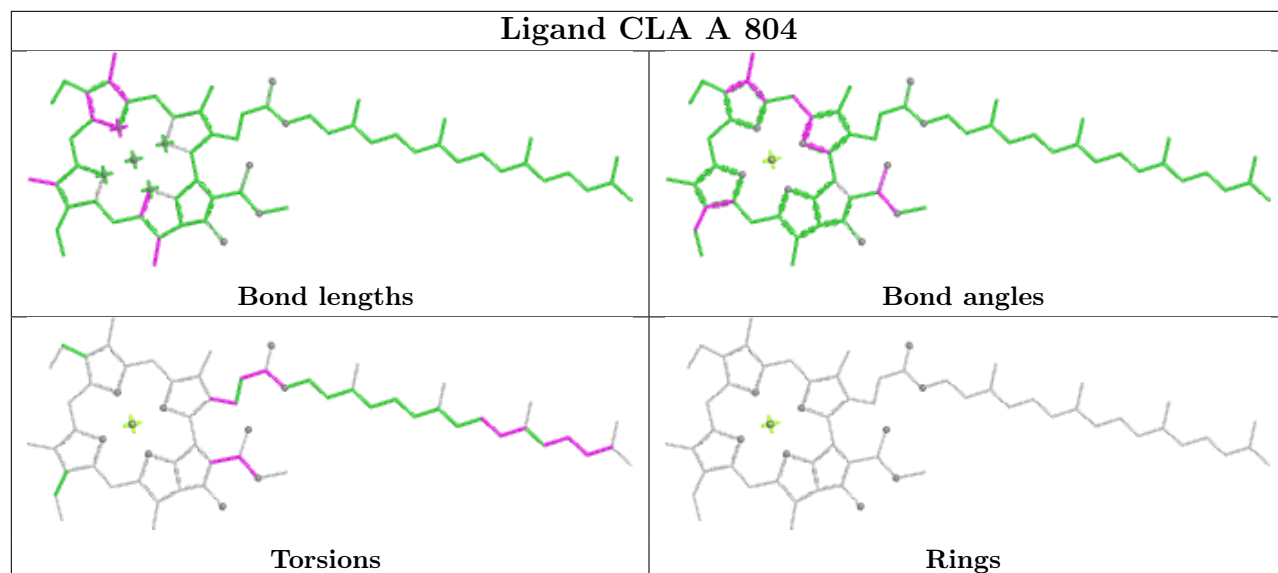
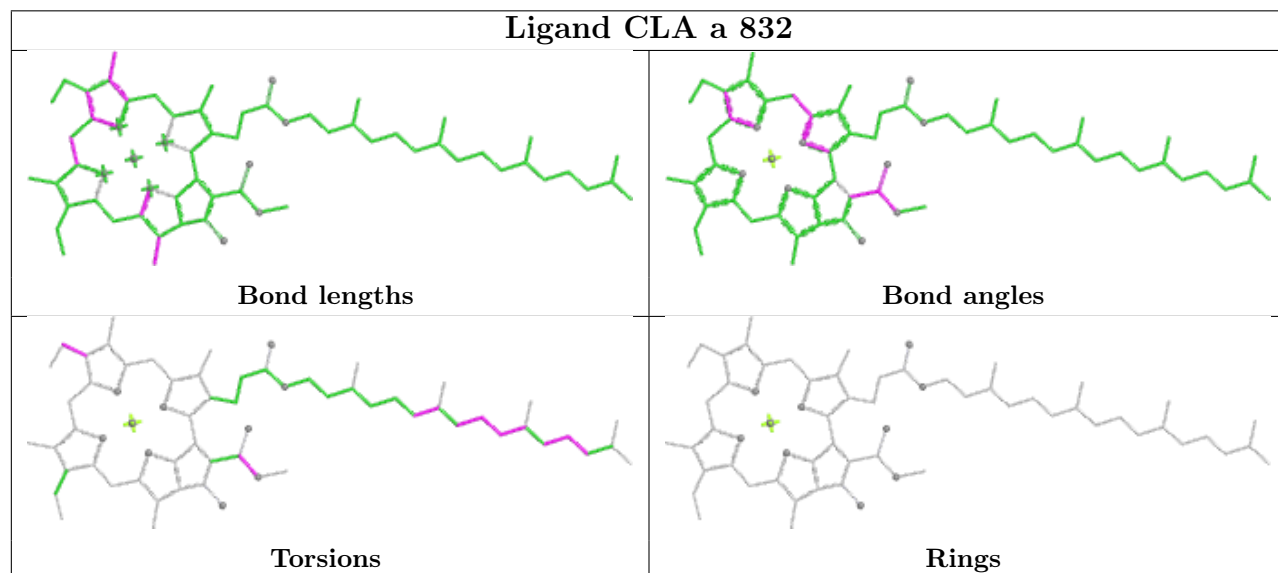
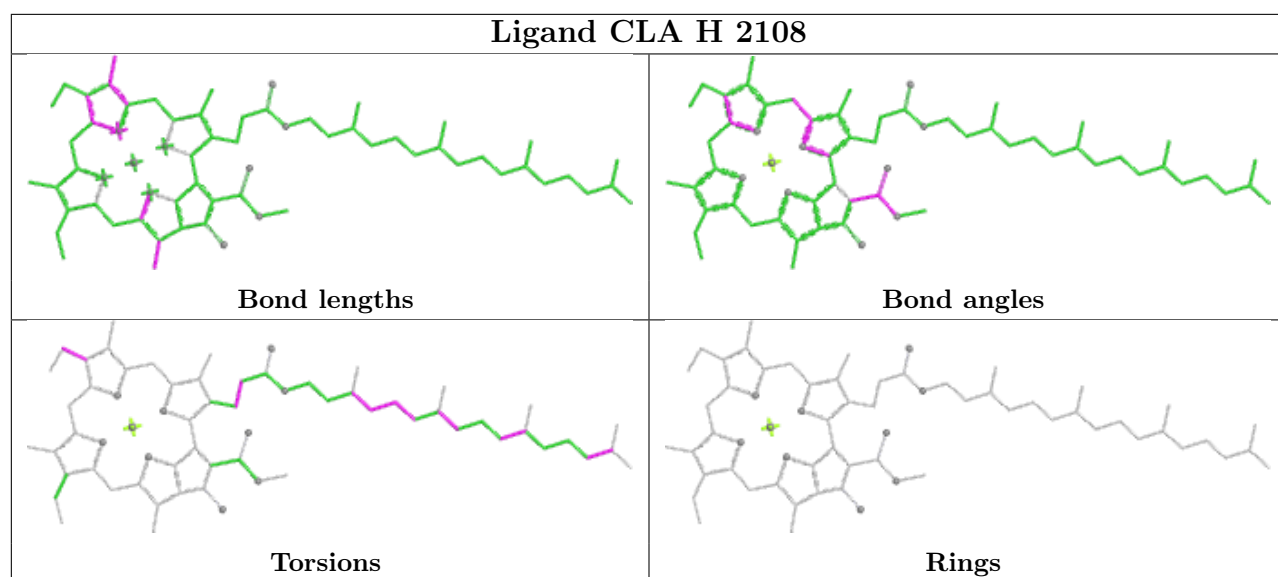


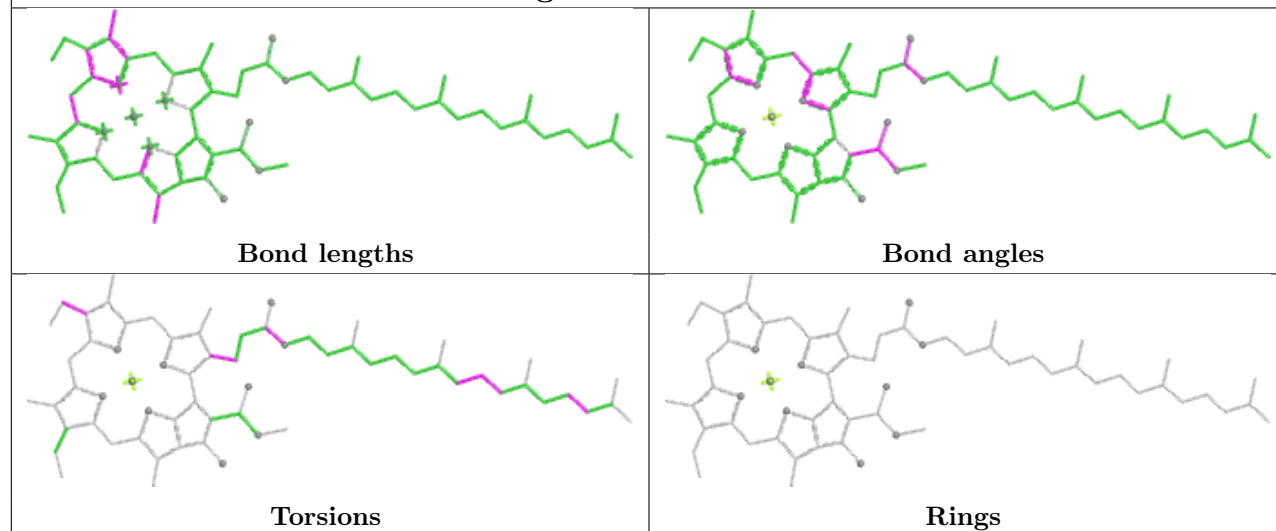
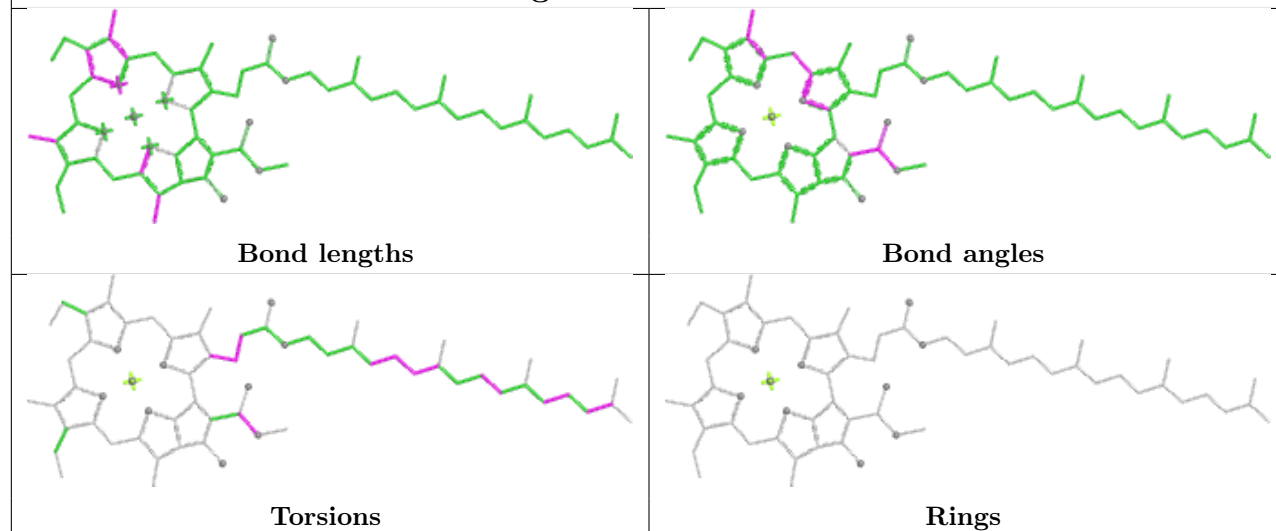


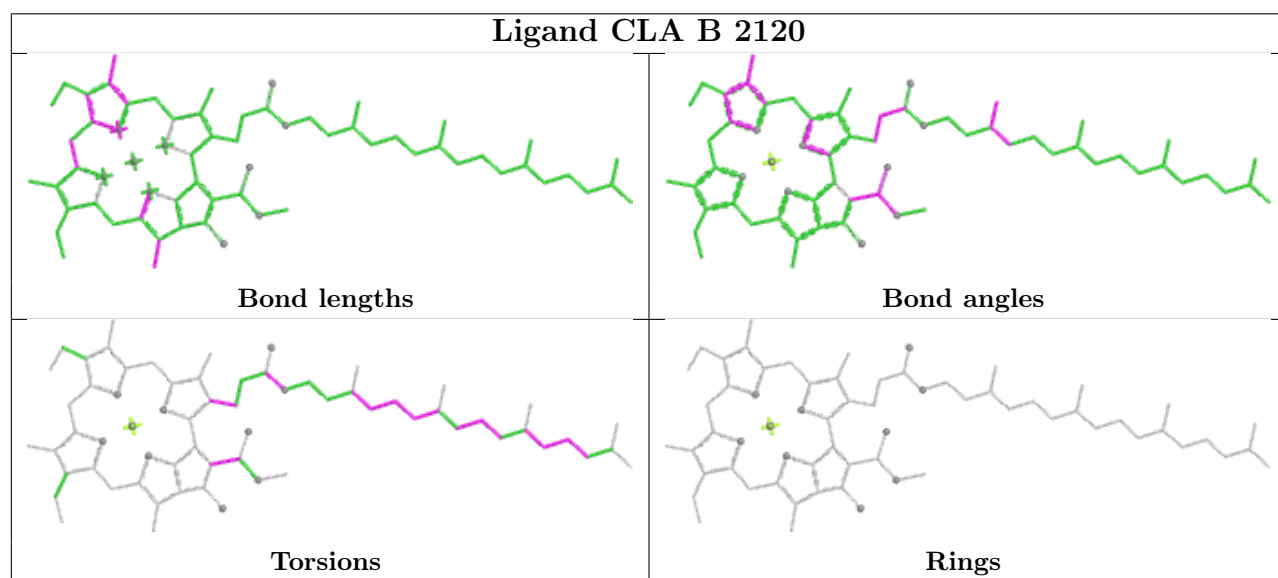
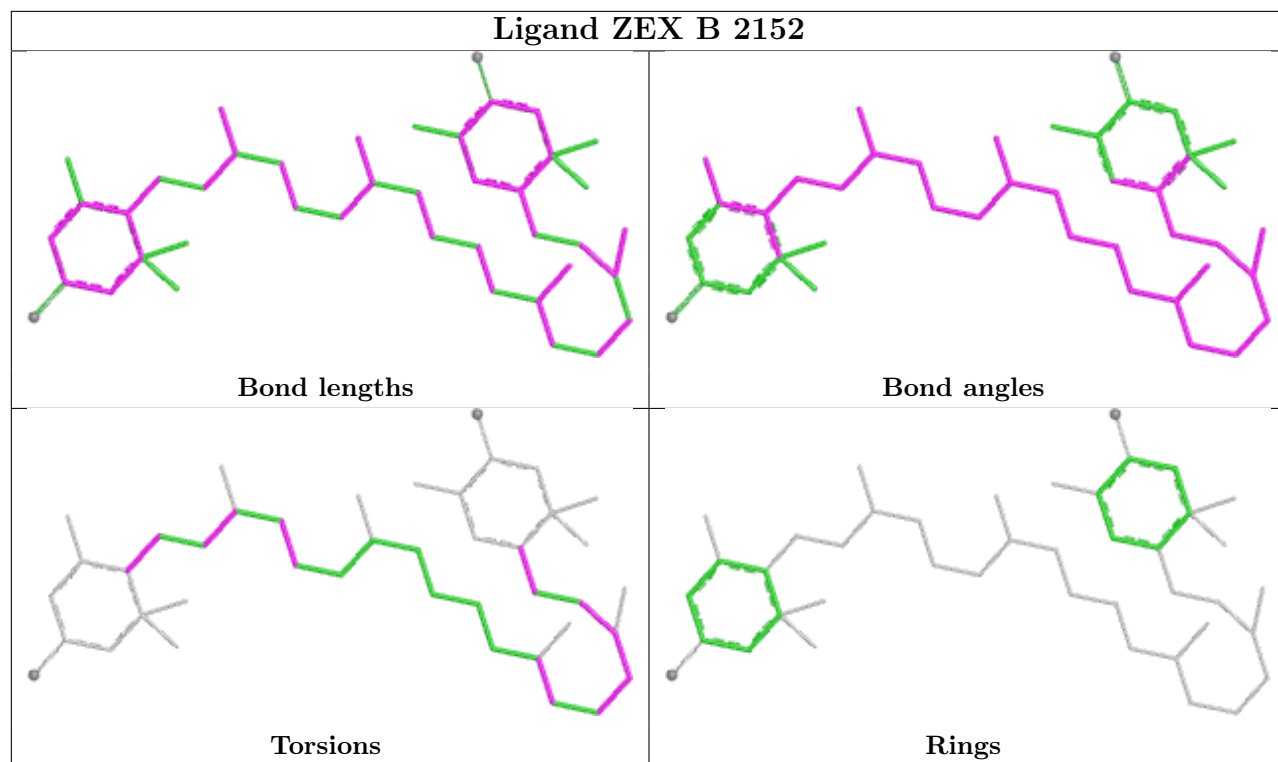


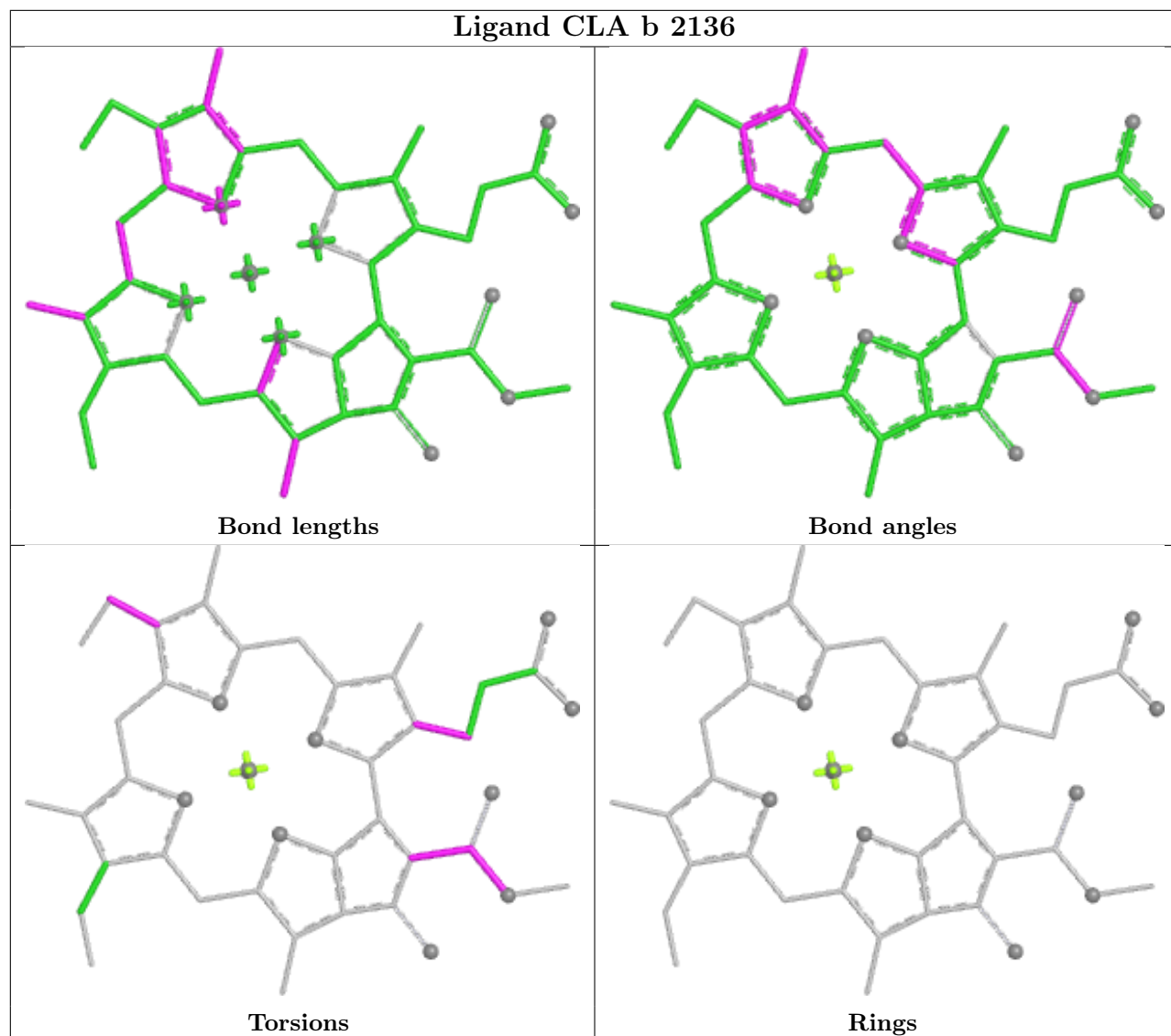




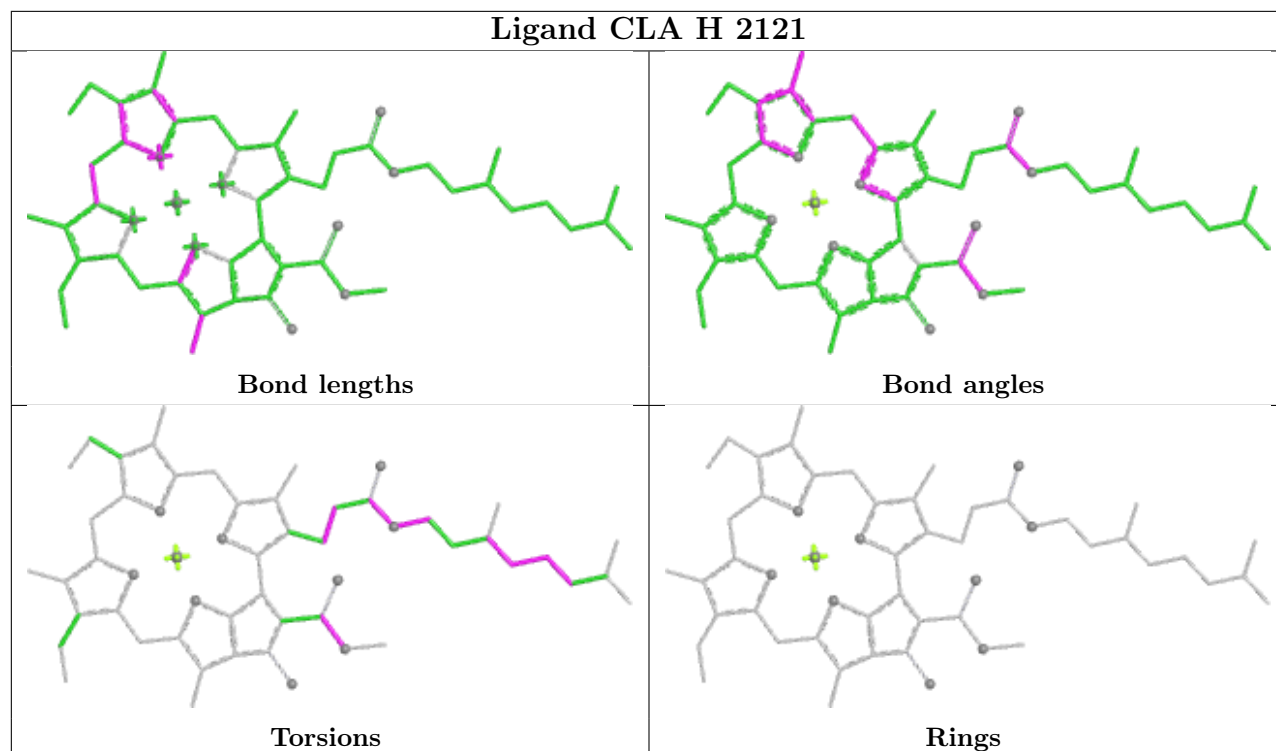


Ligand CLA a 802**Ligand CLA A 829**

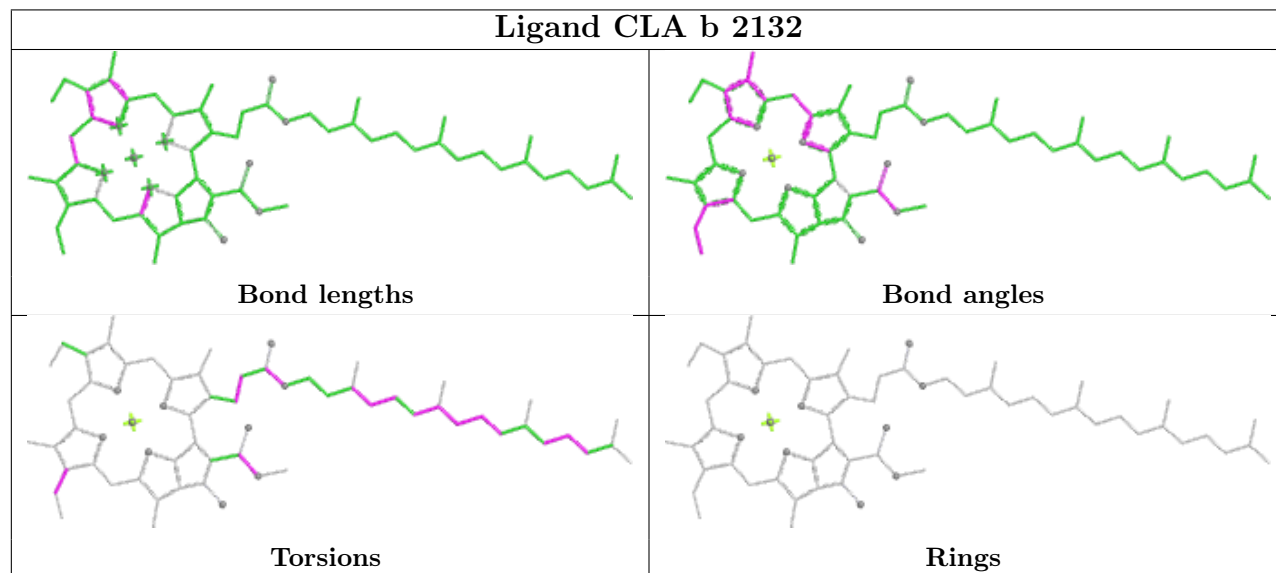




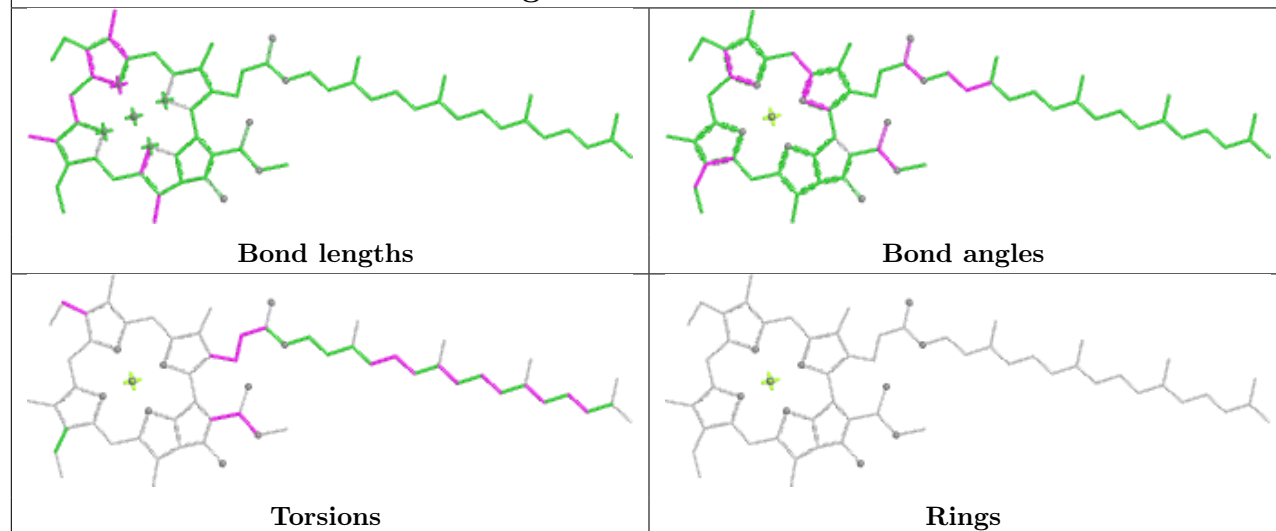
Ligand CLA H 2121



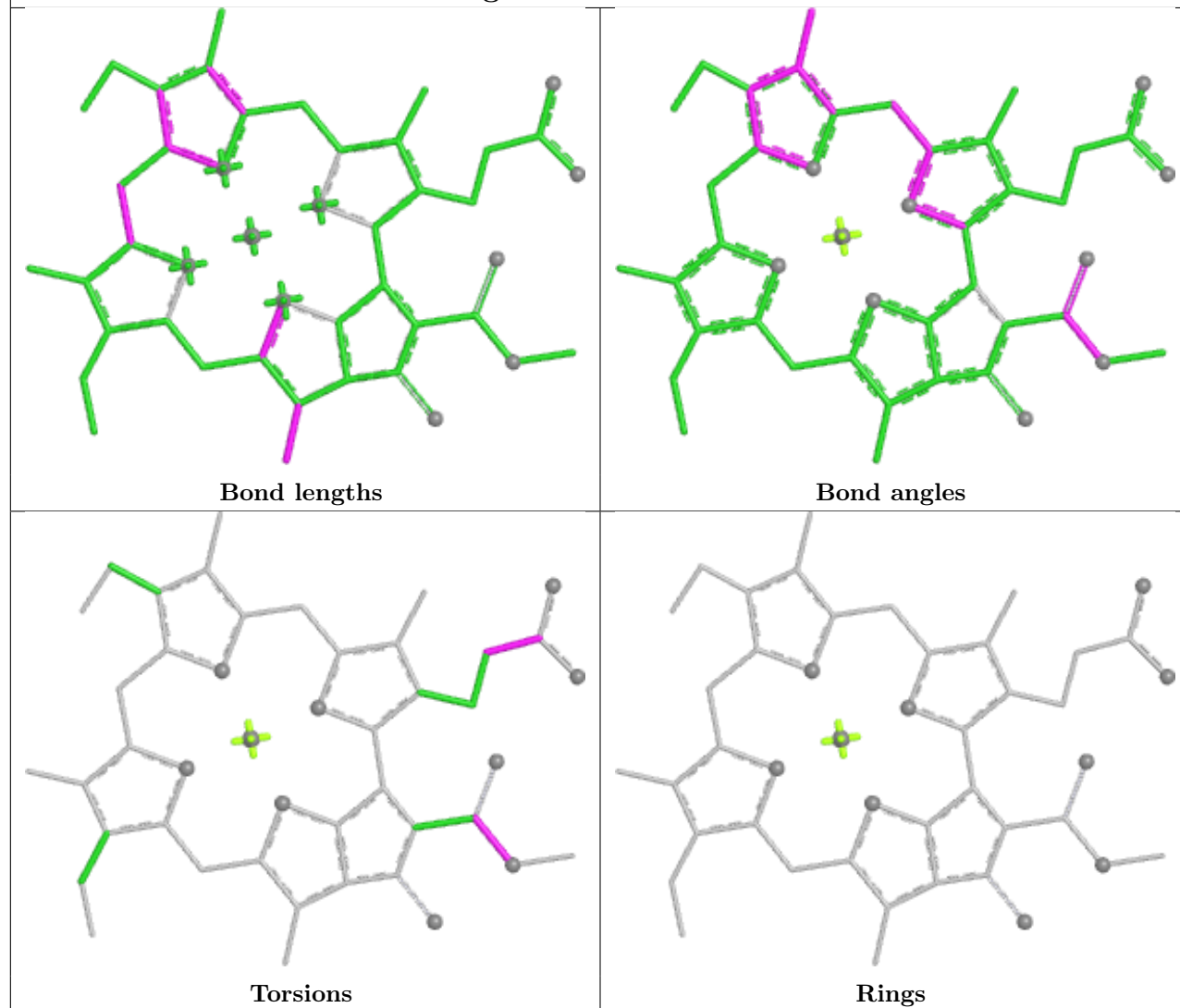
Ligand CLA b 2132



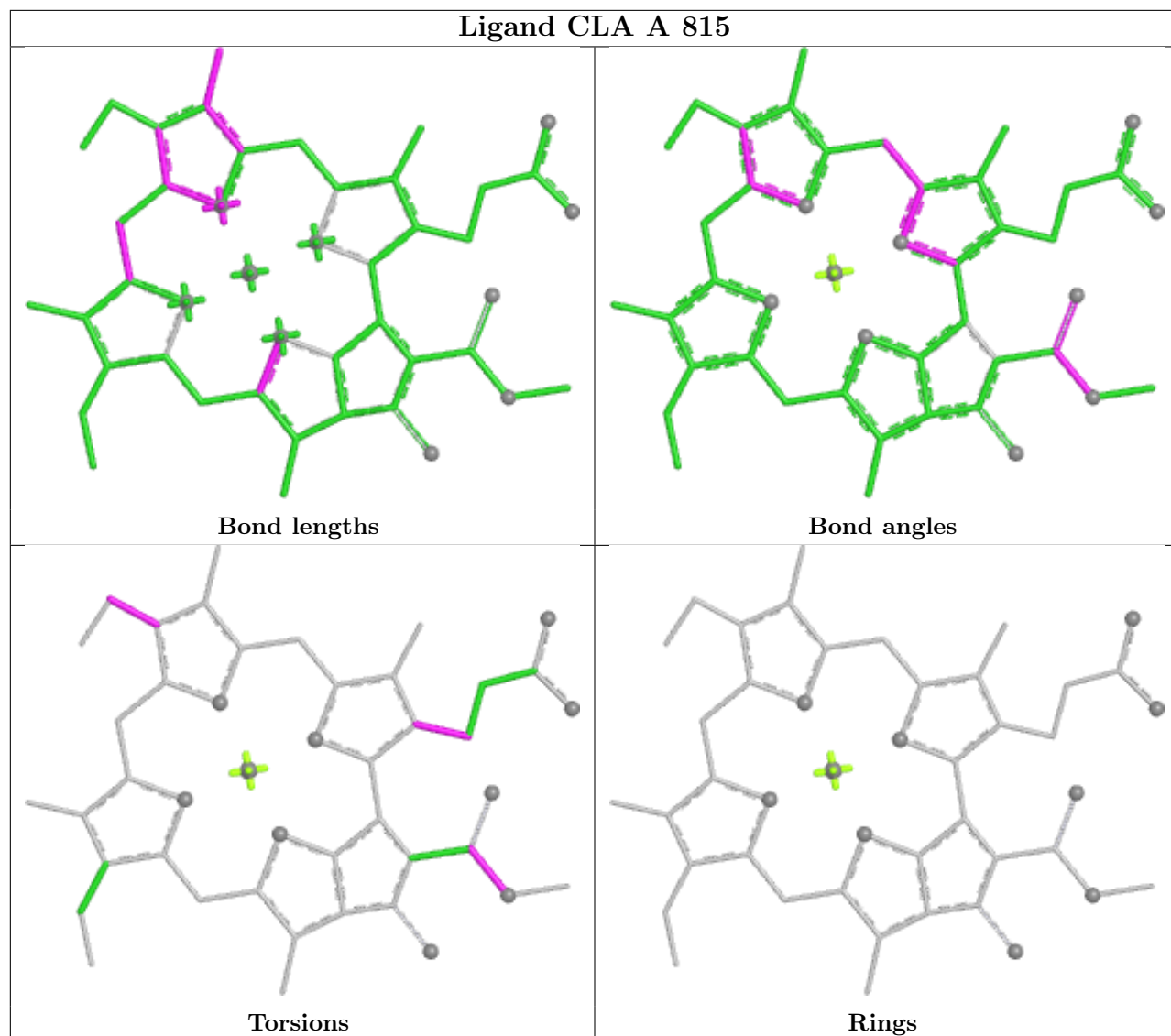
Ligand CLA H 2114



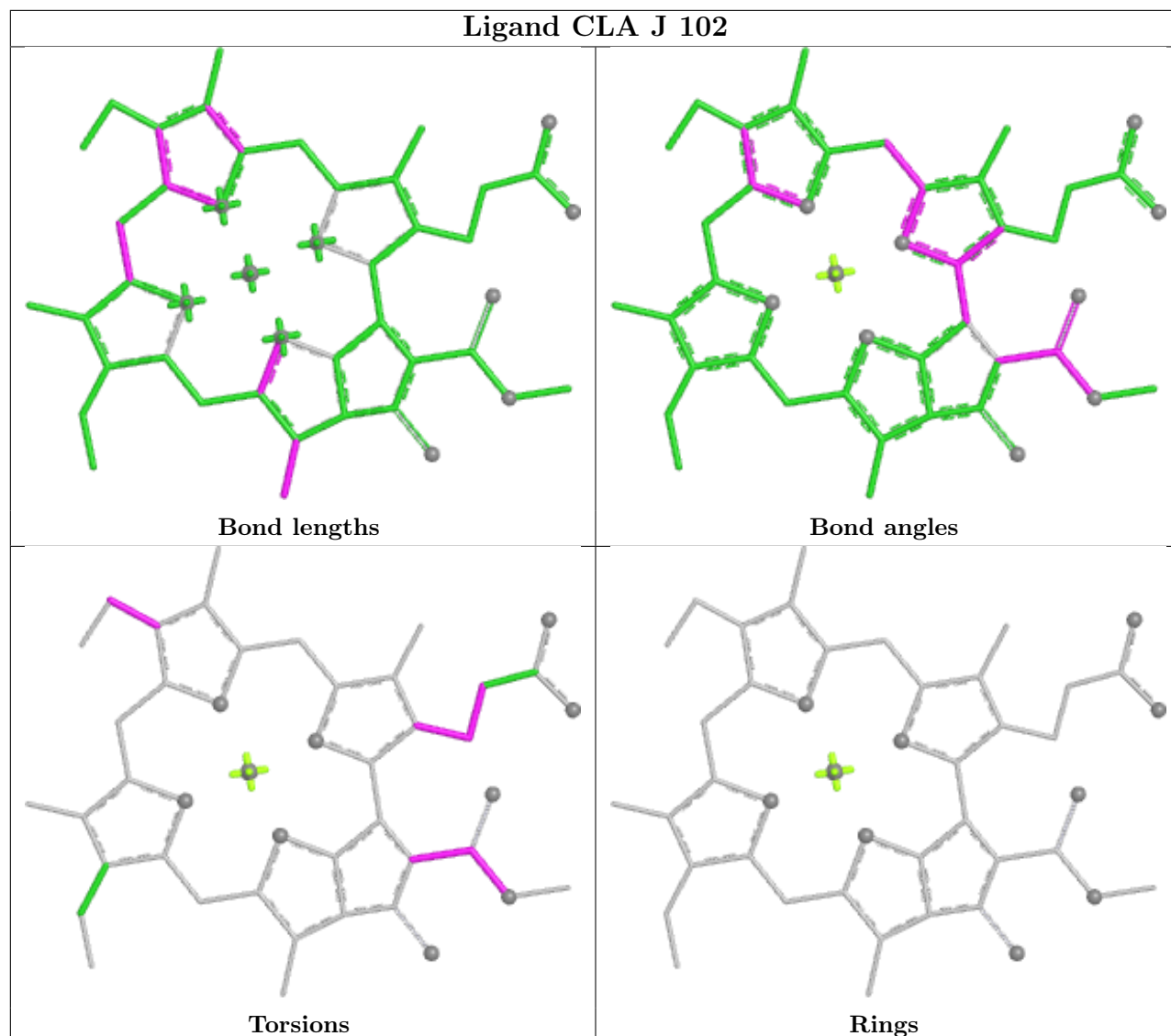
Ligand CLA H 2134



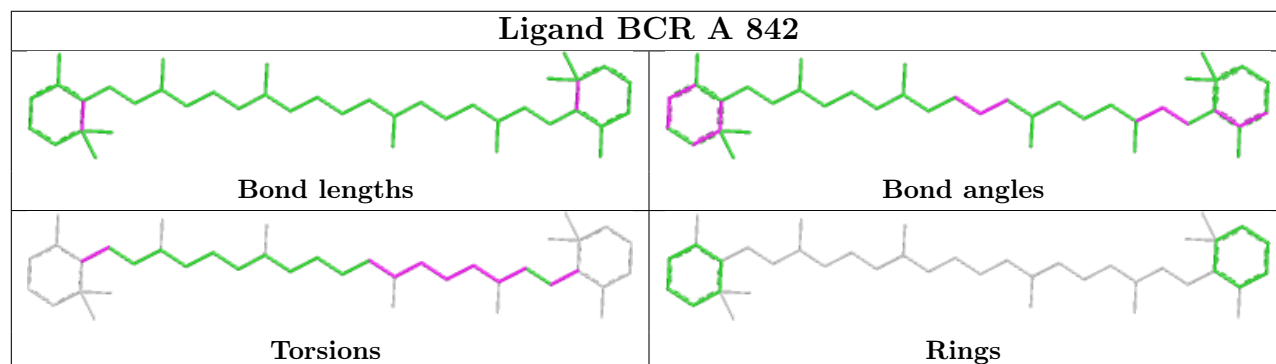
Ligand CLA A 815

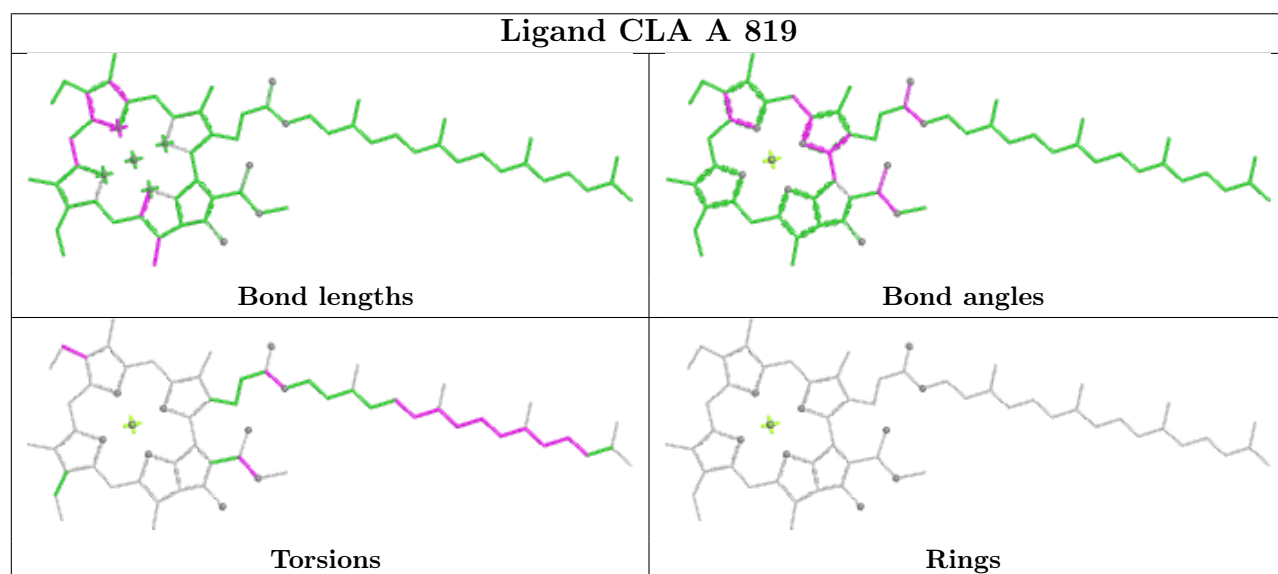
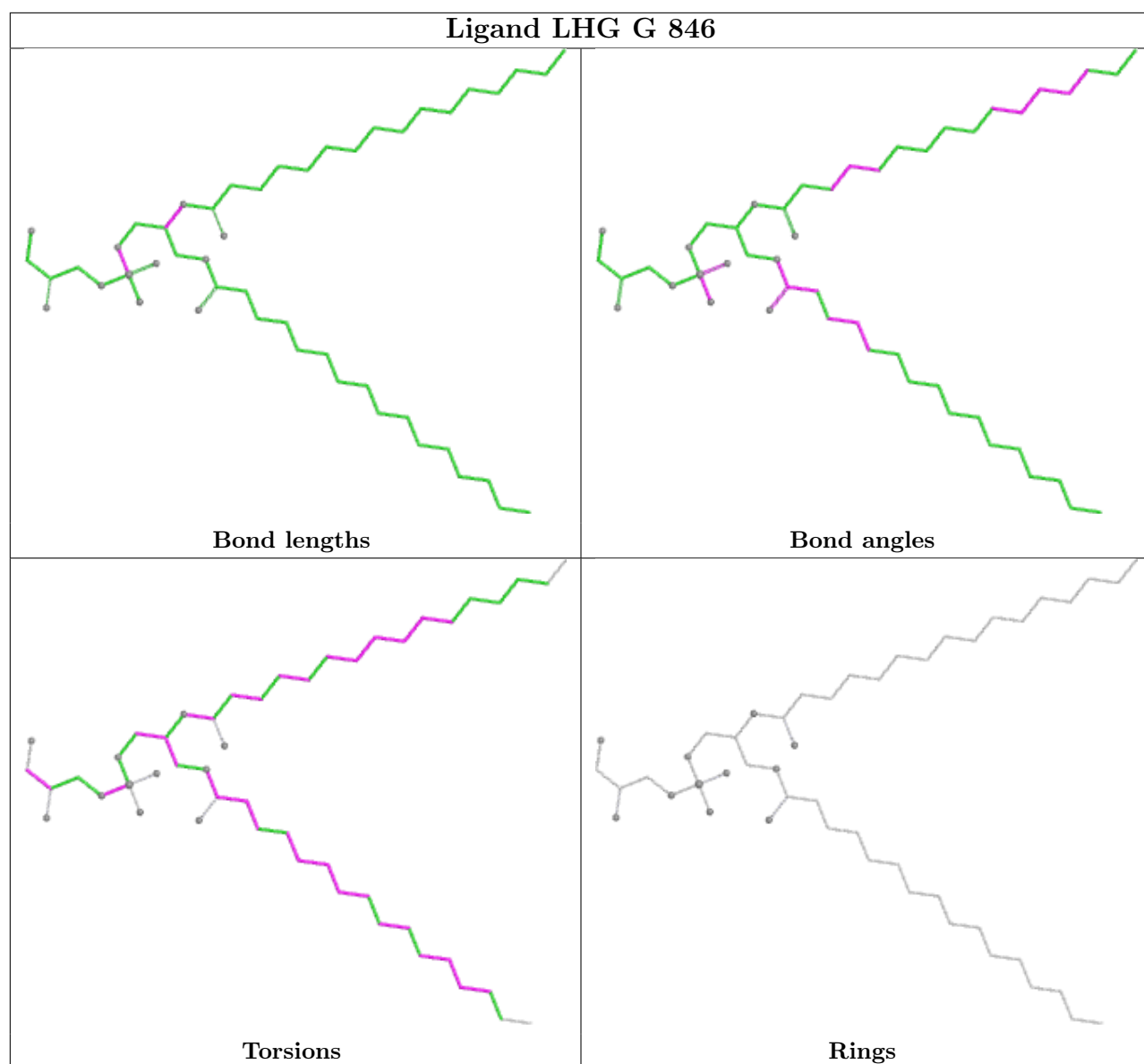


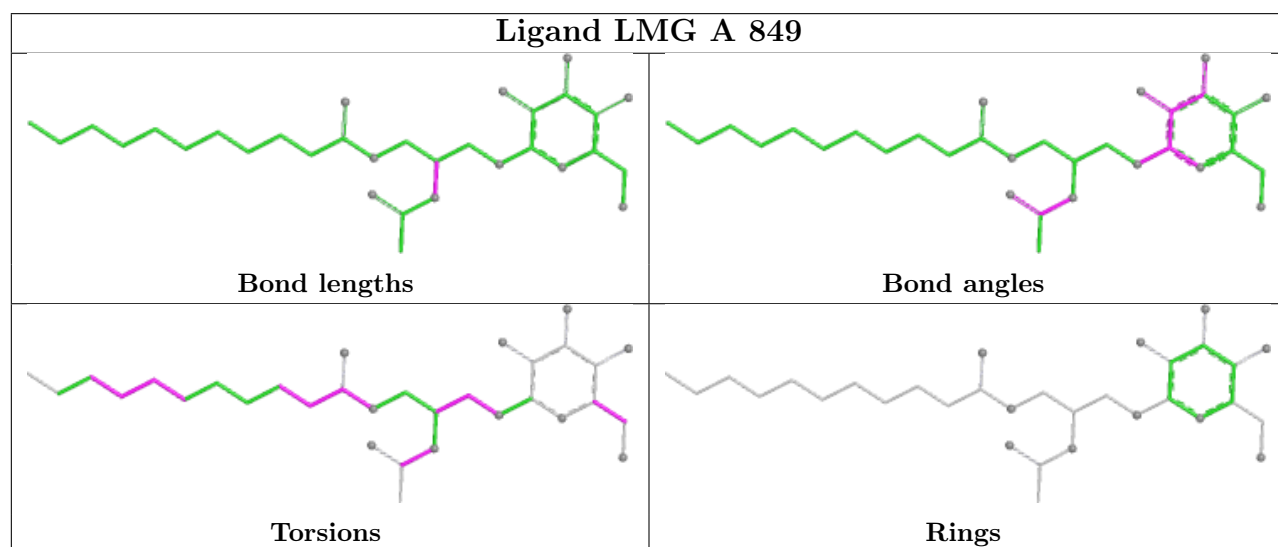
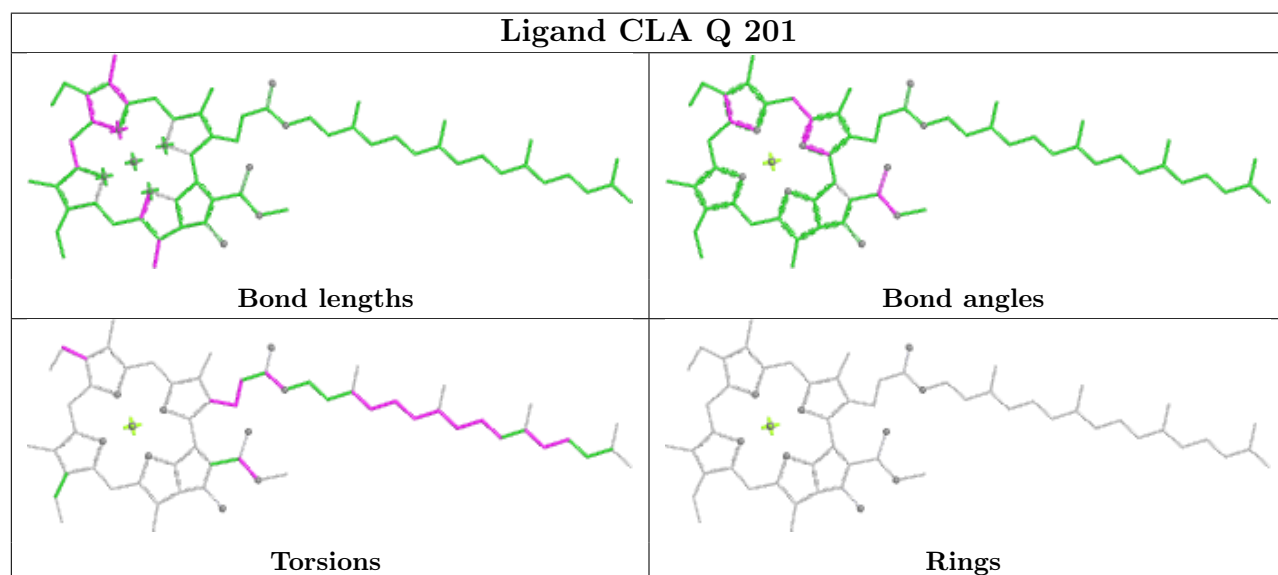
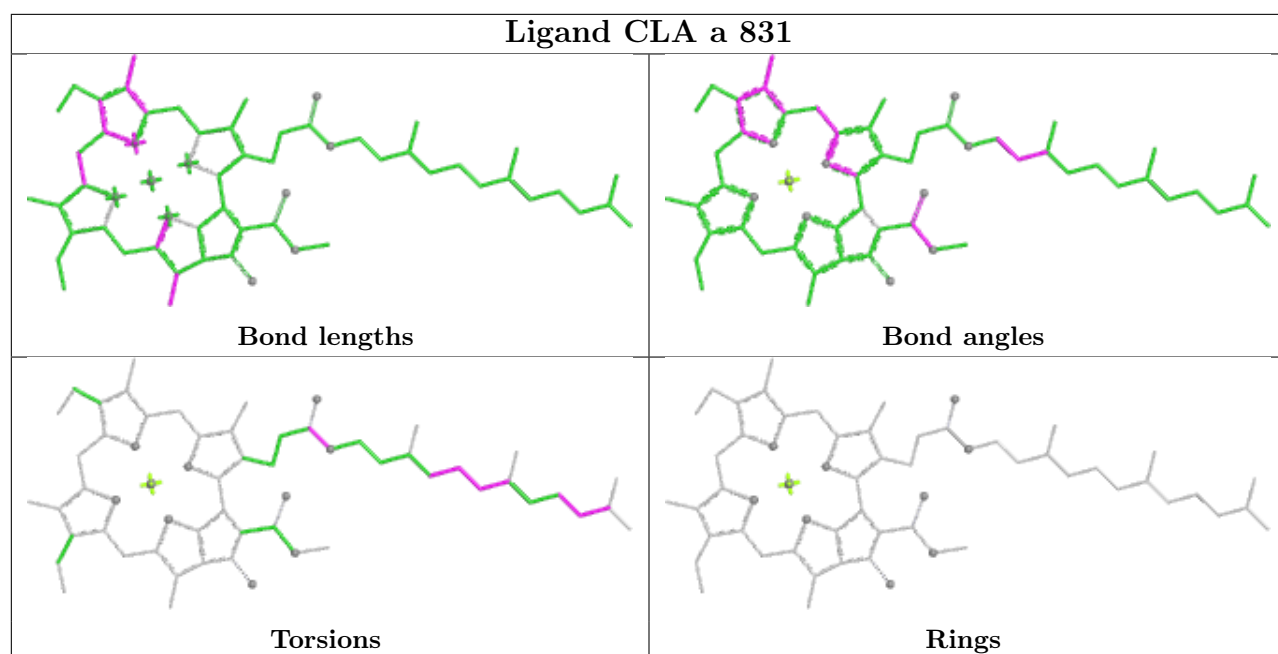
Ligand CLA J 102



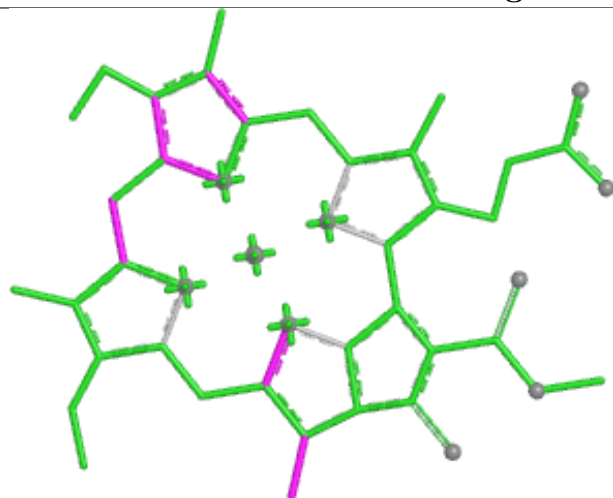
Ligand BCR A 842



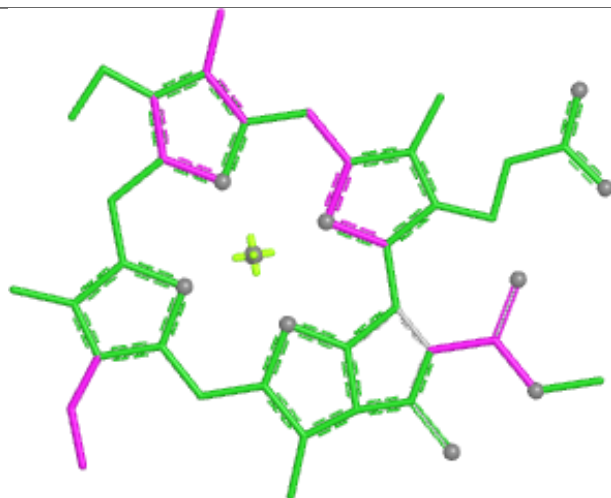




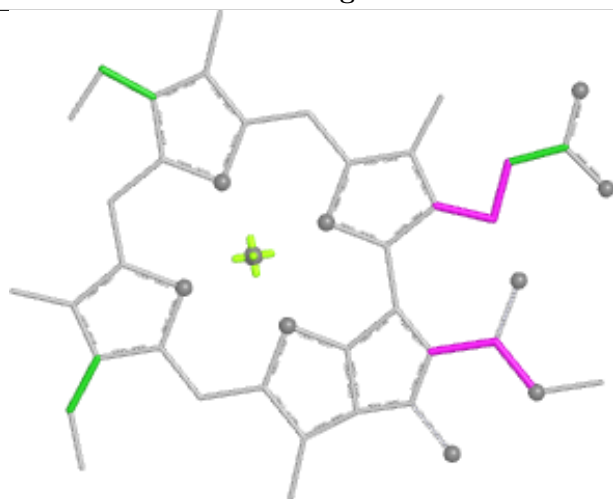
Ligand CLA B 2142



Bond lengths



Bond angles

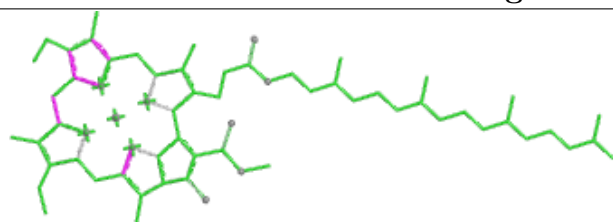


Torsions

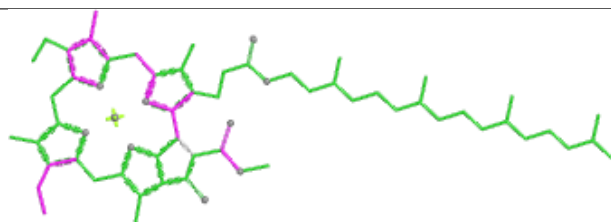


Rings

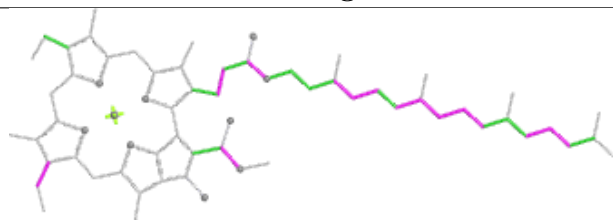
Ligand CLA B 2133



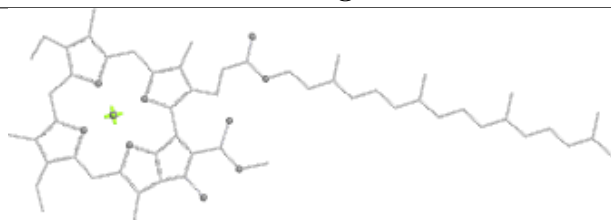
Bond lengths



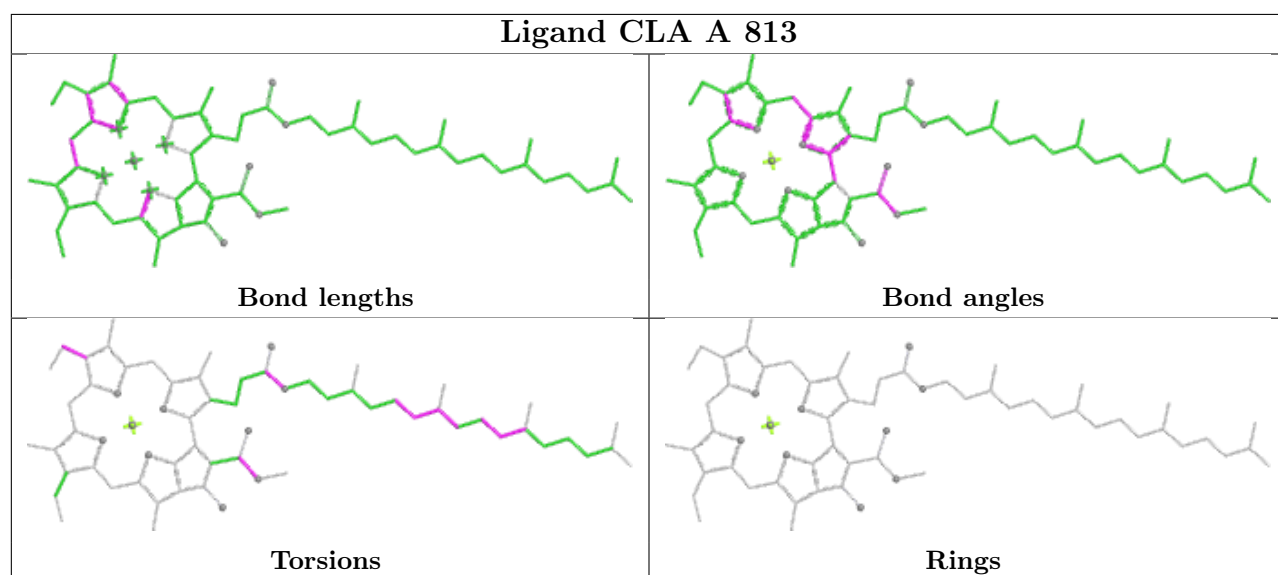
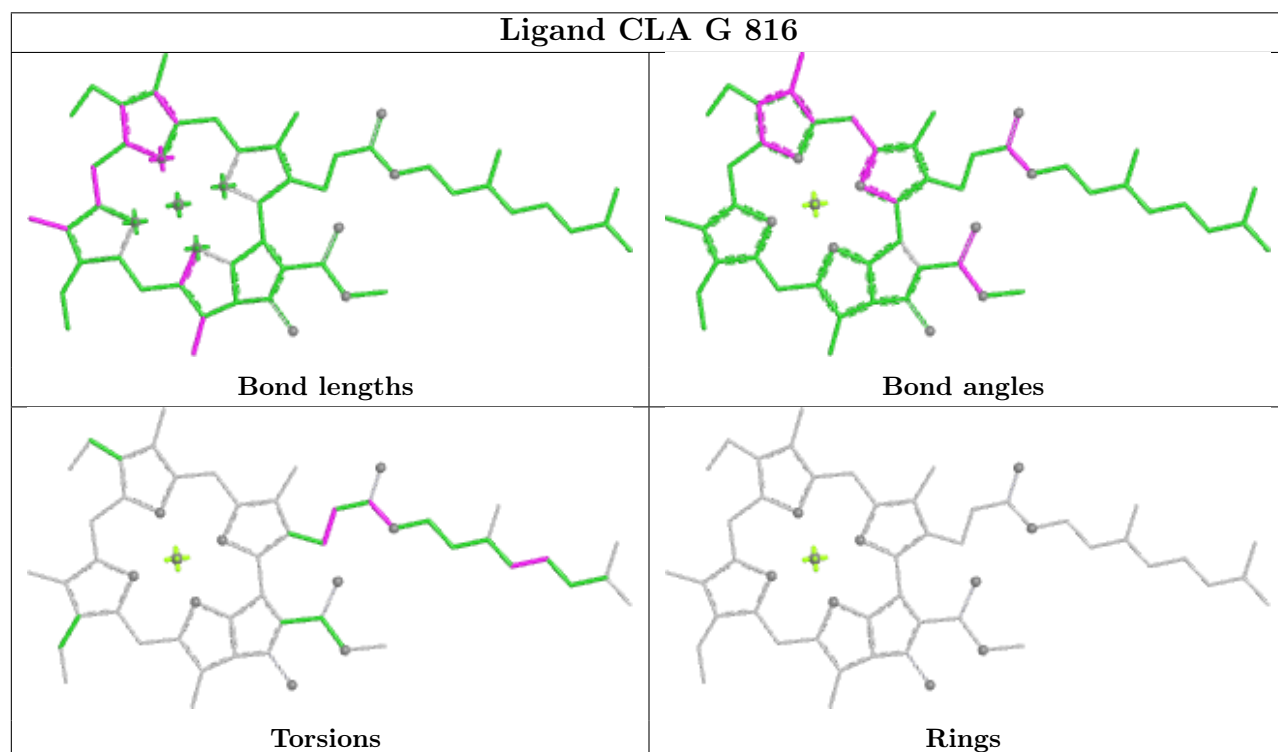
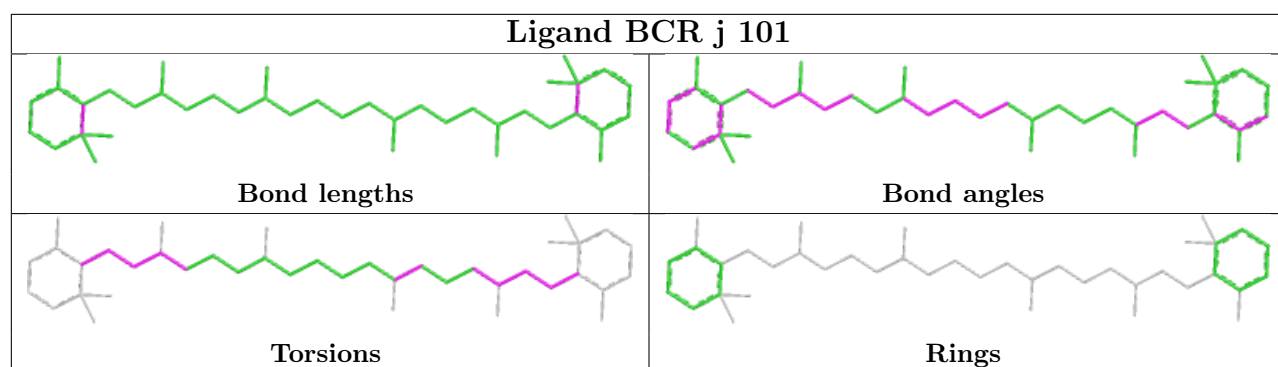
Bond angles

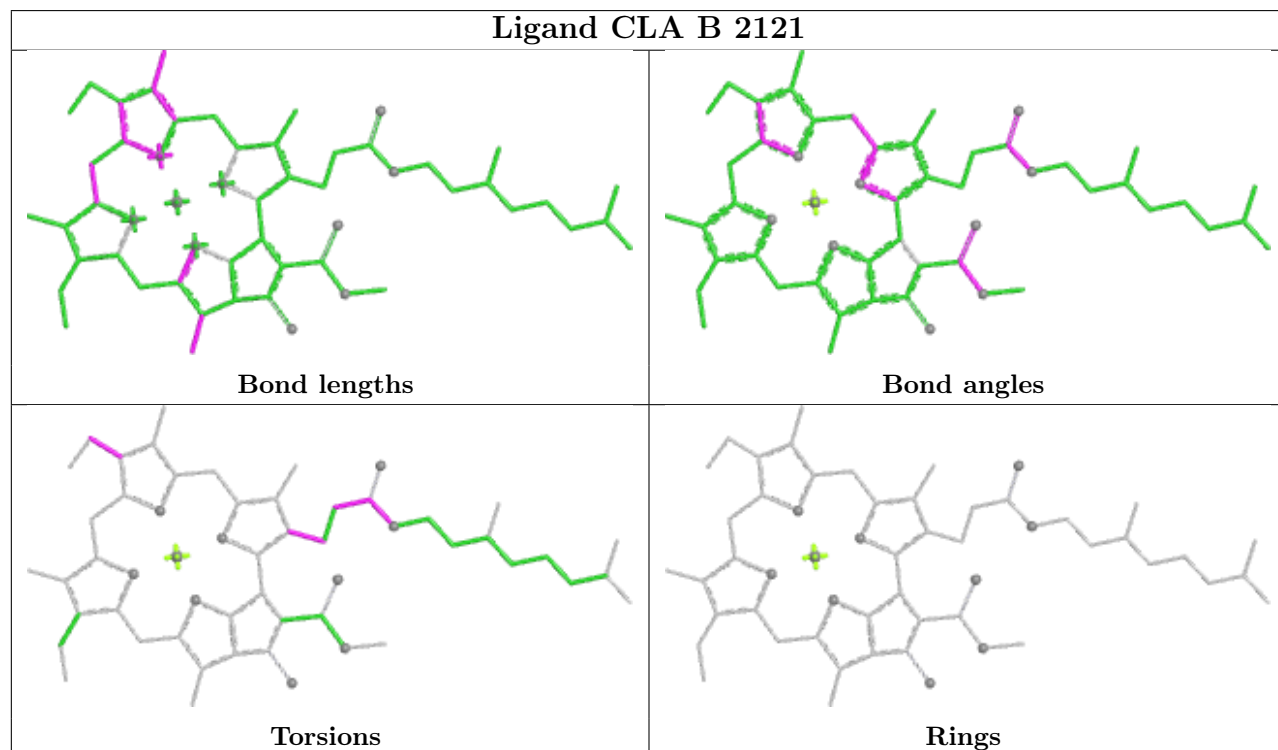
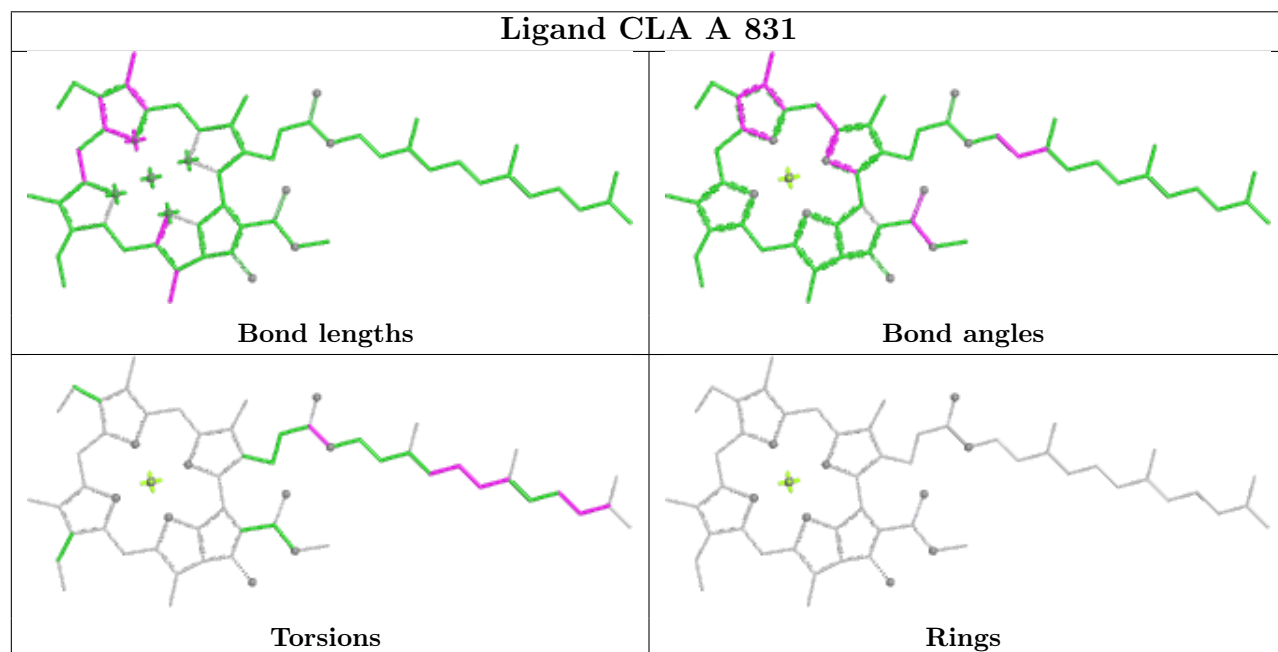
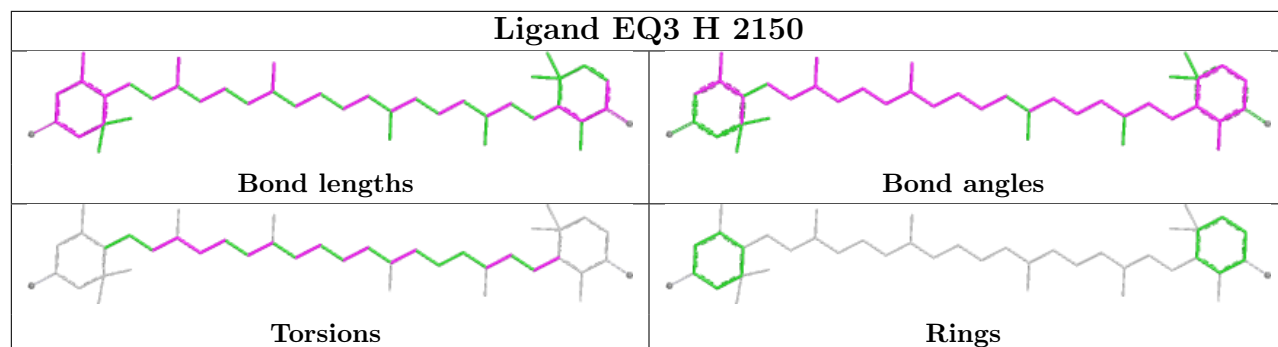


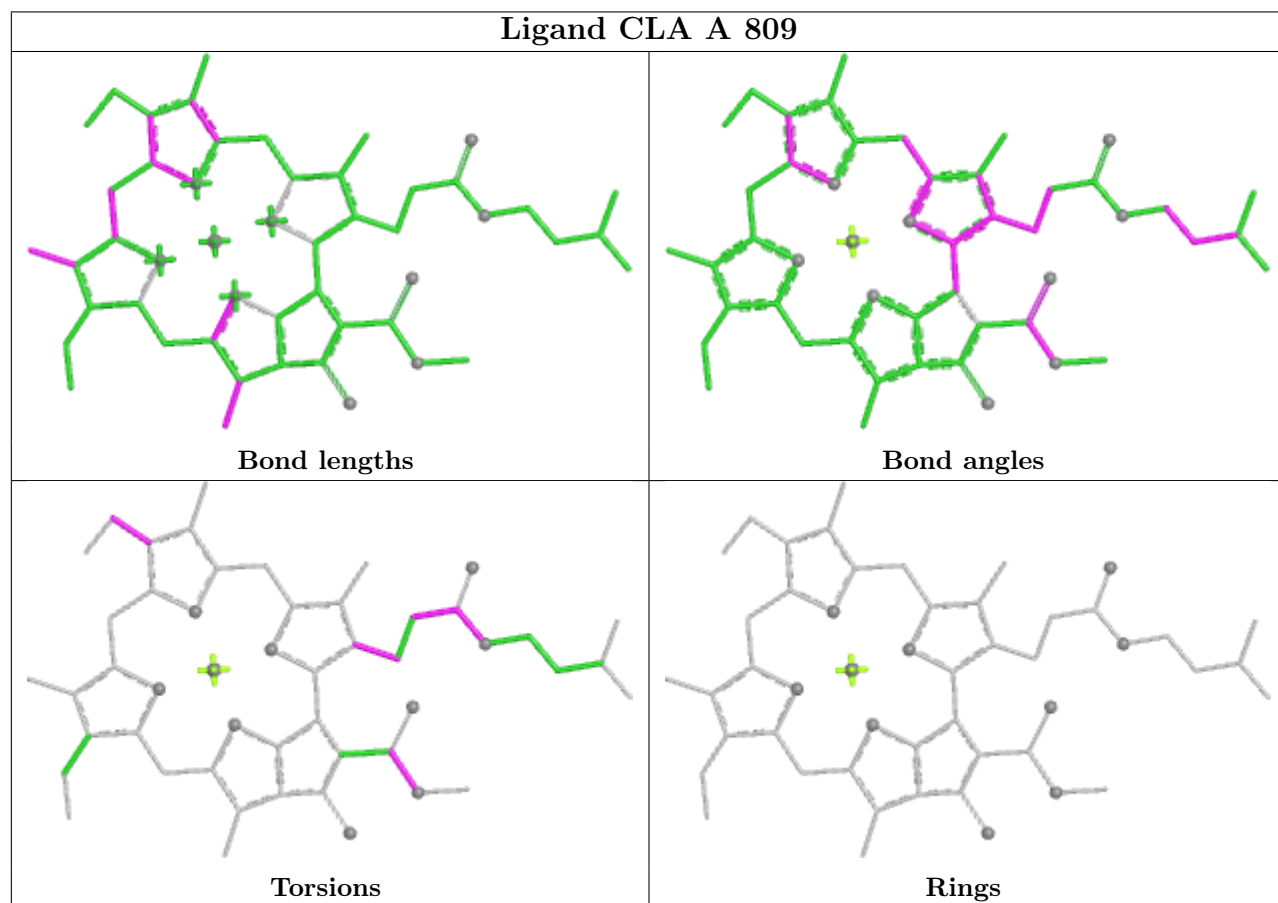
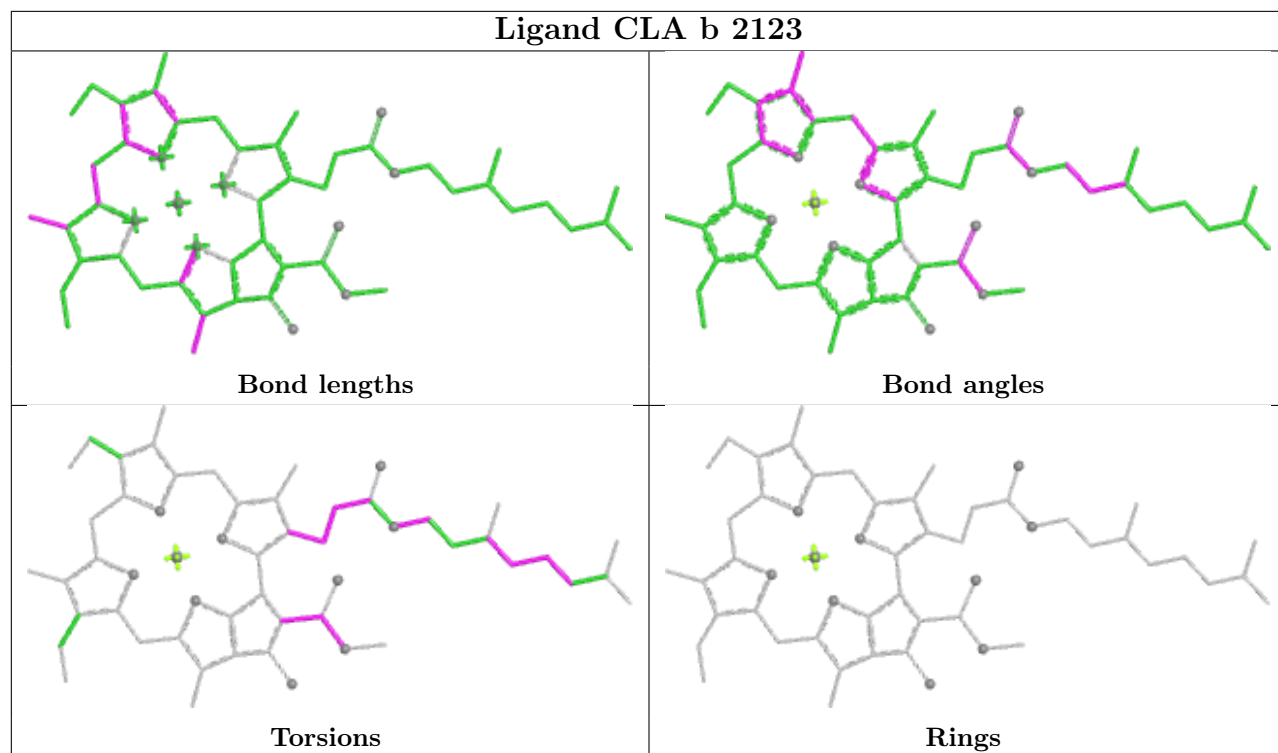
Torsions



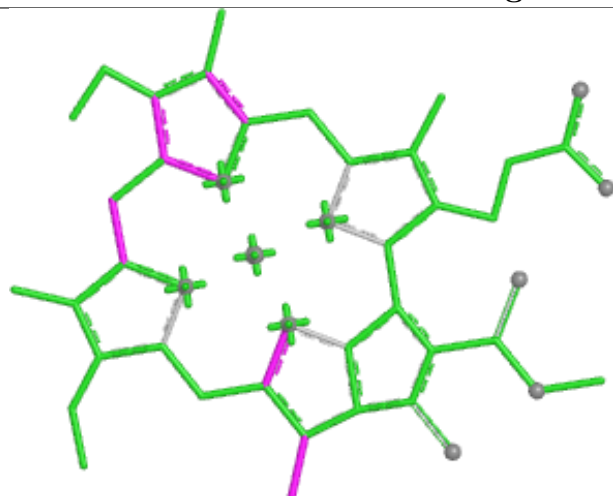
Rings



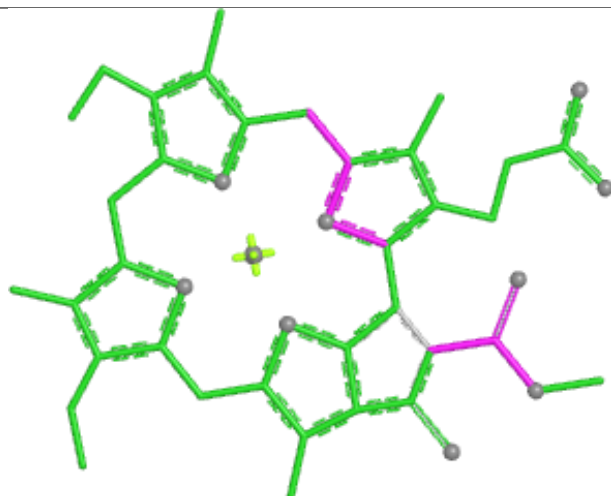




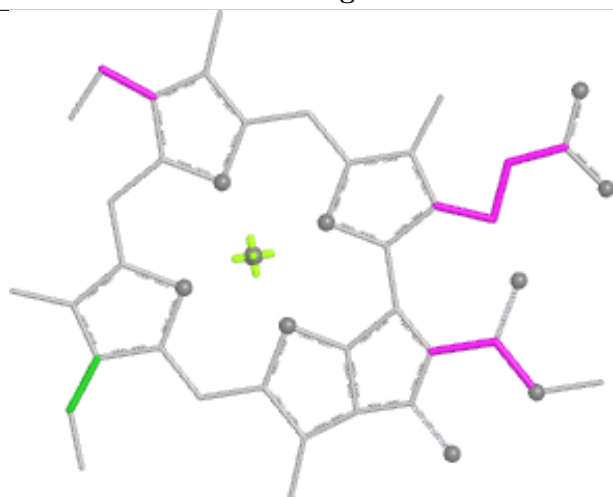
Ligand CLA B 2114



Bond lengths



Bond angles

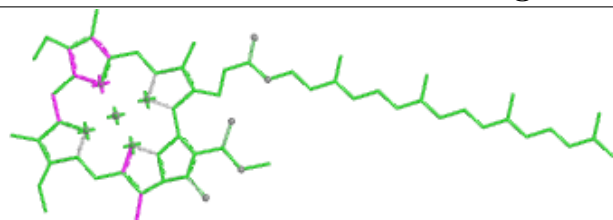


Torsions

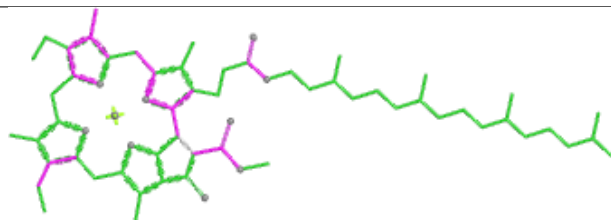


Rings

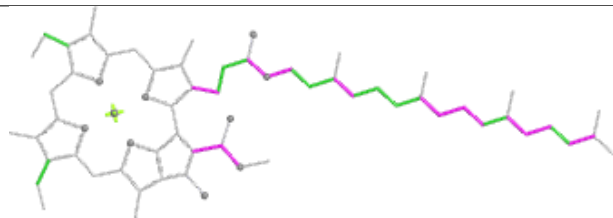
Ligand CLA A 824



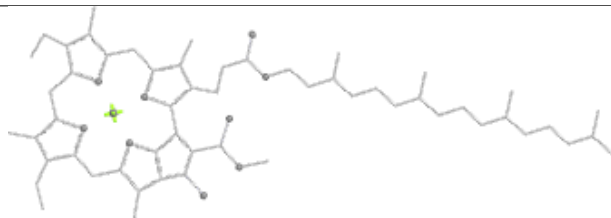
Bond lengths



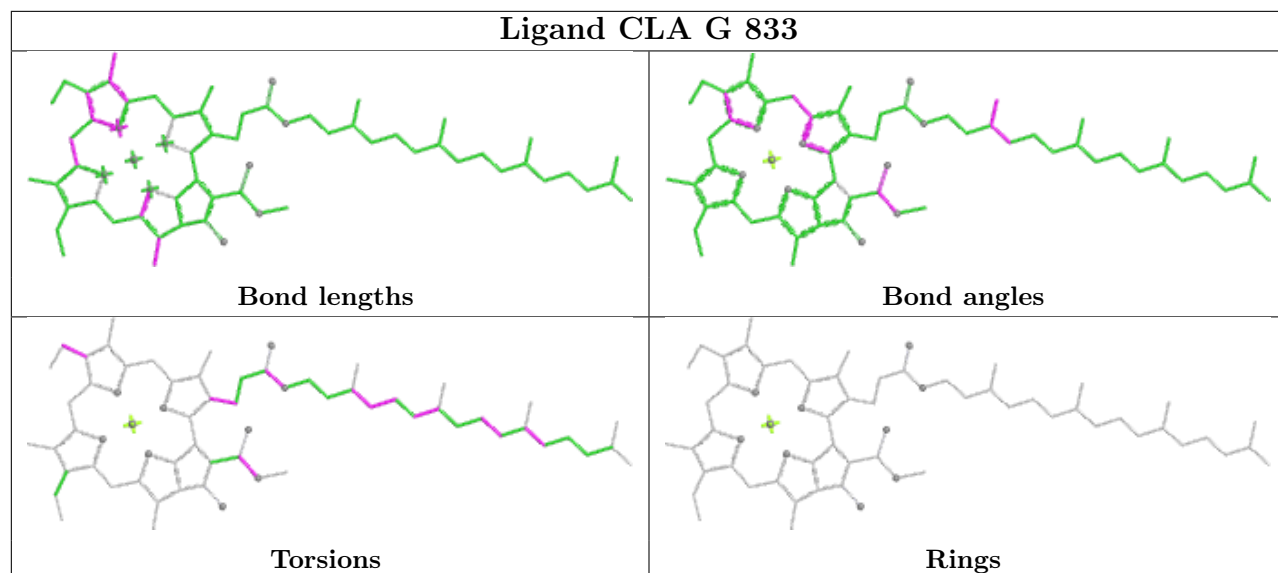
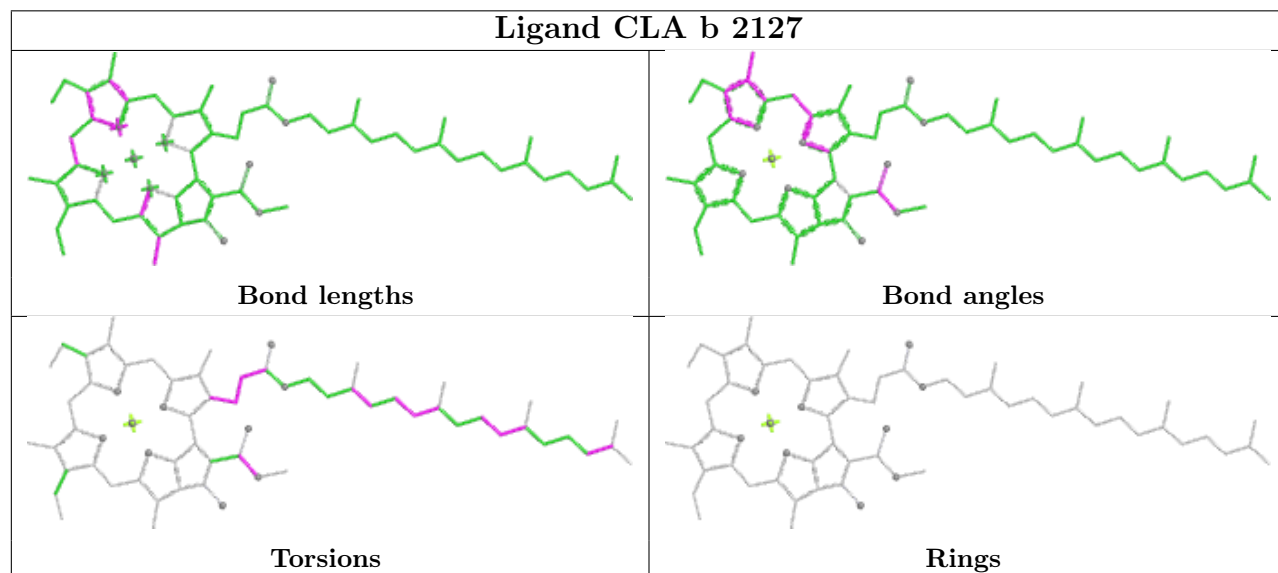
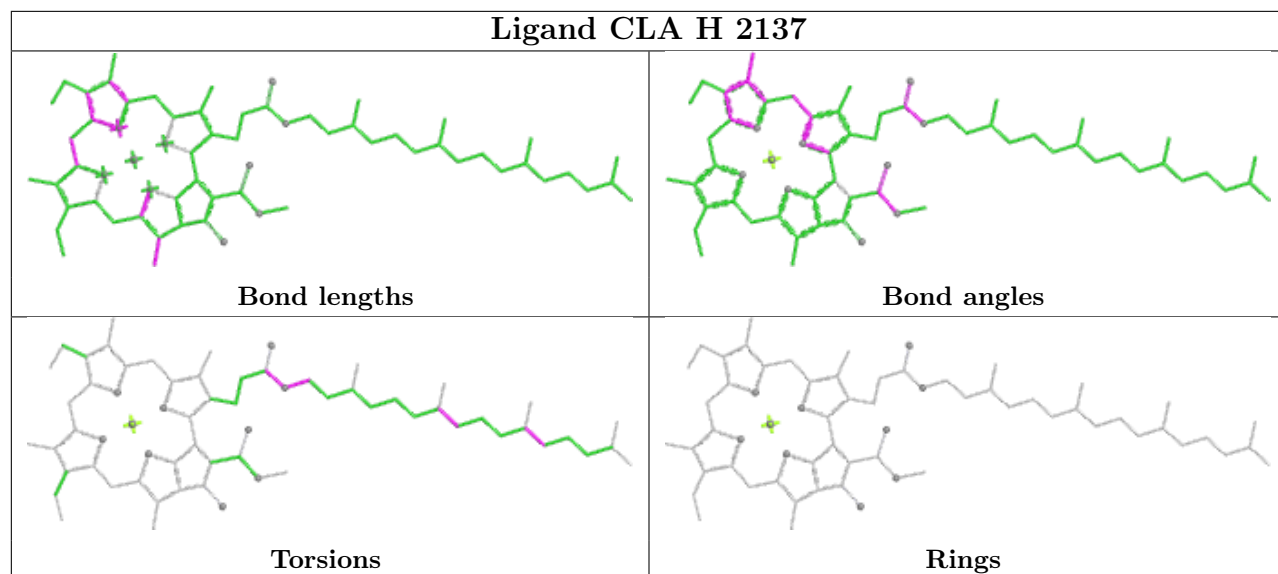
Bond angles

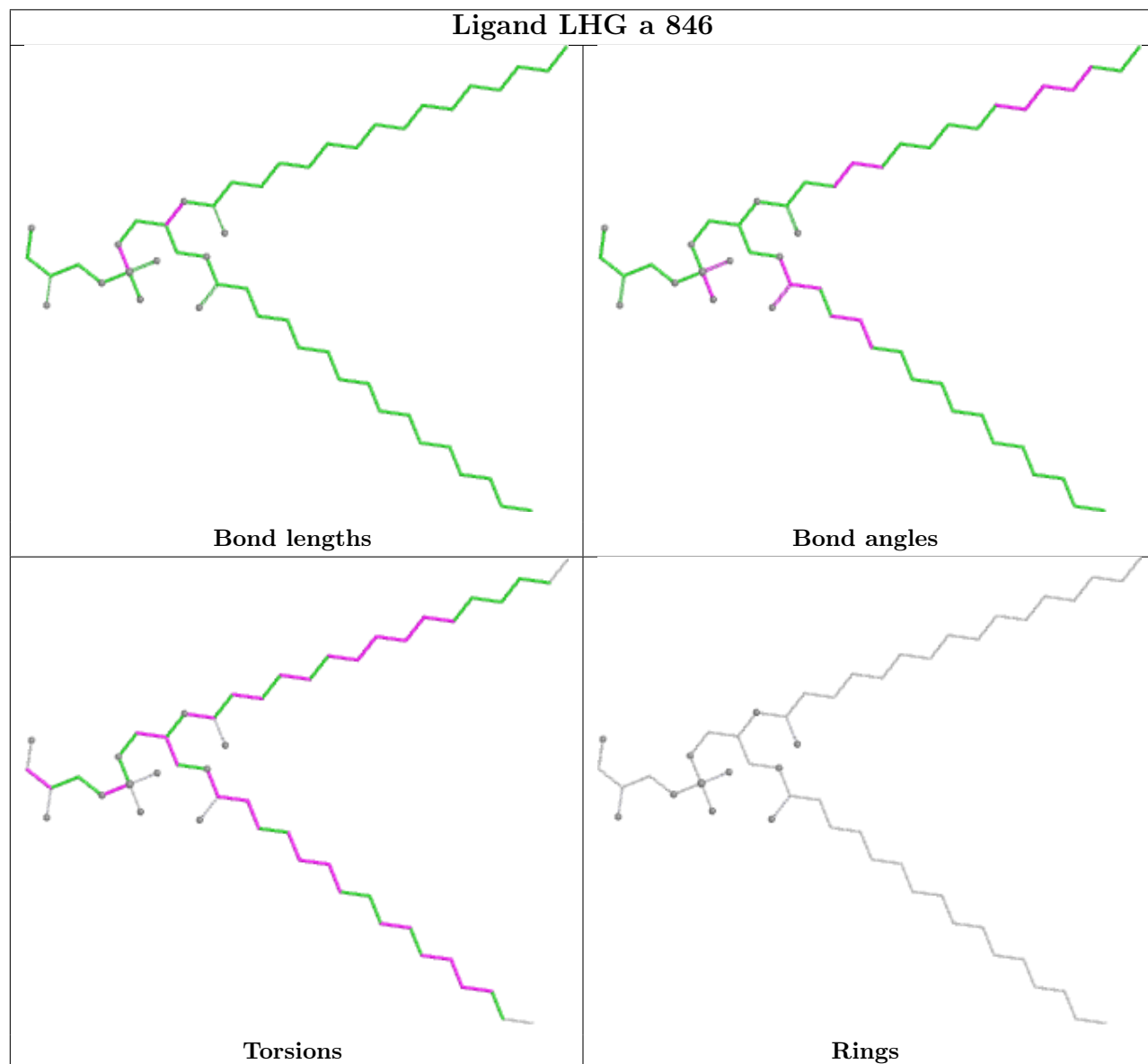
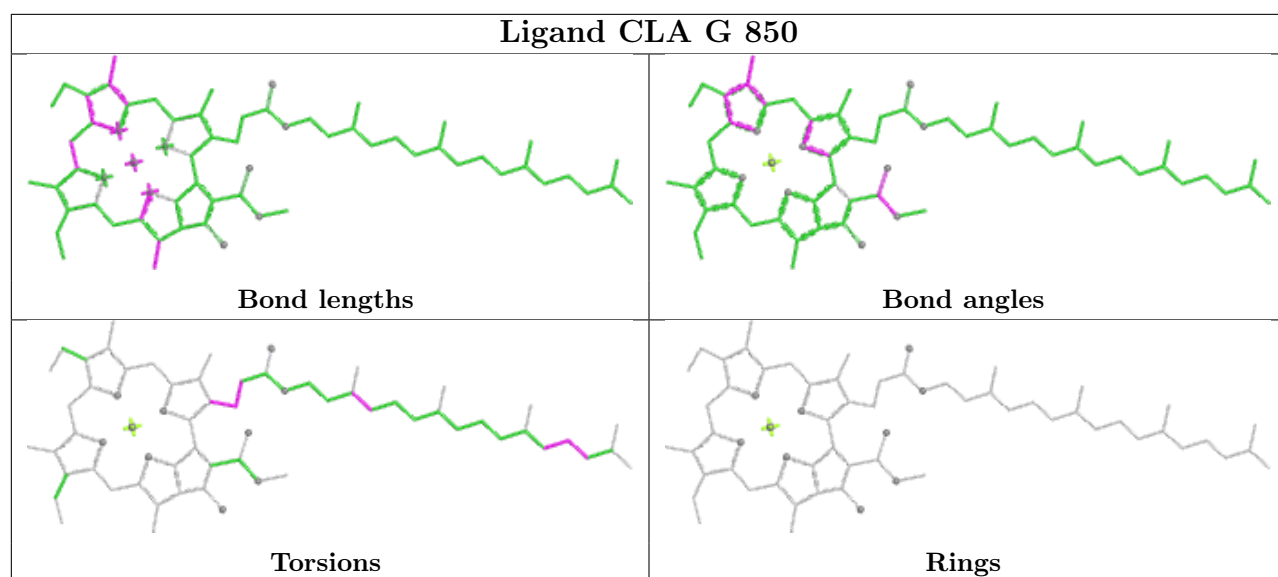


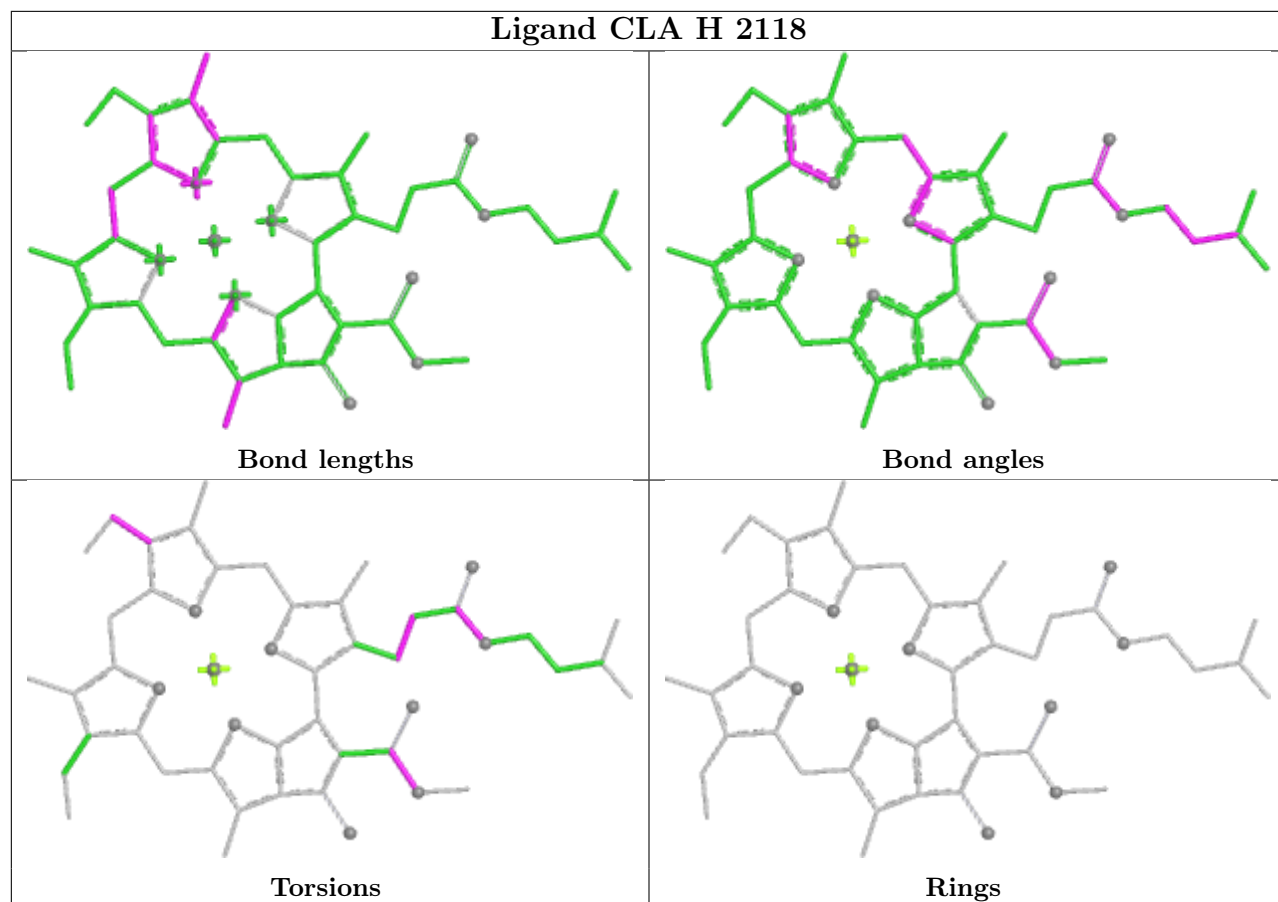
Torsions



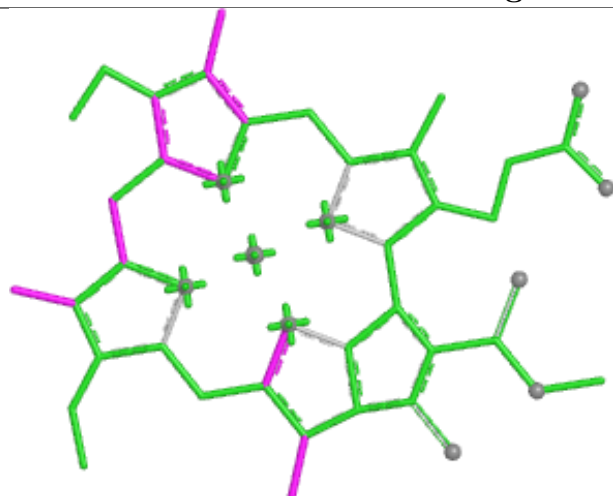
Rings



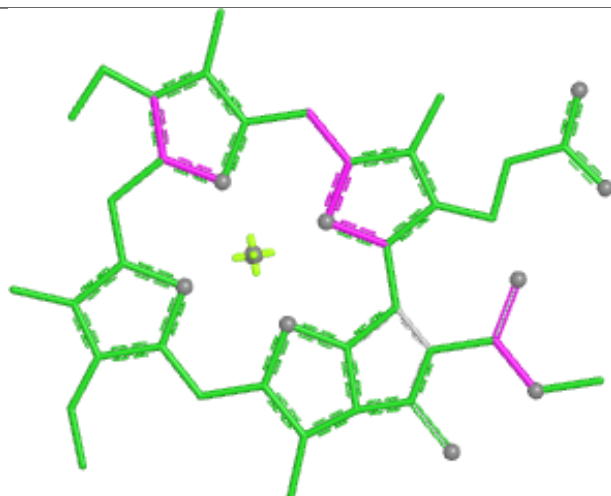




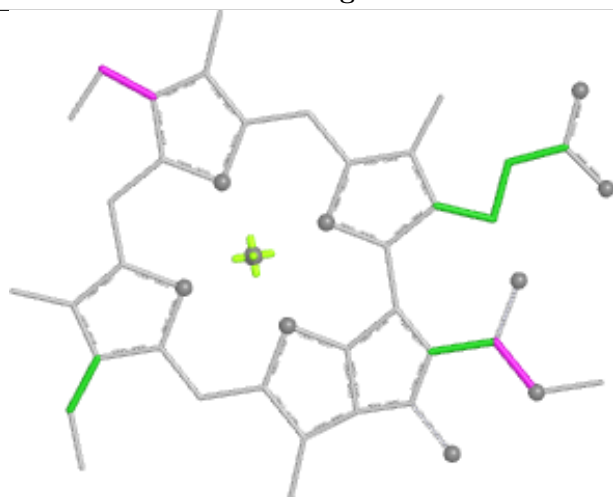
Ligand CLA B 2116



Bond lengths



Bond angles

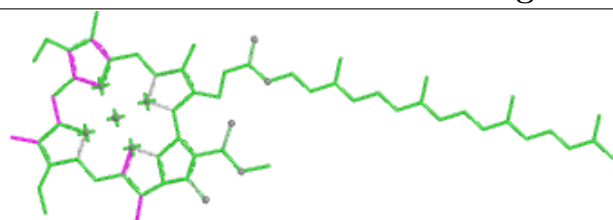


Torsions

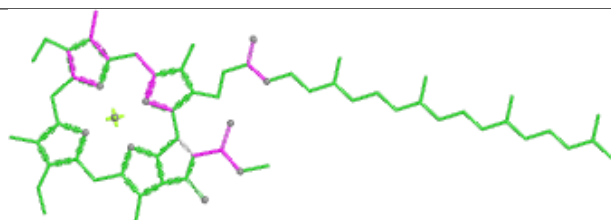


Rings

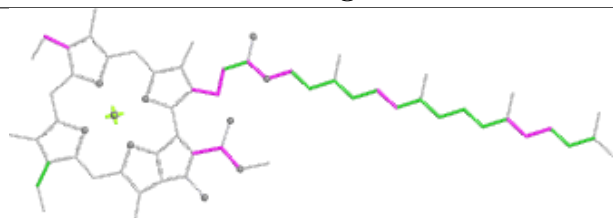
Ligand CLA L 201



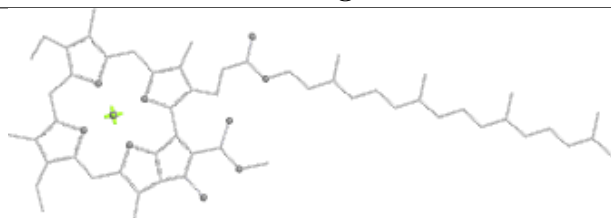
Bond lengths



Bond angles

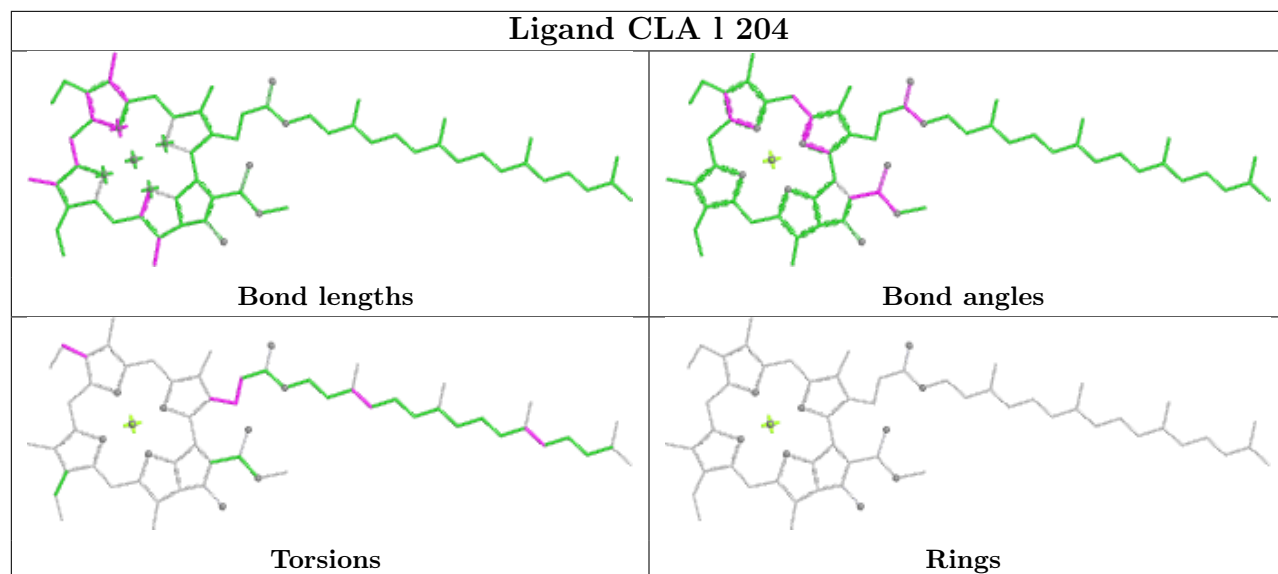


Torsions

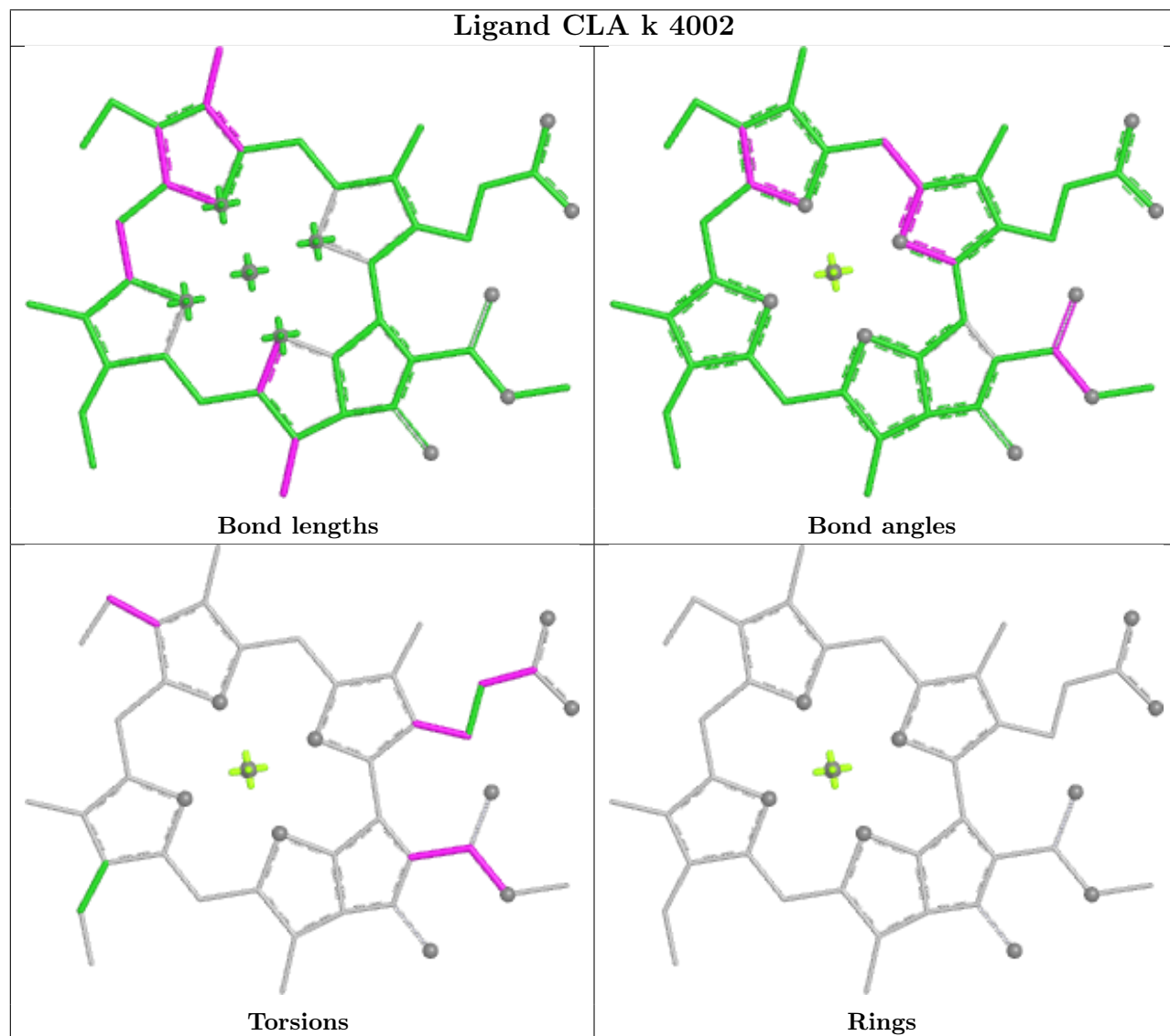


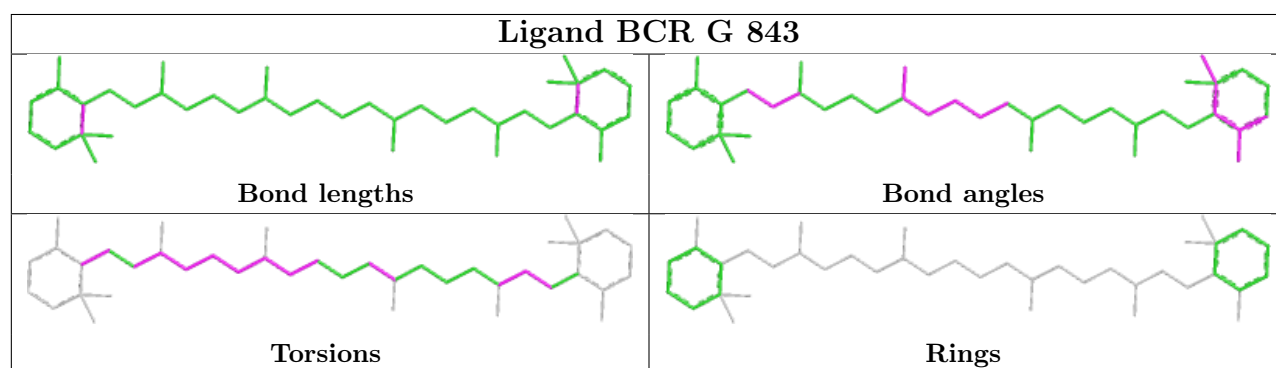
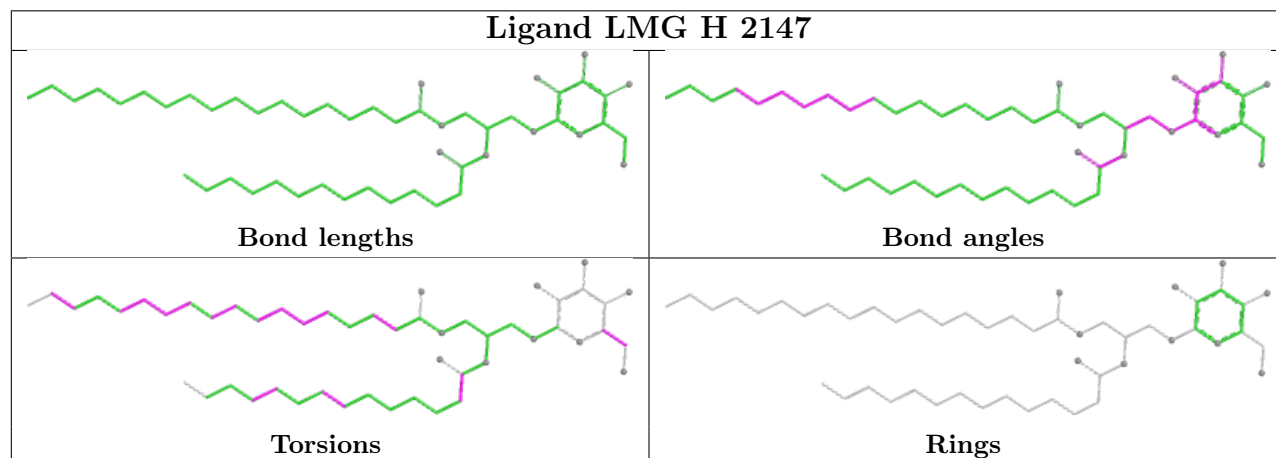
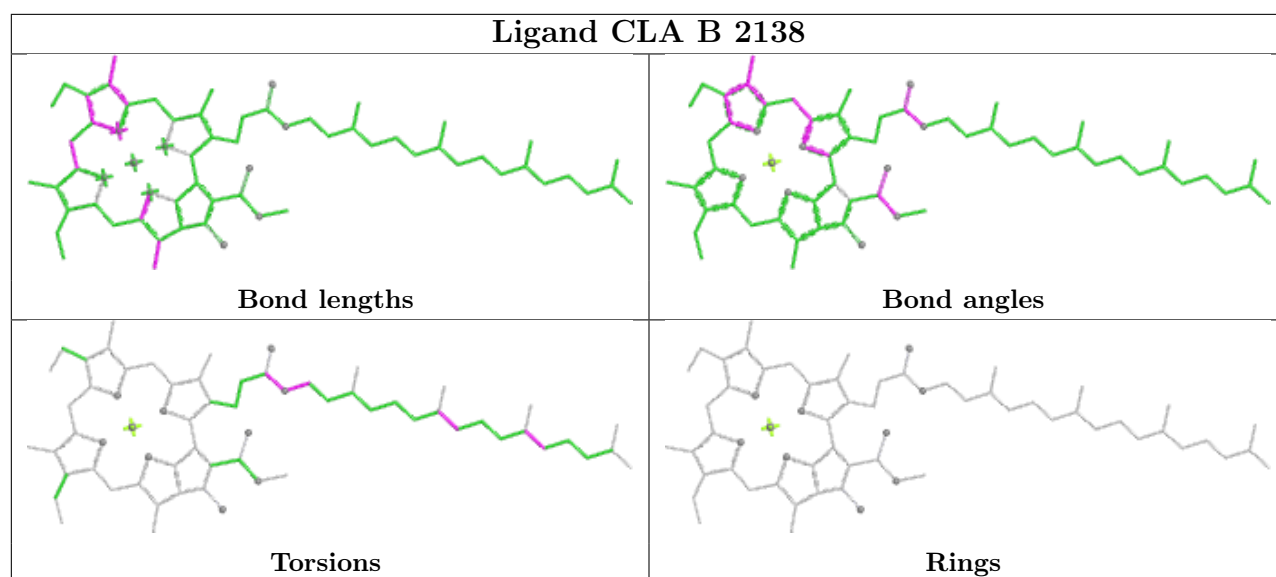
Rings

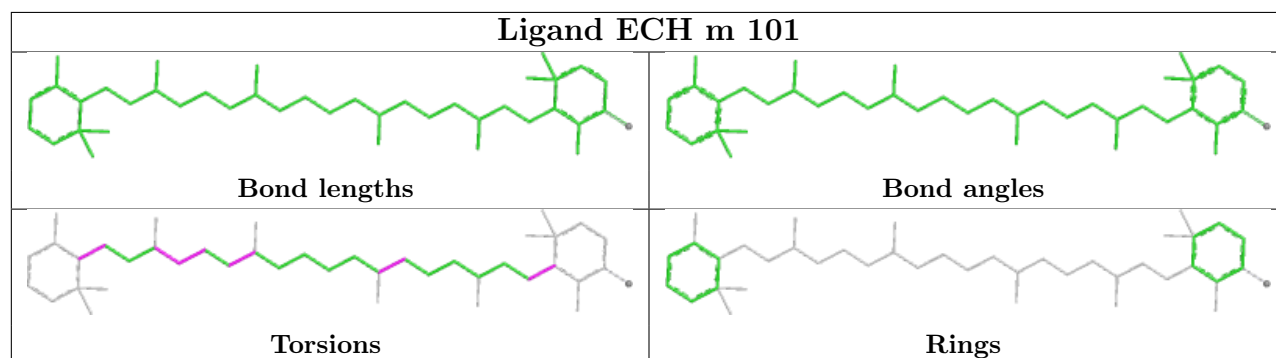
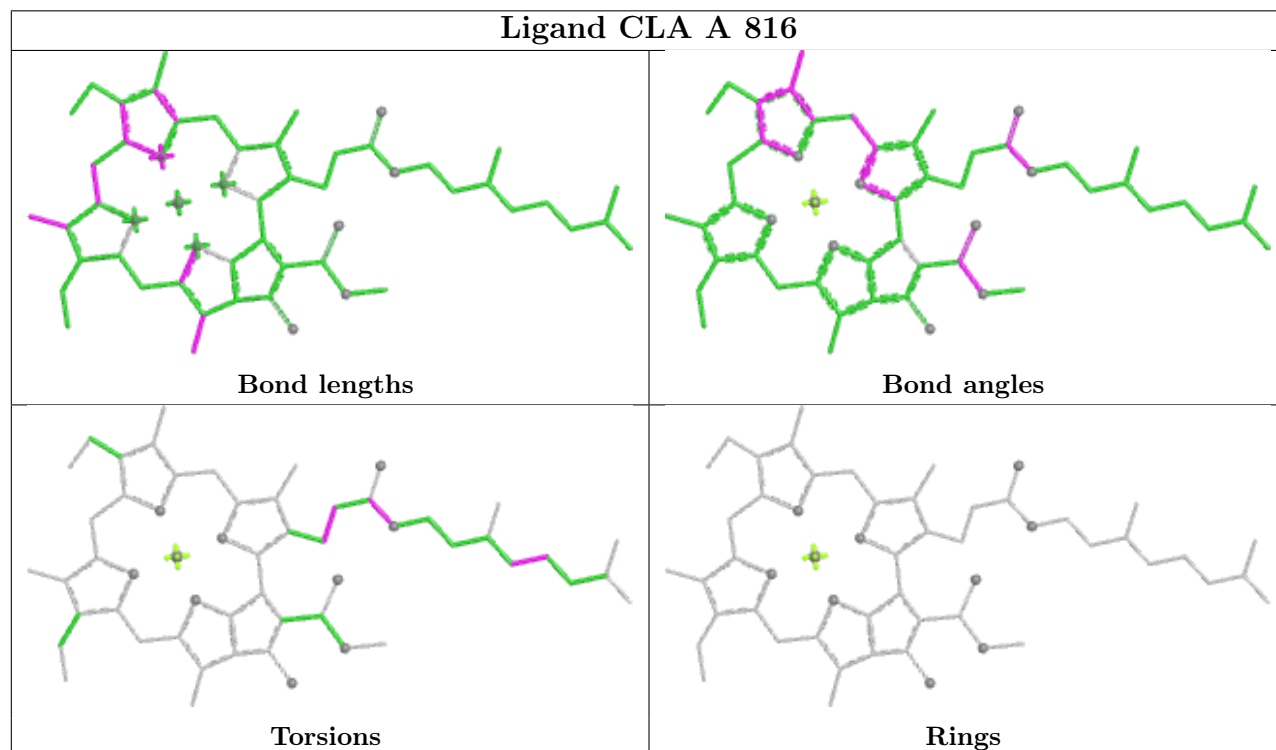
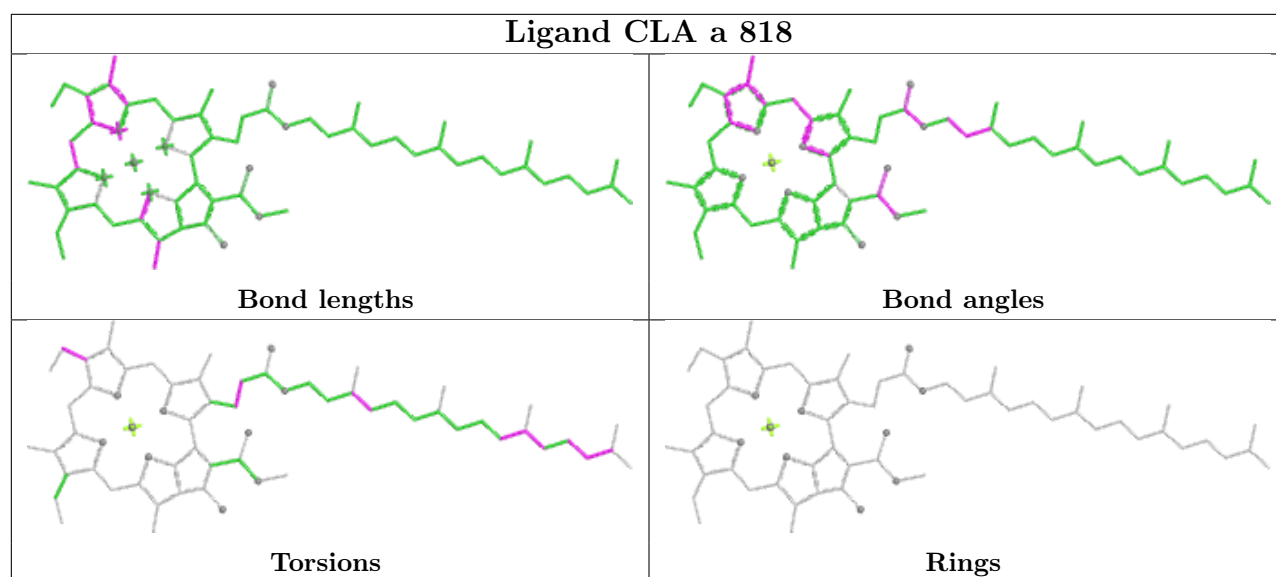
Ligand CLA l 204

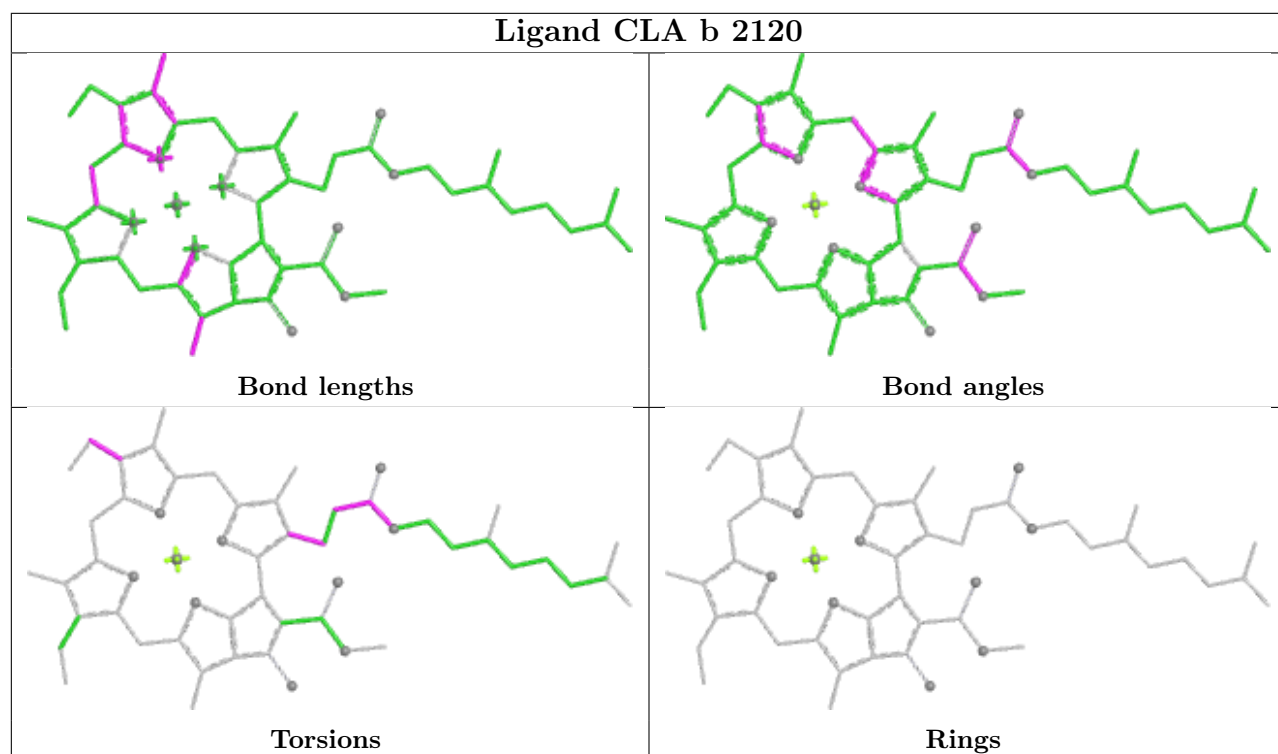
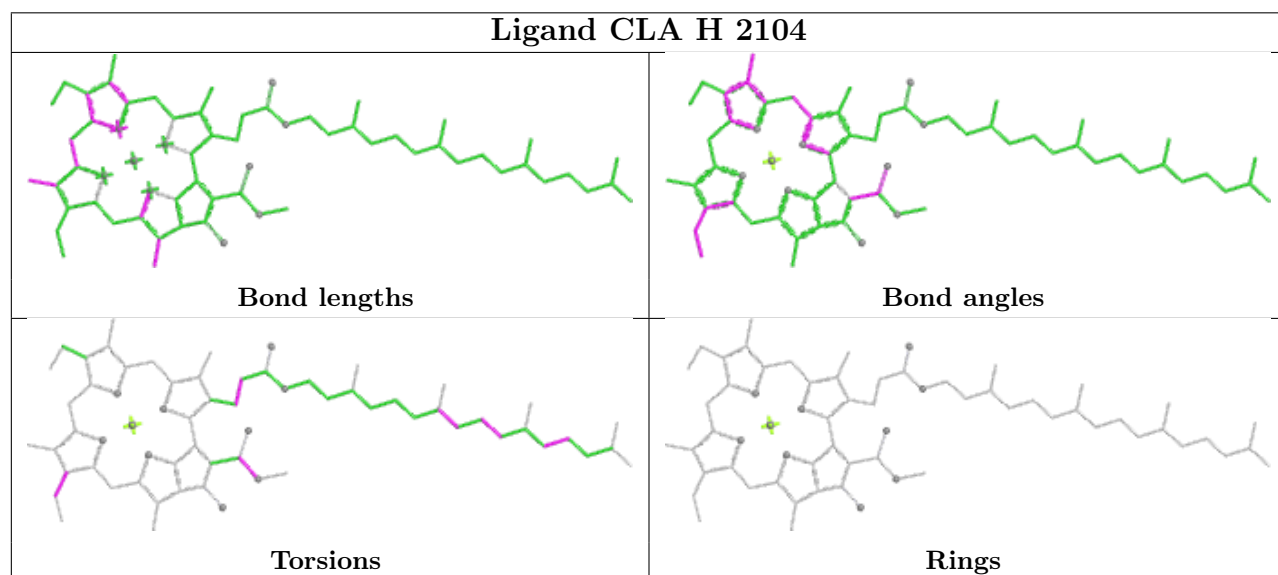
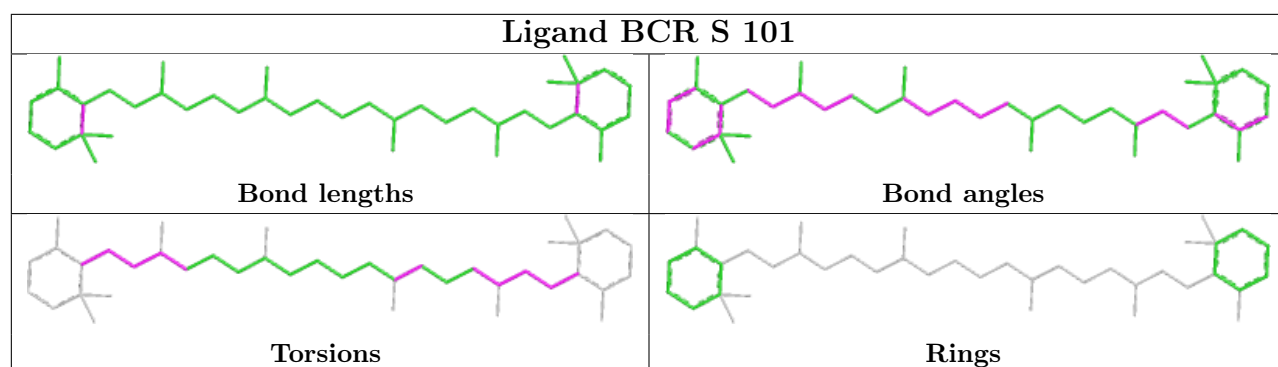


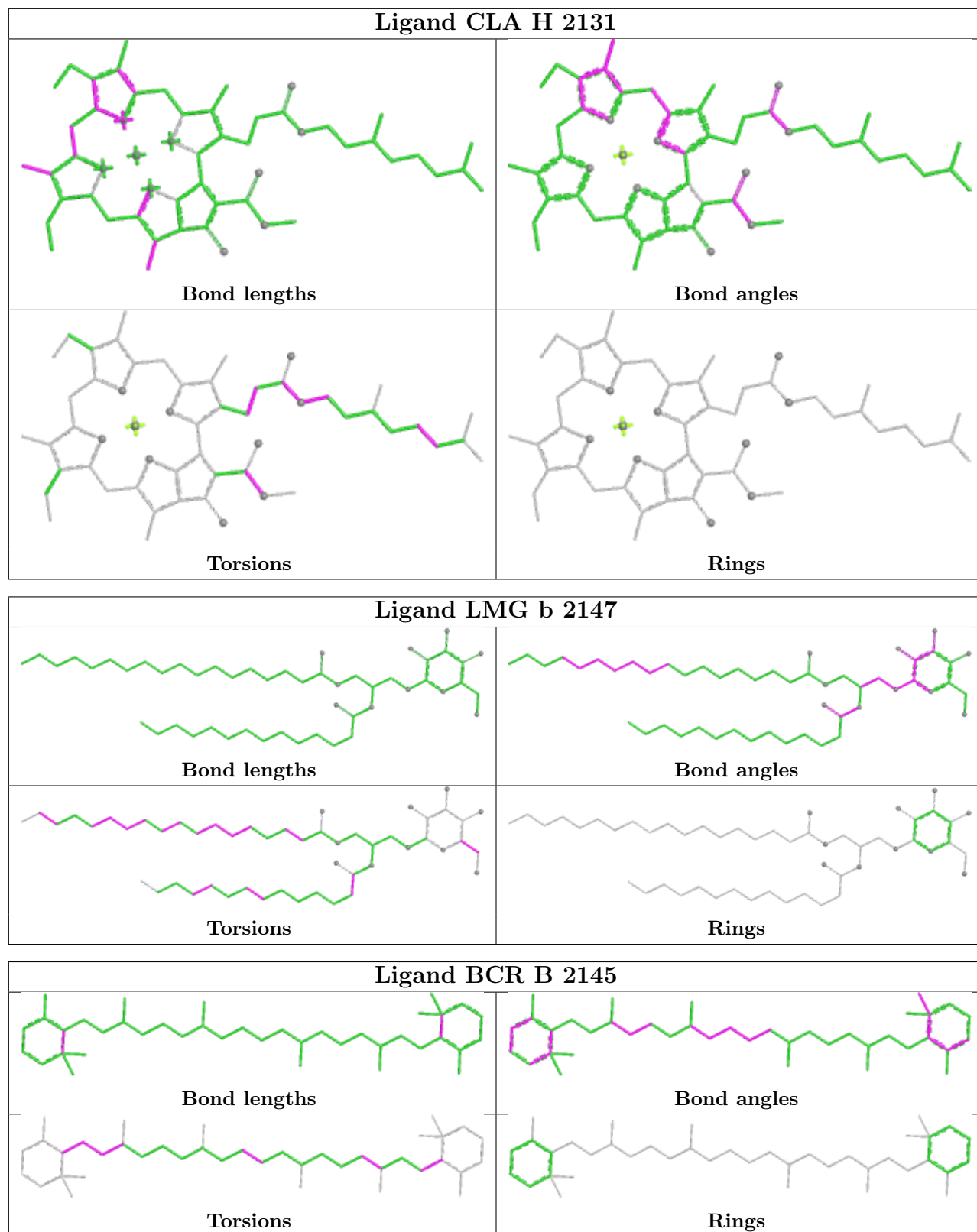
Ligand CLA k 4002

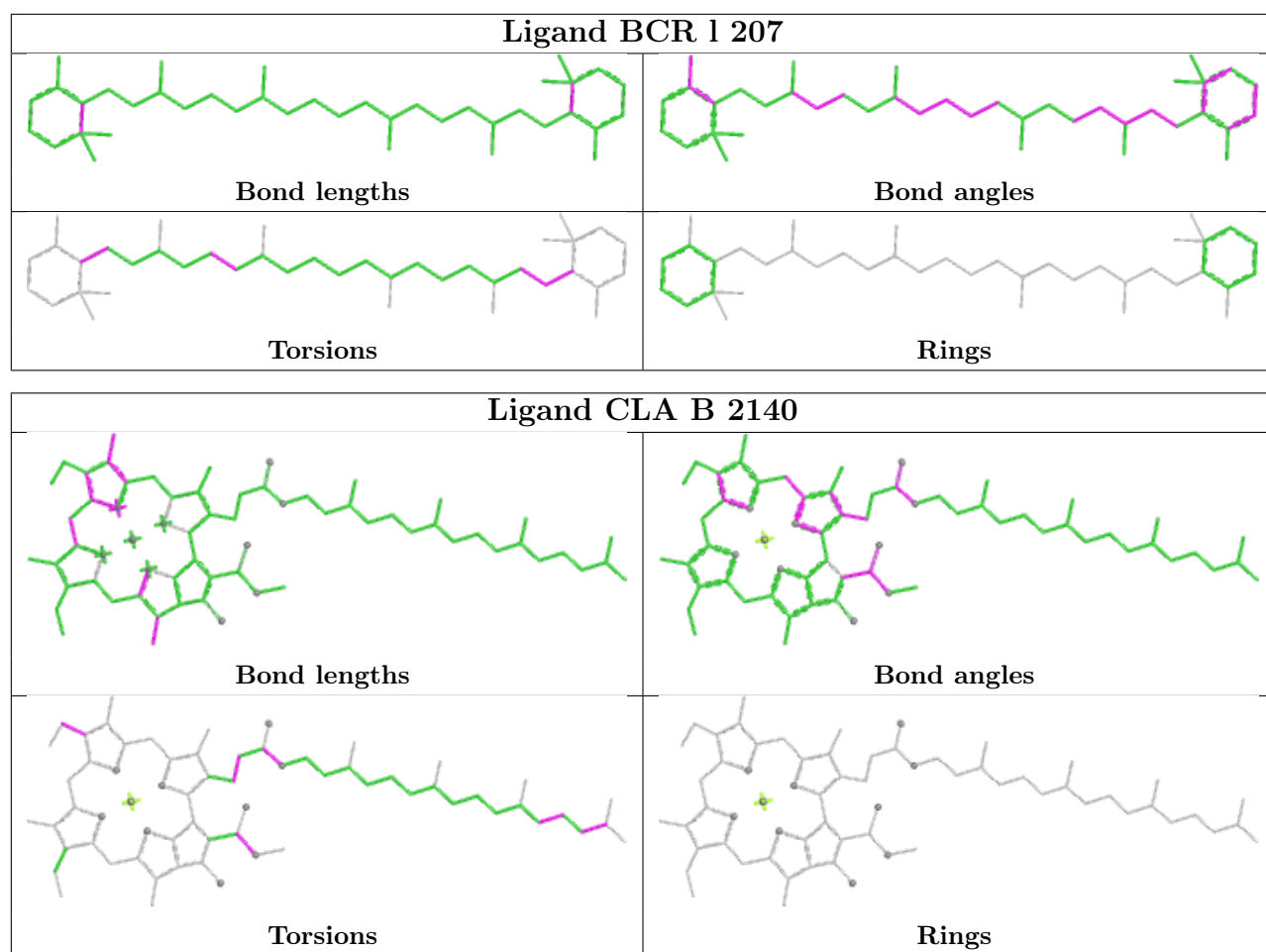


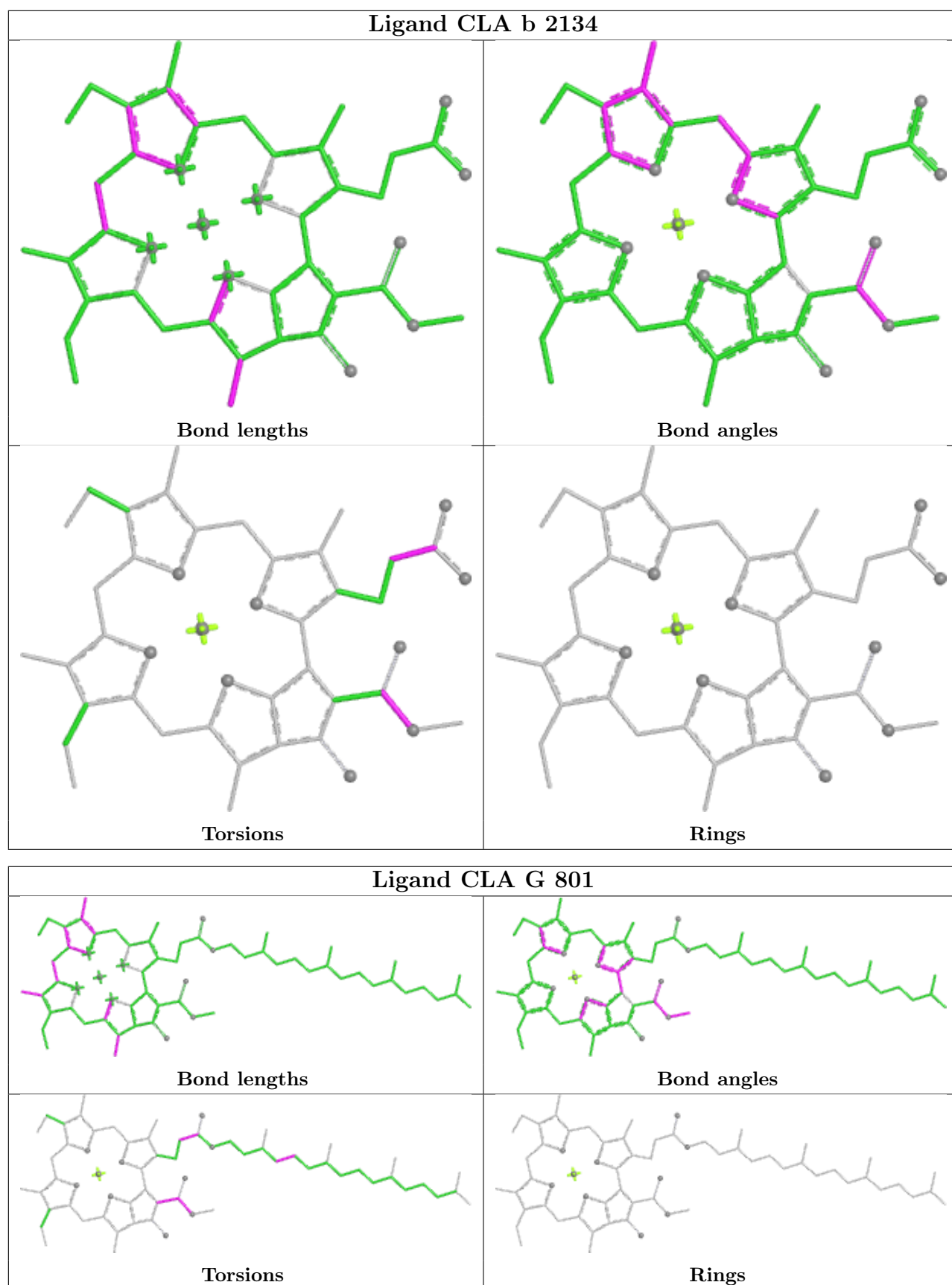


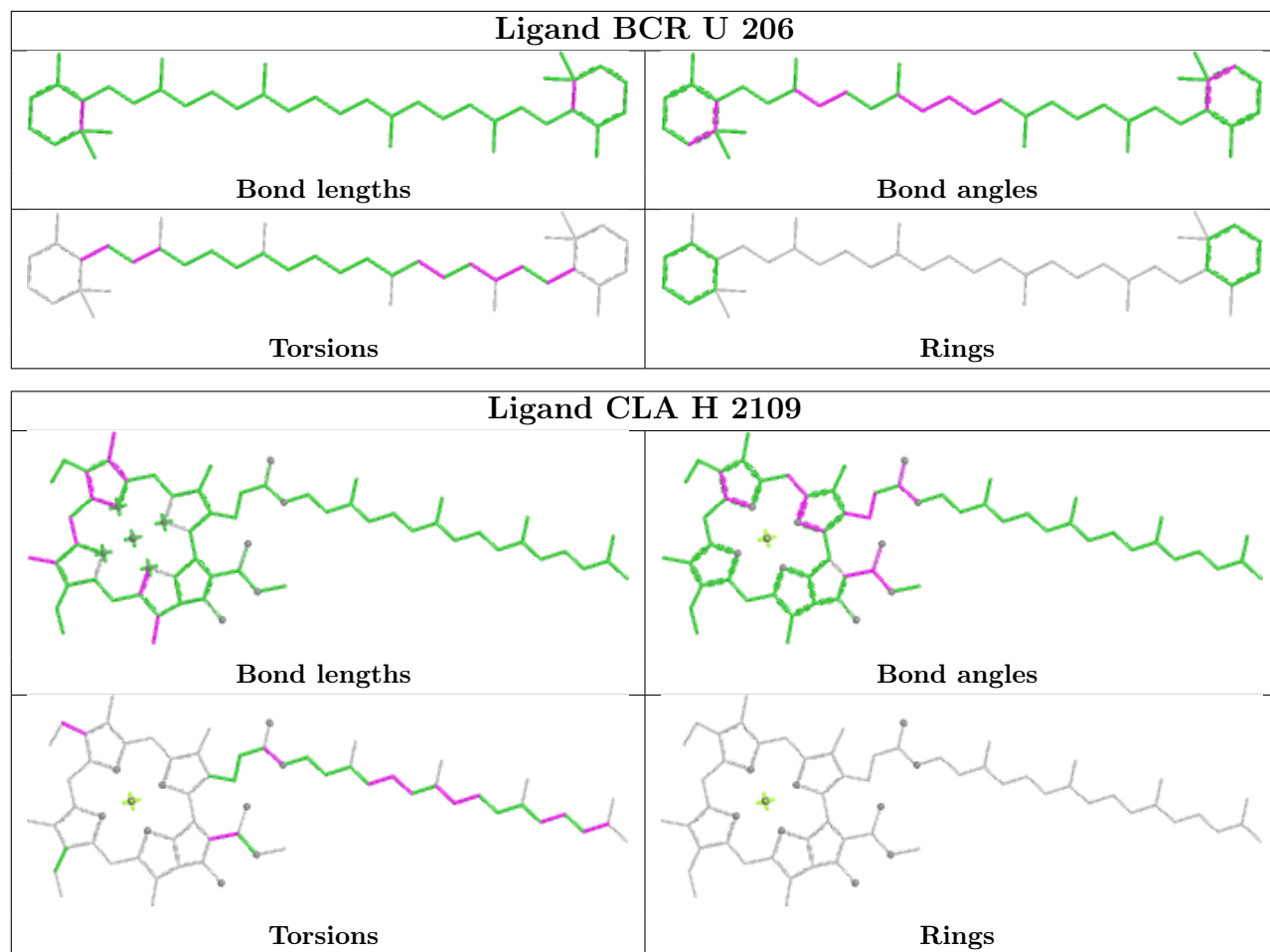




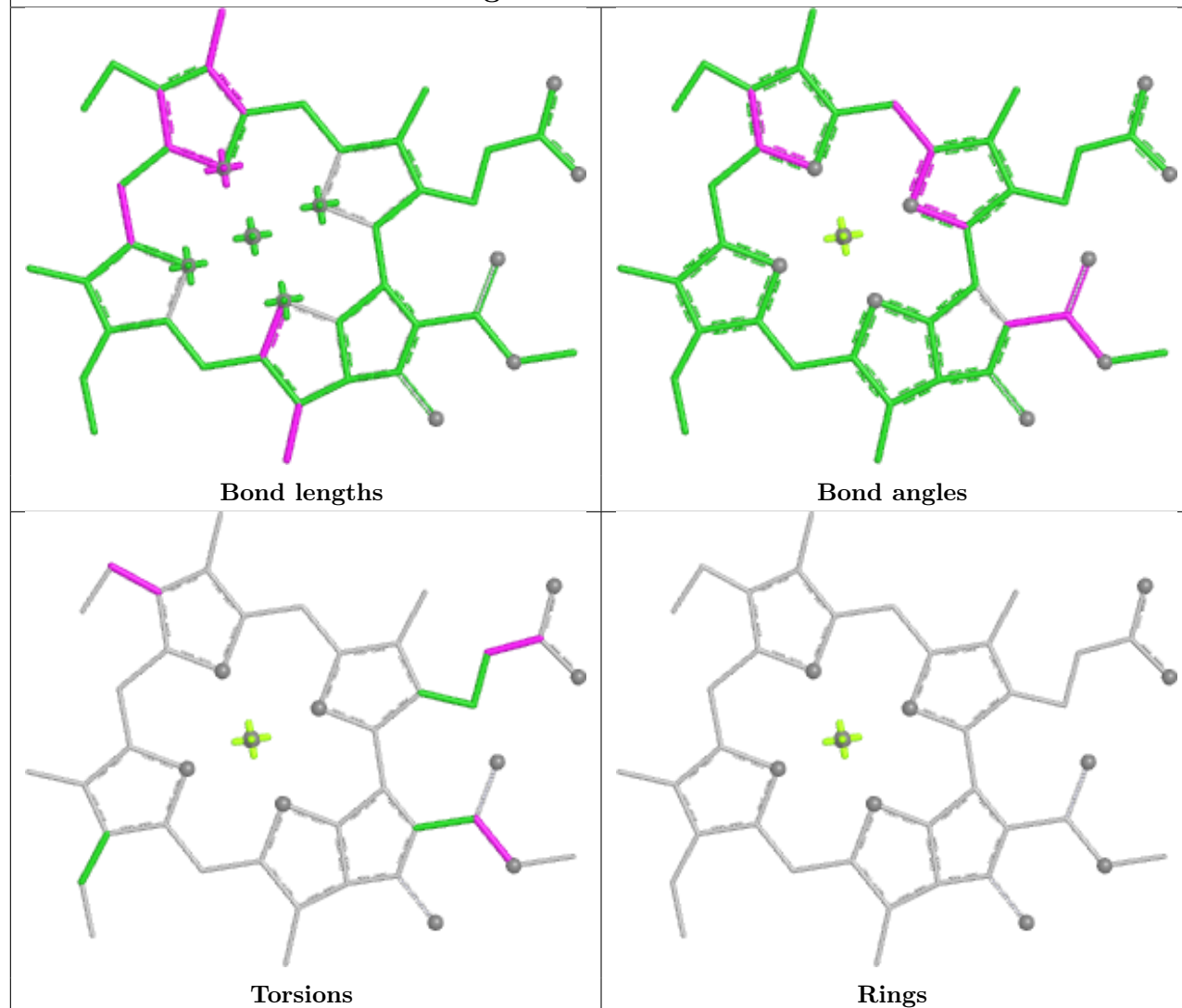




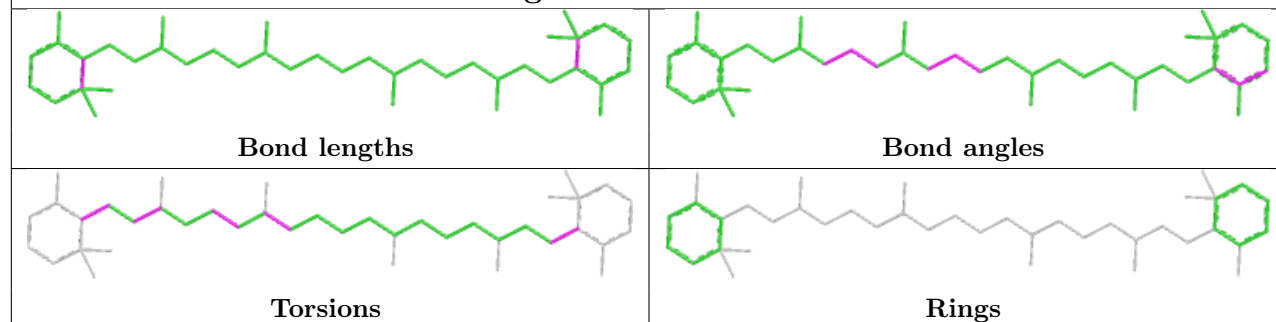


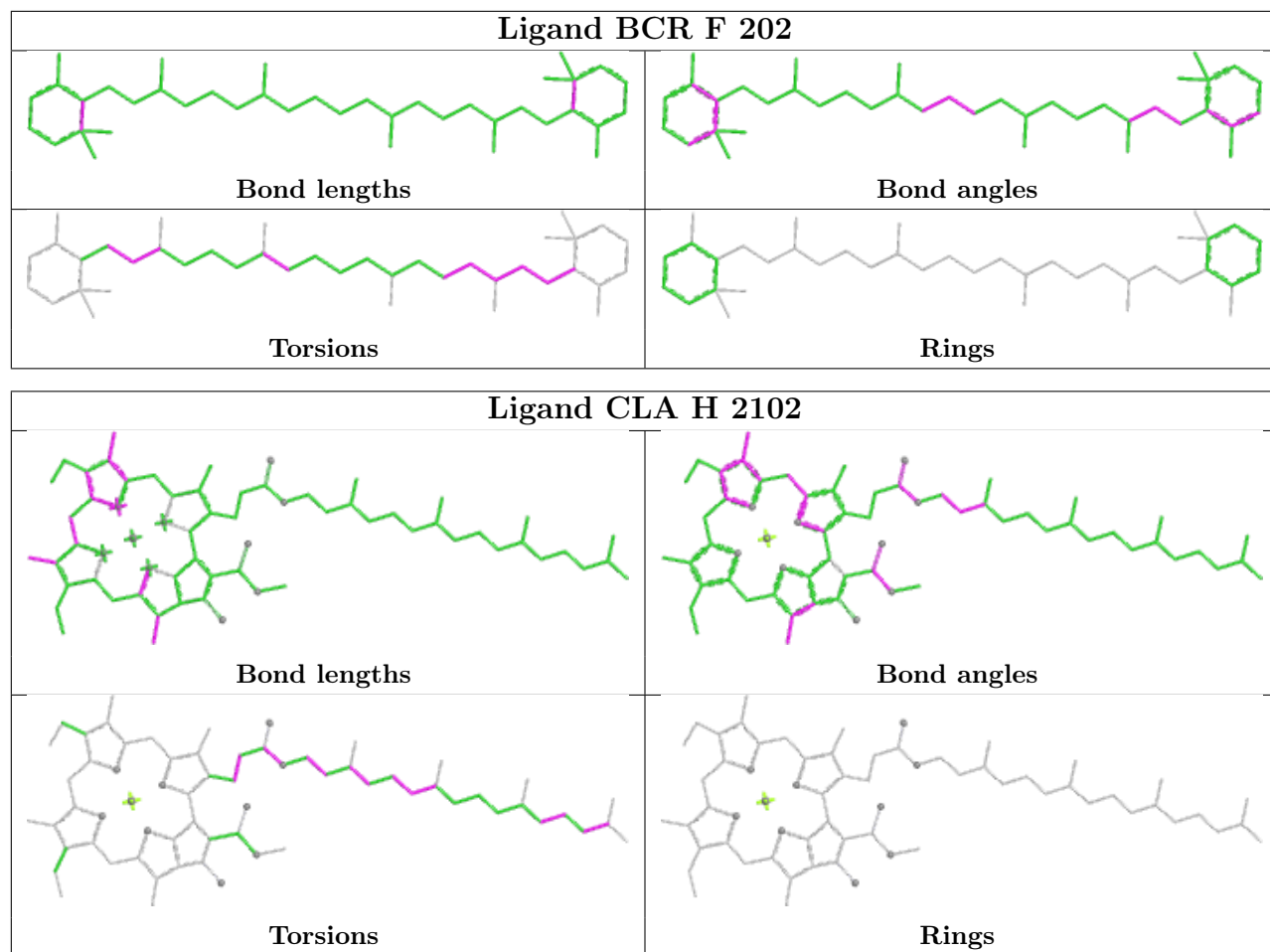


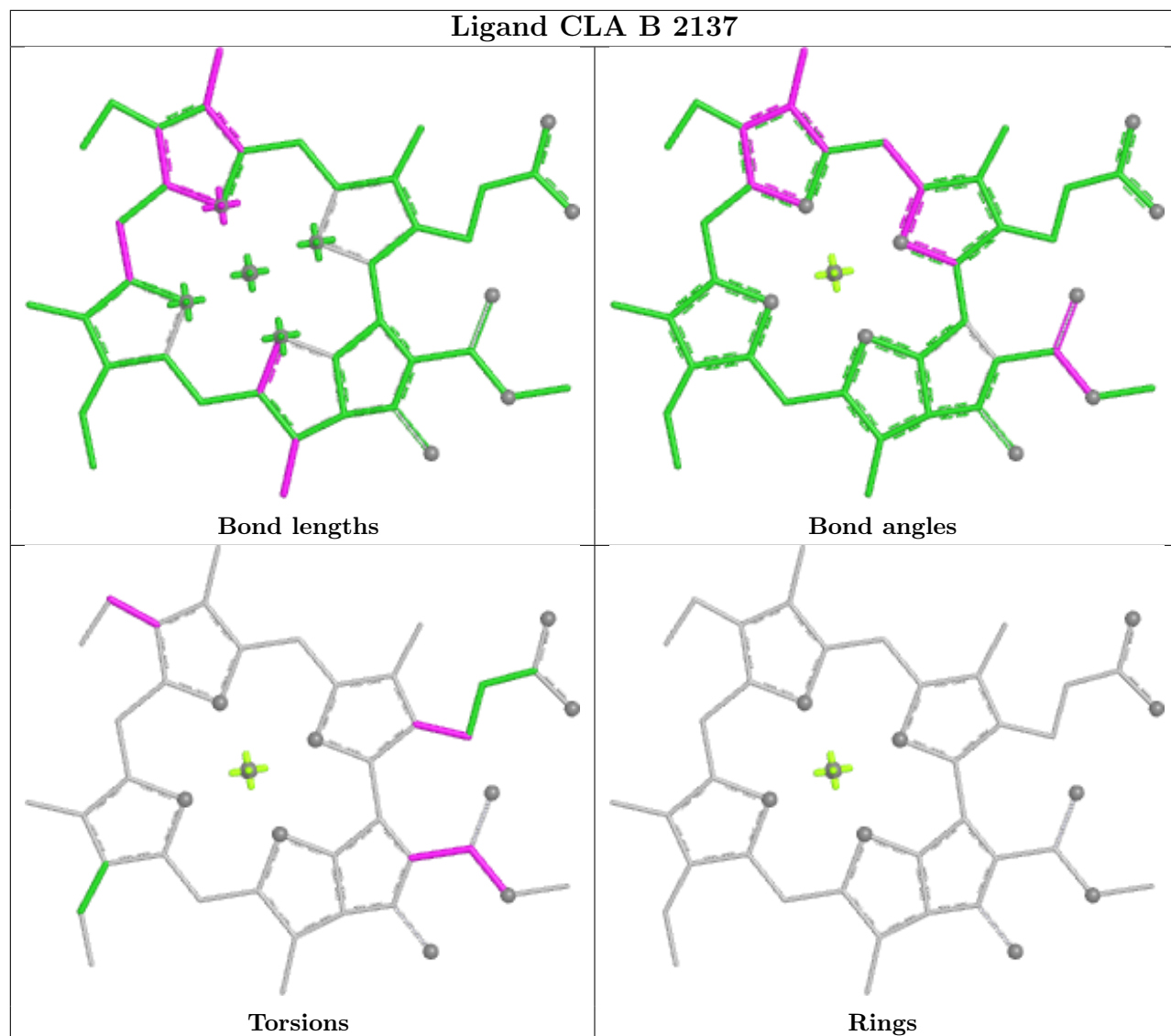
Ligand CLA H 2138

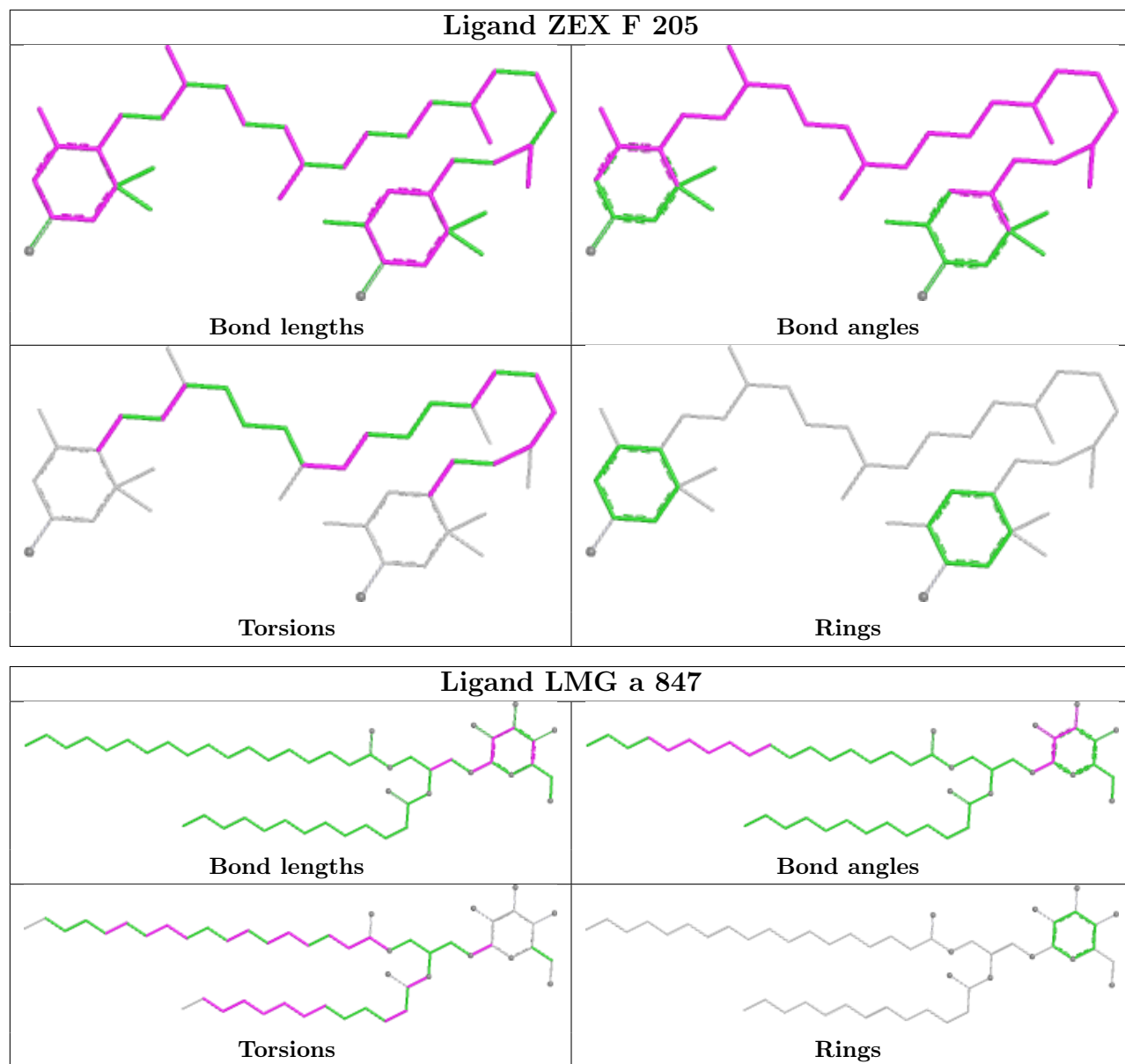


Ligand BCR b 2145

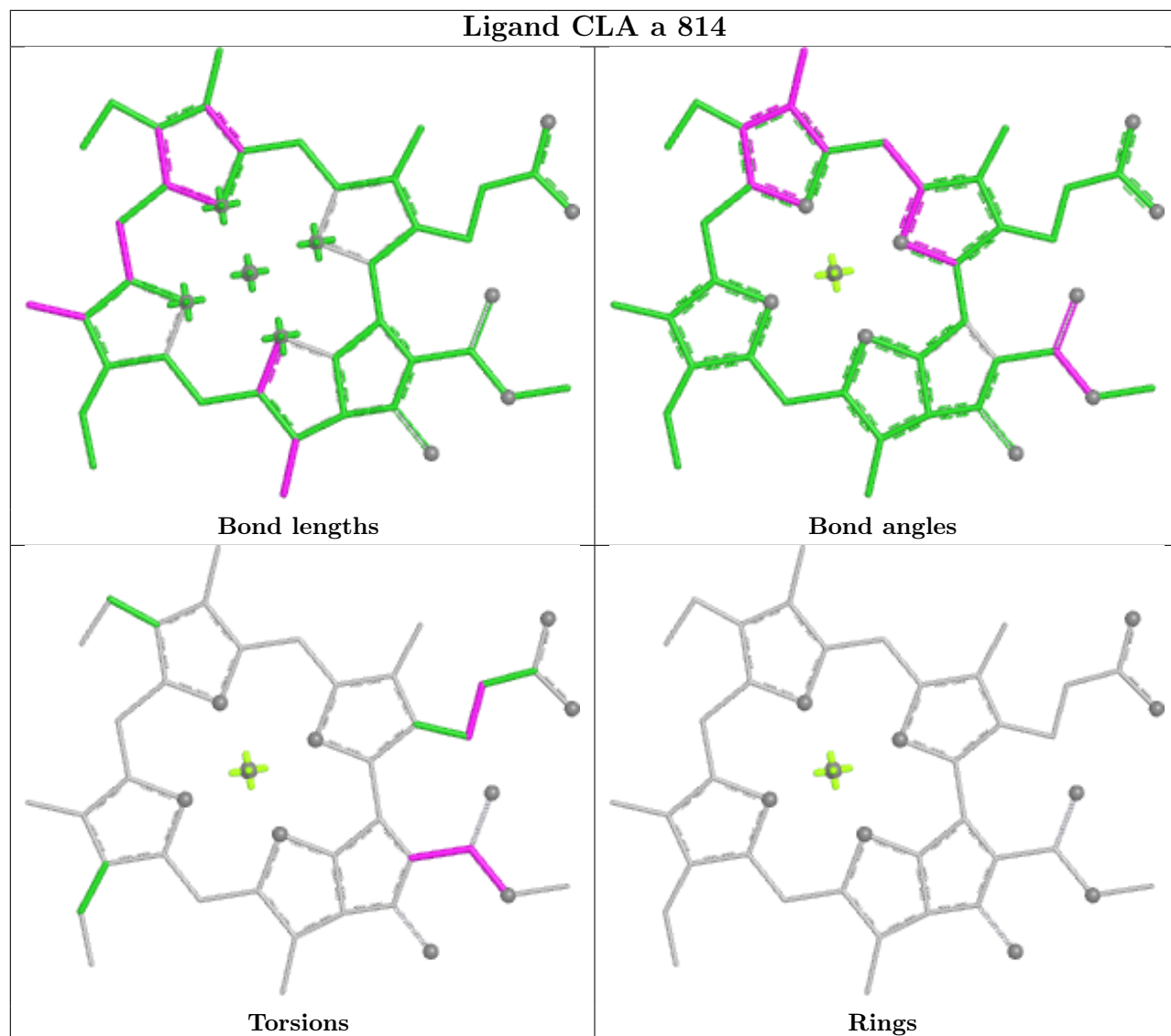


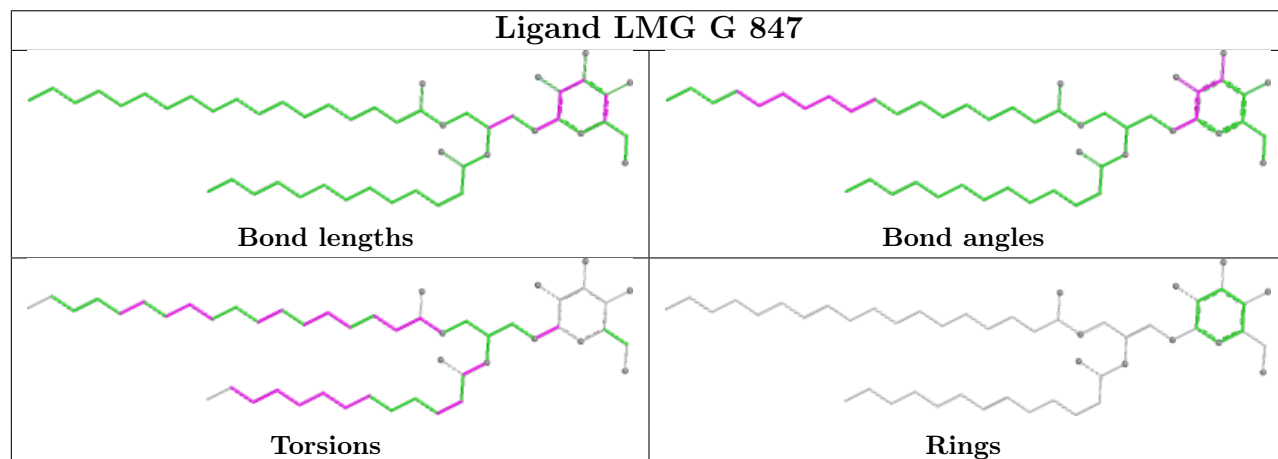
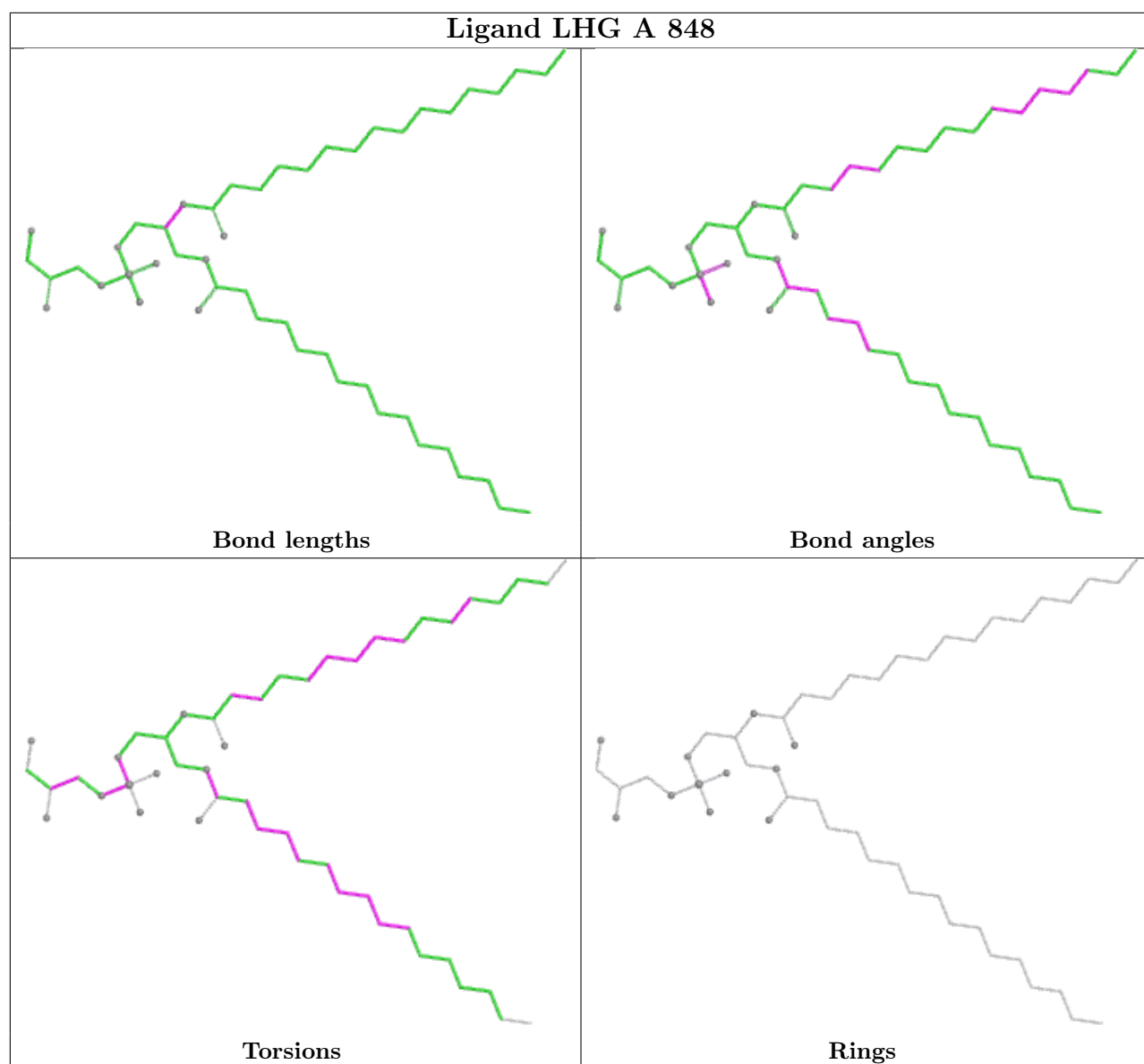


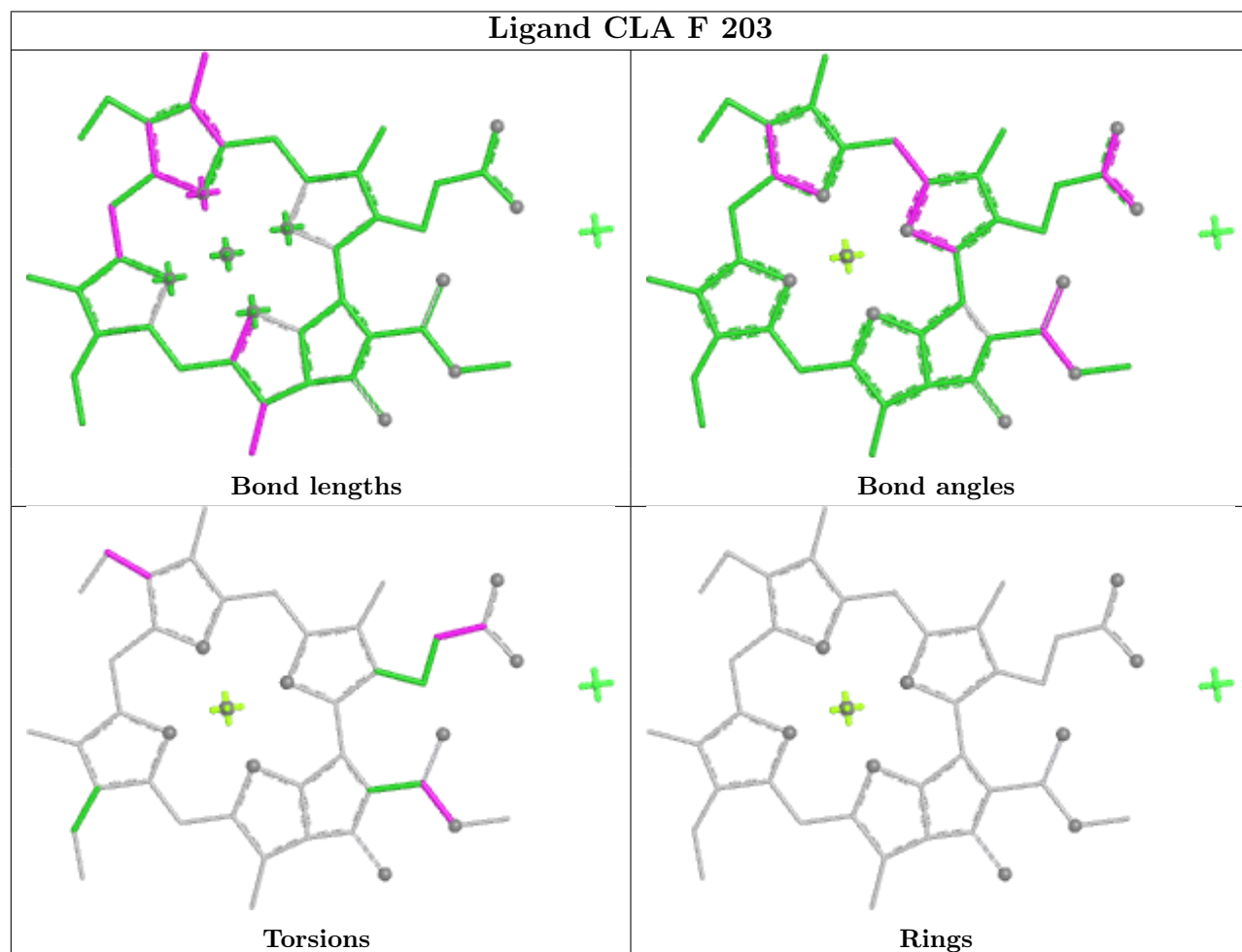
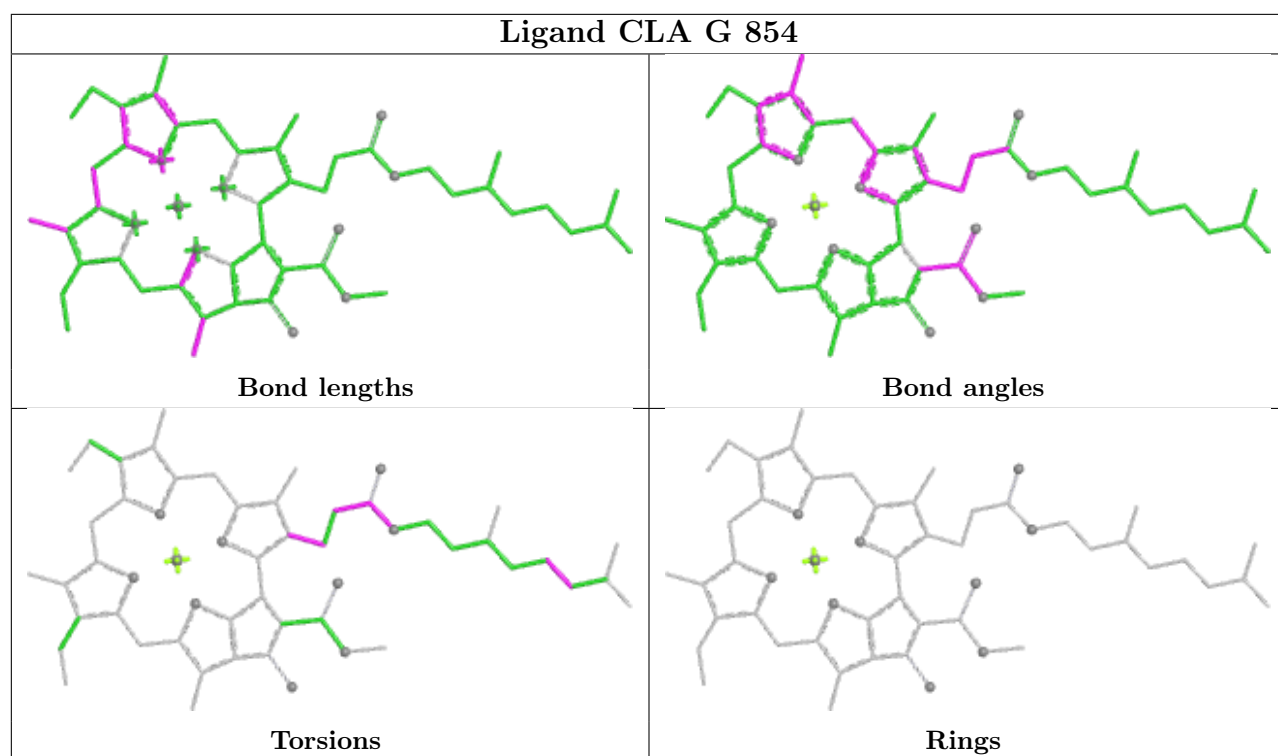


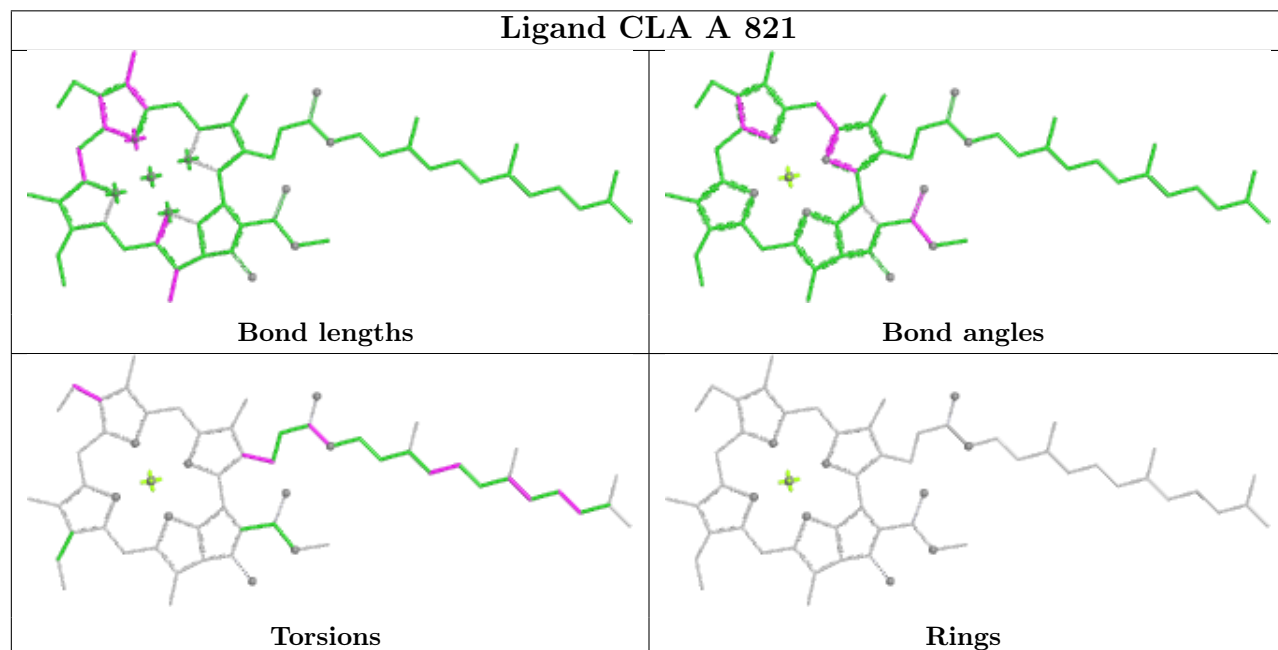
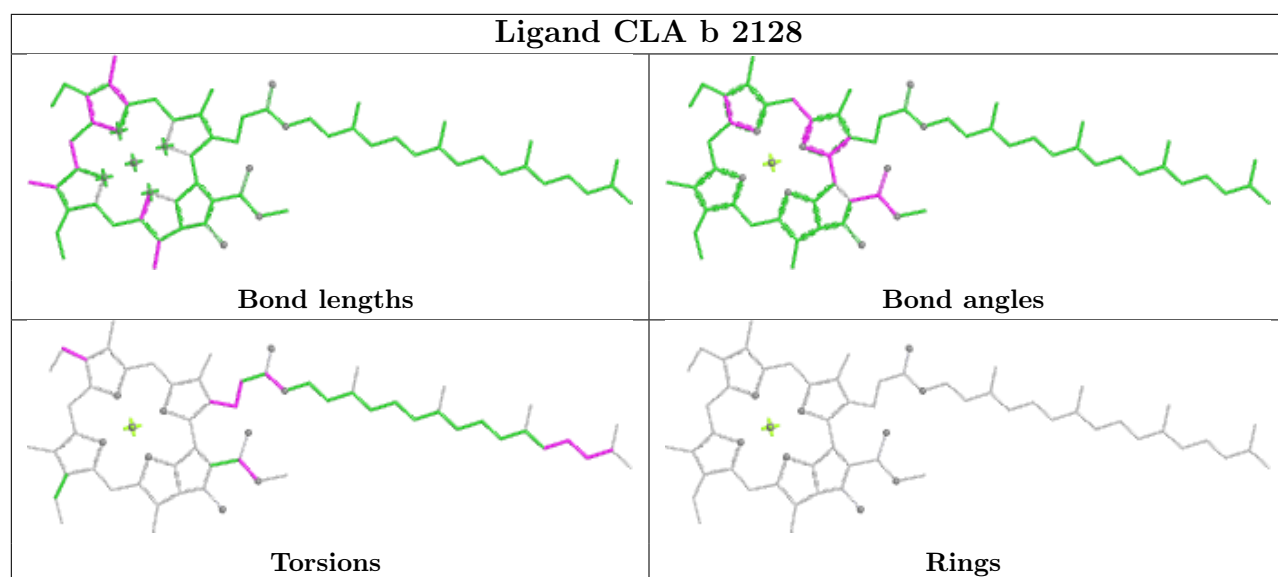


Ligand CLA a 814

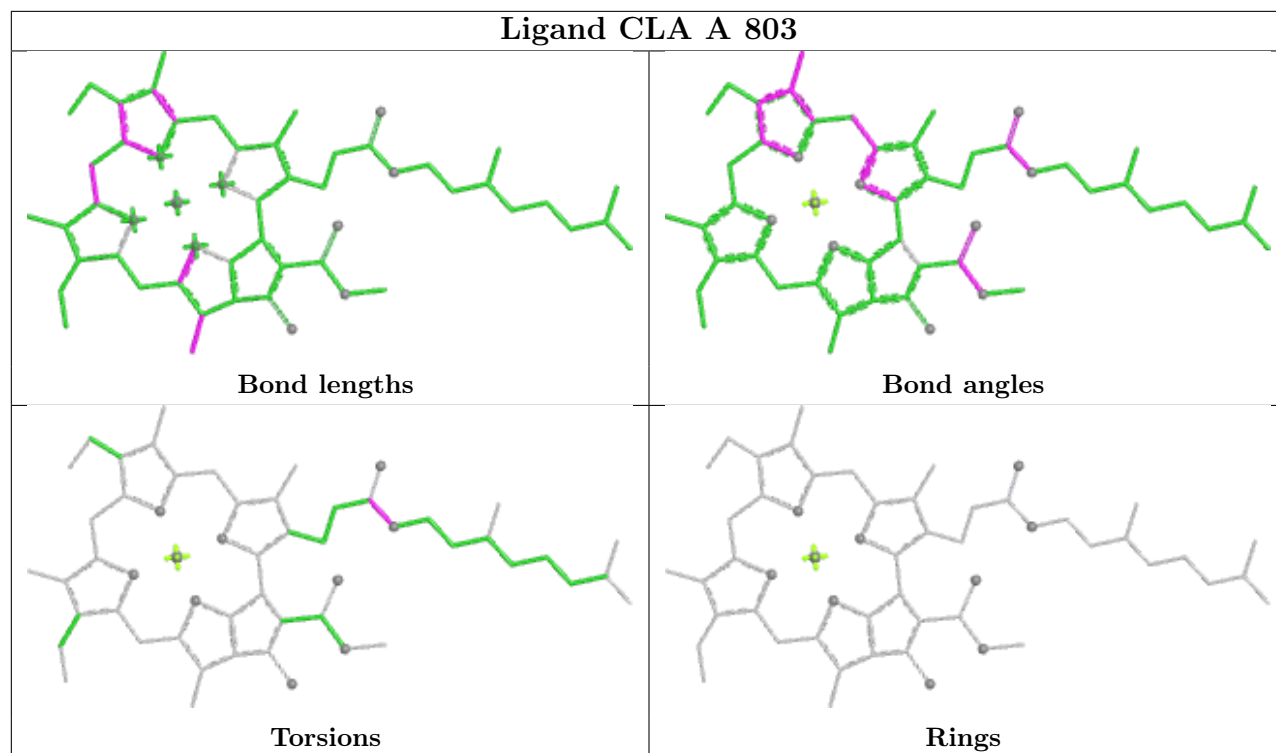




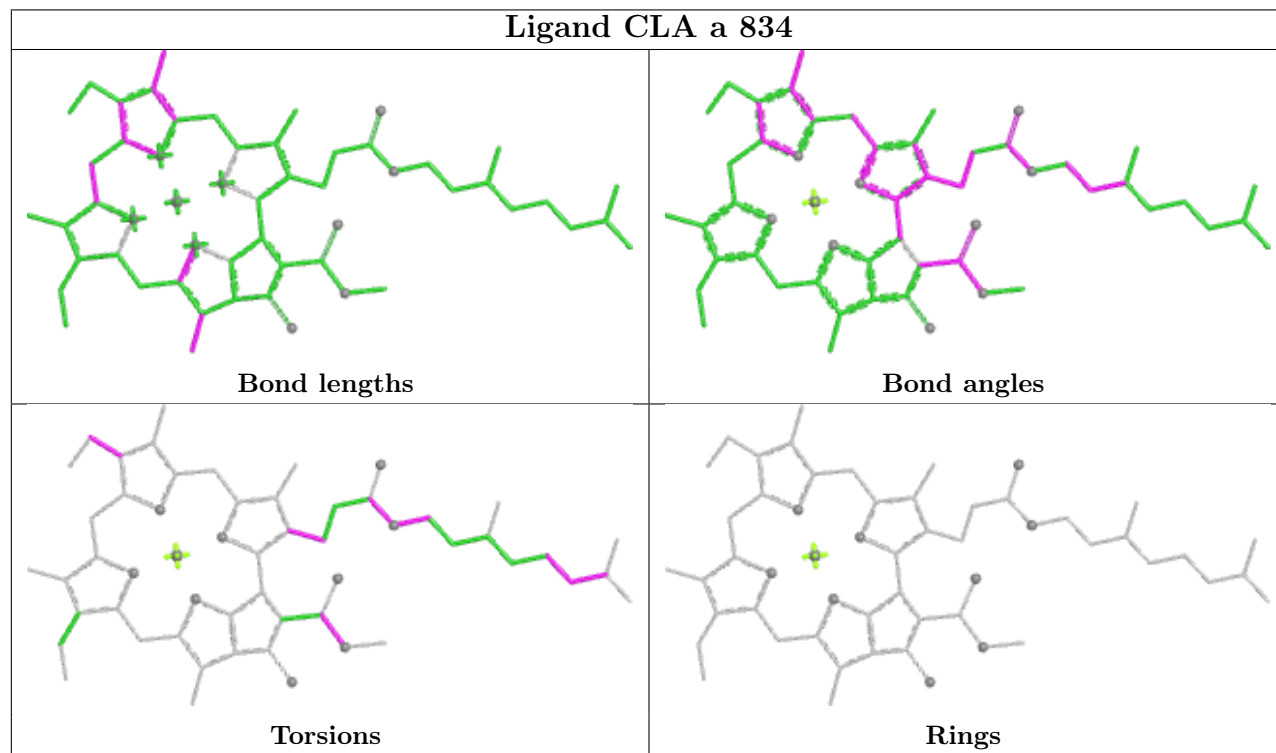


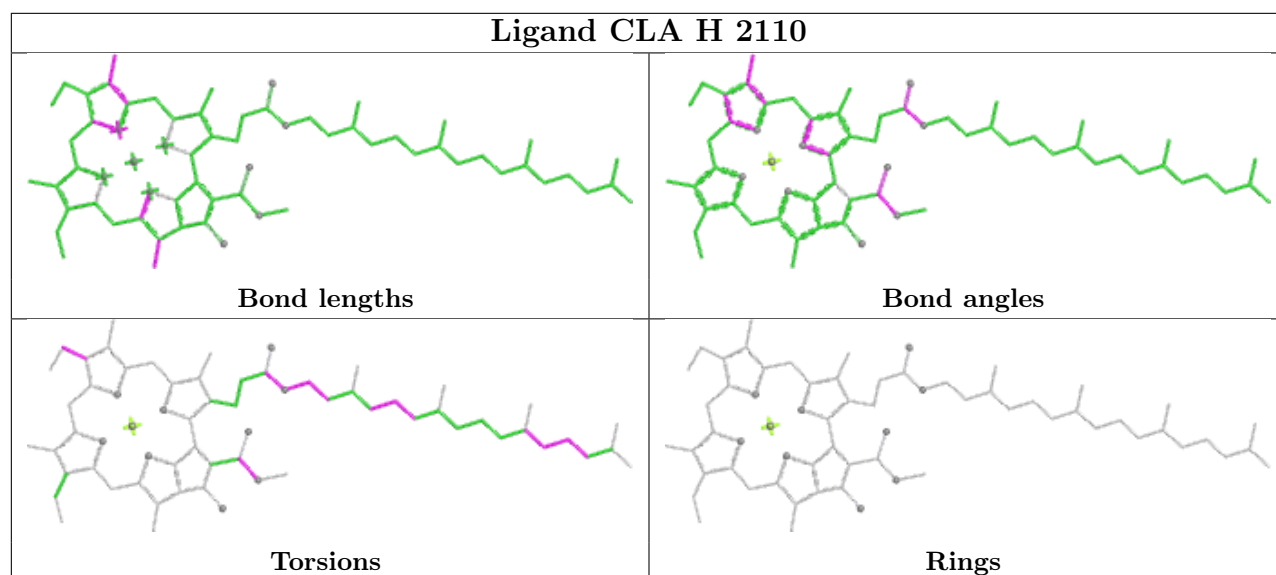
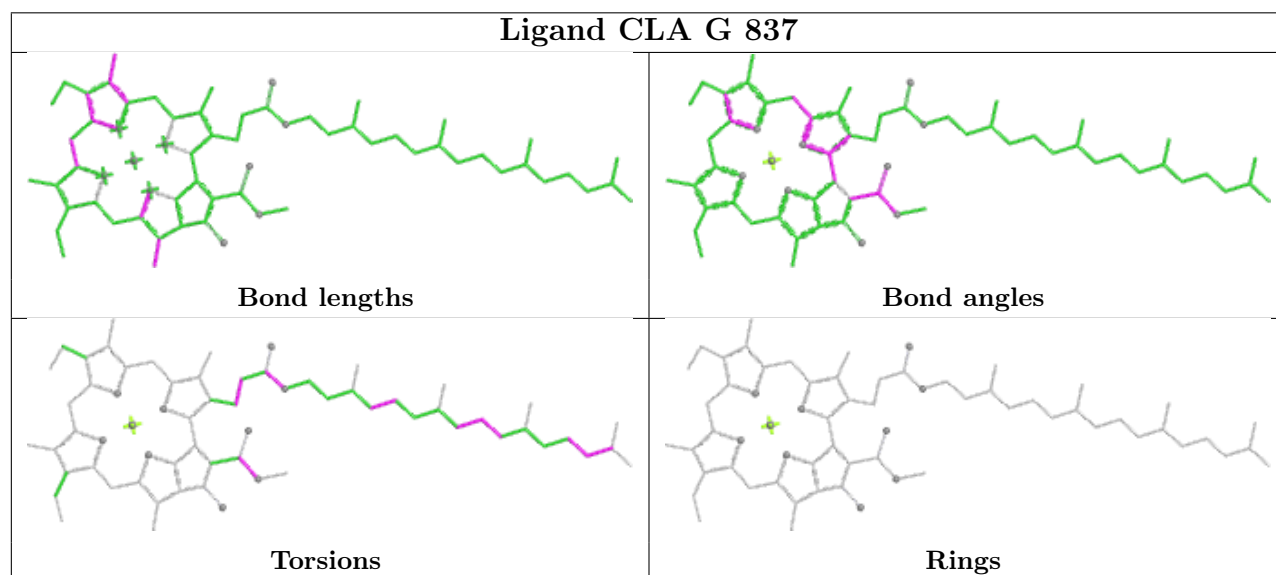
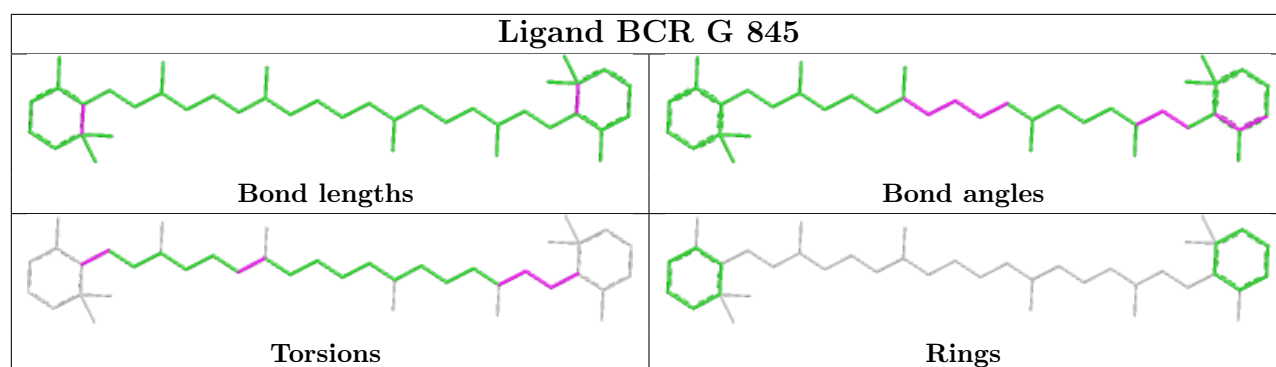


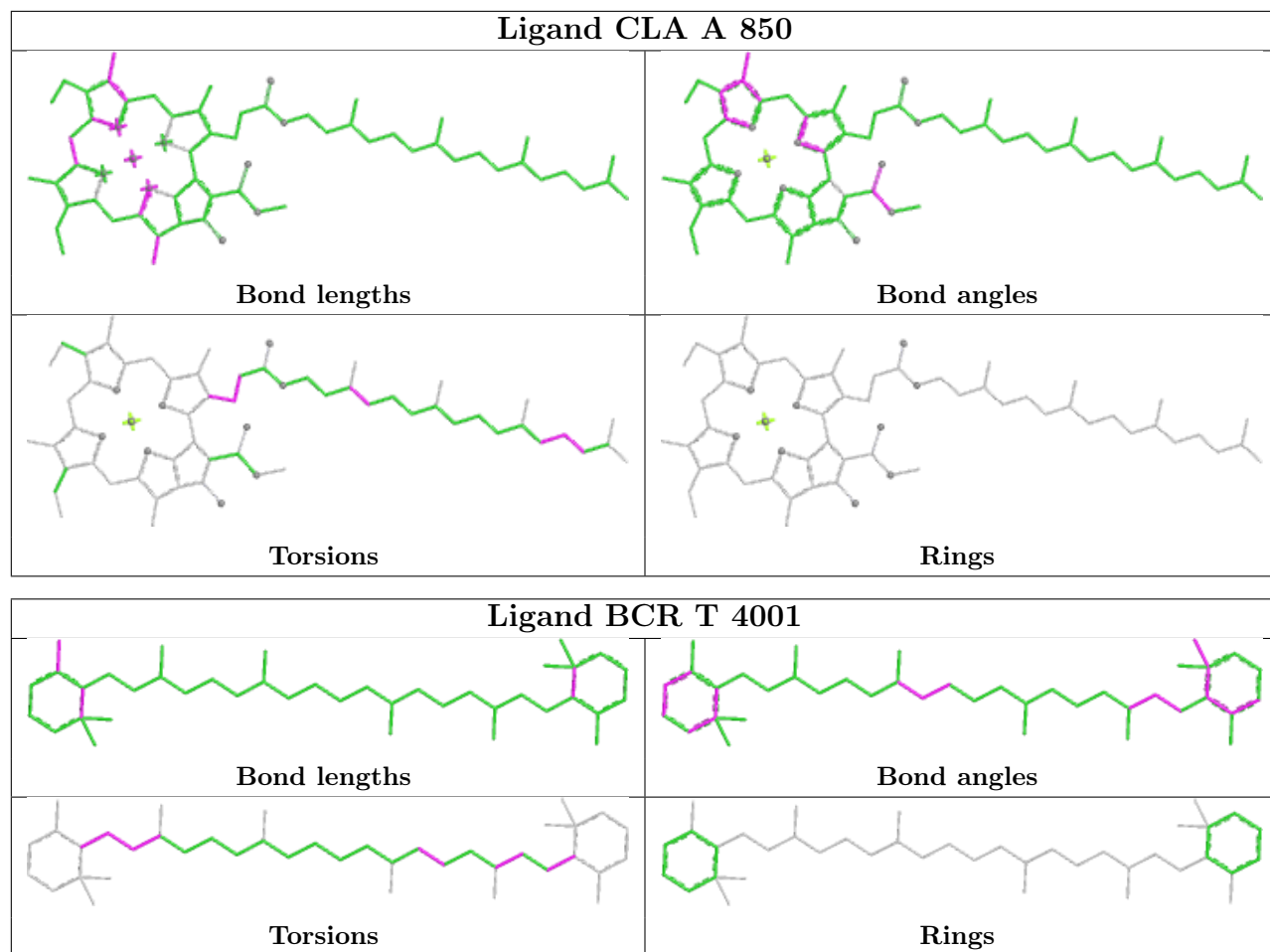
Ligand CLA A 803



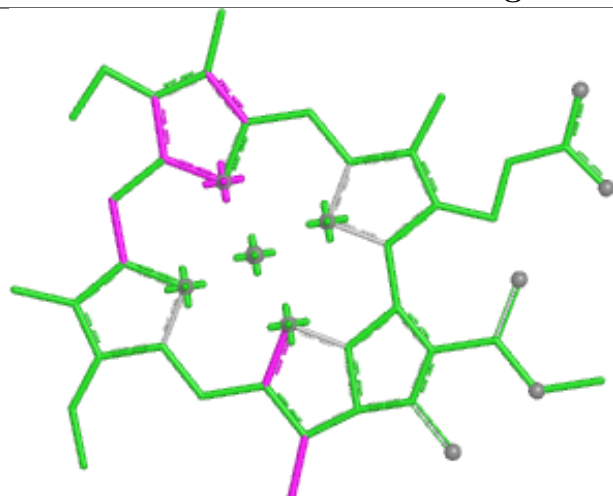
Ligand CLA a 834



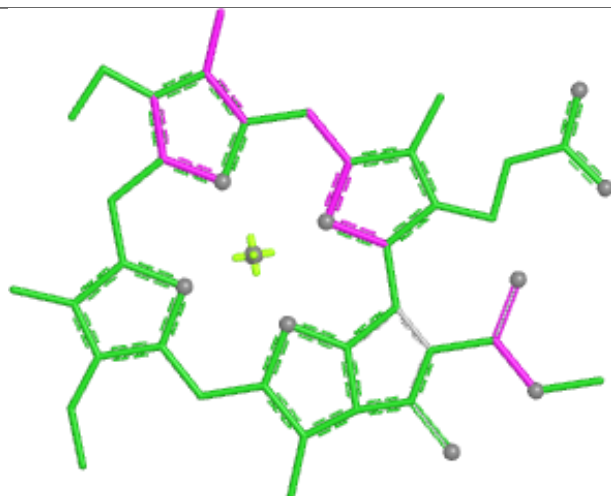




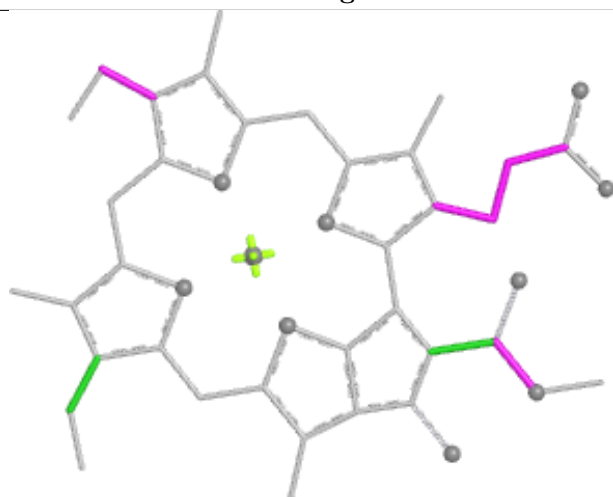
Ligand CLA H 2116



Bond lengths



Bond angles

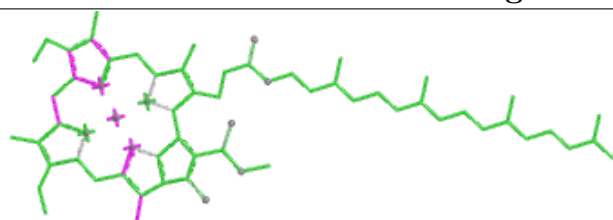


Torsions

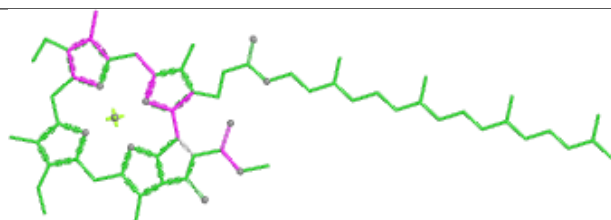


Rings

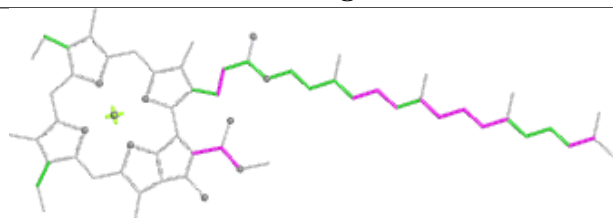
Ligand CLA B 2102



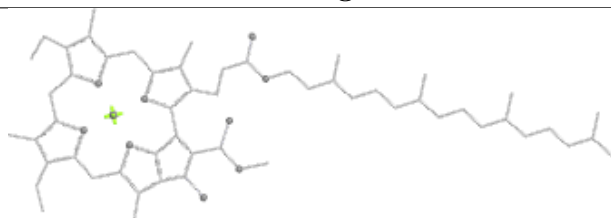
Bond lengths



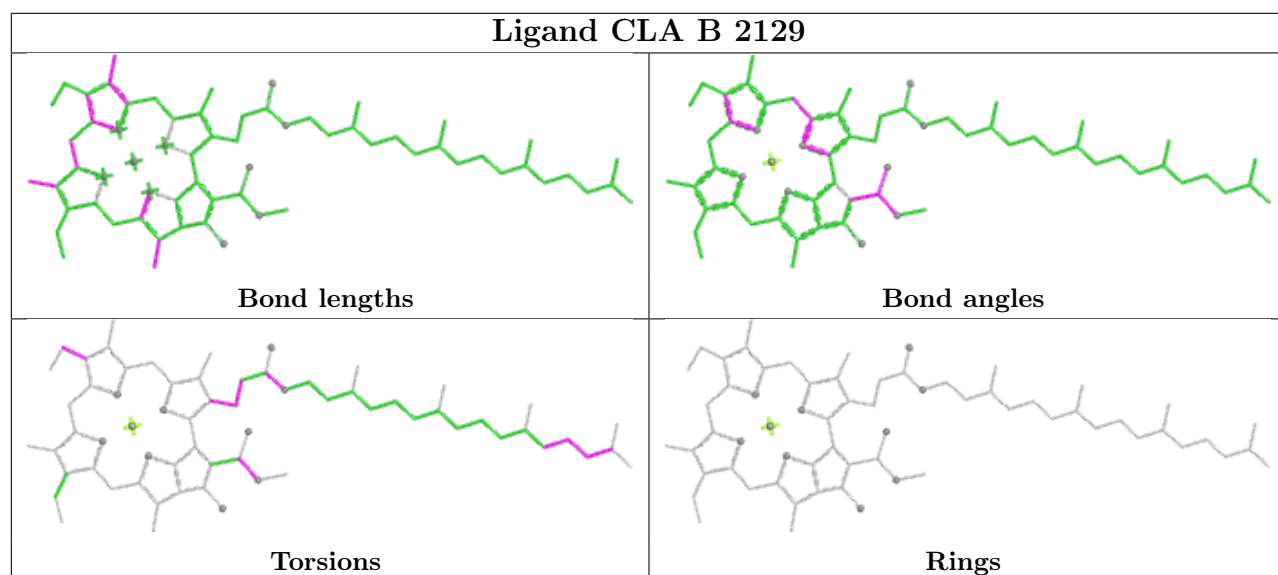
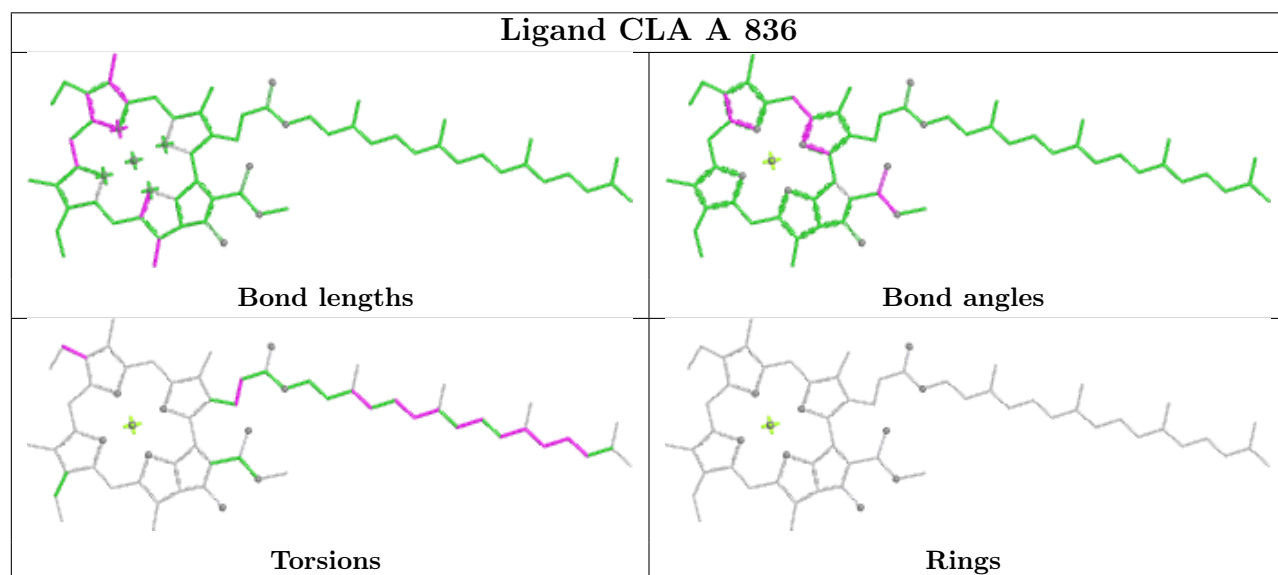
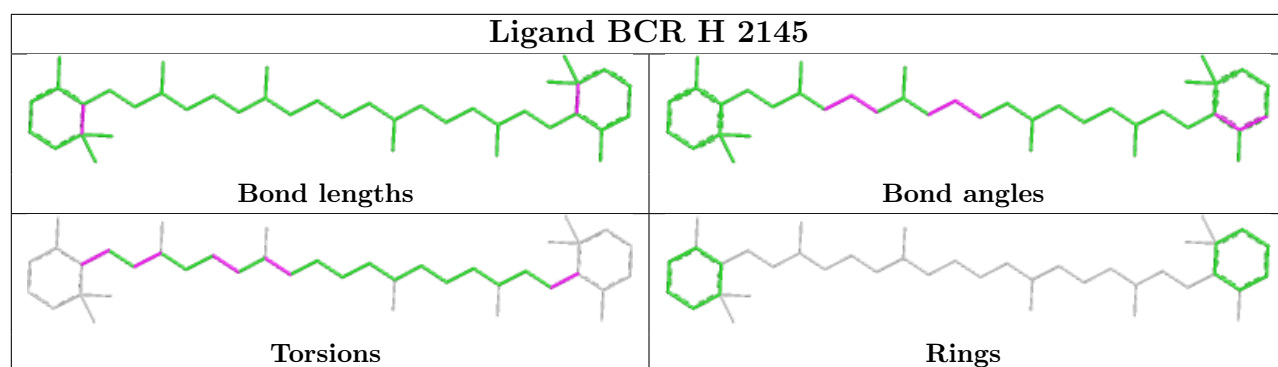
Bond angles

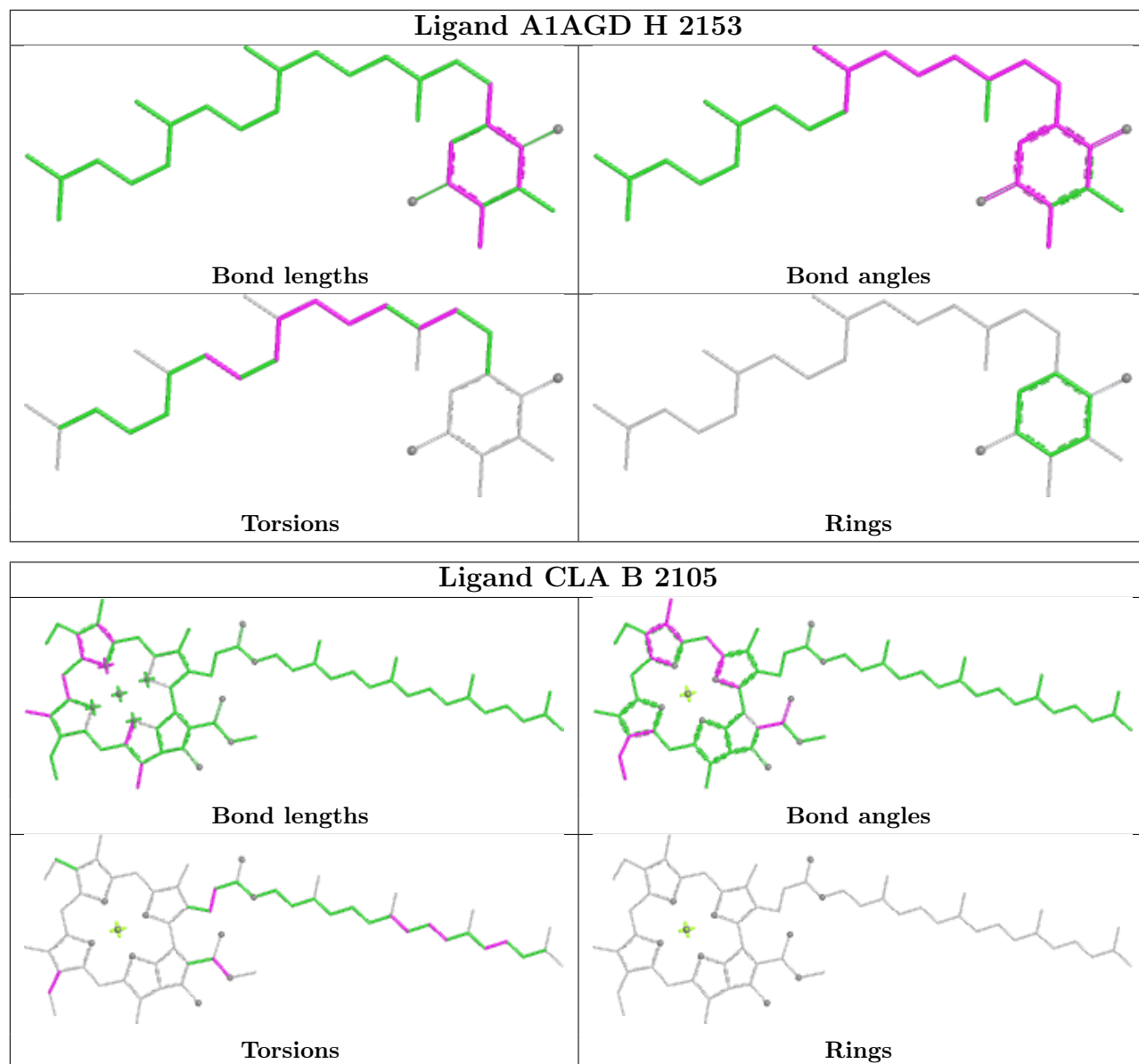


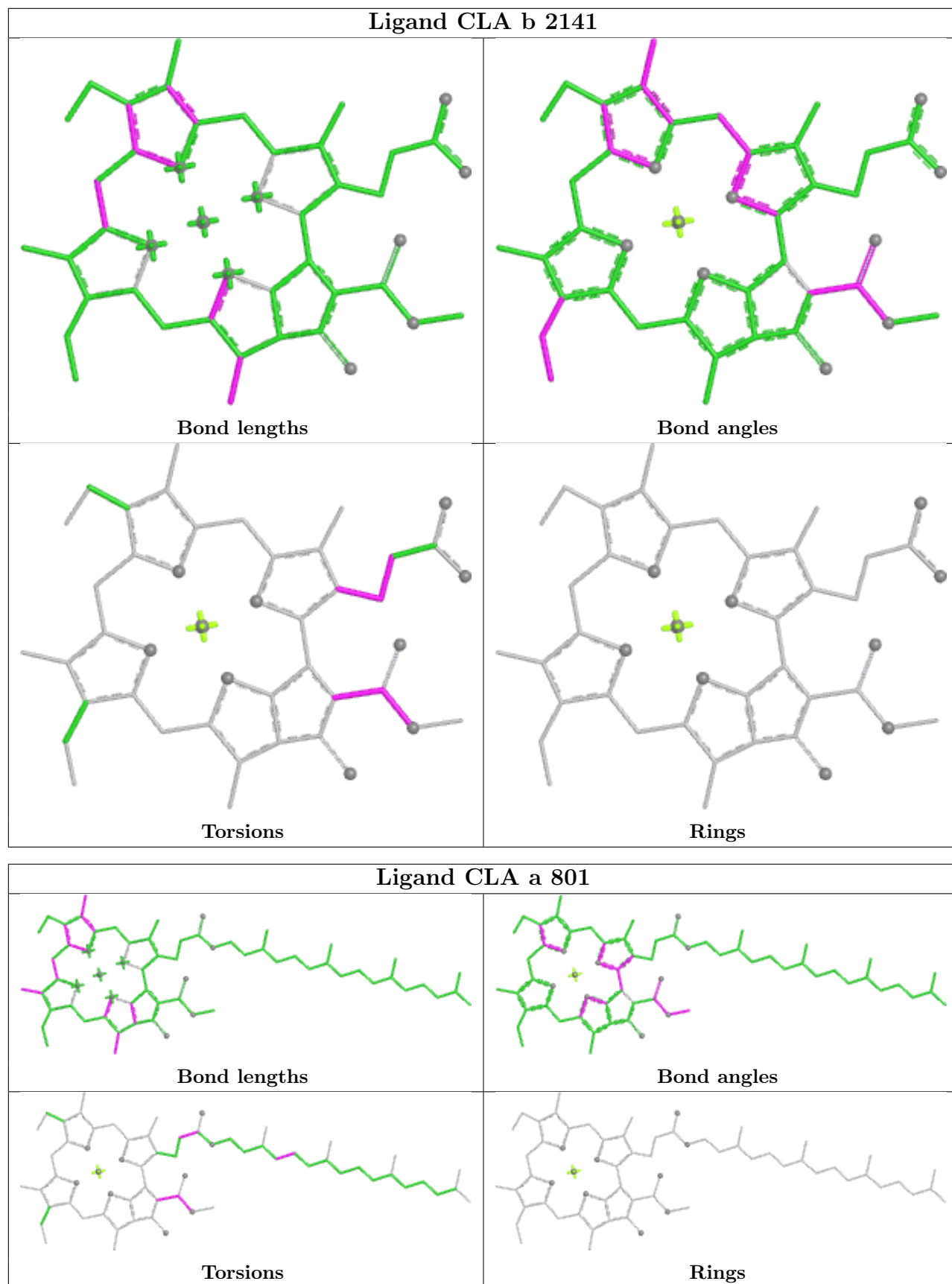
Torsions

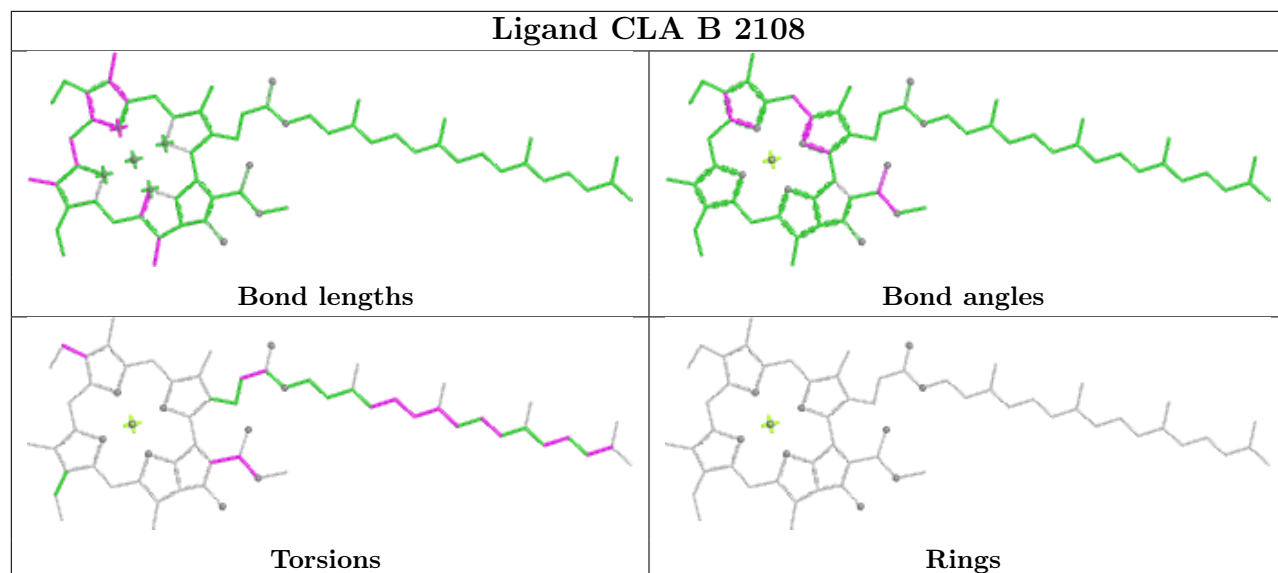
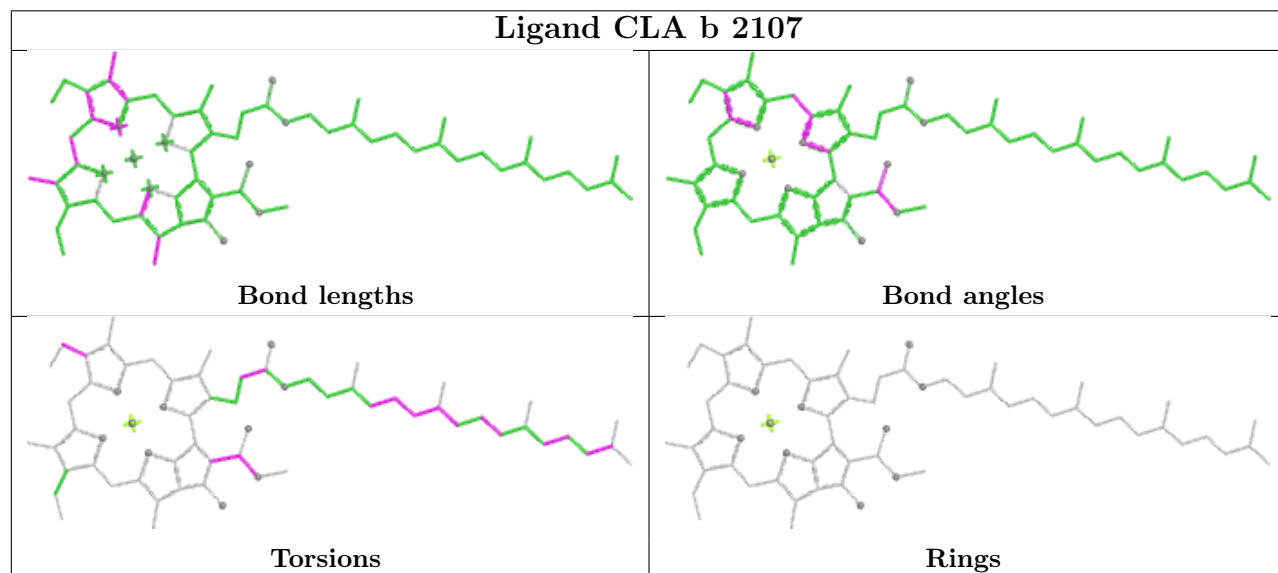
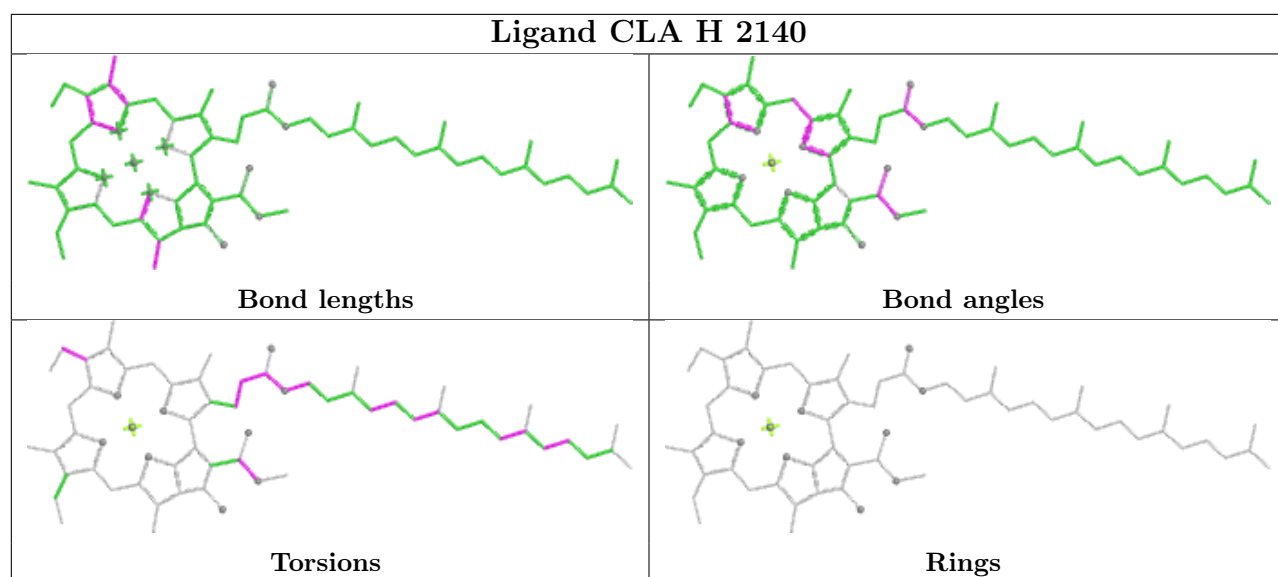


Rings

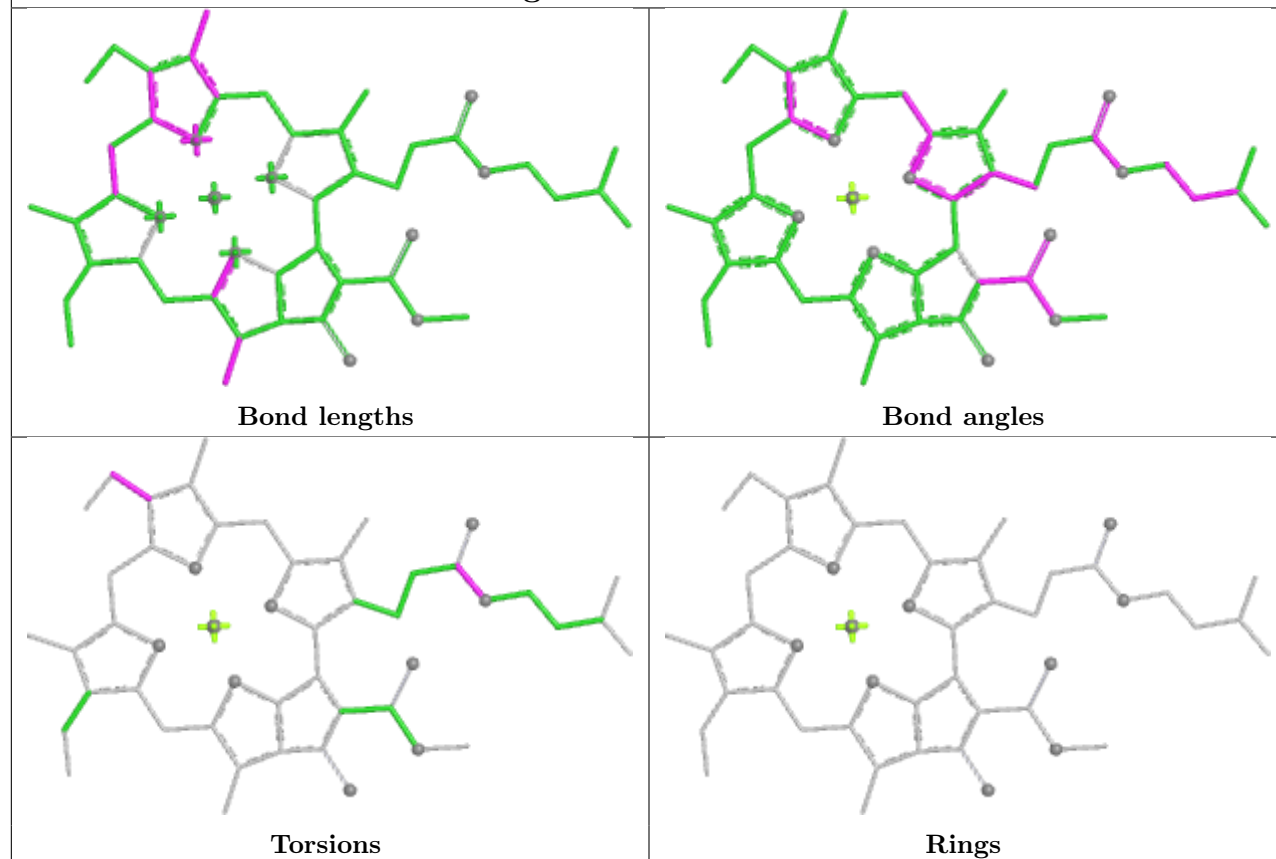




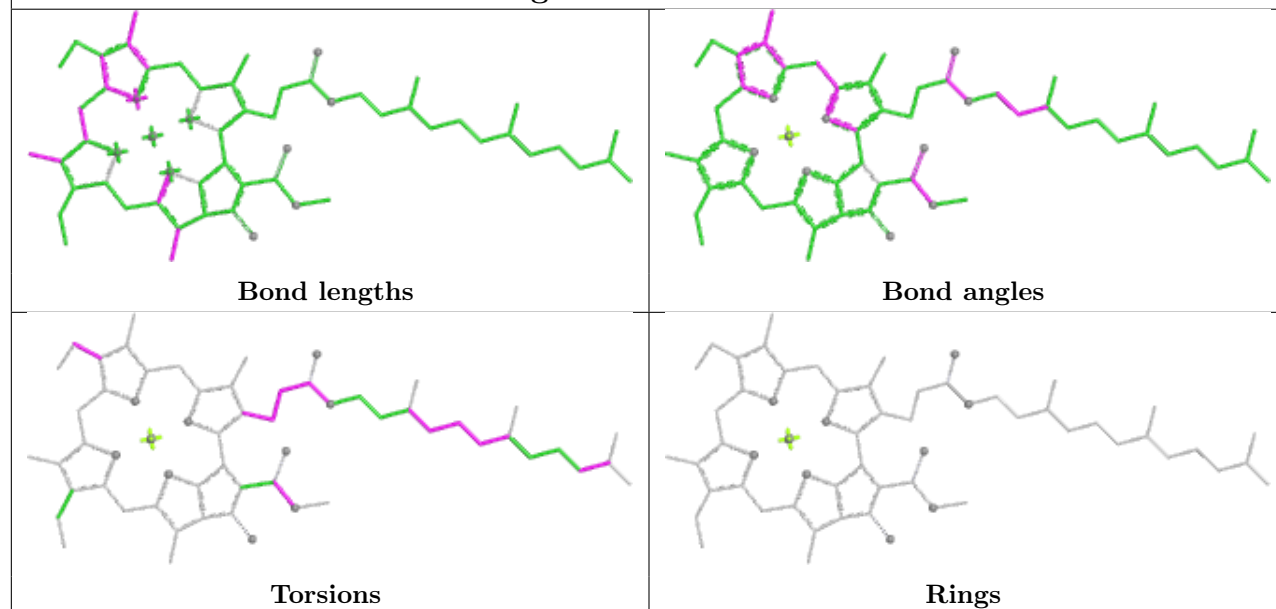


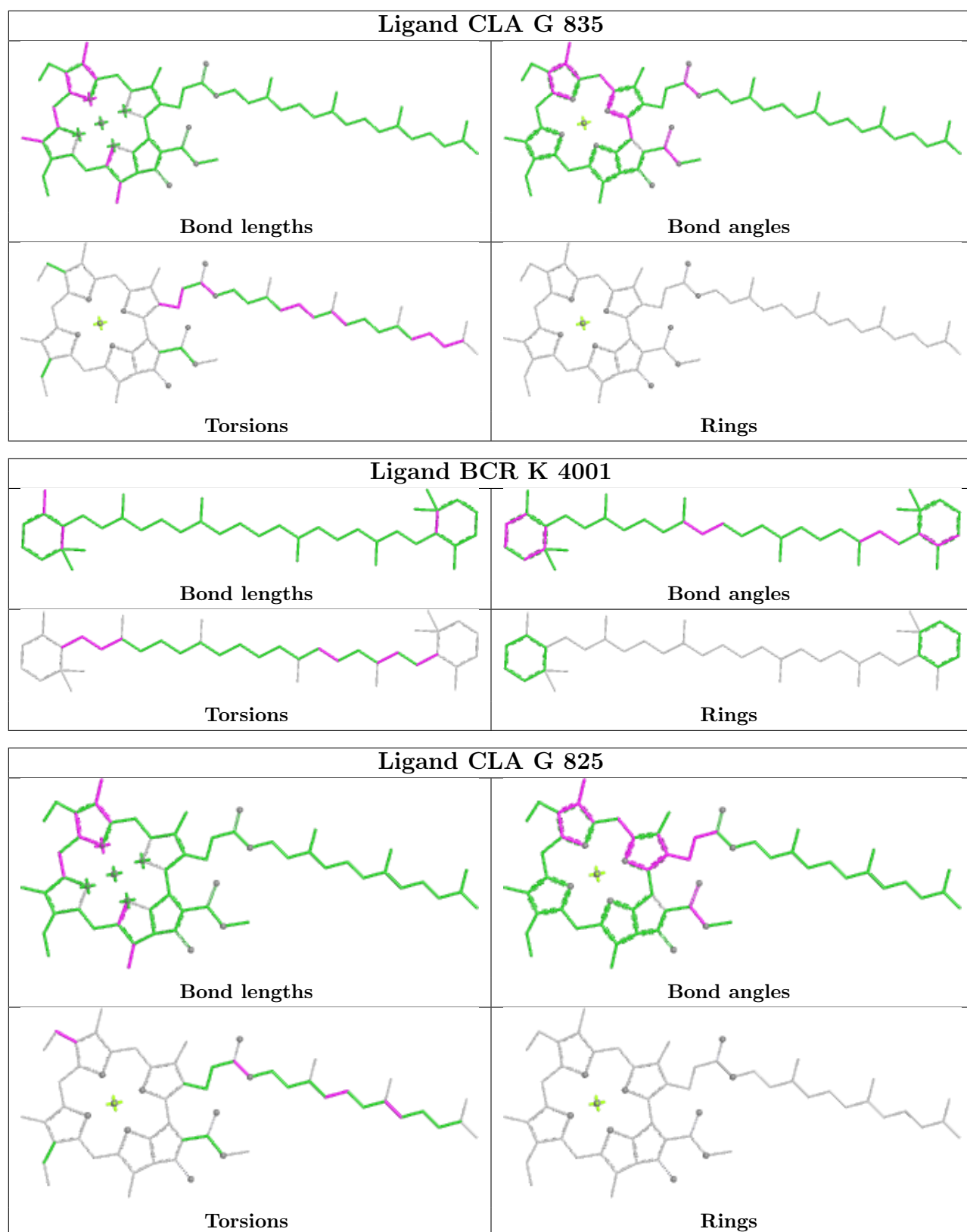


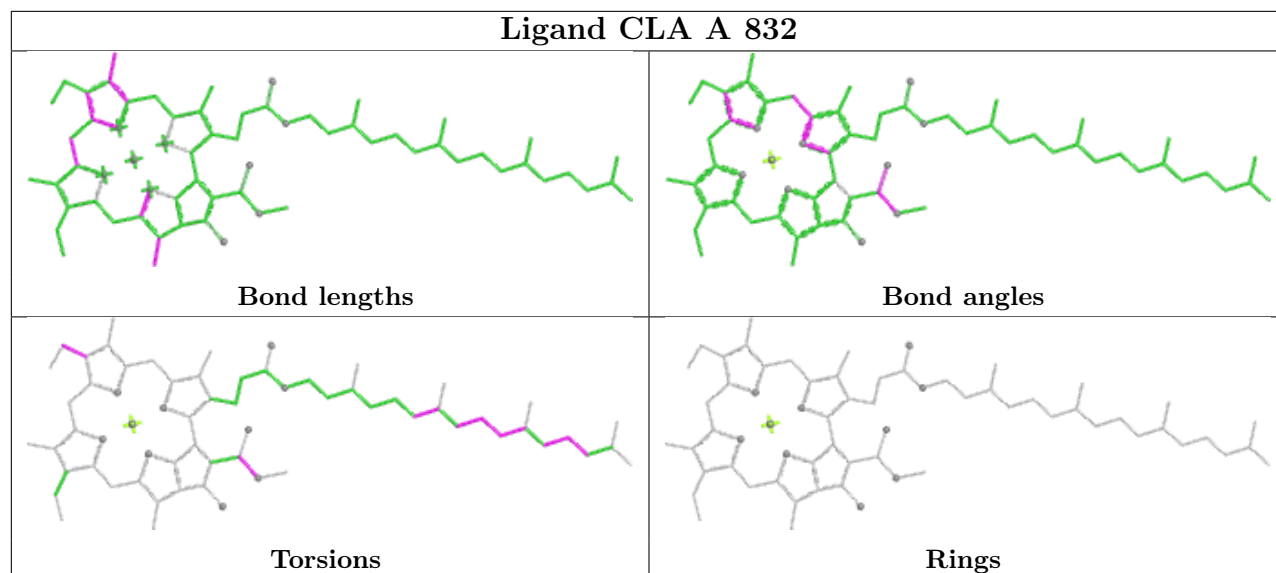
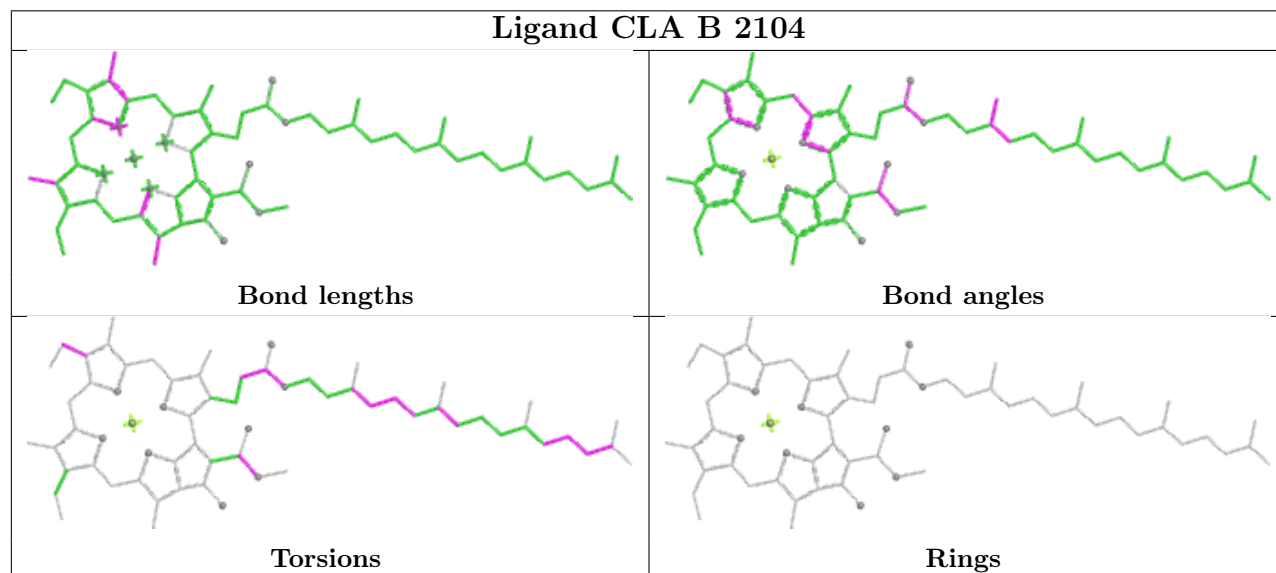
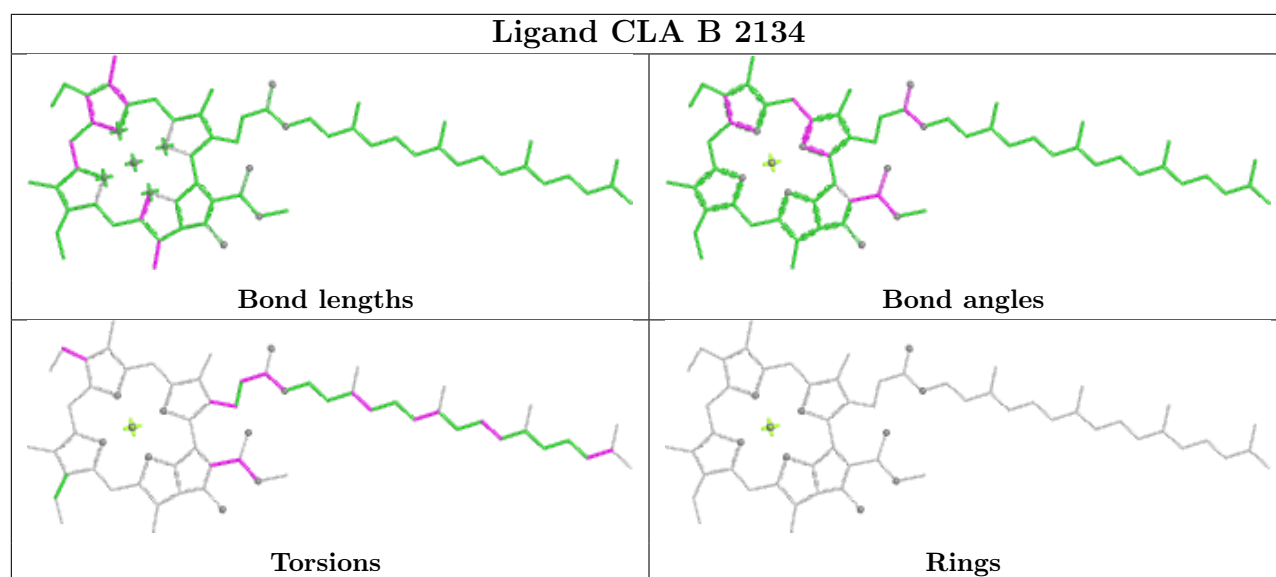
Ligand CLA B 2126

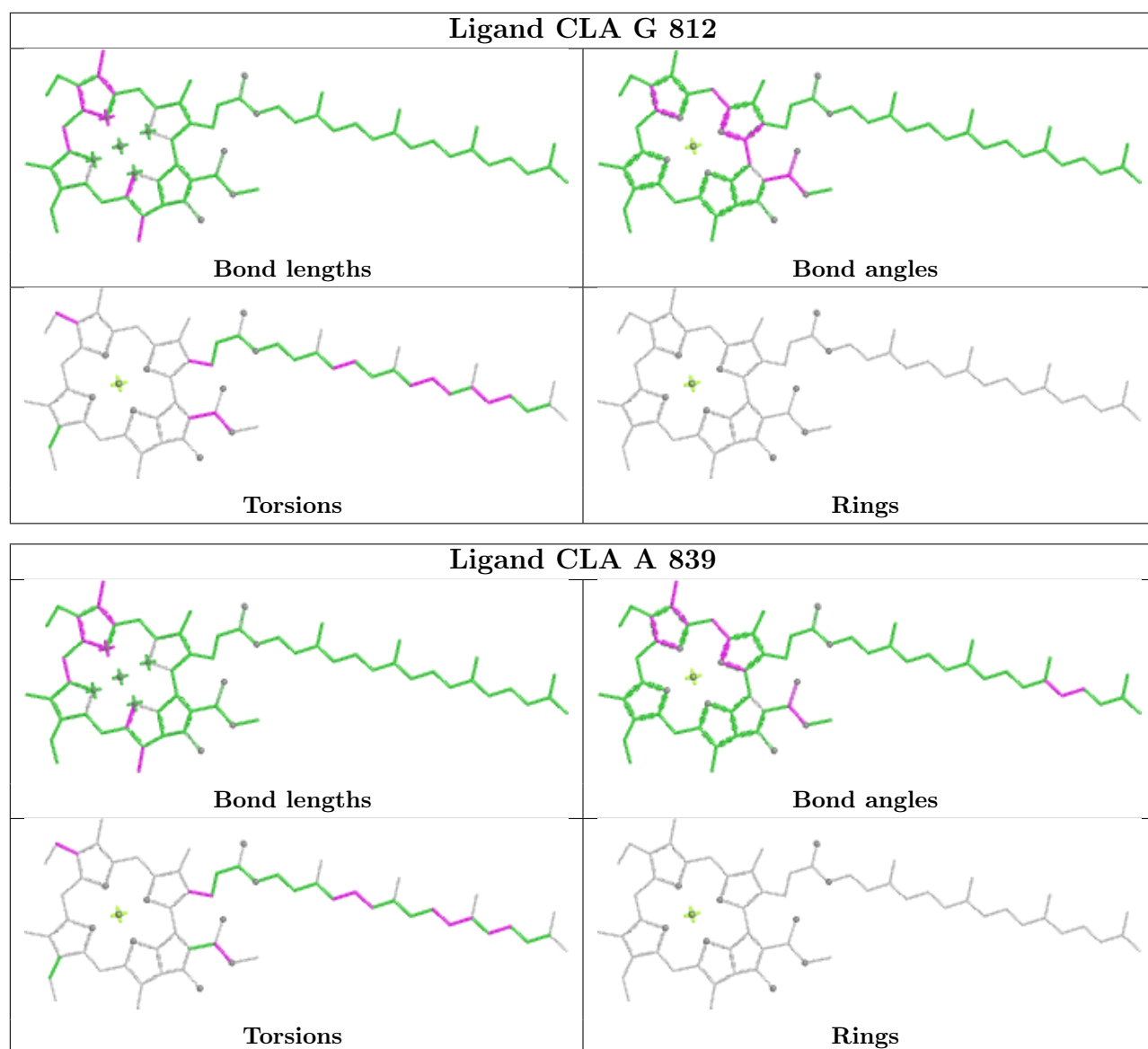


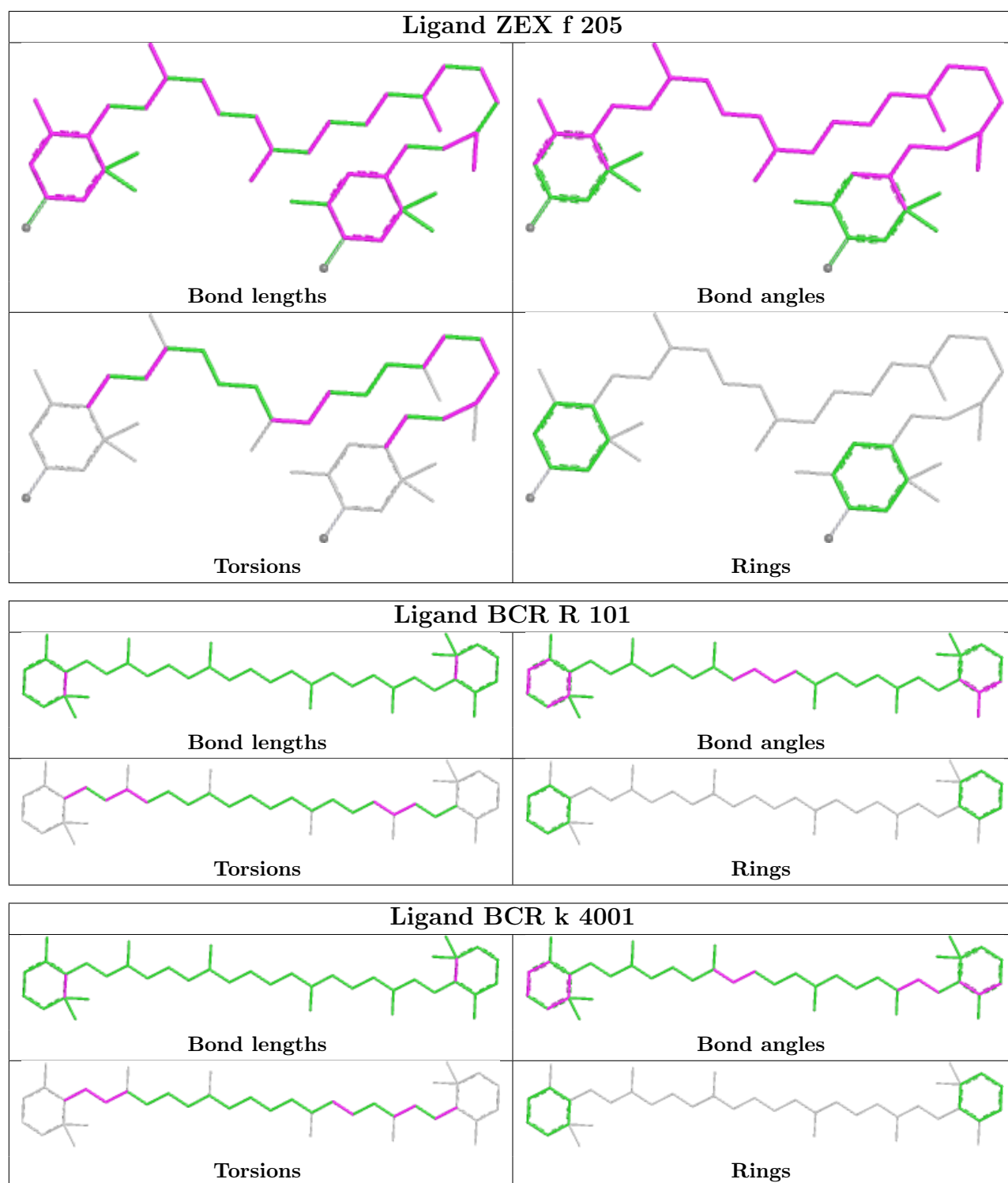
Ligand CLA G 817

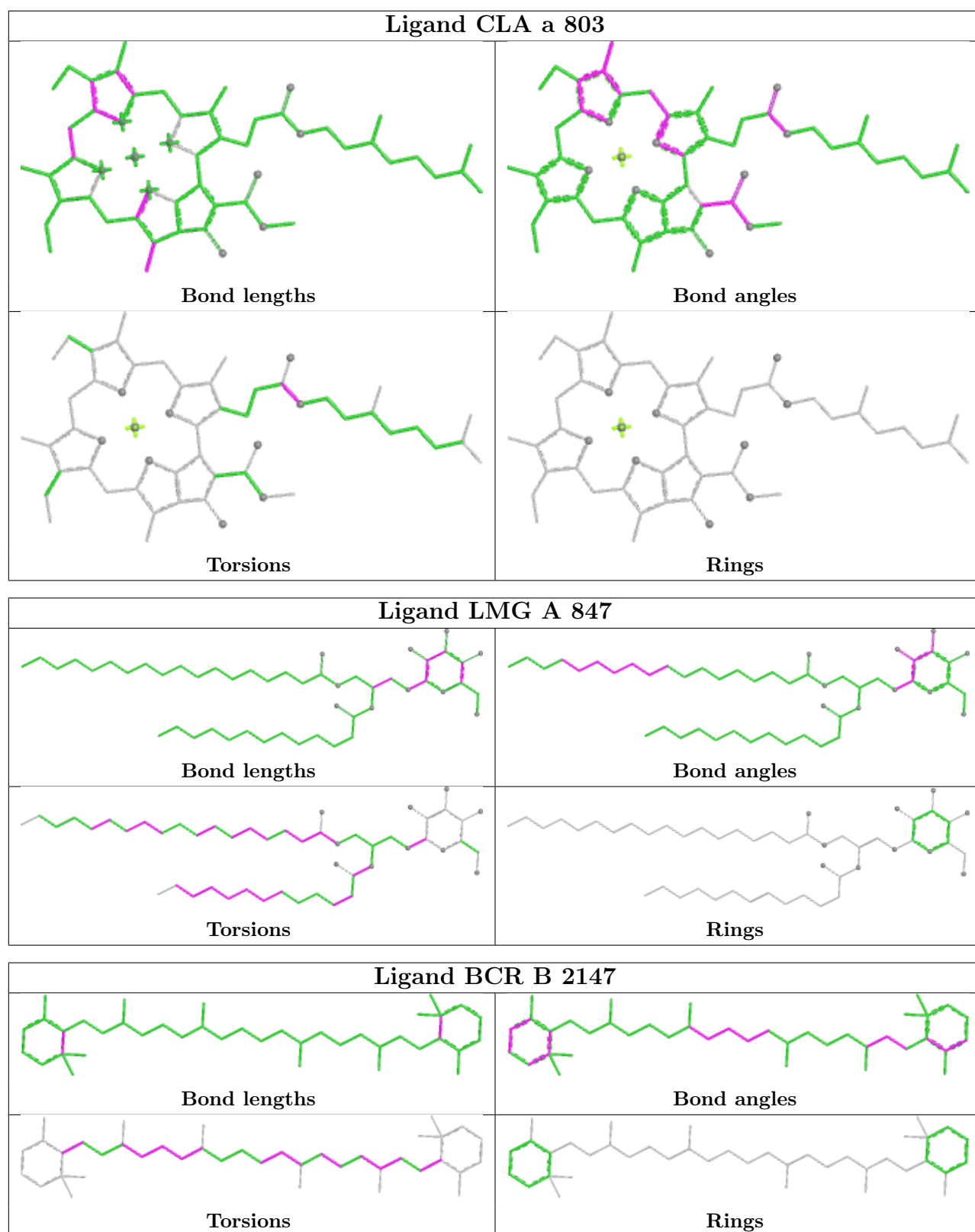


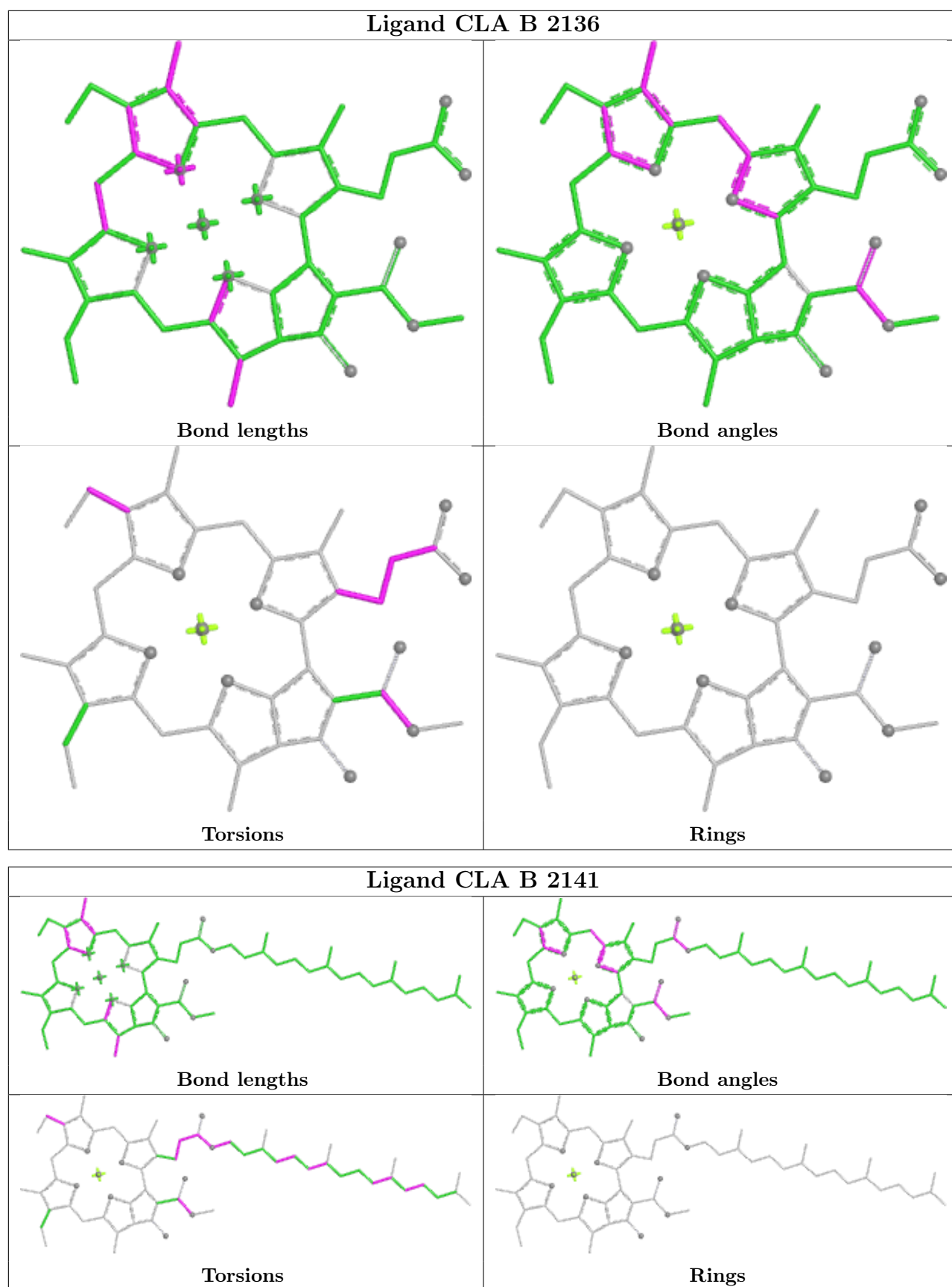


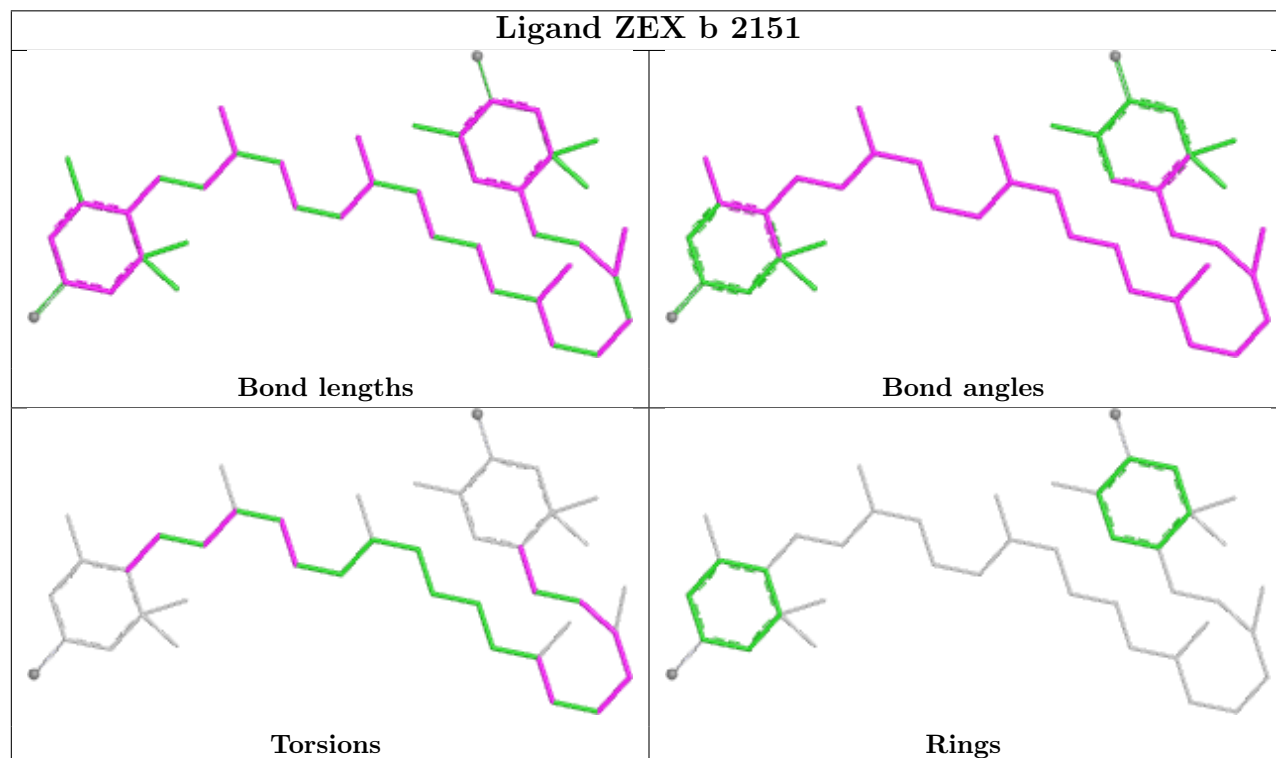
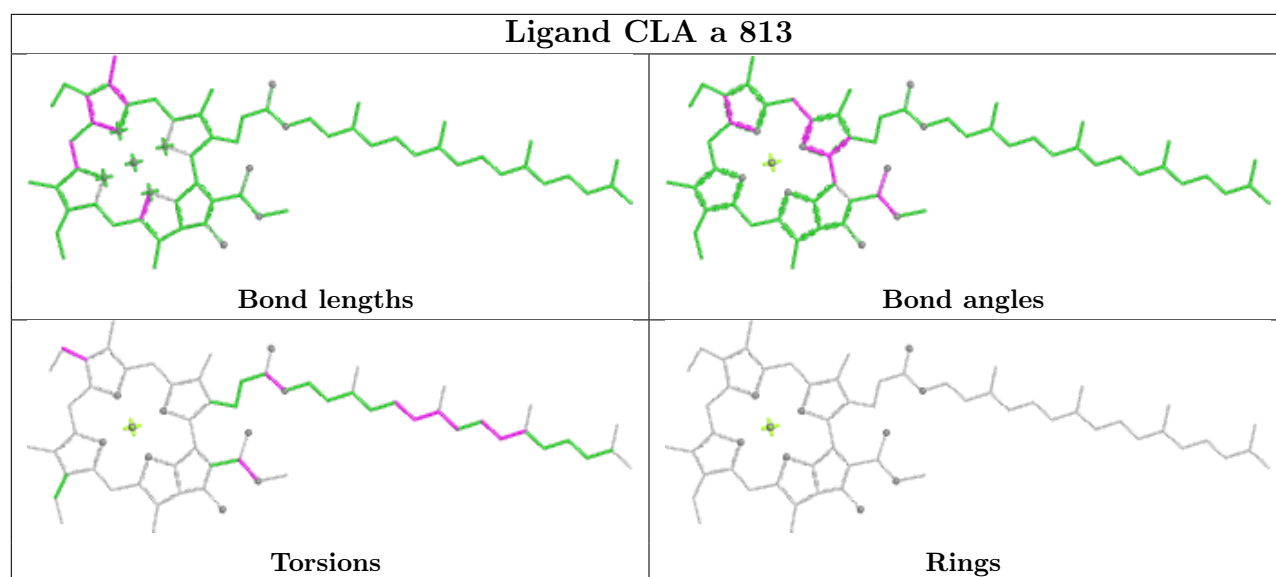


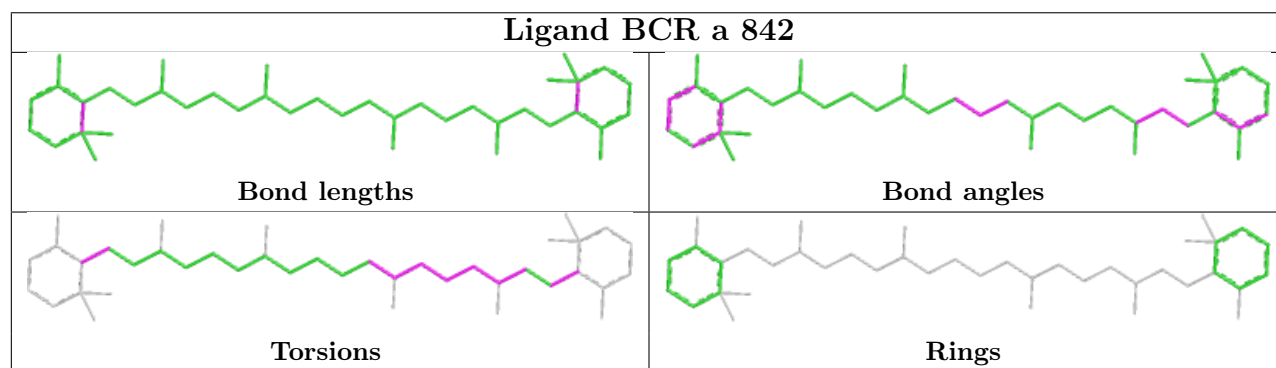
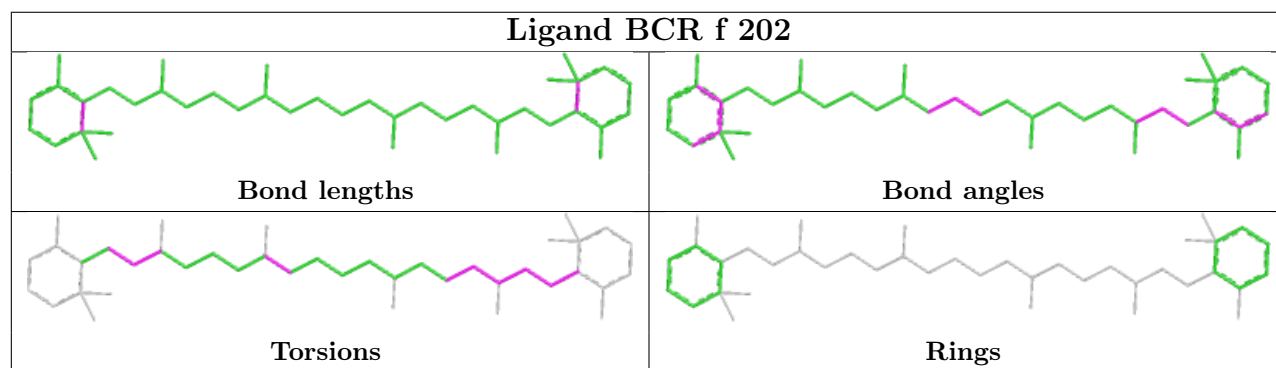
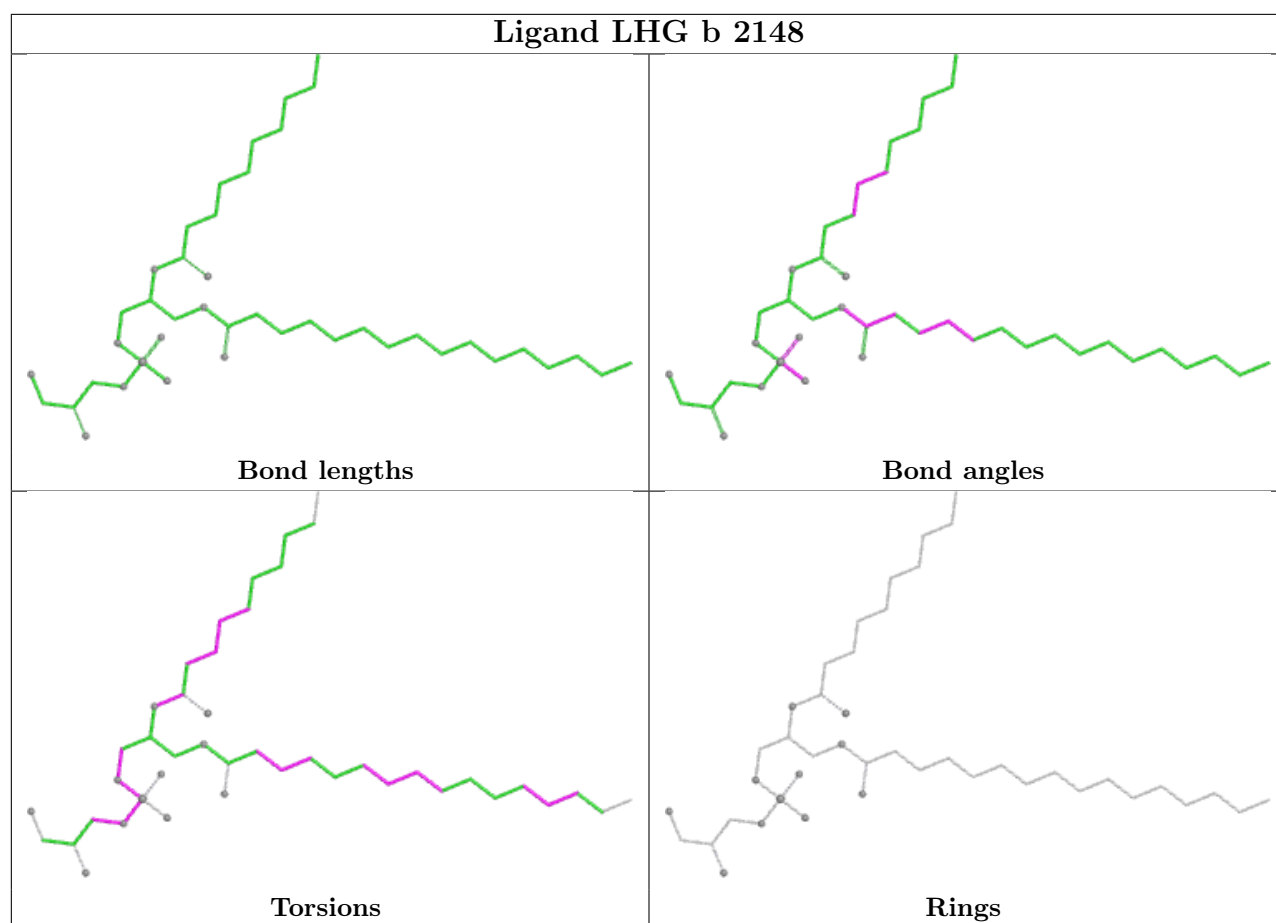


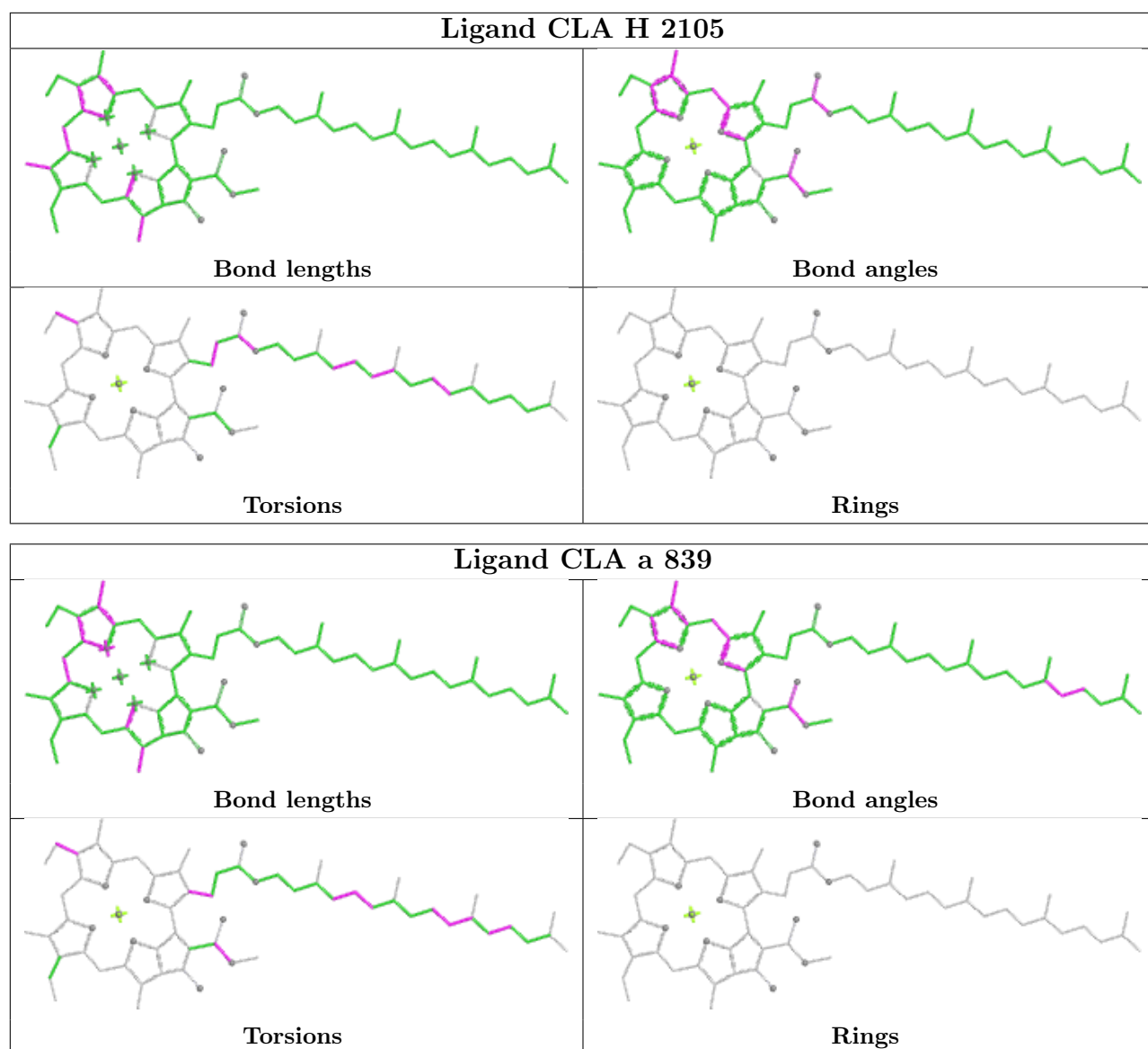


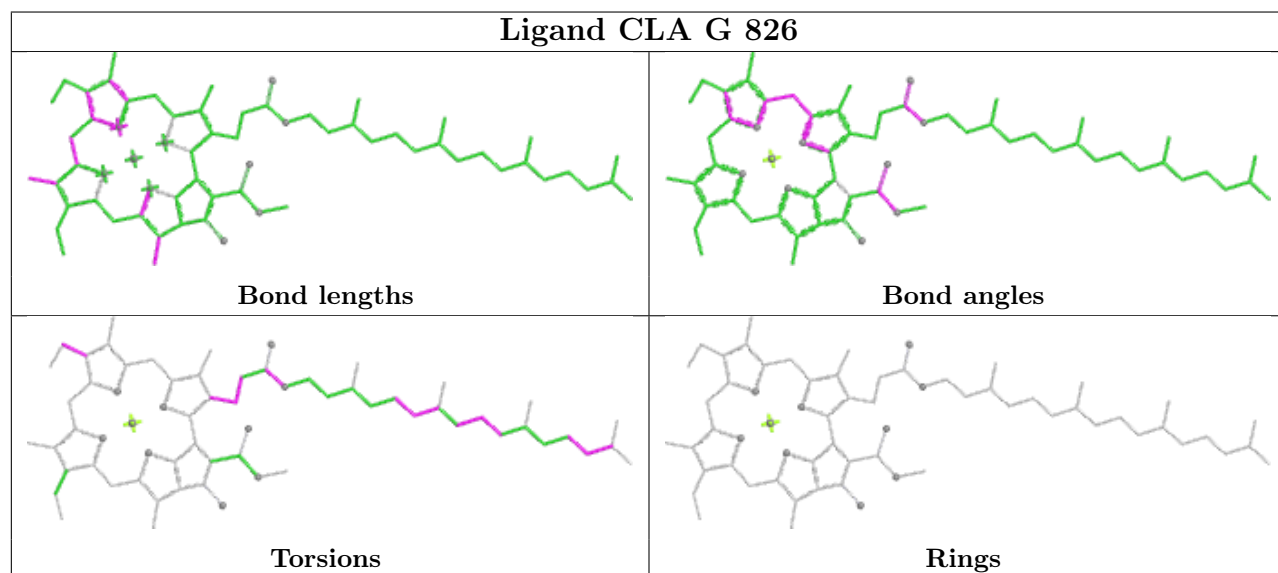
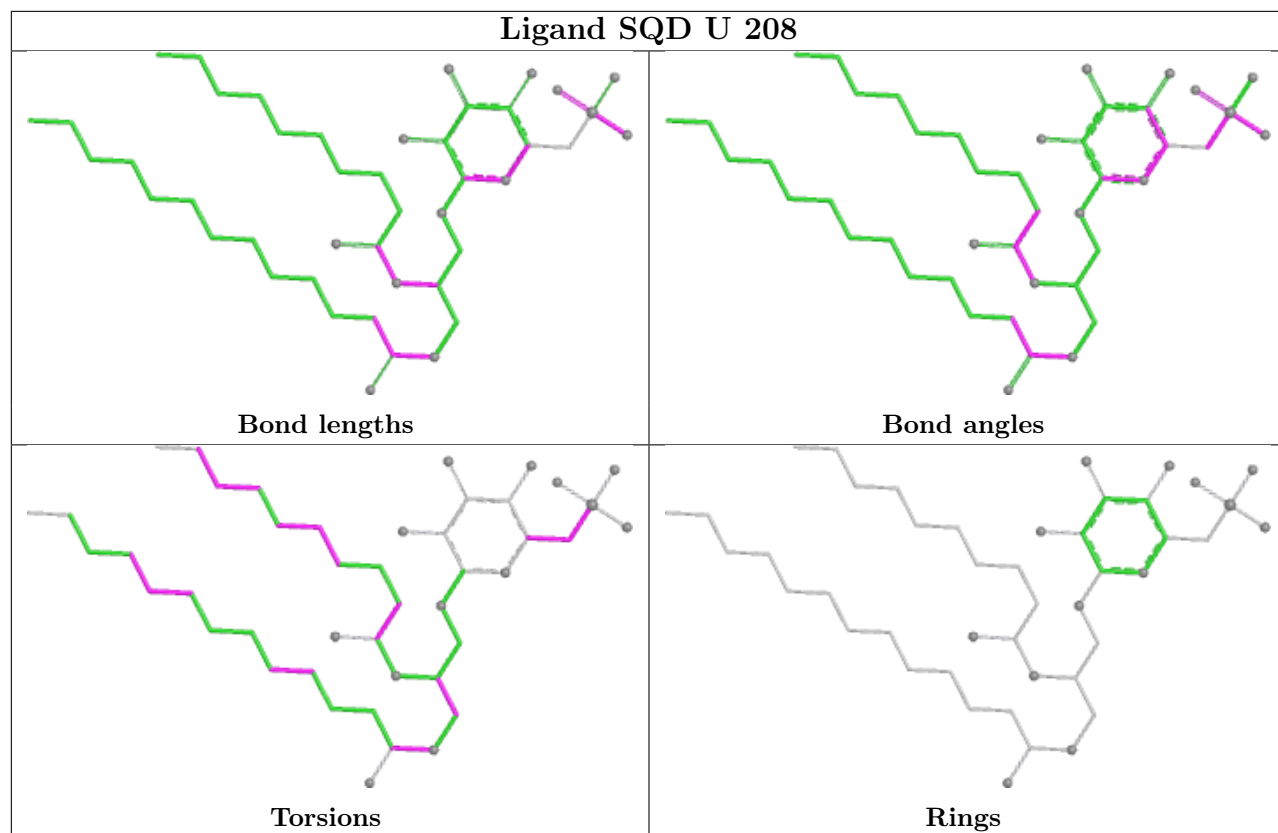


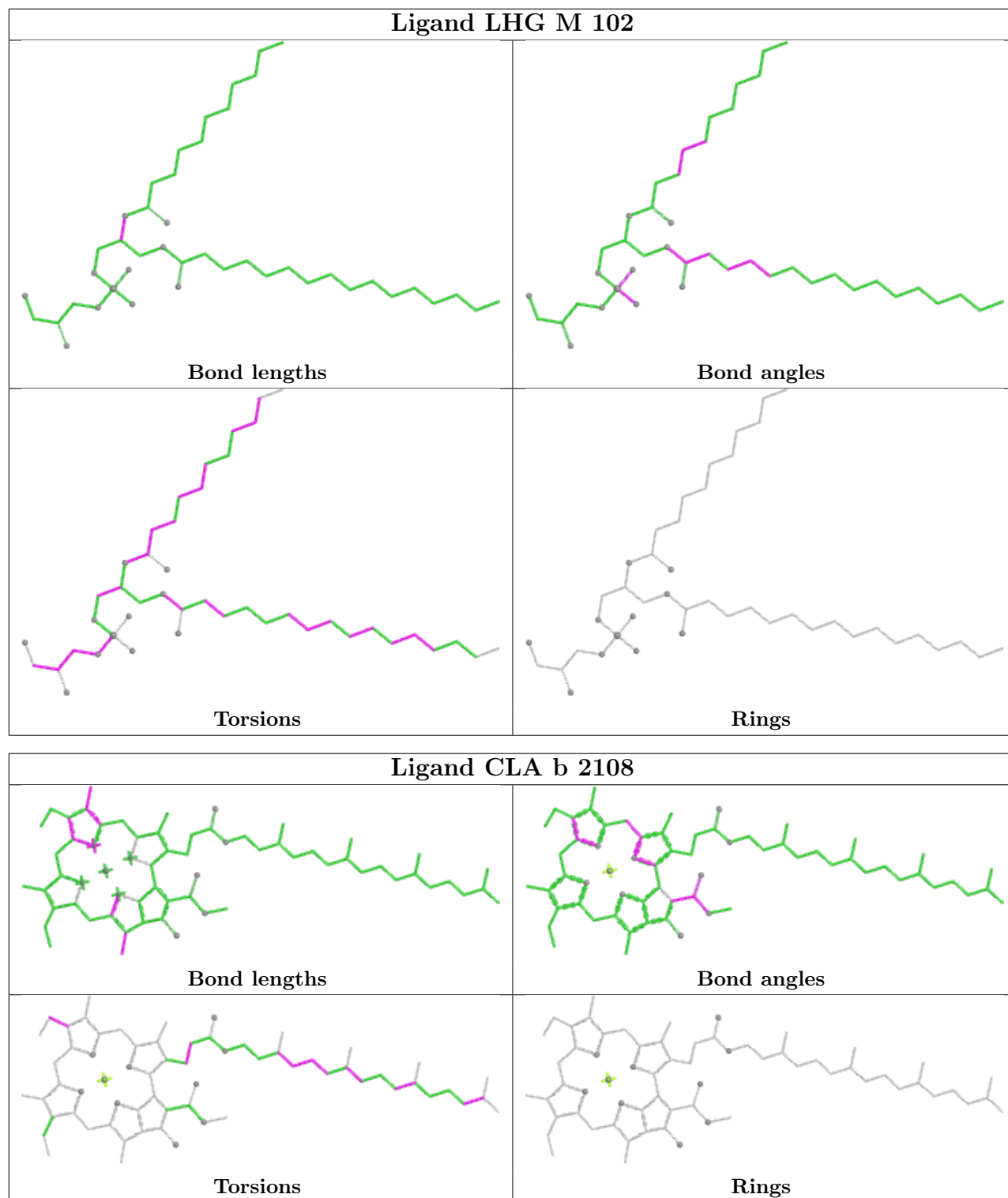


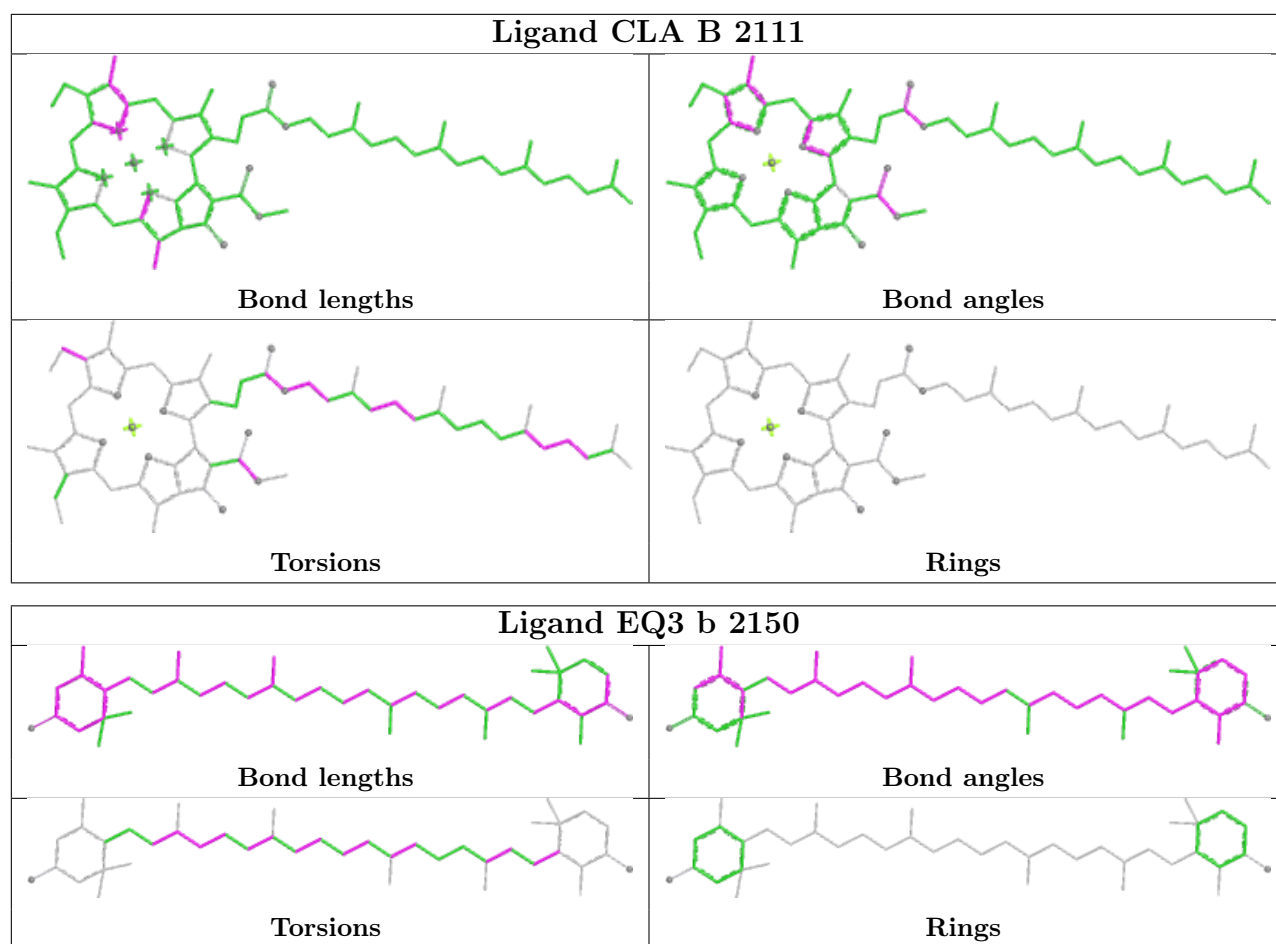


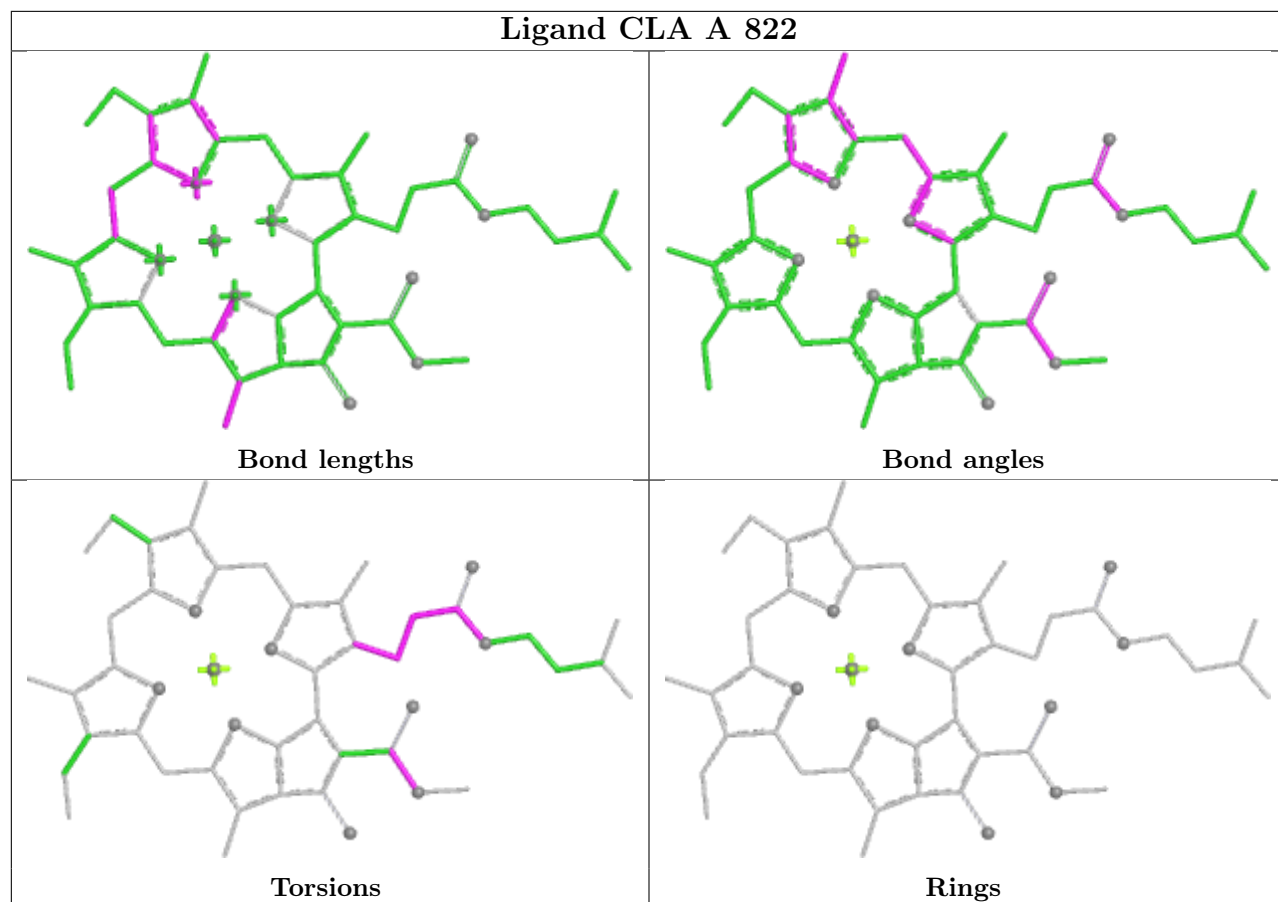


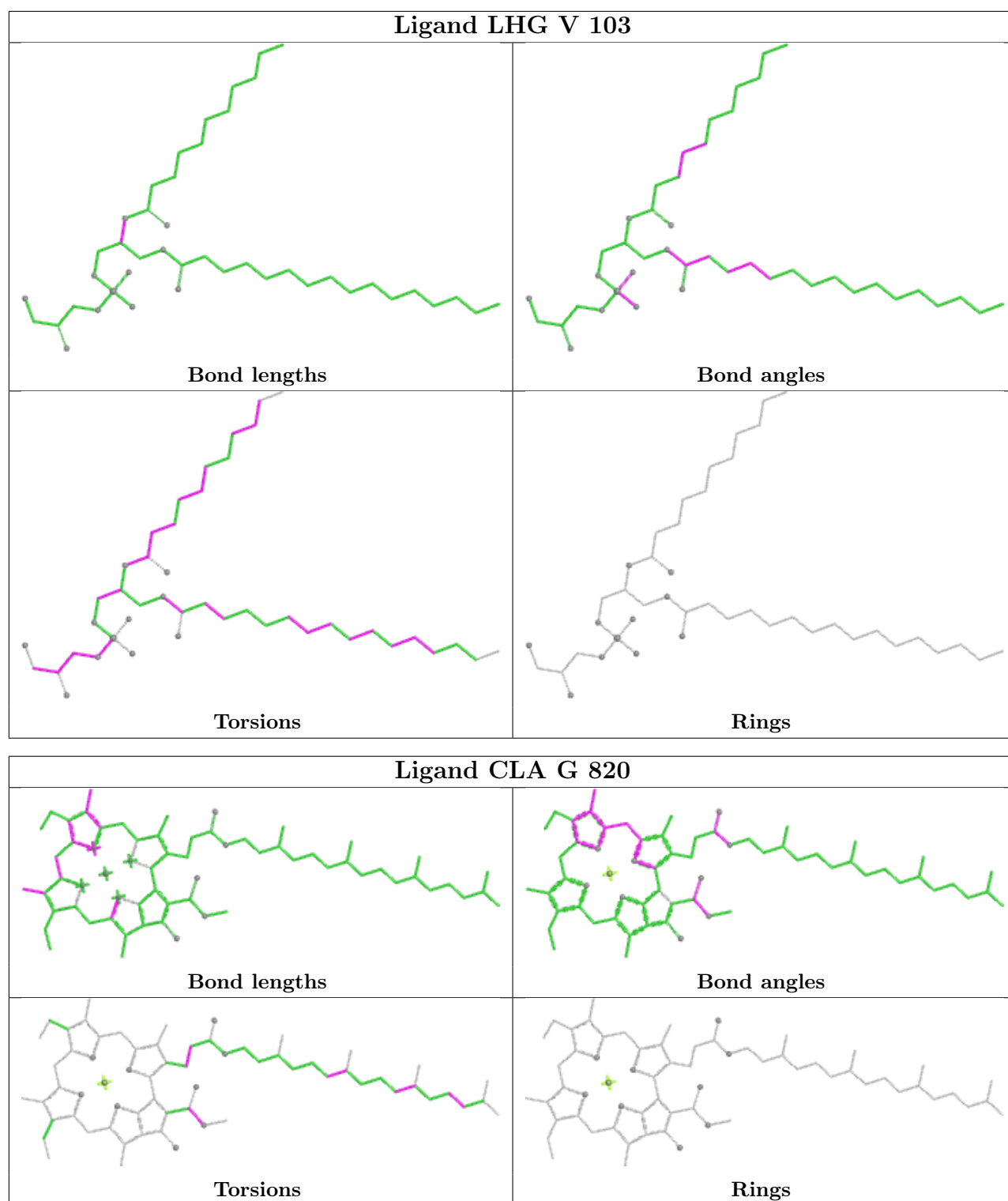


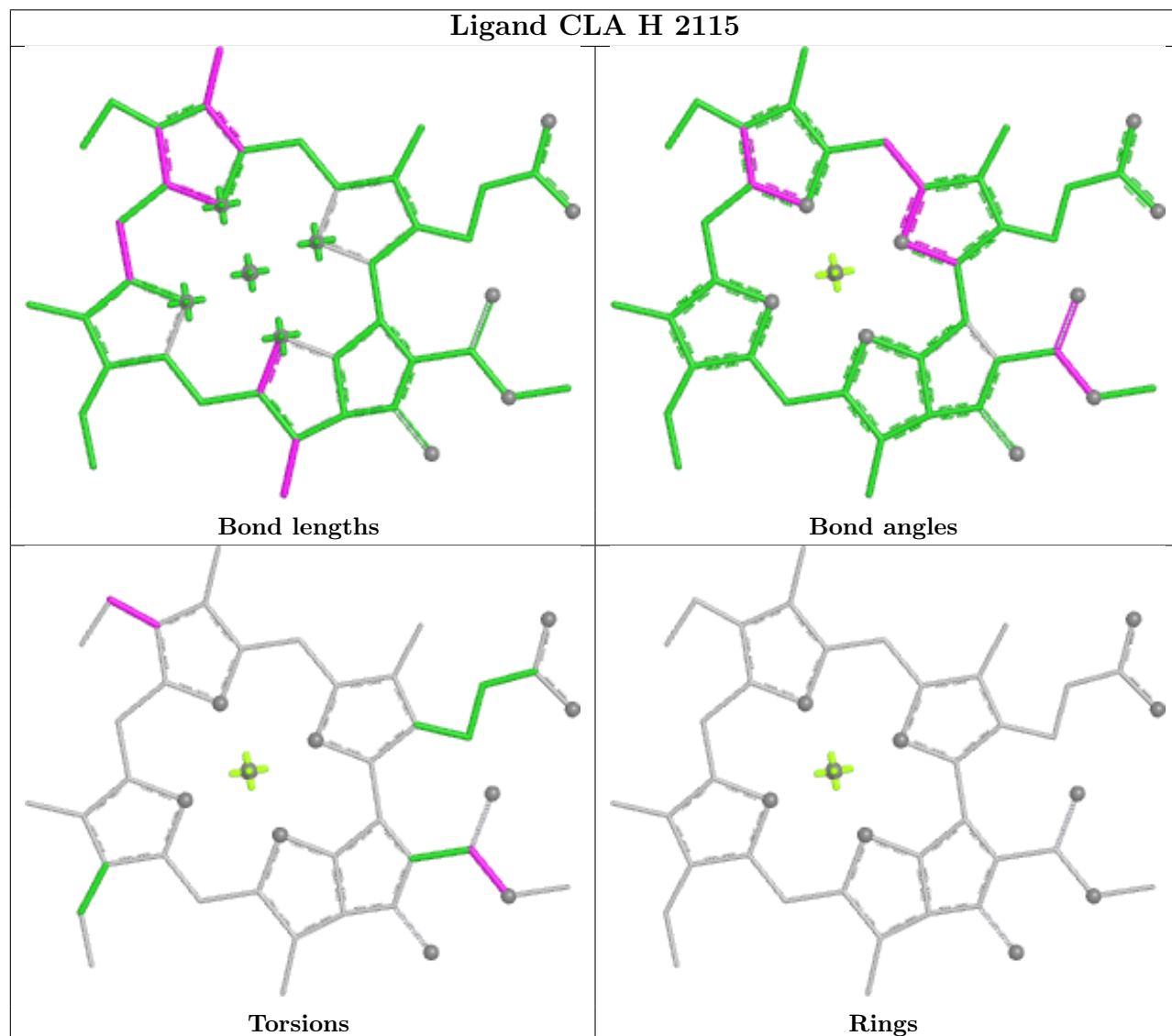
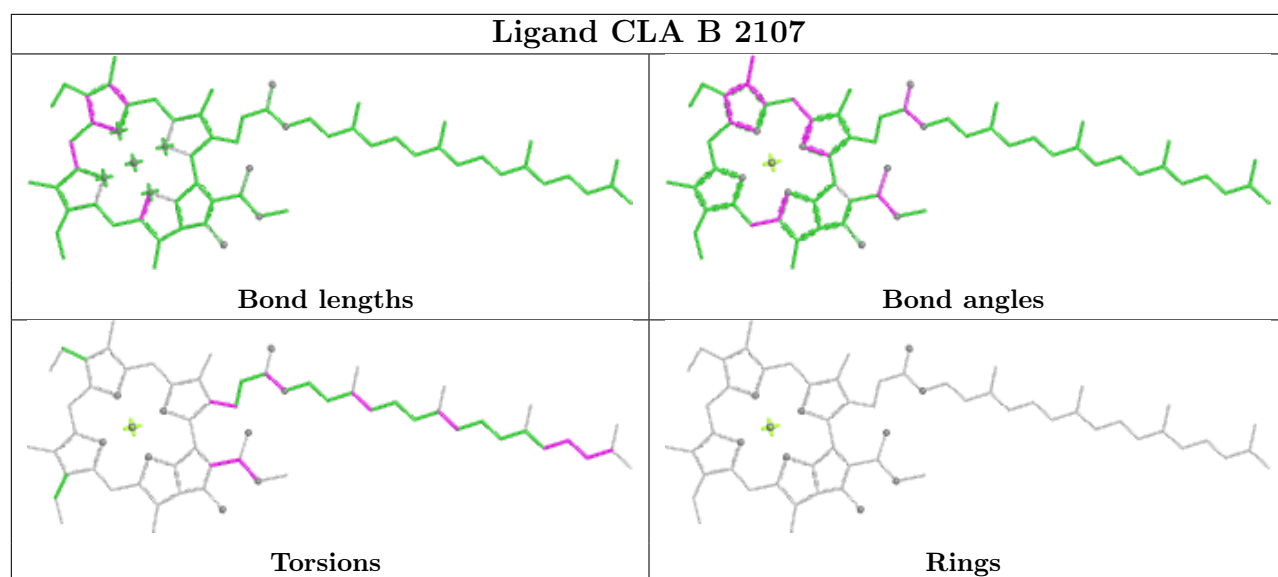


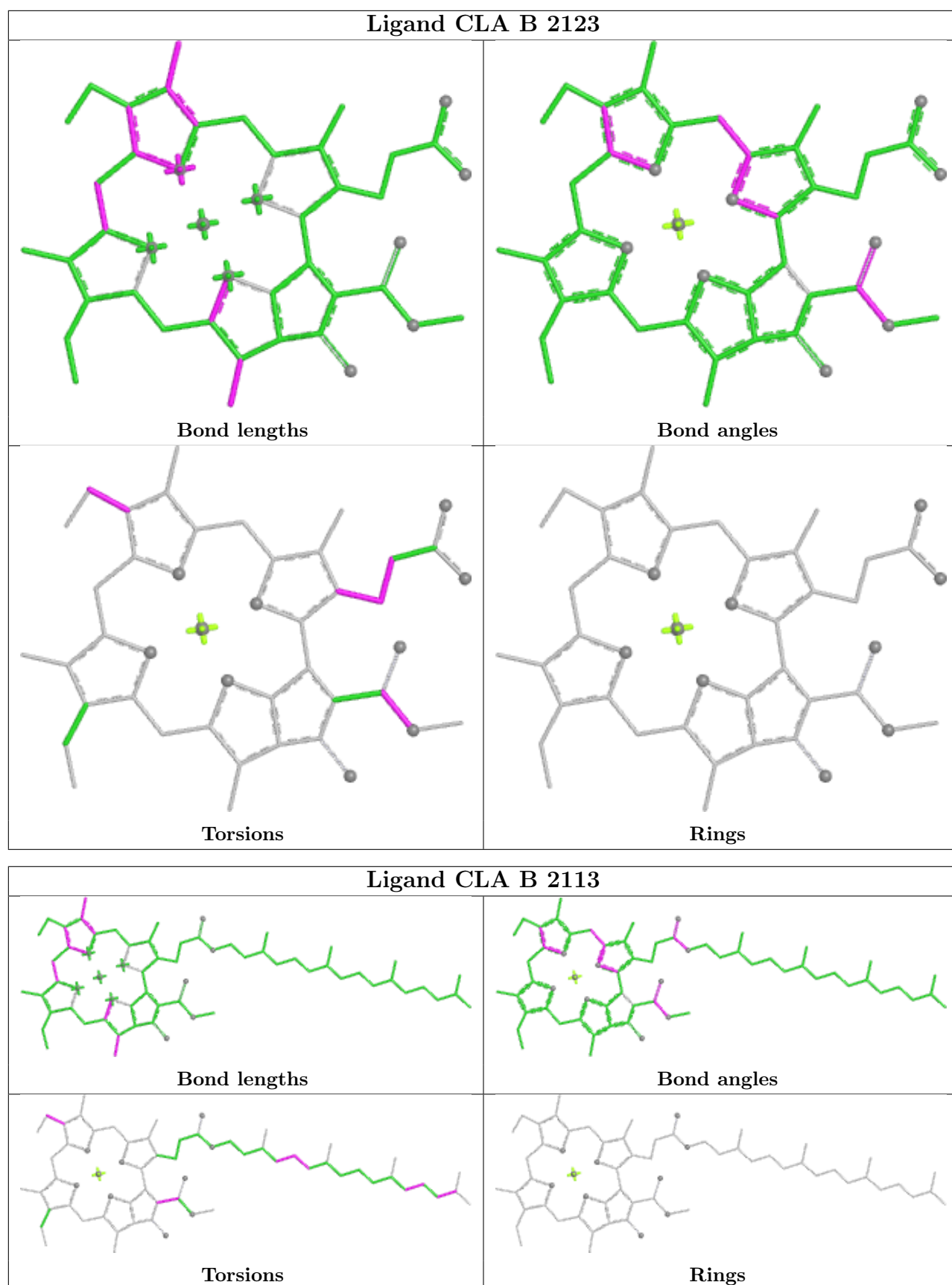


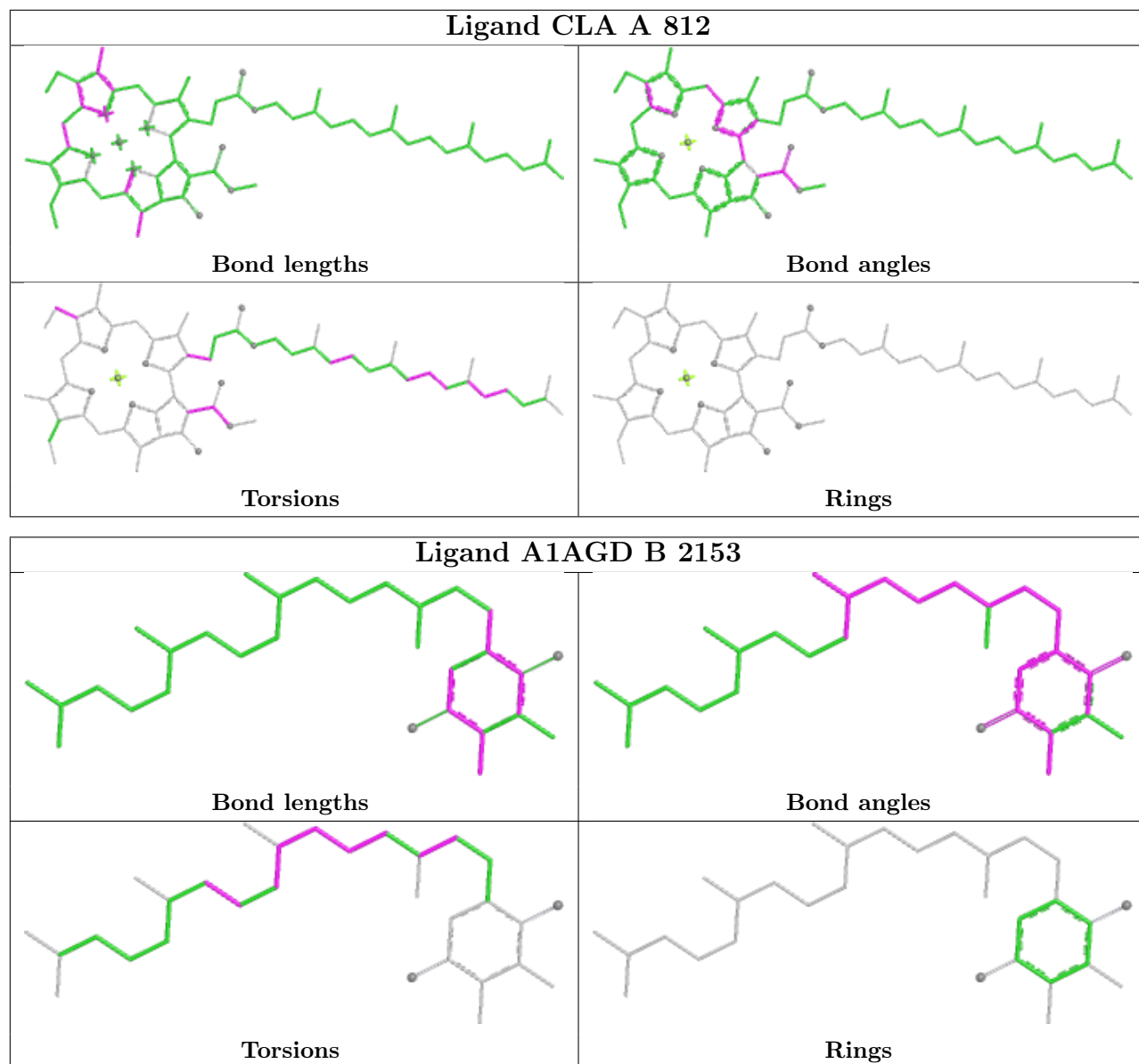




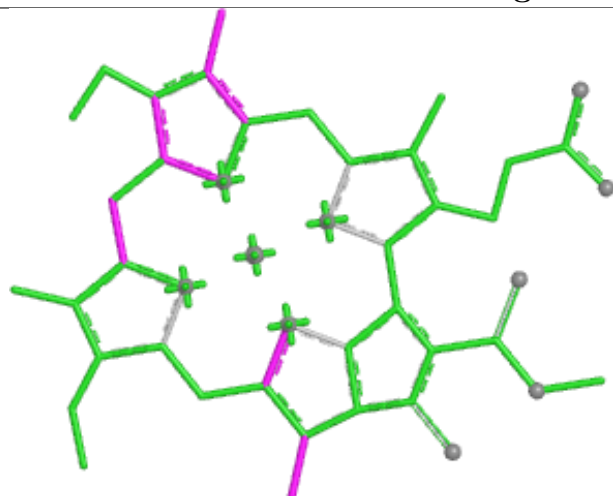




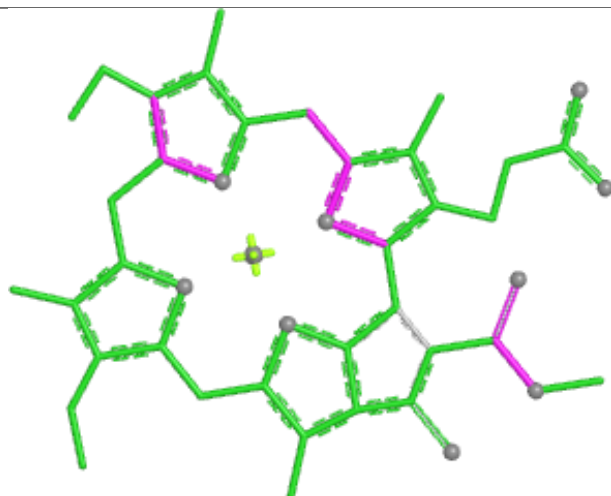




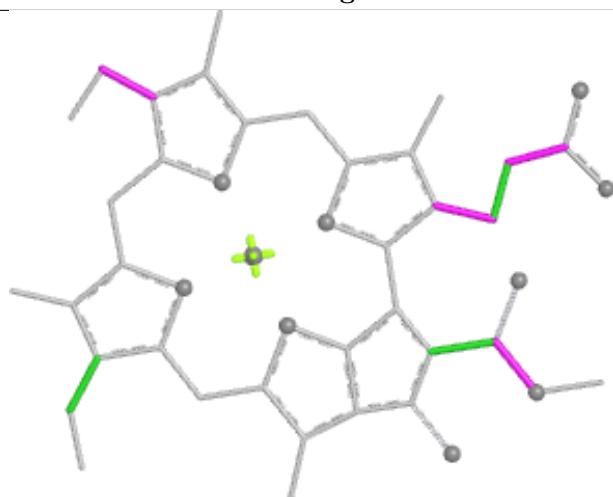
Ligand CLA A 811



Bond lengths



Bond angles

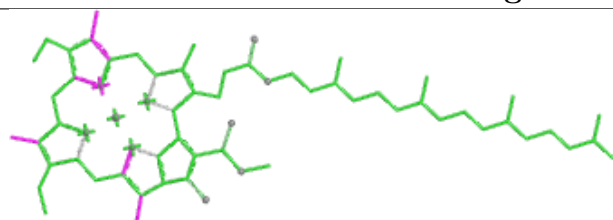


Torsions

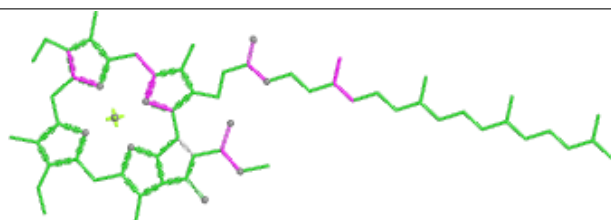


Rings

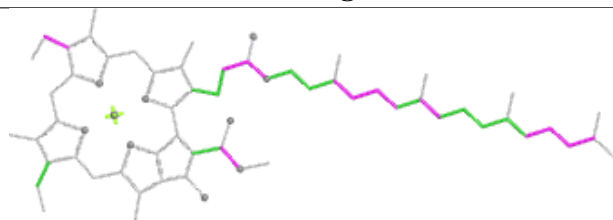
Ligand CLA H 2103



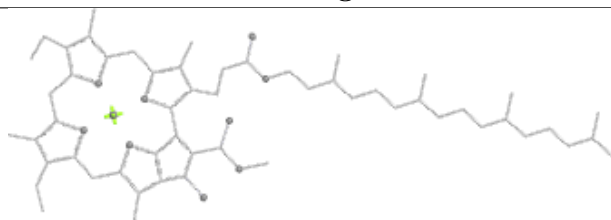
Bond lengths



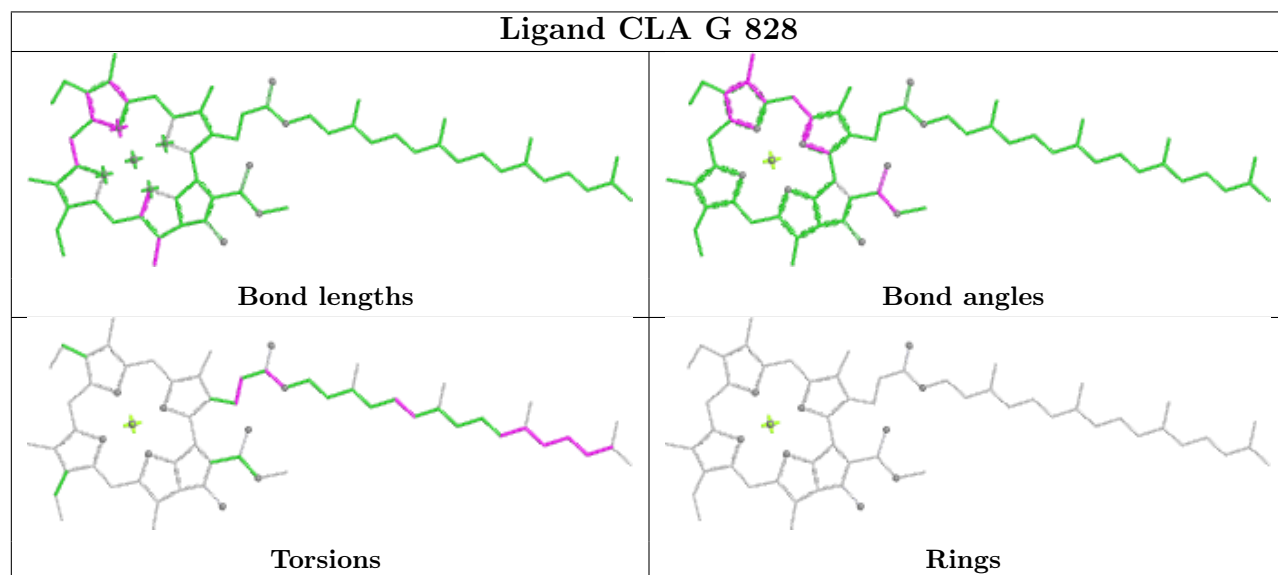
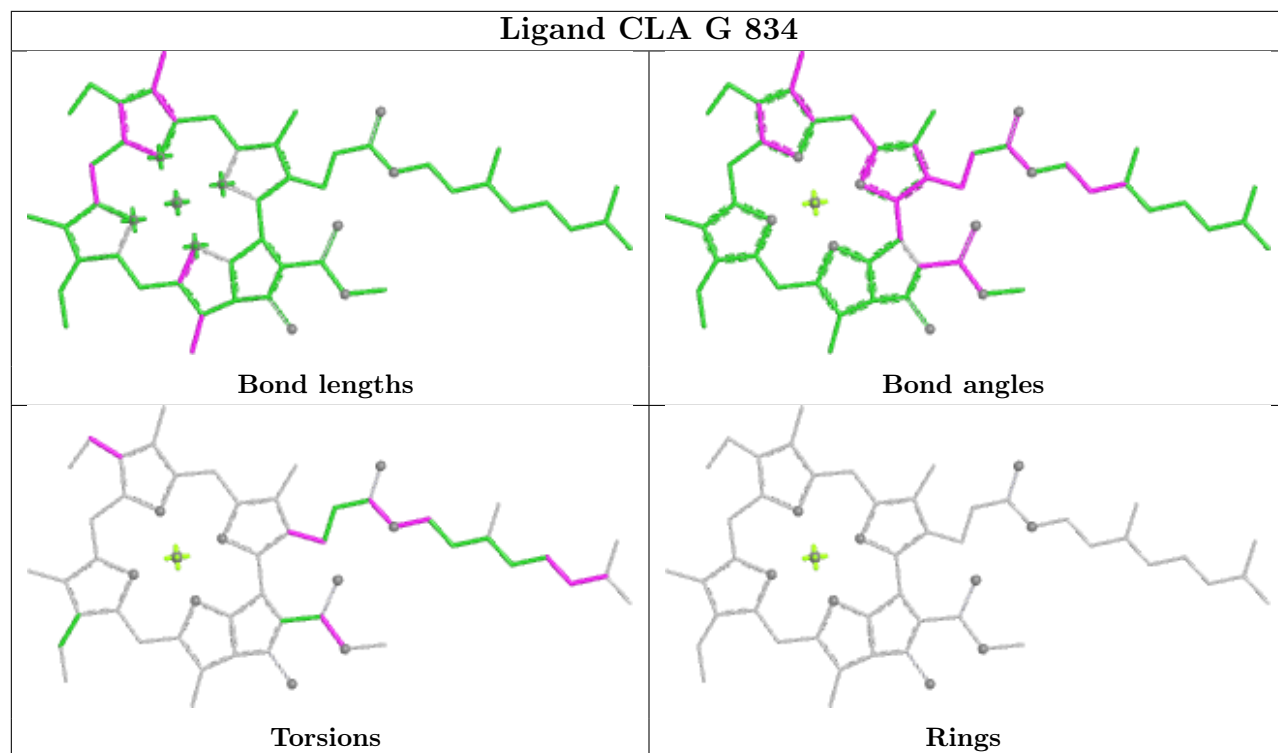
Bond angles

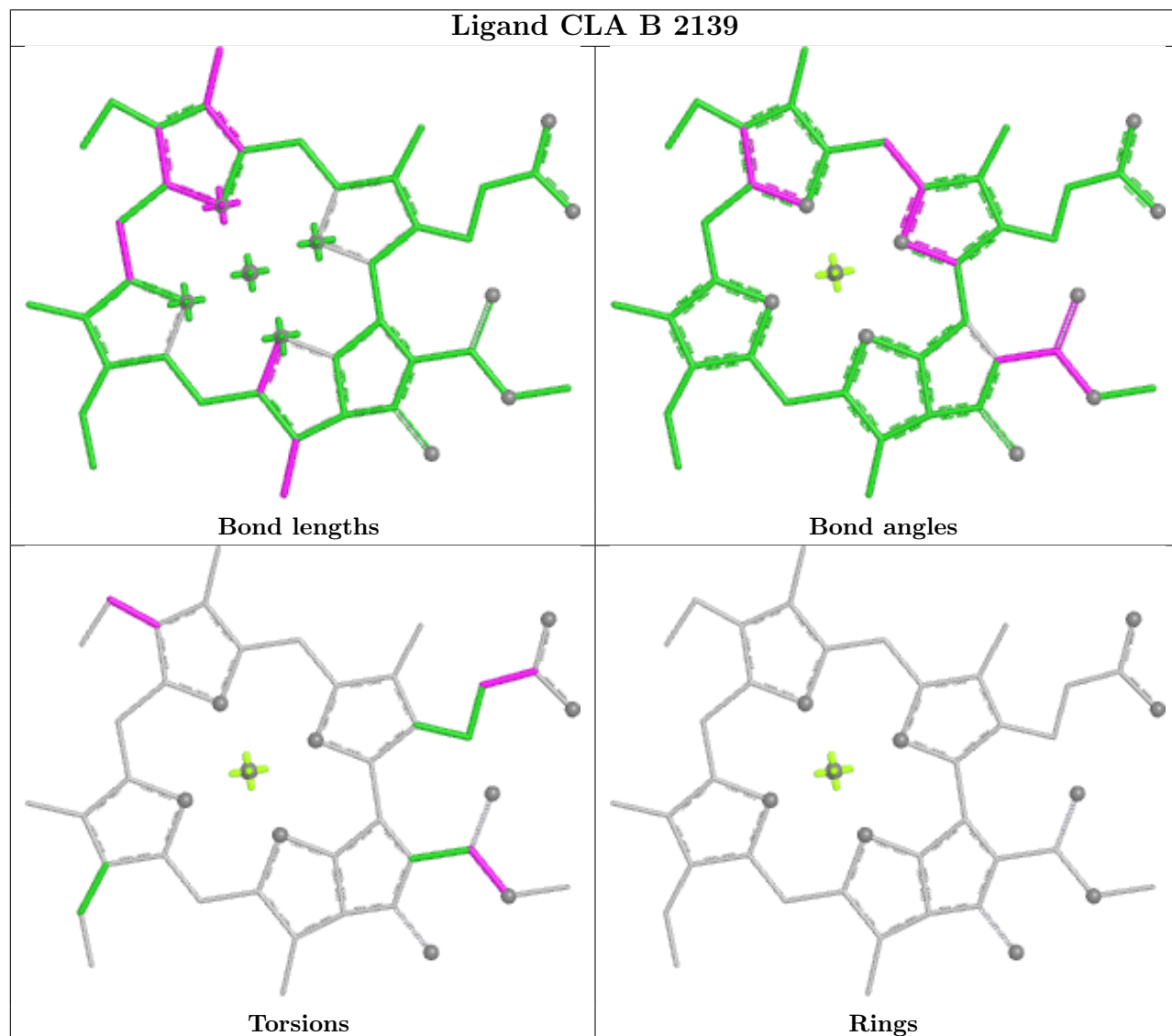
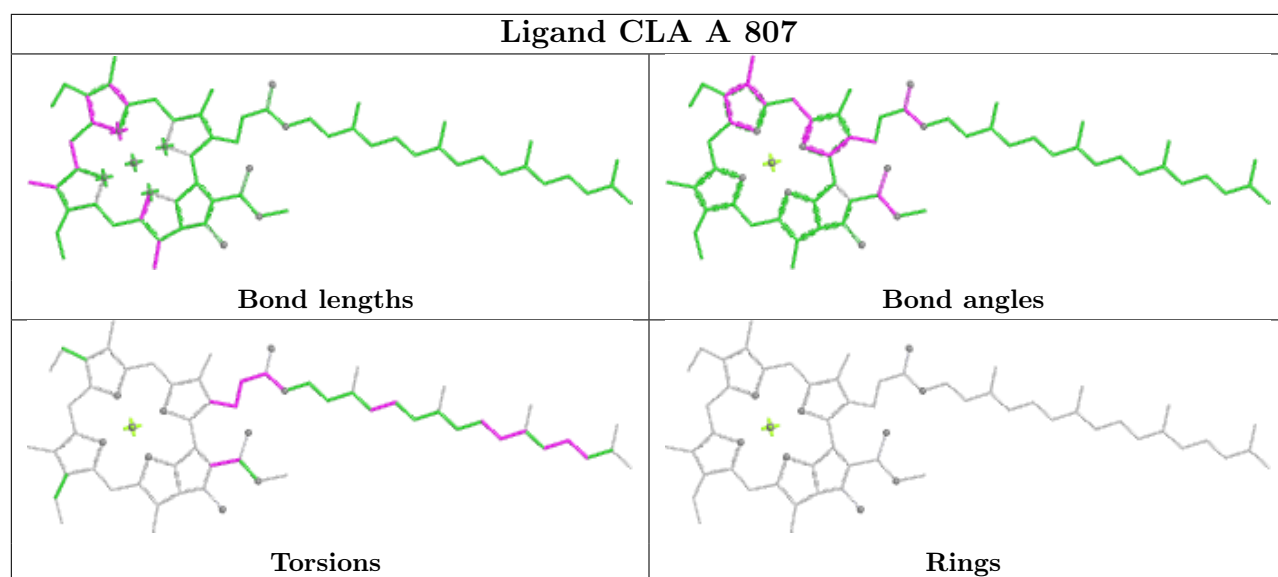


Torsions

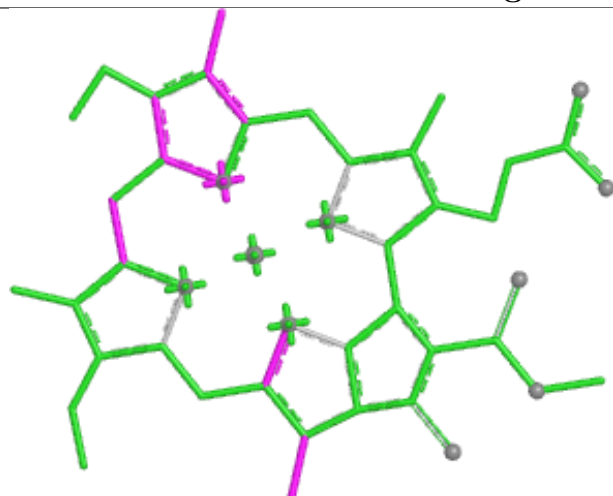


Rings

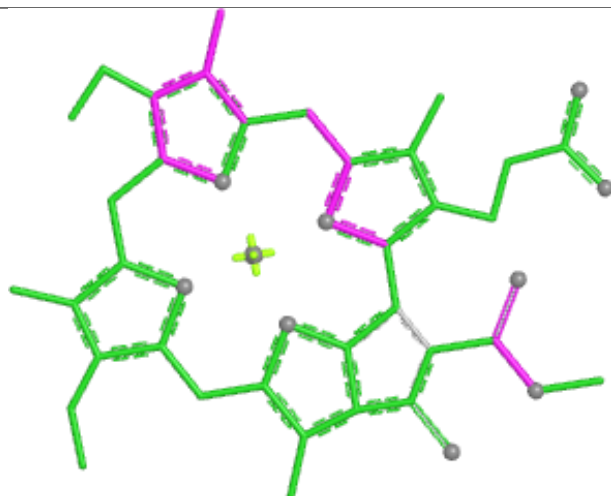




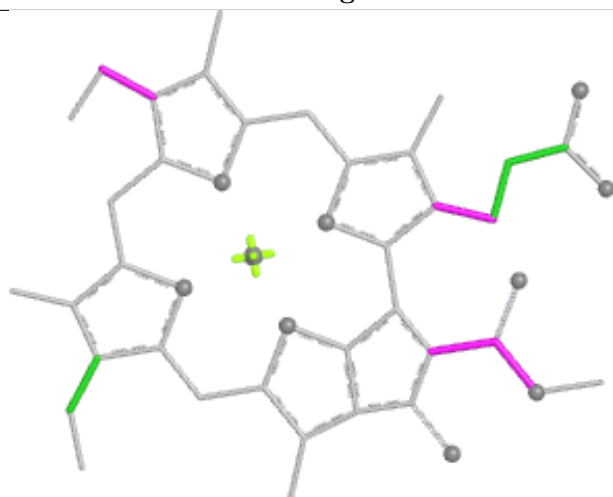
Ligand CLA H 2136



Bond lengths



Bond angles

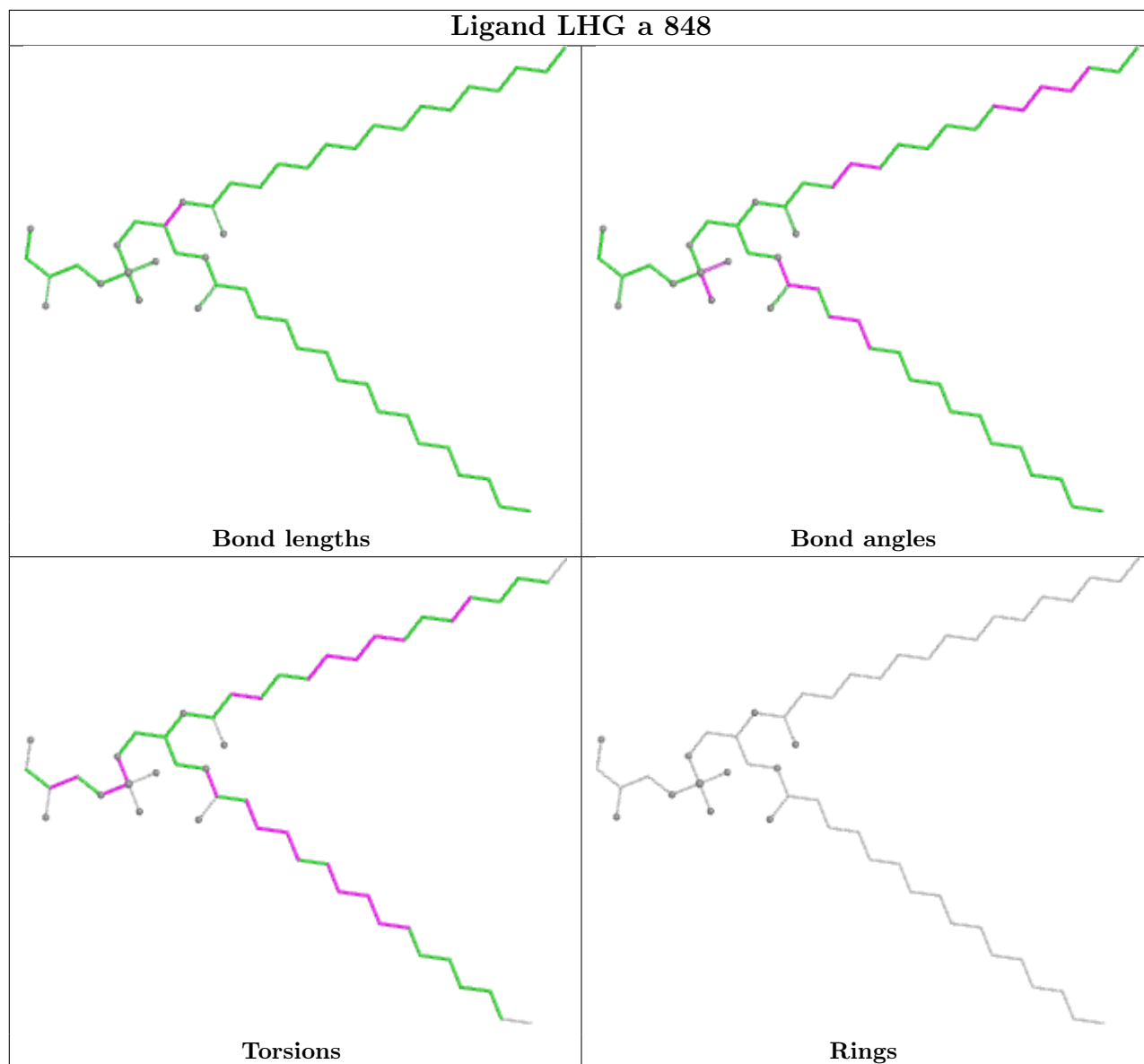


Torsions

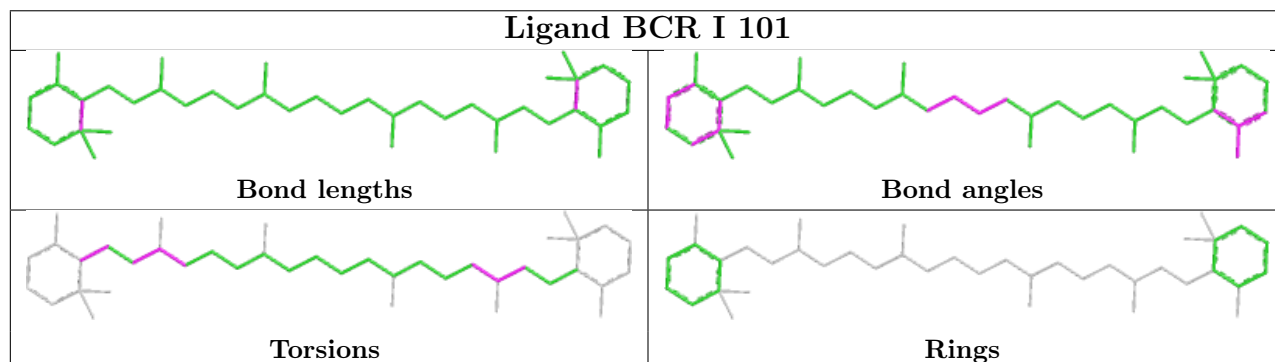


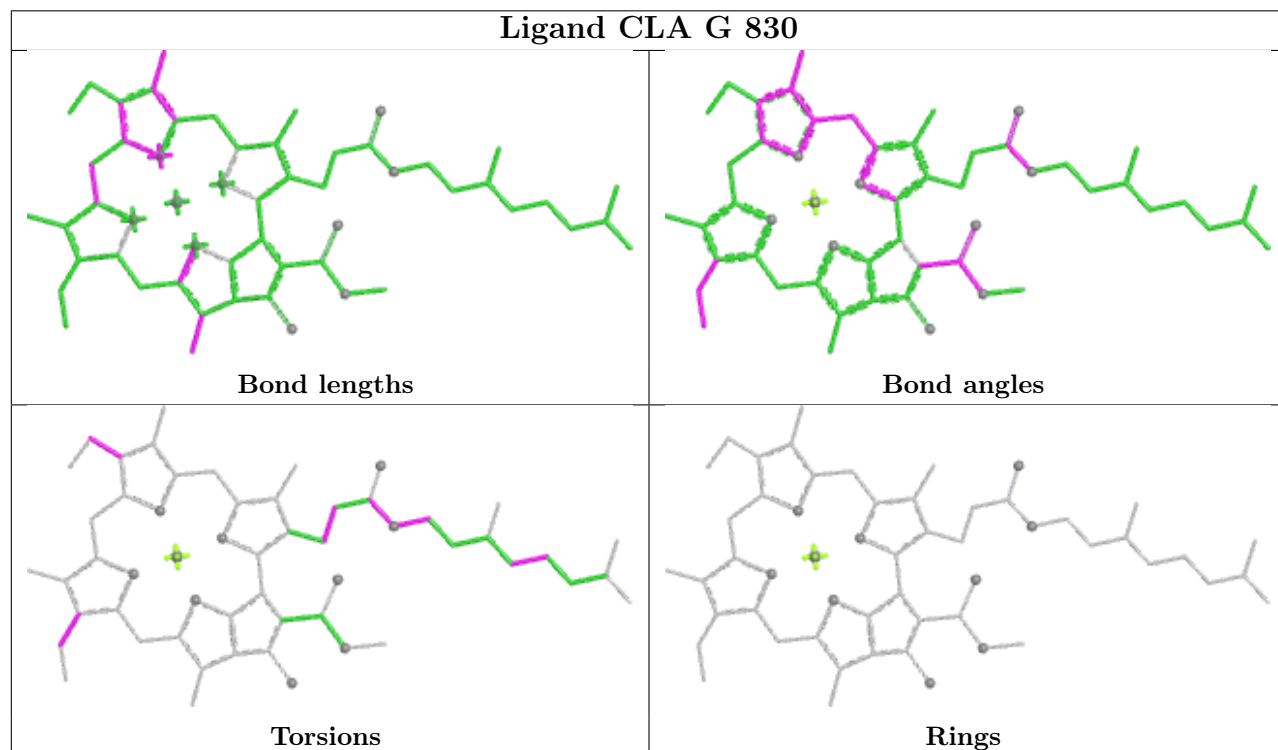
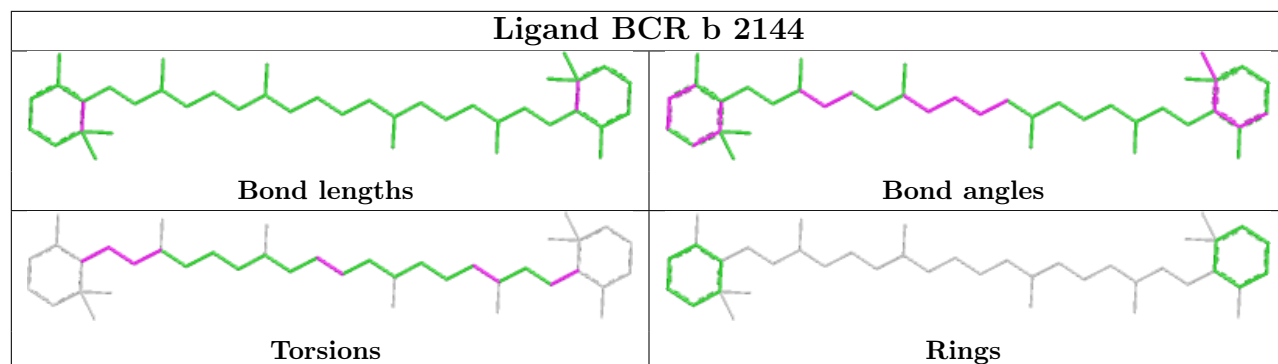
Rings

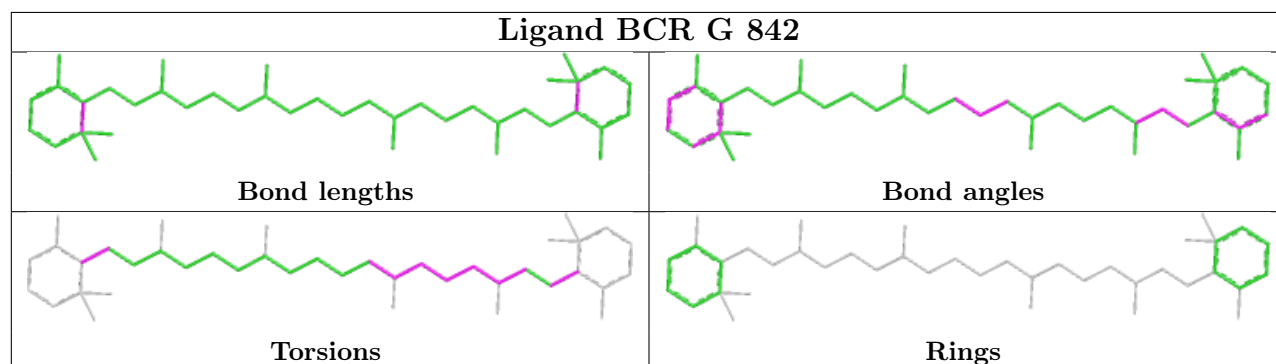
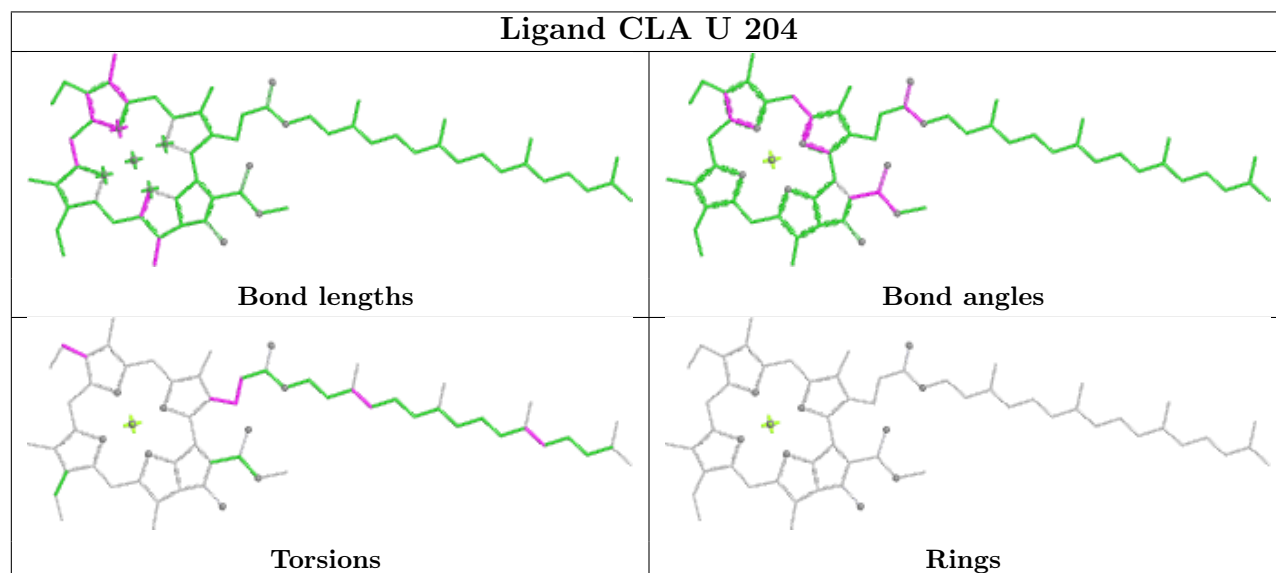
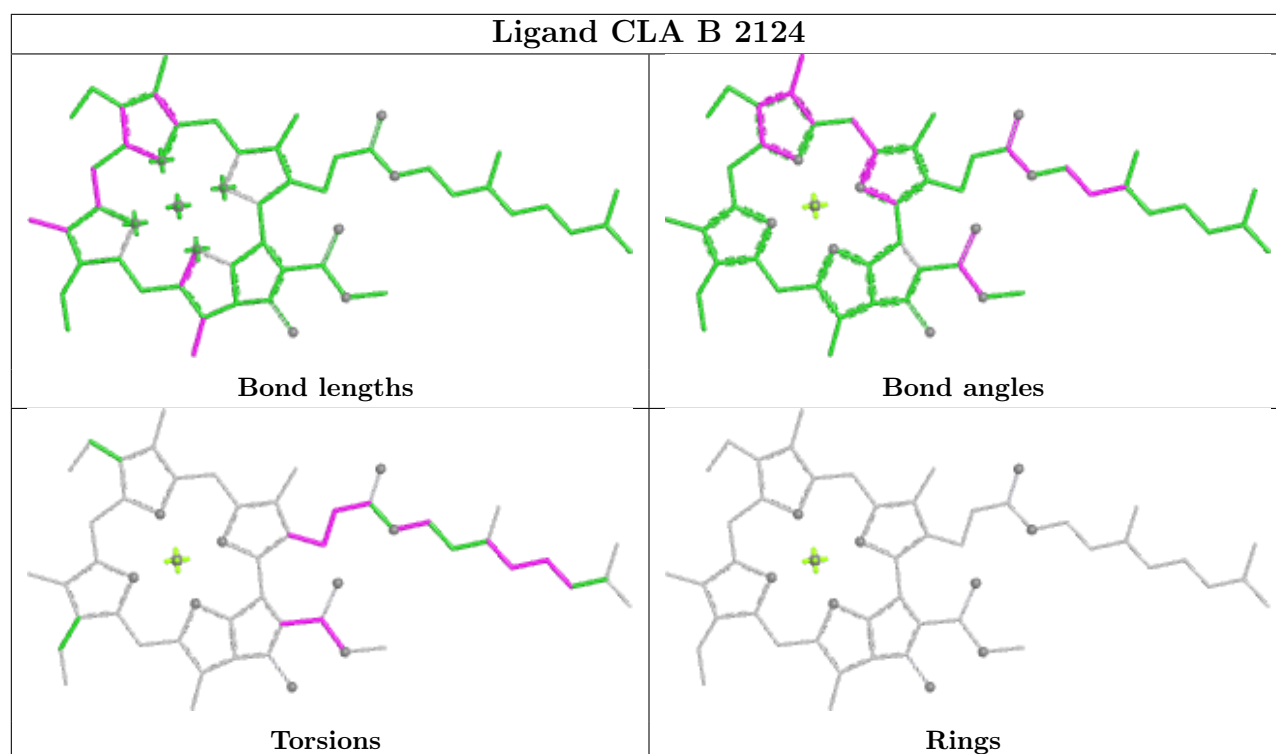
Ligand LHG a 848

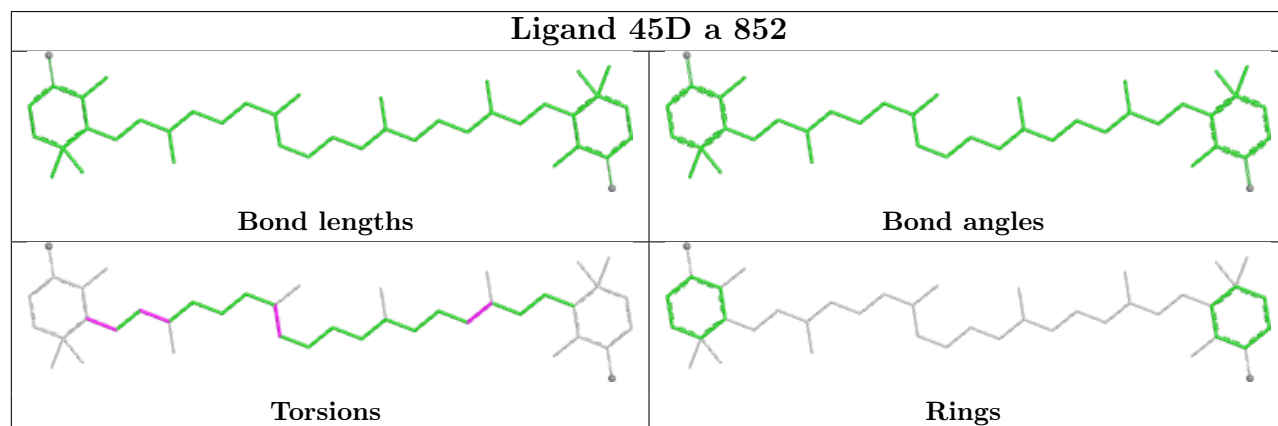
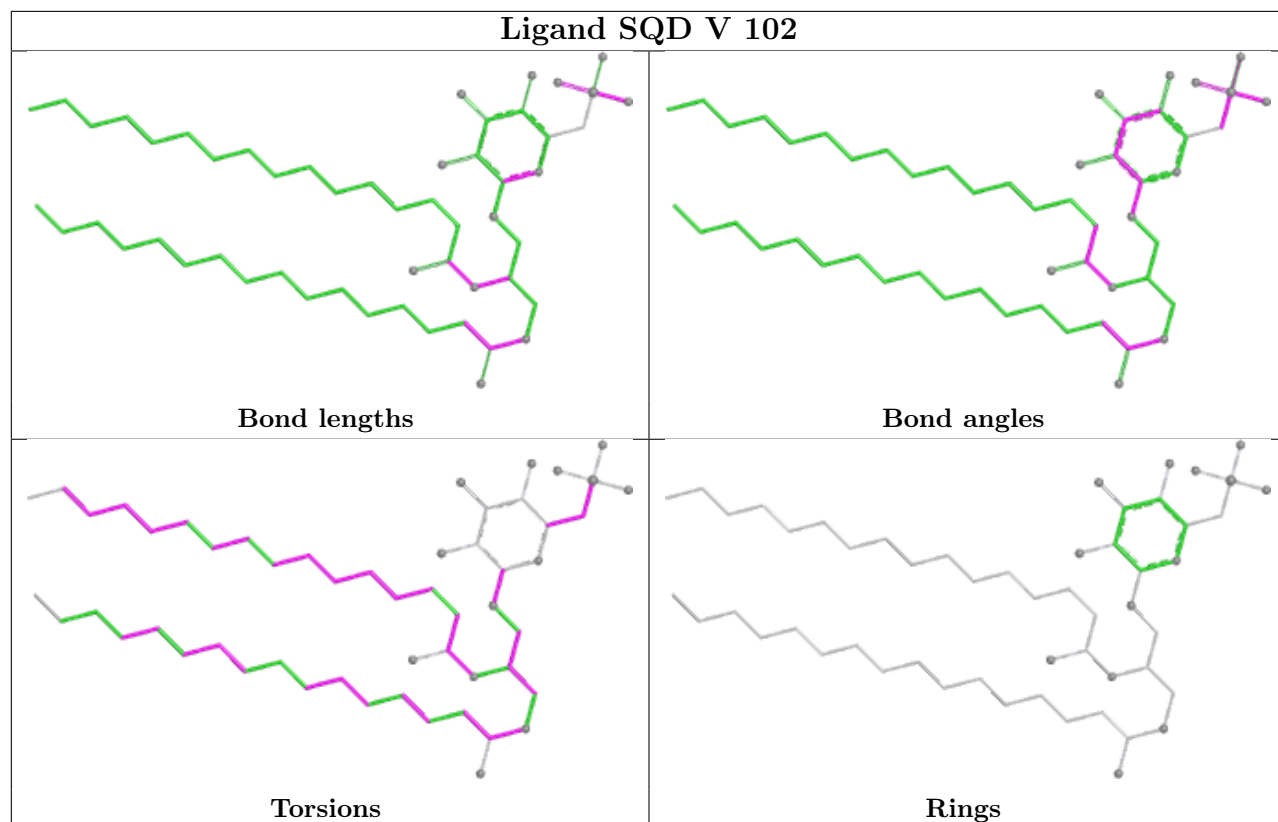


Ligand BCR I 101

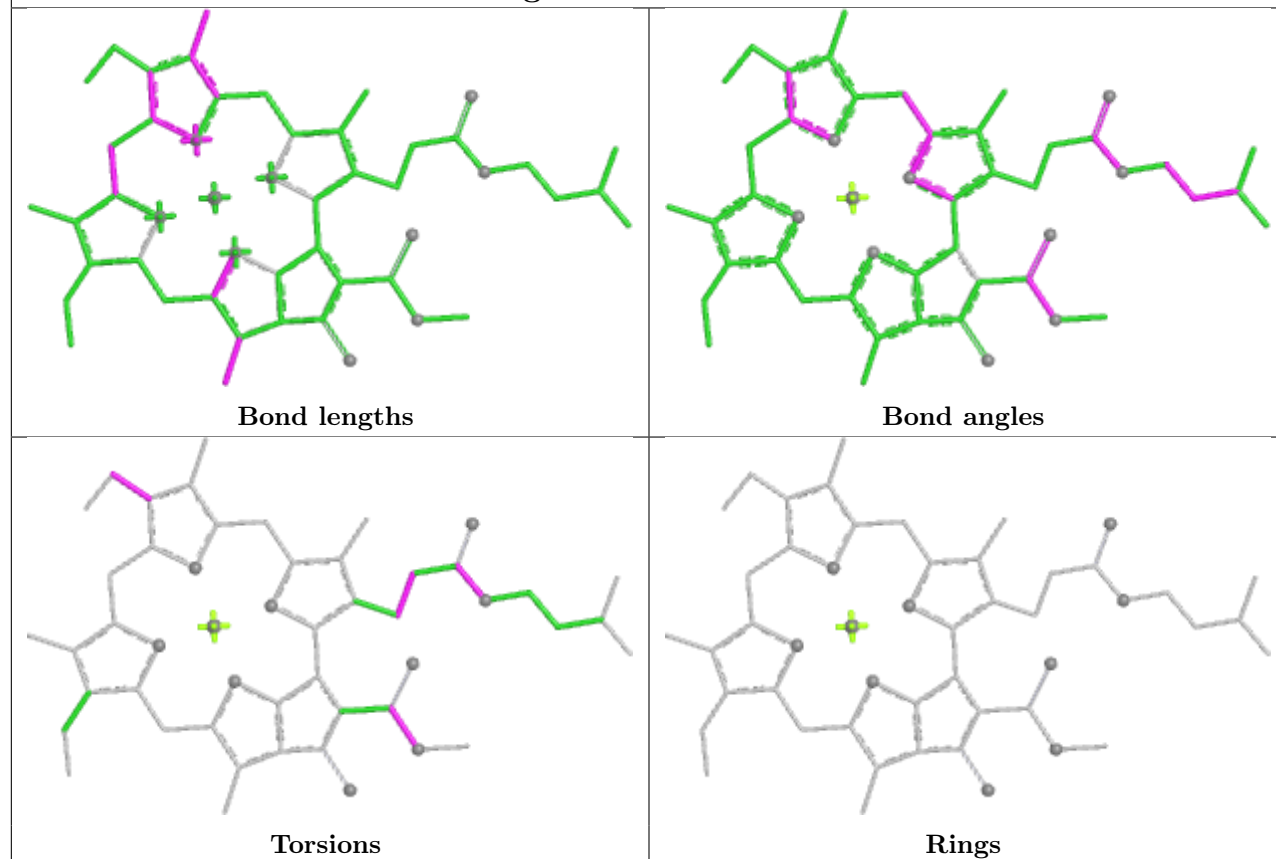




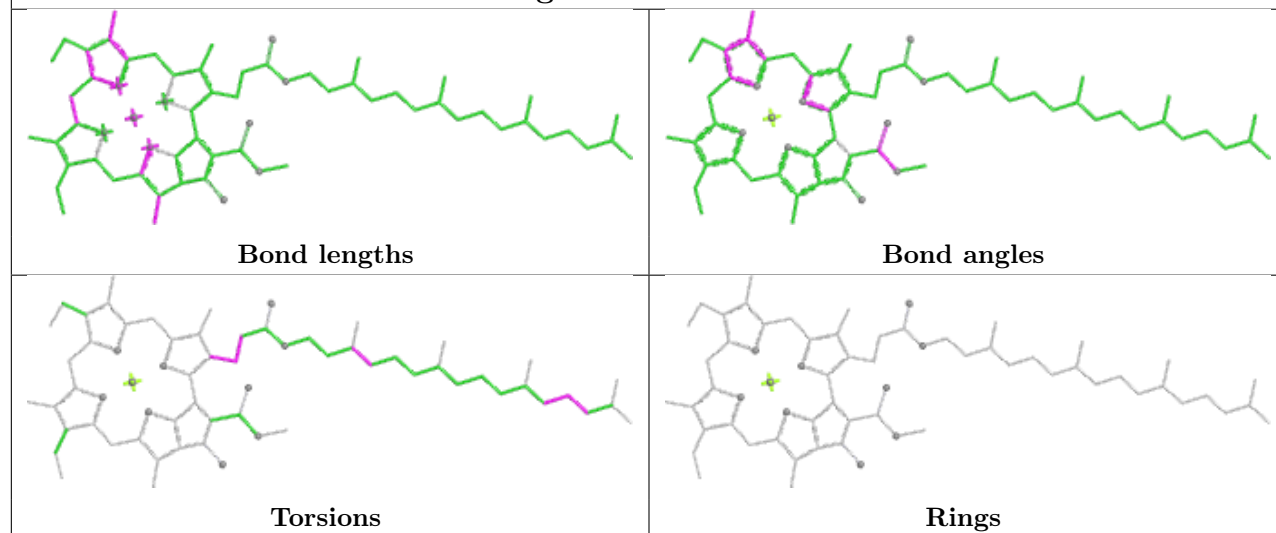


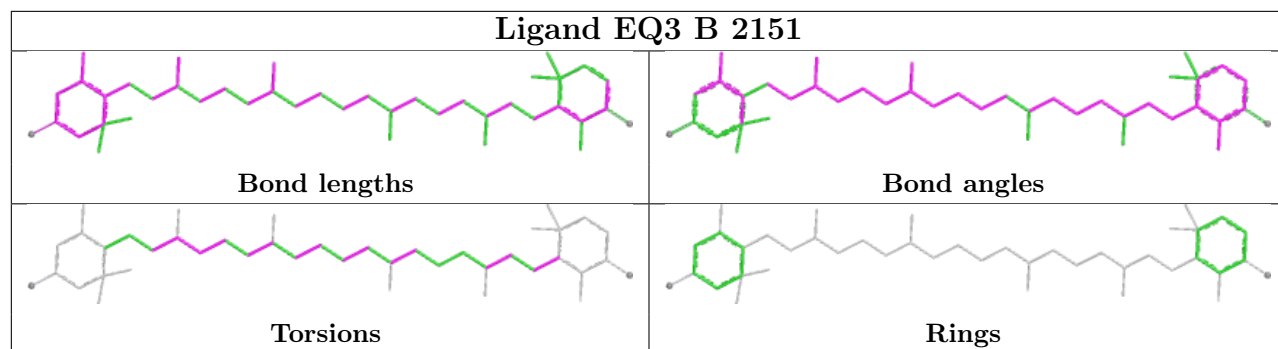
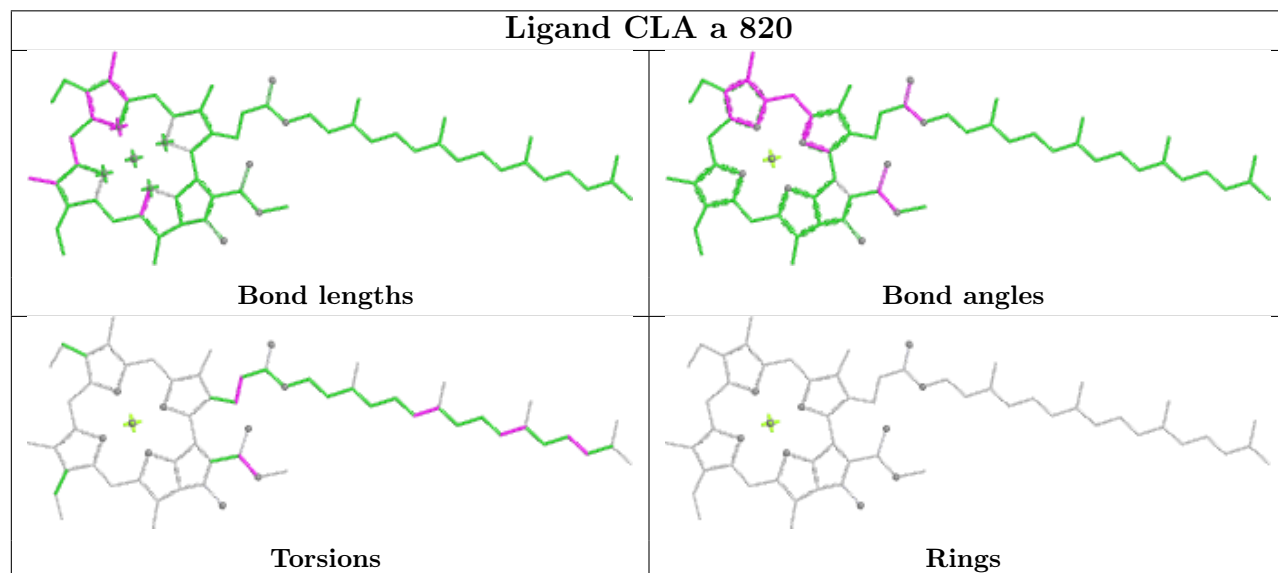
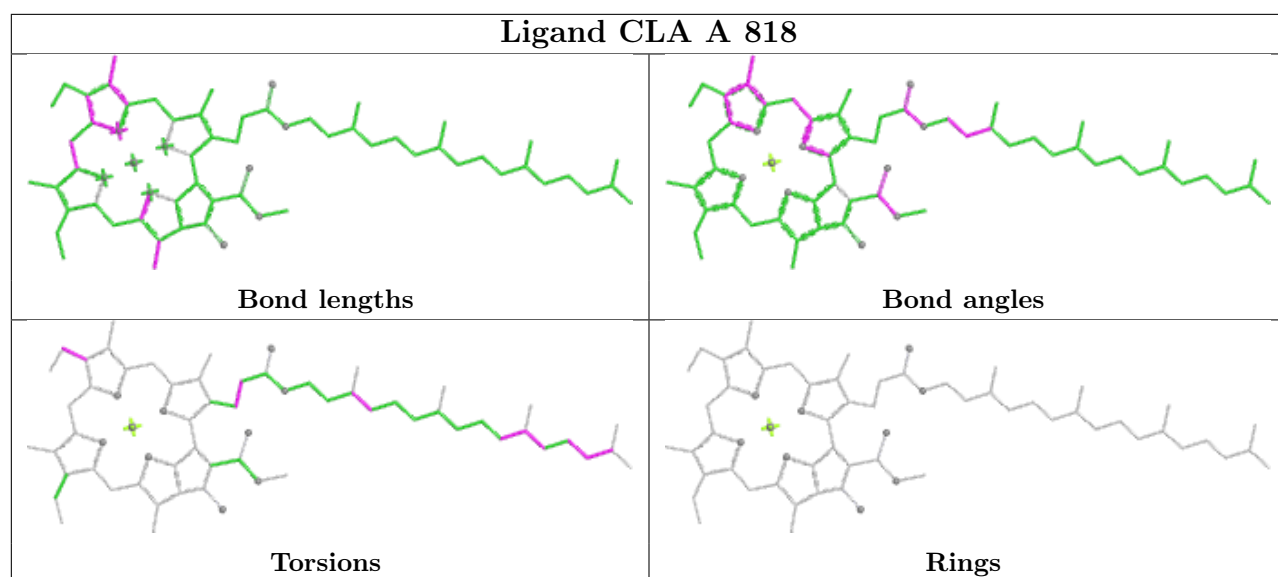


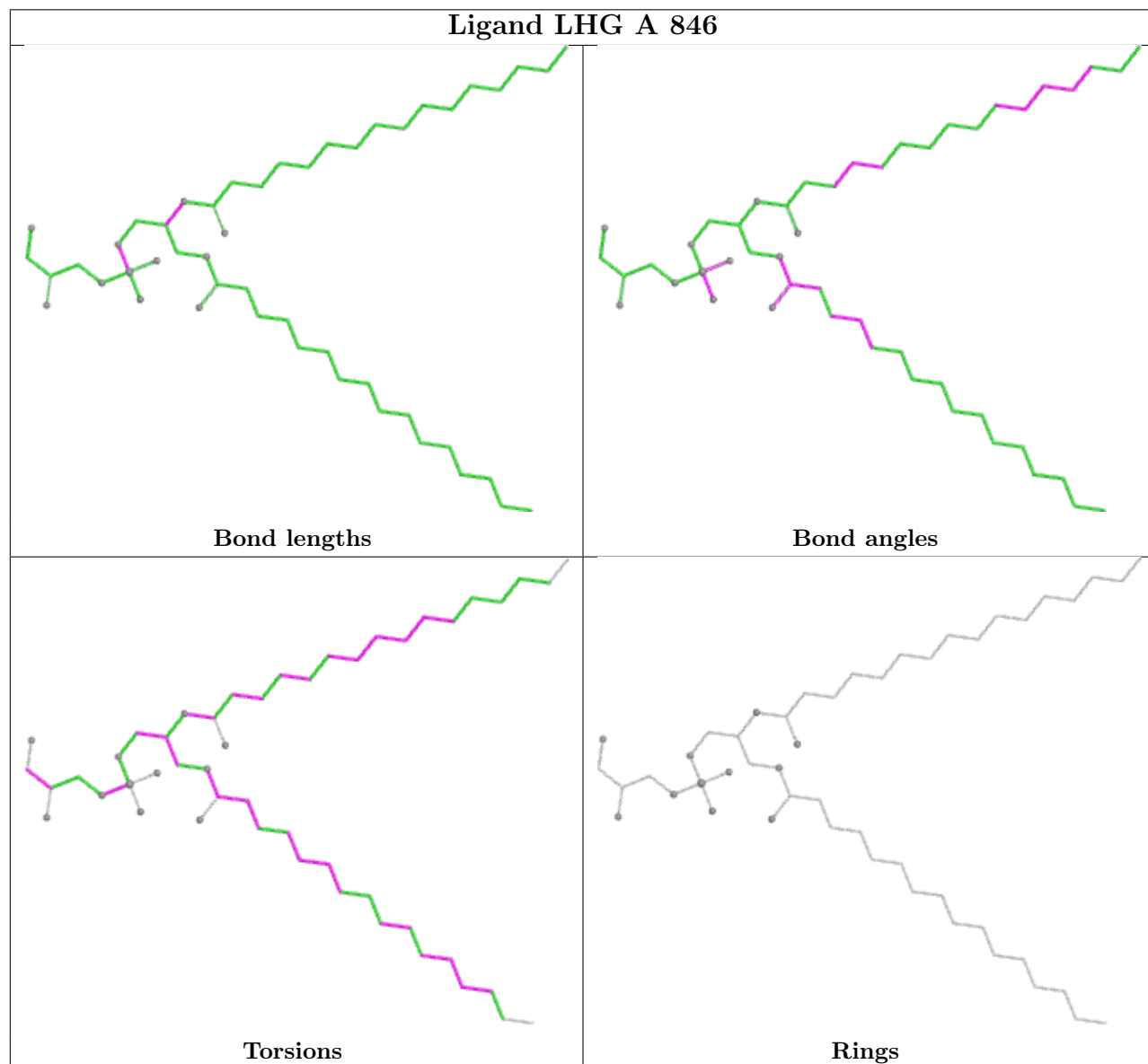
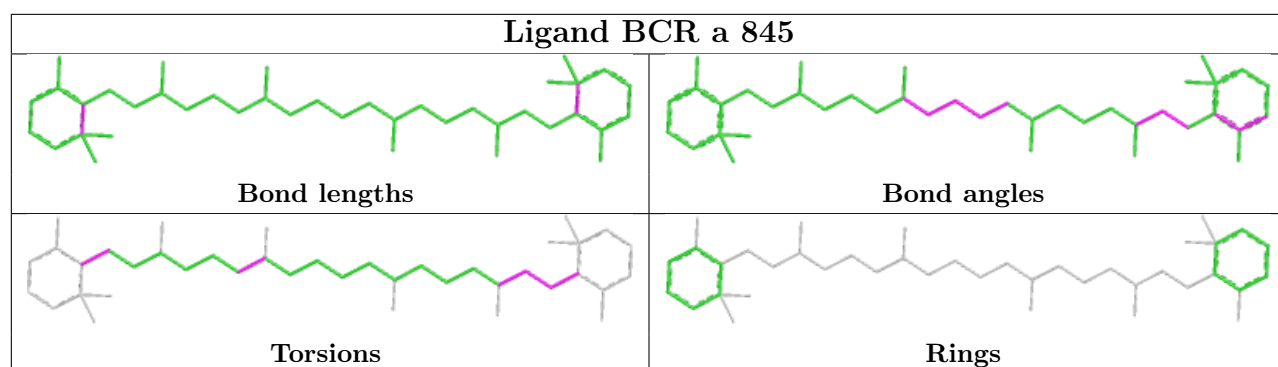
Ligand CLA B 2119

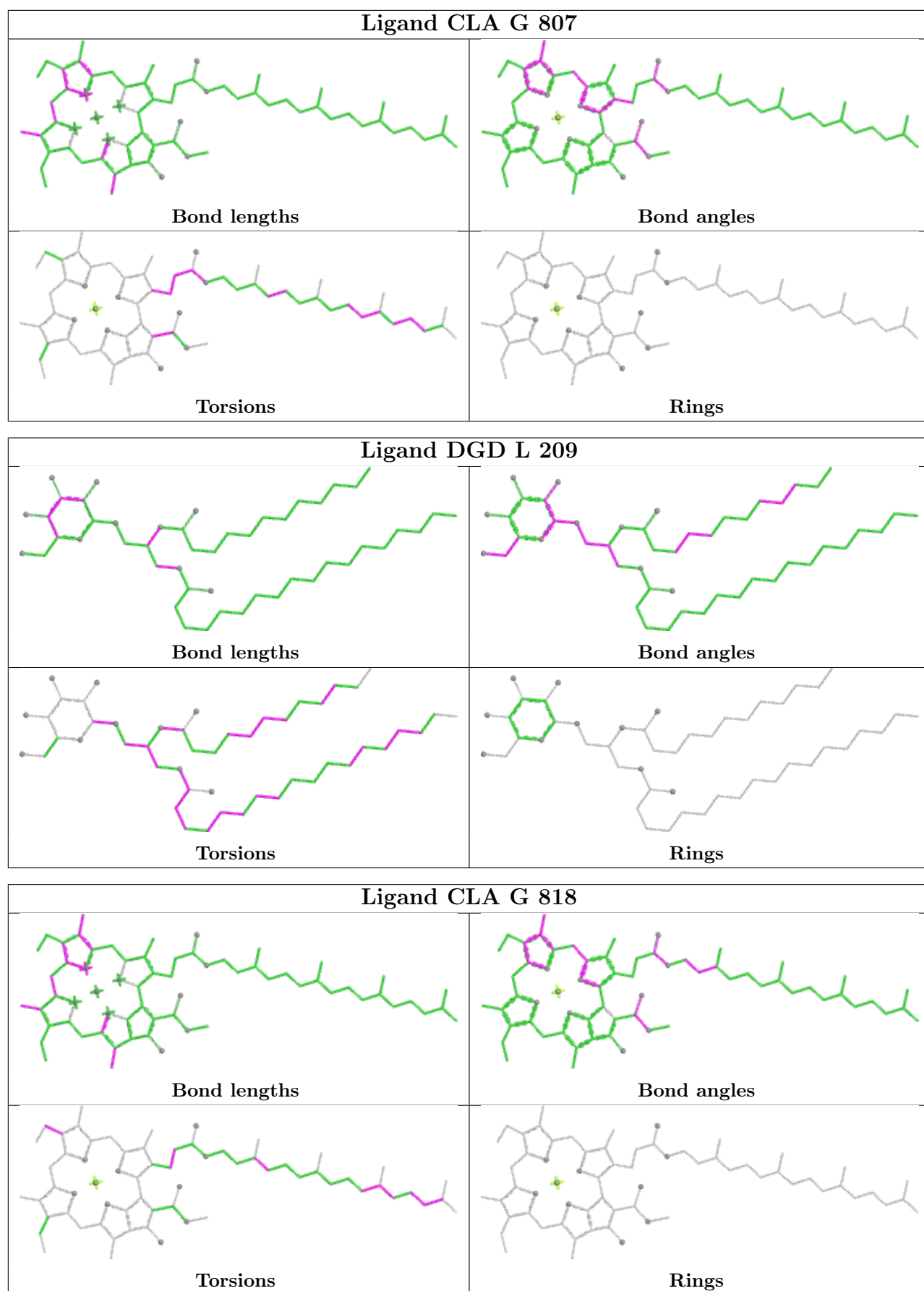


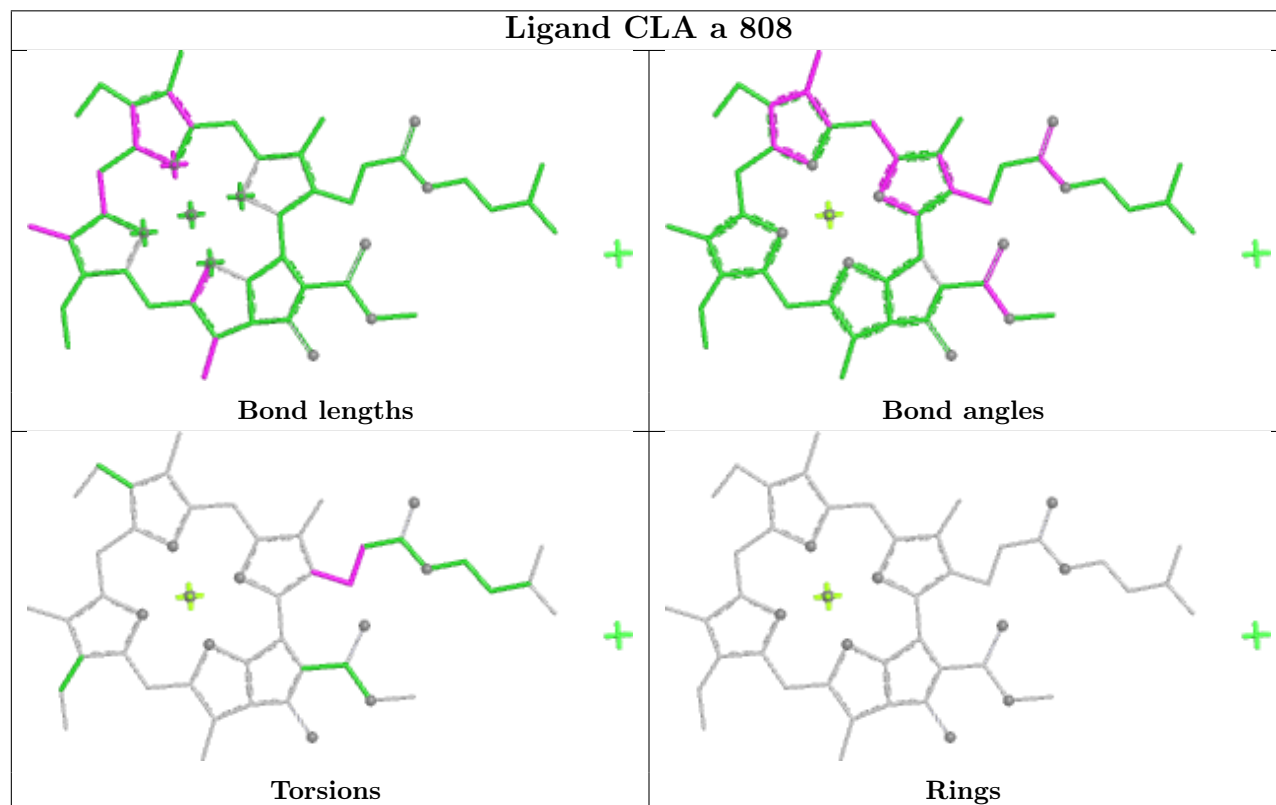
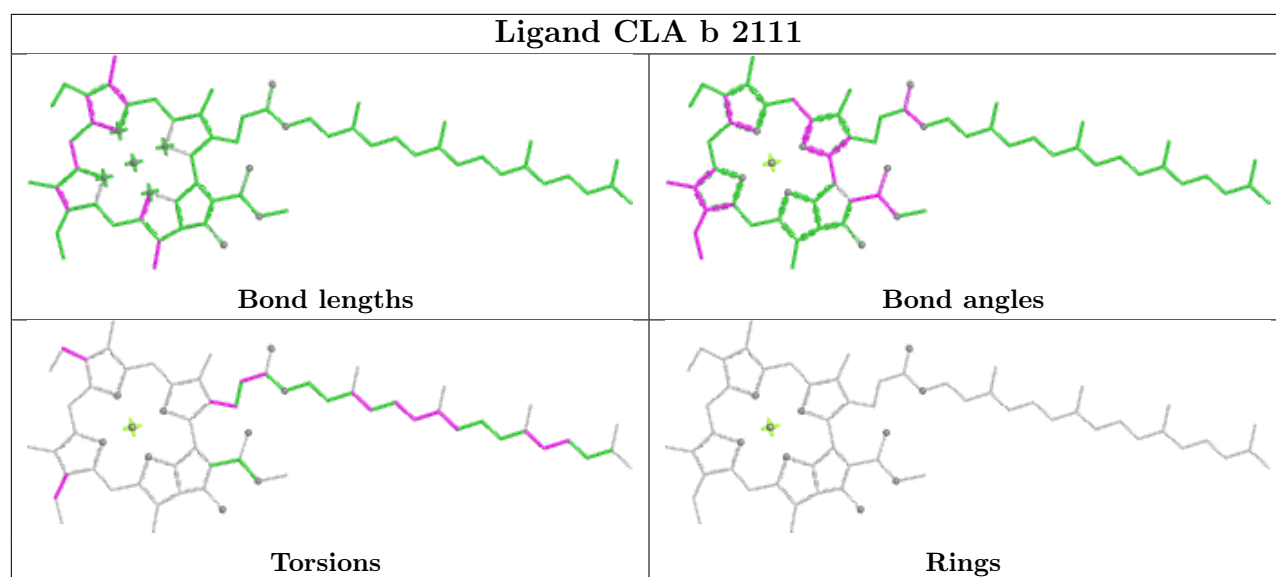
Ligand CLA a 850

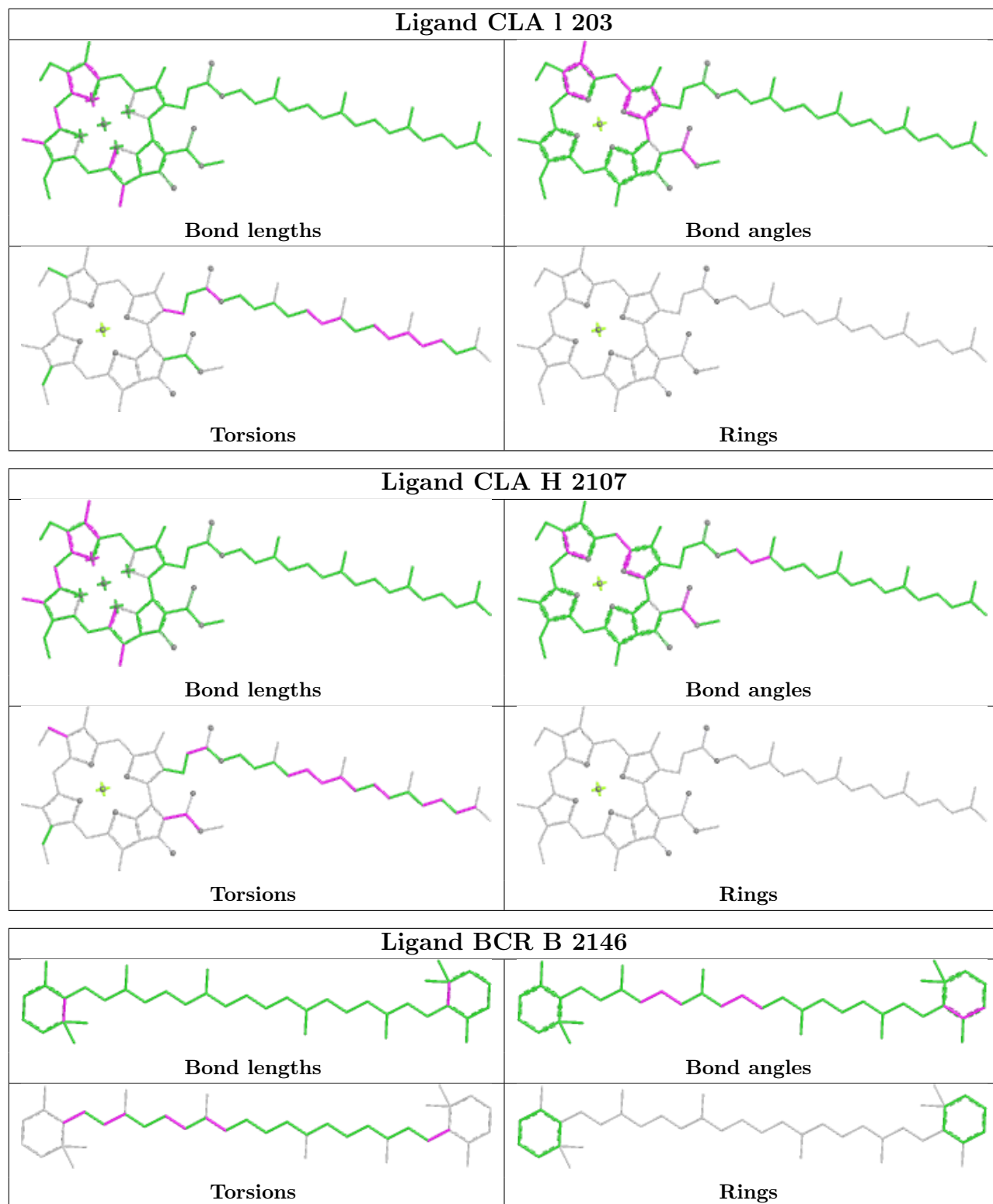


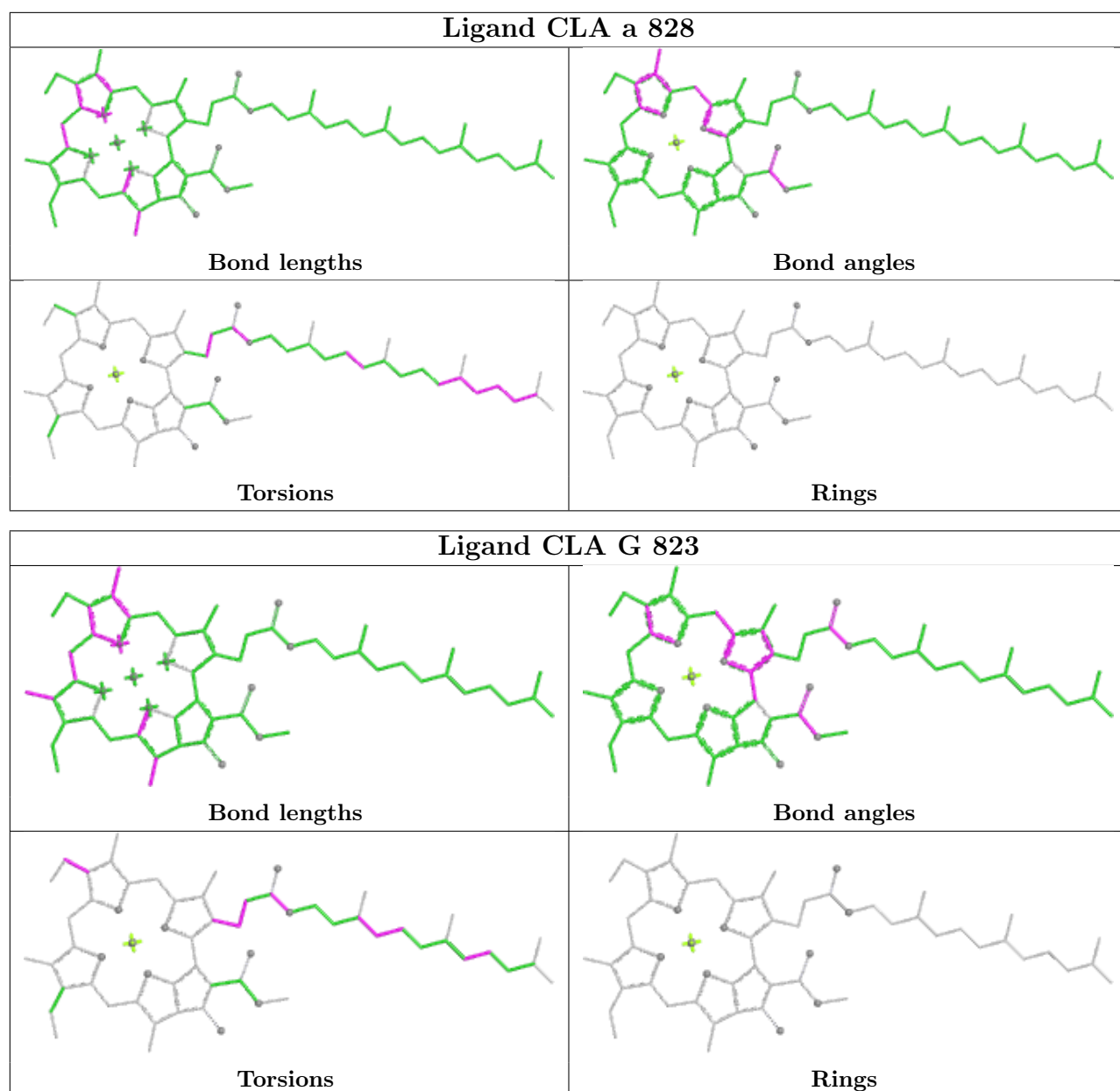




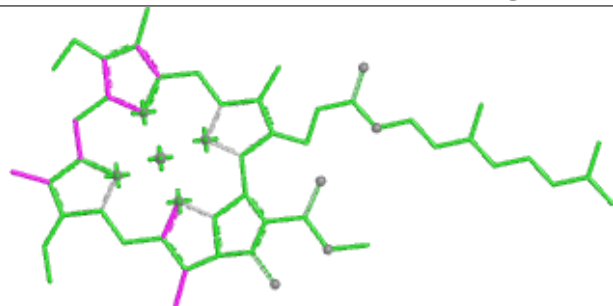




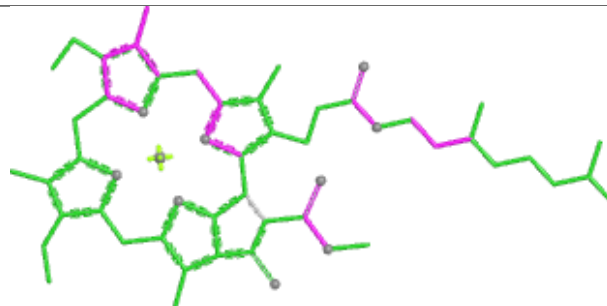




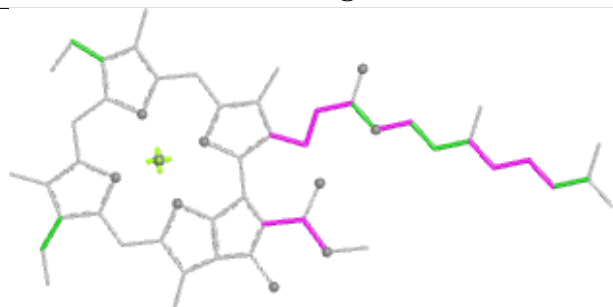
Ligand CLA H 2123



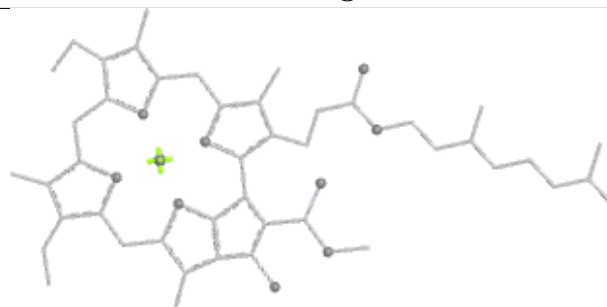
Bond lengths



Bond angles

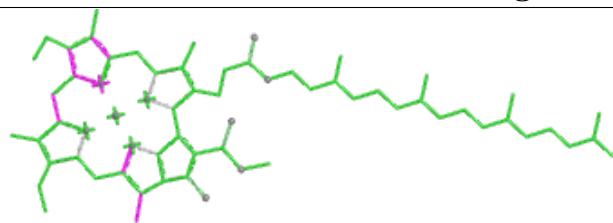


Torsions

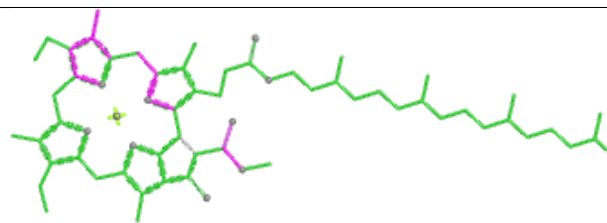


Rings

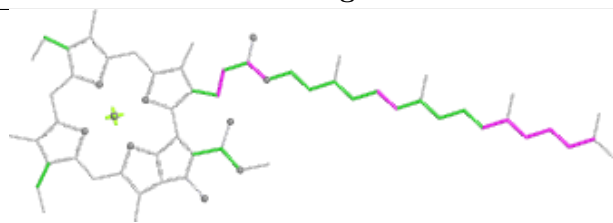
Ligand CLA A 828



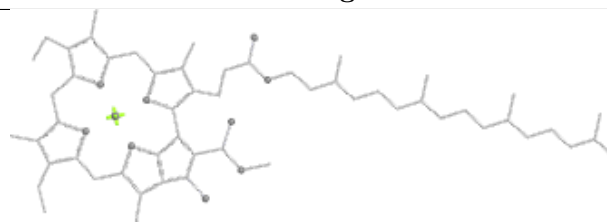
Bond lengths



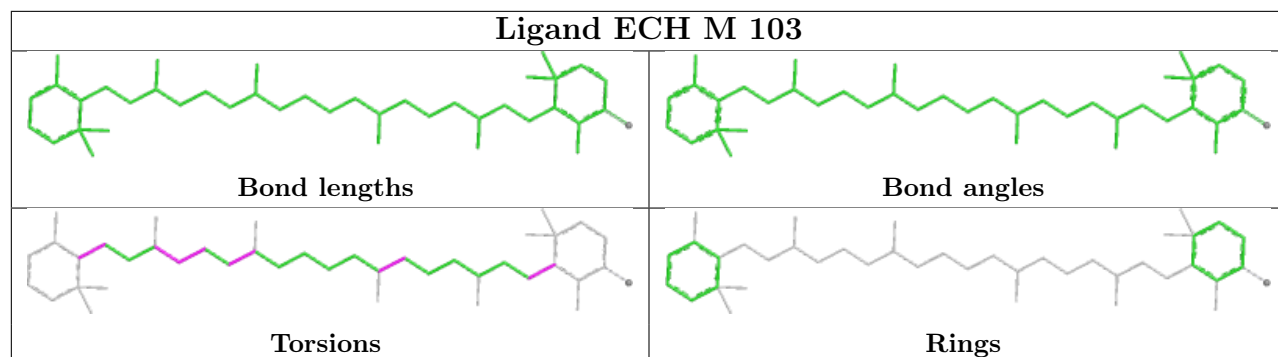
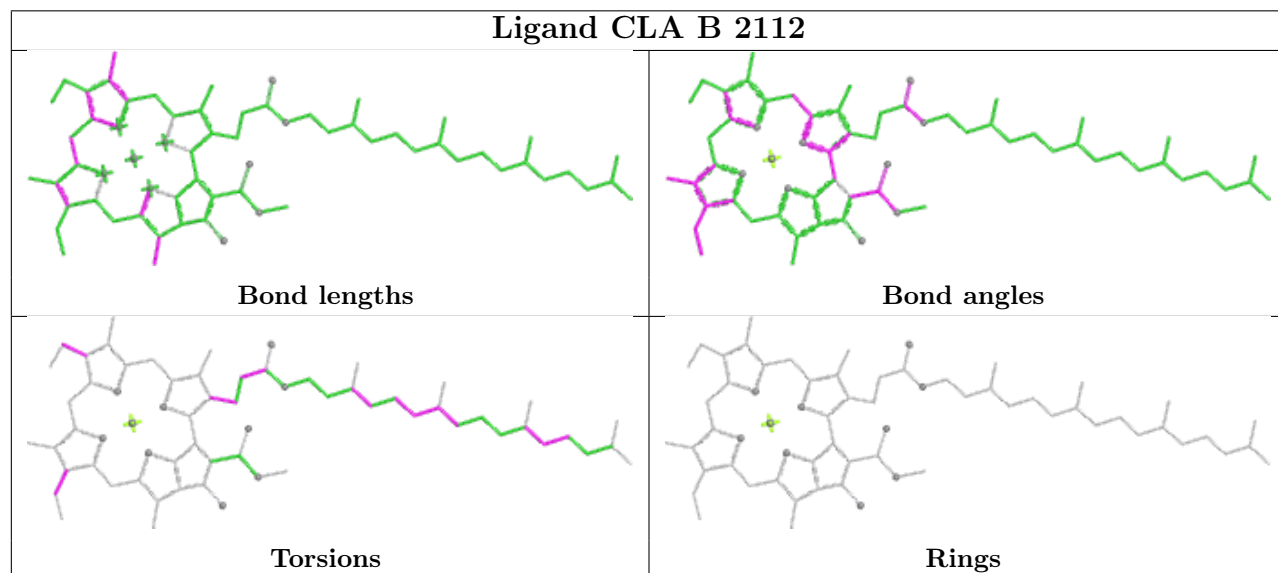
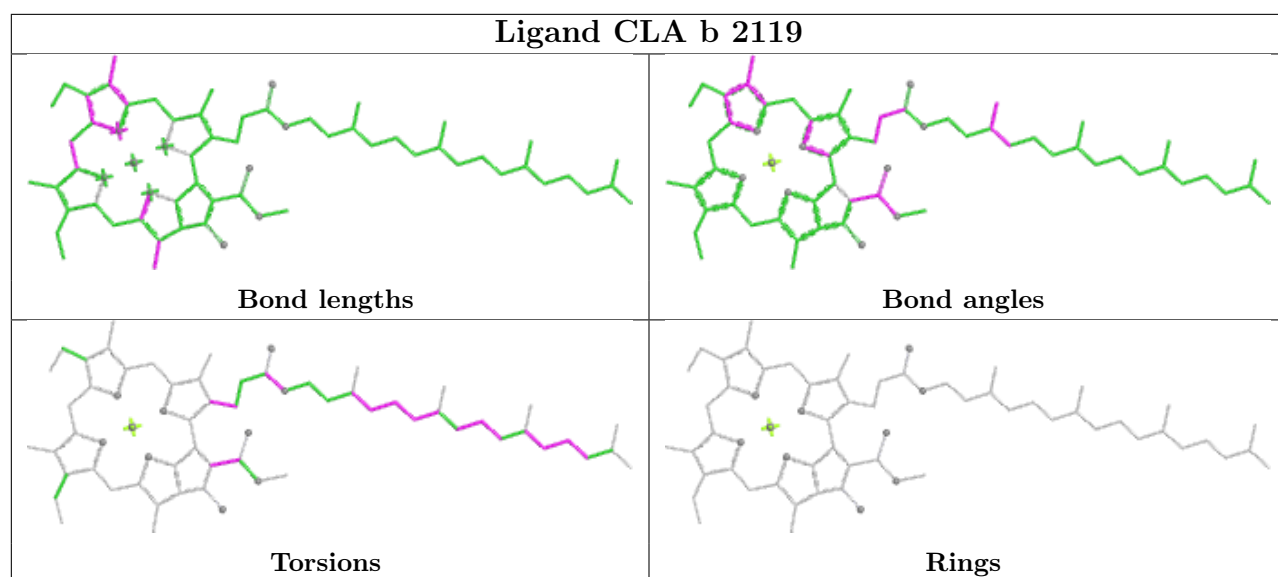
Bond angles

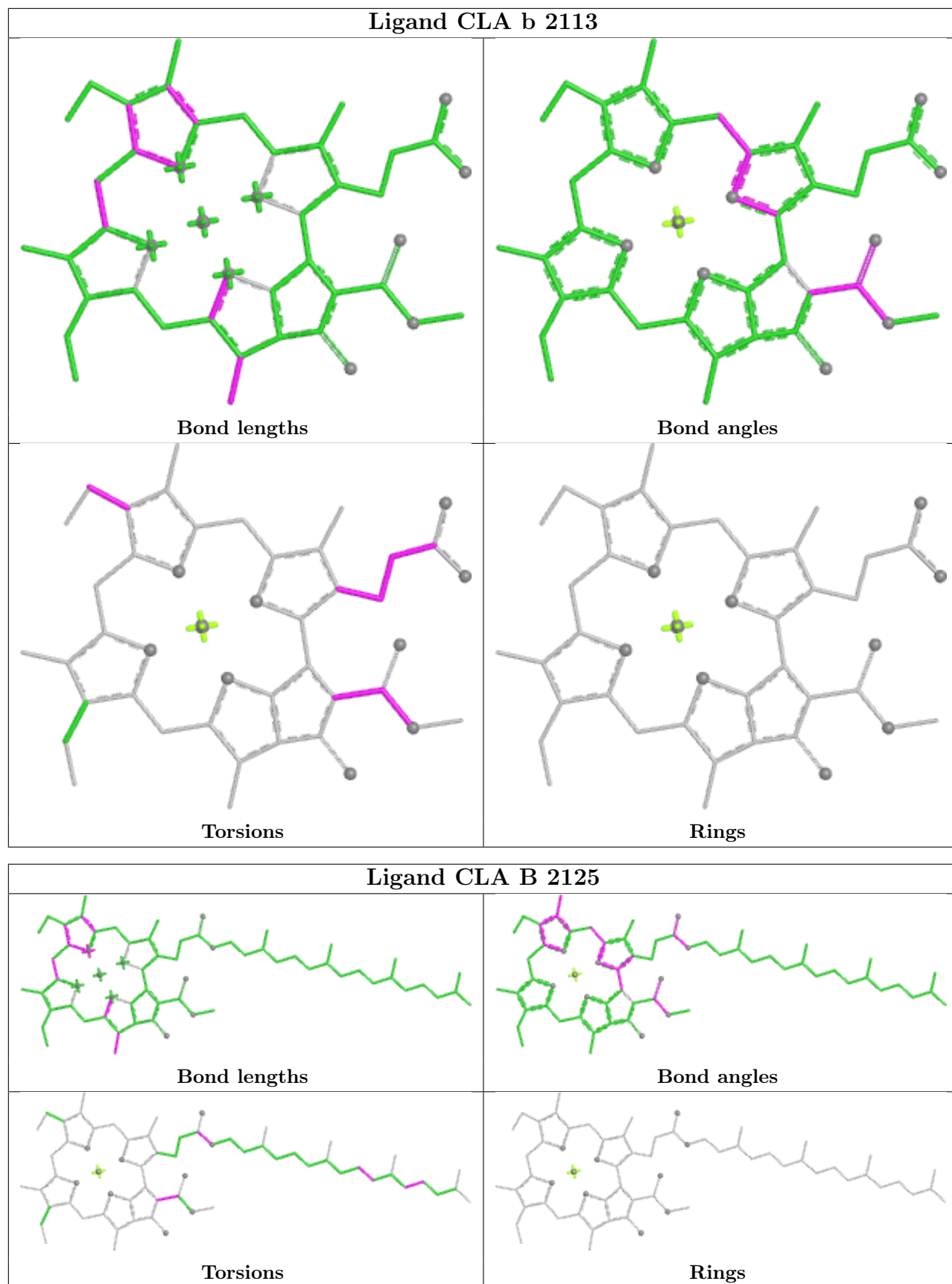


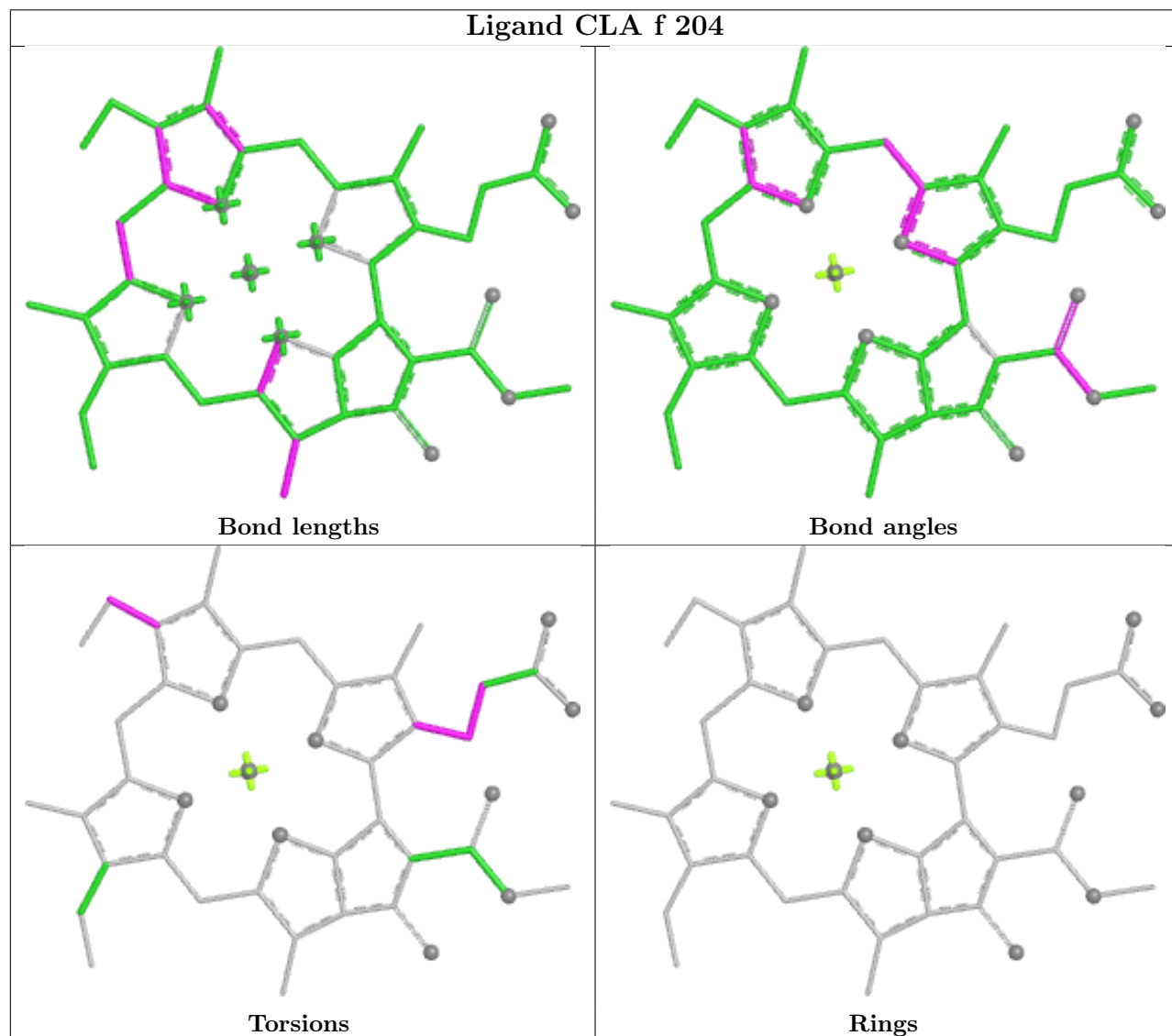
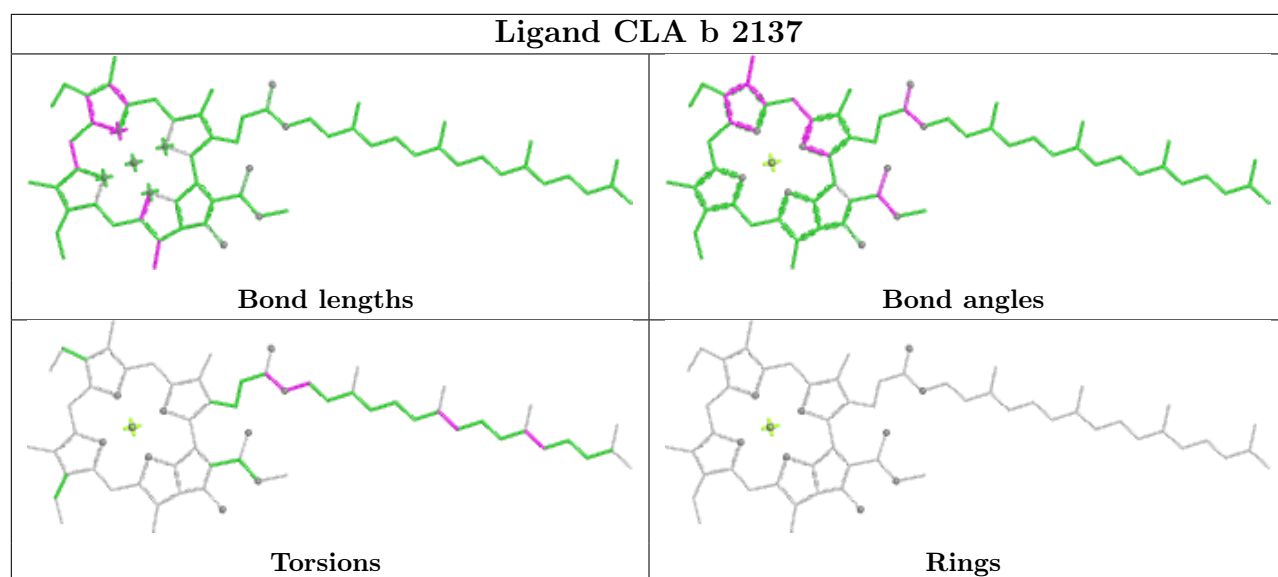
Torsions



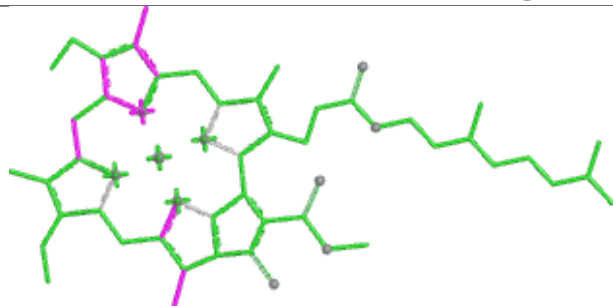
Rings



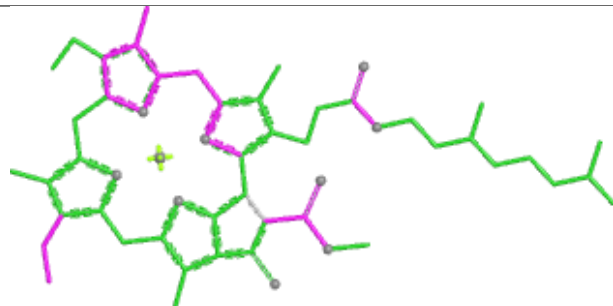




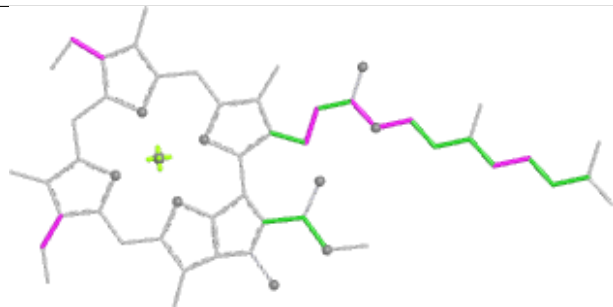
Ligand CLA a 830



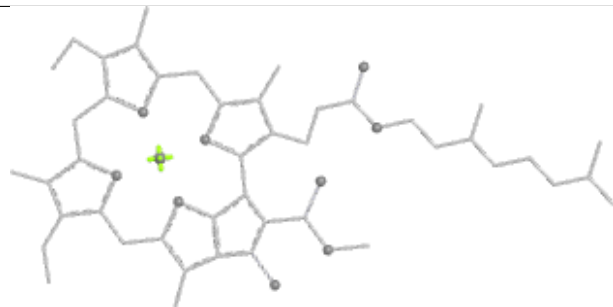
Bond lengths



Bond angles

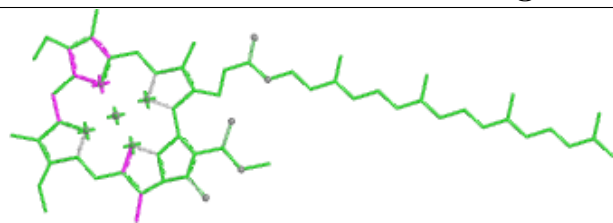


Torsions

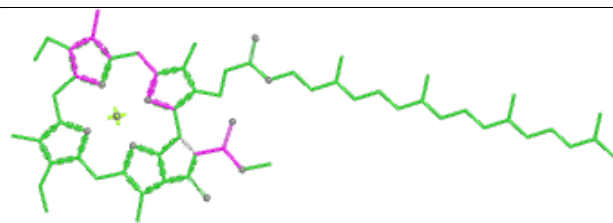


Rings

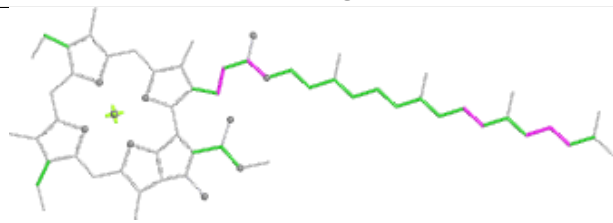
Ligand CLA L 205



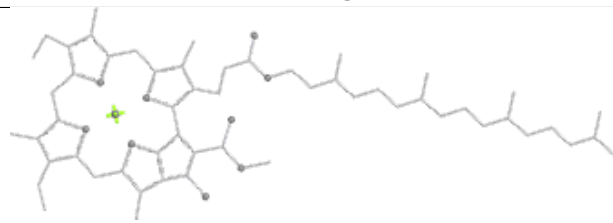
Bond lengths



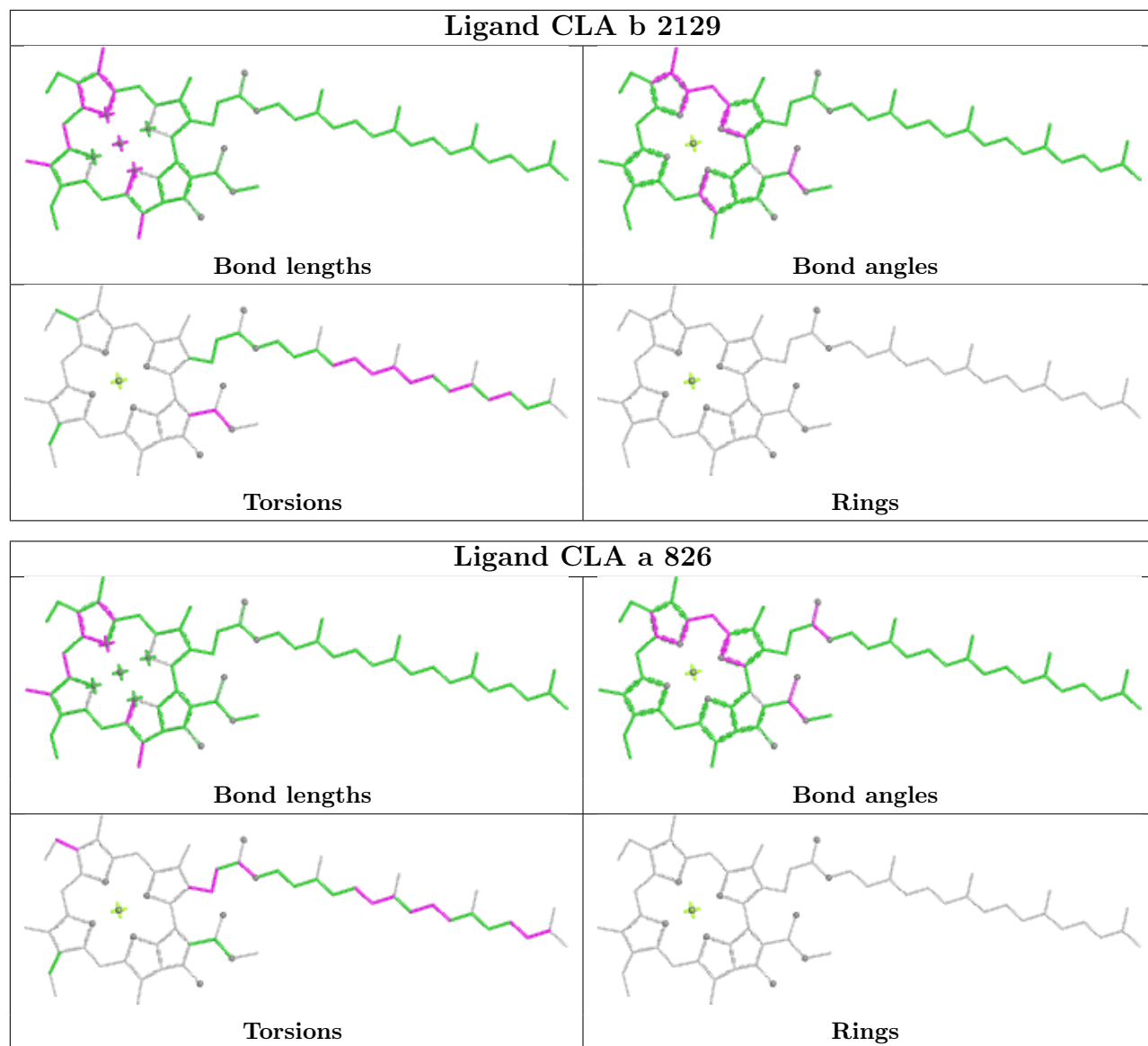
Bond angles



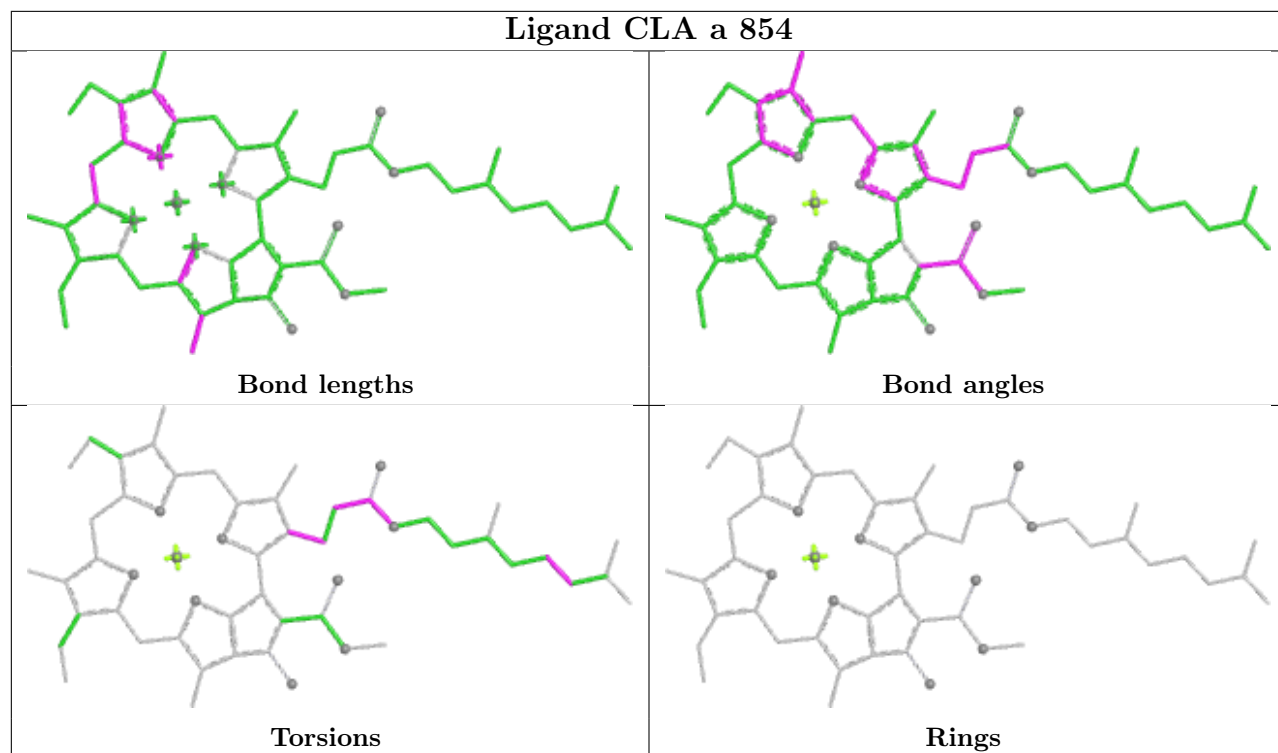
Torsions



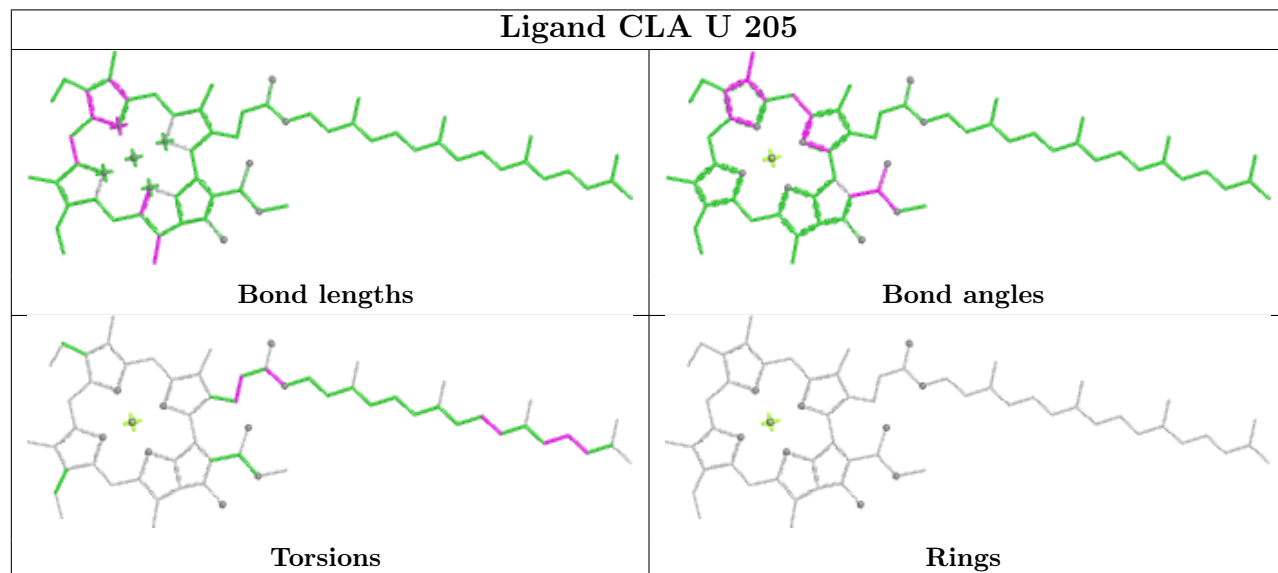
Rings



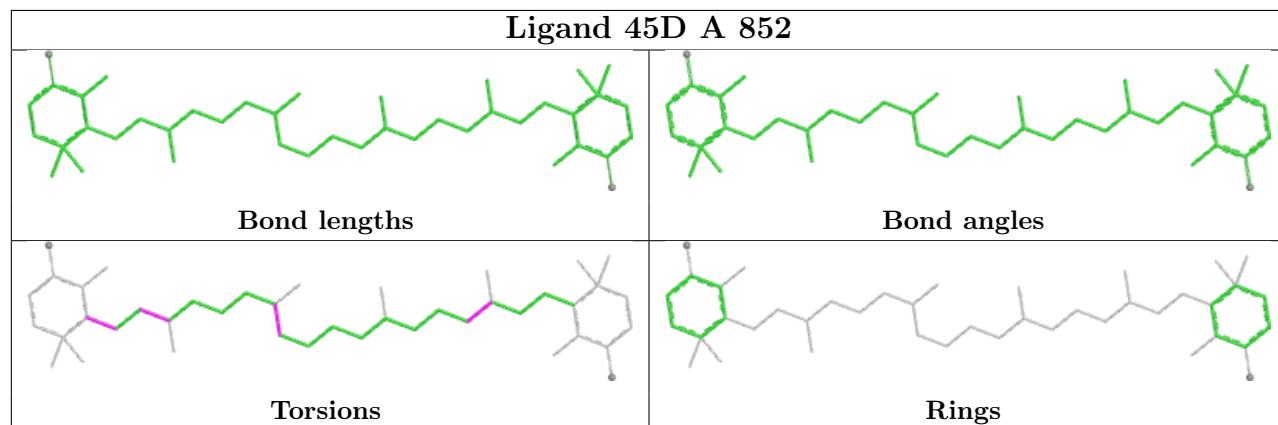
Ligand CLA a 854

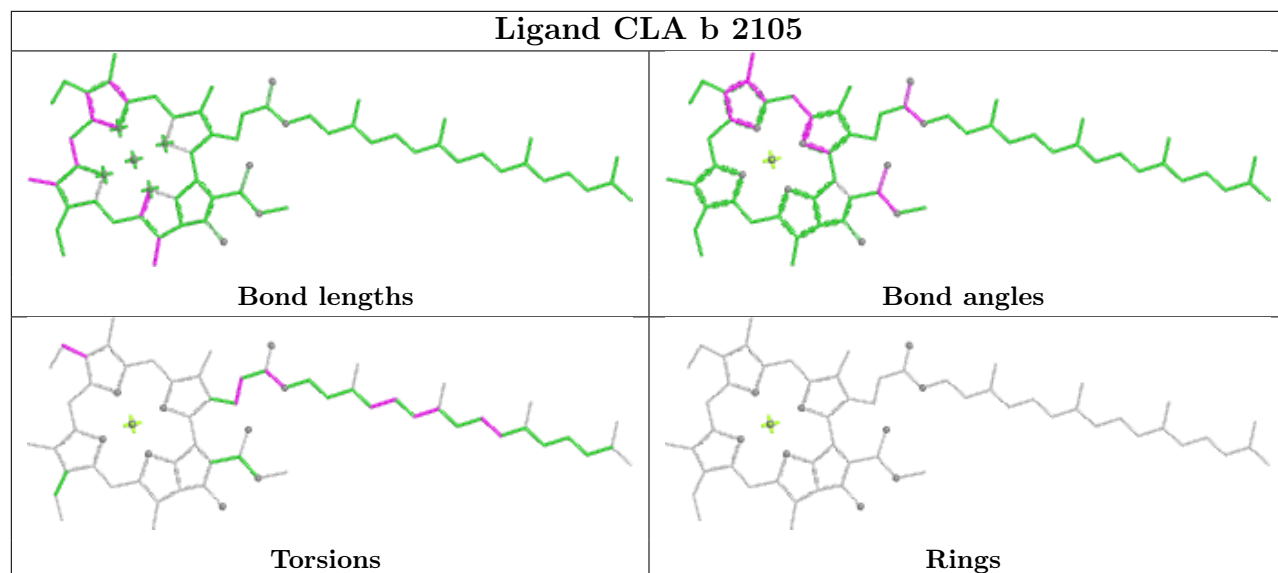
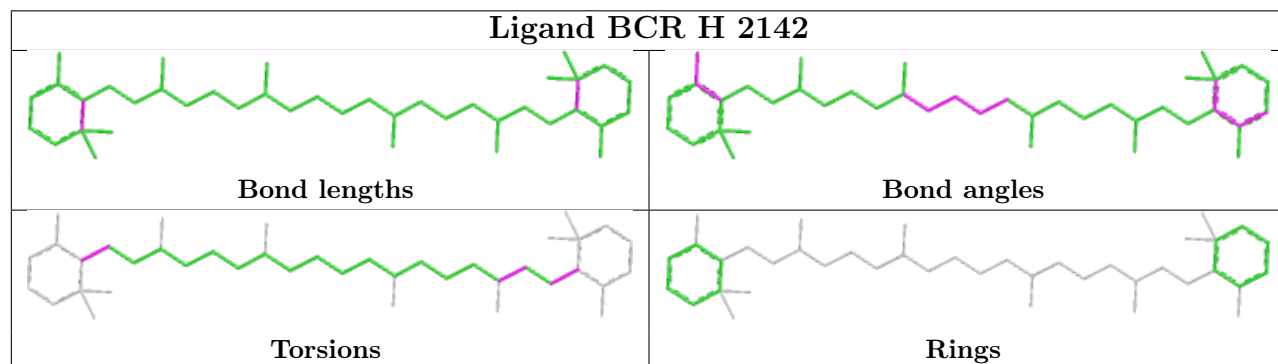
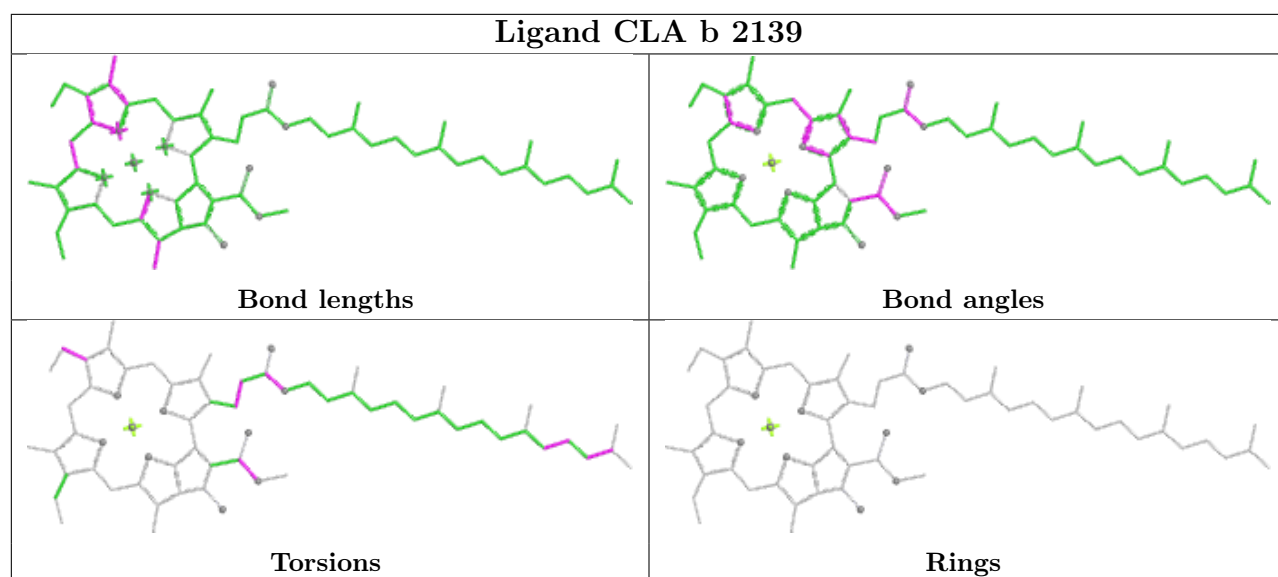


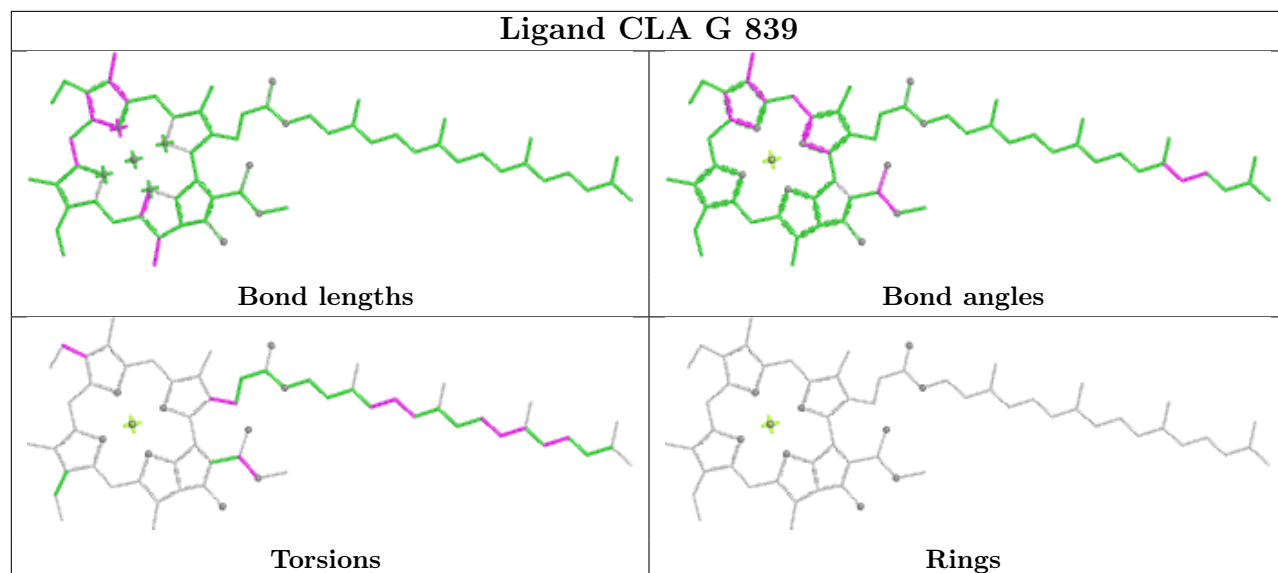
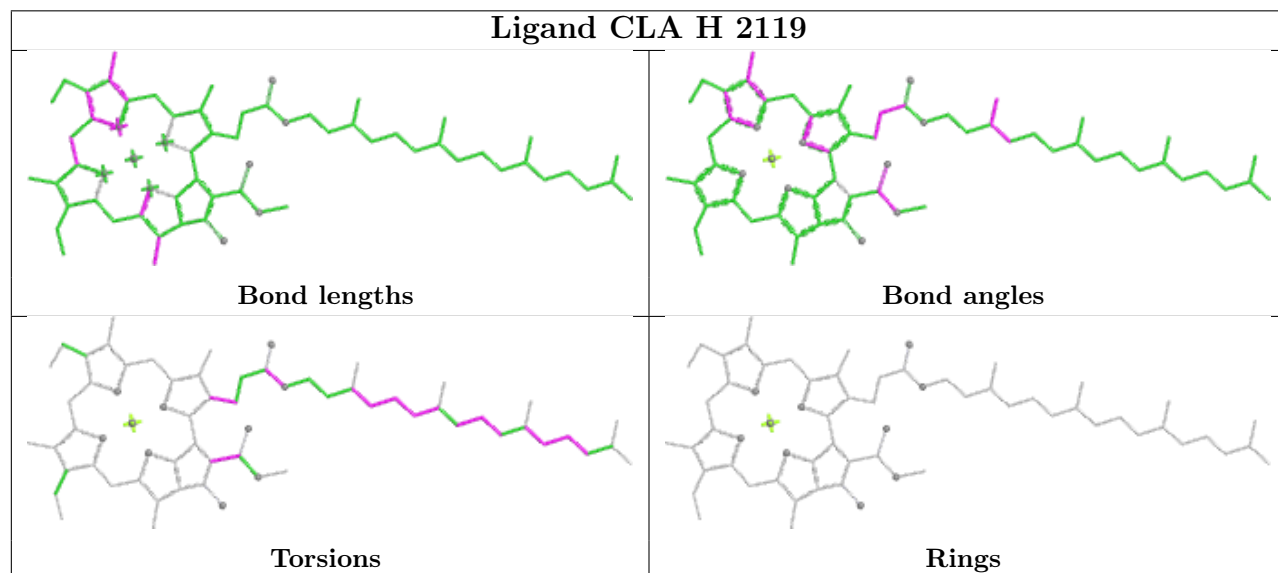
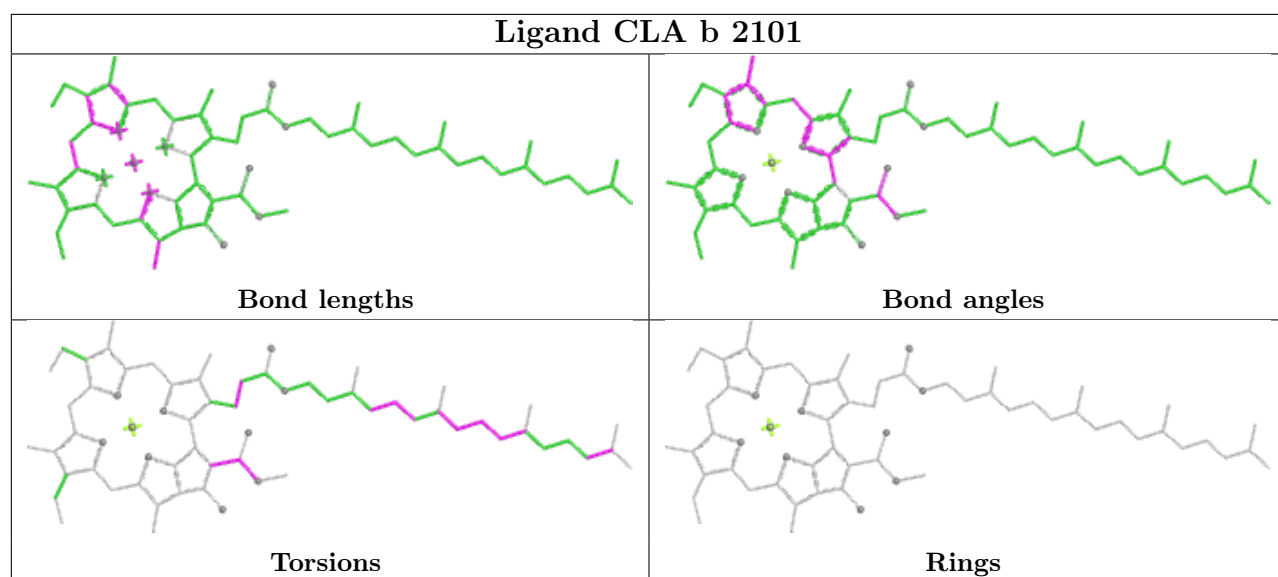
Ligand CLA U 205

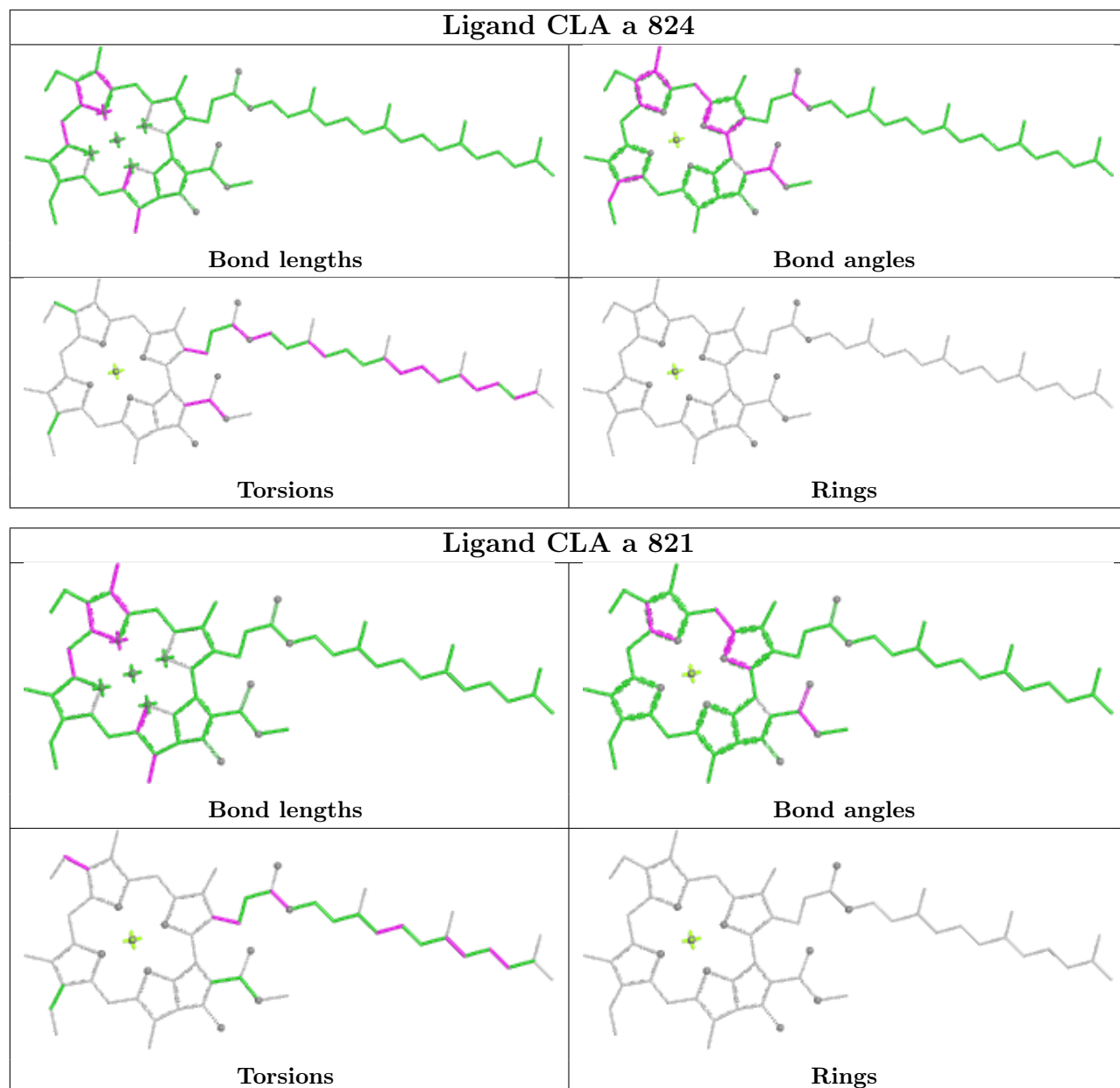


Ligand 45D A 852

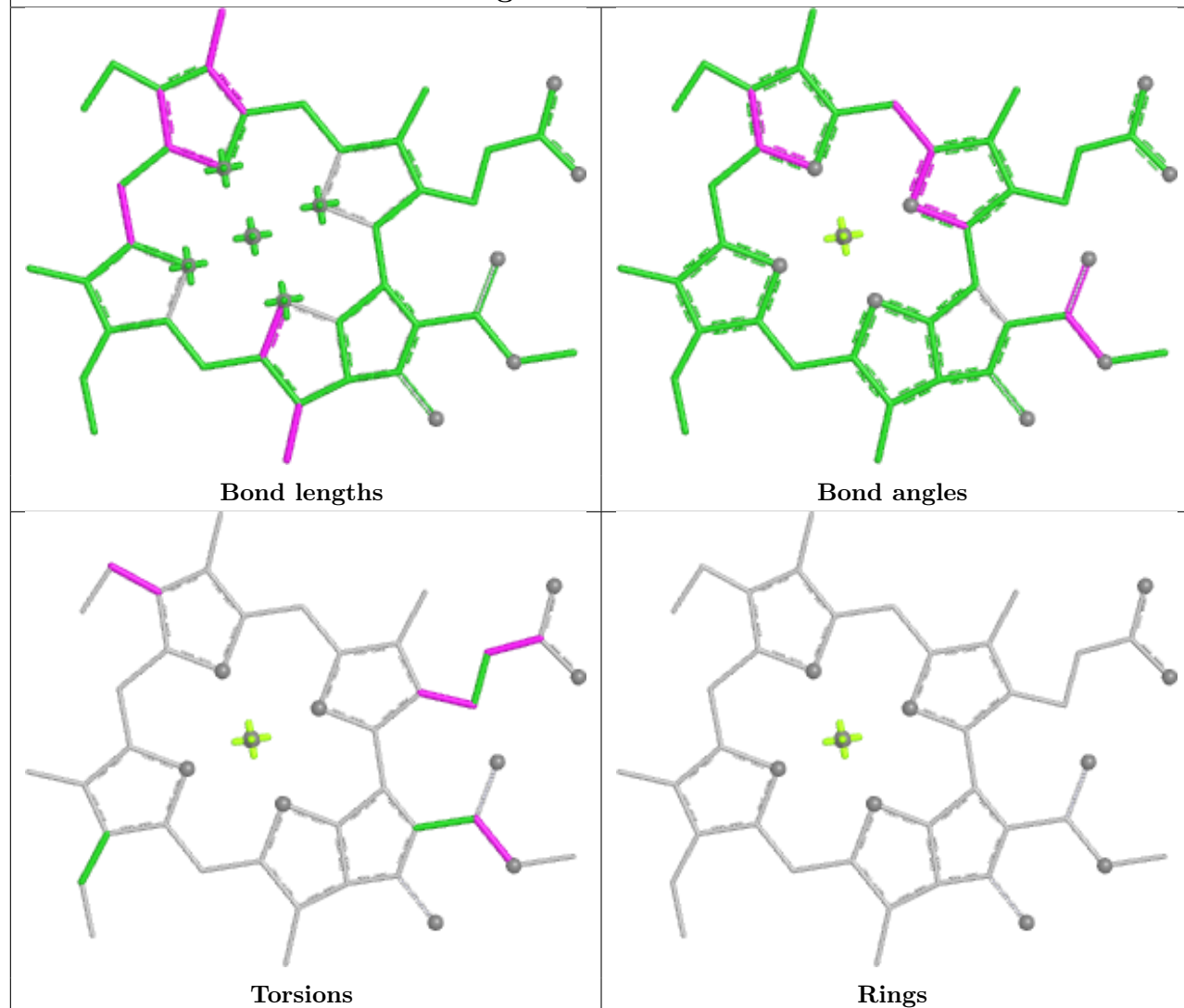




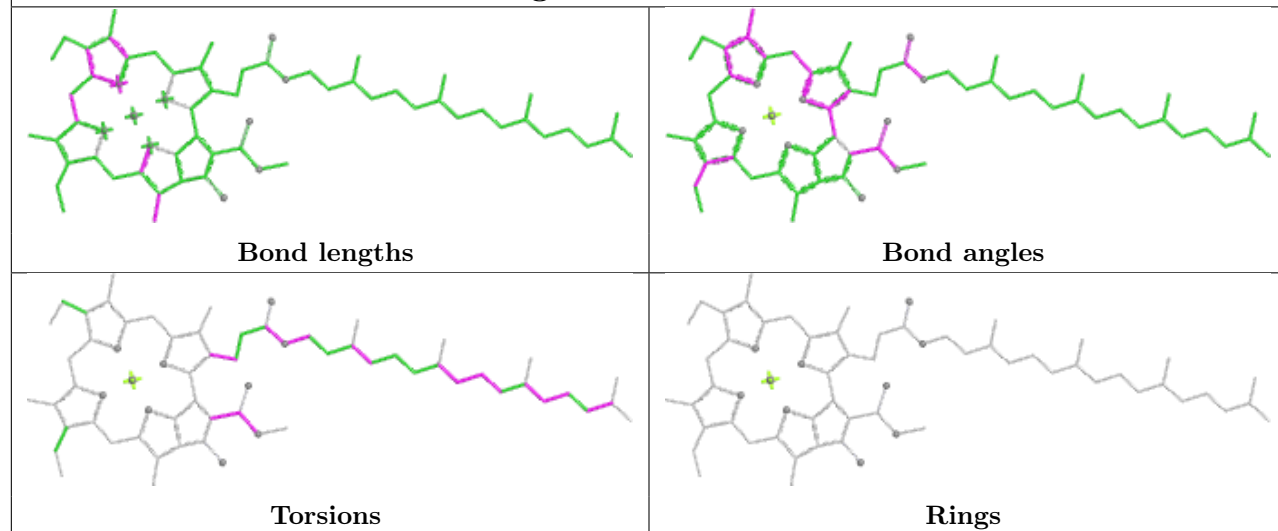


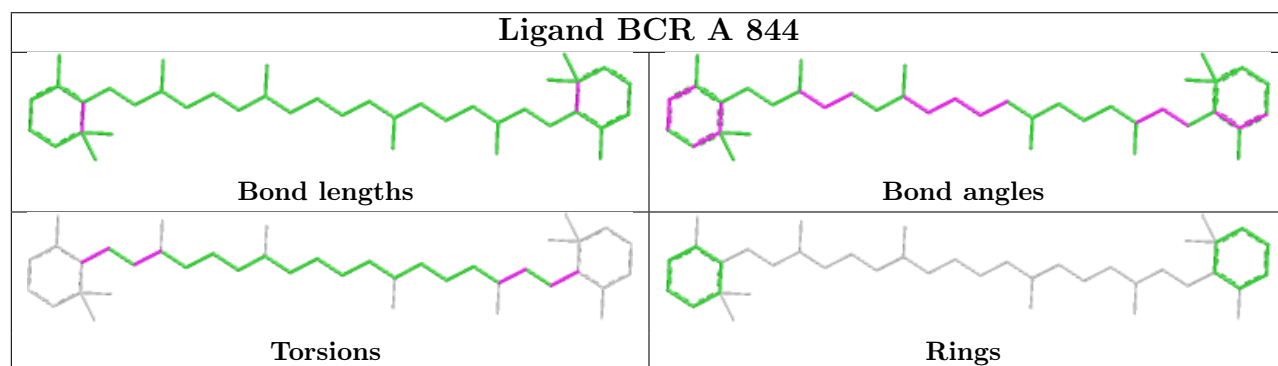
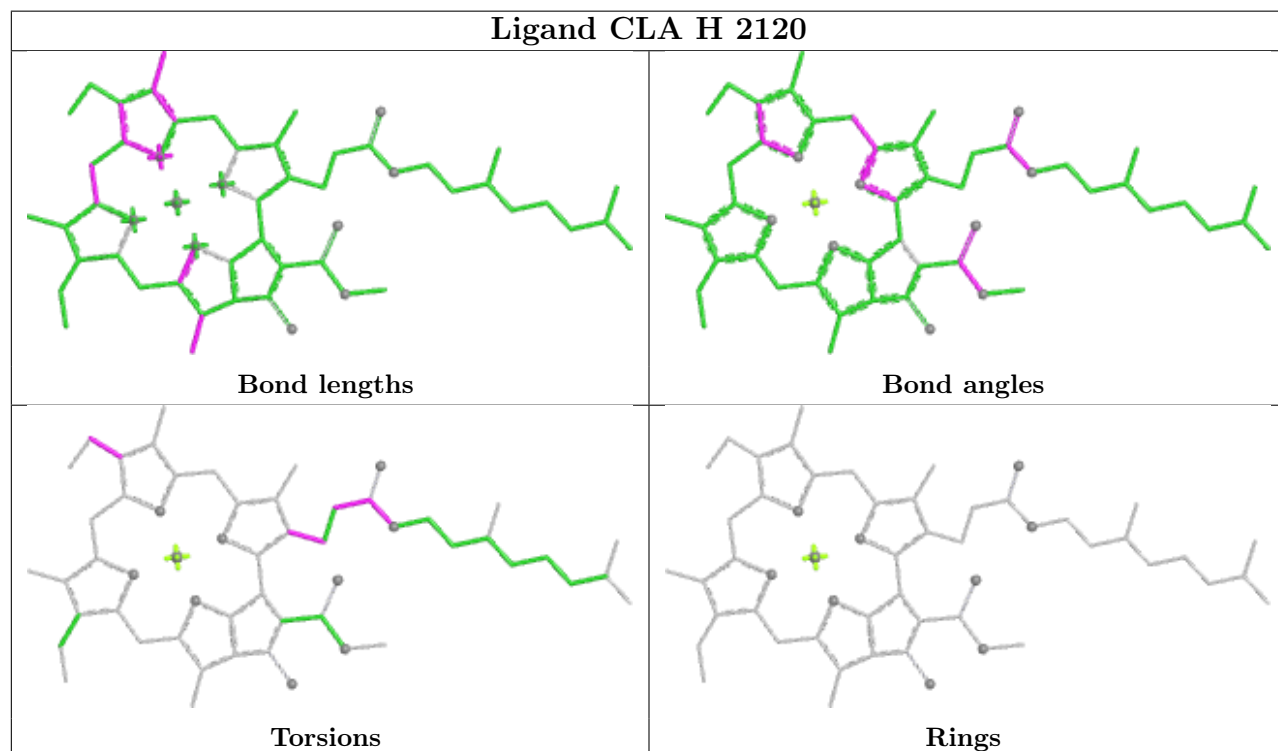
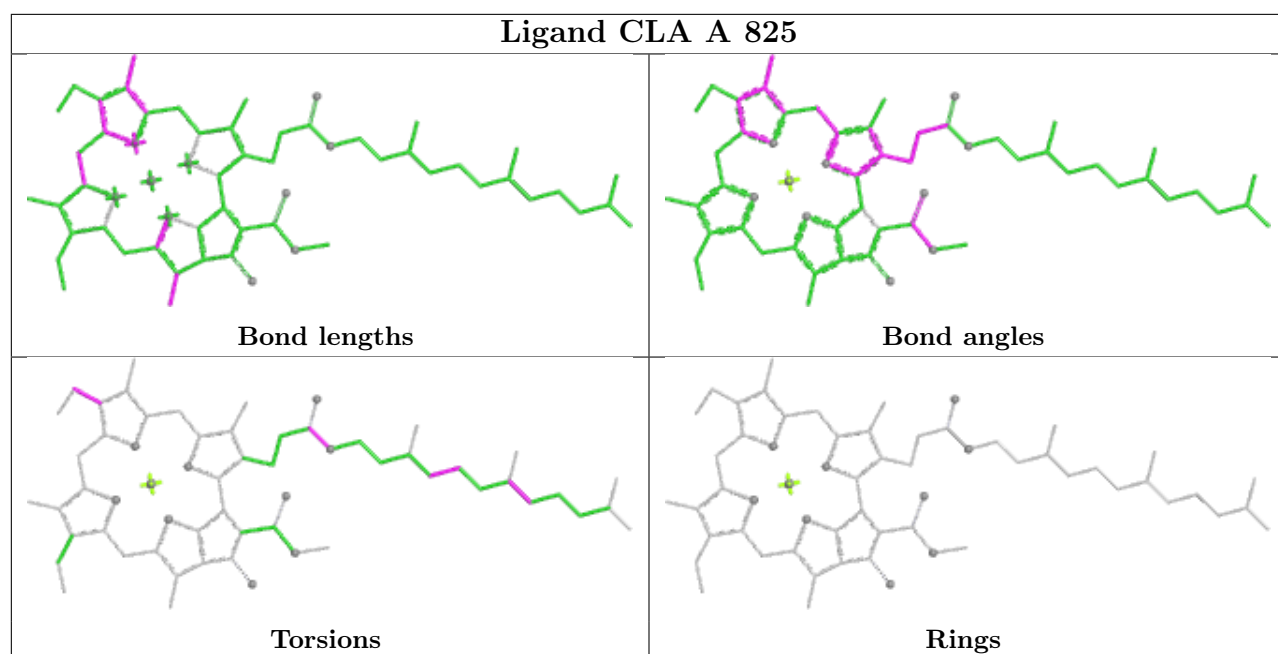


Ligand CLA a 811

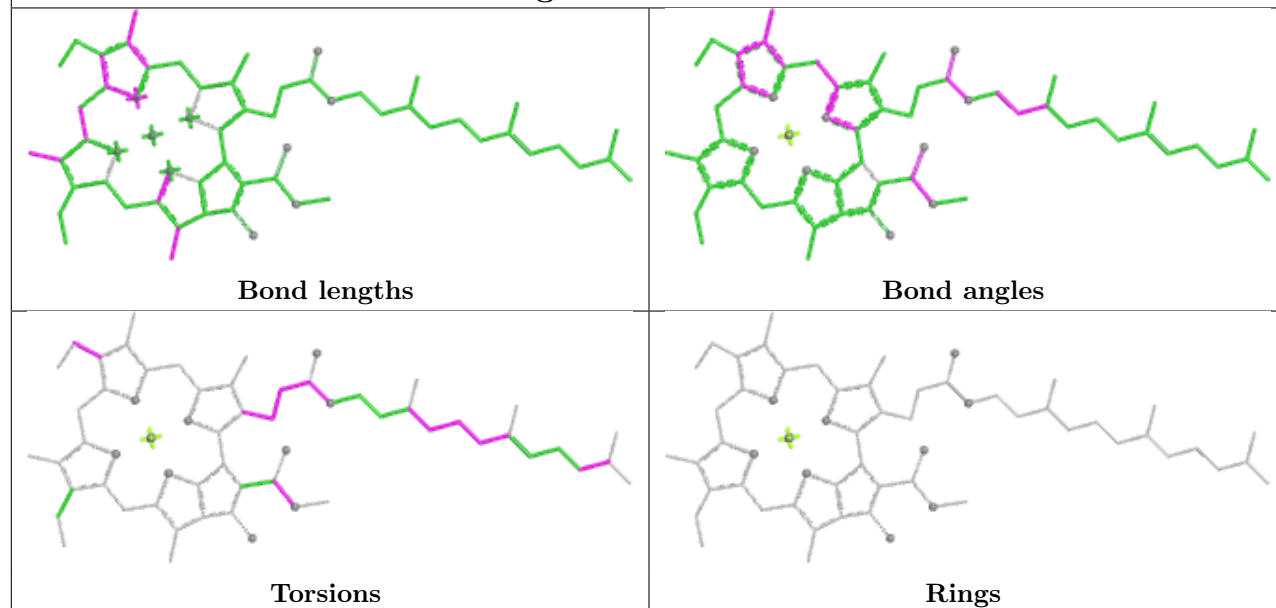


Ligand CLA G 824

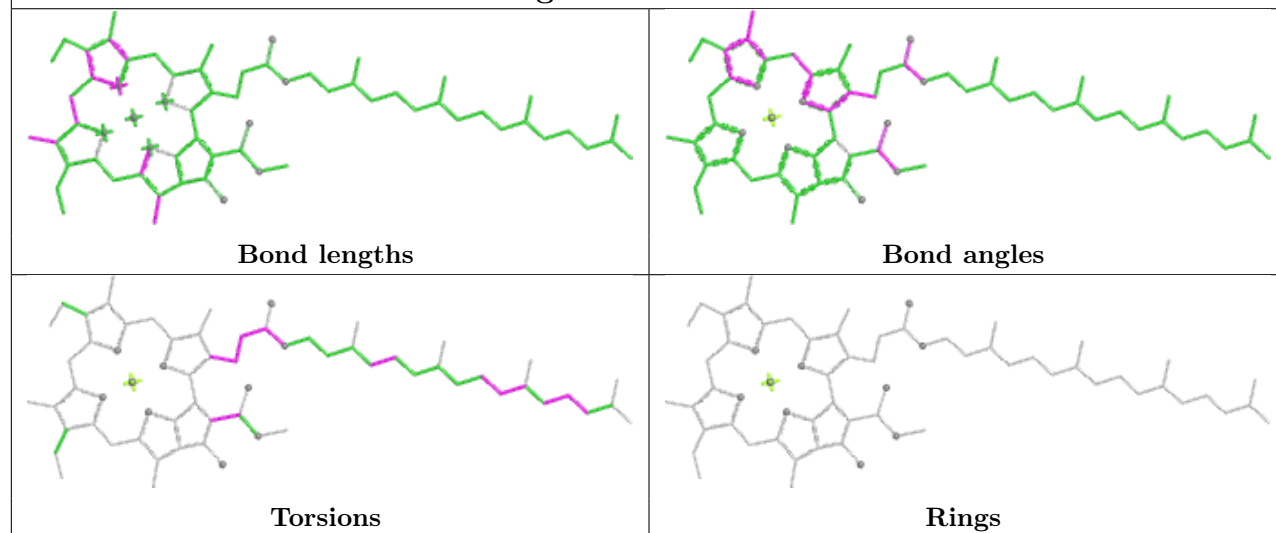


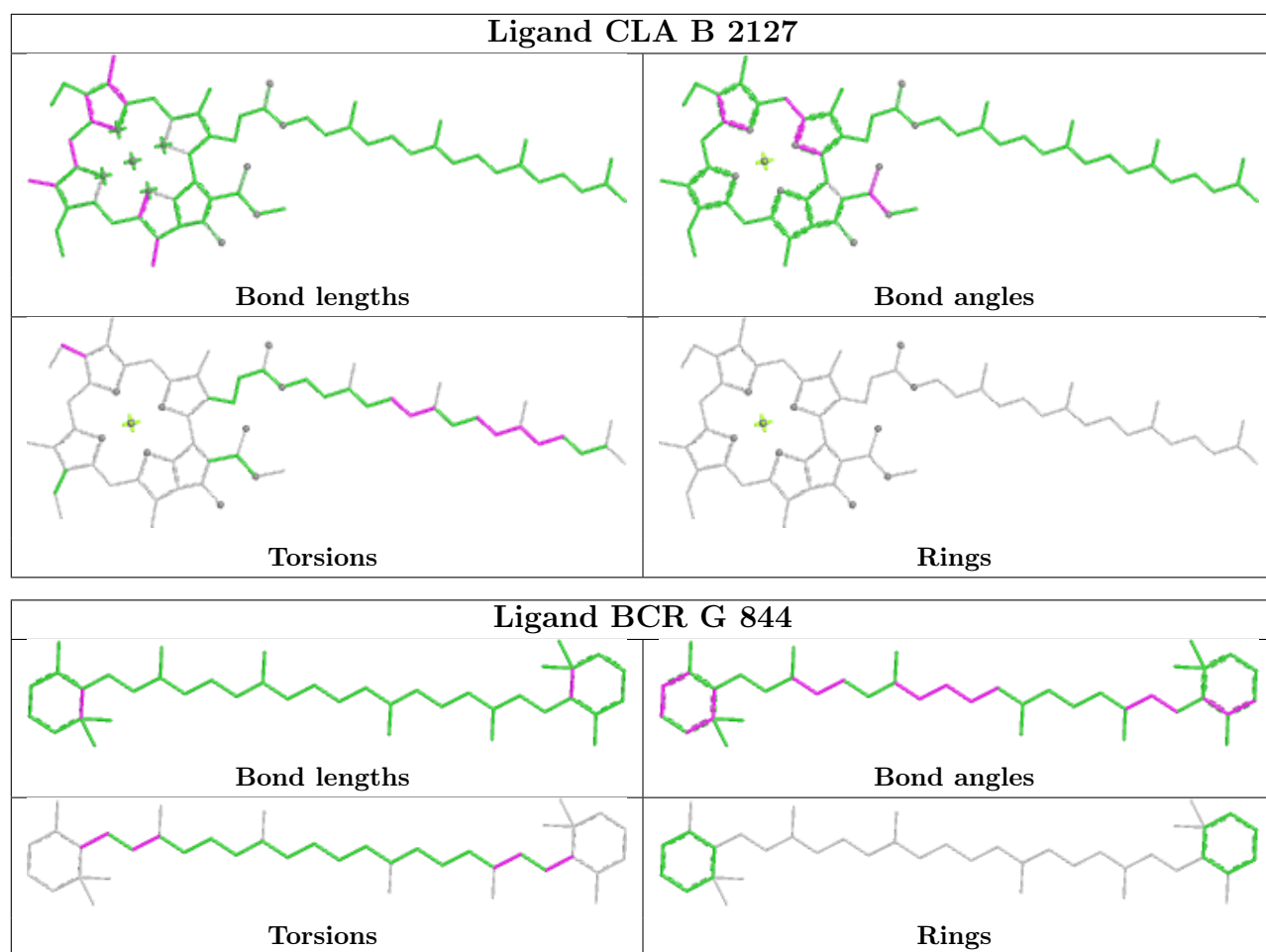


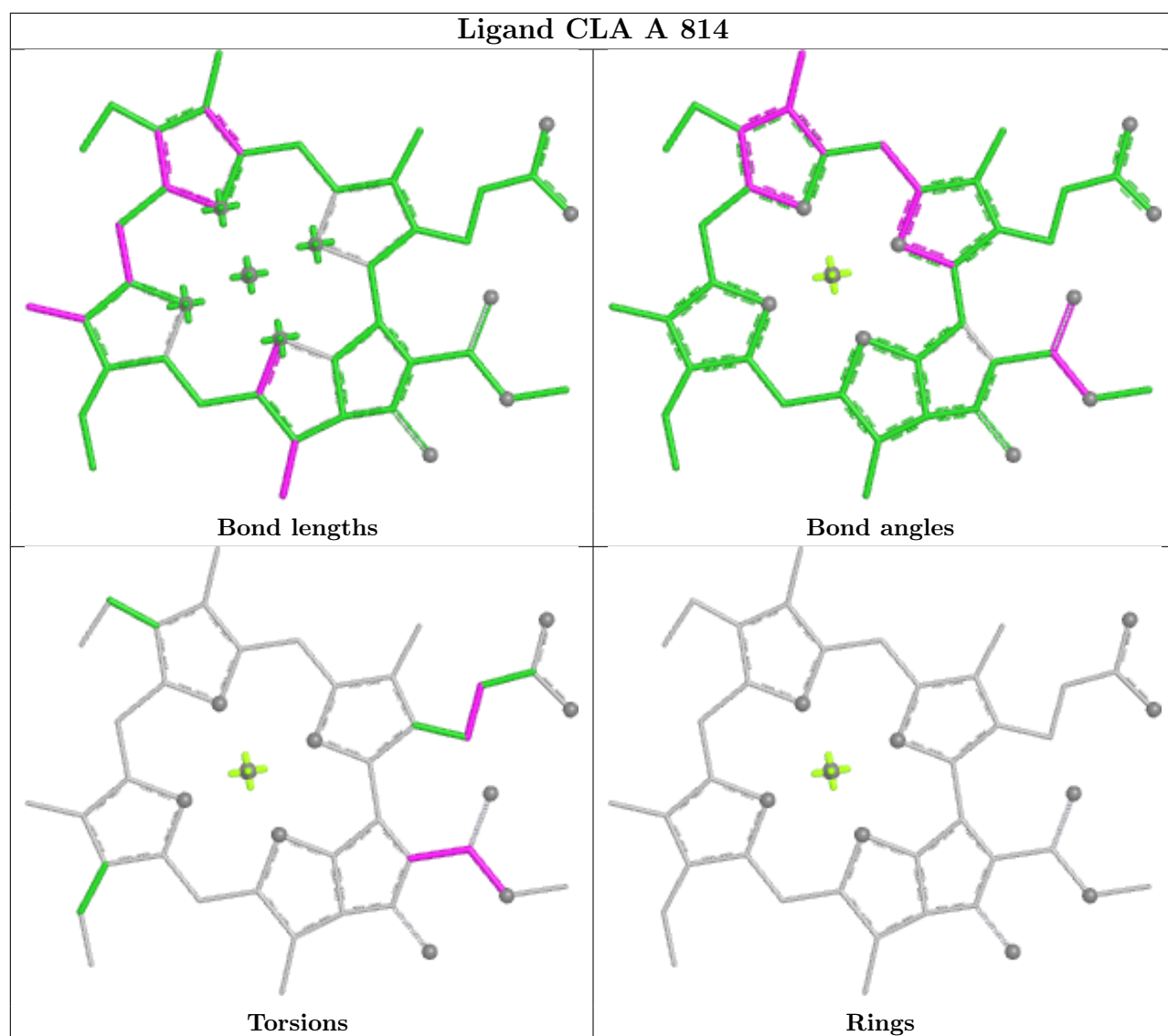
Ligand CLA a 817



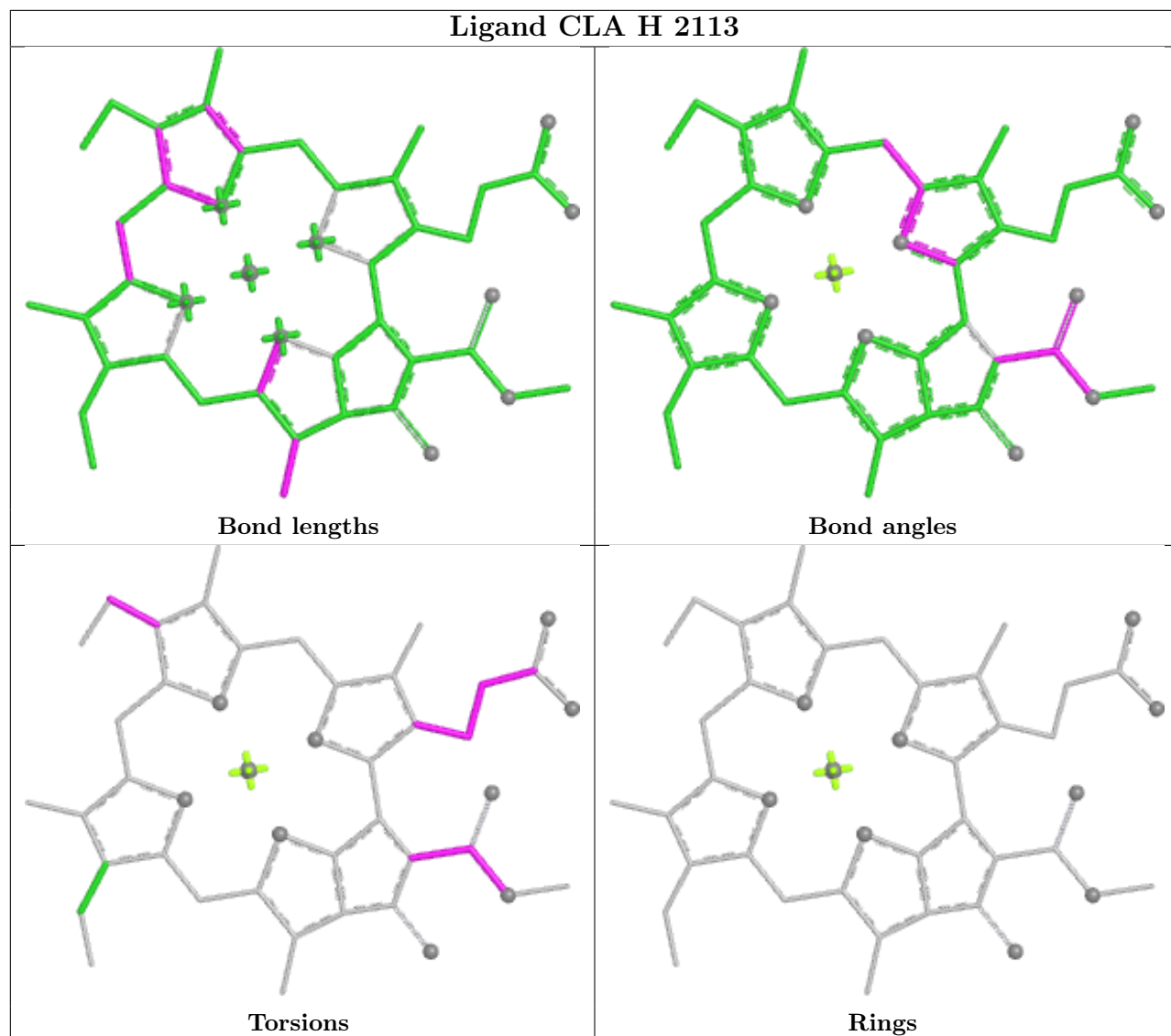
Ligand CLA a 807



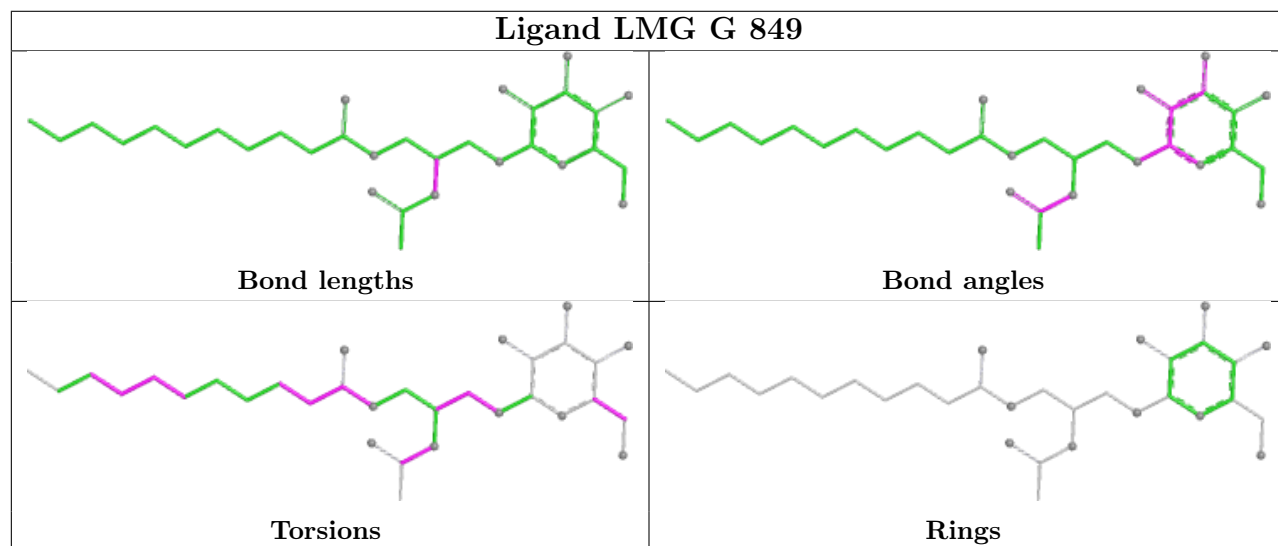




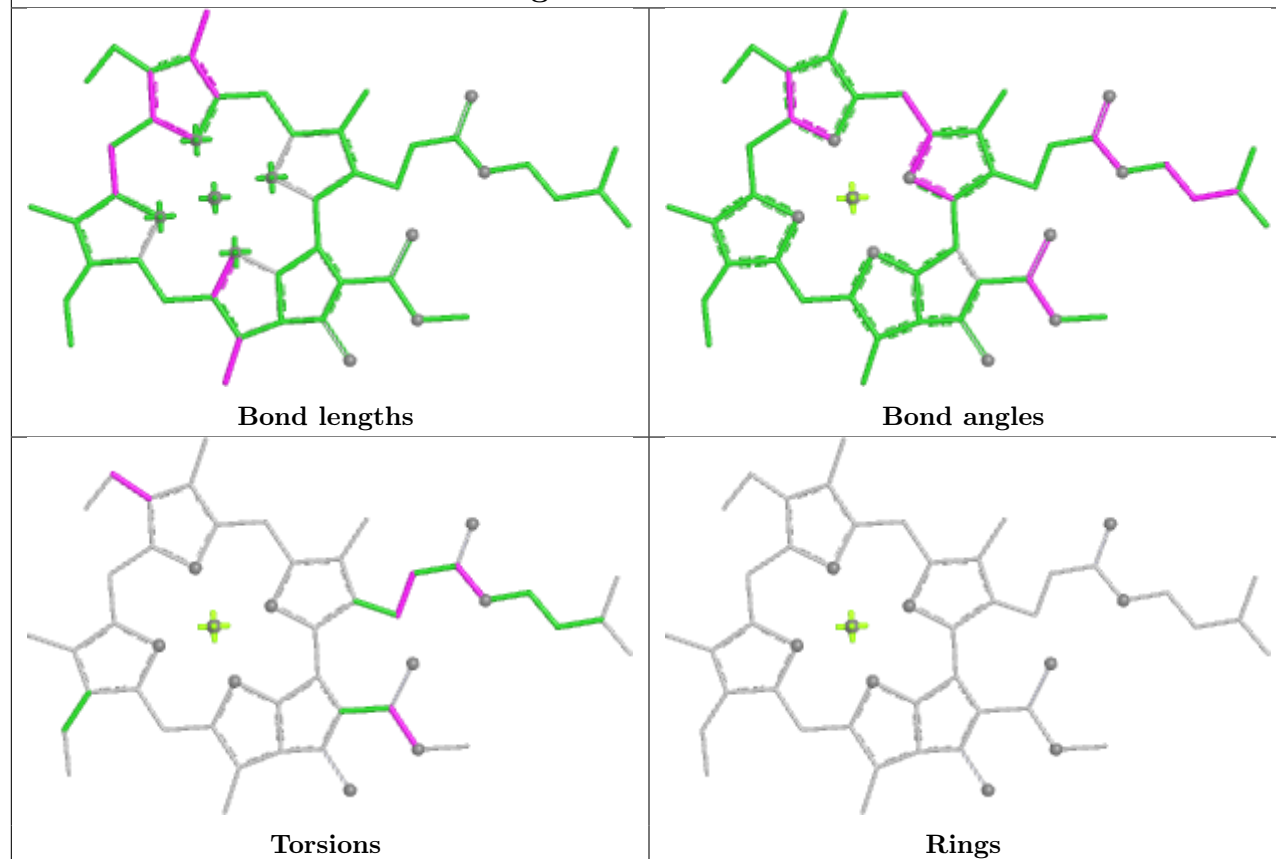
Ligand CLA H 2113



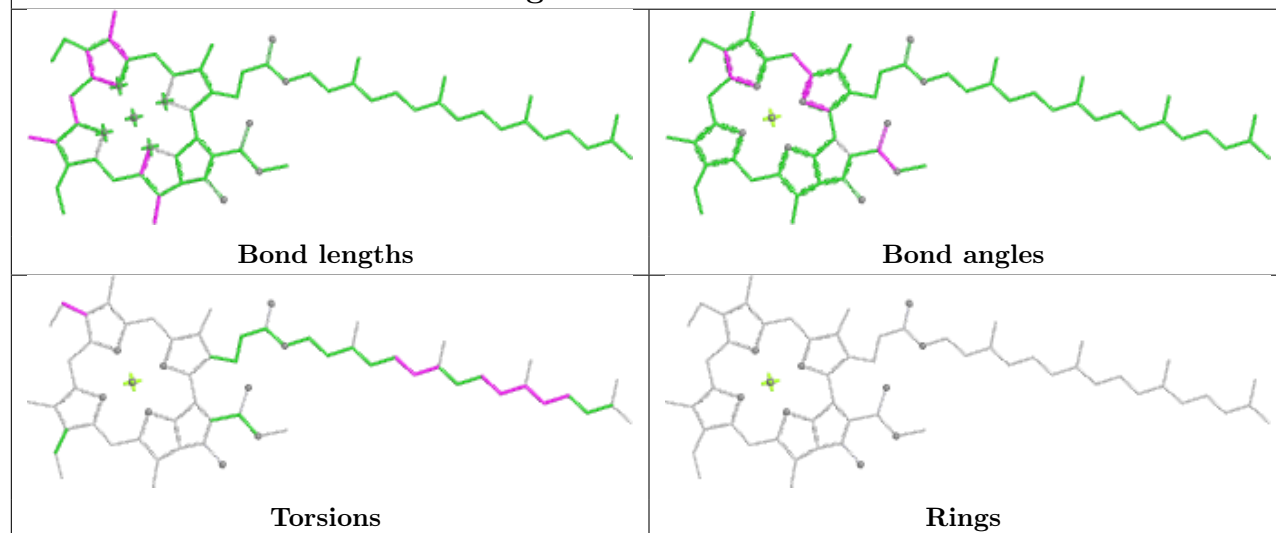
Ligand LMG G 849

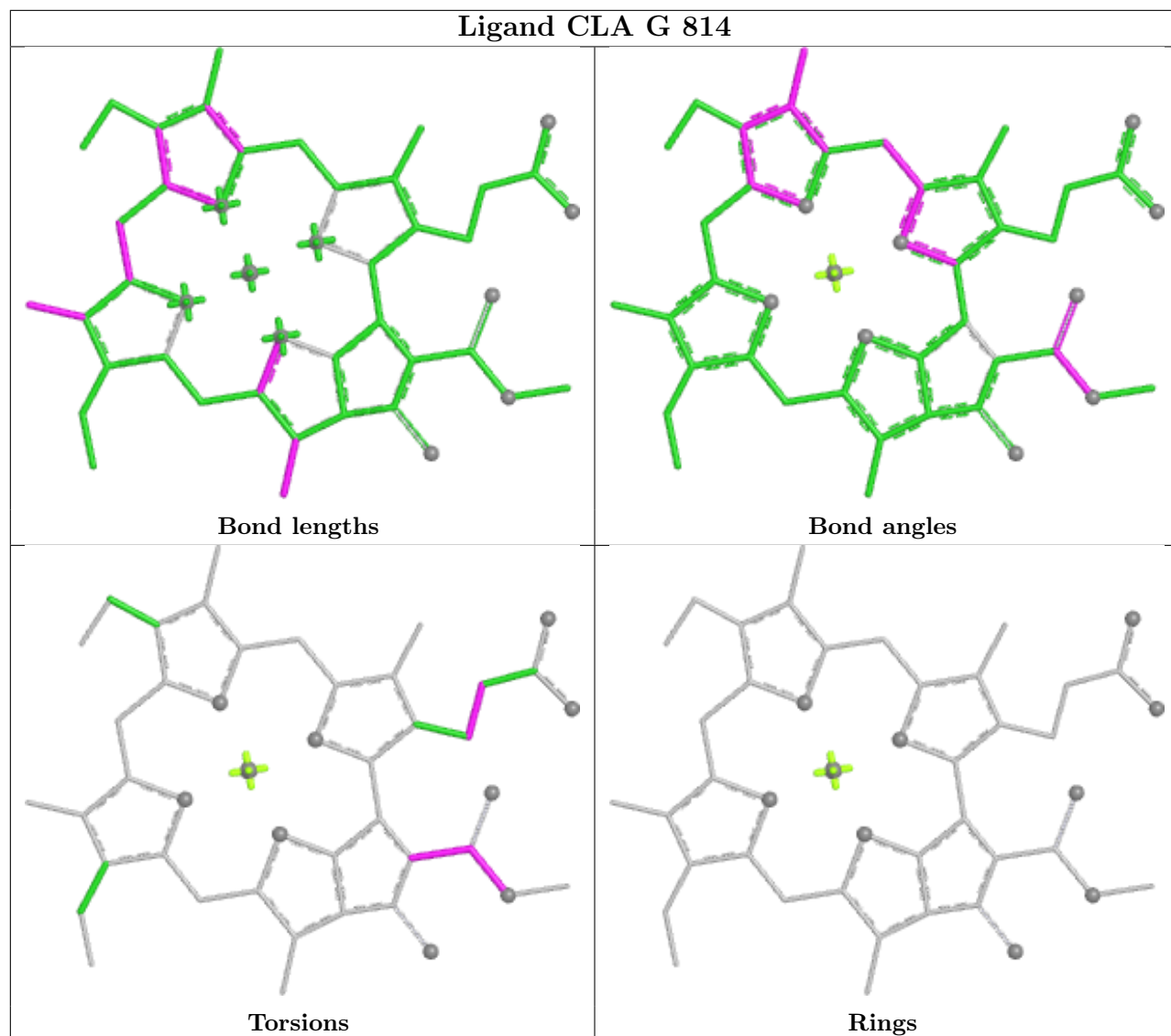


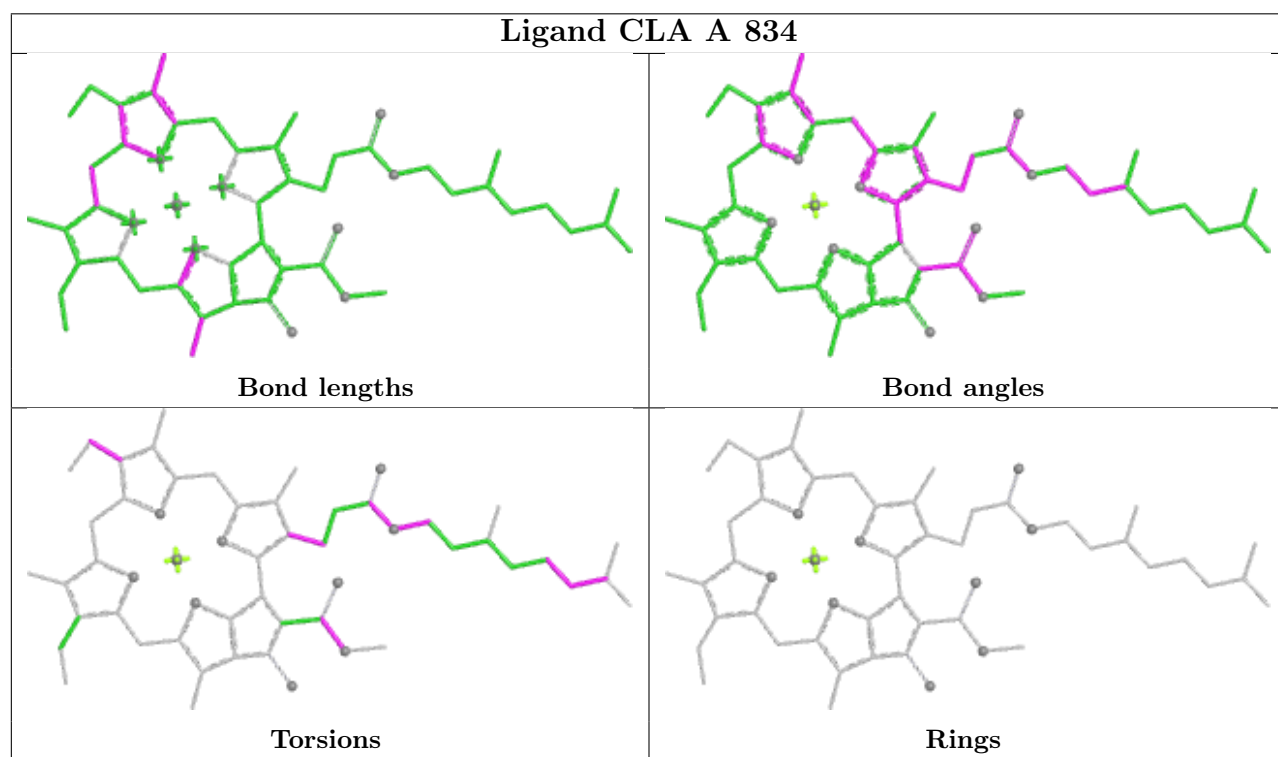
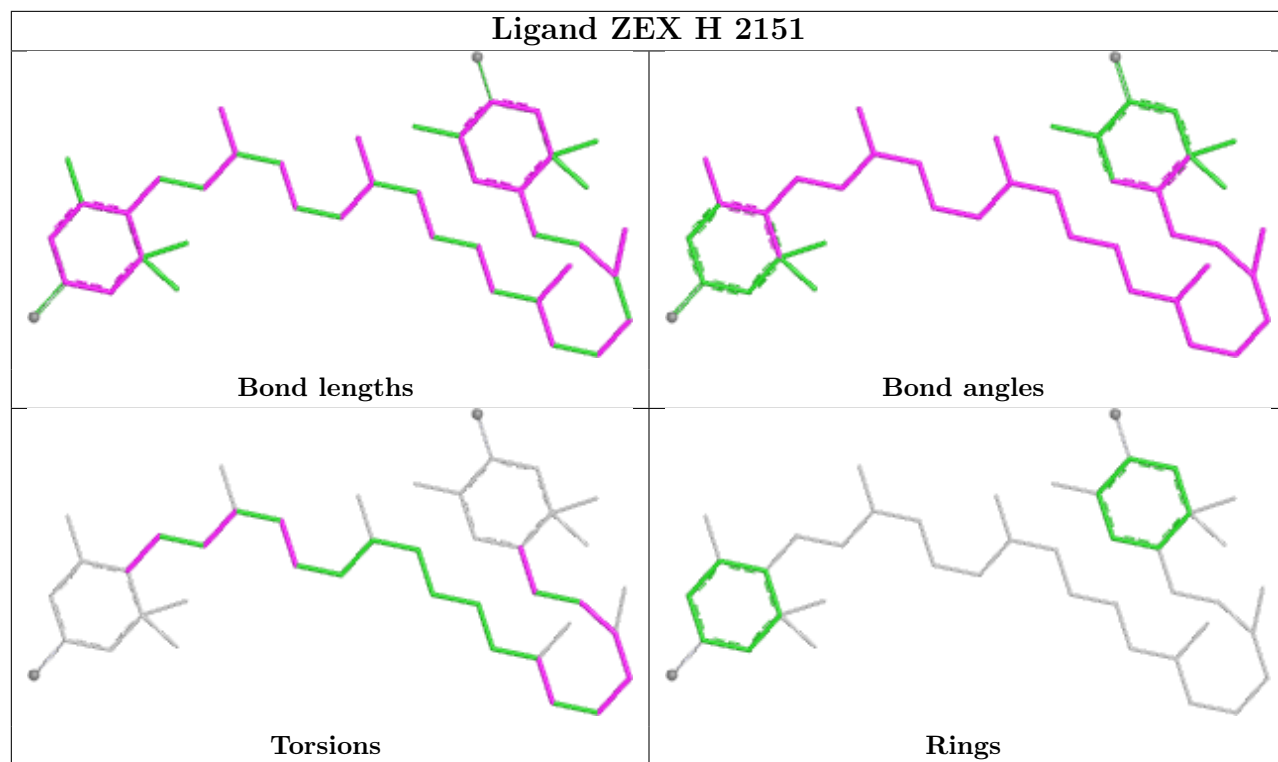
Ligand CLA G 806

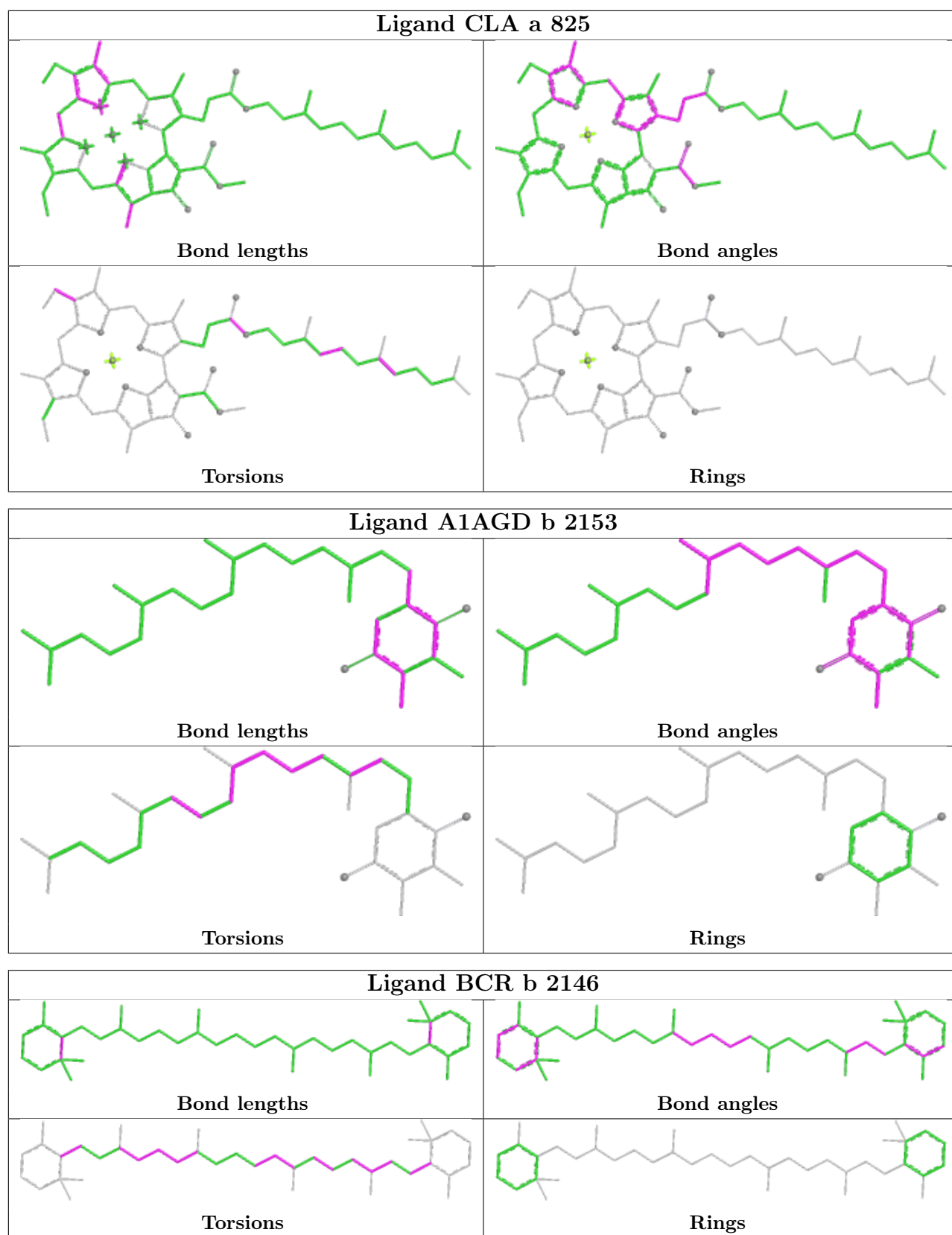


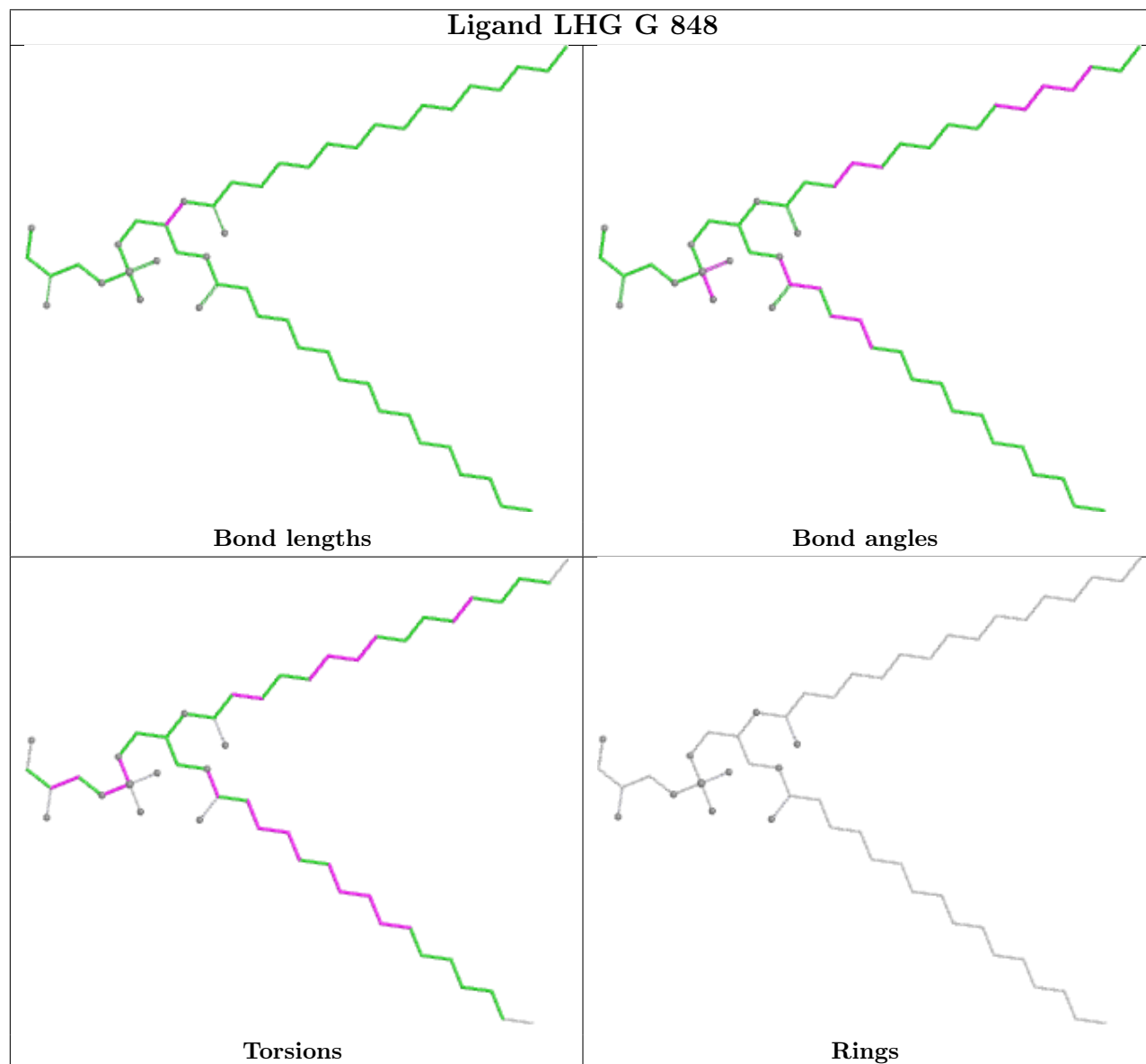
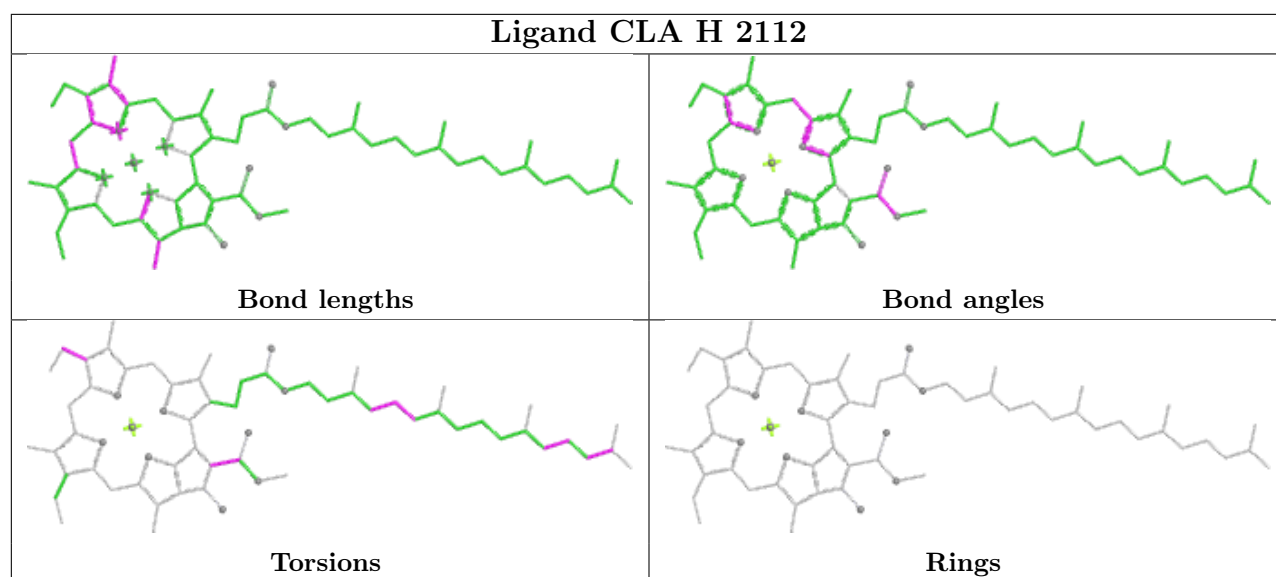
Ligand CLA b 2126

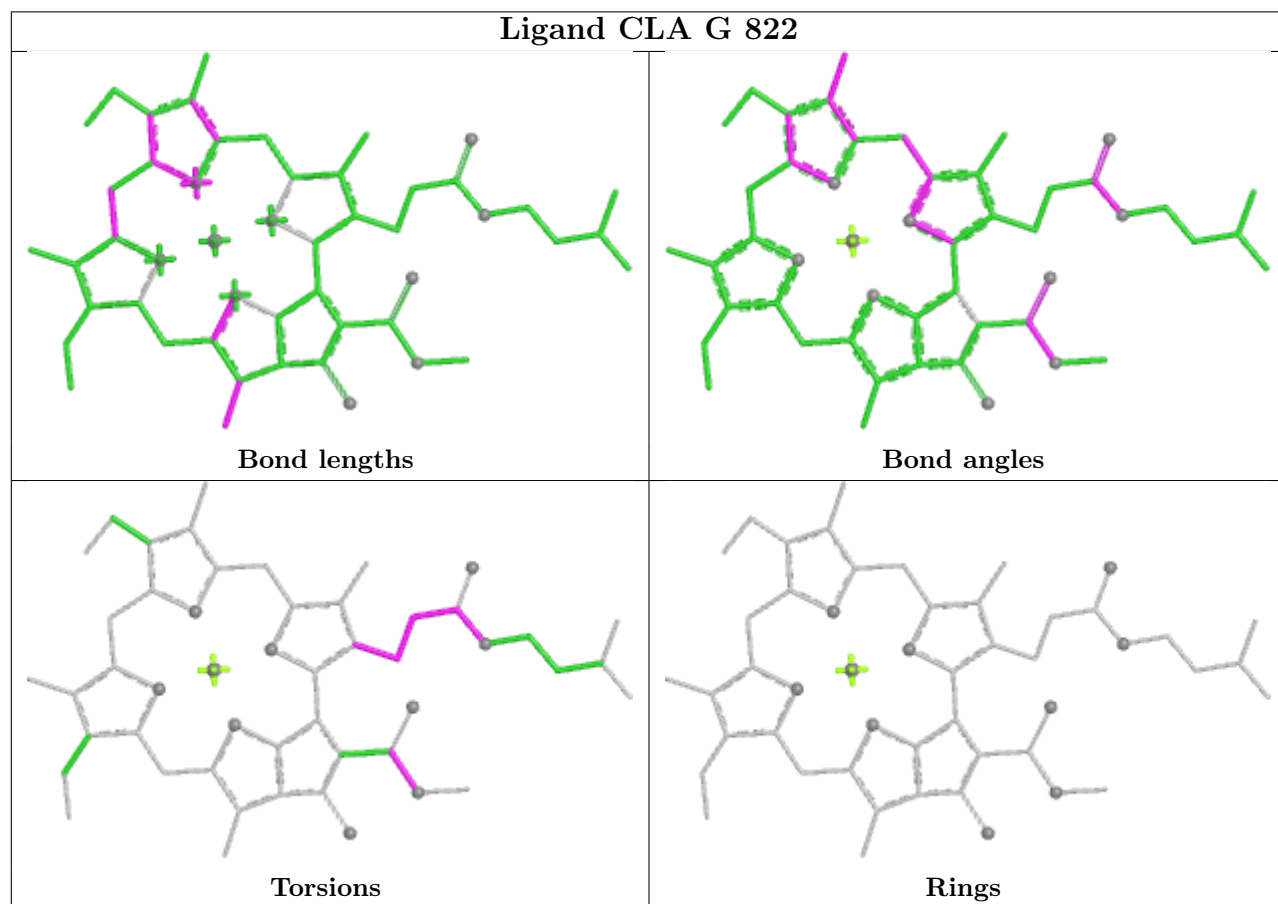
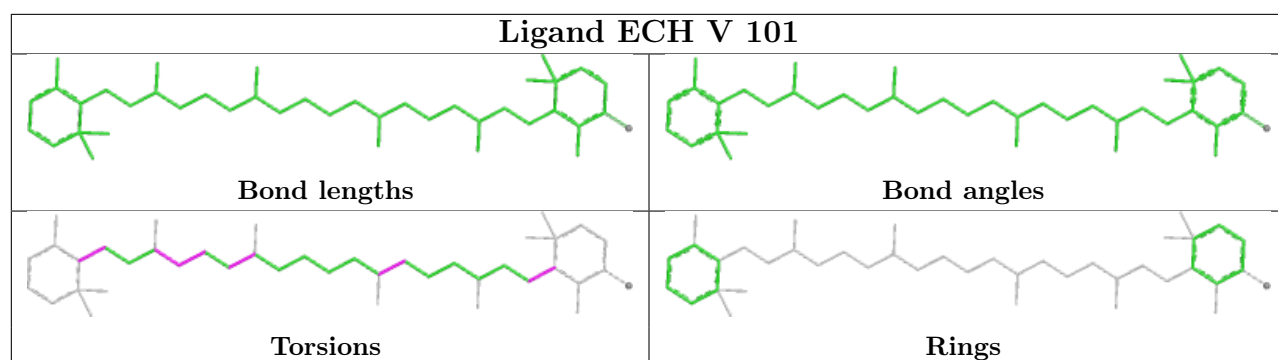


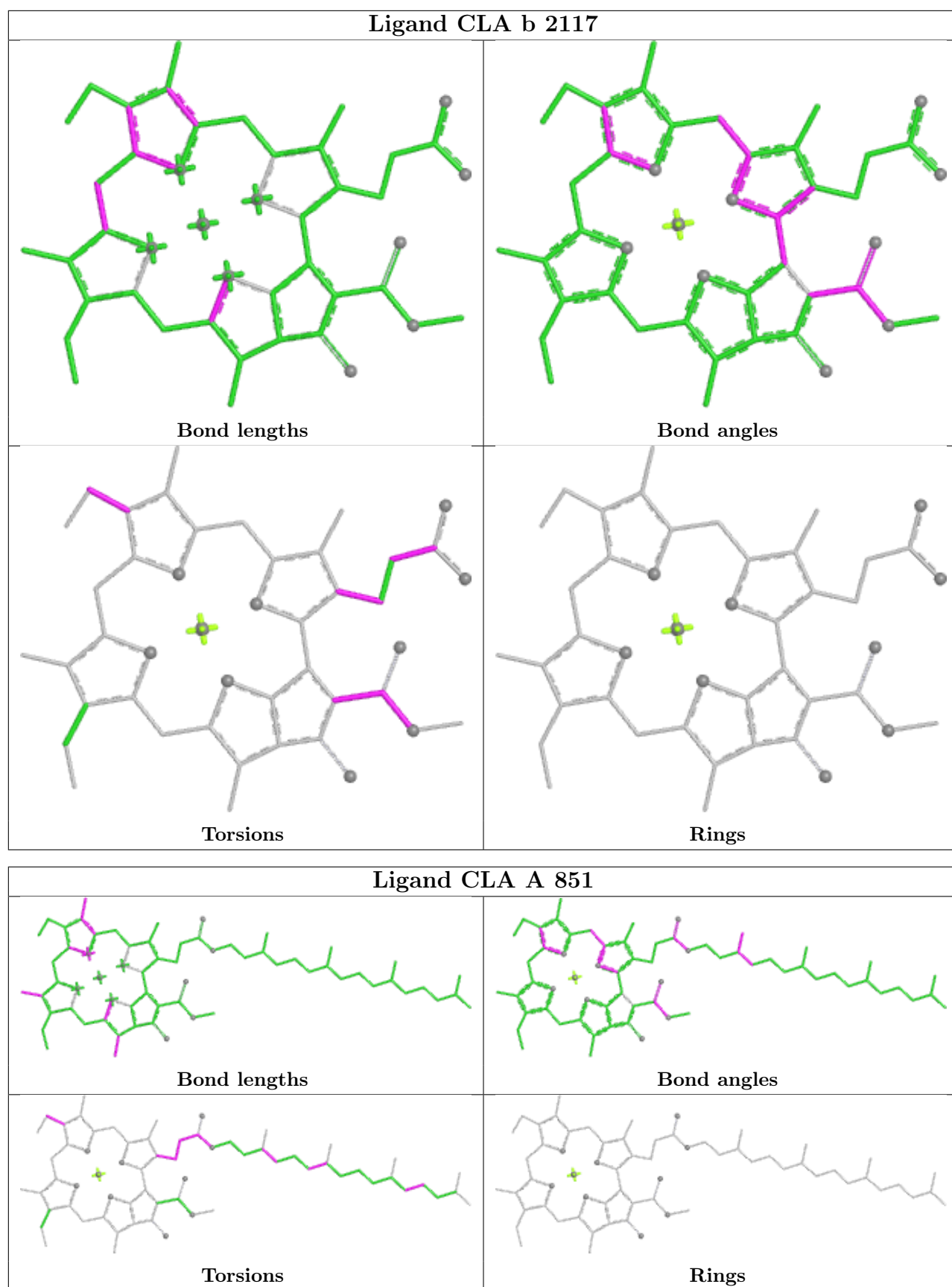


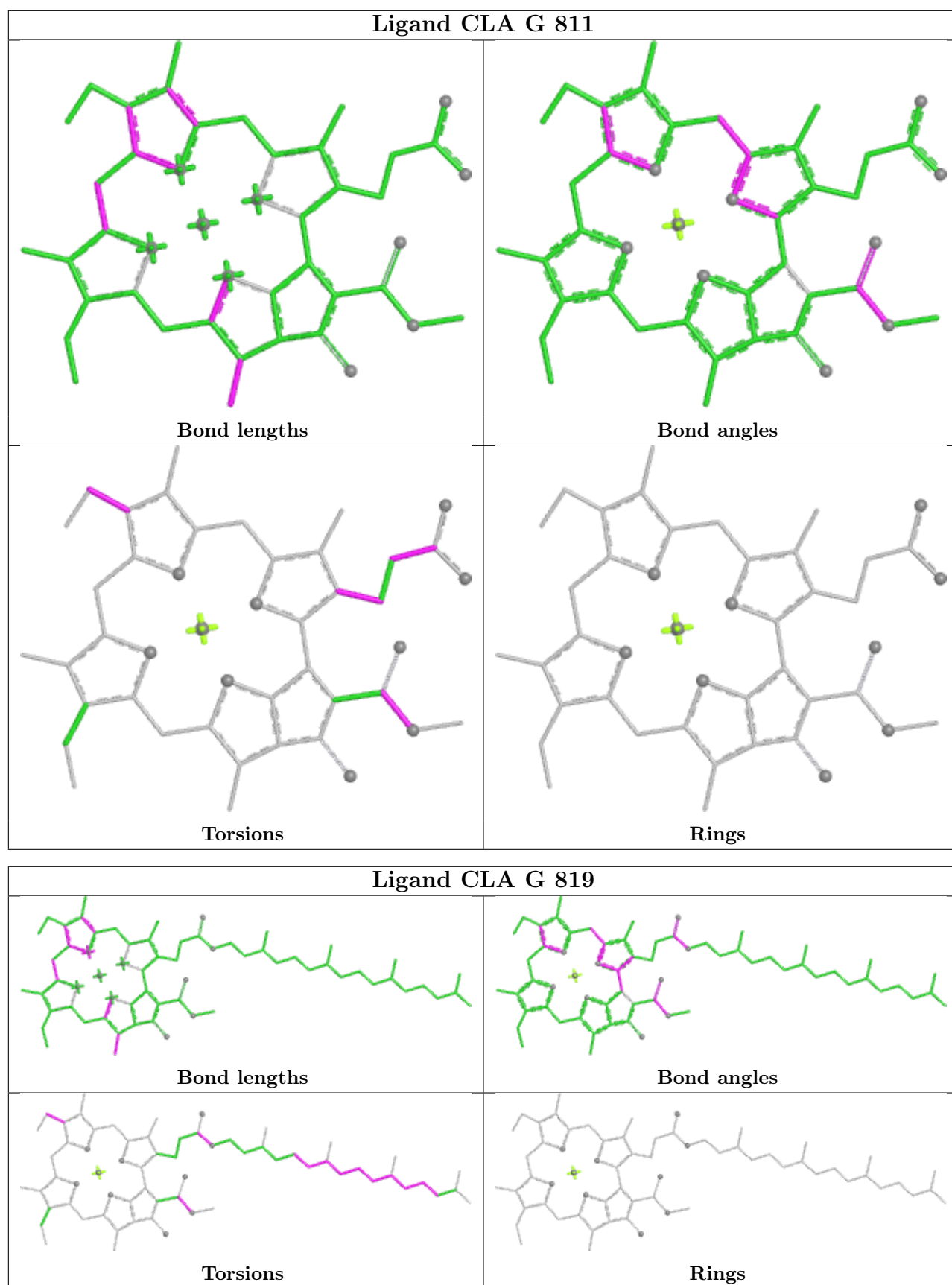


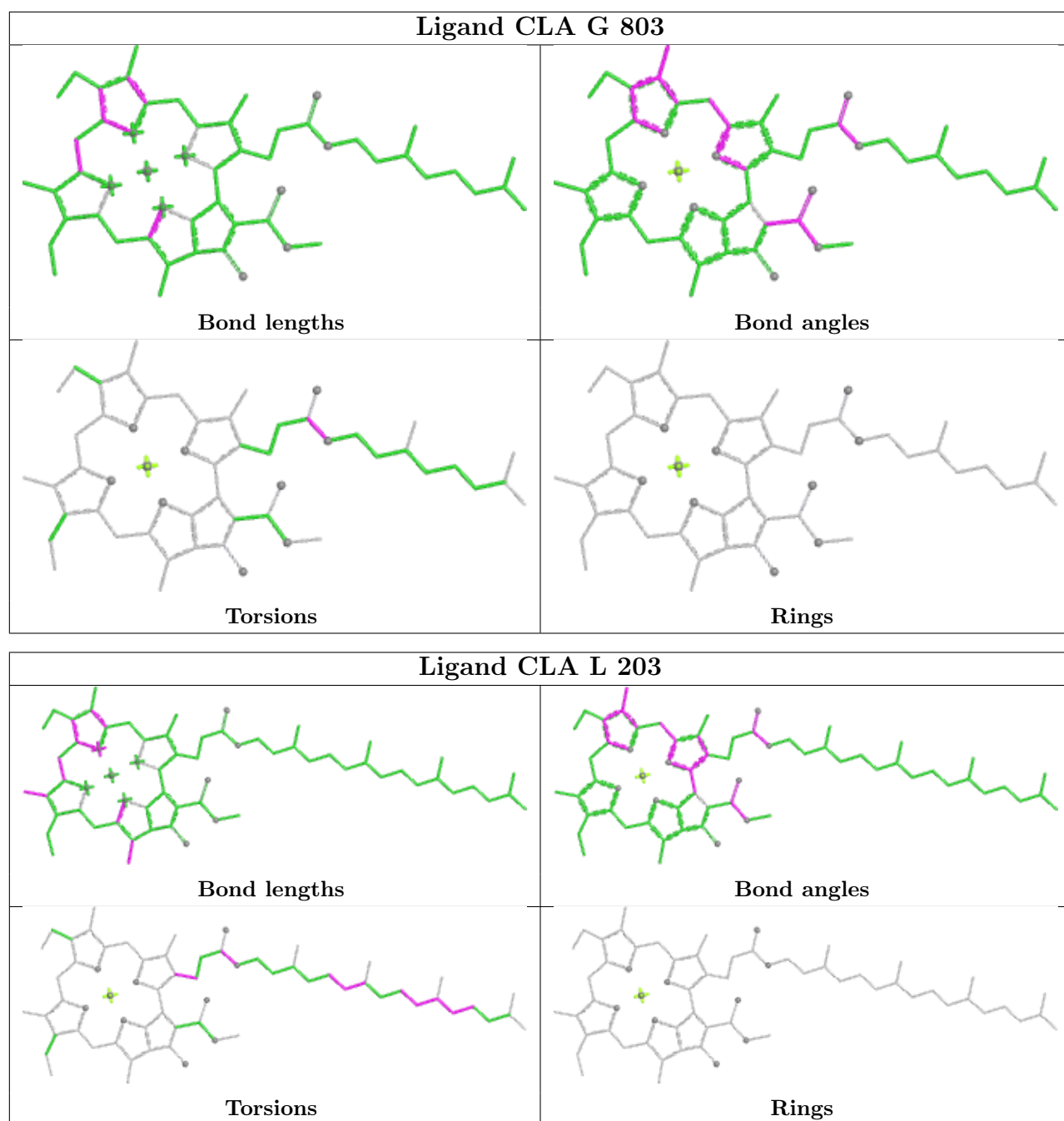


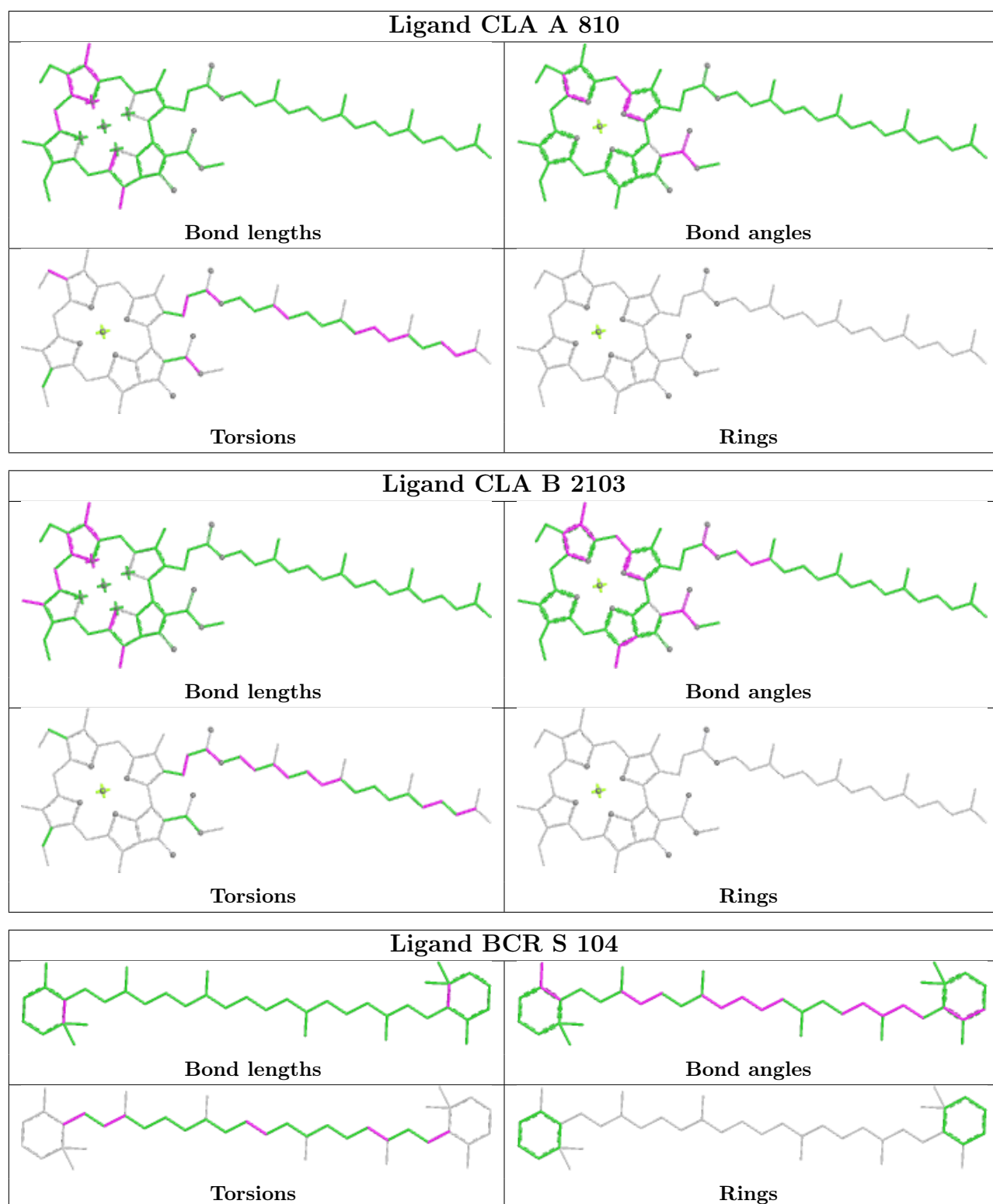


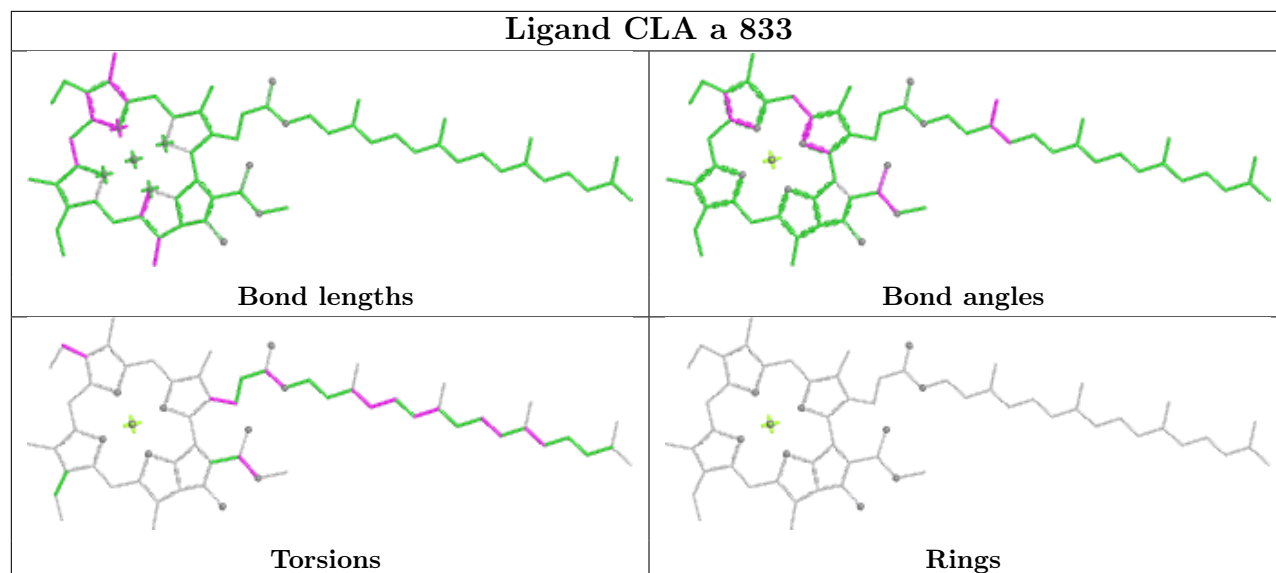
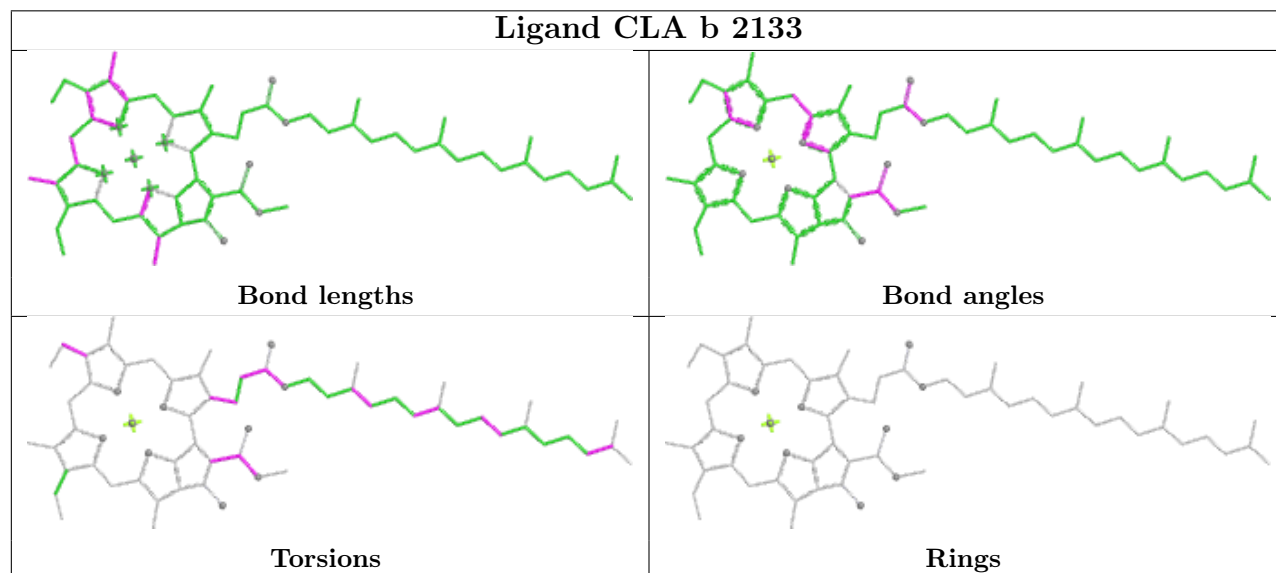
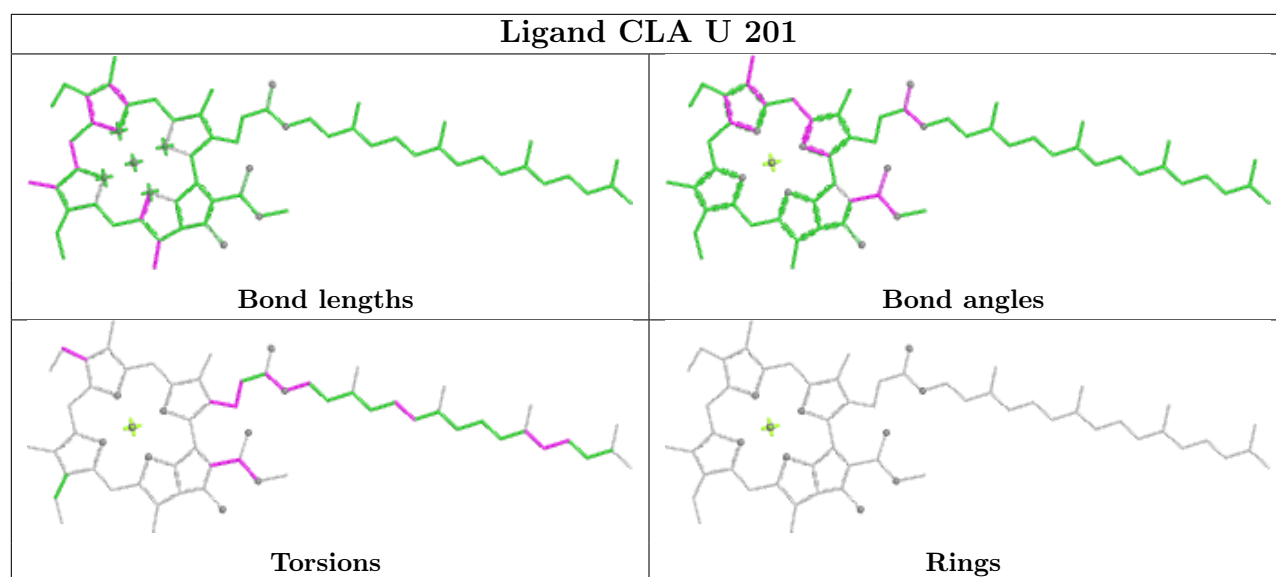


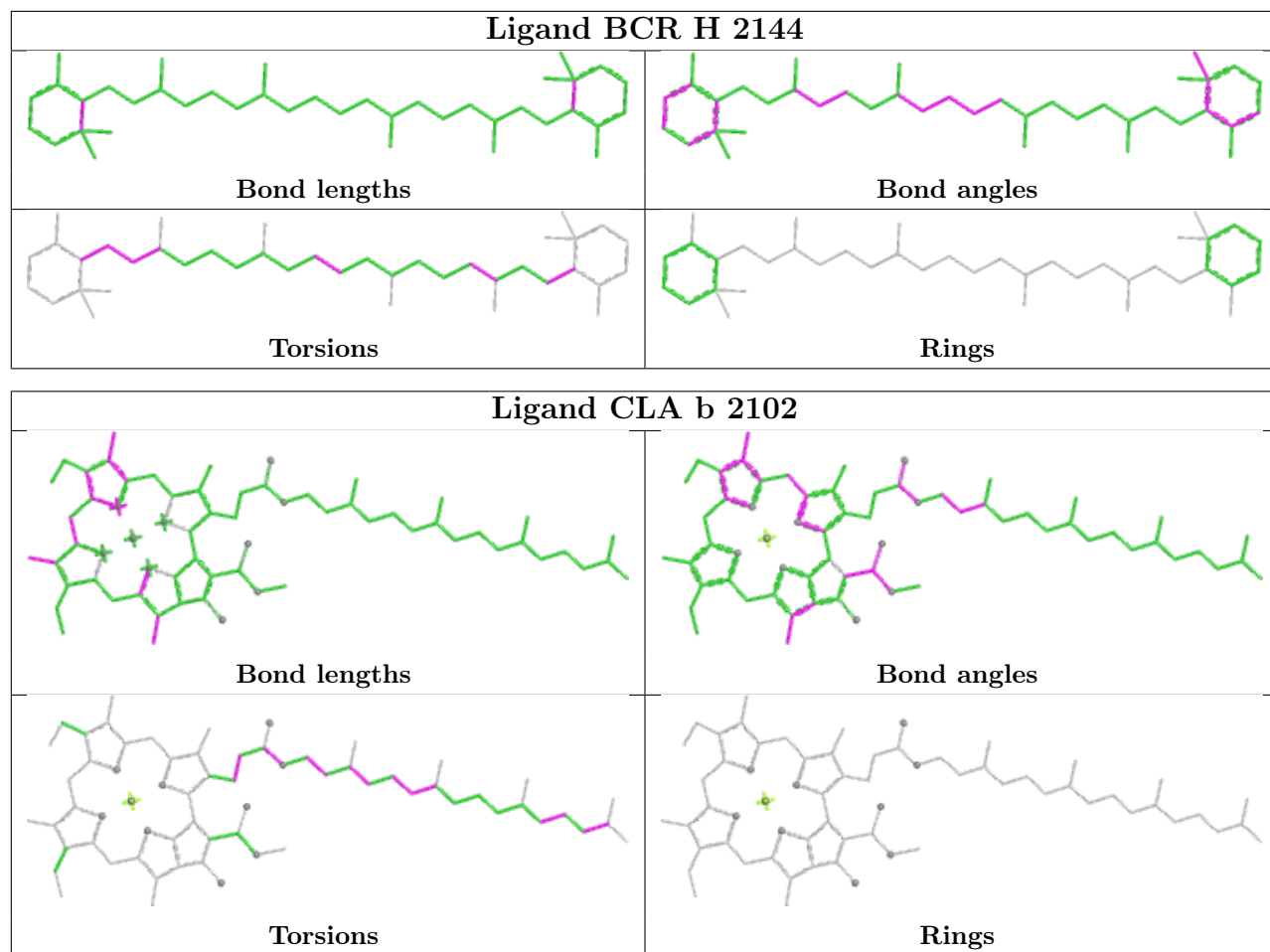




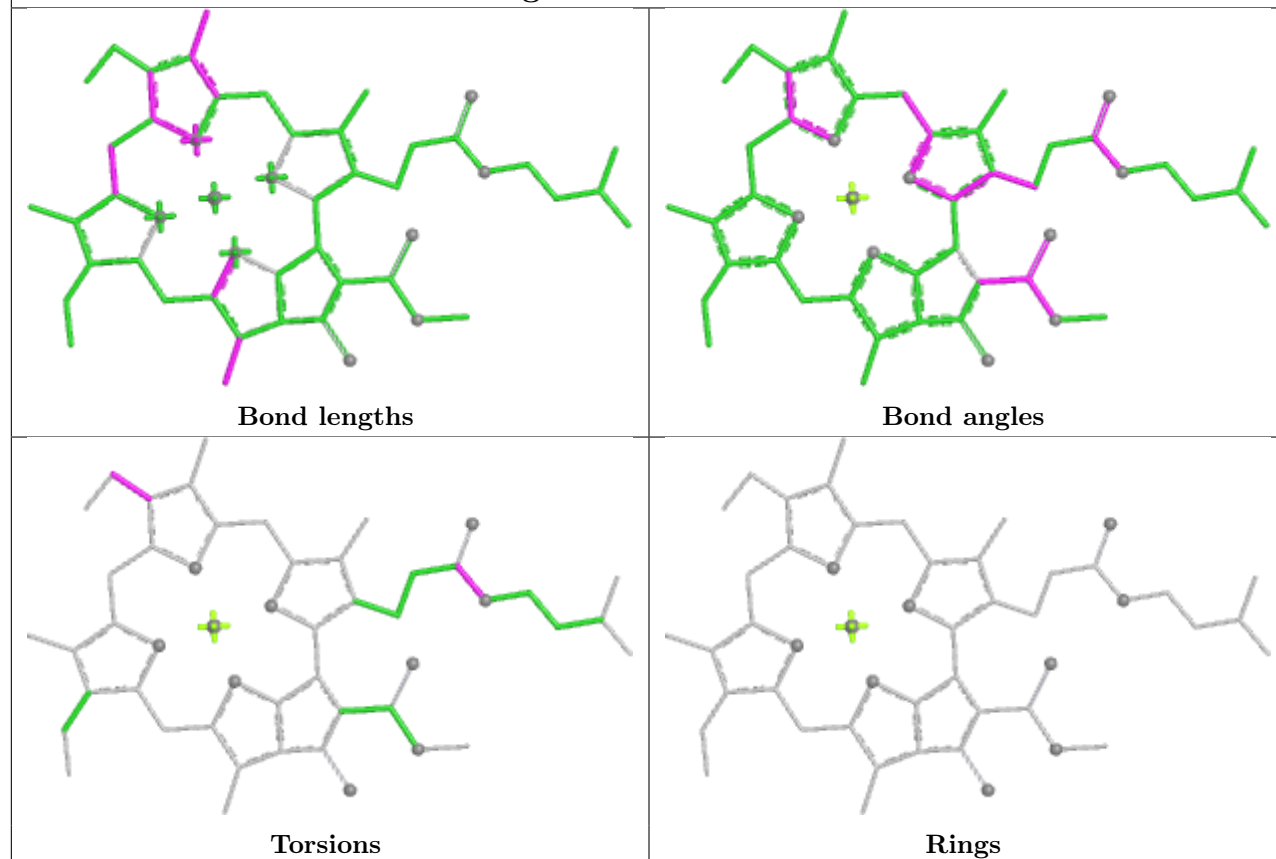




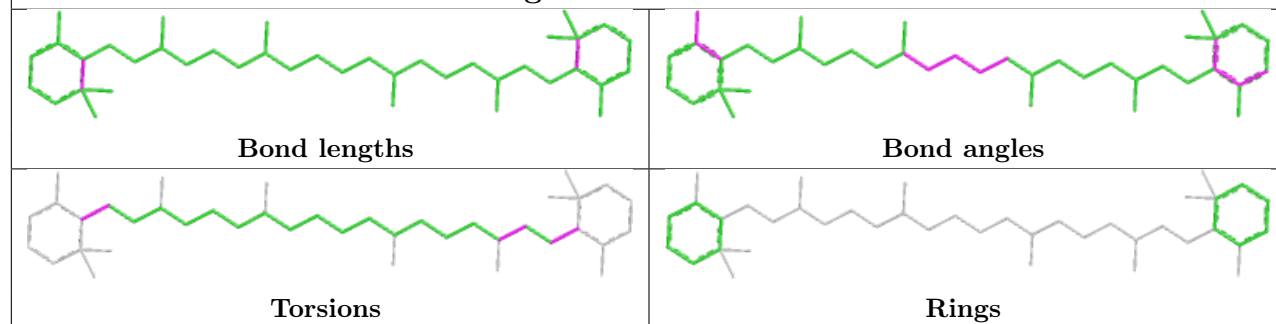




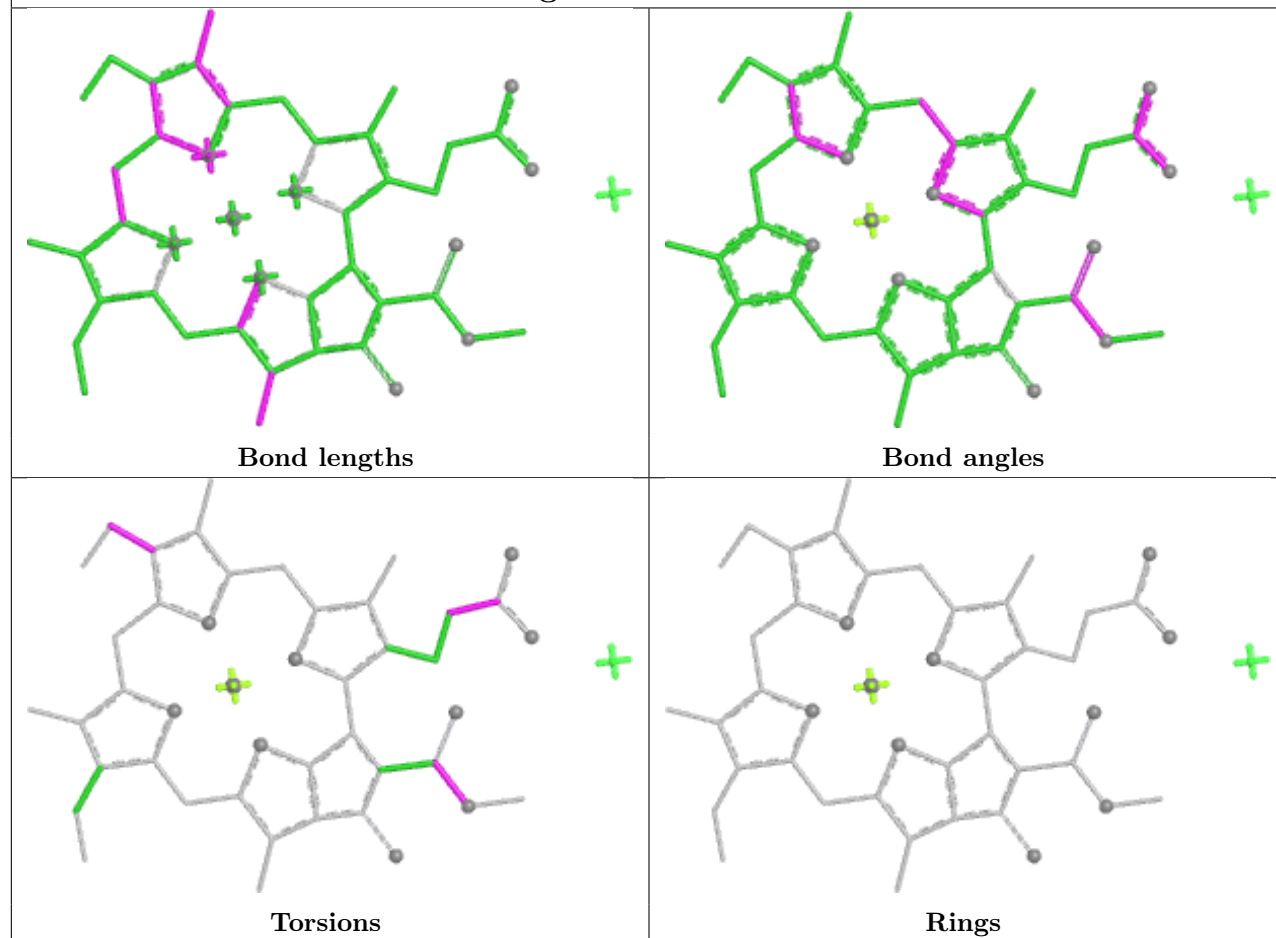
Ligand CLA H 2125



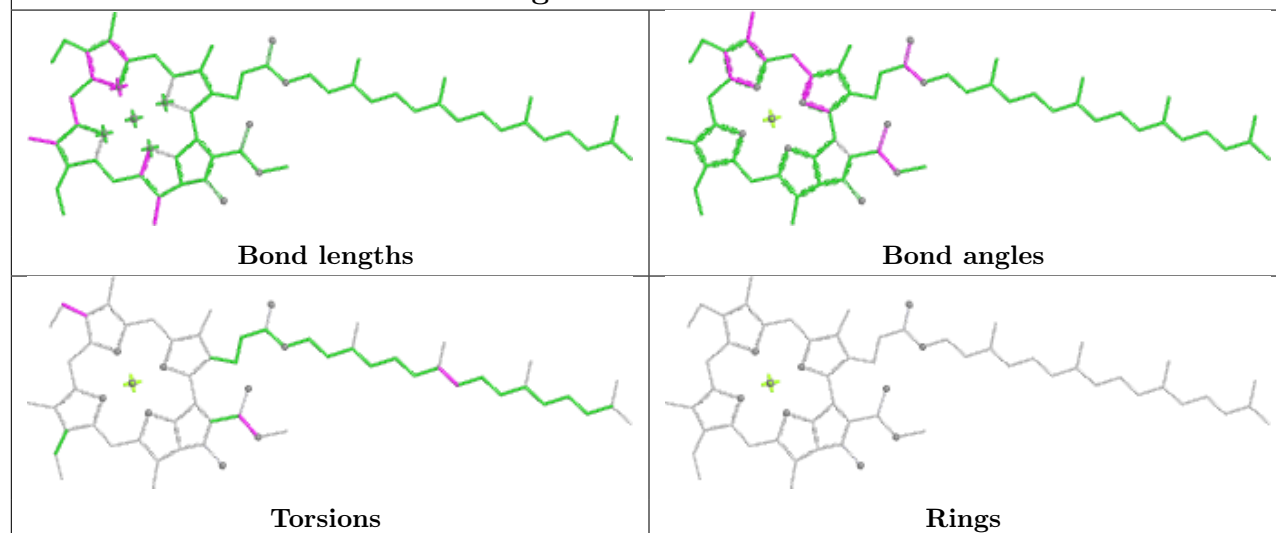
Ligand BCR b 2142



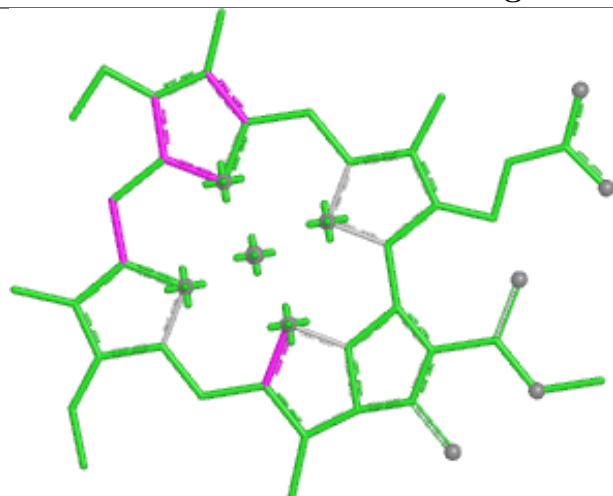
Ligand CLA f 203



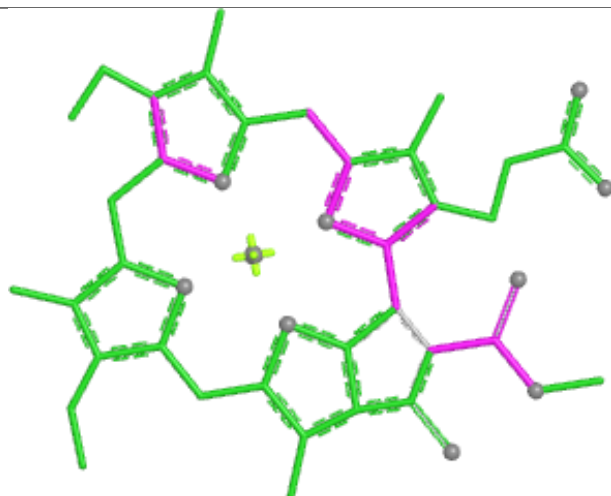
Ligand CLA A 838



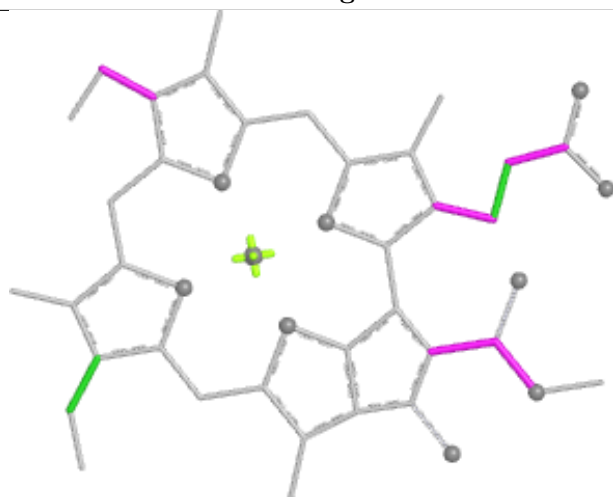
Ligand CLA H 2117



Bond lengths



Bond angles

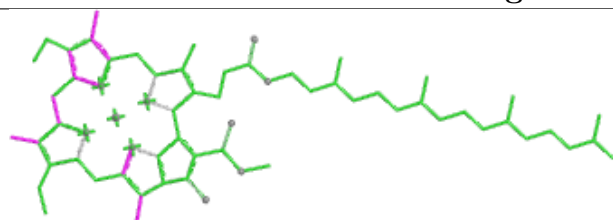


Torsions

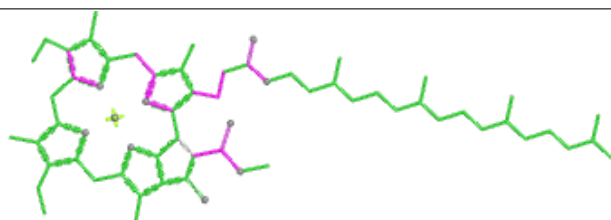


Rings

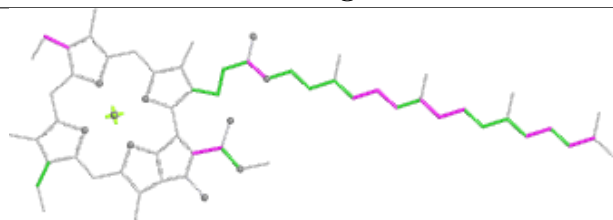
Ligand CLA B 2110



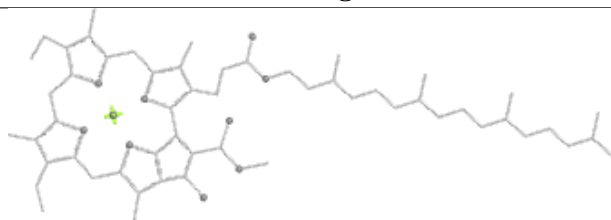
Bond lengths



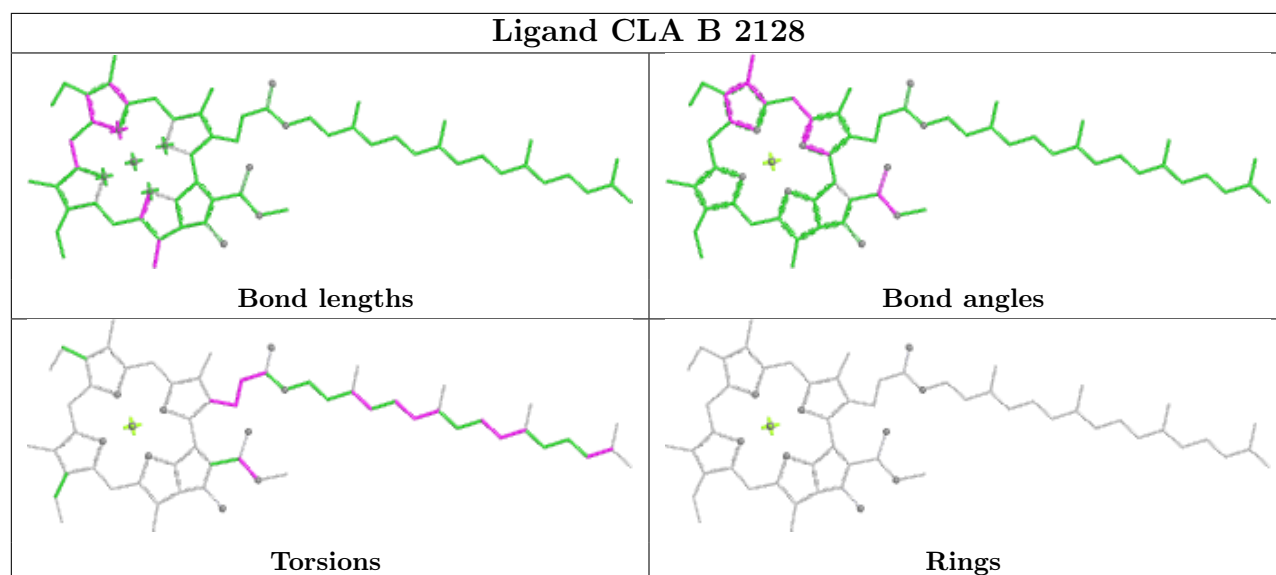
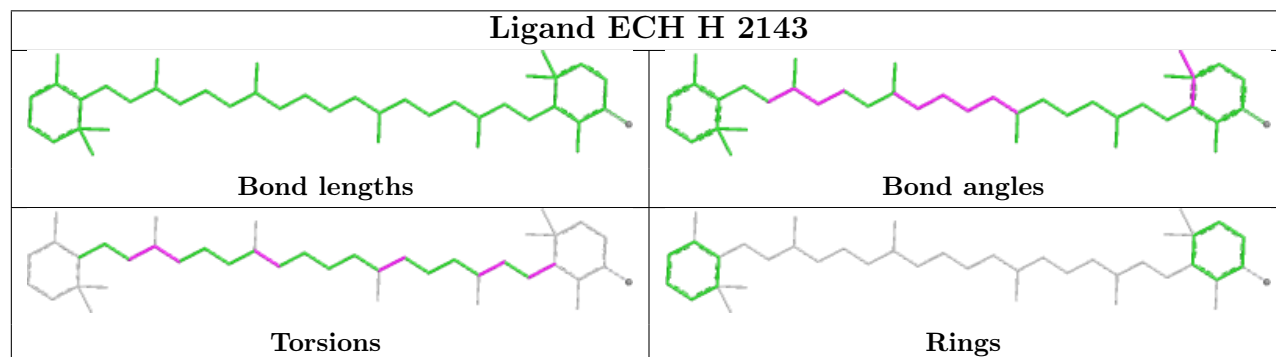
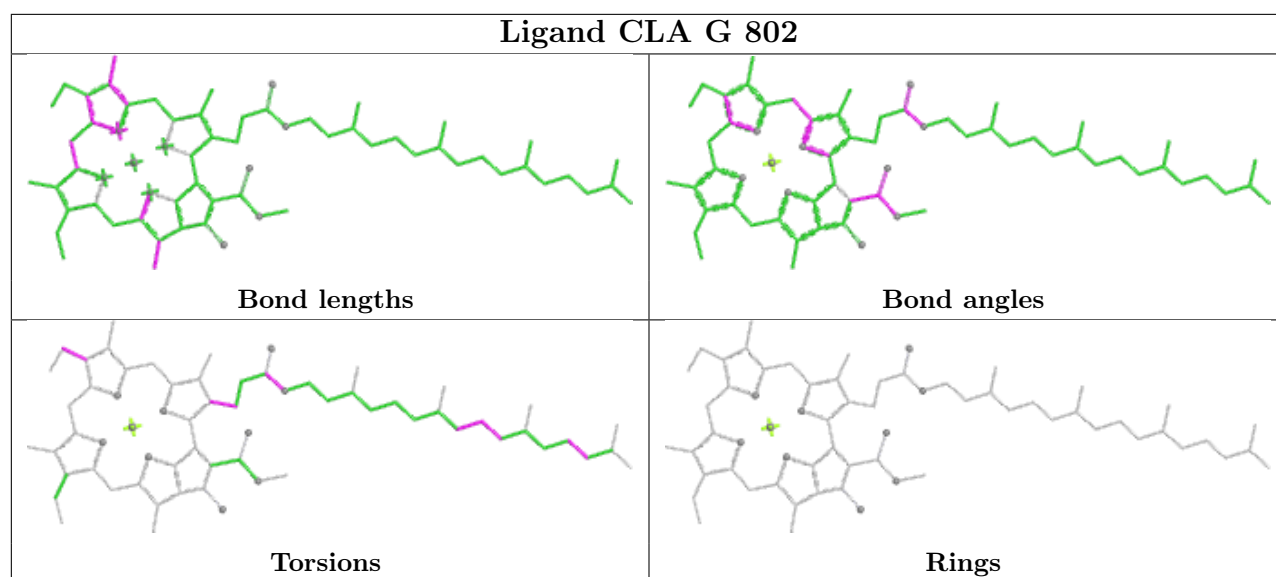
Bond angles

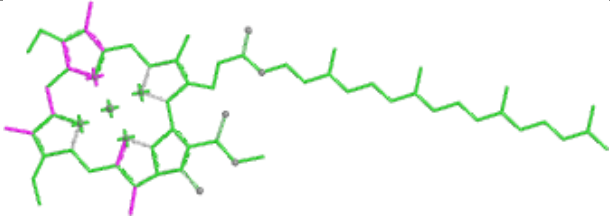
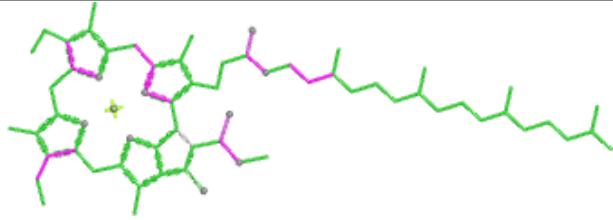
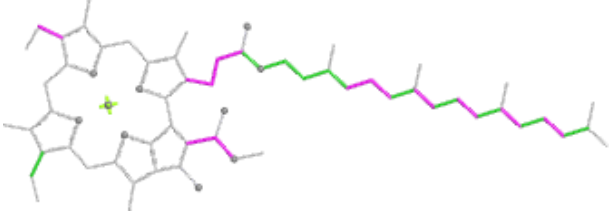
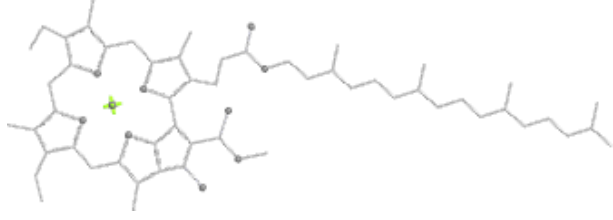
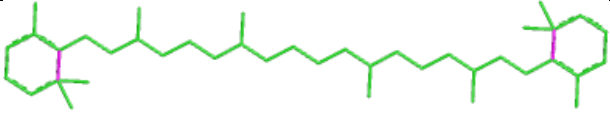
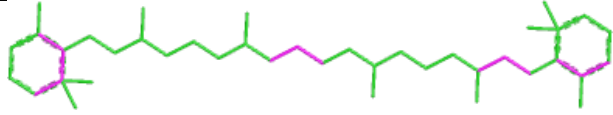
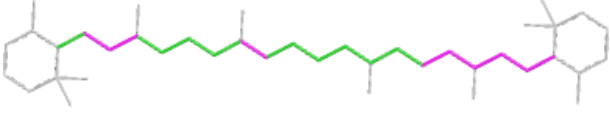
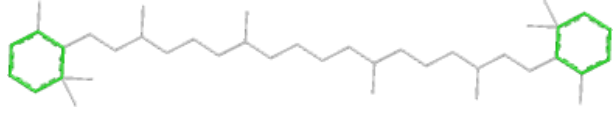
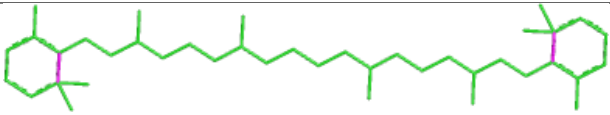
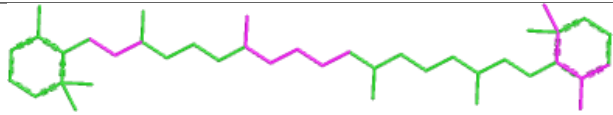
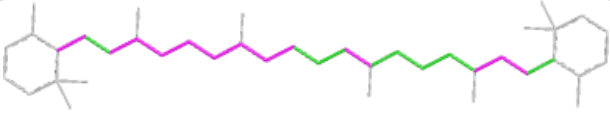
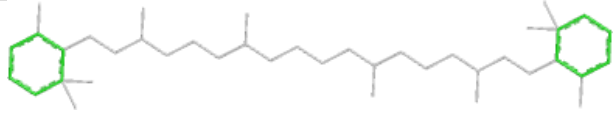


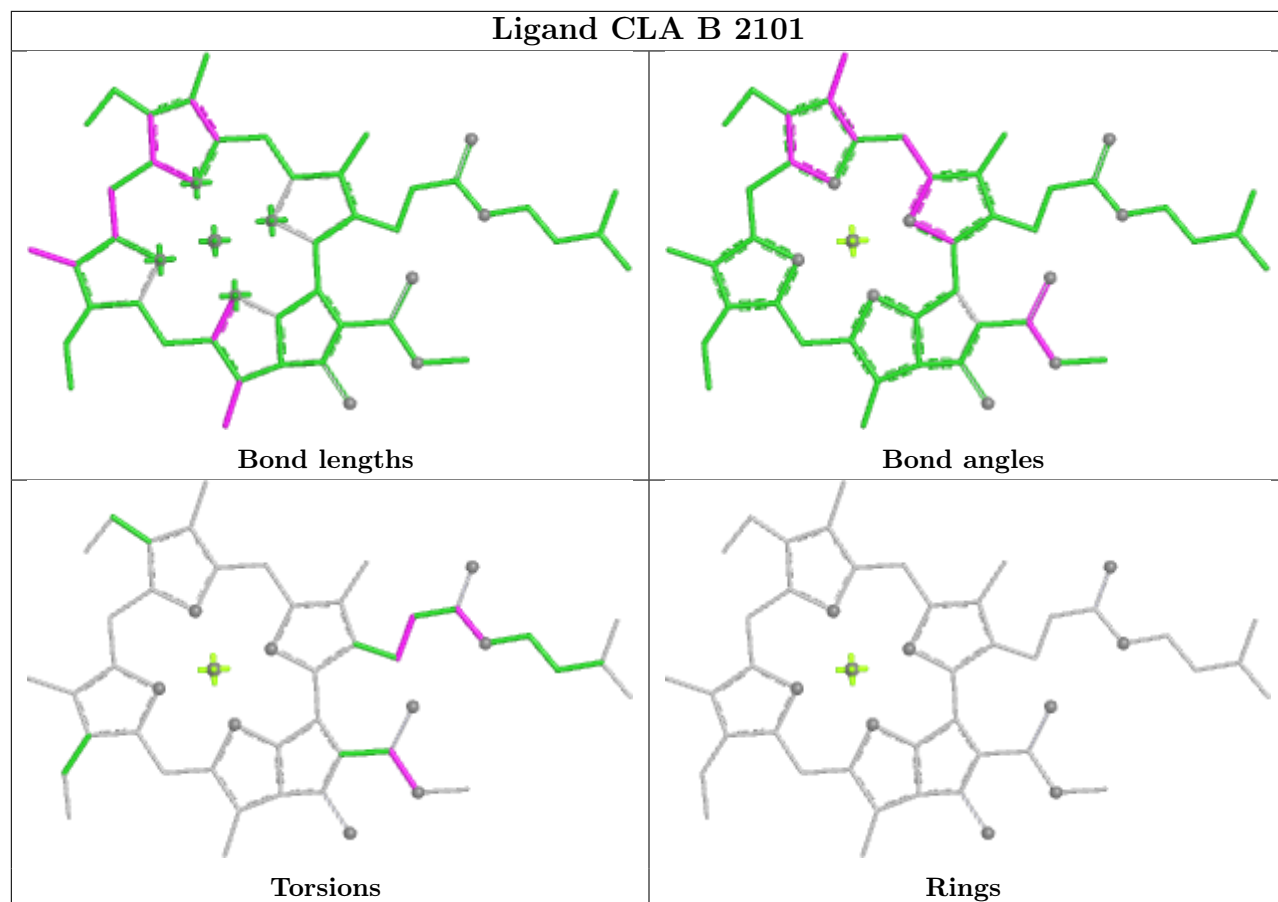
Torsions



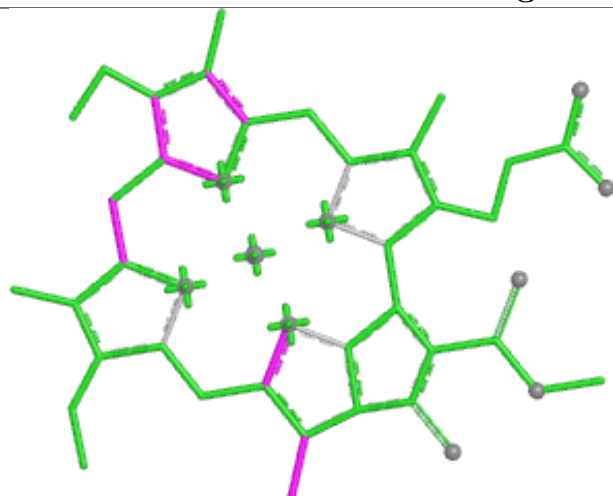
Rings



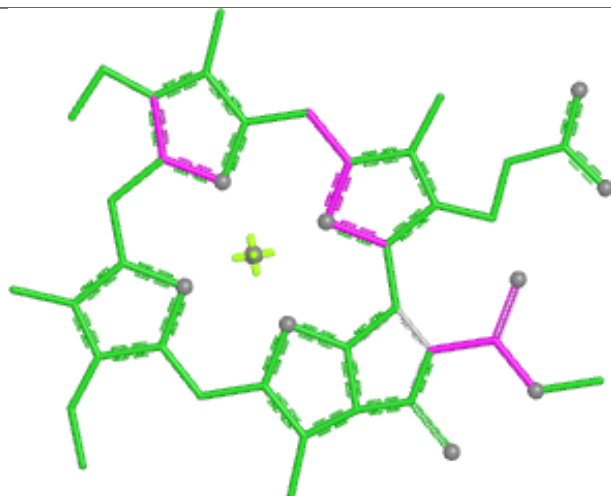
Ligand CLA b 2114	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR Q 202	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR a 843	
 Bond lengths	 Bond angles
 Torsions	 Rings



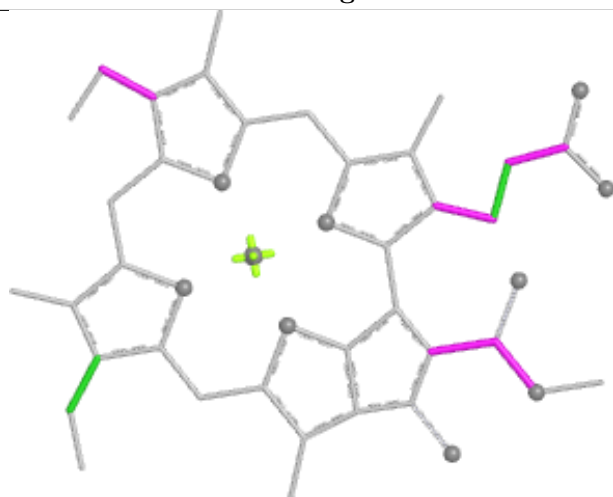
Ligand CLA S 103



Bond lengths



Bond angles

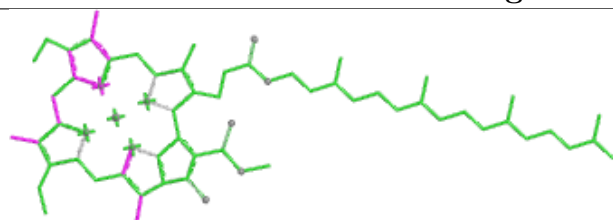


Torsions

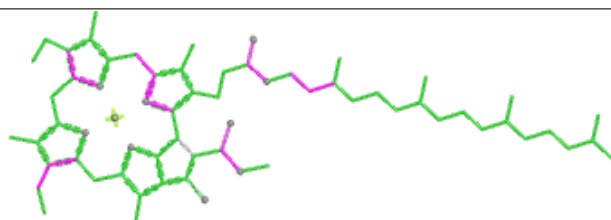


Rings

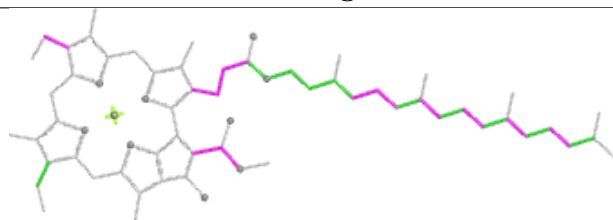
Ligand CLA B 2115



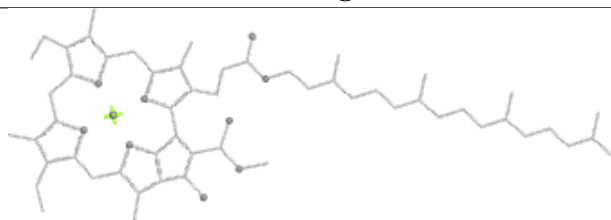
Bond lengths



Bond angles

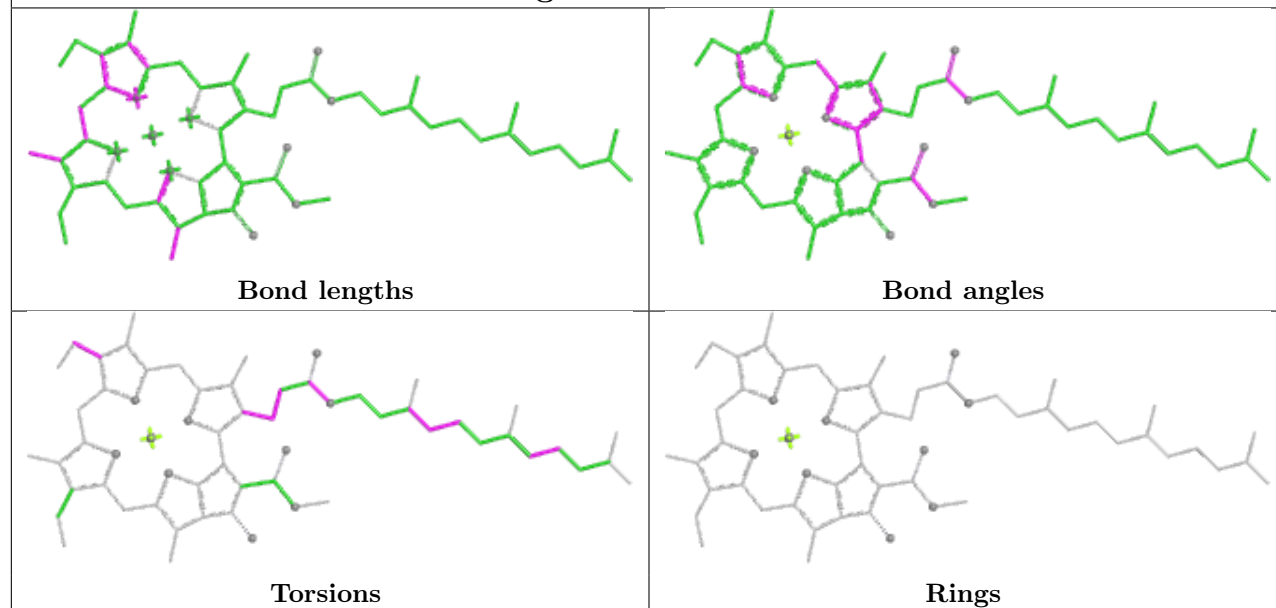


Torsions

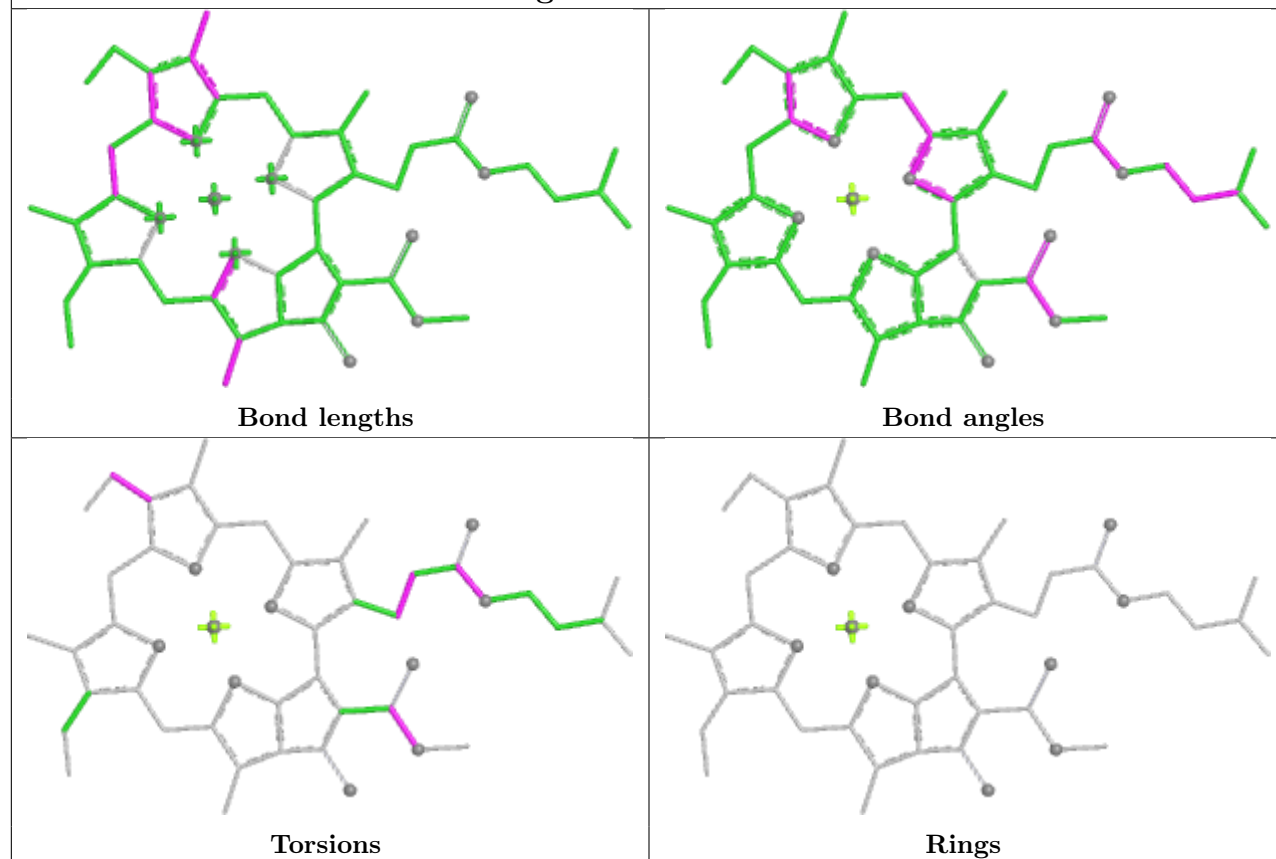


Rings

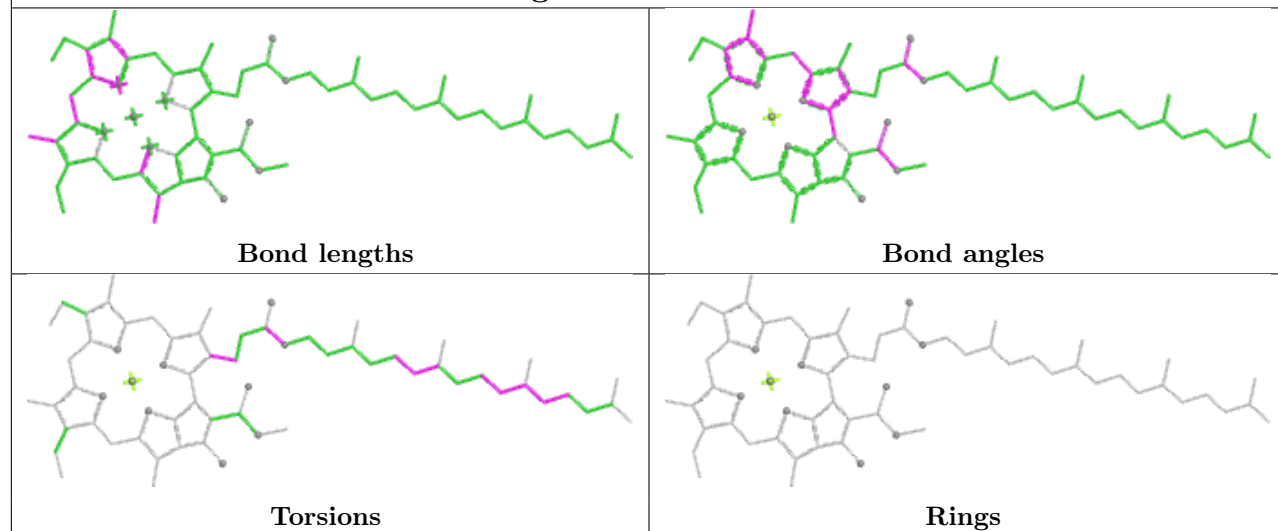
Ligand CLA a 823



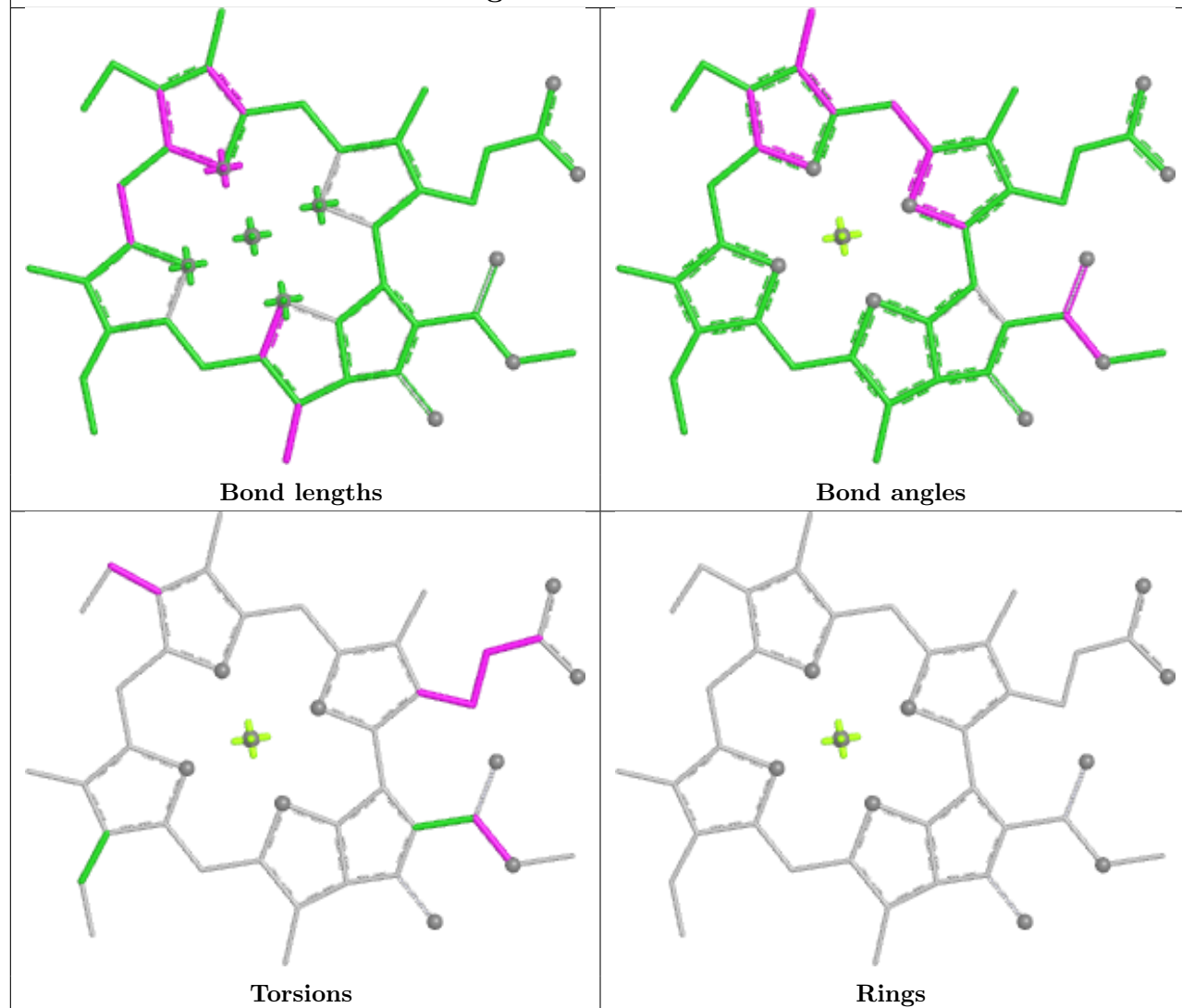
Ligand CLA a 806



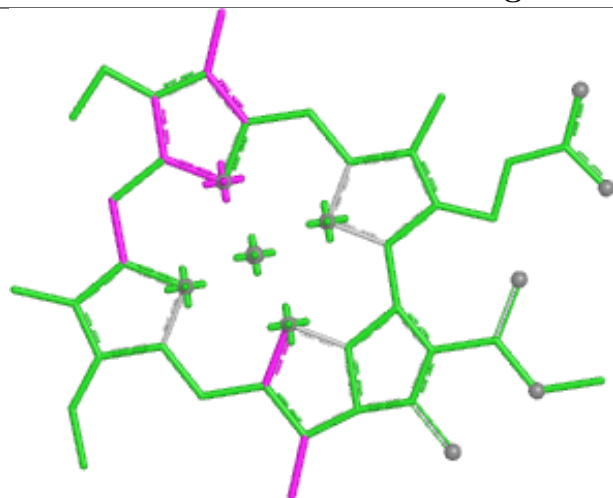
Ligand CLA U 203



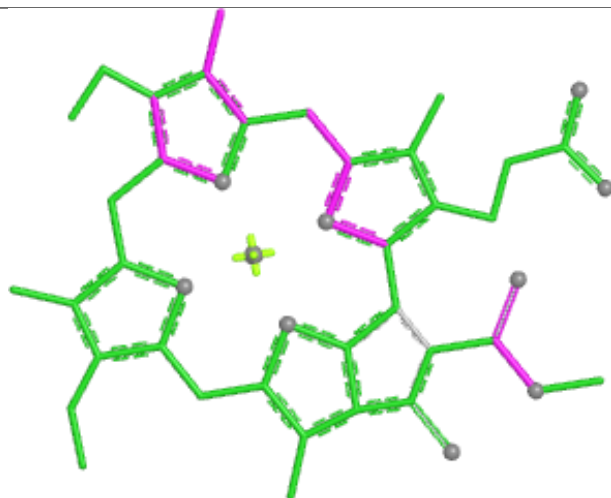
Ligand CLA b 2116



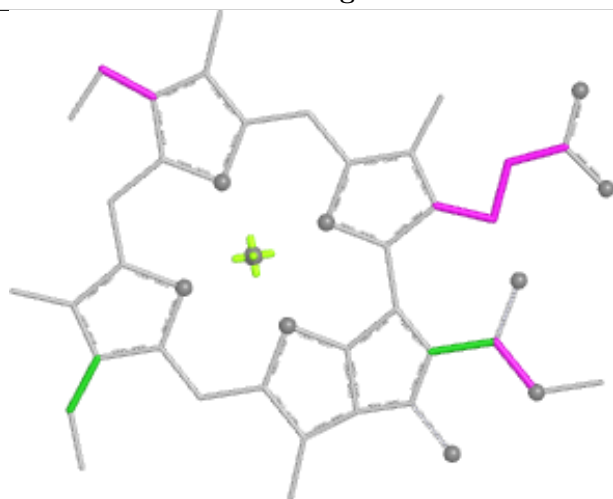
Ligand CLA H 2135



Bond lengths



Bond angles

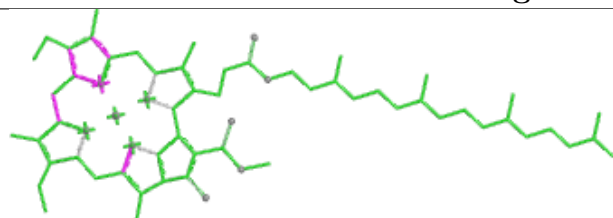


Torsions

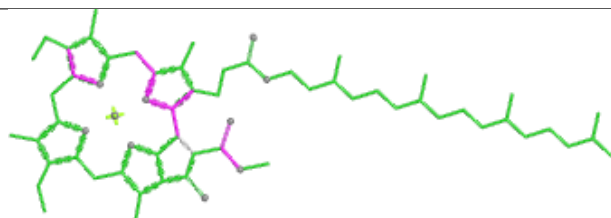


Rings

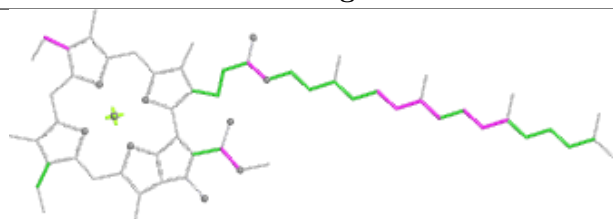
Ligand CLA G 813



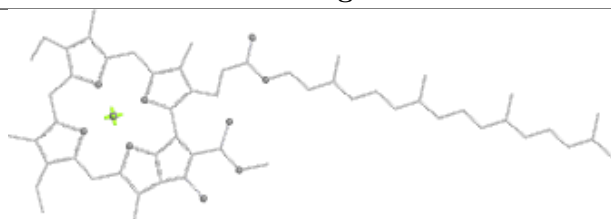
Bond lengths



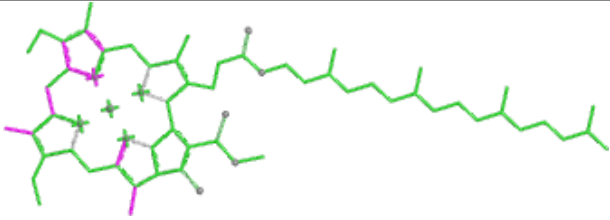
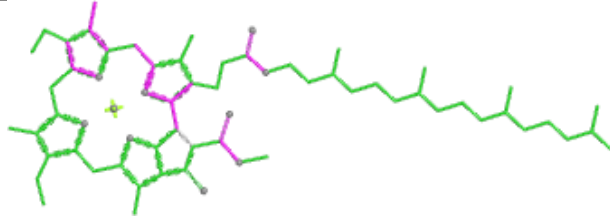
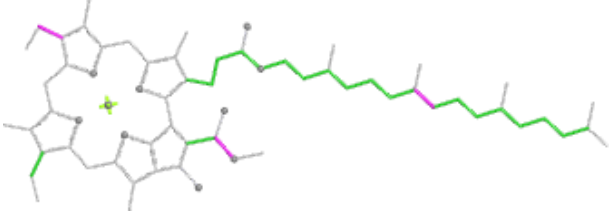
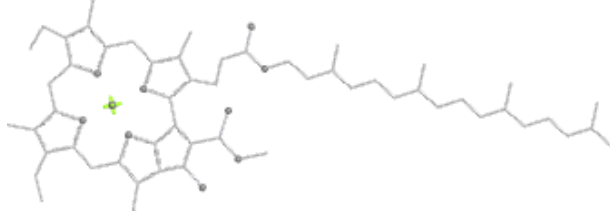
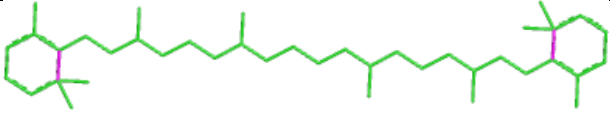
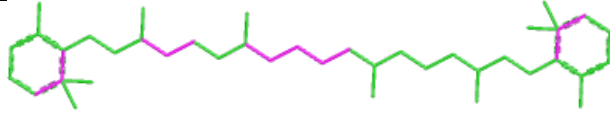
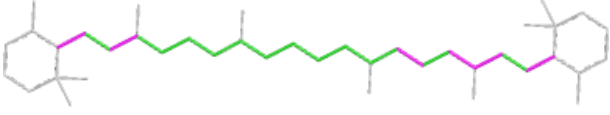
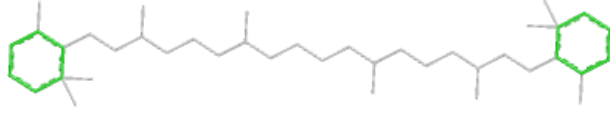
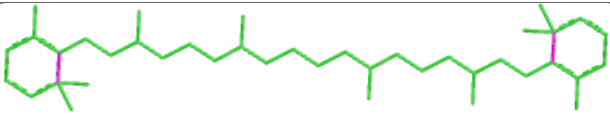
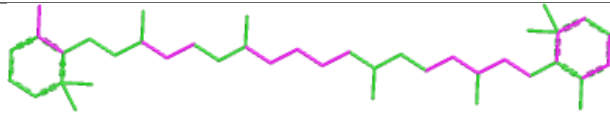
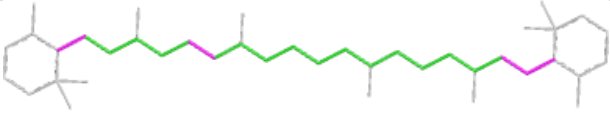
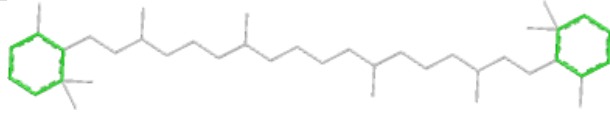
Bond angles



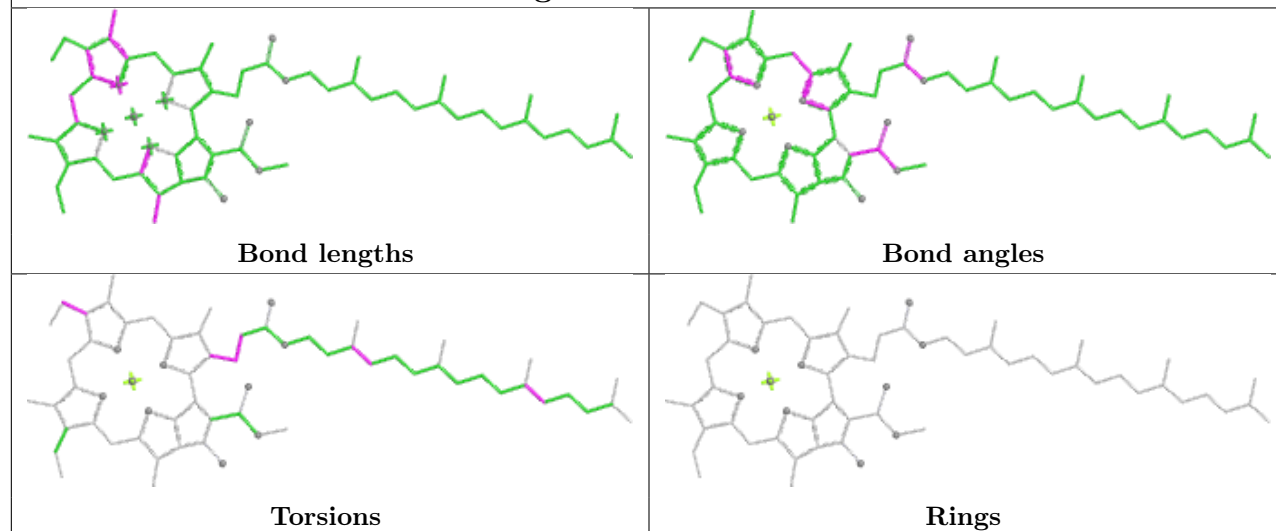
Torsions



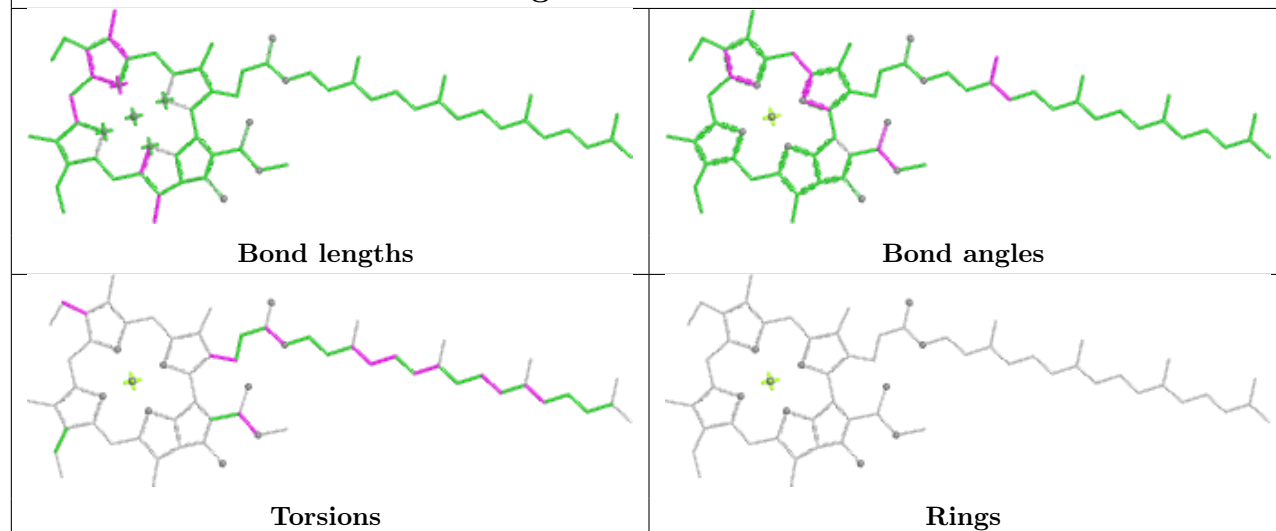
Rings

Ligand CLA G 838	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR L 206	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR U 207	
 Bond lengths	 Bond angles
 Torsions	 Rings

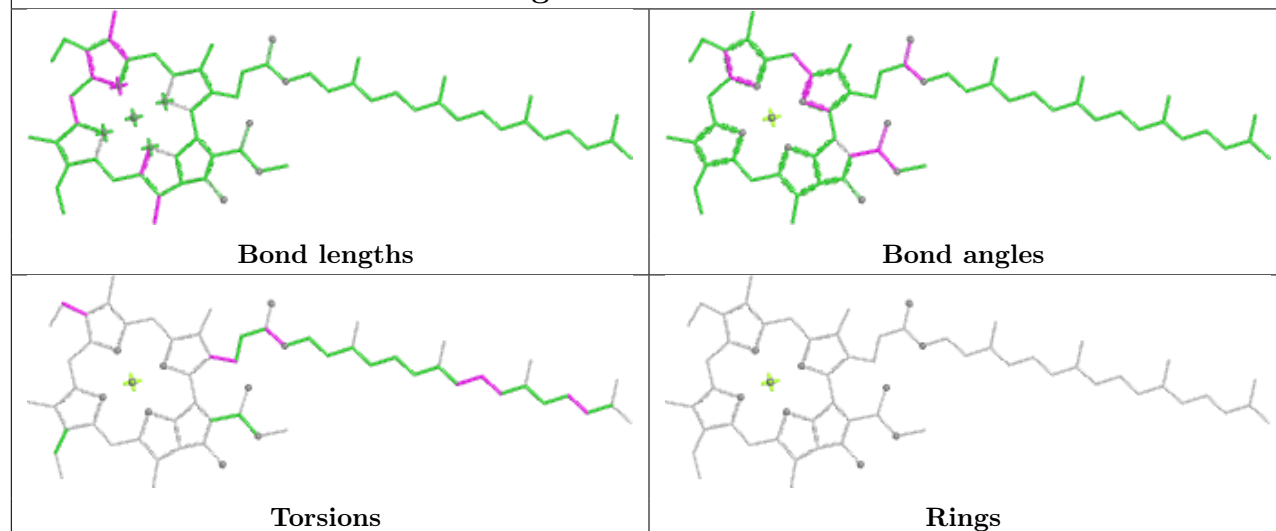
Ligand CLA L 204

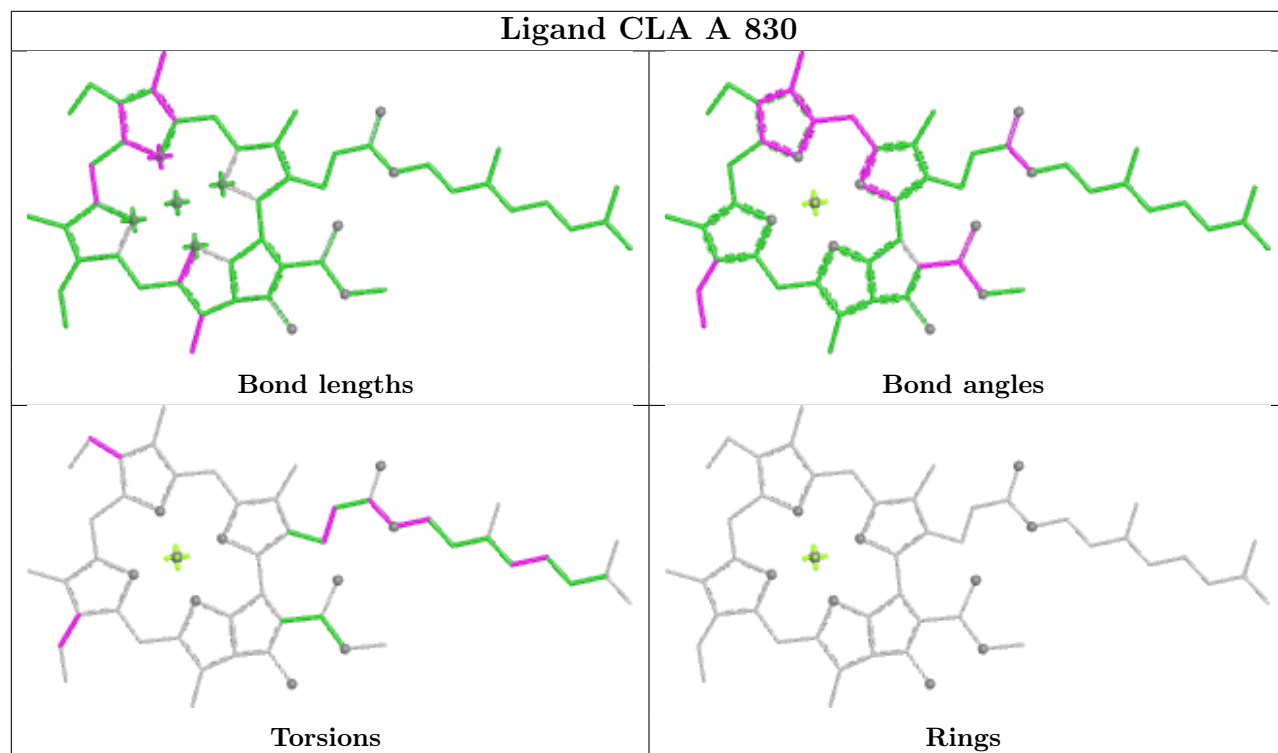


Ligand CLA A 833

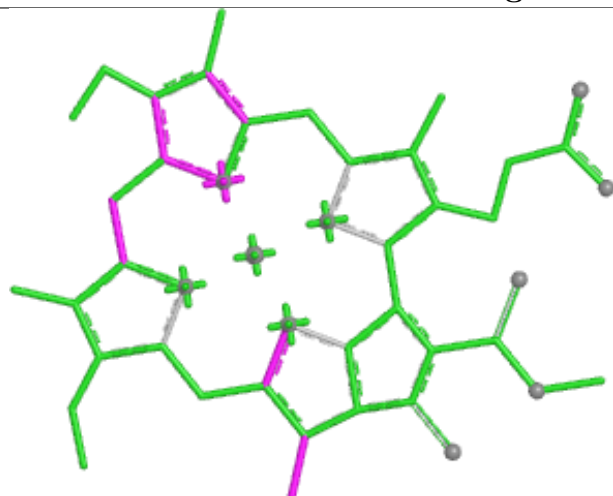


Ligand CLA A 802

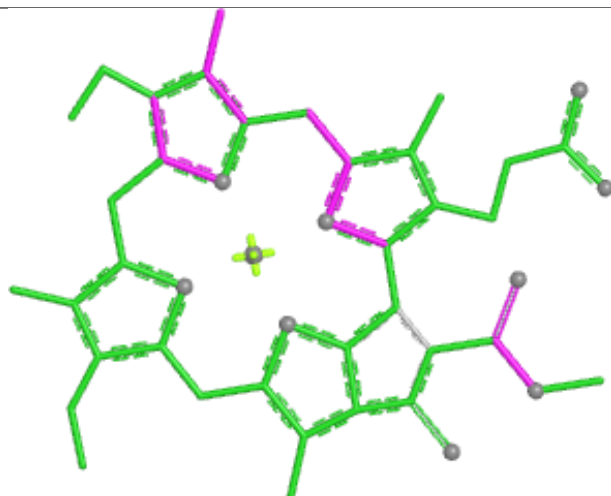




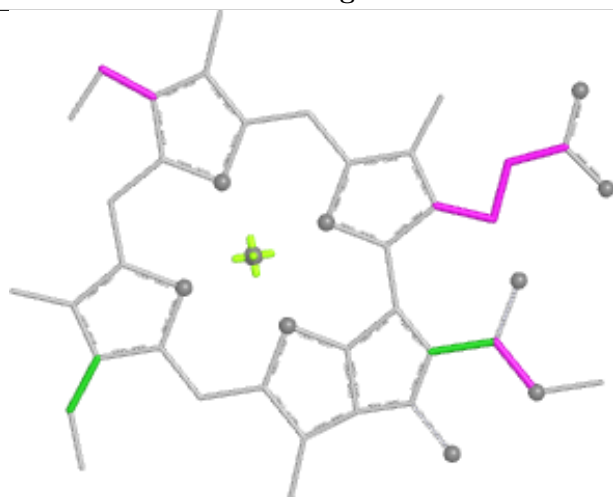
Ligand CLA B 2117



Bond lengths



Bond angles

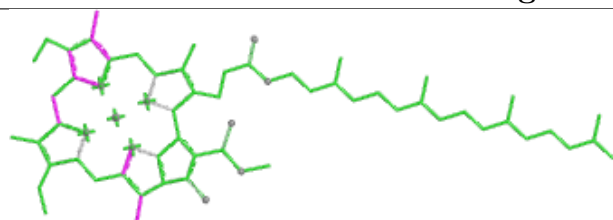


Torsions

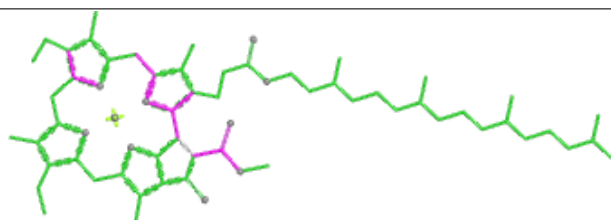


Rings

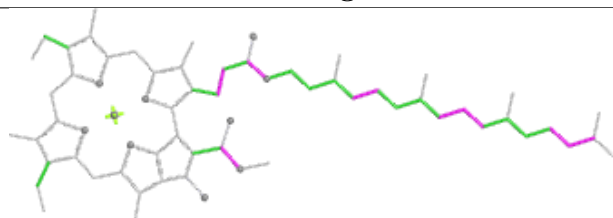
Ligand CLA a 837



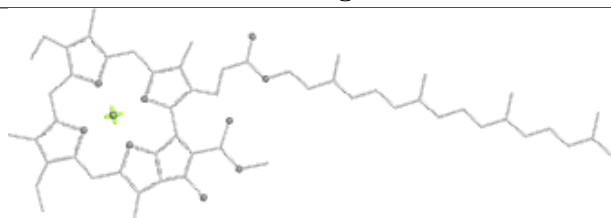
Bond lengths



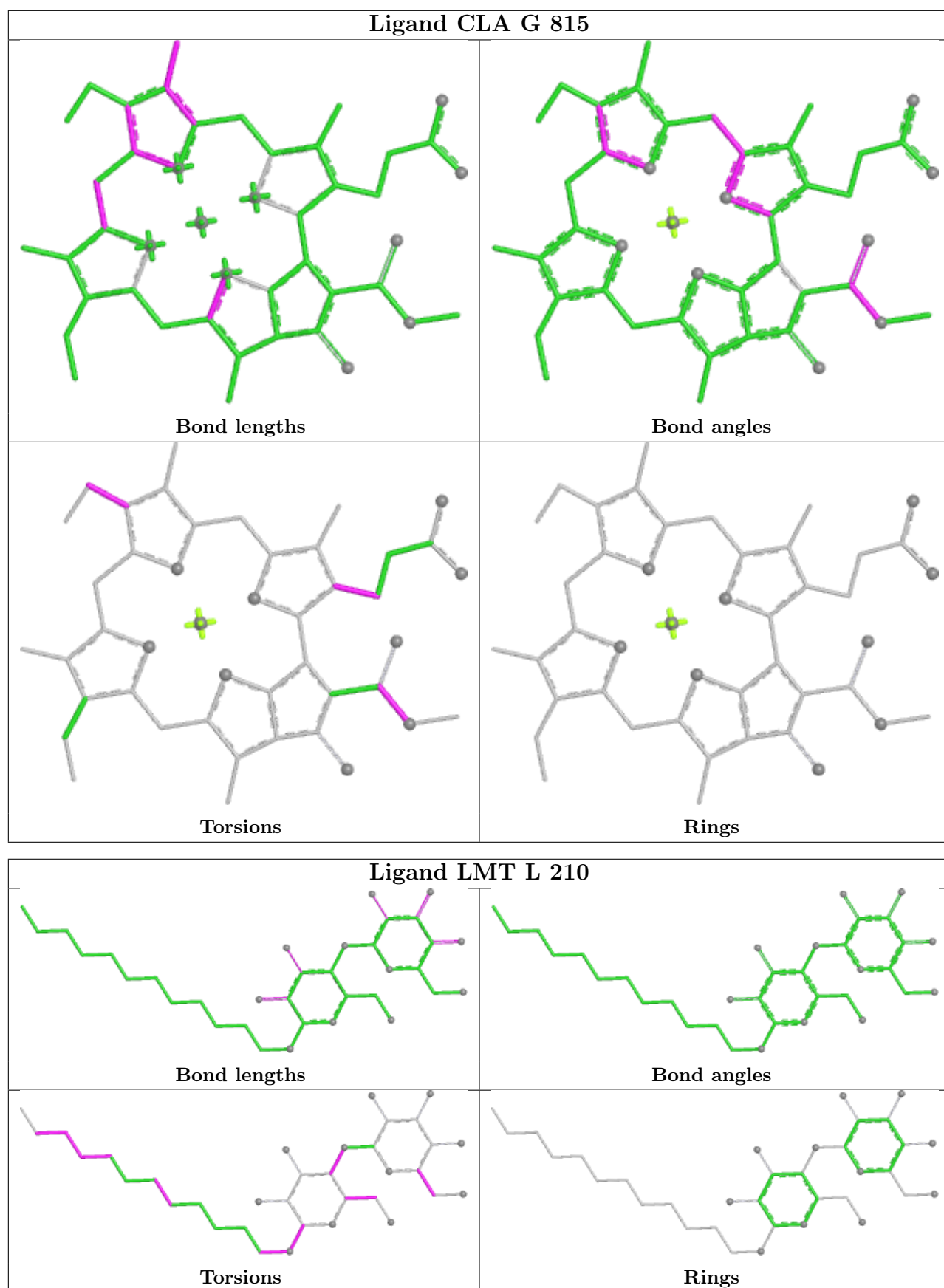
Bond angles

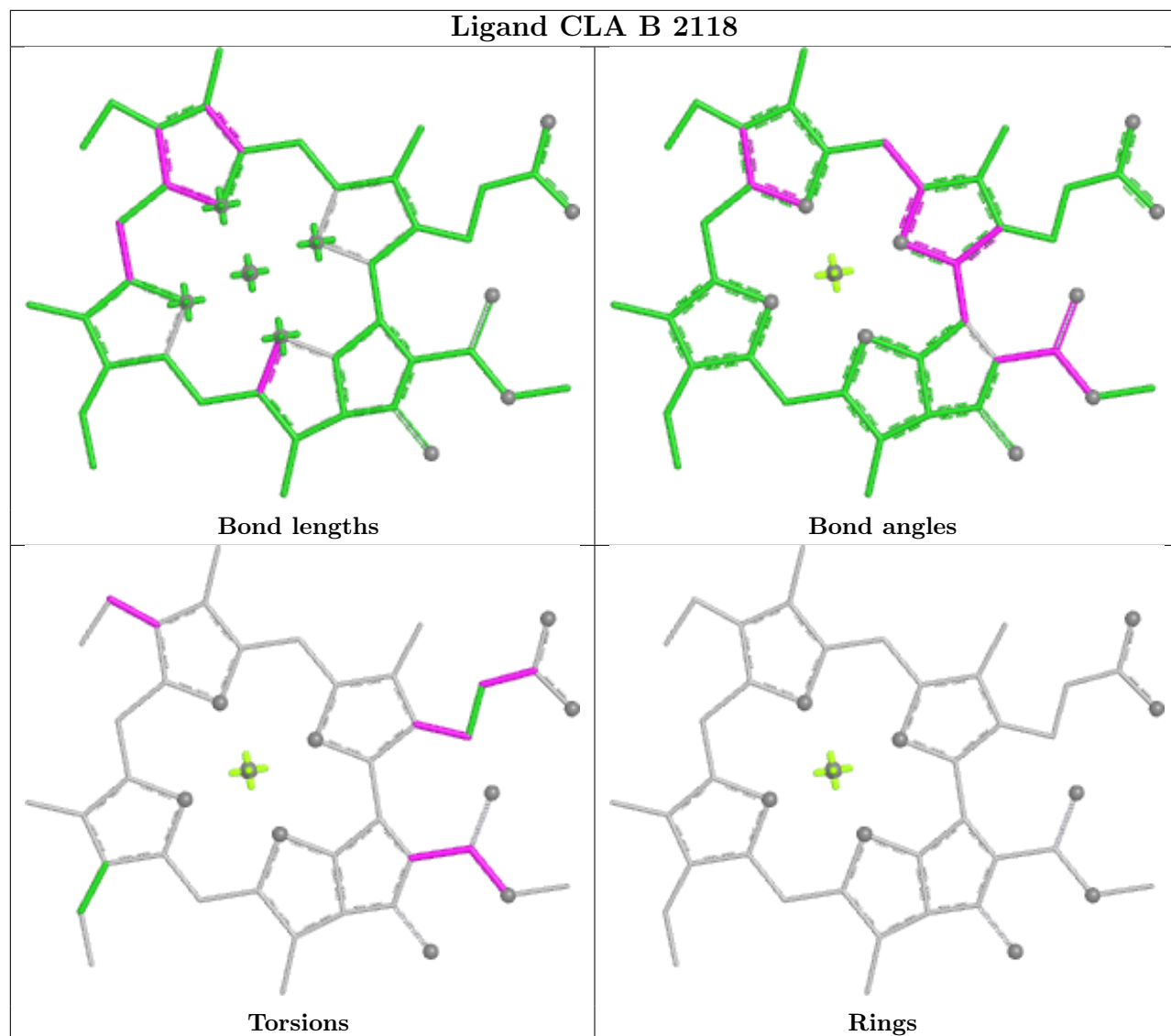


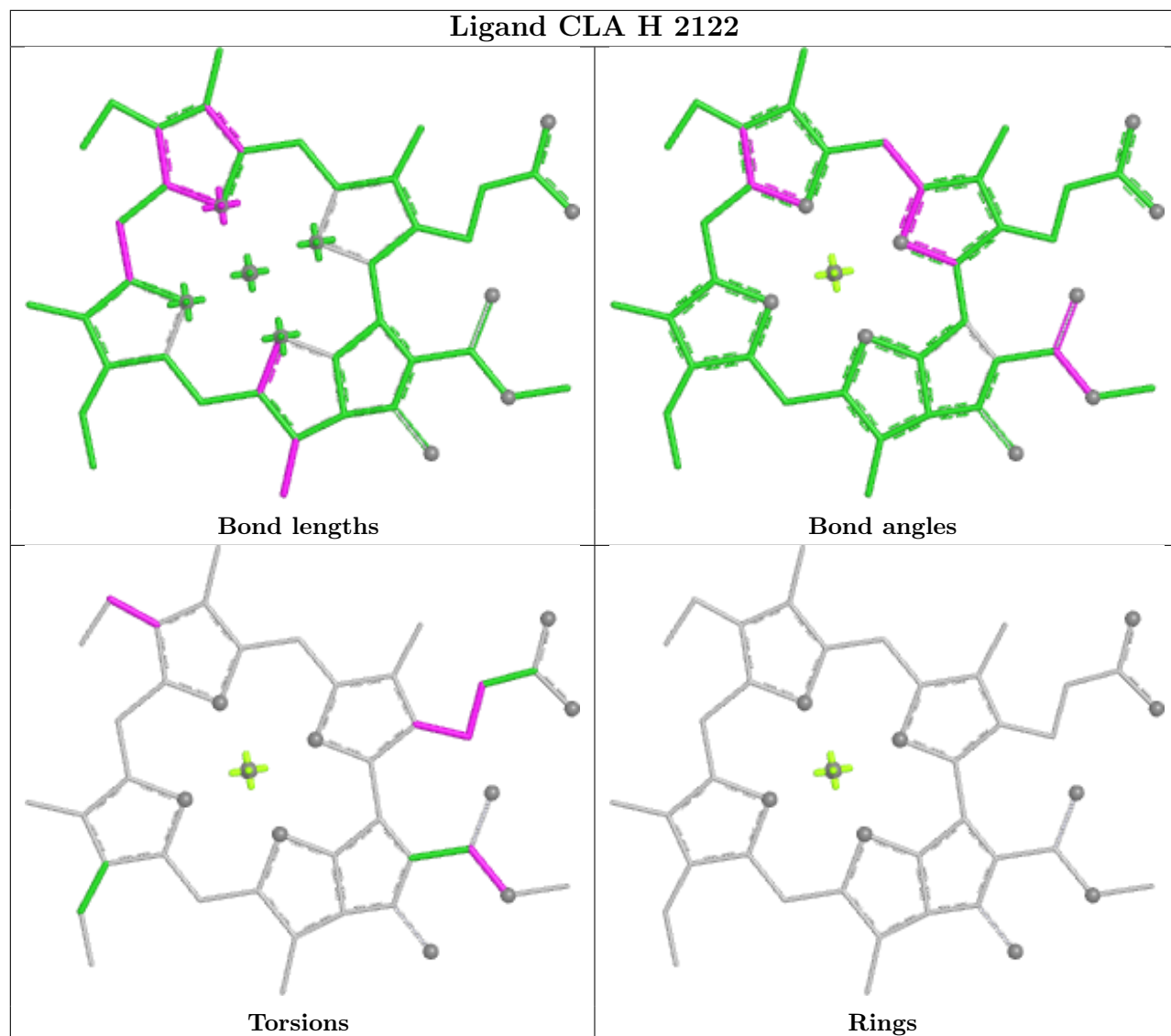
Torsions

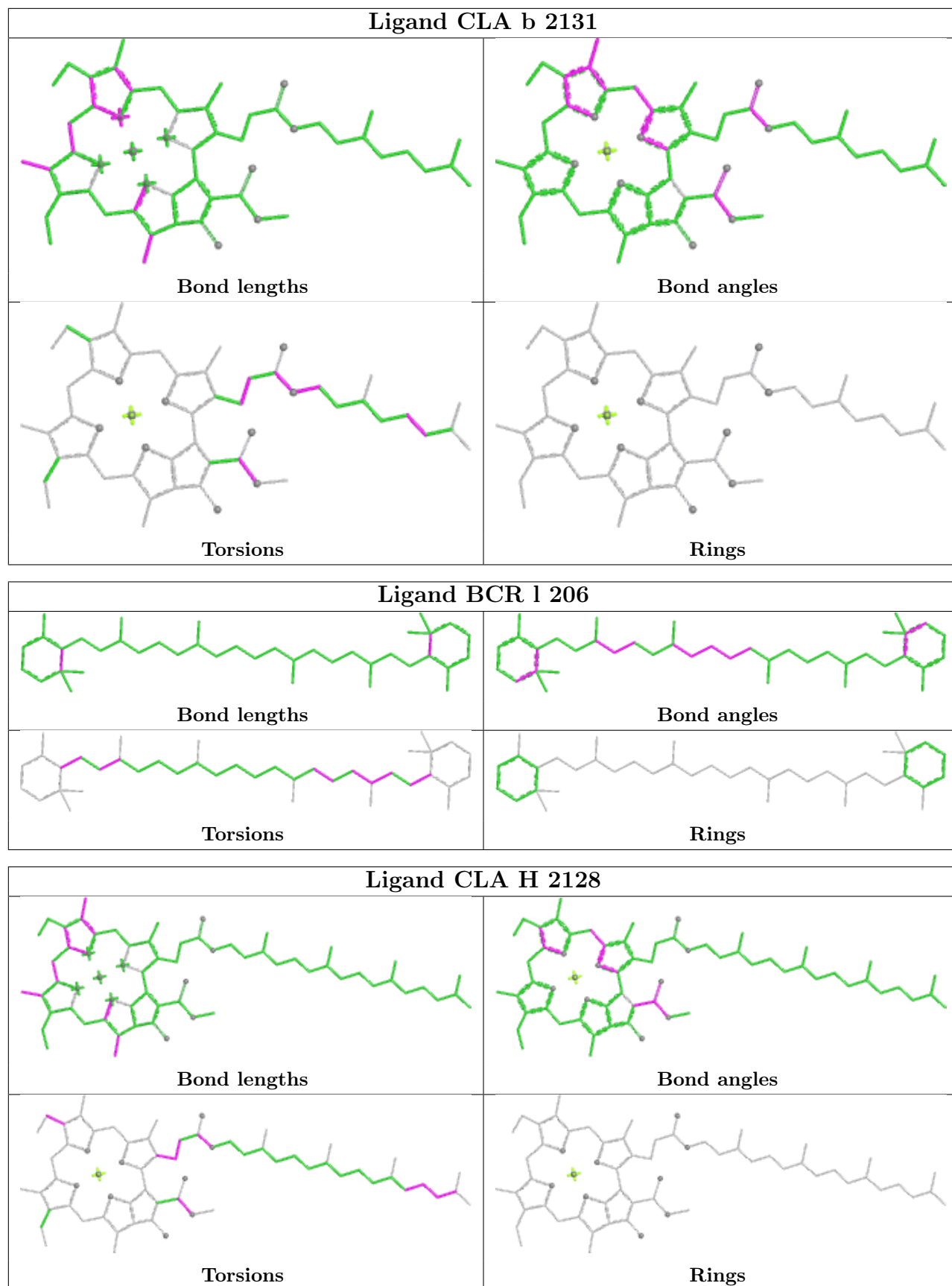


Rings

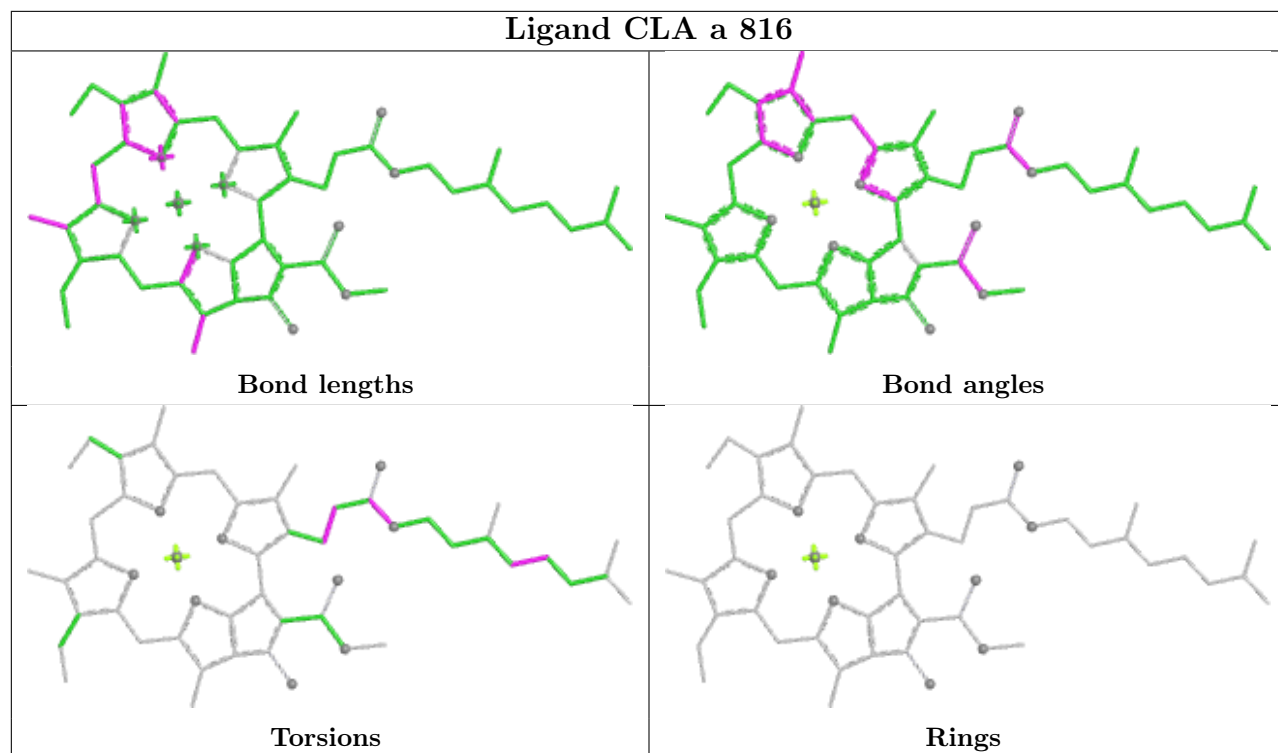




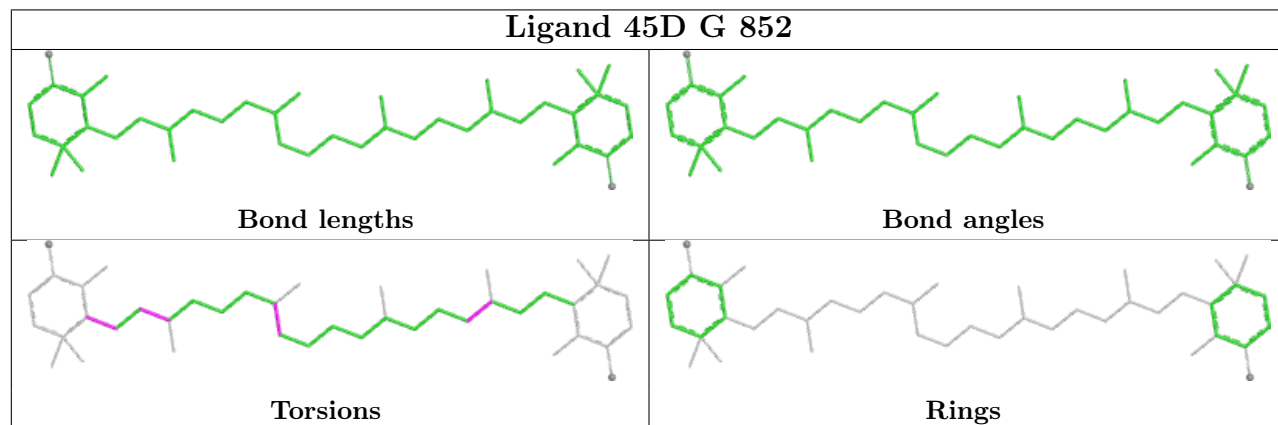




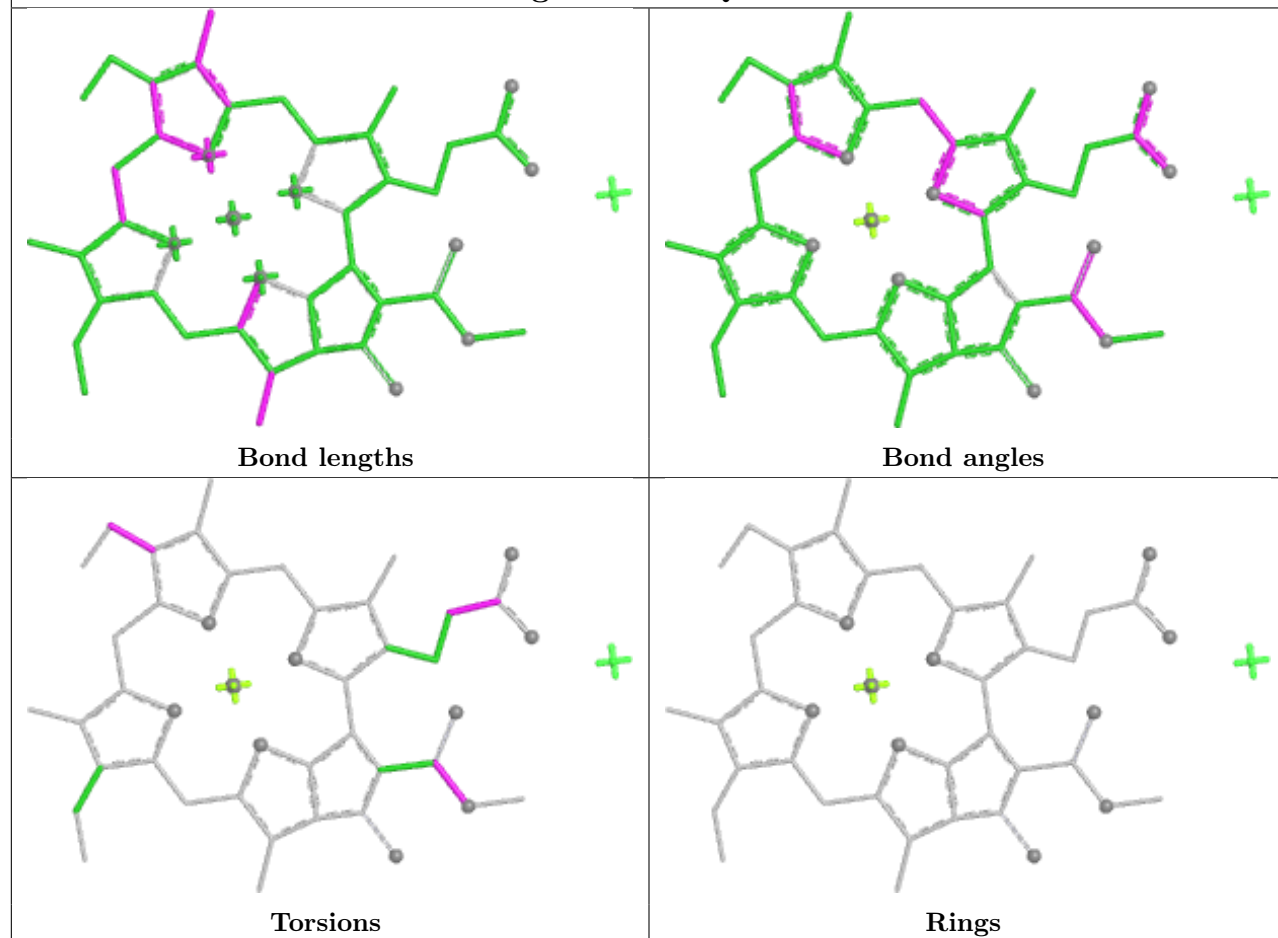
Ligand CLA a 816



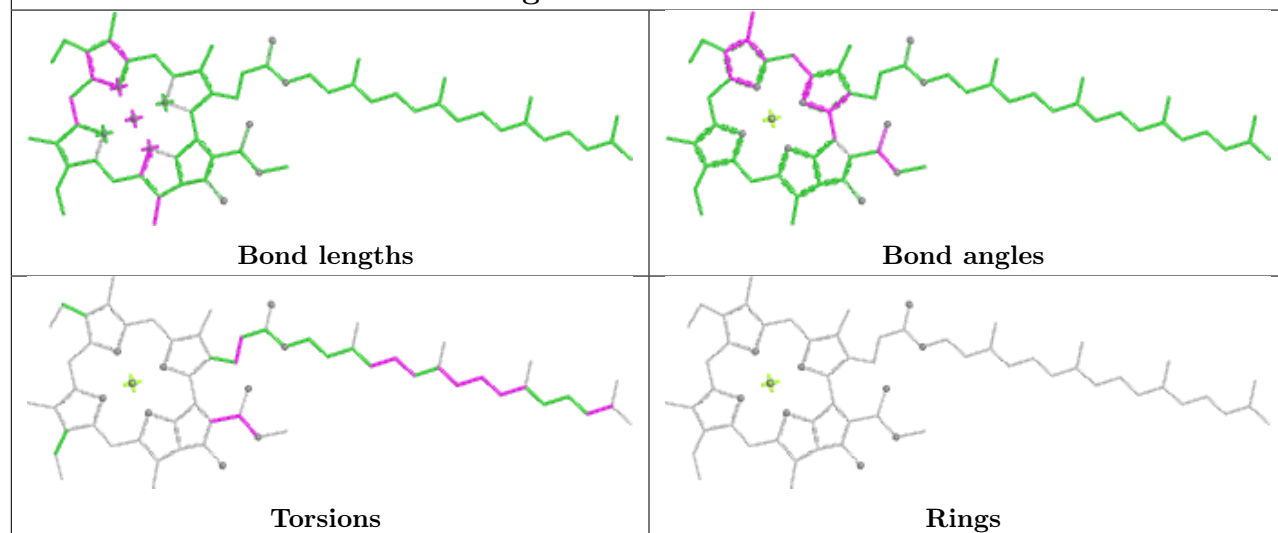
Ligand 45D G 852

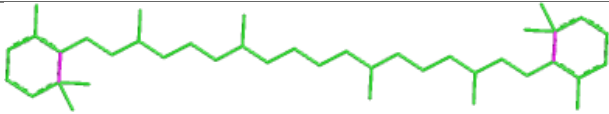
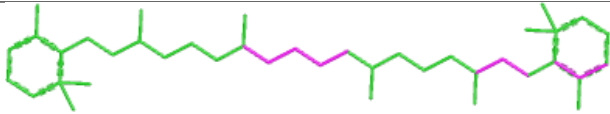
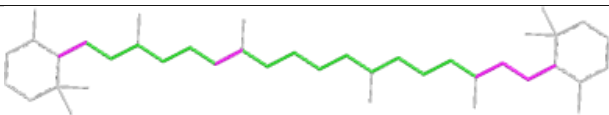
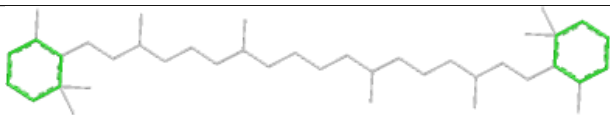


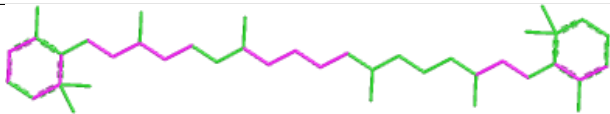
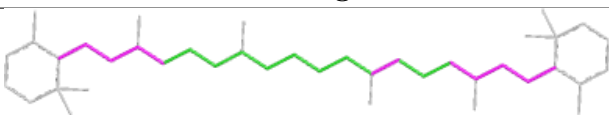
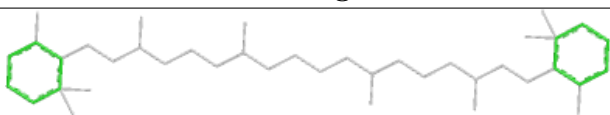
Ligand CLA Q 203

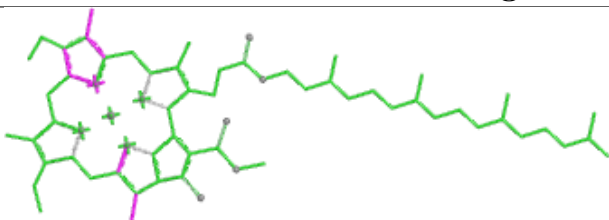
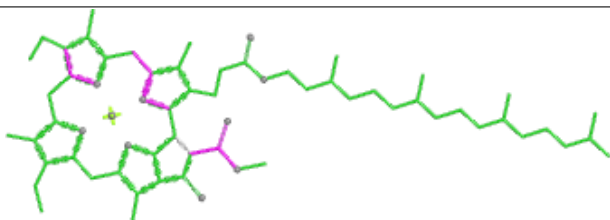
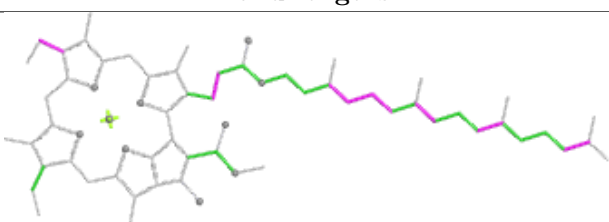
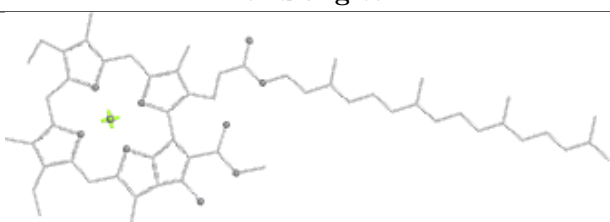


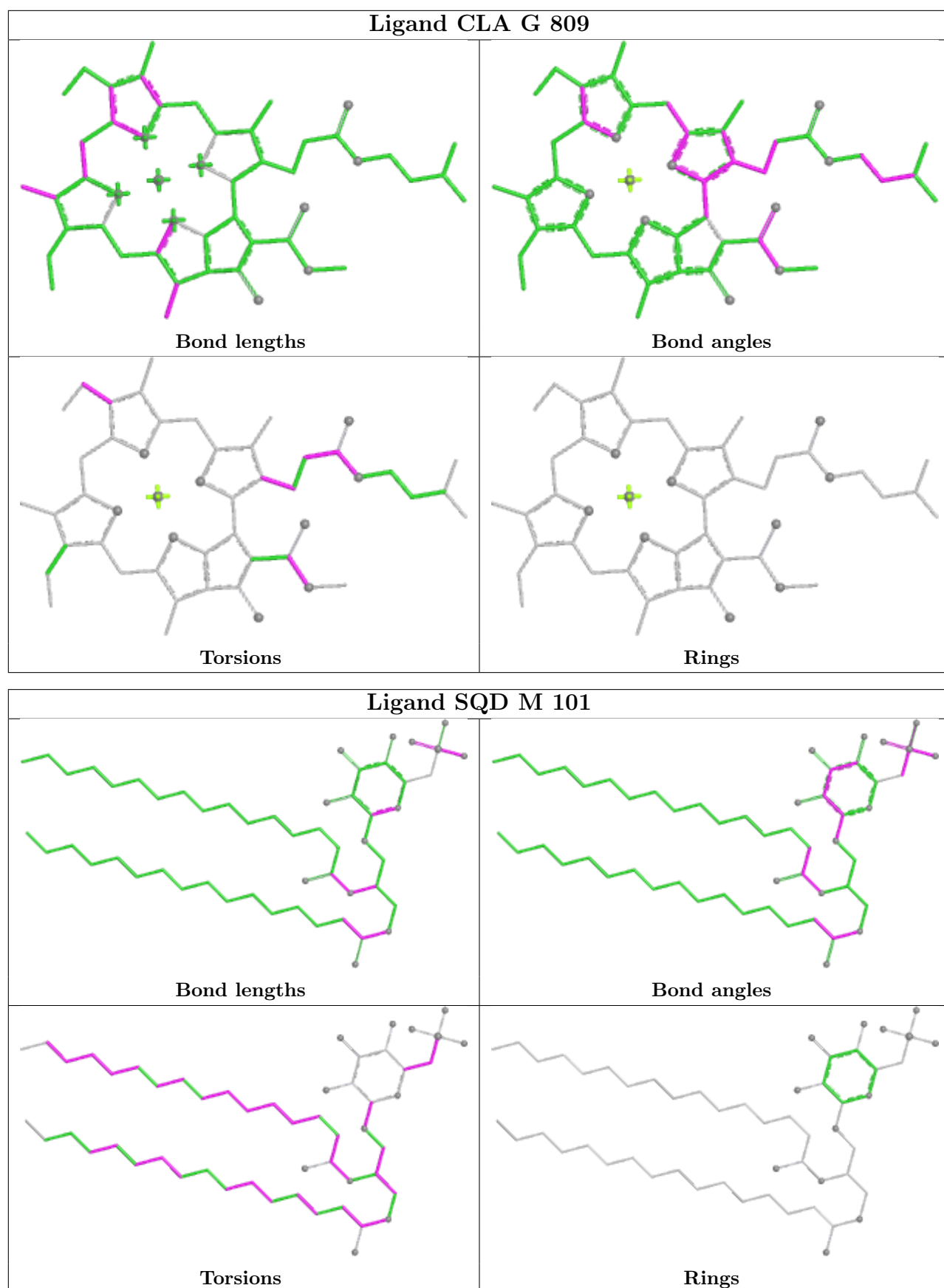
Ligand CLA H 2101

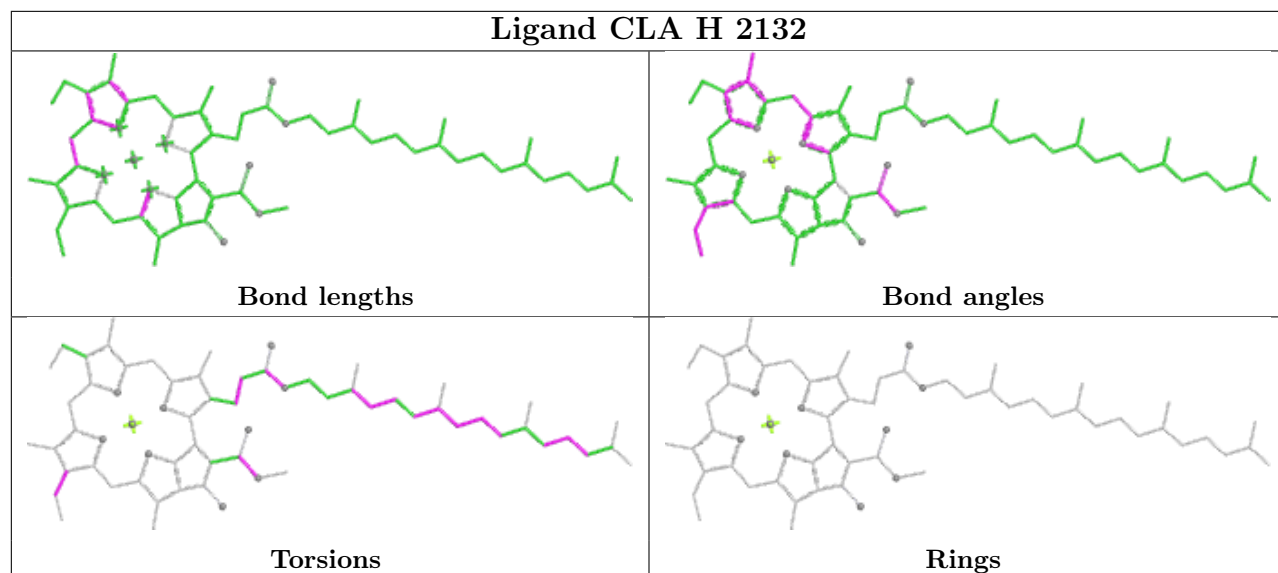
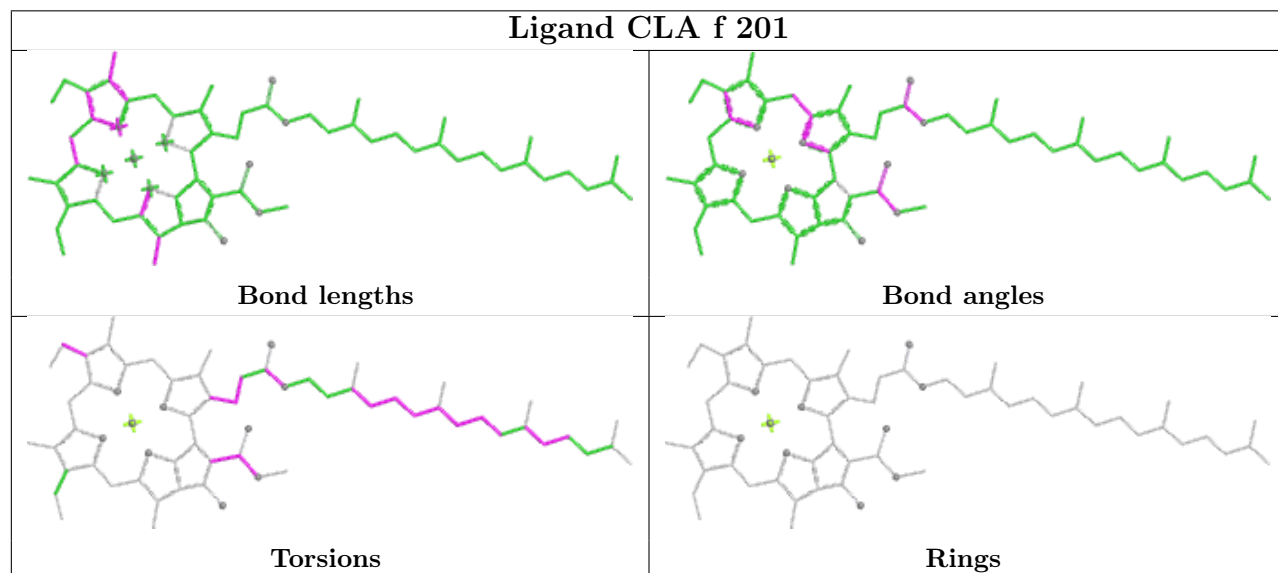
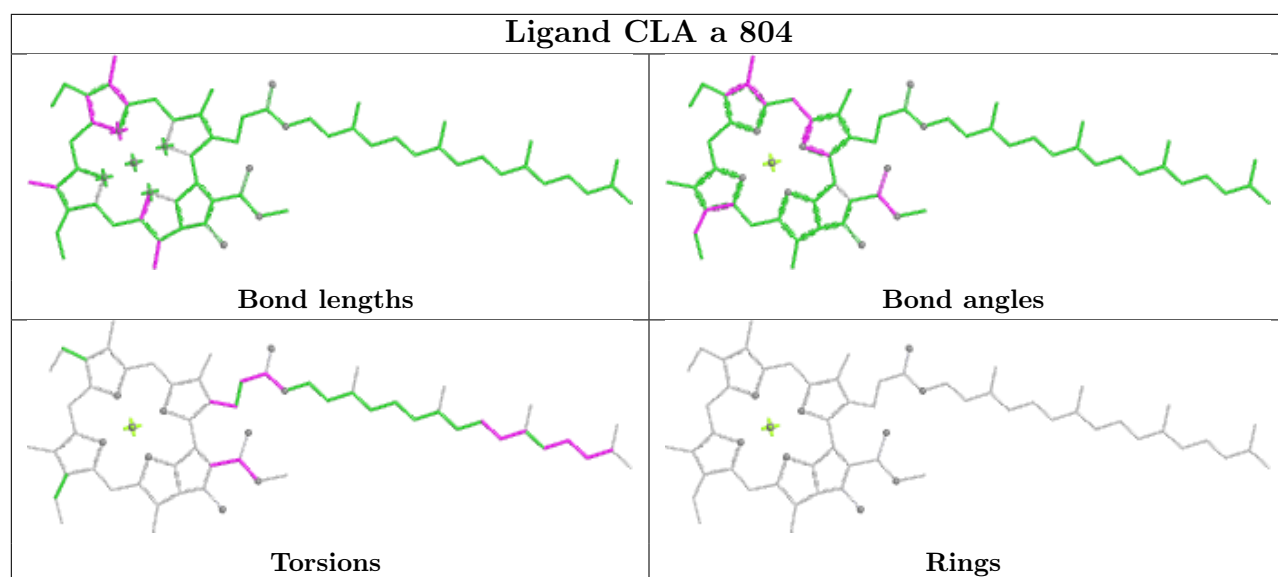


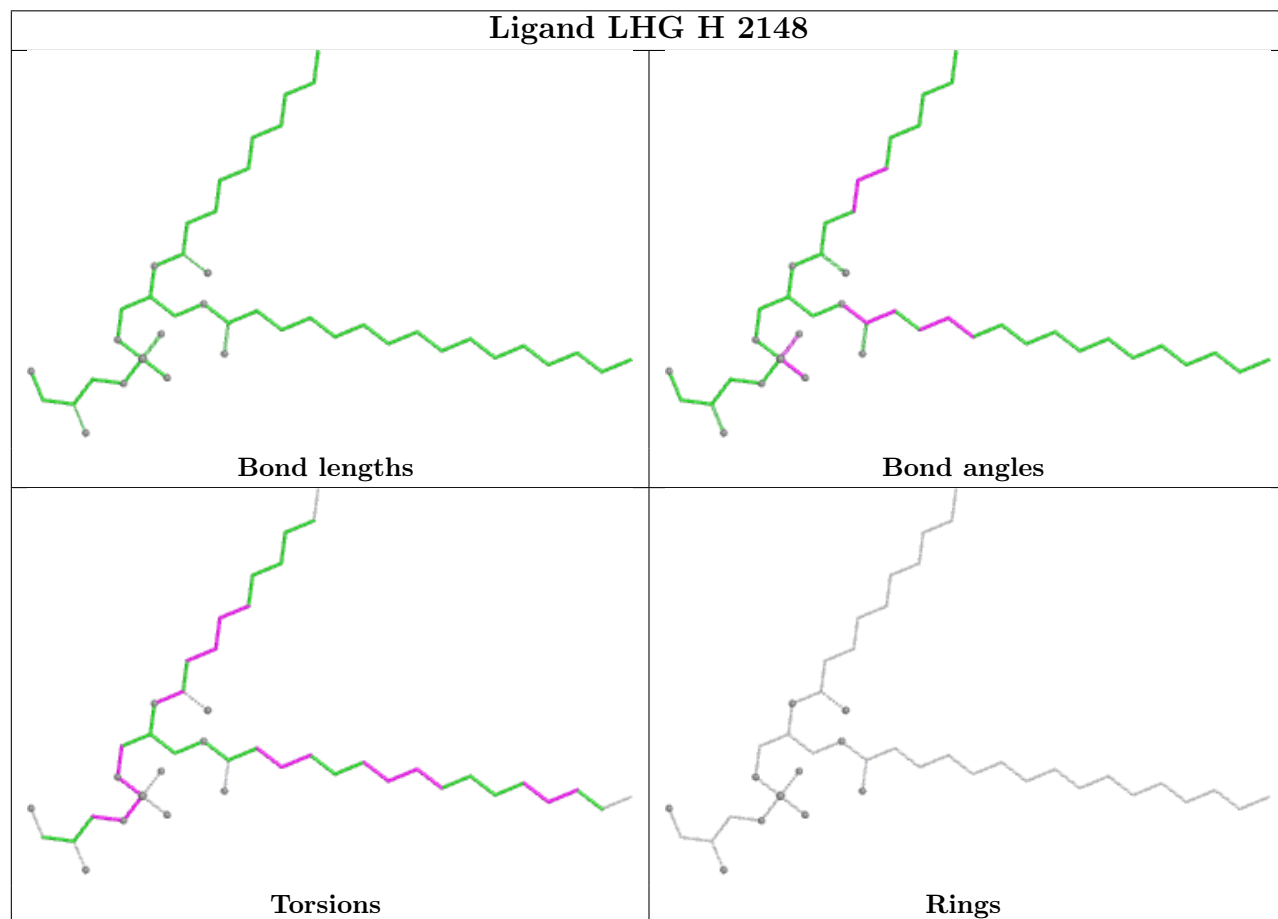
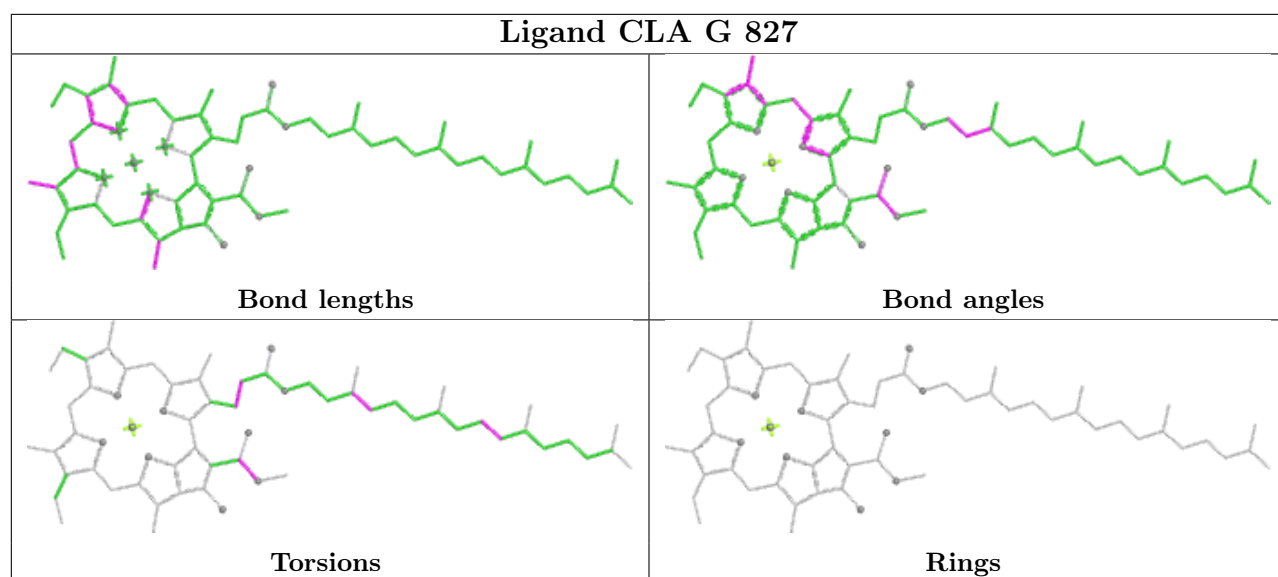
Ligand BCR A 845	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR J 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

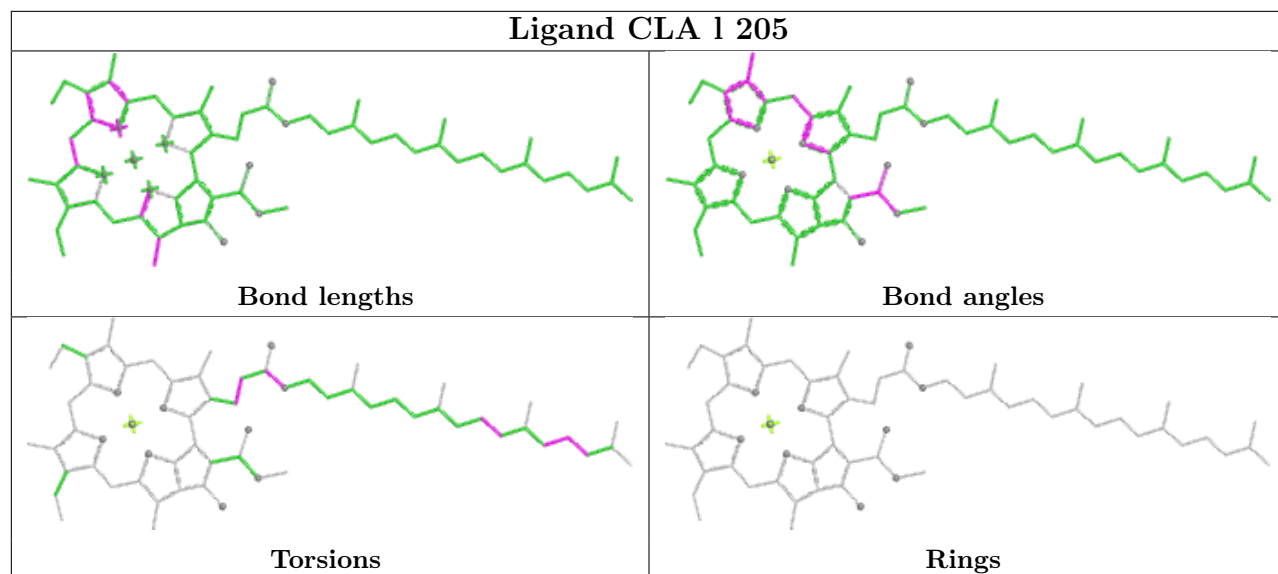
Ligand CLA B 2109	
	
Bond lengths	Bond angles
	
Torsions	Rings



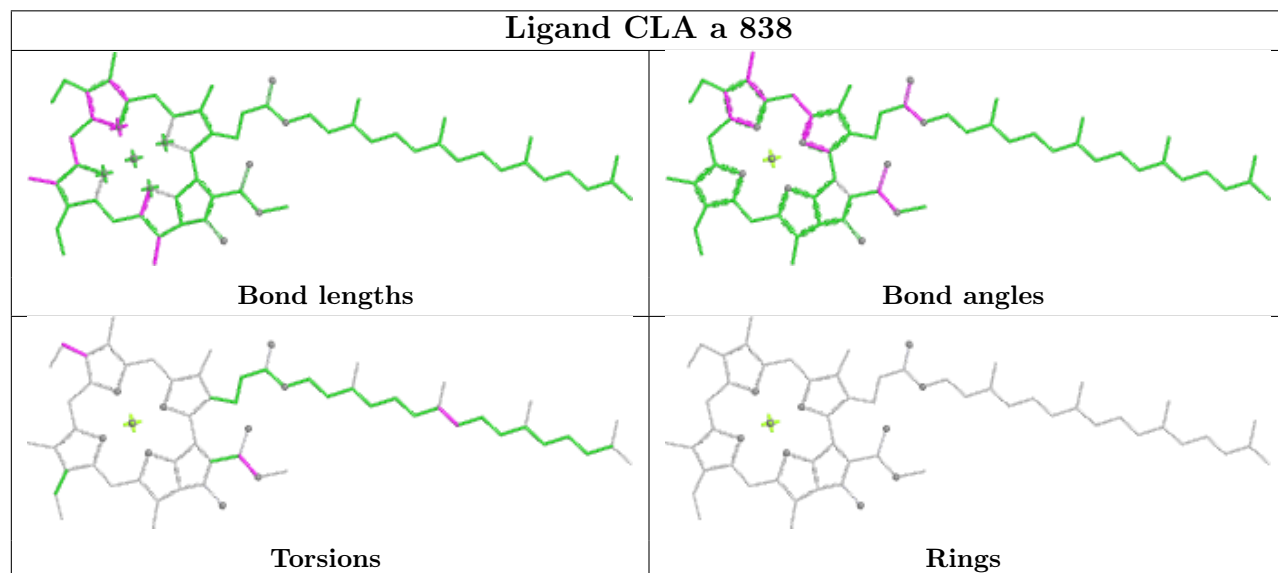




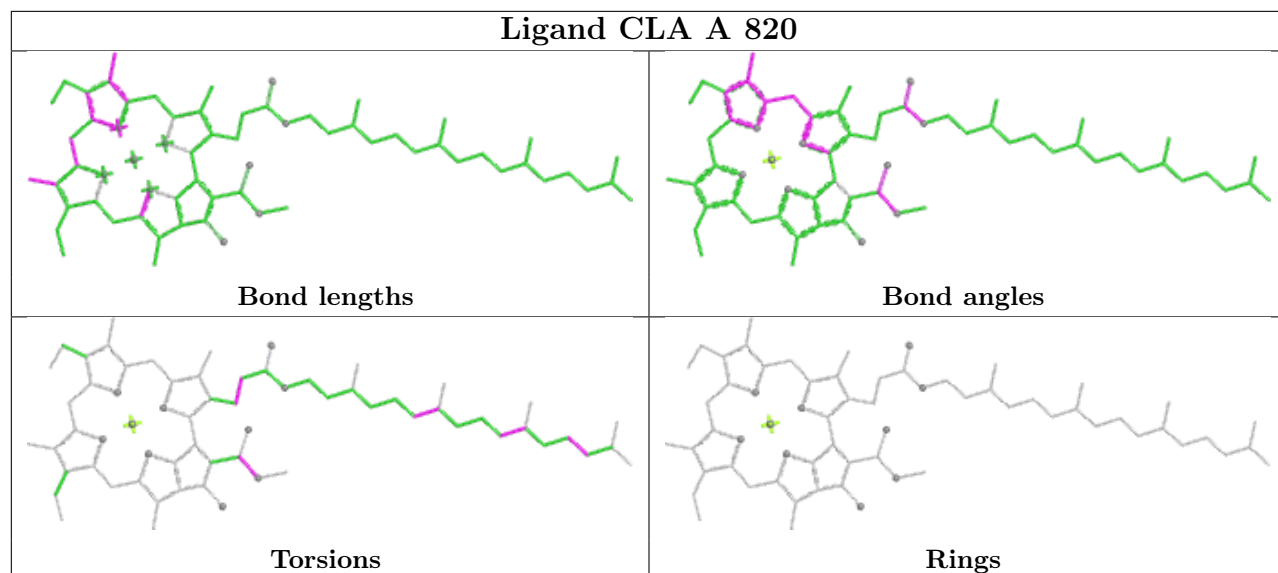
Ligand CLA 1 205

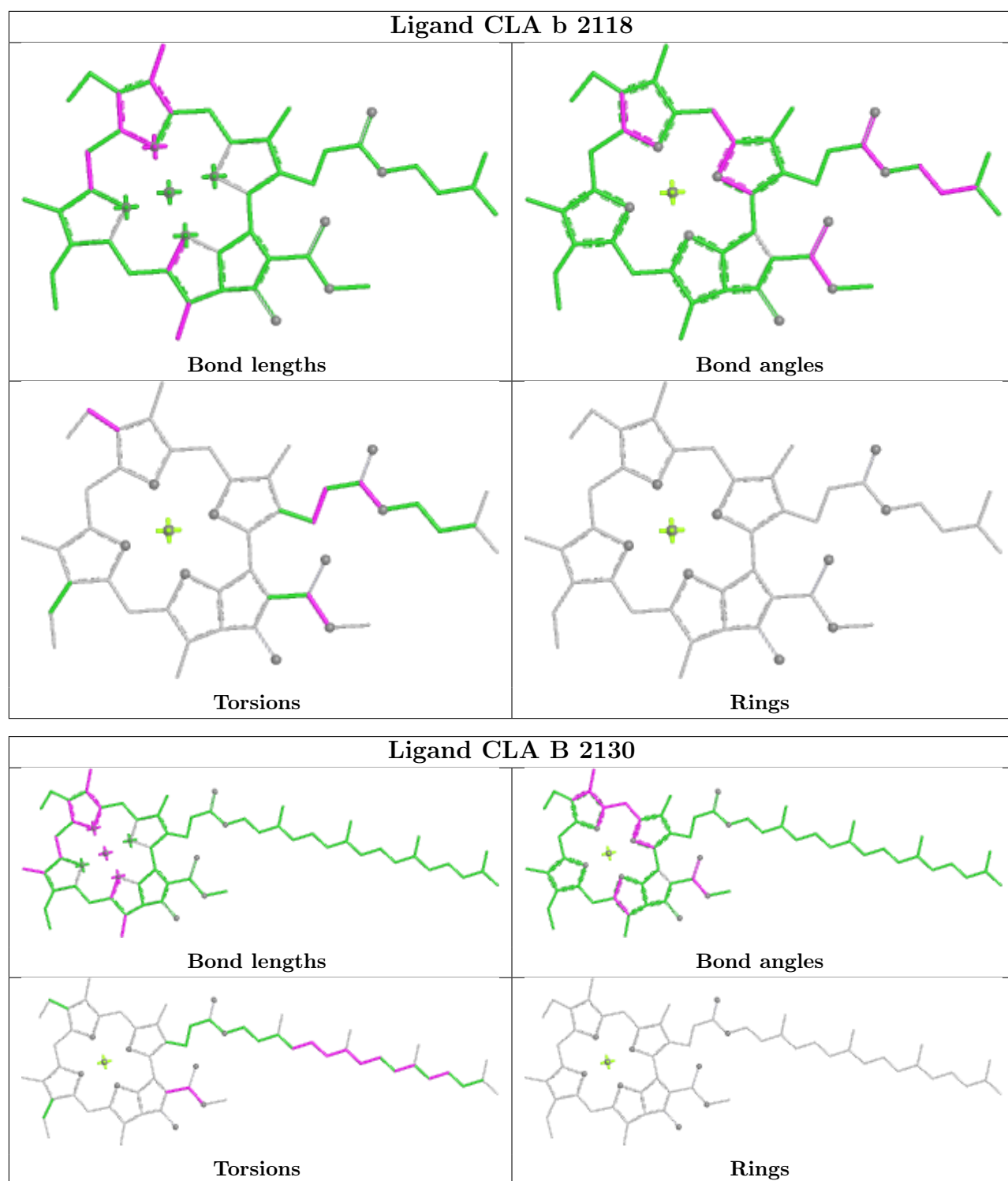


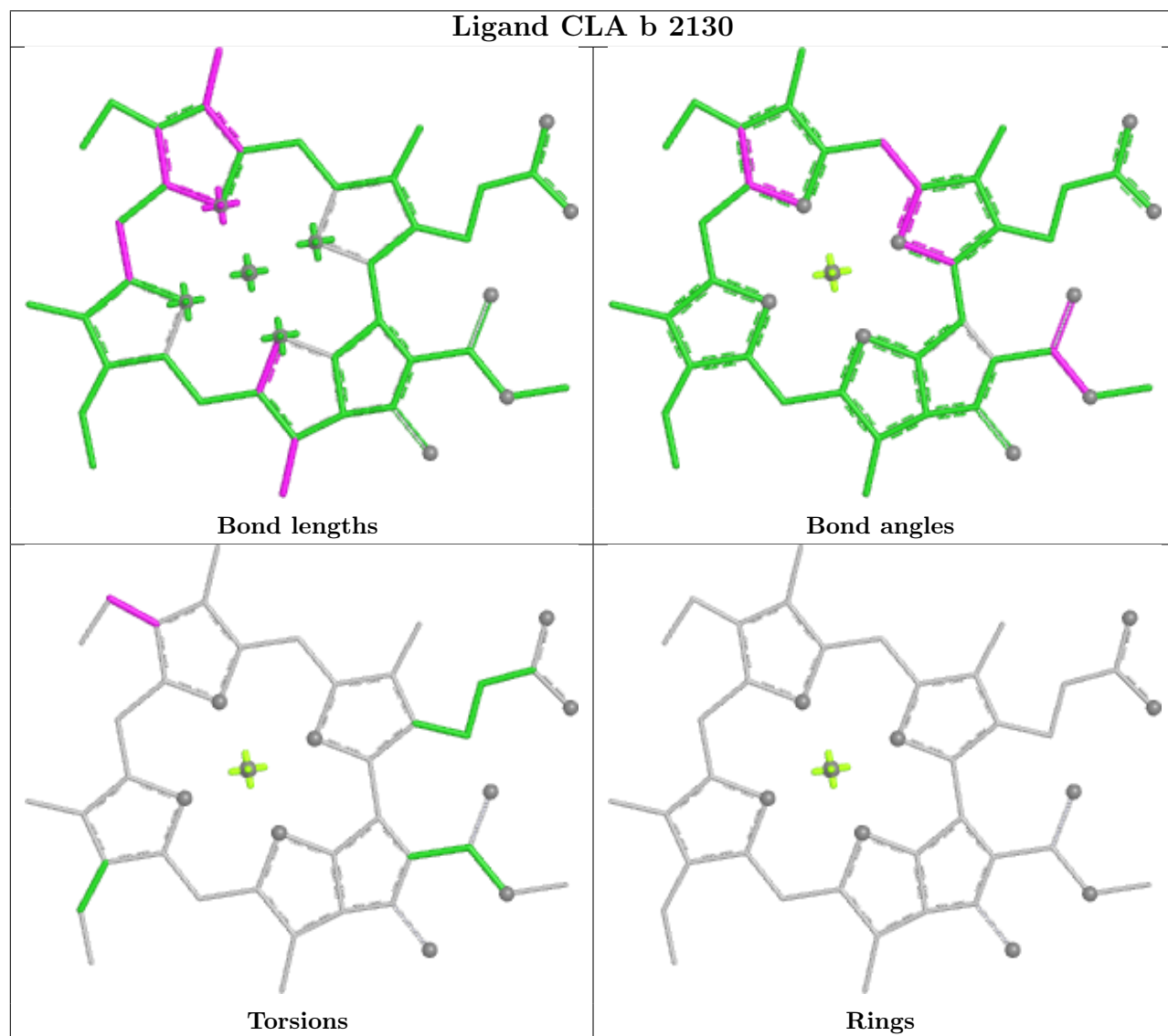
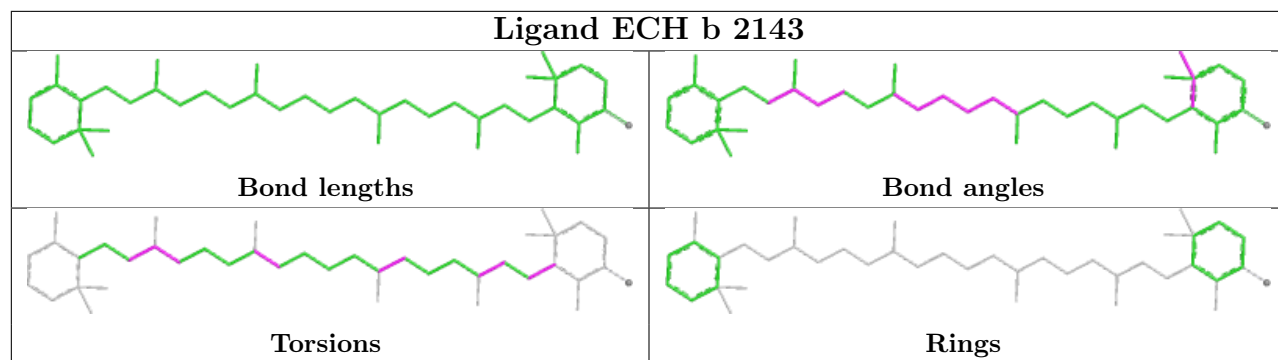
Ligand CLA a 838

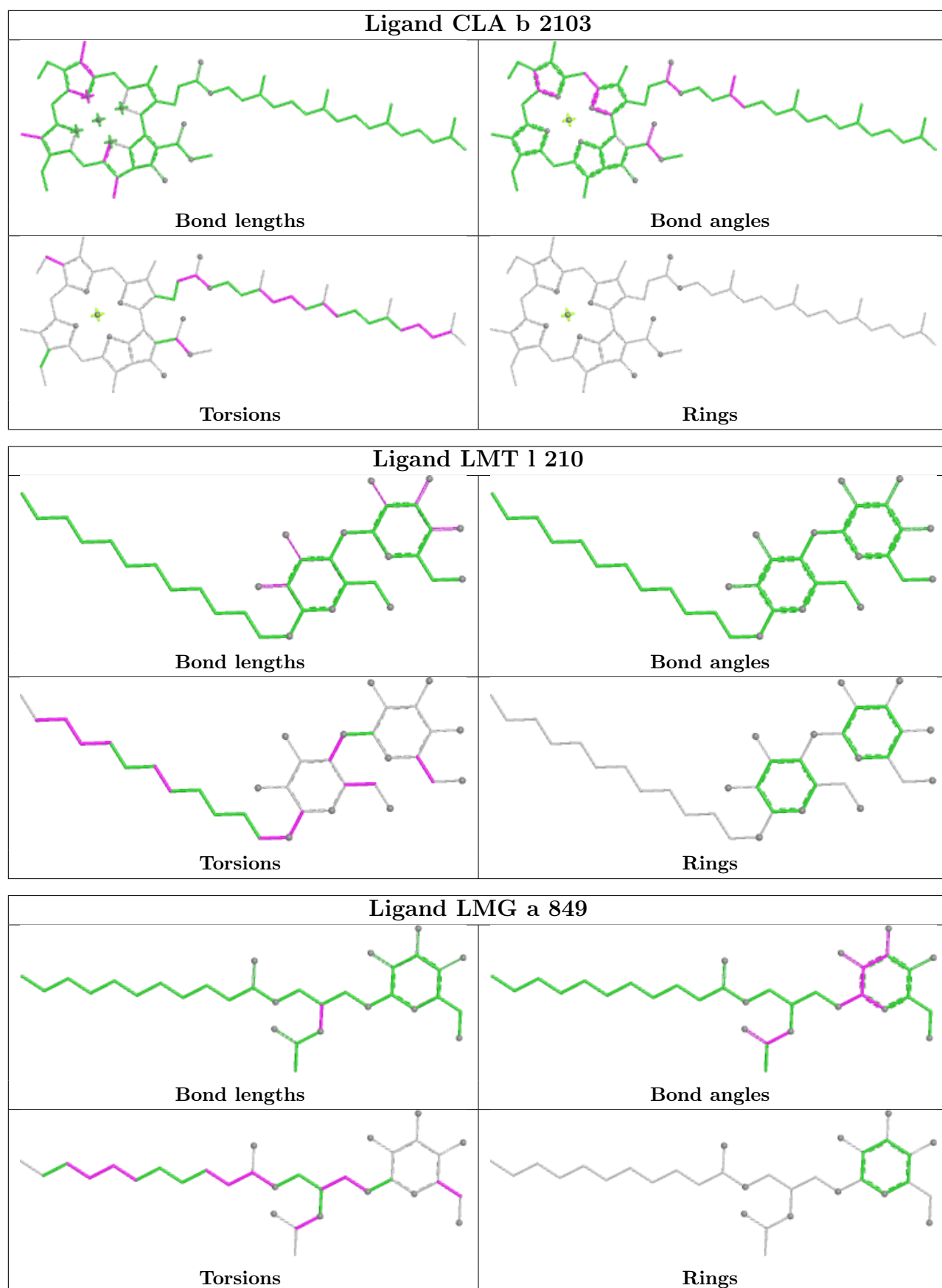


Ligand CLA A 820

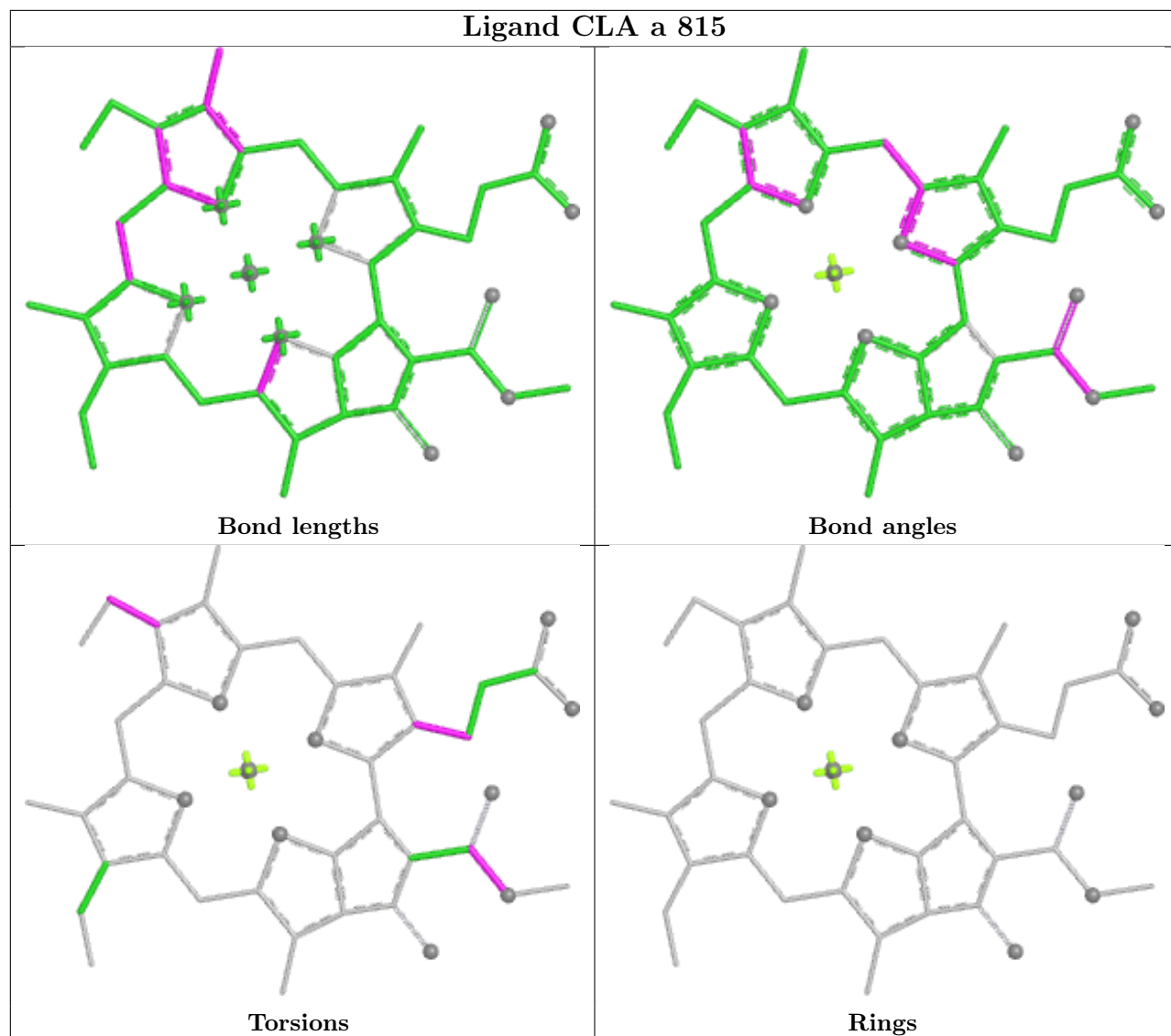




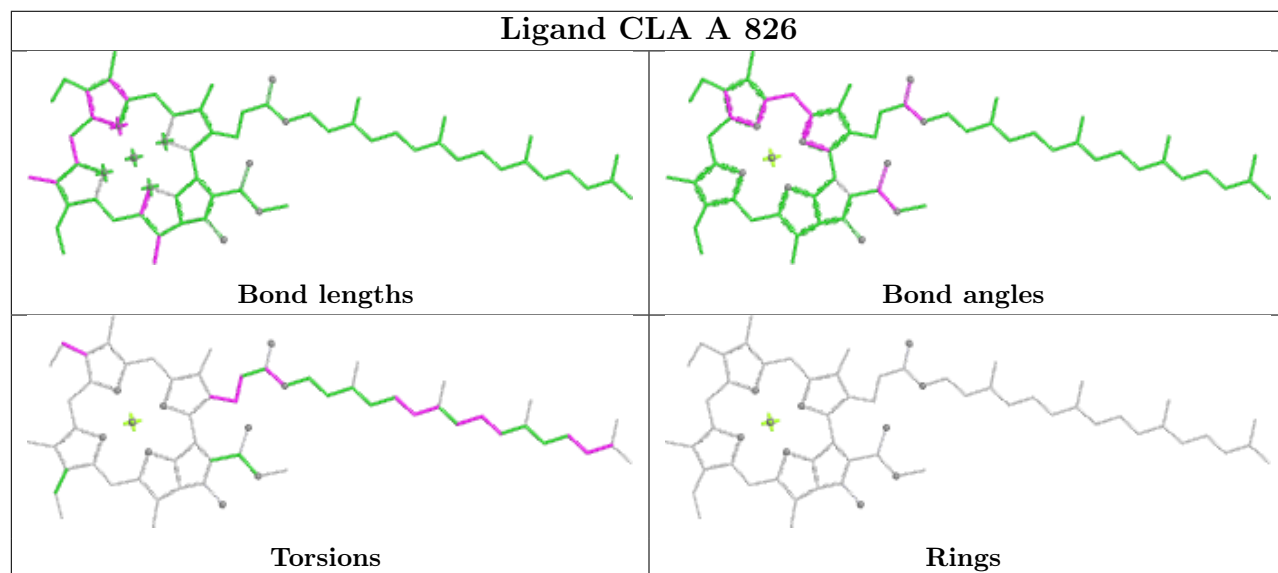




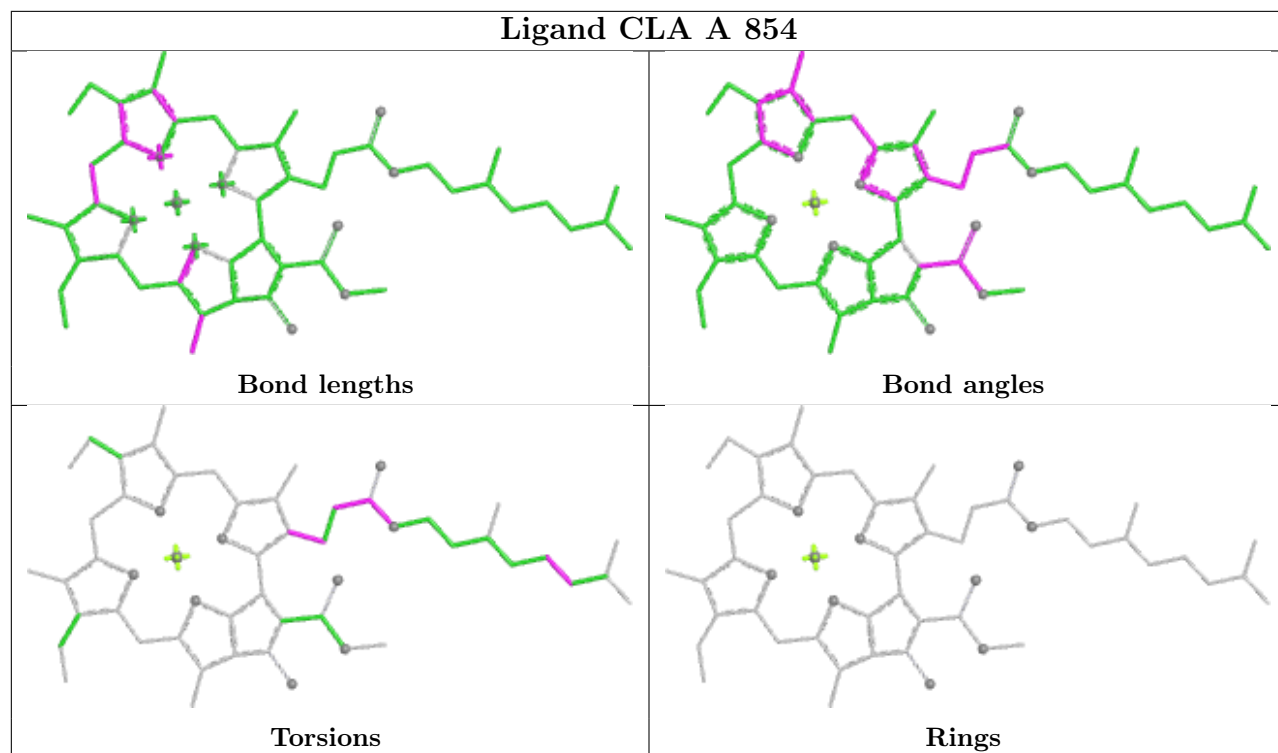
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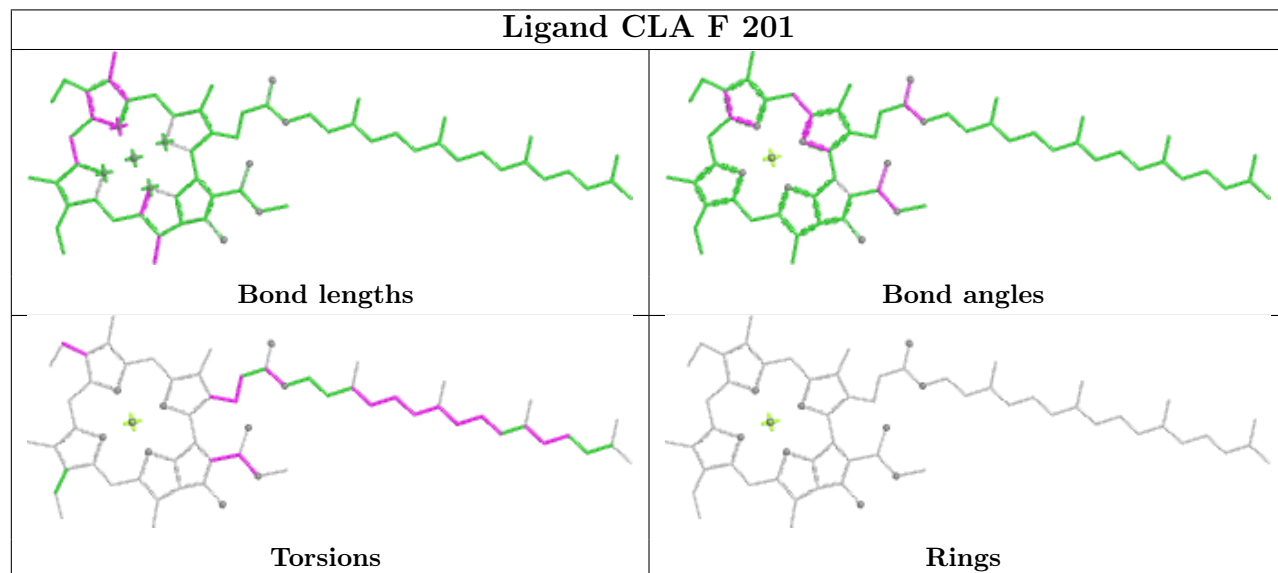
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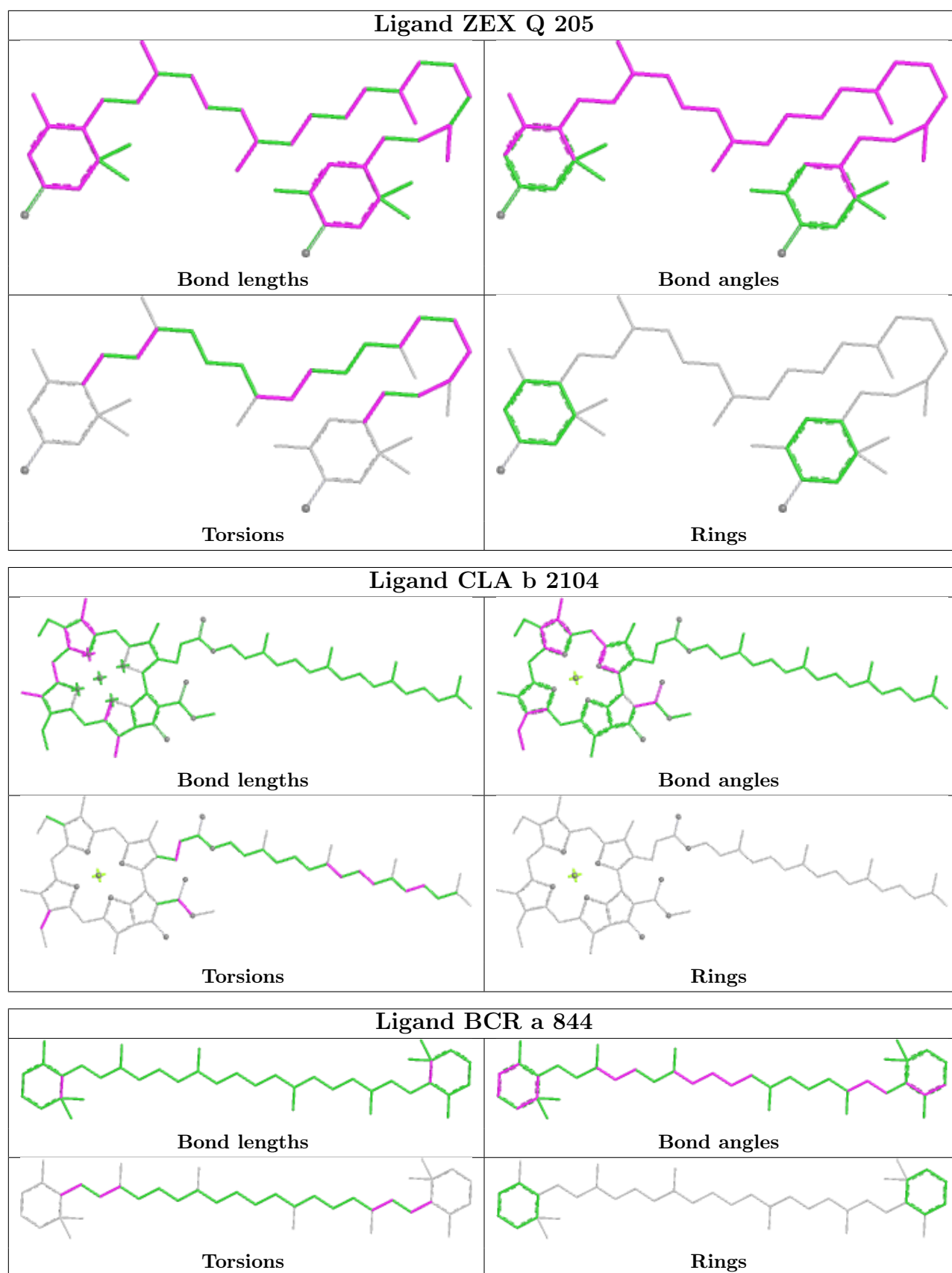


Ligand CLA A 854

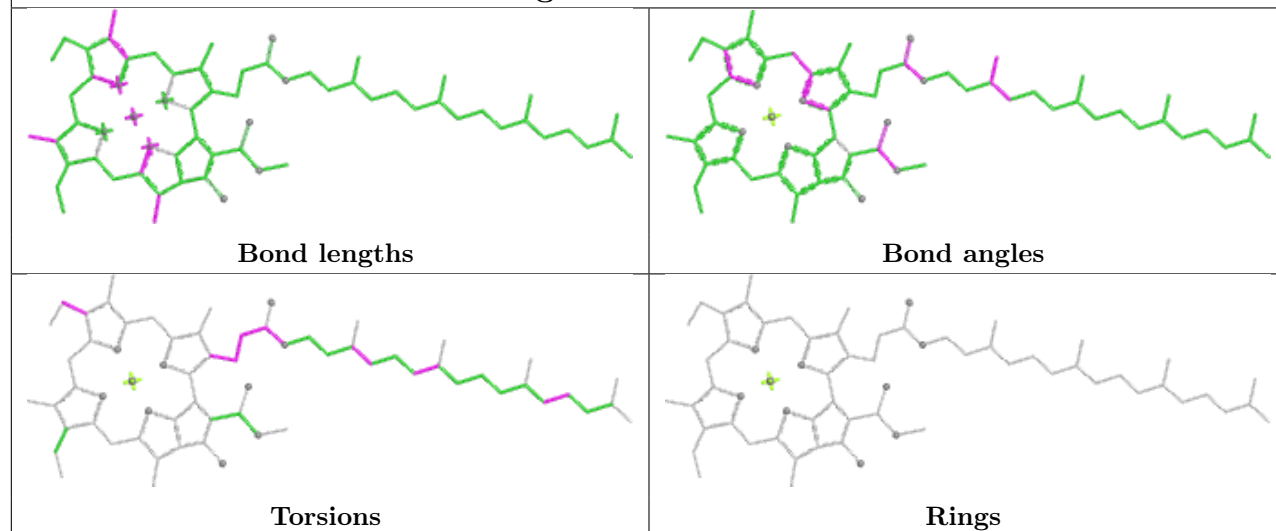


Ligand CLA F 201

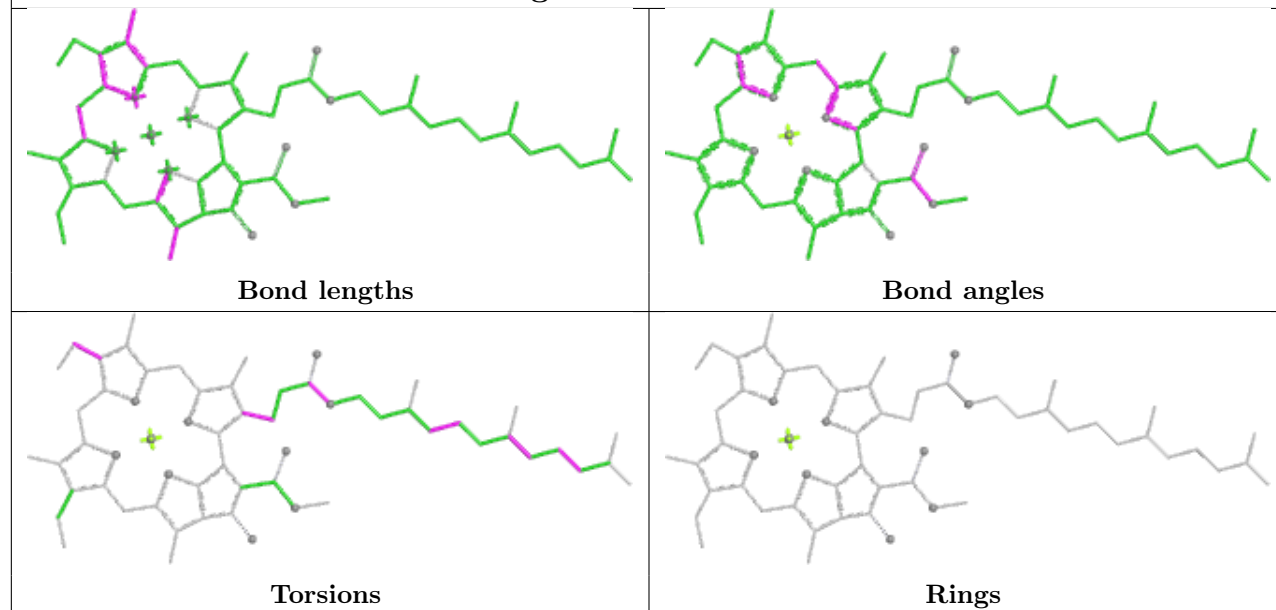


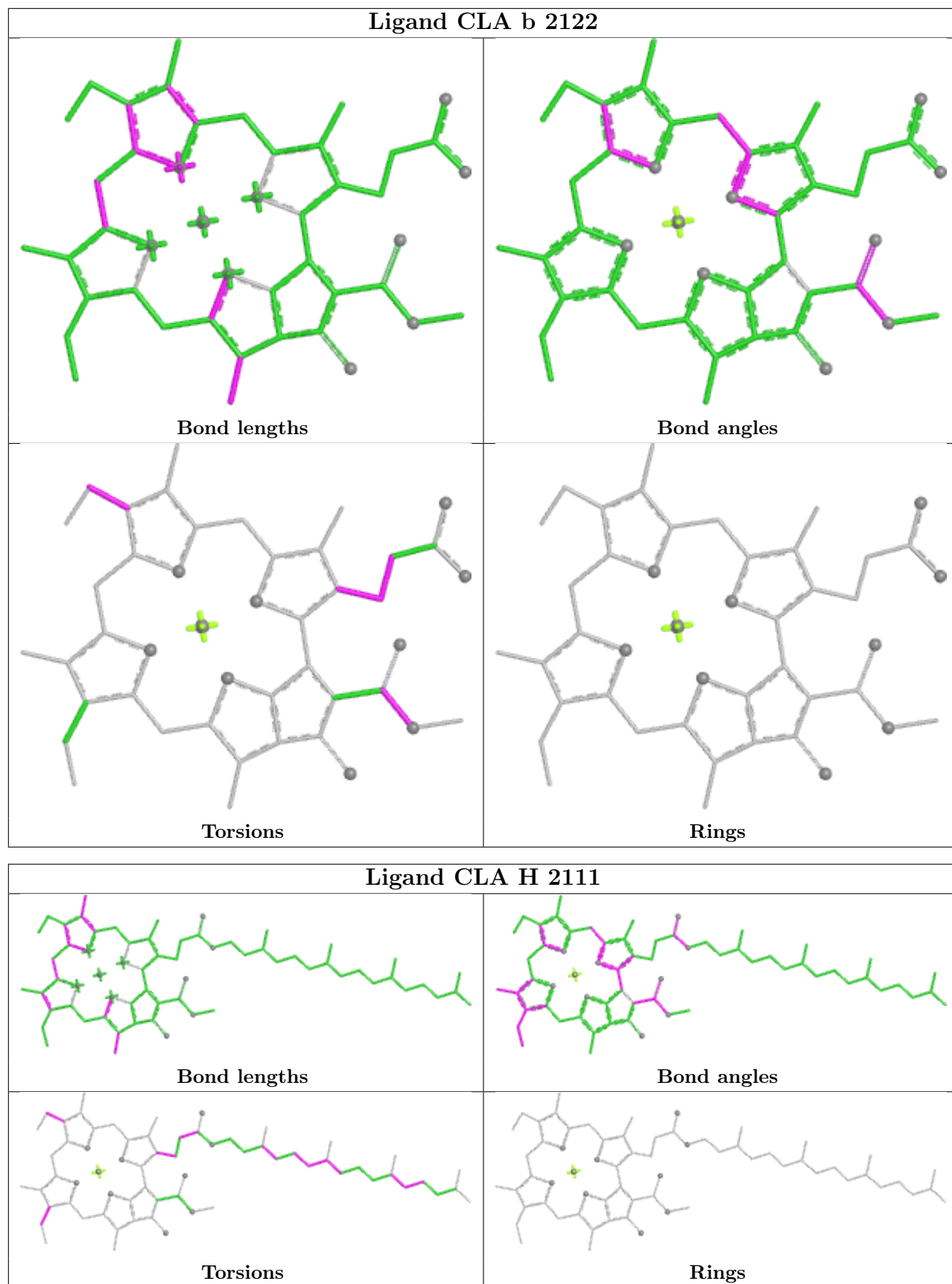


Ligand CLA a 851

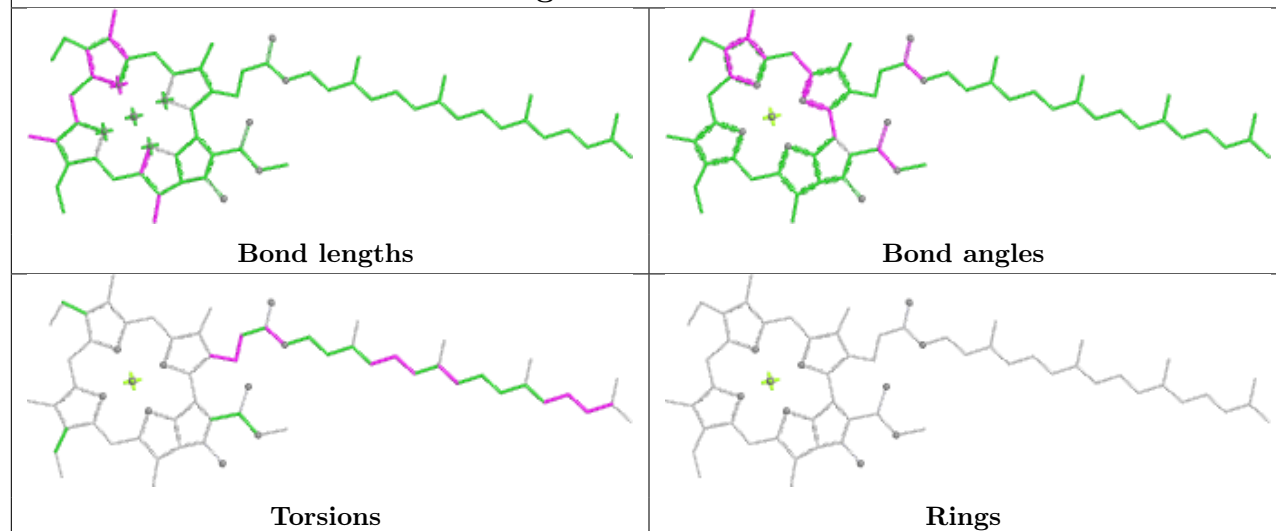


Ligand CLA G 821

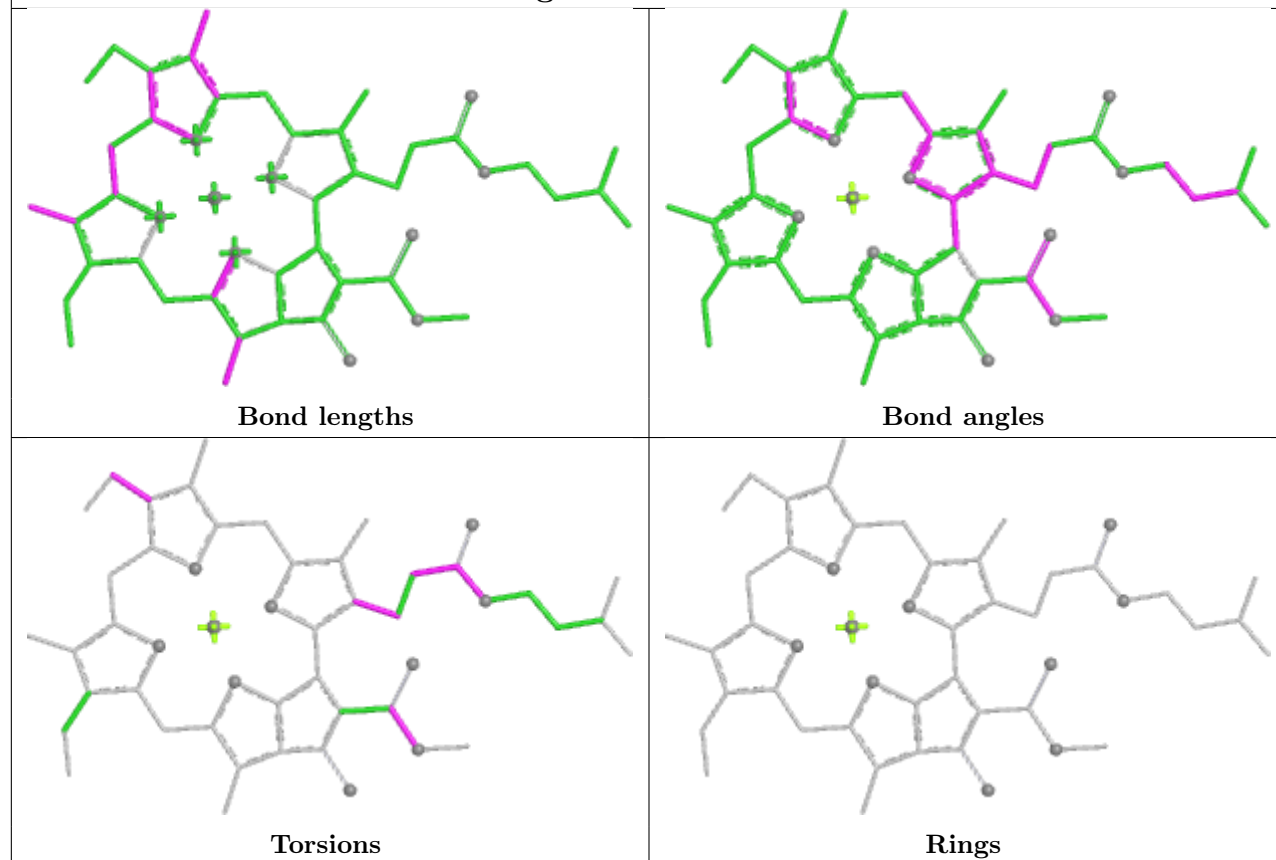


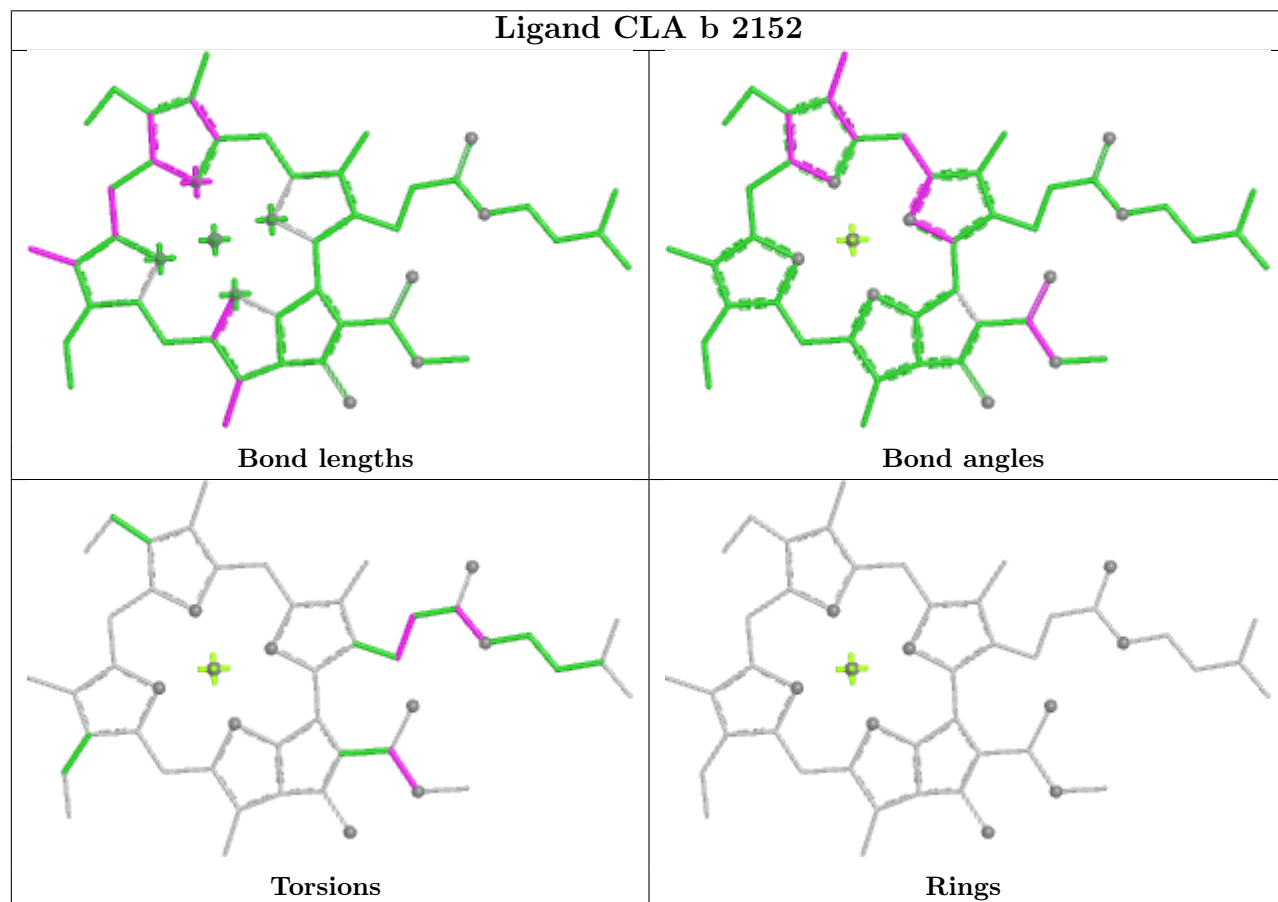
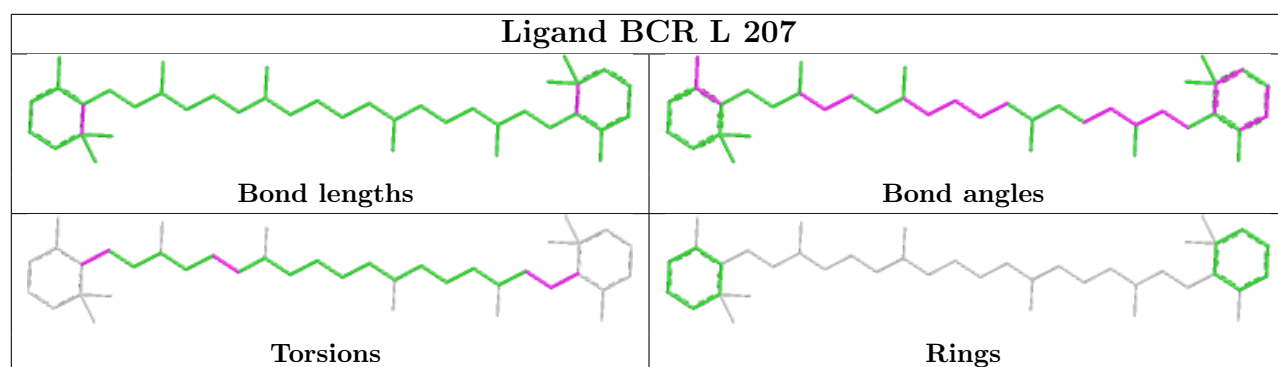


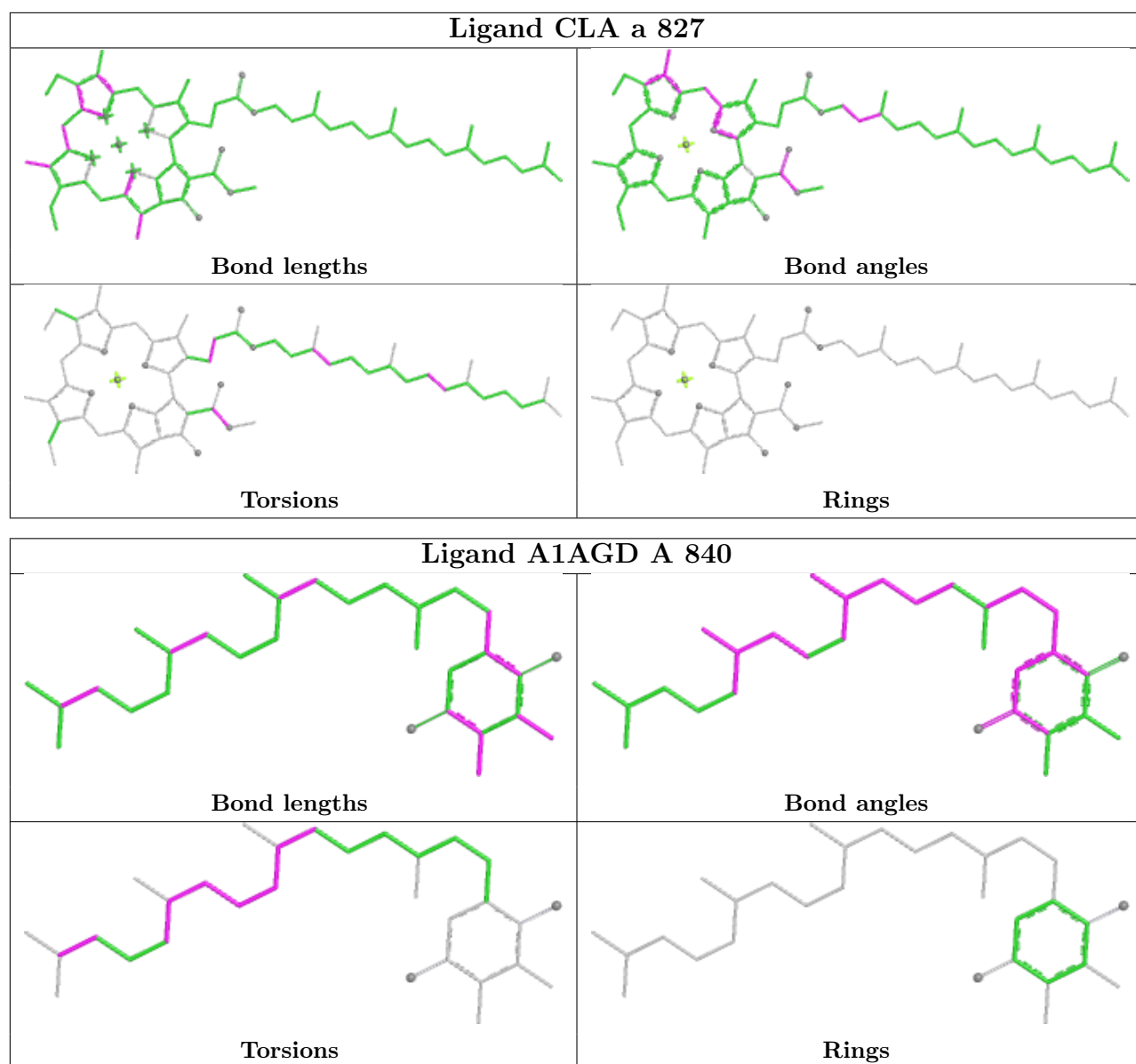
Ligand CLA a 835

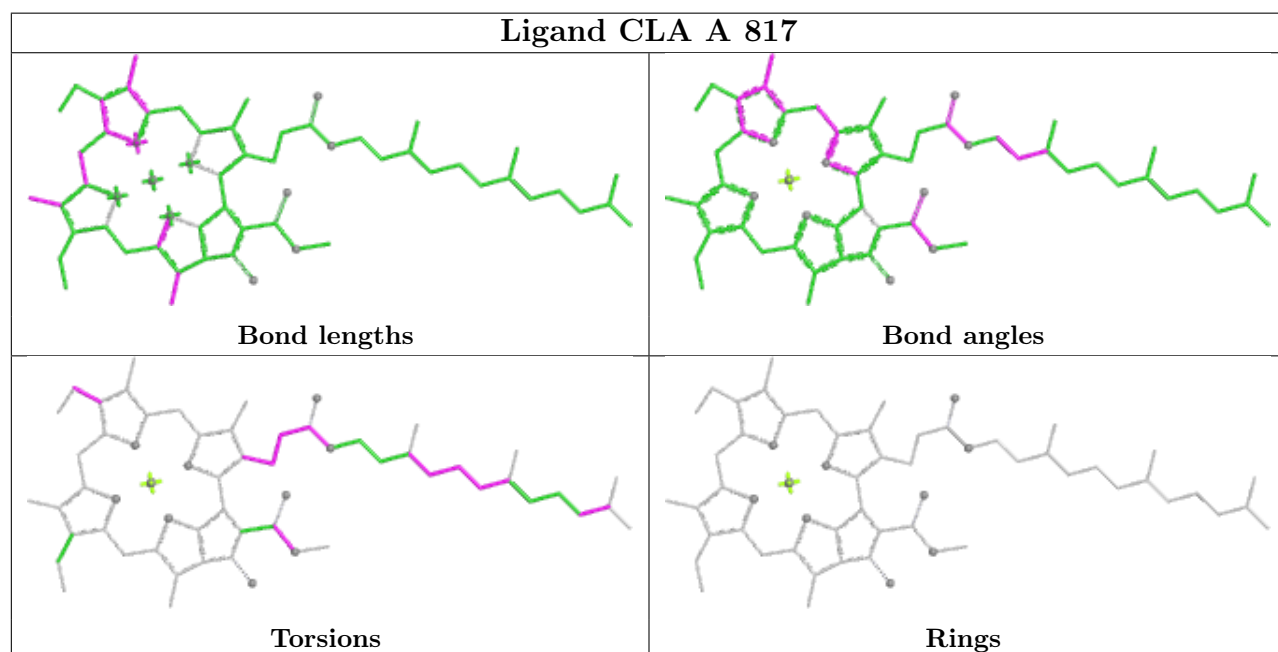
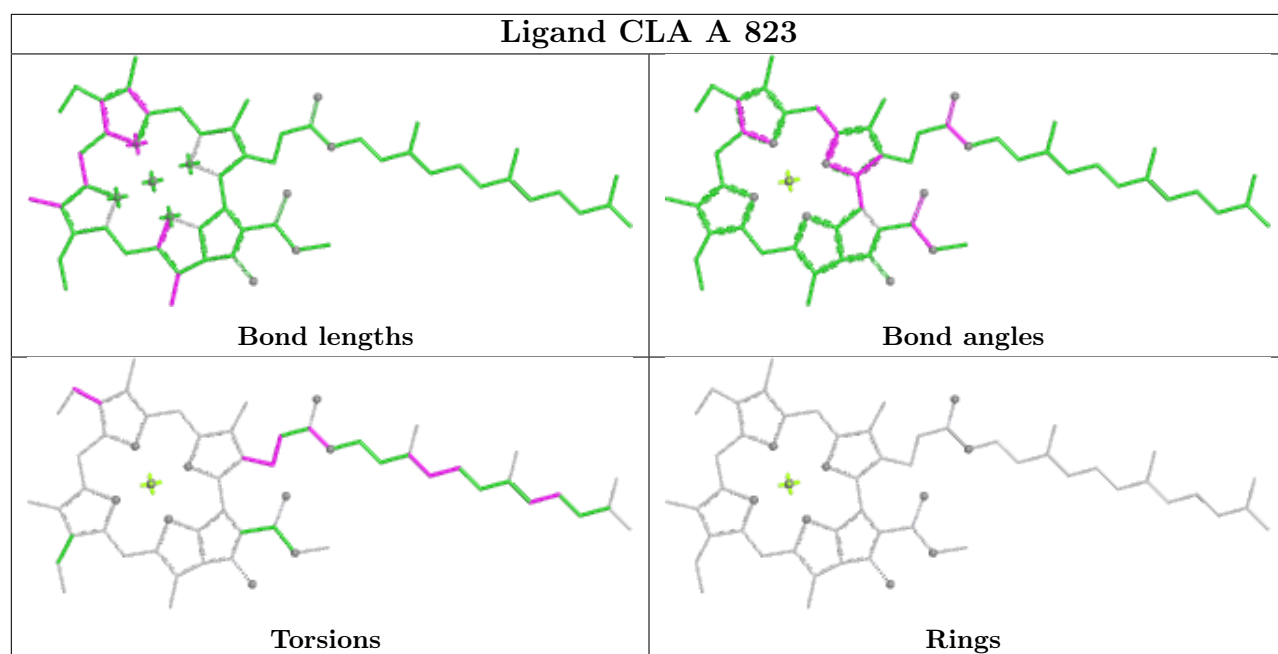


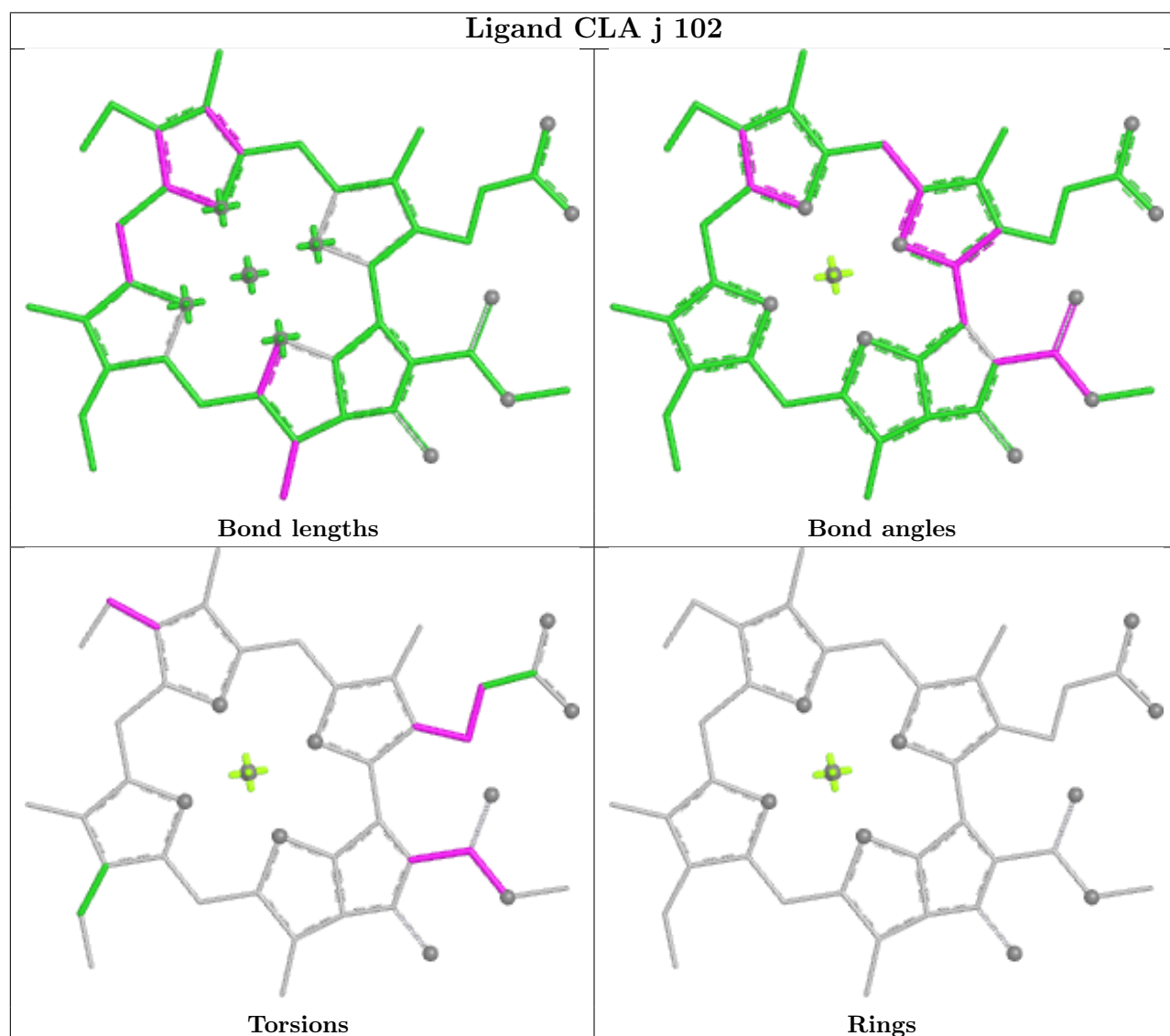
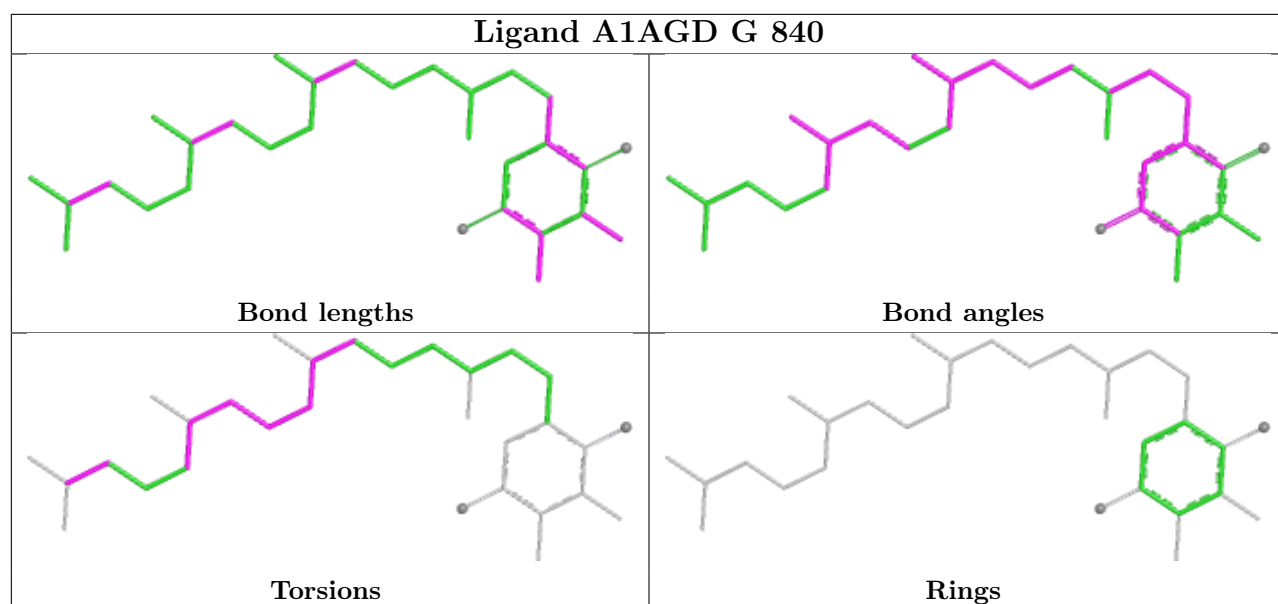
Ligand CLA a 809

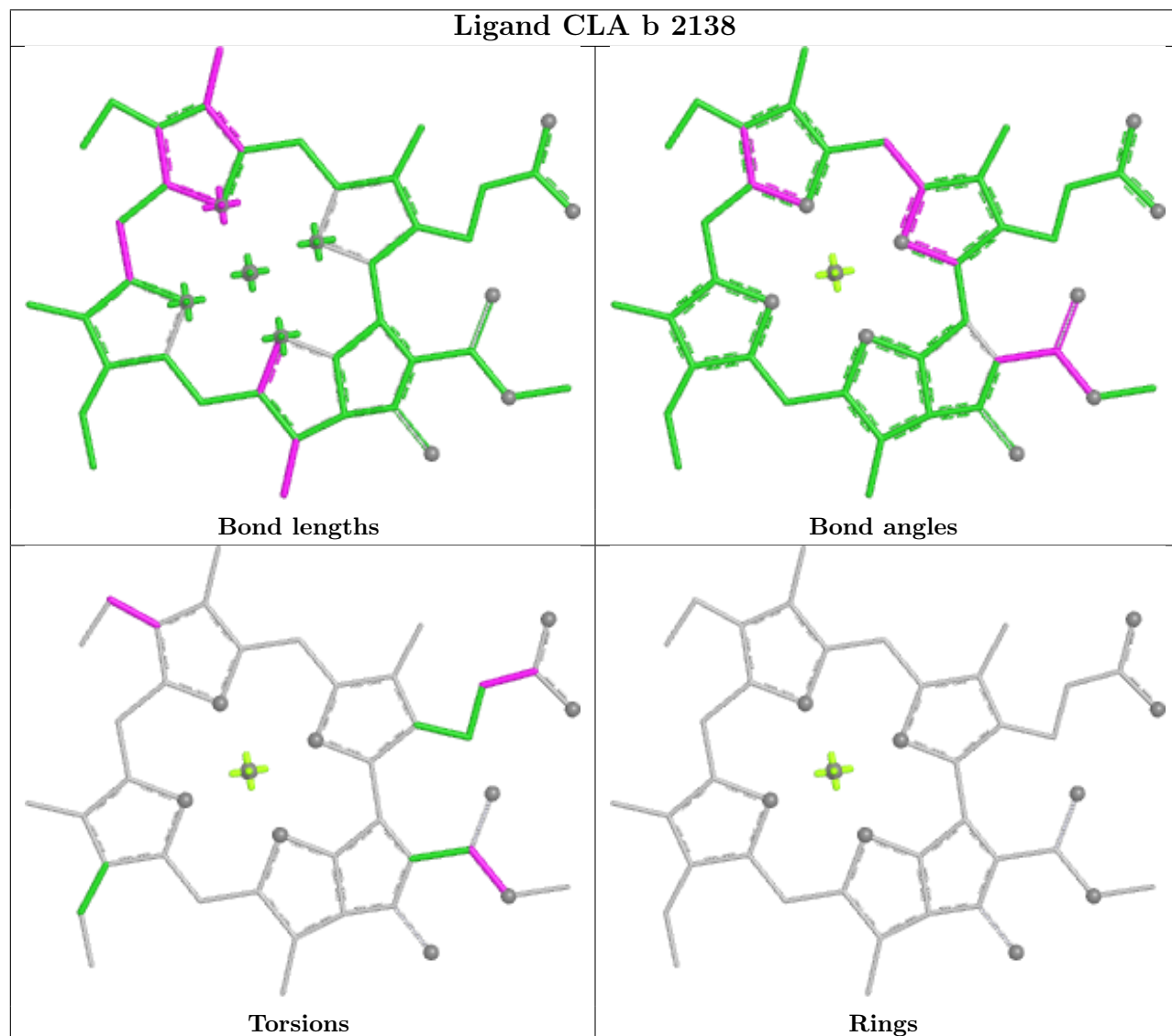
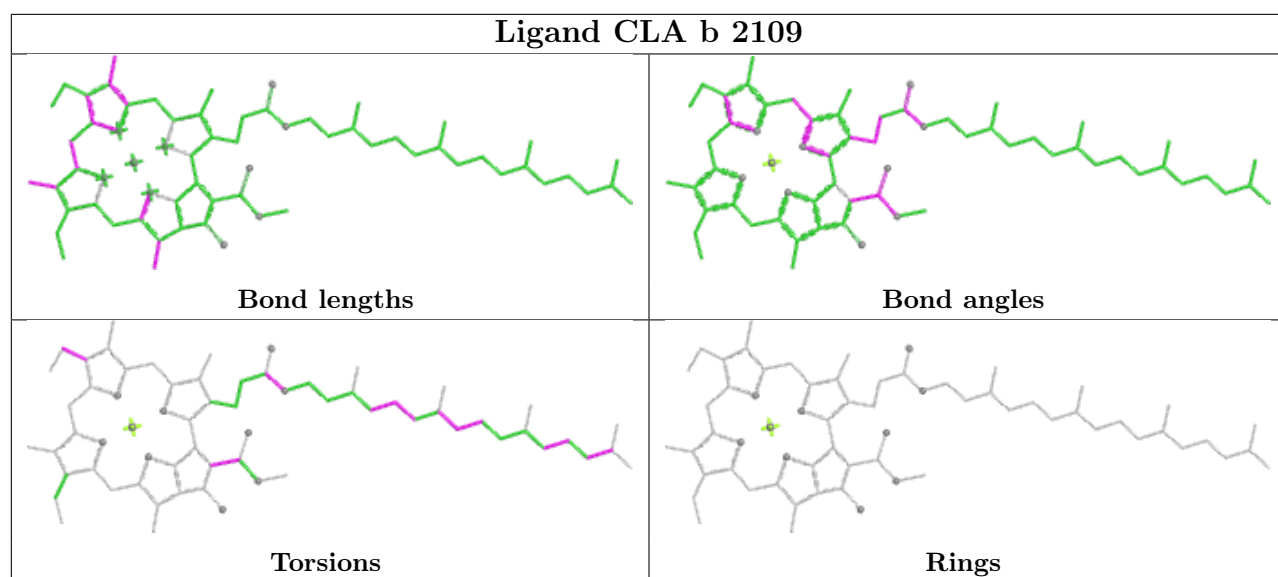


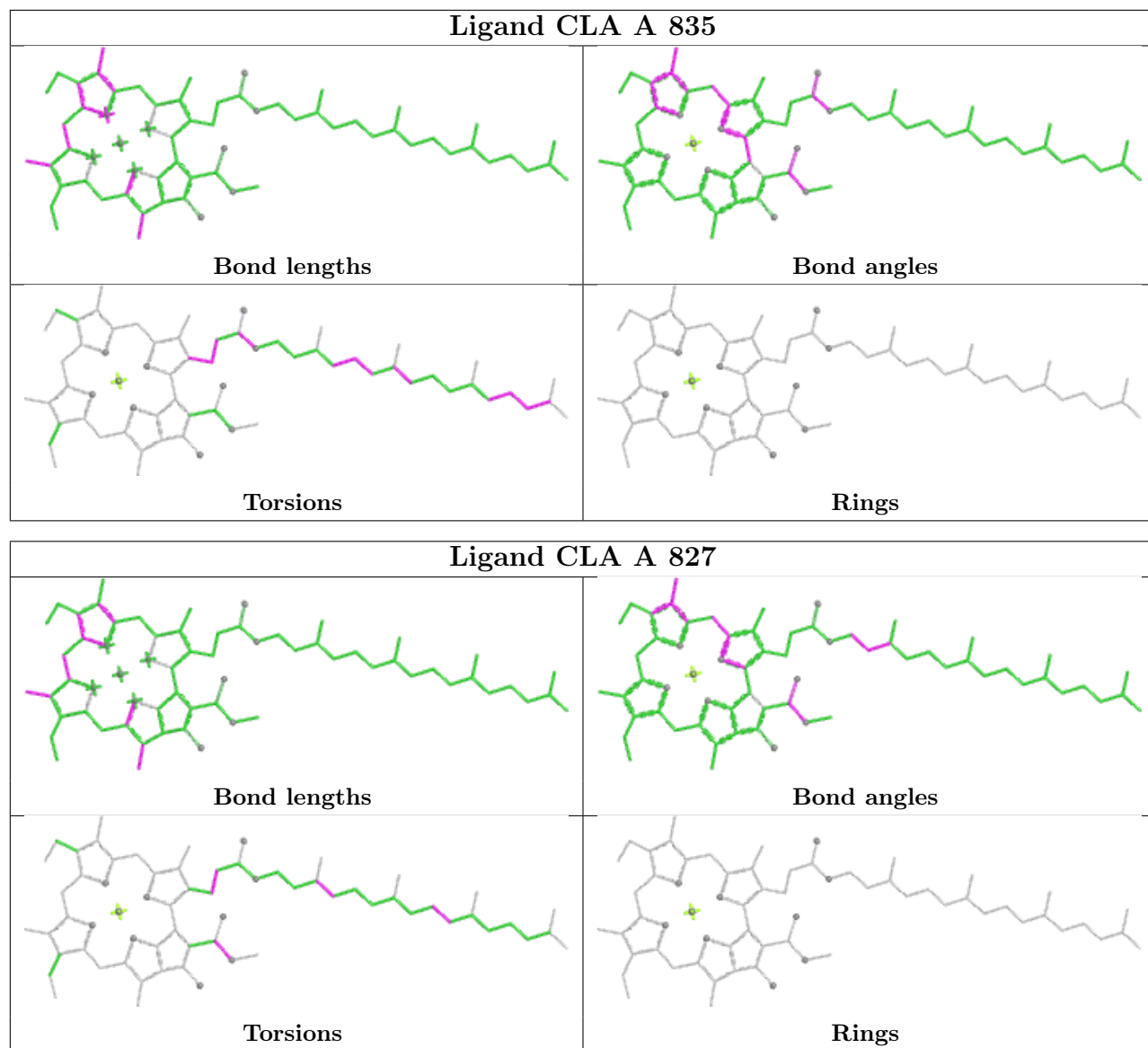


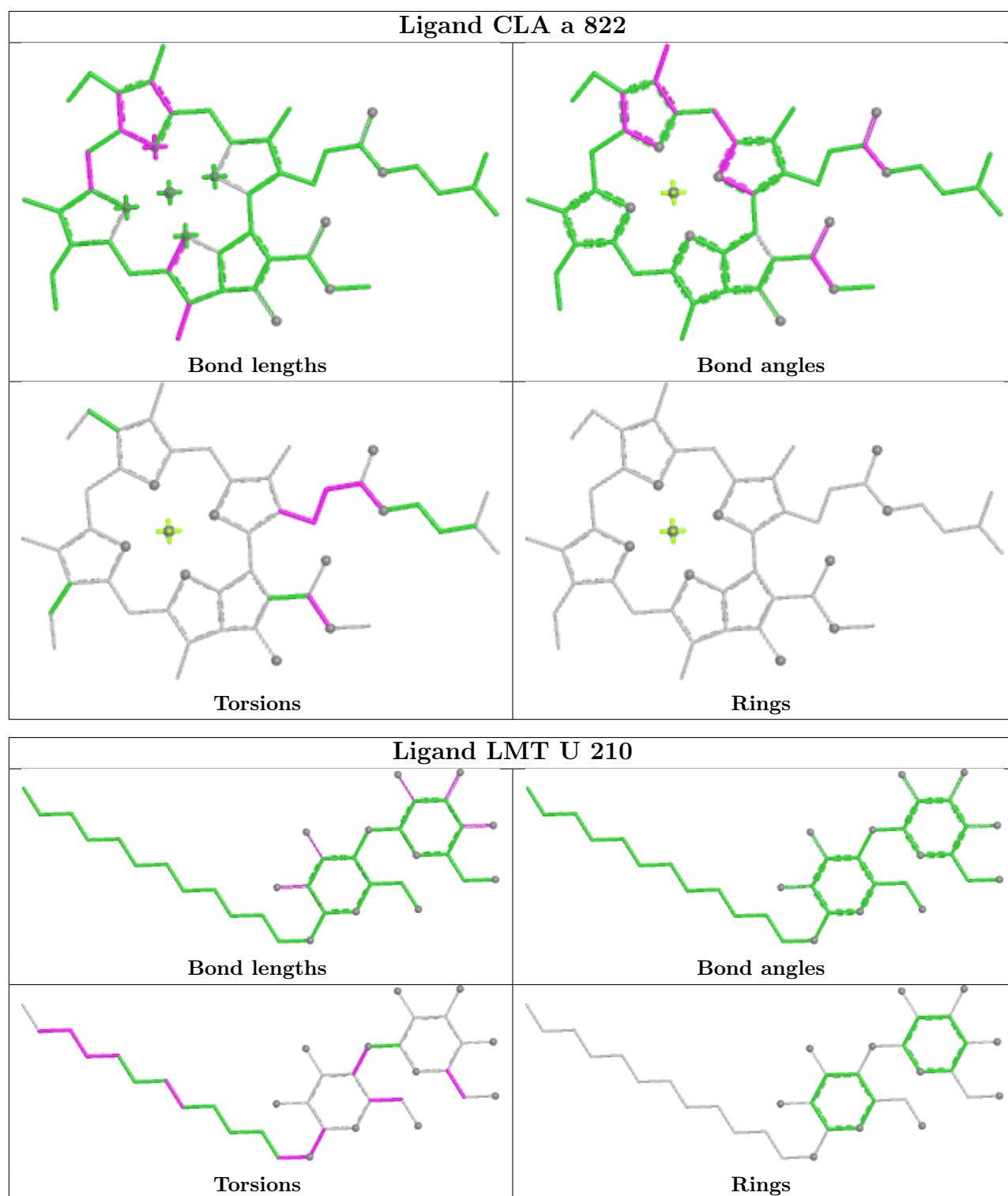












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

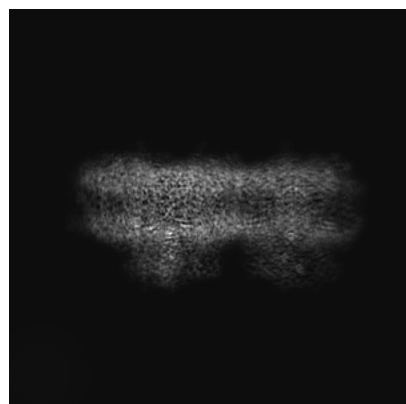
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43843. These allow visual inspection of the internal detail of the map and identification of artifacts.

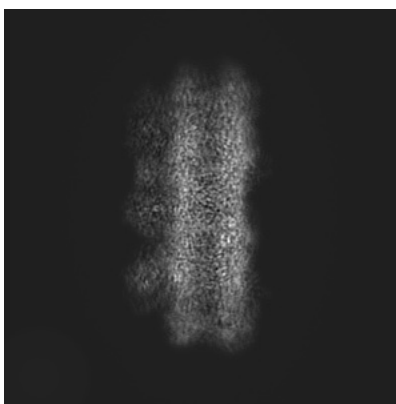
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

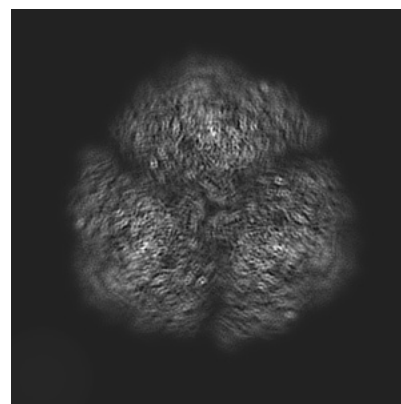
6.1.1 Primary map



X

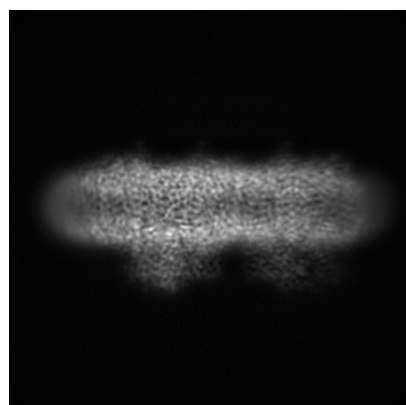


Y

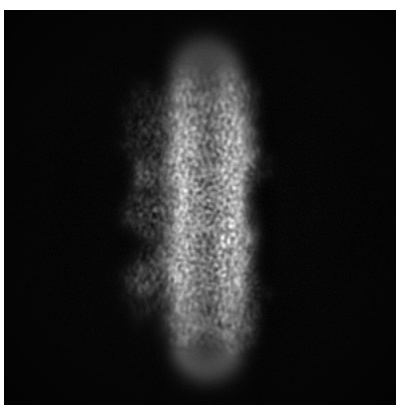


Z

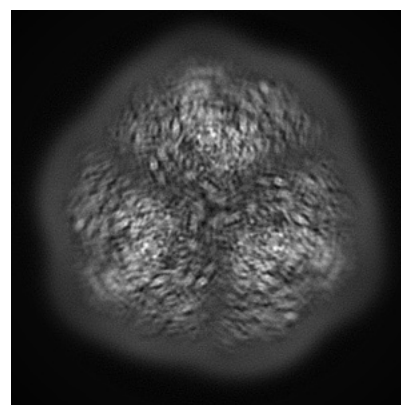
6.1.2 Raw map



X



Y



Z

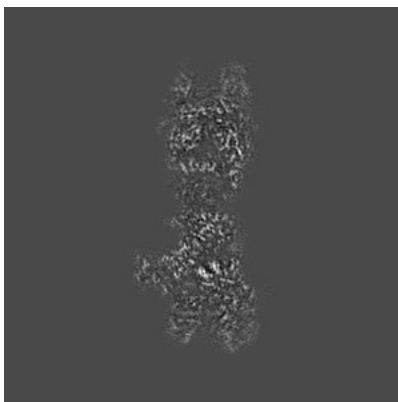
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

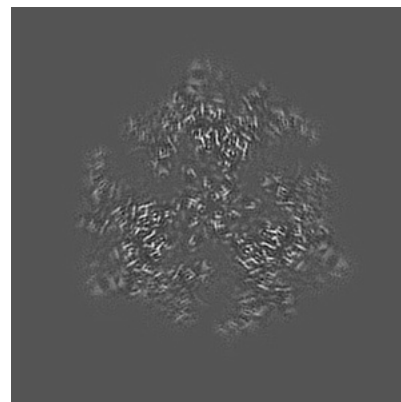
6.2.1 Primary map



X Index: 160

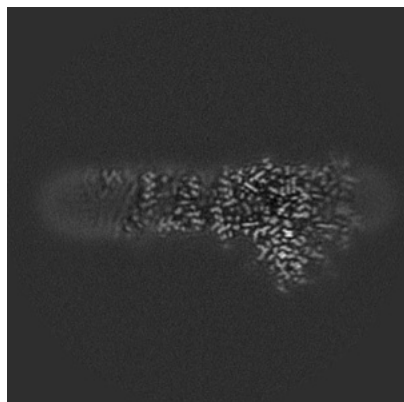


Y Index: 160

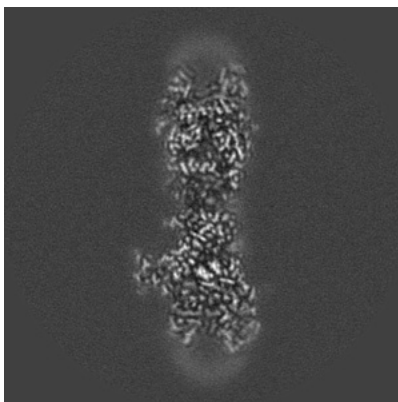


Z Index: 160

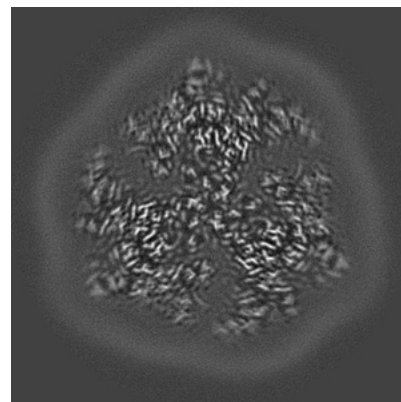
6.2.2 Raw map



X Index: 160



Y Index: 160



Z Index: 160

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

6.3 Largest variance slices [i](#)

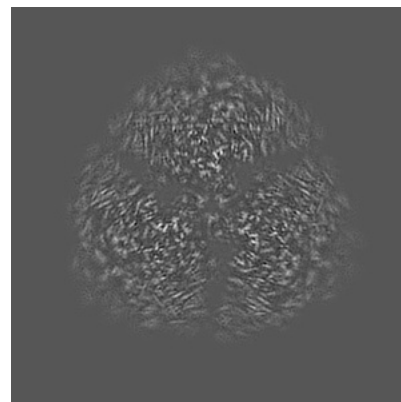
6.3.1 Primary map



X Index: 107

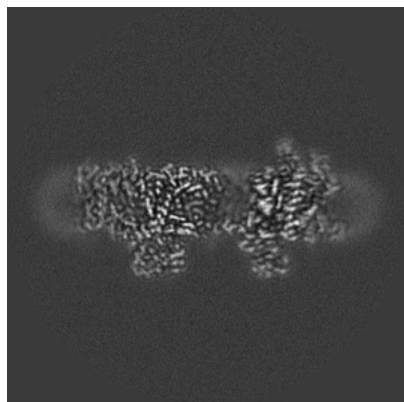


Y Index: 128

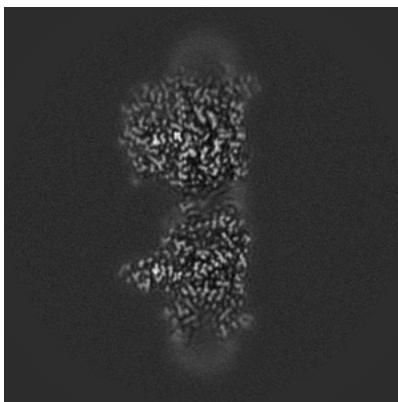


Z Index: 176

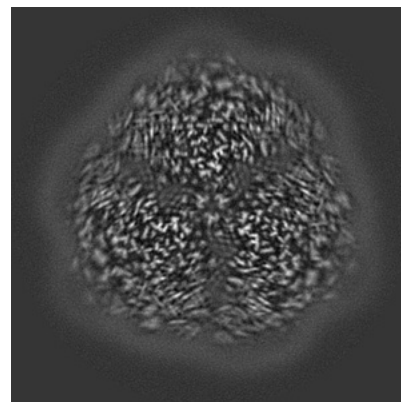
6.3.2 Raw map



X Index: 187



Y Index: 129

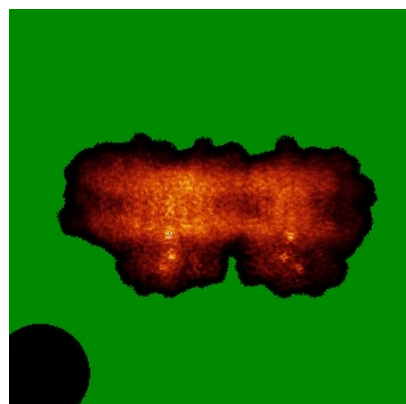


Z Index: 176

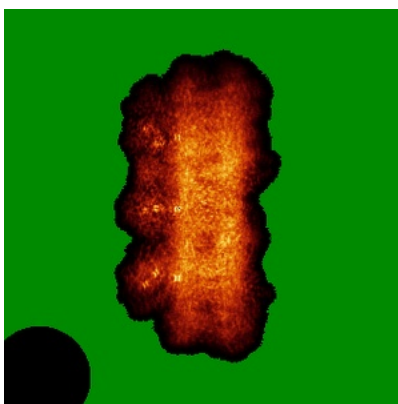
The images above show the largest variance slices of the map in three orthogonal directions.

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

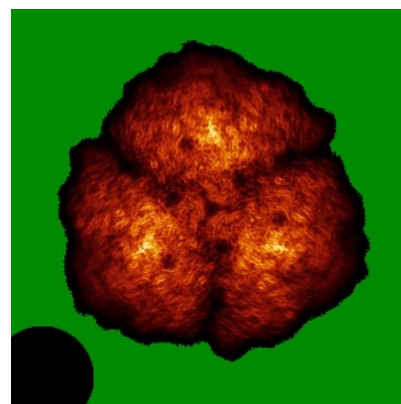
6.4.1 Primary map



X

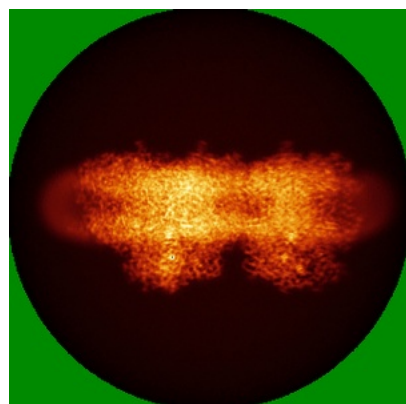


Y

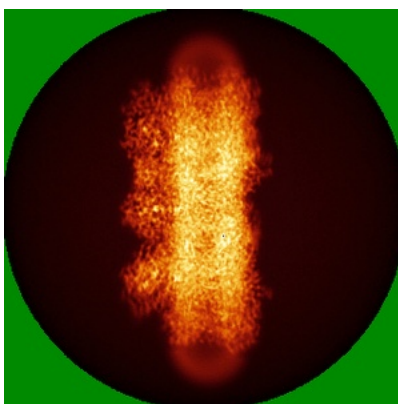


Z

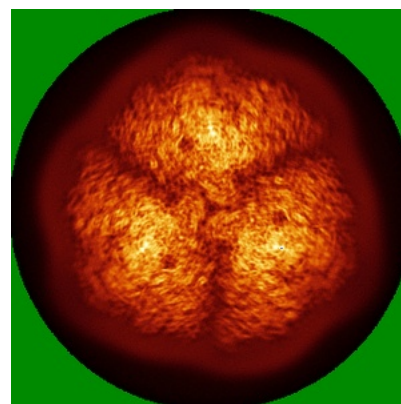
6.4.2 Raw map



X



Y

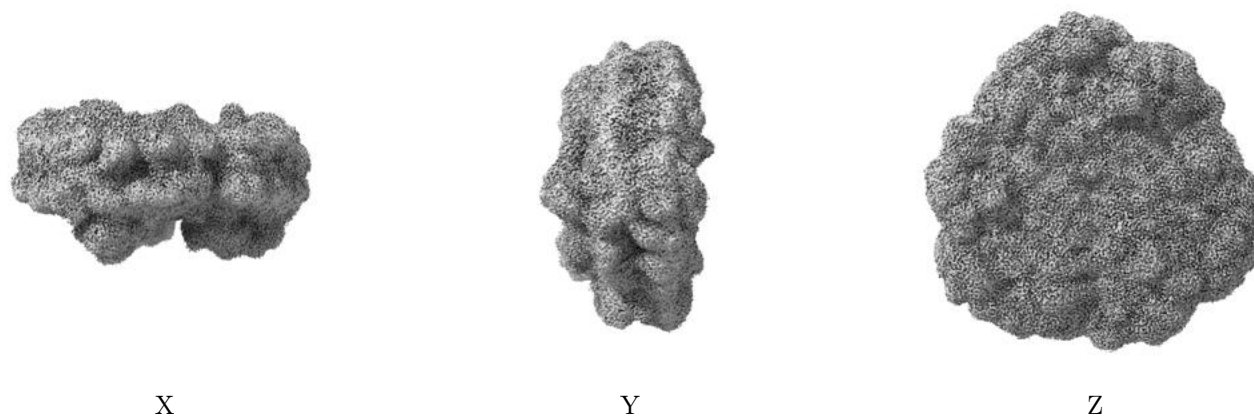


Z

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.

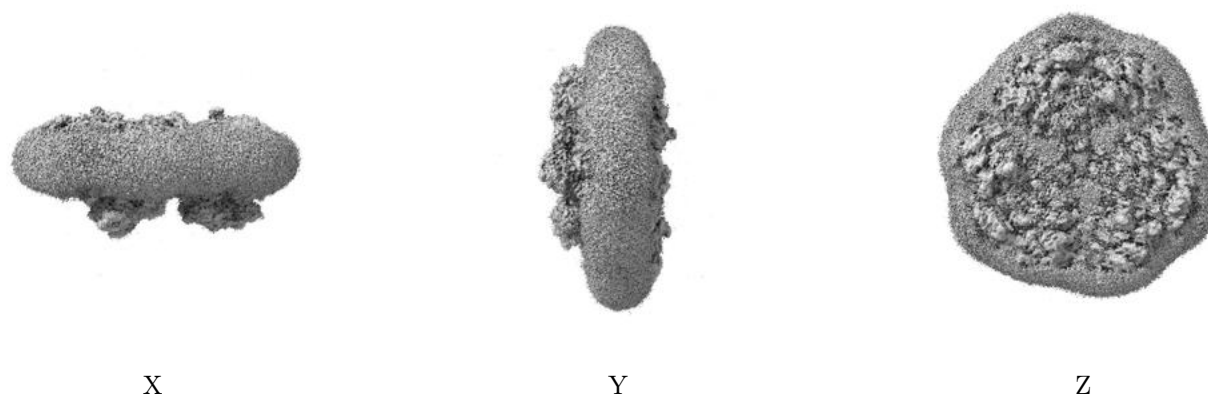
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0149. 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.

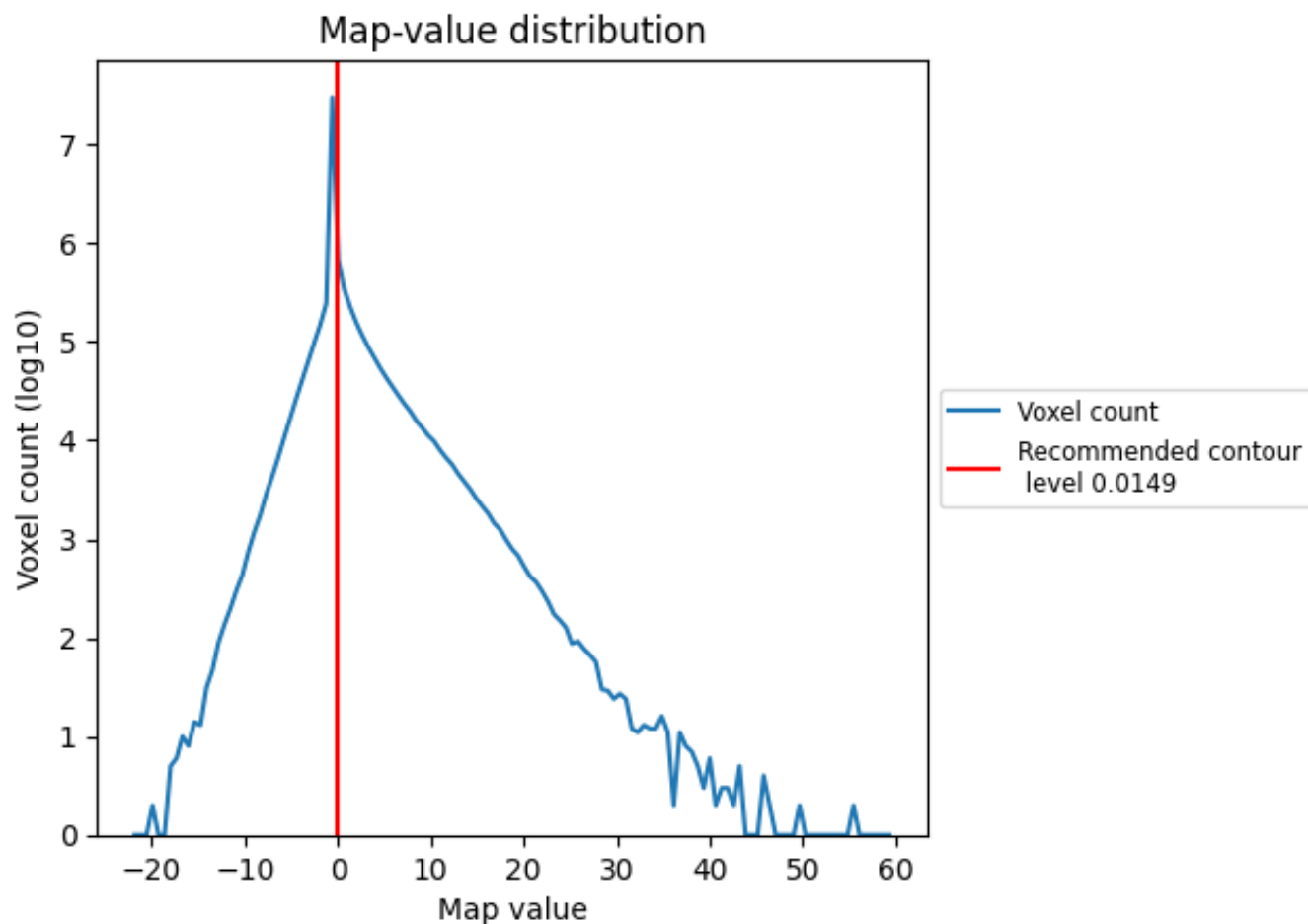
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

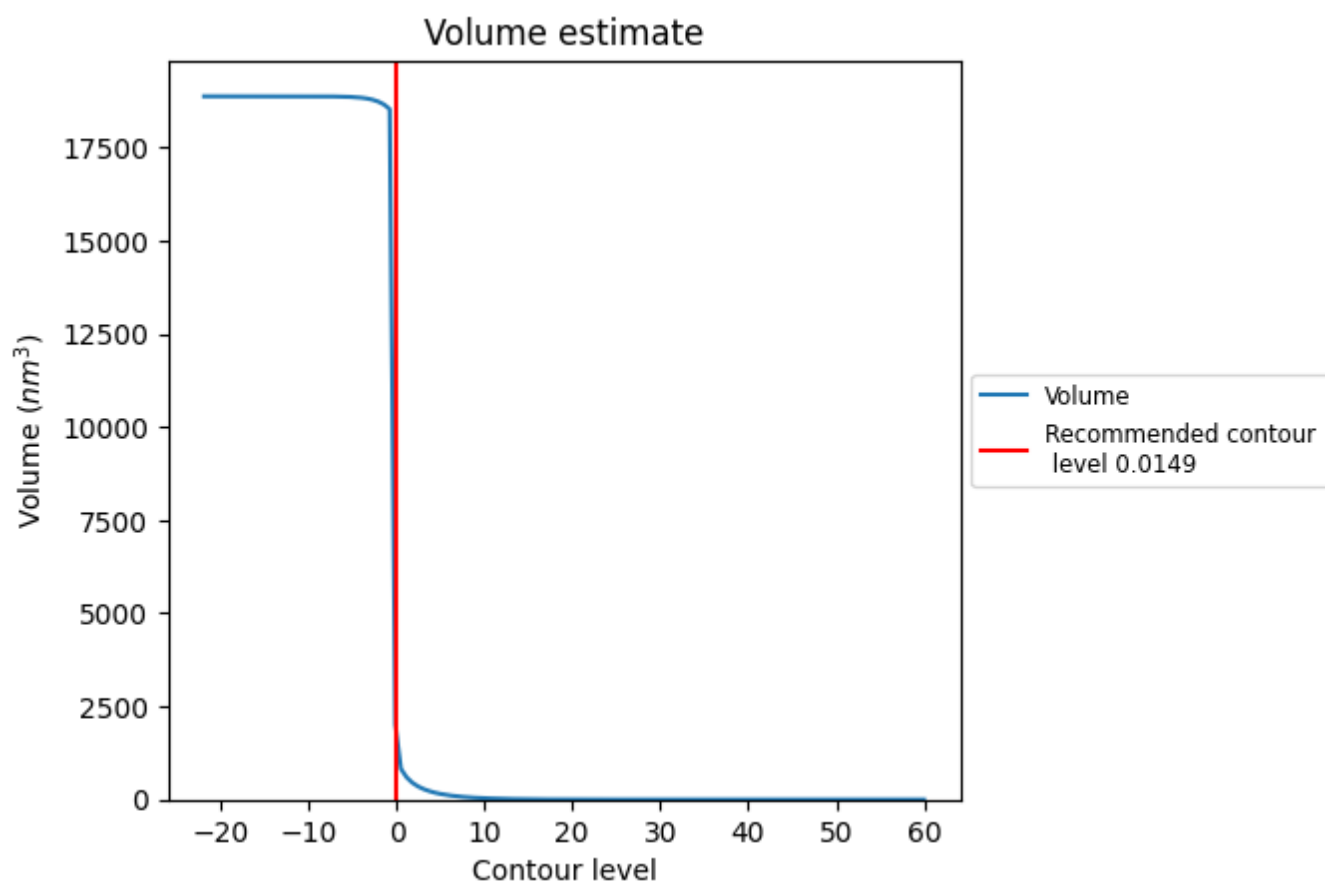
This section contains the results of statistical analysis of the map.

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.

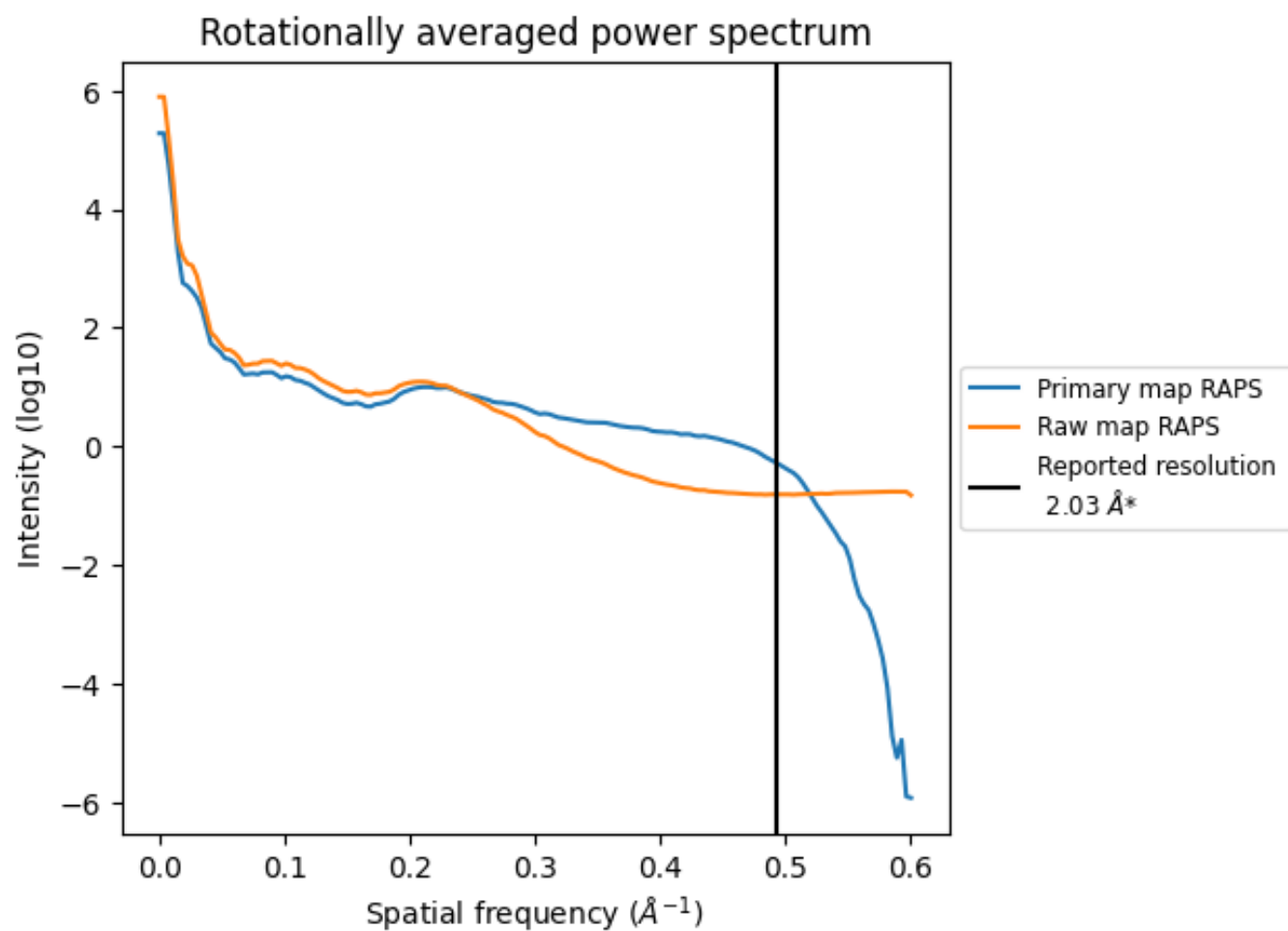
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1809 nm^3 ; this corresponds to an approximate mass of 1634 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 ⓘ

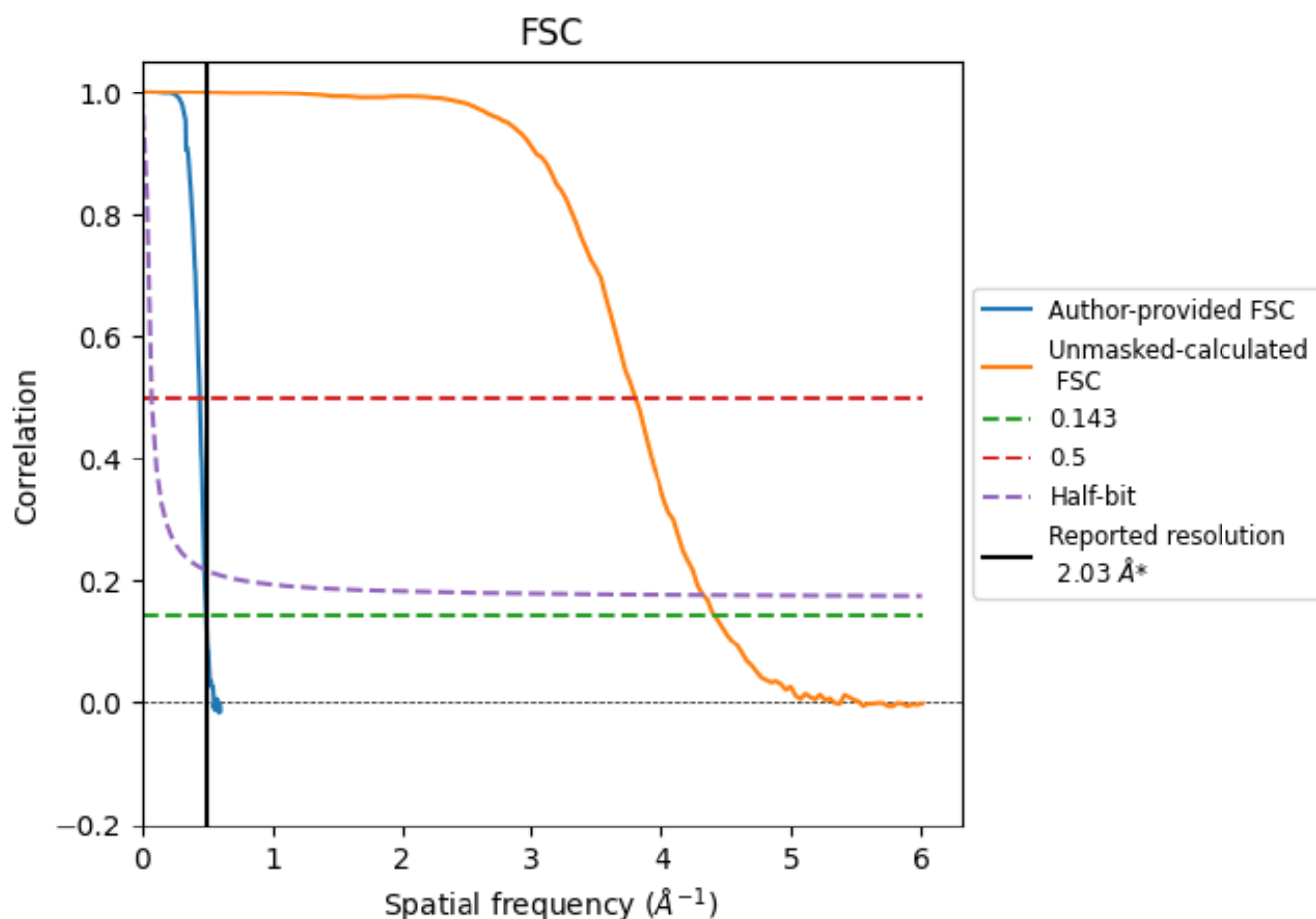


*Reported resolution corresponds to spatial frequency of 0.493 Å⁻¹

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 0.493 Å⁻¹

8.2 Resolution estimates [i](#)

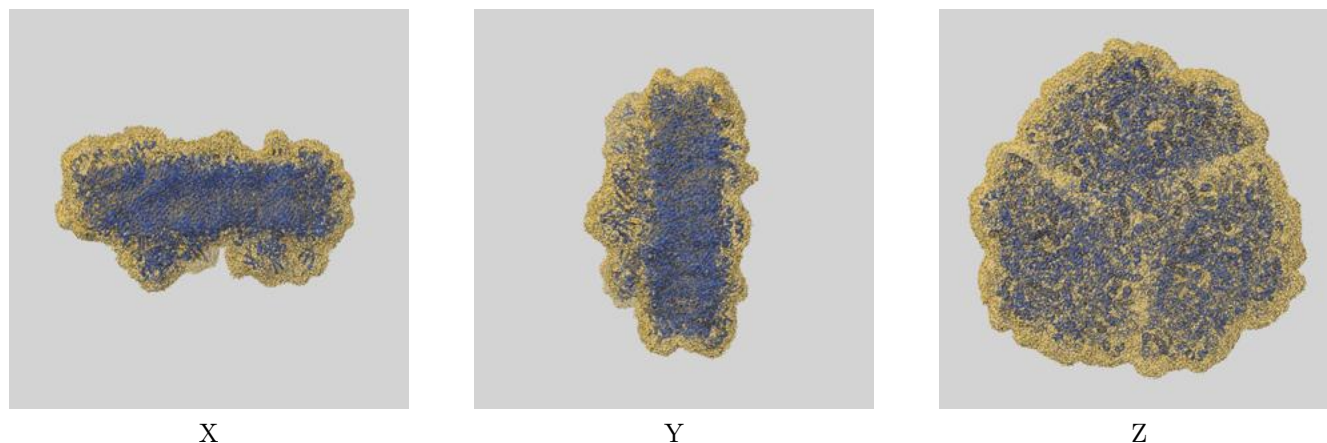
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.03	-	-
Author-provided FSC curve	2.03	2.26	2.06
Unmasked-calculated*	0.23	0.26	0.23

*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 0.23 differs from the reported value 2.03 by more than 10 %

9 Map-model fit [i](#)

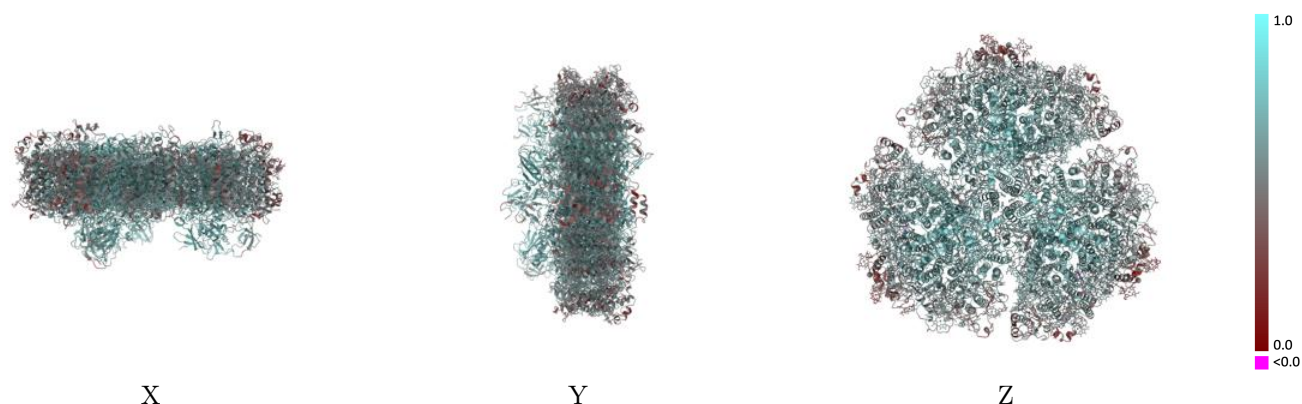
This section contains information regarding the fit between EMDB map EMD-43843 and PDB model 9AU4. Per-residue inclusion information can be found in section [3](#) on page [36](#).

9.1 Map-model overlay [i](#)



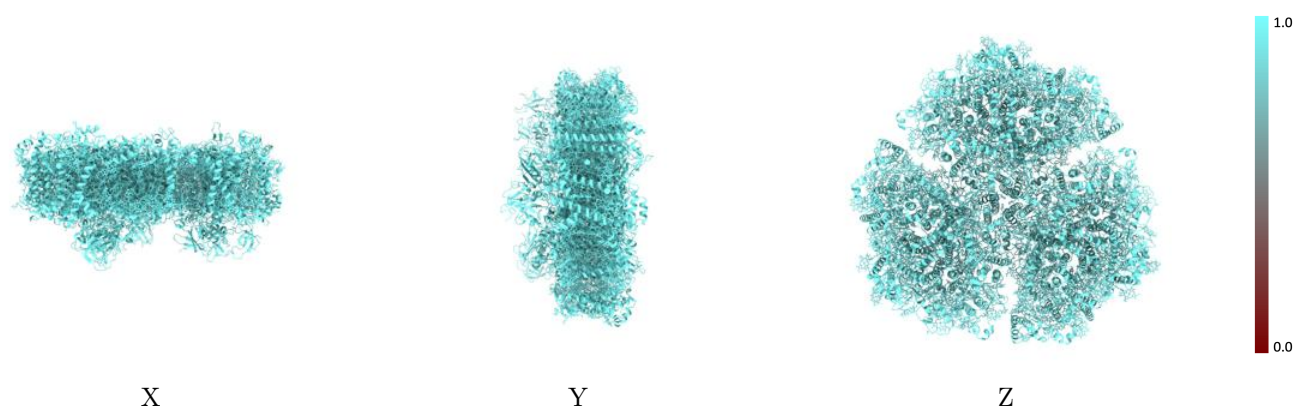
The images above show the 3D surface view of the map at the recommended contour level 0.0149 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



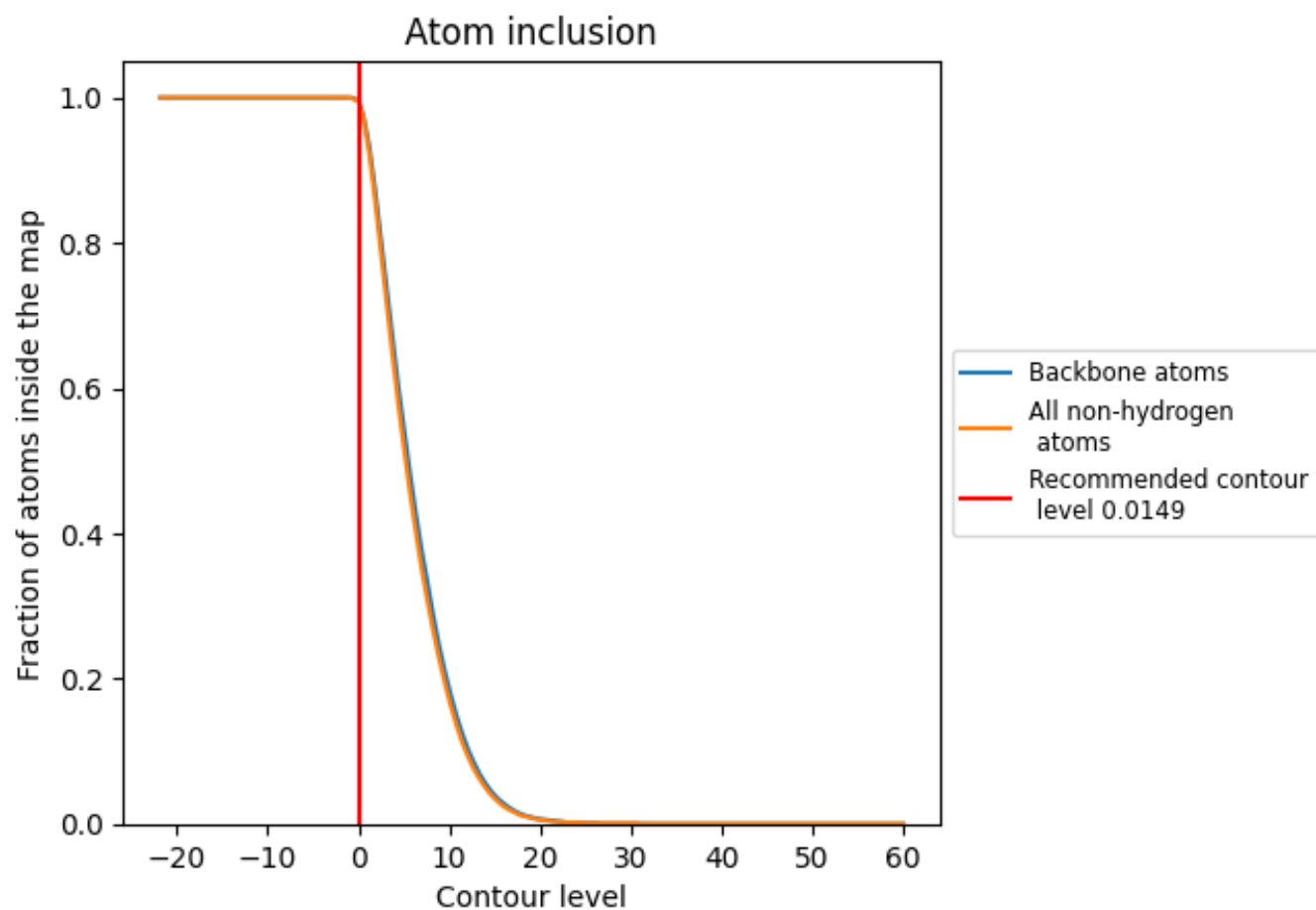
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0149).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.0149) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9950	 0.6100
A	 0.9960	 0.6240
B	 0.9960	 0.6230
C	 0.9970	 0.7170
D	 1.0000	 0.6860
E	 0.9940	 0.5800
F	 0.9880	 0.4410
G	 0.9950	 0.6180
H	 0.9960	 0.6180
I	 1.0000	 0.6990
J	 0.9870	 0.3880
K	 0.9860	 0.4140
L	 0.9990	 0.6850
M	 1.0000	 0.6520
N	 0.9980	 0.7120
O	 0.9990	 0.6740
P	 0.9850	 0.5580
Q	 0.9810	 0.4280
R	 0.9970	 0.6950
S	 0.9830	 0.3800
T	 0.9820	 0.3930
U	 0.9980	 0.6810
V	 1.0000	 0.6530
a	 0.9960	 0.6200
b	 0.9960	 0.6190
c	 0.9970	 0.7150
d	 1.0000	 0.6820
e	 0.9960	 0.5720
f	 0.9880	 0.4310
i	 1.0000	 0.6950
j	 0.9810	 0.3820
k	 0.9880	 0.3970
l	 0.9980	 0.6810
m	 1.0000	 0.6510

