



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 11:12 PM EDT

PDB ID : 6VPV / pdb_00006vpv
EMDB ID : EMD-21320
Title : Trimeric Photosystem I from the High-Light Tolerant Cyanobacteria
Cyanobacterium Aponinum
Authors : Dobson, Z.; Toporik, H.; Vaughn, N.; Lin, S.; Williams, D.; Fromme, P.;
Mazor, Y.
Deposited on : 2020-02-04
Resolution : 2.70 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

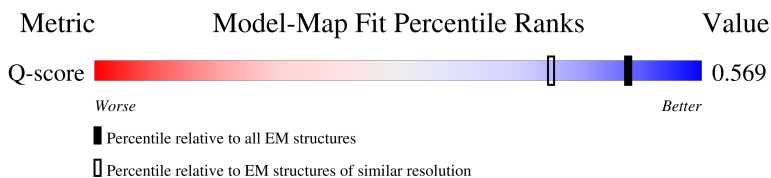
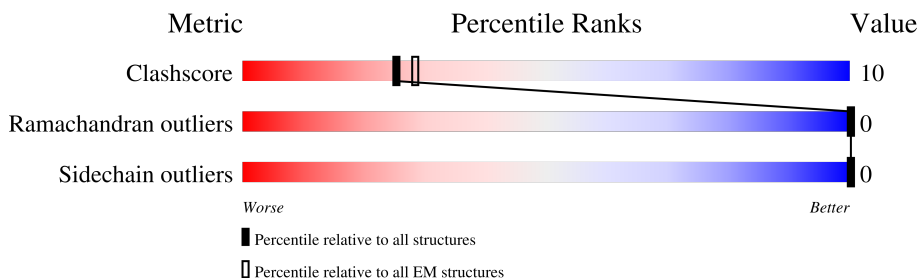
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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	10327 (2.20 - 3.20)

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	1	741	
1	A	741	
1	a	741	
2	2	737	

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Mol	Chain	Length	Quality of chain
2	B	737	
2	b	737	
3	3	80	
3	C	80	
3	c	80	
4	4	139	
4	D	139	
4	d	139	
5	5	68	
5	E	68	
5	e	68	
6	6	141	
6	F	141	
6	f	141	
7	7	38	
7	I	38	
7	i	38	
8	8	39	
8	J	39	
8	j	39	
9	9	78	
9	K	78	
9	k	78	
10	0	160	
10	L	160	

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Mol	Chain	Length	Quality of chain
10	l	160	72% 28%
11	M	30	97%
11	m	30	97%
11	z	30	97%

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 72192 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	741	Total	C	N	O	S	0	0
			5790	3797	983	984	26		
1	a	741	Total	C	N	O	S	0	0
			5790	3797	983	984	26		
1	1	741	Total	C	N	O	S	0	0
			5790	3797	983	984	26		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	320	ASN	SER	conflict	UNP A0A2G3P9X3
A	512	GLU	ASP	conflict	UNP A0A2G3P9X3
a	320	ASN	SER	conflict	UNP A0A2G3P9X3
a	512	GLU	ASP	conflict	UNP A0A2G3P9X3
1	320	ASN	SER	conflict	UNP A0A2G3P9X3
1	512	GLU	ASP	conflict	UNP A0A2G3P9X3

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	737	Total	C	N	O	S	0	0
			5815	3823	978	1000	14		
2	b	737	Total	C	N	O	S	0	0
			5815	3823	978	1000	14		
2	2	737	Total	C	N	O	S	0	0
			5815	3823	978	1000	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			599	368	103	117	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	80	Total	C	N	O	S	0	0
			599	368	103	117	11		
3	3	80	Total	C	N	O	S	0	0
			599	368	103	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	139	Total	C	N	O	S	0	0
			1097	699	185	209	4		
4	d	139	Total	C	N	O	S	0	0
			1097	699	185	209	4		
4	4	139	Total	C	N	O	S	0	0
			1097	699	185	209	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	68	Total	C	N	O	0	0
			539	342	94	103		
5	e	68	Total	C	N	O	0	0
			539	342	94	103		
5	5	68	Total	C	N	O	0	0
			539	342	94	103		

- Molecule 6 is a protein called PSI-F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	141	Total	C	N	O	S	0	0
			1100	708	180	207	5		
6	f	141	Total	C	N	O	S	0	0
			1100	708	180	207	5		
6	6	141	Total	C	N	O	S	0	0
			1100	708	180	207	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	38	Total	C	N	O	S	0	0
			275	186	39	48	2		
7	i	38	Total	C	N	O	S	0	0
			275	186	39	48	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	38	Total	C	N	O	S	0	0
			275	186	39	48	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	39	Total	C	N	O		0	0
			309	212	46	51			
8	j	39	Total	C	N	O		0	0
			309	212	46	51			
8	8	39	Total	C	N	O		0	0
			309	212	46	51			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	78	Total	C	N	O	S	0	0
			544	358	85	97	4		
9	k	78	Total	C	N	O	S	0	0
			544	358	85	97	4		
9	9	78	Total	C	N	O	S	0	0
			544	358	85	97	4		

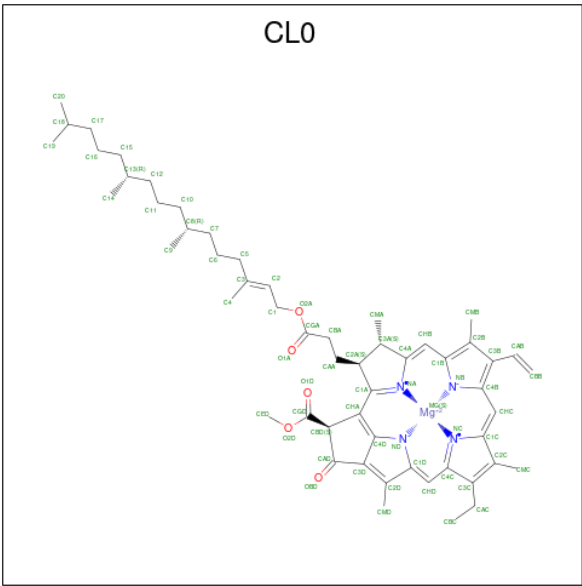
- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	160	Total	C	N	O	S	0	0
			1183	770	193	215	5		
10	l	160	Total	C	N	O	S	0	0
			1183	770	193	215	5		
10	0	160	Total	C	N	O	S	0	0
			1183	770	193	215	5		

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

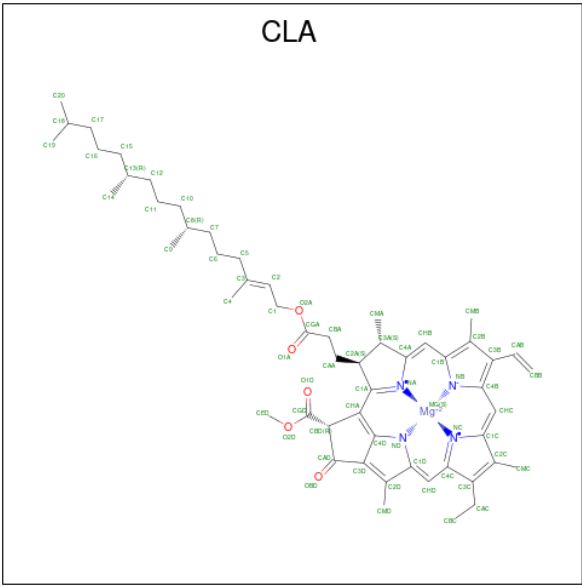
Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	30	Total	C	N	O		0	0
			232	156	35	41			
11	m	30	Total	C	N	O		0	0
			232	156	35	41			
11	z	30	Total	C	N	O		0	0
			232	156	35	41			

- Molecule 12 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

- Molecule 13 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
13	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	B	1	Total 62	C 52	Mg 1	N 4	O 5	0
13	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 40	C 32	Mg 1	N 4	O 3	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	F	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
13	I	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	J	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	J	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
13	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	K	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
13	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
13	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			40	32	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	i	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	j	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	j	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
13	j	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	k	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	k	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
13	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	l	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	l	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
13	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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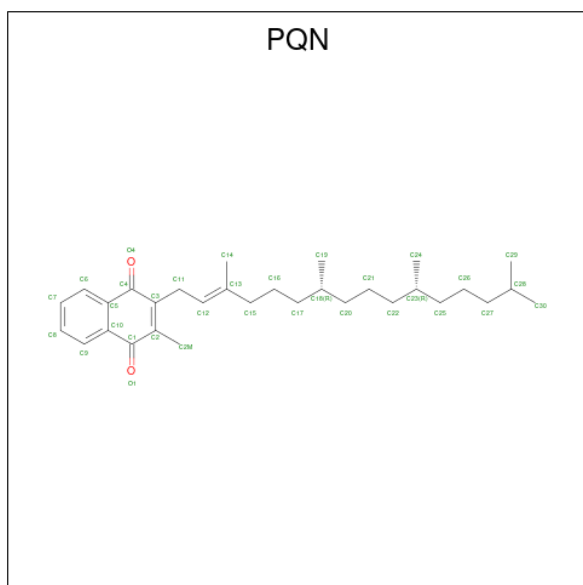
Mol	Chain	Residues	Atoms					AltConf
13	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	2	1	Total 62	C 52	Mg 1	N 4	O 5	0
13	2	1	Total 58	C 48	Mg 1	N 4	O 5	0
13	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	2	1	Total 40	C 32	Mg 1	N 4	O 3	0
13	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
13	7	1	Total 65	C 55	Mg 1	N 4	O 5	0

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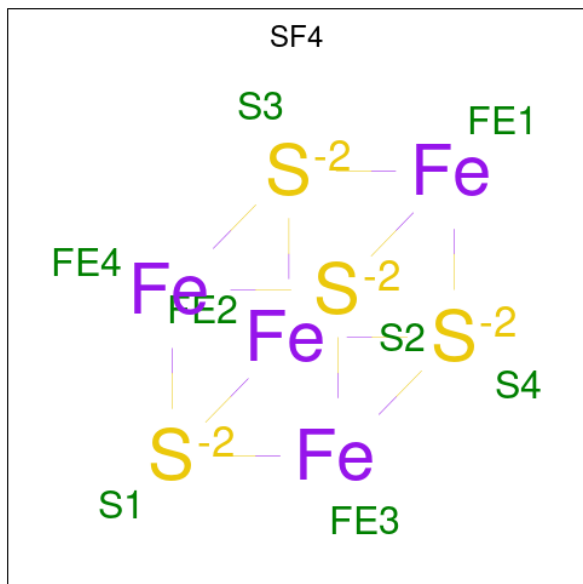
Mol	Chain	Residues	Atoms					AltConf
13	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	8	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
13	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	9	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
13	0	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	0	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	0	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 14 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms			AltConf
14	A	1	Total	C	O	0
			33	31	2	
14	B	1	Total	C	O	0
			33	31	2	
14	a	1	Total	C	O	0
			33	31	2	
14	b	1	Total	C	O	0
			33	31	2	
14	1	1	Total	C	O	0
			33	31	2	
14	2	1	Total	C	O	0
			33	31	2	

- Molecule 15 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



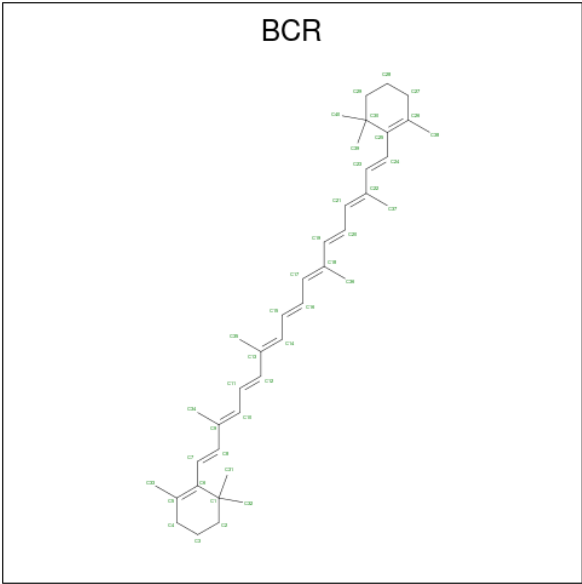
Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	Fe	S	0
			8	4	4	
15	C	1	Total	Fe	S	0
			8	4	4	
15	C	1	Total	Fe	S	0
			8	4	4	
15	a	1	Total	Fe	S	0
			8	4	4	
15	c	1	Total	Fe	S	0
			8	4	4	
15	c	1	Total	Fe	S	0
			8	4	4	

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Mol	Chain	Residues	Atoms			AltConf
15	1	1	Total	Fe	S	0
			8	4	4	
15	3	1	Total	Fe	S	0
			8	4	4	
15	3	1	Total	Fe	S	0
			8	4	4	

- Molecule 16 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



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

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Mol	Chain	Residues	Atoms	AltConf
16	B	1	Total C 40 40	0
16	B	1	Total C 40 40	0
16	B	1	Total C 40 40	0
16	B	1	Total C 40 40	0
16	F	1	Total C 40 40	0
16	F	1	Total C 40 40	0
16	I	1	Total C 40 40	0
16	J	1	Total C 40 40	0
16	J	1	Total C 40 40	0
16	K	1	Total C 40 40	0
16	K	1	Total C 40 40	0
16	L	1	Total C 40 40	0
16	L	1	Total C 40 40	0
16	L	1	Total C 40 40	0
16	M	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	b	1	Total C 40 40	0

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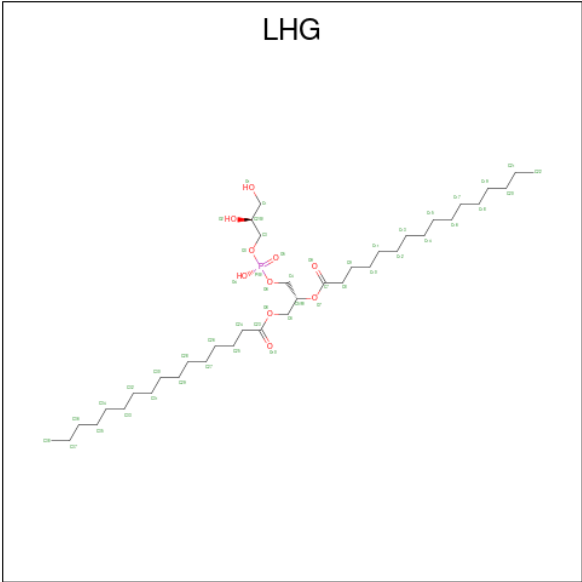
Mol	Chain	Residues	Atoms	AltConf
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	i	1	Total C 40 40	0
16	j	1	Total C 40 40	0
16	j	1	Total C 40 40	0
16	k	1	Total C 40 40	0
16	k	1	Total C 40 40	0
16	l	1	Total C 40 40	0
16	l	1	Total C 40 40	0
16	l	1	Total C 40 40	0
16	m	1	Total C 40 40	0
16	1	1	Total C 40 40	0
16	1	1	Total C 40 40	0
16	1	1	Total C 40 40	0
16	1	1	Total C 40 40	0

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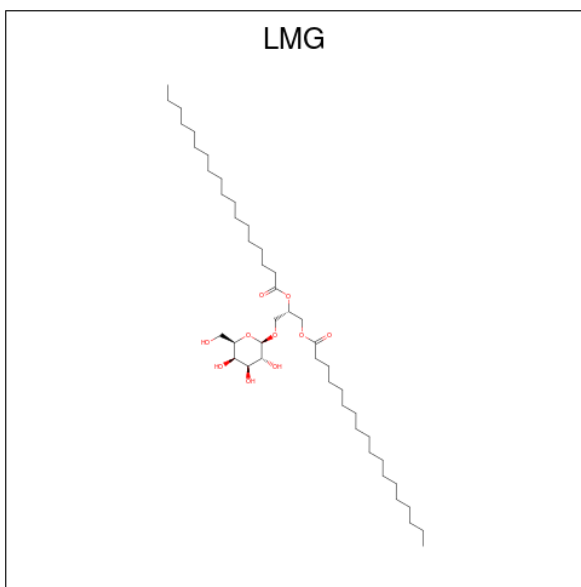
Mol	Chain	Residues	Atoms	AltConf
16	1	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	6	1	Total C 40 40	0
16	6	1	Total C 40 40	0
16	7	1	Total C 40 40	0
16	8	1	Total C 40 40	0
16	8	1	Total C 40 40	0
16	9	1	Total C 40 40	0
16	9	1	Total C 40 40	0
16	0	1	Total C 40 40	0
16	0	1	Total C 40 40	0
16	0	1	Total C 40 40	0
16	z	1	Total C 40 40	0

- Molecule 17 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



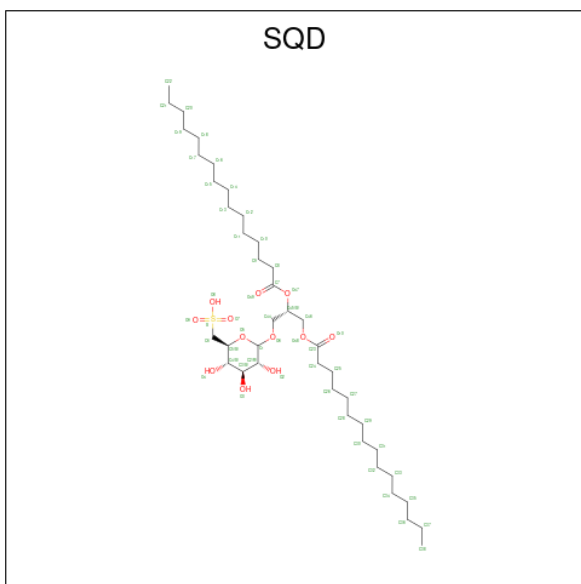
Mol	Chain	Residues	Atoms				AltConf
17	A	1	Total	C	O	P	0
			36	25	10	1	
17	A	1	Total	C	O	P	0
			41	30	10	1	
17	a	1	Total	C	O	P	0
			36	25	10	1	
17	a	1	Total	C	O	P	0
			41	30	10	1	
17	1	1	Total	C	O	P	0
			36	25	10	1	
17	1	1	Total	C	O	P	0
			41	30	10	1	

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
18	B	1	41	31	10	0
18	b	1	41	31	10	0
18	2	1	41	31	10	0

- Molecule 19 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).

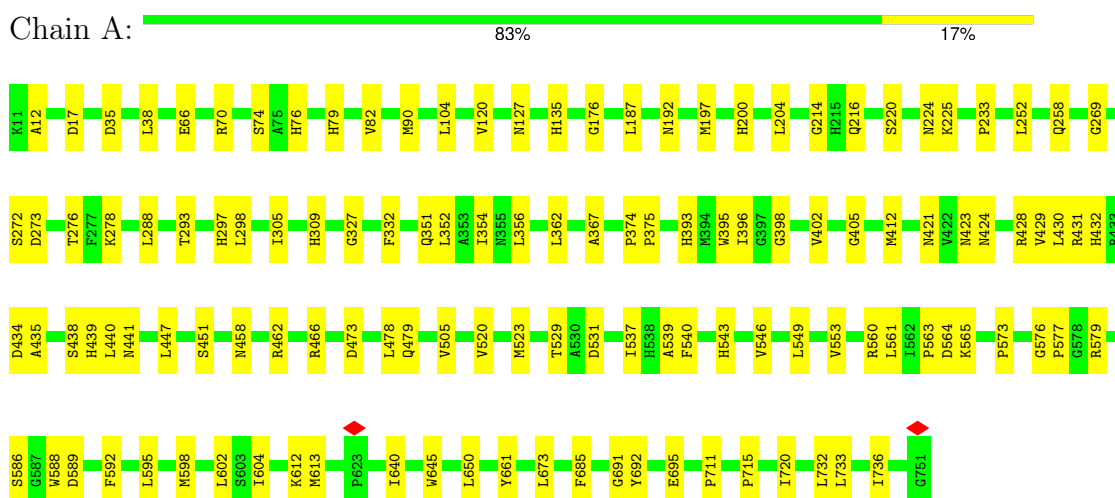


Mol	Chain	Residues	Atoms				AltConf
19	I	1	Total	C	O	S	0
			50	37	12	1	
19	i	1	Total	C	O	S	0
			50	37	12	1	
19	7	1	Total	C	O	S	0
			50	37	12	1	

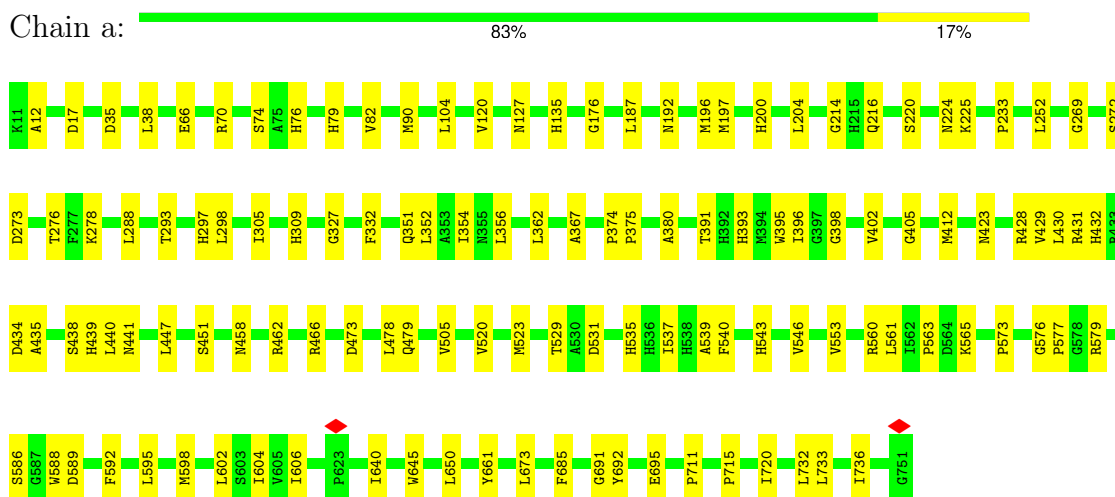
3 Residue-property plots

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.

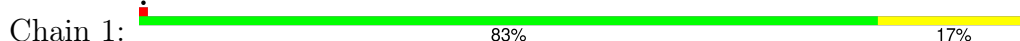
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

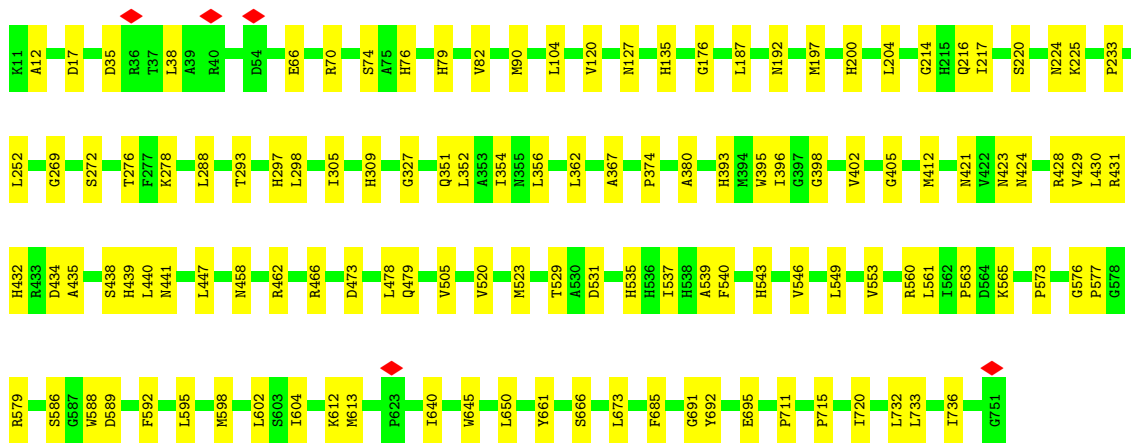


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



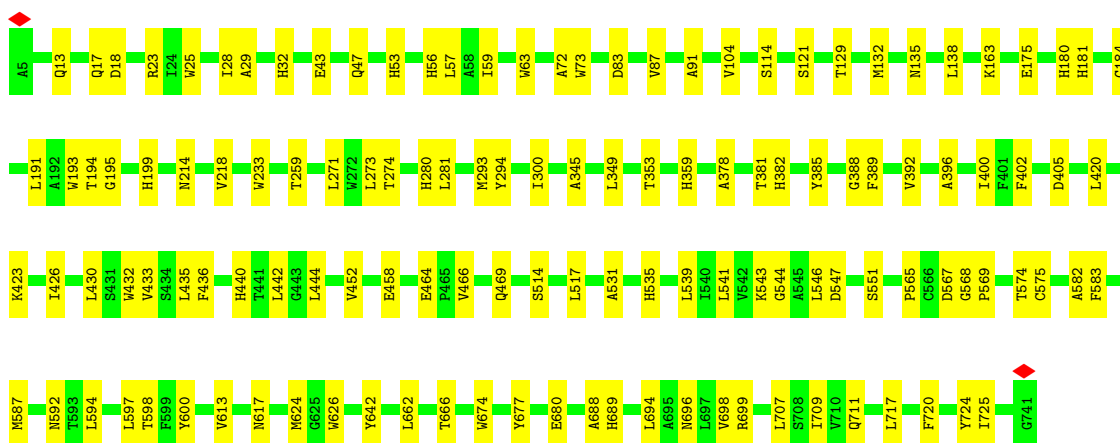
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1





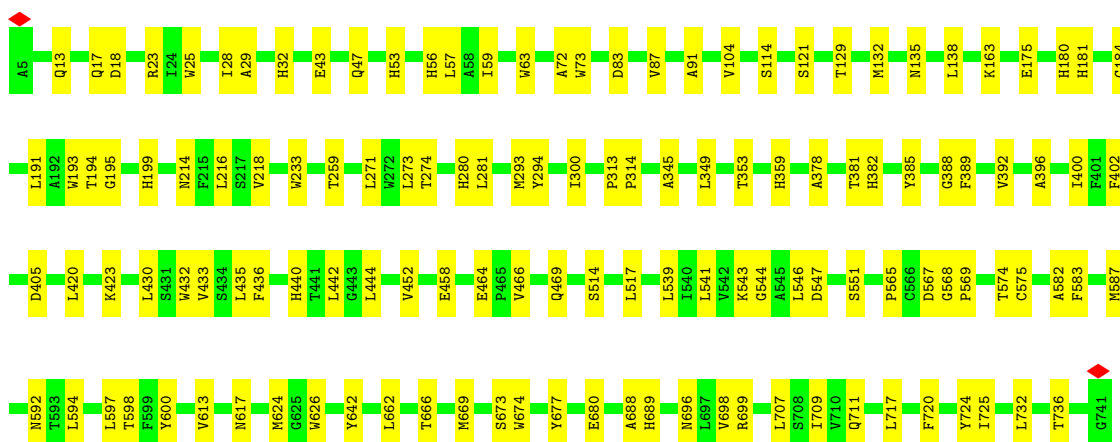
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 83% 17%



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b: 82% 18%



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

G568	G741	A396	G184	A5
P569		I400	L191	Q13
T574		F401	A192	
C575		F402	W193	Q17
A582		D405	T194	D18
F583		L420	G195	
M587		L420	H199	R23
		K423		T24
N592		I426	N214	W25
T593		L430	V218	T28
L594		L430	K219	A29
L597		S431	P220	H32
T598		W432	W233	E43
F599		V433		Q47
V600		S434	T259	
V613		L435	L271	H53
N617		F436	W272	
		H440	L273	H56
M624		T441	T274	L57
G625		L442	H280	A58
W626		G443	L281	I59
		L444		W63
V642		V452	M293	
		A453	Y294	A72
L662		E458	I300	W73
T666		E464	P313	D83
W674		P465	P314	W87
Y677		V466		A91
		Q469	A345	H92
E680		S514	L349	A93
A688		L517	T353	V104
H689			V356	S114
N696		A531	H359	S121
L697		H535	Y366	T129
R699		L539	A378	M132
L707		I540	T381	N135
S708		L541	H382	L138
I709		V542		K163
W710		K543	Y385	E175
Q711		G544		H180
		A545	G388	
L717		L546	F389	
		D547	V392	
F720		P565		
Y724		C566		
T725		D567		

-
- A horizontal bar chart showing the distribution of 20 items across 10 categories. The categories are labeled S2, K6, T15, D24, V25, M28, D32, G33, C34, K35, S41, T45, E55, C58, D61, F62, L63, R66, A71, and V81. The bars are colored yellow, green, or red. A red diamond is placed above the D61 bar.
- | Category | Value | Color |
|----------|-------|--------|
| S2 | 1 | Yellow |
| K6 | 1 | Yellow |
| T15 | 1 | Yellow |
| D24 | 1 | Yellow |
| V25 | 1 | Yellow |
| M28 | 1 | Yellow |
| D32 | 1 | Yellow |
| G33 | 1 | Green |
| C34 | 1 | Yellow |
| K35 | 1 | Yellow |
| S41 | 1 | Yellow |
| T45 | 1 | Yellow |
| E55 | 1 | Yellow |
| C58 | 1 | Yellow |
| D61 | 1 | Red |
| F62 | 1 | Yellow |
| L63 | 1 | Yellow |
| R66 | 1 | Yellow |
| A71 | 1 | Yellow |
| V81 | 1 | Green |

- | |
|-----|
| S2 |
| K6 |
| T15 |
| D24 |
| V25 |
| M28 |
| D32 |
| G33 |
| C34 |
| K35 |
| S41 |
| T45 |
| E55 |
| C58 |
| L63 |
| R66 |
| A71 |
| Y91 |

-
- | Category | Count |
|----------|-------|
| S2 | 1 |
| K6 | 1 |
| T15 | 1 |
| D24 | 1 |
| V25 | 1 |
| M28 | 1 |
| D32 | 1 |
| G33 | 2 |
| C34 | 2 |
| K35 | 1 |
| S41 | 1 |
| T45 | 1 |
| E55 | 1 |
| C58 | 1 |
| L63 | 1 |
| S64 | 1 |
| I65 | 2 |
| R66 | 1 |
| A71 | 1 |
| Y31 | 1 |

-
- | Month | Nodes |
|-------|-------|
| I3 | 100 |
| Q4 | 90 |
| S15 | 80 |
| T16 | 70 |
| R25 | 60 |
| T31 | 50 |
| T32 | 40 |
| P44 | 30 |
| N56 | 20 |
| R62 | 10 |
| K63 | 0 |
| E64 | 10 |
| Q65 | 20 |
| C66 | 30 |
| L67 | 40 |
| A68 | 50 |
| L69 | 60 |
| H99 | 70 |
| H116 | 80 |
| K119 | 90 |
| K133 | 100 |
| D141 | 110 |

- 

Chain d:  87% 13%



- Molecule 4: Photosystem I reaction center subunit II

Chain 4:  88% 12%



- Molecule 5: Photosystem I reaction center subunit IV

Chain E:  87% 13%



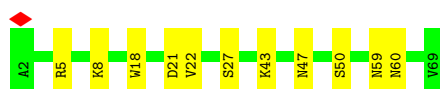
- Molecule 5: Photosystem I reaction center subunit IV

Chain e:  88% 12%



- Molecule 5: Photosystem I reaction center subunit IV

Chain 5:  84% 16%



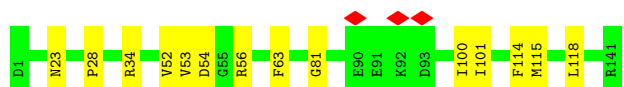
- Molecule 6: PSI-F

Chain F:  89% 11%



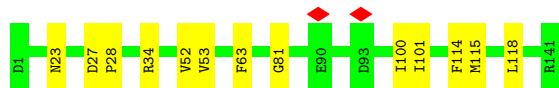
- Molecule 6: PSI-F

Chain f:  90% 10%



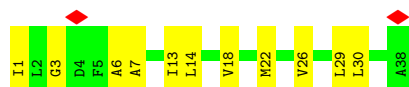
• Molecule 6: PSI-F

Chain 6:  91% 9%



• Molecule 7: Photosystem I reaction center subunit VIII

Chain I:  5% 71% 29%



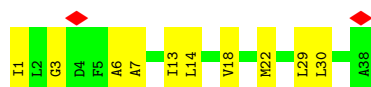
• Molecule 7: Photosystem I reaction center subunit VIII

Chain i:  5% 71% 29%



• Molecule 7: Photosystem I reaction center subunit VIII

Chain 7:  5% 74% 26%



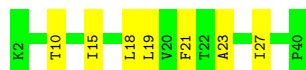
• Molecule 8: Photosystem I reaction center subunit IX

Chain J:  82% 18%



• Molecule 8: Photosystem I reaction center subunit IX

Chain j:  82% 18%

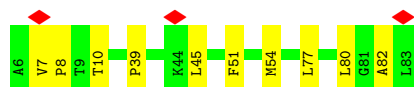
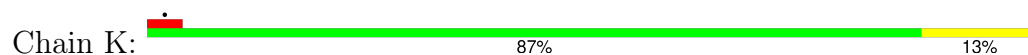


• Molecule 8: Photosystem I reaction center subunit IX

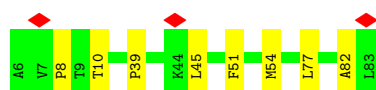
Chain 8:  82% 18%



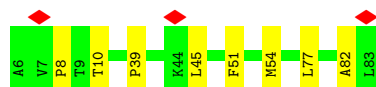
- Molecule 9: Photosystem I reaction center subunit PsaK



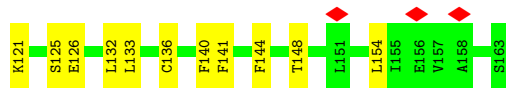
- Molecule 9: Photosystem I reaction center subunit PsaK



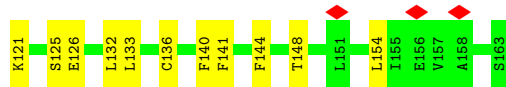
- Molecule 9: Photosystem I reaction center subunit PsaK



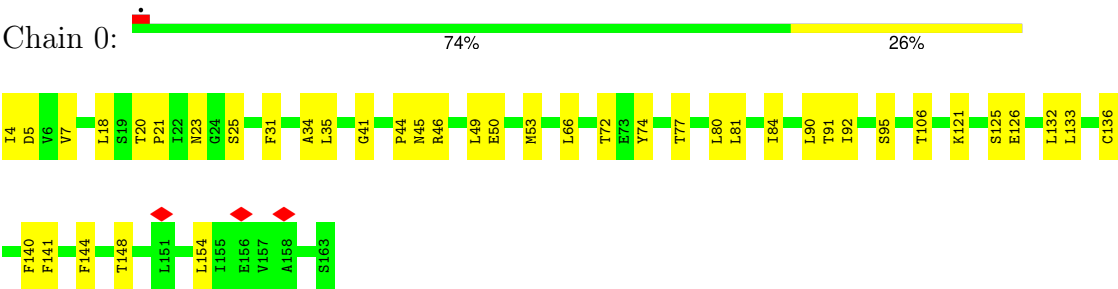
- Molecule 10: Photosystem I reaction center subunit XI



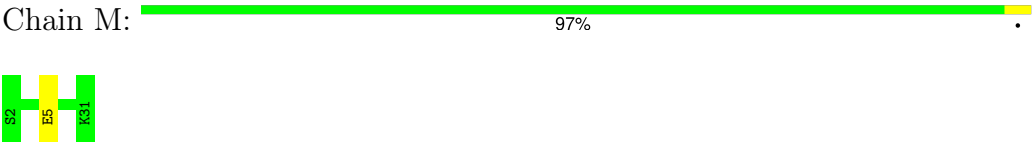
- Molecule 10: Photosystem I reaction center subunit XI



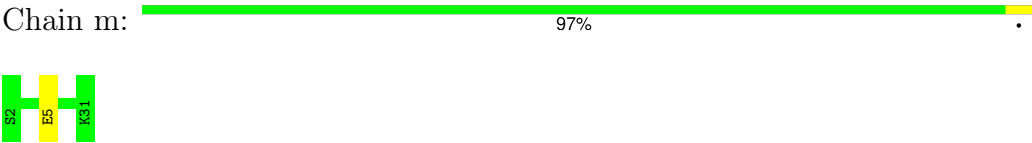
- Molecule 10: Photosystem I reaction center subunit XI



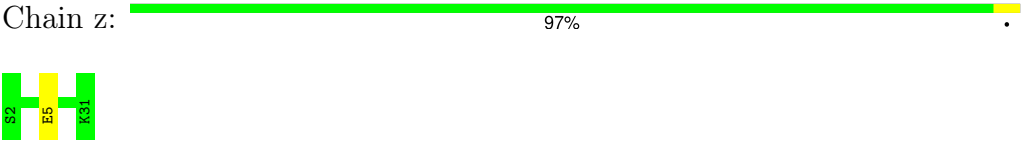
• Molecule 11: Photosystem I reaction center subunit XII



• Molecule 11: Photosystem I reaction center subunit XII



• Molecule 11: Photosystem I reaction center subunit XII



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	75290	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.53	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	37.813	Depositor
Minimum map value	-24.049	Depositor
Average map value	0.001	Depositor
Map value standard deviation	1.148	Depositor
Recommended contour level	2.1	Depositor
Map size (Å)	315.19998, 315.19998, 315.19998	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0506666, 1.0506666, 1.0506666	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.26	0/5986	0.49	0/8157
1	A	0.26	0/5986	0.49	0/8157
1	a	0.26	0/5986	0.49	0/8157
2	2	0.27	0/6026	0.53	0/8237
2	B	0.26	0/6026	0.53	0/8237
2	b	0.27	0/6026	0.53	0/8237
3	3	0.26	0/609	0.54	0/824
3	C	0.26	0/609	0.54	0/824
3	c	0.26	0/609	0.54	0/824
4	4	0.24	0/1123	0.61	0/1514
4	D	0.24	0/1123	0.61	0/1514
4	d	0.25	0/1123	0.61	0/1514
5	5	0.21	0/549	0.48	0/741
5	E	0.21	0/549	0.48	0/741
5	e	0.21	0/549	0.48	0/741
6	6	0.25	0/1130	0.59	0/1533
6	F	0.24	0/1130	0.59	0/1533
6	f	0.25	0/1130	0.59	0/1533
7	7	0.26	0/280	0.66	0/381
7	I	0.26	0/280	0.66	0/381
7	i	0.26	0/280	0.66	0/381
8	8	0.28	0/318	0.43	0/435
8	J	0.28	0/318	0.43	0/435
8	j	0.28	0/318	0.43	0/435
9	9	0.28	0/556	0.67	0/759
9	K	0.28	0/556	0.67	0/759
9	k	0.28	0/556	0.67	0/759
10	0	0.27	0/1215	0.71	0/1659
10	L	0.27	0/1215	0.71	0/1659
10	l	0.27	0/1215	0.71	0/1659
11	M	0.16	0/235	0.37	0/318
11	m	0.16	0/235	0.37	0/318

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	z	0.16	0/235	0.37	0/318
All	All	0.26	0/54081	0.54	0/73674

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	2	0	1
2	B	0	1
2	b	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	674	TRP	Peptide
2	B	674	TRP	Peptide
2	b	674	TRP	Peptide

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	1	5790	0	5666	97	0
1	A	5790	0	5666	102	0
1	a	5790	0	5666	98	0
2	2	5815	0	5585	111	0
2	B	5815	0	5585	110	0
2	b	5815	0	5585	109	0
3	3	599	0	579	13	0
3	C	599	0	579	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c	599	0	579	12	0
4	4	1097	0	1080	15	0
4	D	1097	0	1080	16	0
4	d	1097	0	1080	16	0
5	5	539	0	530	7	0
5	E	539	0	530	6	0
5	e	539	0	530	5	0
6	6	1100	0	1075	19	0
6	F	1100	0	1075	19	0
6	f	1100	0	1075	20	0
7	7	275	0	296	22	0
7	I	275	0	296	23	0
7	i	275	0	296	24	0
8	8	309	0	323	7	0
8	J	309	0	323	7	0
8	j	309	0	323	7	0
9	9	544	0	556	5	0
9	K	544	0	556	7	0
9	k	544	0	556	5	0
10	0	1183	0	1186	111	0
10	L	1183	0	1186	123	0
10	l	1183	0	1186	114	0
11	M	232	0	252	1	0
11	m	232	0	252	1	0
11	z	232	0	252	1	0
12	1	65	0	72	5	0
12	A	65	0	72	5	0
12	a	65	0	72	5	0
13	0	286	0	275	16	0
13	1	2387	0	2270	113	0
13	2	2184	0	2136	88	0
13	6	146	0	115	3	0
13	7	65	0	72	8	0
13	8	135	0	100	3	0
13	9	135	0	96	1	0
13	A	2387	0	2270	107	0
13	B	2249	0	2208	90	0
13	F	146	0	115	6	0
13	I	65	0	72	9	0
13	J	135	0	100	3	0
13	K	135	0	96	0	0
13	L	221	0	203	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	a	2387	0	2270	109	0
13	b	2249	0	2208	90	0
13	f	146	0	115	6	0
13	i	65	0	72	9	0
13	j	135	0	100	3	0
13	k	135	0	96	0	0
13	l	221	0	203	15	0
14	1	33	0	46	2	0
14	2	33	0	46	7	0
14	A	33	0	46	4	0
14	B	33	0	46	7	0
14	a	33	0	46	4	0
14	b	33	0	46	6	0
15	1	8	0	0	0	0
15	3	16	0	0	1	0
15	A	8	0	0	0	0
15	C	16	0	0	0	0
15	a	8	0	0	0	0
15	c	16	0	0	0	0
16	0	120	0	168	10	0
16	1	200	0	280	18	0
16	2	280	0	392	23	0
16	6	80	0	112	4	0
16	7	40	0	56	3	0
16	8	80	0	112	5	0
16	9	80	0	112	5	0
16	A	200	0	280	20	0
16	B	280	0	392	19	0
16	F	80	0	112	5	0
16	I	40	0	56	5	0
16	J	80	0	112	3	0
16	K	80	0	112	2	0
16	L	120	0	168	16	0
16	M	40	0	56	2	0
16	a	200	0	280	17	0
16	b	280	0	392	21	0
16	f	80	0	112	4	0
16	i	40	0	56	5	0
16	j	80	0	112	4	0
16	k	80	0	112	2	0
16	l	120	0	168	12	0
16	m	40	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	z	40	0	56	3	0
17	1	77	0	97	2	0
17	A	77	0	97	2	0
17	a	77	0	97	1	0
18	2	41	0	52	3	0
18	B	41	0	52	3	0
18	b	41	0	52	3	0
19	7	50	0	64	12	0
19	I	50	0	64	13	0
19	i	50	0	64	12	0
All	All	72192	0	71571	1491	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 10.

All (1491) 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)
6:6:115:MET:CE	6:6:118:LEU:HD12	1.29	1.59
6:F:115:MET:CE	6:F:118:LEU:HD12	1.29	1.58
6:f:115:MET:CE	6:f:118:LEU:HD12	1.29	1.56
7:i:30:LEU:HD21	19:i:101:SQD:C29	1.37	1.52
7:I:30:LEU:HD21	19:I:103:SQD:C29	1.40	1.46
7:7:30:LEU:HD21	19:7:101:SQD:C29	1.45	1.44
6:F:115:MET:CE	6:F:118:LEU:CD1	2.04	1.36
6:f:115:MET:CE	6:f:118:LEU:CD1	2.04	1.35
6:6:115:MET:CE	6:6:118:LEU:CD1	2.04	1.34
7:i:30:LEU:CD2	19:i:101:SQD:H292	1.59	1.32
7:i:30:LEU:CD2	19:i:101:SQD:C29	2.12	1.28
7:I:30:LEU:CD2	19:I:103:SQD:H292	1.68	1.24
7:7:30:LEU:CD2	19:7:101:SQD:H292	1.69	1.23
7:I:30:LEU:CD2	19:I:103:SQD:C29	2.17	1.21
7:7:30:LEU:CD2	19:7:101:SQD:C29	2.22	1.18
7:i:30:LEU:HD21	19:i:101:SQD:H291	1.17	1.15
7:7:30:LEU:HD21	19:7:101:SQD:H291	1.24	1.14
7:I:30:LEU:HD21	19:I:103:SQD:H291	1.18	1.14
10:l:136:CYS:SG	16:l:201:BCR:H24C	1.91	1.09
10:L:144:PHE:CZ	10:L:80:LEU:HD23	1.89	1.08
7:7:30:LEU:HD21	19:7:101:SQD:H292	1.20	1.08
6:F:115:MET:HE1	6:F:118:LEU:CD1	1.83	1.07
6:f:115:MET:HE1	6:f:118:LEU:CD1	1.83	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:i:30:LEU:HD21	19:i:101:SQD:H292	1.12	1.04
7:I:30:LEU:HD21	19:I:103:SQD:H292	1.21	1.04
6:6:115:MET:HE1	6:6:118:LEU:CD1	1.83	1.04
10:L:136:CYS:SG	16:L:207:BCR:H24C	2.00	1.02
10:0:136:CYS:SG	16:0:201:BCR:H24C	2.00	1.00
10:l:154:LEU:CD2	7:7:13:ILE:HD11	1.92	1.00
7:I:13:ILE:HD11	10:0:154:LEU:CD2	1.94	0.98
10:l:144:PHE:CZ	10:0:80:LEU:HD23	1.99	0.97
6:F:115:MET:HE3	6:F:118:LEU:CD1	1.81	0.97
6:F:115:MET:HE1	6:F:118:LEU:HD11	1.45	0.97
10:L:154:LEU:CD2	7:i:13:ILE:HD11	1.95	0.97
6:f:115:MET:HE3	6:f:118:LEU:CD1	1.81	0.96
6:f:115:MET:HE1	6:f:118:LEU:HD11	1.45	0.96
10:L:77:THR:HG21	10:0:148:THR:CG2	1.95	0.95
10:L:4:ILE:HD13	2:b:163:LYS:HZ1	1.29	0.95
6:6:115:MET:HE1	6:6:118:LEU:HD11	1.45	0.95
6:F:115:MET:HE3	6:F:118:LEU:HD12	0.95	0.95
10:L:80:LEU:HD23	10:0:144:PHE:CZ	2.02	0.94
6:6:115:MET:HE3	6:6:118:LEU:HD12	0.95	0.94
10:l:4:ILE:HD13	2:2:163:LYS:HZ1	1.33	0.94
2:B:163:LYS:NZ	10:0:4:ILE:HD13	1.82	0.94
10:L:133:LEU:HD21	10:0:49:LEU:CD1	1.98	0.94
6:6:115:MET:HE3	6:6:118:LEU:CD1	1.81	0.94
6:f:115:MET:HE2	6:f:118:LEU:HD12	1.48	0.93
10:L:77:THR:HG23	10:0:144:PHE:CZ	2.04	0.93
6:f:115:MET:HE3	6:f:118:LEU:HD12	0.95	0.93
10:L:148:THR:CG2	10:l:77:THR:HG21	1.98	0.92
10:L:49:LEU:CD1	10:l:133:LEU:HD21	1.98	0.92
10:L:140:PHE:CZ	10:0:140:PHE:HE2	1.86	0.92
6:f:114:PHE:CE2	6:f:115:MET:HG2	2.05	0.92
7:i:30:LEU:HD23	19:i:101:SQD:H292	1.51	0.91
6:6:115:MET:HE2	6:6:118:LEU:HD12	1.48	0.91
6:F:114:PHE:CE2	6:F:115:MET:HG2	2.05	0.91
10:L:74:TYR:CE1	10:0:148:THR:O	2.24	0.91
10:L:133:LEU:HD21	10:0:49:LEU:HD13	1.51	0.91
6:F:115:MET:HE2	6:F:118:LEU:HD12	1.48	0.90
6:6:114:PHE:CE2	6:6:115:MET:HG2	2.05	0.90
10:L:132:LEU:HD22	13:0:205:CLA:HED2	1.54	0.90
10:L:81:LEU:HD21	10:0:144:PHE:HD2	1.36	0.90
10:l:4:ILE:HD13	2:2:163:LYS:NZ	1.90	0.87
7:I:30:LEU:HD23	19:I:103:SQD:H292	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:77:THR:CG2	10:0:148:THR:HG21	2.04	0.87
10:l:148:THR:CG2	10:0:77:THR:HG21	2.05	0.87
10:l:144:PHE:HD2	10:0:81:LEU:HD21	1.39	0.87
10:L:140:PHE:HE2	10:l:140:PHE:CZ	1.93	0.86
10:l:49:LEU:CD1	10:0:133:LEU:HD21	2.04	0.86
10:L:144:PHE:HD2	10:l:81:LEU:HD21	1.42	0.85
10:L:140:PHE:CZ	10:0:140:PHE:CE2	2.65	0.85
10:L:148:THR:O	10:l:74:TYR:CE1	2.30	0.85
10:L:4:ILE:HD13	2:b:163:LYS:NZ	1.91	0.84
10:L:49:LEU:HD13	10:l:133:LEU:HD21	1.59	0.84
7:I:29:LEU:HD21	19:I:103:SQD:H92	1.60	0.84
10:L:148:THR:HG21	10:l:77:THR:CG2	2.07	0.84
7:I:13:ILE:HD11	10:0:154:LEU:HD22	1.60	0.83
10:l:140:PHE:HE2	10:0:140:PHE:CZ	1.97	0.83
10:l:49:LEU:HD13	10:0:133:LEU:HD21	1.62	0.82
10:L:148:THR:HG22	10:l:77:THR:HG21	1.61	0.82
2:B:163:LYS:HZ1	10:0:4:ILE:HD13	1.42	0.81
10:l:136:CYS:SG	16:l:201:BCR:C24	2.68	0.81
10:L:77:THR:HG21	10:0:148:THR:HG22	1.61	0.81
10:l:144:PHE:CZ	10:0:77:THR:HG23	2.16	0.81
10:L:140:PHE:CE2	10:l:140:PHE:CZ	2.70	0.80
10:l:148:THR:O	10:0:74:TYR:CE1	2.34	0.80
10:l:154:LEU:HD21	7:7:13:ILE:HD11	1.61	0.79
7:7:30:LEU:HD23	19:7:101:SQD:H292	1.60	0.79
10:L:81:LEU:HD21	10:0:144:PHE:CD2	2.19	0.79
10:L:154:LEU:HD21	7:i:13:ILE:HD11	1.65	0.79
7:i:29:LEU:HD21	19:i:101:SQD:H92	1.65	0.78
10:l:148:THR:HG21	10:0:77:THR:CG2	2.14	0.78
10:l:154:LEU:HD22	7:7:13:ILE:HD11	1.64	0.78
10:L:136:CYS:SG	16:L:207:BCR:C24	2.72	0.78
10:l:144:PHE:CD2	10:0:81:LEU:HD21	2.19	0.78
13:l:204:CLA:HED2	10:0:132:LEU:HD22	1.64	0.77
10:L:53:MET:SD	10:l:132:LEU:HD21	2.25	0.77
7:7:29:LEU:HD21	19:7:101:SQD:H92	1.66	0.77
10:L:144:PHE:CZ	10:l:77:THR:HG23	2.21	0.76
10:l:148:THR:HG22	10:0:77:THR:HG21	1.68	0.76
13:L:203:CLA:HED2	10:l:132:LEU:HD22	1.66	0.75
10:L:154:LEU:HD22	7:i:13:ILE:HD11	1.67	0.75
10:0:136:CYS:SG	16:0:201:BCR:C24	2.74	0.75
10:L:49:LEU:HD11	10:l:133:LEU:HD21	1.67	0.74
7:I:30:LEU:CD2	19:I:103:SQD:C28	2.64	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:77:THR:HG21	10:0:148:THR:HG21	1.66	0.74
10:L:144:PHE:CD2	10:l:81:LEU:HD21	2.22	0.74
10:l:140:PHE:CE2	10:0:140:PHE:CZ	2.75	0.74
2:B:163:LYS:NZ	10:0:4:ILE:CD1	2.51	0.73
10:L:74:TYR:HE1	10:0:148:THR:O	1.72	0.73
10:L:148:THR:CG2	10:l:77:THR:CG2	2.65	0.73
7:I:13:ILE:HD11	10:0:154:LEU:HD21	1.68	0.73
7:i:30:LEU:CD2	19:i:101:SQD:C28	2.67	0.73
7:I:30:LEU:HD22	19:I:103:SQD:H281	1.70	0.73
6:F:100:ILE:HG12	8:J:10:THR:HG22	1.71	0.72
10:L:132:LEU:HD21	10:0:53:MET:SD	2.30	0.72
6:6:100:ILE:HG12	8:8:10:THR:HG22	1.71	0.71
7:i:30:LEU:HD22	19:i:101:SQD:H281	1.72	0.71
6:f:100:ILE:HG12	8:j:10:THR:HG22	1.71	0.71
10:L:148:THR:O	10:l:74:TYR:HE1	1.72	0.71
13:b:808:CLA:HBB2	13:b:810:CLA:HMA3	1.74	0.70
10:l:53:MET:SD	10:0:132:LEU:HD21	2.32	0.70
13:2:835:CLA:H2	13:2:836:CLA:H121	1.74	0.70
13:B:808:CLA:HBB2	13:B:810:CLA:HMA3	1.74	0.70
13:2:807:CLA:HBB2	13:2:809:CLA:HMA3	1.74	0.69
13:B:836:CLA:H2	13:B:837:CLA:H121	1.74	0.69
2:b:195:GLY:O	2:b:199:HIS:HB2	1.93	0.69
13:b:836:CLA:H2	13:b:837:CLA:H121	1.74	0.69
10:l:136:CYS:HB3	16:l:201:BCR:H393	1.74	0.69
2:2:195:GLY:O	2:2:199:HIS:HB2	1.93	0.68
2:B:163:LYS:HD2	10:0:4:ILE:HD11	1.76	0.68
2:B:195:GLY:O	2:B:199:HIS:HB2	1.93	0.68
7:7:30:LEU:CD2	19:7:101:SQD:C28	2.72	0.67
13:1:826:CLA:H51	13:1:836:CLA:H2	1.76	0.67
10:L:132:LEU:HD21	10:0:53:MET:CE	2.25	0.67
10:l:49:LEU:HD11	10:0:133:LEU:HD21	1.75	0.67
3:3:24:ASP:HB2	4:4:67:LEU:HD21	1.77	0.67
13:a:831:CLA:HMC3	13:a:838:CLA:HBB1	1.76	0.67
13:A:831:CLA:HMC3	13:A:838:CLA:HBB1	1.76	0.67
10:L:95:SER:OG	10:0:46:ARG:NH2	2.23	0.67
1:A:398:GLY:HA3	1:A:602:LEU:HD11	1.76	0.67
3:c:24:ASP:HB2	4:d:67:LEU:HD21	1.77	0.67
3:C:24:ASP:HB2	4:D:67:LEU:HD21	1.76	0.67
6:F:114:PHE:CD2	6:F:115:MET:HG2	2.29	0.67
1:a:398:GLY:HA3	1:a:602:LEU:HD11	1.77	0.67
6:6:114:PHE:CD2	6:6:115:MET:HG2	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:826:CLA:H51	13:A:836:CLA:H2	1.76	0.66
13:a:826:CLA:H51	13:a:836:CLA:H2	1.76	0.66
10:l:4:ILE:HD11	2:2:163:LYS:HD2	1.77	0.66
2:B:544:GLY:HA3	2:B:582:ALA:HB2	1.78	0.66
6:f:114:PHE:CD2	6:f:115:MET:HG2	2.30	0.66
2:2:544:GLY:HA3	2:2:582:ALA:HB2	1.78	0.66
13:1:831:CLA:HMC3	13:1:838:CLA:HBB1	1.77	0.65
10:l:148:THR:O	10:0:74:TYR:HE1	1.79	0.65
7:I:30:LEU:CD2	19:I:103:SQD:H281	2.24	0.65
1:1:398:GLY:HA3	1:1:602:LEU:HD11	1.76	0.65
10:l:4:ILE:CD1	2:2:163:LYS:NZ	2.59	0.65
7:7:30:LEU:HD22	19:7:101:SQD:H281	1.77	0.65
10:L:77:THR:CG2	10:0:144:PHE:CZ	2.78	0.65
2:b:544:GLY:HA3	2:b:582:ALA:HB2	1.78	0.64
10:L:133:LEU:HD21	10:0:49:LEU:HD11	1.75	0.64
2:b:385:TYR:HA	2:b:594:LEU:HD13	1.80	0.64
10:L:133:LEU:CD2	10:0:49:LEU:CD1	2.75	0.64
10:L:53:MET:CE	10:l:132:LEU:HD21	2.28	0.64
13:1:826:CLA:H61	13:1:838:CLA:H42	1.80	0.64
10:L:49:LEU:HD11	10:l:133:LEU:CD2	2.28	0.64
13:1:839:CLA:H41	16:6:202:BCR:H21C	1.80	0.64
10:L:46:ARG:NH2	10:l:95:SER:OG	2.31	0.64
13:A:826:CLA:H61	13:A:838:CLA:H42	1.80	0.63
10:L:4:ILE:CD1	2:b:163:LYS:NZ	2.61	0.63
10:L:77:THR:HG23	10:0:144:PHE:HZ	1.58	0.63
13:a:839:CLA:H41	16:f:202:BCR:H21C	1.80	0.63
13:b:805:CLA:HMB2	13:b:826:CLA:HBB2	1.80	0.63
13:1:802:CLA:H101	16:1:848:BCR:H23C	1.81	0.63
13:A:802:CLA:H101	16:A:848:BCR:H23C	1.81	0.63
13:a:826:CLA:H61	13:a:838:CLA:H42	1.80	0.63
13:a:802:CLA:H101	16:a:848:BCR:H23C	1.81	0.62
14:b:839:PQN:H142	16:b:845:BCR:H271	1.81	0.62
1:A:478:LEU:HB2	1:A:529:THR:HG23	1.81	0.62
13:A:839:CLA:H41	16:F:202:BCR:H21C	1.80	0.62
10:L:133:LEU:HD11	10:0:133:LEU:HB3	1.80	0.62
13:a:826:CLA:H2	13:a:834:CLA:HBB2	1.81	0.62
10:0:136:CYS:HB3	16:0:201:BCR:H393	1.81	0.62
1:a:478:LEU:HB2	1:a:529:THR:HG23	1.81	0.62
14:2:838:PQN:H142	16:2:844:BCR:H271	1.82	0.62
1:A:736:ILE:HG23	13:A:828:CLA:HAB	1.81	0.62
2:B:385:TYR:HA	2:B:594:LEU:HD13	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:696:ASN:HB2	10:l:106:THR:HB	1.82	0.62
13:1:826:CLA:H2	13:1:834:CLA:HBB2	1.82	0.62
2:2:385:TYR:HA	2:2:594:LEU:HD13	1.80	0.62
9:k:39:PRO:HB2	9:k:54:MET:HG2	1.81	0.62
10:l:46:ARG:NH2	10:0:95:SER:OG	2.31	0.62
13:A:826:CLA:H2	13:A:834:CLA:HBB2	1.82	0.62
13:L:203:CLA:HMD3	10:l:95:SER:HB2	1.82	0.62
9:9:39:PRO:HB2	9:9:54:MET:HG2	1.80	0.62
13:B:805:CLA:HMB2	13:B:826:CLA:HBB2	1.81	0.62
1:1:478:LEU:HB2	1:1:529:THR:HG23	1.81	0.62
1:1:736:ILE:HG23	13:1:828:CLA:HAB	1.81	0.62
2:B:163:LYS:HZ2	10:0:4:ILE:CD1	2.11	0.61
3:3:15:THR:HA	3:3:28:MET:HE3	1.82	0.61
2:B:696:ASN:HB2	10:L:106:THR:HB	1.82	0.61
14:B:839:PQN:H142	16:B:845:BCR:H271	1.82	0.61
2:b:436:PHE:O	2:b:440:HIS:ND1	2.30	0.61
1:A:520:VAL:HG11	1:A:523:MET:HG3	1.83	0.61
9:K:39:PRO:HB2	9:K:54:MET:HG2	1.81	0.61
2:2:696:ASN:HB2	10:0:106:THR:HB	1.82	0.61
2:2:436:PHE:O	2:2:440:HIS:ND1	2.30	0.61
3:c:15:THR:HA	3:c:28:MET:HE3	1.83	0.61
3:C:15:THR:HA	3:C:28:MET:HE3	1.83	0.61
4:D:62:ARG:NH2	4:D:64:GLU:OE1	2.34	0.61
10:L:95:SER:HB2	13:0:205:CLA:HMD3	1.83	0.61
1:a:736:ILE:HG23	13:a:828:CLA:HAB	1.81	0.61
1:1:520:VAL:HG11	1:1:523:MET:HG3	1.83	0.61
13:2:805:CLA:HMB2	13:2:825:CLA:HBB2	1.81	0.61
7:i:30:LEU:CD2	19:i:101:SQD:H281	2.31	0.60
4:4:62:ARG:NH2	4:4:64:GLU:OE1	2.34	0.60
10:L:4:ILE:HD11	2:b:163:LYS:HD2	1.84	0.60
1:a:595:LEU:HB3	1:a:732:LEU:HD11	1.83	0.60
2:B:436:PHE:O	2:B:440:HIS:ND1	2.30	0.60
2:B:13:GLN:O	2:B:17:GLN:NE2	2.35	0.60
2:B:32:HIS:ND1	13:B:805:CLA:O1A	2.35	0.60
9:K:77:LEU:HB3	9:K:82:ALA:HB3	1.84	0.60
13:a:840:CLA:H91	8:j:19:LEU:HD12	1.84	0.60
13:1:810:CLA:HBB2	13:1:813:CLA:HMA3	1.84	0.60
1:1:120:VAL:HG21	8:8:27:ILE:HG23	1.83	0.60
13:1:840:CLA:H91	8:8:19:LEU:HD12	1.84	0.60
2:2:32:HIS:ND1	13:2:805:CLA:O1A	2.35	0.60
13:B:823:CLA:H72	16:B:844:BCR:H362	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:13:GLN:O	2:b:17:GLN:NE2	2.35	0.60
13:b:825:CLA:H8	16:b:841:BCR:H21C	1.84	0.60
1:1:595:LEU:HB3	1:1:732:LEU:HD11	1.83	0.60
1:A:595:LEU:HB3	1:A:732:LEU:HD11	1.83	0.60
1:a:120:VAL:HG21	8:j:27:ILE:HG23	1.83	0.60
1:a:520:VAL:HG11	1:a:523:MET:HG3	1.83	0.59
2:b:32:HIS:ND1	13:b:805:CLA:O1A	2.35	0.59
13:B:825:CLA:H8	16:B:841:BCR:H21C	1.84	0.59
2:2:13:GLN:O	2:2:17:GLN:NE2	2.35	0.59
4:d:62:ARG:NH2	4:d:64:GLU:OE1	2.34	0.59
13:2:824:CLA:H8	16:2:840:BCR:H21C	1.84	0.59
10:L:133:LEU:CD2	10:0:49:LEU:HD11	2.31	0.59
2:b:29:ALA:HB2	18:b:846:LMG:H141	1.84	0.59
13:b:823:CLA:H72	16:b:844:BCR:H362	1.84	0.59
1:a:351:GLN:HG3	13:a:825:CLA:H122	1.84	0.59
13:A:839:CLA:H172	13:F:201:CLA:HED2	1.85	0.59
13:a:810:CLA:HBB2	13:a:813:CLA:HMA3	1.84	0.59
16:a:848:BCR:H16C	13:a:852:CLA:H8	1.85	0.59
7:7:30:LEU:CD2	19:7:101:SQD:H281	2.33	0.59
9:9:77:LEU:HB3	9:9:82:ALA:HB3	1.84	0.59
4:D:32:THR:HA	4:D:56:ASN:O	2.03	0.58
1:a:435:ALA:O	1:a:439:HIS:ND1	2.35	0.58
2:b:194:THR:HG21	2:b:281:LEU:HB2	1.85	0.58
16:1:848:BCR:H16C	13:1:852:CLA:H8	1.85	0.58
2:2:29:ALA:HB2	18:2:845:LMG:H141	1.84	0.58
2:2:18:ASP:HB3	2:2:23:ARG:HB2	1.85	0.58
1:A:120:VAL:HG21	8:J:27:ILE:HG23	1.83	0.58
1:A:351:GLN:HG3	13:A:825:CLA:H122	1.84	0.58
1:1:351:GLN:HG3	13:1:825:CLA:H122	1.84	0.58
1:1:553:VAL:HG21	16:1:847:BCR:HC32	1.85	0.58
10:L:144:PHE:CE2	10:l:80:LEU:HD23	2.38	0.58
13:1:839:CLA:H172	13:6:201:CLA:HED2	1.85	0.58
13:A:810:CLA:HBB2	13:A:813:CLA:HMA3	1.84	0.58
13:A:840:CLA:H91	8:J:19:LEU:HD12	1.84	0.58
2:2:194:THR:HG21	2:2:281:LEU:HB2	1.85	0.58
1:a:553:VAL:HG21	16:a:847:BCR:HC32	1.85	0.58
13:b:802:CLA:H122	16:b:845:BCR:H362	1.85	0.58
2:B:18:ASP:HB3	2:B:23:ARG:HB2	1.85	0.58
13:B:802:CLA:H122	16:B:845:BCR:H362	1.85	0.58
8:J:21:PHE:HA	13:J:1103:CLA:HBB2	1.86	0.58
10:L:49:LEU:CD1	10:l:133:LEU:CD2	2.77	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:447:LEU:HB3	1:a:540:PHE:HB2	1.86	0.58
9:k:77:LEU:HB3	9:k:82:ALA:HB3	1.84	0.58
10:l:53:MET:CE	10:0:132:LEU:HD21	2.33	0.58
2:B:29:ALA:HB2	18:B:846:LMG:H141	1.85	0.58
13:a:839:CLA:H172	13:f:201:CLA:HED2	1.85	0.58
16:A:848:BCR:H16C	13:A:852:CLA:H8	1.85	0.58
1:1:76:HIS:ND1	13:1:813:CLA:OBD	2.35	0.58
2:b:18:ASP:HB3	2:b:23:ARG:HB2	1.86	0.57
13:1:837:CLA:H121	13:0:208:CLA:H161	1.86	0.57
1:A:79:HIS:HB2	13:A:805:CLA:HMB2	1.86	0.57
13:A:803:CLA:H172	13:B:847:CLA:HMB2	1.86	0.57
5:e:18:TRP:HB3	5:e:21:ASP:HB3	1.86	0.57
1:a:79:HIS:HB2	13:a:805:CLA:HMB2	1.87	0.57
8:j:21:PHE:HA	13:j:1103:CLA:HBB2	1.86	0.57
13:2:822:CLA:H72	16:2:843:BCR:H362	1.84	0.57
8:8:21:PHE:HA	13:8:1103:CLA:HBB2	1.86	0.57
13:a:803:CLA:H172	13:b:847:CLA:HMB2	1.86	0.57
16:a:848:BCR:H271	13:b:829:CLA:HHB	1.87	0.57
4:d:32:THR:HA	4:d:56:ASN:O	2.03	0.57
13:1:841:CLA:H111	10:0:90:LEU:HD21	1.87	0.57
1:A:553:VAL:HG21	16:A:847:BCR:HC32	1.85	0.57
10:L:92:ILE:HD11	13:0:205:CLA:HBA2	1.86	0.57
13:A:808:CLA:HBA2	13:A:828:CLA:H12	1.87	0.57
13:A:832:CLA:H151	14:B:839:PQN:H191	1.87	0.57
13:a:808:CLA:HBA2	13:a:828:CLA:H12	1.87	0.57
13:a:832:CLA:H151	14:b:839:PQN:H191	1.87	0.57
1:1:447:LEU:HB3	1:1:540:PHE:HB2	1.86	0.57
16:1:848:BCR:H271	13:2:828:CLA:HHB	1.87	0.57
2:2:707:LEU:HD21	14:2:838:PQN:H151	1.87	0.57
13:2:802:CLA:H122	16:2:844:BCR:H362	1.85	0.57
4:4:32:THR:HA	4:4:56:ASN:O	2.03	0.57
2:B:194:THR:HG21	2:B:281:LEU:HB2	1.85	0.57
10:l:35:LEU:HD22	13:l:207:CLA:HBD	1.87	0.57
13:A:841:CLA:H111	10:L:90:LEU:HD21	1.87	0.57
10:L:45:ASN:ND2	10:0:45:ASN:ND2	2.53	0.57
1:1:435:ALA:O	1:1:439:HIS:ND1	2.35	0.57
2:2:43:GLU:OE2	2:2:47:GLN:NE2	2.38	0.57
1:A:447:LEU:HB3	1:A:540:PHE:HB2	1.86	0.56
2:B:43:GLU:OE2	2:B:47:GLN:NE2	2.38	0.56
1:a:76:HIS:ND1	13:a:813:CLA:OBD	2.35	0.56
13:b:806:CLA:H3A	13:i:102:CLA:HMB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:803:CLA:H172	13:2:846:CLA:HMB2	1.86	0.56
2:B:707:LEU:HD21	14:B:839:PQN:H151	1.87	0.56
13:A:837:CLA:H121	13:L:206:CLA:H161	1.86	0.56
2:B:725:ILE:HG12	13:B:824:CLA:HMC2	1.87	0.56
5:E:18:TRP:HB3	5:E:21:ASP:HB3	1.86	0.56
1:1:79:HIS:HB2	13:1:805:CLA:HMB2	1.87	0.56
2:2:725:ILE:HG12	13:2:823:CLA:HMC2	1.87	0.56
5:5:18:TRP:HB3	5:5:21:ASP:HB3	1.86	0.56
4:D:62:ARG:HB2	4:D:65:GLN:HG3	1.88	0.56
13:a:837:CLA:H121	13:l:207:CLA:H161	1.86	0.56
13:2:806:CLA:H3A	13:7:102:CLA:HMB3	1.86	0.56
1:A:441:ASN:ND2	13:A:841:CLA:OBD	2.39	0.56
13:B:806:CLA:H3A	13:I:101:CLA:HMB3	1.86	0.56
10:L:35:LEU:HD22	13:L:206:CLA:HBD	1.87	0.56
13:1:808:CLA:HBA2	13:1:828:CLA:H12	1.87	0.56
10:L:95:SER:CB	10:0:46:ARG:HH21	2.18	0.56
13:a:841:CLA:H111	10:l:90:LEU:HD21	1.87	0.56
10:l:144:PHE:HZ	10:0:77:THR:HG23	1.67	0.56
2:b:707:LEU:HD21	14:b:839:PQN:H151	1.87	0.56
3:3:24:ASP:OD2	4:4:99:HIS:ND1	2.39	0.56
4:d:62:ARG:HB2	4:d:65:GLN:HG3	1.87	0.56
7:i:14:LEU:HD13	13:i:102:CLA:H2	1.88	0.56
1:1:441:ASN:ND2	13:1:841:CLA:OBD	2.39	0.56
10:L:53:MET:CE	10:l:132:LEU:CD2	2.84	0.56
2:b:43:GLU:OE2	2:b:47:GLN:NE2	2.38	0.56
3:c:24:ASP:OD2	4:d:99:HIS:ND1	2.39	0.56
13:1:831:CLA:HBB2	13:1:838:CLA:HMC2	1.88	0.56
2:2:423:LYS:NZ	2:2:547:ASP:OD1	2.39	0.56
10:0:35:LEU:HD22	13:0:208:CLA:HBD	1.87	0.56
2:b:423:LYS:NZ	2:b:547:ASP:OD1	2.39	0.56
13:1:832:CLA:H151	14:2:838:PQN:H191	1.87	0.56
1:A:435:ALA:O	1:A:439:HIS:ND1	2.35	0.55
3:C:24:ASP:OD2	4:D:99:HIS:ND1	2.39	0.55
1:A:434:ASP:OD1	1:A:560:ARG:NH1	2.40	0.55
2:b:725:ILE:HG12	13:b:824:CLA:HMC2	1.87	0.55
1:a:434:ASP:OD1	1:a:560:ARG:NH1	2.40	0.55
10:l:49:LEU:HD11	10:0:133:LEU:CD2	2.36	0.55
16:A:848:BCR:H271	13:B:829:CLA:HHB	1.87	0.55
2:B:184:GLY:HA3	13:B:810:CLA:HBB1	1.89	0.55
13:1:808:CLA:HAB	13:1:828:CLA:H101	1.88	0.55
13:L:203:CLA:HBA2	10:l:92:ILE:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:l:91:THR:HG21	10:l:132:LEU:HB2	1.89	0.55
1:1:434:ASP:OD1	1:1:560:ARG:NH1	2.40	0.55
13:A:819:CLA:HAB	13:A:819:CLA:H8	1.89	0.55
1:a:395:TRP:HB3	13:a:828:CLA:HMC3	1.88	0.55
2:2:184:GLY:HA3	13:2:809:CLA:HBB1	1.89	0.55
1:a:441:ASN:ND2	13:a:841:CLA:OBD	2.39	0.55
1:A:395:TRP:HB3	13:A:828:CLA:HMC3	1.88	0.55
13:A:808:CLA:HAB	13:A:828:CLA:H101	1.88	0.55
13:b:808:CLA:H121	16:b:841:BCR:H341	1.89	0.55
2:B:423:LYS:NZ	2:B:547:ASP:OD1	2.39	0.54
13:B:808:CLA:H121	16:B:841:BCR:H341	1.89	0.54
13:a:808:CLA:HAB	13:a:828:CLA:H101	1.88	0.54
13:A:806:CLA:H161	13:A:829:CLA:HBB2	1.90	0.54
13:a:806:CLA:H161	13:a:829:CLA:HBB2	1.90	0.54
13:2:807:CLA:H121	16:2:840:BCR:H341	1.88	0.54
13:A:831:CLA:HBB2	13:A:838:CLA:HMC2	1.88	0.54
10:L:91:THR:HG21	10:L:132:LEU:HB2	1.89	0.54
13:a:831:CLA:HBB2	13:a:838:CLA:HMC2	1.88	0.54
2:b:184:GLY:HA3	13:b:810:CLA:HBB1	1.89	0.54
10:l:144:PHE:CZ	10:0:77:THR:CG2	2.89	0.54
1:A:565:LYS:NZ	2:B:680:GLU:OE1	2.41	0.54
1:1:395:TRP:HB3	13:1:828:CLA:HMC3	1.88	0.54
2:B:613:VAL:O	2:B:617:ASN:ND2	2.41	0.54
1:a:565:LYS:NZ	2:b:680:GLU:OE1	2.41	0.54
13:a:819:CLA:HAB	13:a:819:CLA:H8	1.89	0.54
1:A:586:SER:OG	1:A:589:ASP:OD2	2.25	0.54
7:I:14:LEU:HD13	13:I:101:CLA:H2	1.88	0.54
10:L:77:THR:CG2	10:0:148:THR:CG2	2.66	0.54
2:2:423:LYS:HB2	2:2:546:LEU:HB3	1.90	0.54
4:4:62:ARG:HB2	4:4:65:GLN:HG3	1.88	0.54
1:A:405:GLY:HA2	16:A:847:BCR:HC31	1.90	0.54
13:l:204:CLA:HMD3	10:0:95:SER:HB2	1.89	0.54
13:1:806:CLA:H161	13:1:829:CLA:HBB2	1.89	0.54
10:0:91:THR:HG21	10:0:132:LEU:HB2	1.89	0.54
1:A:423:ASN:OD1	1:A:431:ARG:NH2	2.41	0.54
1:1:225:LYS:HD3	1:1:252:LEU:HD12	1.90	0.54
2:2:613:VAL:O	2:2:617:ASN:ND2	2.41	0.54
1:A:458:ASN:HD22	1:A:640:ILE:HB	1.74	0.54
2:B:587:MET:HB2	2:B:717:LEU:HD11	1.90	0.54
10:L:132:LEU:CD2	10:0:53:MET:CE	2.85	0.54
1:a:405:GLY:HA2	16:a:847:BCR:HC31	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:565:LYS:NZ	2:2:680:GLU:OE1	2.41	0.53
2:2:25:TRP:HE1	13:2:835:CLA:HBB1	1.72	0.53
2:2:587:MET:HB2	2:2:717:LEU:HD11	1.90	0.53
2:b:587:MET:HB2	2:b:717:LEU:HD11	1.90	0.53
13:1:819:CLA:H61	13:1:829:CLA:H91	1.90	0.53
1:A:225:LYS:HD3	1:A:252:LEU:HD12	1.90	0.53
1:a:214:GLY:HA3	13:a:815:CLA:HAB	1.90	0.53
13:b:820:CLA:HMD3	13:b:821:CLA:HHC	1.90	0.53
10:l:49:LEU:CD1	10:0:133:LEU:CD2	2.83	0.53
13:1:819:CLA:H8	13:1:819:CLA:HAB	1.89	0.53
2:2:458:GLU:OE2	6:6:34:ARG:NE	2.40	0.53
7:7:14:LEU:HD13	13:7:102:CLA:H2	1.88	0.53
2:B:423:LYS:HB2	2:B:546:LEU:HB3	1.90	0.53
1:a:458:ASN:HD22	1:a:640:ILE:HB	1.74	0.53
13:a:819:CLA:H61	13:a:829:CLA:H91	1.90	0.53
2:b:25:TRP:HE1	13:b:836:CLA:HBB1	1.72	0.53
1:A:76:HIS:ND1	13:A:813:CLA:OBD	2.35	0.53
1:A:214:GLY:HA3	13:A:815:CLA:HAB	1.90	0.53
1:a:440:LEU:HD21	1:a:546:VAL:HG12	1.90	0.53
13:2:819:CLA:HMD3	13:2:820:CLA:HHC	1.90	0.53
2:B:25:TRP:HE1	13:B:836:CLA:HBB1	1.72	0.53
2:B:121:SER:HA	13:B:824:CLA:HMA2	1.90	0.53
13:b:837:CLA:HBC2	14:b:839:PQN:H171	1.90	0.53
1:1:586:SER:OG	1:1:589:ASP:OD2	2.25	0.53
1:a:104:LEU:HB3	1:a:233:PRO:HG2	1.91	0.53
1:a:423:ASN:OD1	1:a:431:ARG:NH2	2.41	0.53
2:b:423:LYS:HB2	2:b:546:LEU:HB3	1.90	0.53
1:1:423:ASN:OD1	1:1:431:ARG:NH2	2.41	0.53
2:2:121:SER:HA	13:2:823:CLA:HMA2	1.90	0.53
1:1:104:LEU:HB3	1:1:233:PRO:HG2	1.91	0.53
1:1:405:GLY:HA2	16:1:847:BCR:HC31	1.90	0.53
13:2:806:CLA:HMB3	13:7:102:CLA:H3A	1.91	0.53
1:A:440:LEU:HD21	1:A:546:VAL:HG12	1.90	0.53
3:c:2:SER:N	3:c:71:ALA:O	2.42	0.53
1:1:197:MET:HE1	13:1:821:CLA:HMB3	1.91	0.53
1:1:214:GLY:HA3	13:1:815:CLA:HAB	1.90	0.53
10:l:136:CYS:HB3	16:l:201:BCR:C25	2.38	0.53
1:1:17:ASP:OD2	1:1:70:ARG:NH2	2.41	0.53
13:2:836:CLA:HBC2	14:2:838:PQN:H171	1.90	0.53
10:l:46:ARG:NH1	10:l:50:GLU:OE1	2.38	0.52
1:A:412:MET:HE1	1:A:430:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:820:CLA:HBB2	16:A:845:BCR:H402	1.91	0.52
13:B:806:CLA:HMB3	13:I:101:CLA:H3A	1.91	0.52
1:a:197:MET:HE1	13:a:821:CLA:HMB3	1.91	0.52
5:e:18:TRP:HE1	5:e:43:LYS:HB2	1.74	0.52
1:1:458:ASN:HD22	1:1:640:ILE:HB	1.74	0.52
13:1:820:CLA:HBB2	16:1:845:BCR:H402	1.91	0.52
1:A:104:LEU:HB3	1:A:233:PRO:HG2	1.91	0.52
1:A:736:ILE:HG21	13:A:828:CLA:HMC2	1.91	0.52
3:C:2:SER:N	3:C:71:ALA:O	2.42	0.52
13:1:822:CLA:HMD2	16:9:4001:BCR:H24C	1.91	0.52
13:B:820:CLA:HMD3	13:B:821:CLA:HHC	1.90	0.52
5:E:18:TRP:HE1	5:E:43:LYS:HB2	1.74	0.52
1:a:586:SER:OG	1:a:589:ASP:OD2	2.25	0.52
13:a:820:CLA:HBB2	16:a:845:BCR:H402	1.90	0.52
13:b:806:CLA:HMB3	13:i:102:CLA:H3A	1.91	0.52
1:1:440:LEU:HD21	1:1:546:VAL:HG12	1.90	0.52
6:6:101:ILE:HD12	13:6:201:CLA:HED1	1.91	0.52
13:l:204:CLA:HBA2	10:0:92:ILE:HD11	1.91	0.52
5:5:18:TRP:HE1	5:5:43:LYS:HB2	1.74	0.52
13:A:819:CLA:H61	13:A:829:CLA:H91	1.90	0.52
13:A:821:CLA:H171	13:A:831:CLA:HBC1	1.92	0.52
1:a:736:ILE:HG21	13:a:828:CLA:HMC2	1.91	0.52
6:F:101:ILE:HD12	13:F:201:CLA:HED1	1.91	0.52
1:a:225:LYS:HD3	1:a:252:LEU:HD12	1.90	0.52
13:b:806:CLA:H43	13:b:824:CLA:H11	1.91	0.52
10:l:46:ARG:HH21	10:0:95:SER:CB	2.22	0.52
1:1:736:ILE:HG21	13:1:828:CLA:HMC2	1.91	0.52
13:A:817:CLA:HAA1	9:K:8:PRO:HG2	1.92	0.52
13:A:832:CLA:HBB2	10:L:66:LEU:HD13	1.91	0.52
2:b:121:SER:HA	13:b:824:CLA:HMA2	1.90	0.52
13:B:837:CLA:HBC2	14:B:839:PQN:H171	1.90	0.52
13:L:203:CLA:HMD3	10:l:95:SER:CB	2.38	0.52
13:a:832:CLA:HBB2	10:l:66:LEU:HD13	1.91	0.52
3:c:55:GLU:OE2	3:c:66:ARG:NH1	2.43	0.52
1:1:127:ASN:HB3	1:1:135:HIS:HB3	1.91	0.52
13:A:828:CLA:H171	13:A:852:CLA:H121	1.92	0.51
13:A:841:CLA:H13	10:L:90:LEU:HD11	1.92	0.51
10:L:77:THR:HG22	10:0:148:THR:HG21	1.91	0.51
1:a:327:GLY:HA3	13:a:823:CLA:HED3	1.92	0.51
1:a:428:ARG:O	1:a:432:HIS:ND1	2.34	0.51
12:a:801:CL0:H15	13:a:852:CLA:HED1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:821:CLA:H171	13:a:831:CLA:HBC1	1.92	0.51
3:3:55:GLU:OE2	3:3:66:ARG:NH1	2.43	0.51
1:A:595:LEU:HD21	13:A:830:CLA:HBC1	1.93	0.51
1:A:604:ILE:HD12	12:A:801:CL0:H57	1.93	0.51
6:F:53:VAL:HG12	6:F:63:PHE:HB2	1.93	0.51
1:a:595:LEU:HD21	13:a:830:CLA:HBC1	1.93	0.51
13:1:832:CLA:HBB2	10:0:66:LEU:HD13	1.91	0.51
3:3:2:SER:N	3:3:71:ALA:O	2.42	0.51
13:a:804:CLA:HBC2	13:a:830:CLA:H42	1.93	0.51
13:a:841:CLA:H13	10:l:90:LEU:HD11	1.92	0.51
2:b:613:VAL:O	2:b:617:ASN:ND2	2.41	0.51
10:l:133:LEU:HB3	10:0:133:LEU:HD11	1.91	0.51
10:l:148:THR:CG2	10:0:77:THR:CG2	2.73	0.51
13:1:828:CLA:H171	13:1:852:CLA:H121	1.93	0.51
2:2:359:HIS:ND1	13:2:813:CLA:OBD	2.40	0.51
13:7:102:CLA:H72	16:7:103:BCR:HC41	1.92	0.51
1:A:197:MET:HE1	13:A:821:CLA:HMB3	1.91	0.51
7:I:13:ILE:CD1	10:0:154:LEU:HD21	2.40	0.51
10:L:133:LEU:HB3	10:l:133:LEU:HD11	1.92	0.51
10:L:136:CYS:HB3	16:L:207:BCR:H393	1.91	0.51
1:a:127:ASN:HB3	1:a:135:HIS:HB3	1.91	0.51
10:l:44:PRO:HB2	10:l:126:GLU:HB2	1.93	0.51
10:L:46:ARG:HG2	10:l:125:SER:HB3	1.92	0.51
1:a:17:ASP:OD2	1:a:70:ARG:NH2	2.41	0.51
13:a:822:CLA:HMD2	16:k:4001:BCR:H24C	1.91	0.51
13:1:817:CLA:HAA1	9:9:8:PRO:HG2	1.92	0.51
10:L:44:PRO:HB2	10:L:126:GLU:HB2	1.93	0.51
10:L:141:PHE:CE1	10:l:84:ILE:HG21	2.45	0.51
13:a:828:CLA:H171	13:a:852:CLA:H121	1.93	0.51
13:b:810:CLA:H42	16:b:841:BCR:H19C	1.93	0.51
1:1:604:ILE:HD12	12:1:801:CL0:H57	1.93	0.51
10:0:44:PRO:HB2	10:0:126:GLU:HB2	1.93	0.51
13:A:822:CLA:HMD2	16:K:4001:BCR:H24C	1.91	0.51
10:L:136:CYS:HB3	16:L:207:BCR:C25	2.41	0.51
1:a:402:VAL:HG21	1:a:598:MET:HG2	1.93	0.51
1:a:604:ILE:HD12	12:a:801:CL0:H57	1.93	0.51
6:f:101:ILE:HD12	13:f:201:CLA:HED1	1.91	0.51
1:1:402:VAL:HG21	1:1:598:MET:HG2	1.93	0.51
2:2:57:LEU:HD12	13:2:809:CLA:HED1	1.93	0.51
13:B:806:CLA:H43	13:B:824:CLA:H11	1.91	0.51
10:L:140:PHE:HE2	10:l:140:PHE:CE2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:412:MET:HE1	1:a:430:LEU:HD11	1.92	0.51
13:a:852:CLA:HBC2	2:b:592:ASN:HB2	1.93	0.51
2:b:233:TRP:HZ3	13:b:813:CLA:H102	1.75	0.51
13:2:806:CLA:H43	13:2:823:CLA:H11	1.91	0.51
1:A:127:ASN:HB3	1:A:135:HIS:HB3	1.91	0.51
10:L:5:ASP:OD1	10:L:5:ASP:N	2.44	0.51
10:l:45:ASN:ND2	10:0:45:ASN:ND2	2.59	0.51
13:1:821:CLA:H171	13:1:831:CLA:HBC1	1.92	0.51
13:1:841:CLA:H13	10:0:90:LEU:HD11	1.92	0.51
13:1:852:CLA:HBC2	2:2:592:ASN:HB2	1.93	0.51
6:6:53:VAL:HG12	6:6:63:PHE:HB2	1.93	0.51
13:B:815:CLA:H171	13:B:823:CLA:H3A	1.93	0.51
3:C:55:GLU:OE2	3:C:66:ARG:NH1	2.43	0.51
13:I:101:CLA:H72	16:I:102:BCR:HC41	1.92	0.51
13:a:817:CLA:HAA1	9:k:8:PRO:HG2	1.92	0.51
1:1:327:GLY:HA3	13:1:823:CLA:HED3	1.92	0.51
1:1:412:MET:HE1	1:1:430:LEU:HD11	1.91	0.51
13:1:804:CLA:HBC2	13:1:830:CLA:H42	1.93	0.51
13:B:806:CLA:HBB1	13:B:806:CLA:H8	1.93	0.50
3:C:41:SER:HB2	4:D:116:HIS:H	1.76	0.50
13:b:815:CLA:H171	13:b:823:CLA:H3A	1.93	0.50
7:i:30:LEU:HD22	19:i:101:SQD:C28	2.36	0.50
13:1:825:CLA:HBA1	13:1:829:CLA:H193	1.93	0.50
13:2:806:CLA:HBB1	13:2:806:CLA:H8	1.93	0.50
1:A:327:GLY:HA3	13:A:823:CLA:HED3	1.92	0.50
2:B:57:LEU:HD12	13:B:810:CLA:HED1	1.93	0.50
2:b:385:TYR:HB3	13:b:824:CLA:HMC3	1.93	0.50
2:b:402:PHE:HE2	16:b:844:BCR:H381	1.77	0.50
13:a:823:CLA:HHB	13:a:842:CLA:HBC3	1.93	0.50
3:c:41:SER:HB2	4:d:116:HIS:H	1.76	0.50
13:i:102:CLA:H72	16:i:103:BCR:HC41	1.92	0.50
2:2:402:PHE:HE2	16:2:843:BCR:H381	1.77	0.50
3:C:58:CYS:O	5:E:47:ASN:ND2	2.44	0.50
13:a:825:CLA:HBA1	13:a:829:CLA:H193	1.93	0.50
2:b:466:VAL:HG11	6:f:52:VAL:HG13	1.94	0.50
13:b:806:CLA:H8	13:b:806:CLA:HBB1	1.93	0.50
1:1:595:LEU:HD21	13:1:830:CLA:HBC1	1.93	0.50
13:A:804:CLA:HBC2	13:A:830:CLA:H42	1.93	0.50
2:B:464:GLU:OE2	2:B:469:GLN:NE2	2.36	0.50
13:1:823:CLA:HHB	13:1:842:CLA:HBC3	1.93	0.50
2:2:233:TRP:HZ3	13:2:812:CLA:H102	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:TRP:HZ3	13:B:813:CLA:H102	1.75	0.50
2:B:402:PHE:HE2	16:B:844:BCR:H381	1.77	0.50
2:B:458:GLU:OE2	6:F:34:ARG:NE	2.40	0.50
2:B:466:VAL:HG11	6:F:52:VAL:HG13	1.93	0.50
2:B:711:GLN:HA	18:B:846:LMG:H112	1.94	0.50
10:L:81:LEU:HG	10:0:144:PHE:HE2	1.76	0.50
6:f:53:VAL:HG12	6:f:63:PHE:HB2	1.93	0.50
3:3:58:CYS:O	5:5:47:ASN:ND2	2.44	0.50
13:A:852:CLA:HBC2	2:B:592:ASN:HB2	1.93	0.50
1:a:560:ARG:NH2	4:d:16:THR:O	2.45	0.50
13:1:852:CLA:HMB2	2:2:442:LEU:HD13	1.94	0.50
2:2:699:ARG:NH1	10:0:106:THR:OG1	2.41	0.50
3:3:41:SER:HB2	4:4:116:HIS:H	1.76	0.50
13:A:825:CLA:HBA1	13:A:829:CLA:H193	1.93	0.50
2:b:699:ARG:NH1	10:l:106:THR:OG1	2.42	0.50
13:b:829:CLA:HMC3	16:b:848:BCR:H10C	1.94	0.50
13:1:838:CLA:H102	16:1:846:BCR:H23C	1.94	0.50
1:A:17:ASP:OD2	1:A:70:ARG:NH2	2.41	0.50
1:A:402:VAL:HG21	1:A:598:MET:HG2	1.93	0.50
13:A:806:CLA:HAA1	13:A:830:CLA:HMB2	1.94	0.50
16:A:848:BCR:H14C	13:A:852:CLA:H111	1.94	0.50
10:L:18:LEU:O	10:L:23:ASN:ND2	2.44	0.50
2:b:57:LEU:HD12	13:b:810:CLA:HED1	1.93	0.50
13:b:804:CLA:H112	13:b:821:CLA:HBA1	1.94	0.50
1:1:560:ARG:NH2	4:4:16:THR:O	2.45	0.50
12:1:801:CL0:H15	13:1:852:CLA:HED1	1.93	0.50
13:1:806:CLA:HAA1	13:1:830:CLA:HMB2	1.94	0.50
2:2:385:TYR:HB3	13:2:823:CLA:HMC3	1.93	0.50
13:2:805:CLA:H72	18:2:845:LMG:H331	1.94	0.50
13:2:809:CLA:H42	16:2:840:BCR:H19C	1.93	0.50
10:L:46:ARG:HH21	10:l:95:SER:CB	2.25	0.49
13:a:841:CLA:HAB	2:b:698:VAL:HG11	1.94	0.49
2:b:711:GLN:HA	18:b:846:LMG:H112	1.94	0.49
16:i:103:BCR:H402	16:l:203:BCR:H353	1.94	0.49
13:2:828:CLA:HMC3	16:2:847:BCR:H10C	1.93	0.49
1:A:539:ALA:HB1	13:A:837:CLA:HMB3	1.93	0.49
12:A:801:CL0:H15	13:A:852:CLA:HED1	1.92	0.49
10:L:45:ASN:ND2	10:l:45:ASN:ND2	2.59	0.49
13:a:818:CLA:HAC1	13:a:834:CLA:H42	1.94	0.49
13:2:814:CLA:H171	13:2:822:CLA:H3A	1.93	0.49
13:A:838:CLA:H102	16:A:846:BCR:H23C	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:810:CLA:H42	16:B:841:BCR:H19C	1.93	0.49
13:B:827:CLA:HMC2	13:B:838:CLA:H142	1.94	0.49
10:L:136:CYS:HB3	16:L:207:BCR:C26	2.42	0.49
10:l:5:ASP:OD1	10:l:5:ASP:N	2.44	0.49
10:l:34:ALA:HB1	13:l:204:CLA:HBC2	1.95	0.49
2:2:567:ASP:HB3	2:2:574:THR:HG21	1.94	0.49
13:2:826:CLA:HMC2	13:2:837:CLA:H142	1.94	0.49
1:A:429:VAL:HG11	13:A:821:CLA:H202	1.95	0.49
1:A:563:PRO:HB3	4:D:44:PRO:HB3	1.94	0.49
13:A:841:CLA:HAB	2:B:698:VAL:HG11	1.94	0.49
9:K:45:LEU:HD13	9:K:51:PHE:HD1	1.77	0.49
10:L:154:LEU:HD21	7:i:13:ILE:CD1	2.38	0.49
3:c:58:CYS:O	5:e:47:ASN:ND2	2.44	0.49
13:1:841:CLA:HAB	2:2:698:VAL:HG11	1.94	0.49
2:2:420:LEU:HA	2:2:423:LYS:HB3	1.94	0.49
1:A:352:LEU:O	1:A:356:LEU:HB2	2.13	0.49
1:a:352:LEU:O	1:a:356:LEU:HB2	2.13	0.49
1:1:539:ALA:HB1	13:1:837:CLA:HMB3	1.93	0.49
2:2:271:LEU:HD13	13:2:813:CLA:HMA2	1.94	0.49
13:A:818:CLA:HAC1	13:A:834:CLA:H42	1.94	0.49
13:A:823:CLA:HHB	13:A:842:CLA:HBC3	1.93	0.49
2:b:59:ILE:HD11	16:m:101:BCR:HC7	1.95	0.49
2:b:420:LEU:HA	2:b:423:LYS:HB3	1.94	0.49
16:7:103:BCR:H402	16:0:204:BCR:H353	1.94	0.49
1:A:428:ARG:O	1:A:432:HIS:ND1	2.34	0.49
1:A:447:LEU:O	1:A:451:SER:OG	2.30	0.49
13:b:805:CLA:H72	18:b:846:LMG:H331	1.94	0.49
16:1:848:BCR:H14C	13:1:852:CLA:H111	1.94	0.49
2:B:271:LEU:HD13	13:B:814:CLA:HMA2	1.94	0.49
13:B:804:CLA:H112	13:B:821:CLA:HBA1	1.94	0.49
1:a:220:SER:O	1:a:224:ASN:HB2	2.13	0.49
2:b:567:ASP:HB3	2:b:574:THR:HG21	1.94	0.49
1:1:220:SER:O	1:1:224:ASN:HB2	2.13	0.49
2:B:59:ILE:HD11	16:M:101:BCR:HC7	1.95	0.49
2:B:385:TYR:HB3	13:B:824:CLA:HMC3	1.93	0.49
2:B:567:ASP:HB3	2:B:574:THR:HG21	1.94	0.49
2:B:677:TYR:OH	13:B:802:CLA:OBD	2.29	0.49
2:B:699:ARG:NH1	10:L:106:THR:OG1	2.42	0.49
13:B:829:CLA:HMC3	16:B:848:BCR:H10C	1.94	0.49
13:a:806:CLA:HAA1	13:a:830:CLA:HMB2	1.94	0.49
13:a:852:CLA:HMB2	2:b:442:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:l:53:MET:CE	10:0:132:LEU:CD2	2.91	0.49
1:A:560:ARG:NH2	4:D:16:THR:O	2.45	0.49
13:b:827:CLA:HMC2	13:b:838:CLA:H142	1.95	0.49
1:1:462:ARG:HG2	2:2:642:TYR:HD2	1.78	0.49
13:1:824:CLA:H141	17:1:850:LHG:H182	1.94	0.49
2:2:466:VAL:HG11	6:6:52:VAL:HG13	1.93	0.49
9:9:45:LEU:HD13	9:9:51:PHE:HD1	1.77	0.49
13:A:852:CLA:HMB2	2:B:442:LEU:HD13	1.94	0.48
13:B:805:CLA:H72	18:B:846:LMG:H331	1.94	0.48
10:L:34:ALA:HB1	13:L:203:CLA:HBC2	1.95	0.48
1:a:539:ALA:HB1	13:a:837:CLA:HMB3	1.93	0.48
16:a:848:BCR:H14C	13:a:852:CLA:H111	1.94	0.48
2:b:271:LEU:HD13	13:b:814:CLA:HMA2	1.94	0.48
2:b:464:GLU:OE2	2:b:469:GLN:NE2	2.36	0.48
2:b:677:TYR:OH	13:b:802:CLA:OBD	2.29	0.48
1:1:531:ASP:O	1:1:535:HIS:ND1	2.36	0.48
13:1:808:CLA:HMC2	13:1:828:CLA:H71	1.94	0.48
2:2:711:GLN:HA	18:2:845:LMG:H112	1.94	0.48
2:B:349:LEU:O	2:B:353:THR:OG1	2.30	0.48
13:B:815:CLA:H192	13:B:823:CLA:HMA1	1.95	0.48
1:a:429:VAL:HG11	13:a:821:CLA:H202	1.95	0.48
13:b:815:CLA:H192	13:b:823:CLA:HMA1	1.95	0.48
10:l:21:PRO:HA	10:l:25:SER:HB3	1.95	0.48
1:1:563:PRO:HB3	4:4:44:PRO:HB3	1.94	0.48
10:0:34:ALA:HB1	13:0:205:CLA:HBC2	1.94	0.48
13:A:808:CLA:HMC2	13:A:828:CLA:H71	1.94	0.48
13:a:838:CLA:H102	16:a:846:BCR:H23C	1.94	0.48
14:a:843:PQN:H272	13:j:1101:CLA:HBA1	1.95	0.48
13:2:804:CLA:H112	13:2:820:CLA:HBA1	1.94	0.48
2:B:359:HIS:ND1	13:B:814:CLA:OBD	2.40	0.48
13:a:802:CLA:H3A	13:a:802:CLA:H12	1.95	0.48
1:1:352:LEU:O	1:1:356:LEU:HB2	2.13	0.48
10:L:31:PHE:HB2	19:i:101:SQD:H81	1.96	0.48
1:a:462:ARG:HG2	2:b:642:TYR:HD2	1.78	0.48
13:a:808:CLA:HMC2	13:a:828:CLA:H71	1.94	0.48
13:1:818:CLA:HAC1	13:1:834:CLA:H42	1.94	0.48
6:6:115:MET:HE2	6:6:118:LEU:CD1	2.21	0.48
1:A:220:SER:O	1:A:224:ASN:HB2	2.13	0.48
13:A:802:CLA:H3A	13:A:802:CLA:H12	1.96	0.48
2:B:420:LEU:HA	2:B:423:LYS:HB3	1.94	0.48
10:L:45:ASN:HD21	10:0:45:ASN:ND2	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:140:PHE:CE2	10:l:140:PHE:CE2	3.01	0.48
13:a:824:CLA:H141	17:a:850:LHG:H182	1.94	0.48
10:l:154:LEU:HD21	7:7:13:ILE:CD1	2.35	0.48
16:I:102:BCR:H402	16:L:202:BCR:H353	1.94	0.48
10:L:21:PRO:HA	10:L:25:SER:HB3	1.94	0.48
13:b:815:CLA:H101	13:b:821:CLA:H41	1.96	0.48
6:f:114:PHE:CE2	6:f:115:MET:CG	2.90	0.48
13:1:802:CLA:H3A	13:1:802:CLA:H12	1.96	0.48
2:2:405:ASP:OD1	4:4:133:LYS:NZ	2.41	0.48
2:2:531:ALA:O	2:2:535:HIS:ND1	2.37	0.48
1:A:462:ARG:HG2	2:B:642:TYR:HD2	1.78	0.48
13:A:824:CLA:H141	17:A:850:LHG:H182	1.94	0.48
2:B:73:TRP:NE1	7:I:6:ALA:O	2.33	0.48
13:B:835:CLA:H12	16:B:844:BCR:H352	1.95	0.48
2:b:175:GLU:HG3	2:b:294:TYR:HB3	1.96	0.48
2:b:349:LEU:O	2:b:353:THR:OG1	2.30	0.48
10:0:21:PRO:HA	10:0:25:SER:HB3	1.94	0.48
13:A:806:CLA:H51	13:A:806:CLA:HMA2	1.96	0.48
19:I:103:SQD:H81	10:0:31:PHE:HB2	1.96	0.48
2:b:91:ALA:HA	13:b:806:CLA:HED2	1.96	0.48
2:b:458:GLU:OE2	6:f:34:ARG:NE	2.40	0.48
2:2:293:MET:HA	13:2:817:CLA:HHD	1.96	0.48
6:F:114:PHE:CE2	6:F:115:MET:CG	2.90	0.48
1:a:269:GLY:H	9:k:10:THR:HG21	1.79	0.48
1:a:573:PRO:HB3	1:a:720:ILE:HB	1.96	0.48
9:k:45:LEU:HD13	9:k:51:PHE:HD1	1.77	0.48
1:1:429:VAL:HG11	13:1:821:CLA:H202	1.95	0.48
13:8:1103:CLA:HBA2	13:8:1103:CLA:H3A	1.59	0.48
1:A:269:GLY:H	9:K:10:THR:HG21	1.79	0.47
1:a:563:PRO:HB3	4:d:44:PRO:HB3	1.94	0.47
13:b:835:CLA:H12	16:b:844:BCR:H352	1.95	0.47
3:c:32:ASP:OD1	3:c:32:ASP:N	2.47	0.47
13:A:818:CLA:HBA2	13:A:818:CLA:H3A	1.51	0.47
13:A:833:CLA:HBB1	16:I:102:BCR:H282	1.96	0.47
13:B:806:CLA:HMB3	13:I:101:CLA:HHB	1.96	0.47
10:L:53:MET:HE1	10:l:132:LEU:CD2	2.43	0.47
2:b:293:MET:HA	13:b:818:CLA:HHD	1.96	0.47
2:b:669:MET:O	2:b:673:SER:OG	2.28	0.47
14:1:843:PQN:H272	13:8:1101:CLA:HBA1	1.95	0.47
2:2:175:GLU:HG3	2:2:294:TYR:HB3	1.96	0.47
10:0:46:ARG:NH1	10:0:50:GLU:OE1	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:MET:HA	13:B:818:CLA:HHD	1.96	0.47
1:a:505:VAL:HG13	13:a:834:CLA:HED3	1.96	0.47
13:a:833:CLA:HBB1	16:i:103:BCR:H282	1.96	0.47
13:b:804:CLA:HBD	13:b:804:CLA:H143	1.96	0.47
13:b:837:CLA:HBA1	16:b:845:BCR:H352	1.95	0.47
1:1:573:PRO:HB3	1:1:720:ILE:HB	1.96	0.47
2:B:91:ALA:HA	13:B:806:CLA:HED2	1.96	0.47
2:B:392:VAL:HG22	2:B:541:LEU:HD11	1.96	0.47
2:b:392:VAL:HG22	2:b:541:LEU:HD11	1.96	0.47
1:1:269:GLY:H	9:9:10:THR:HG21	1.80	0.47
10:0:7:VAL:HG13	10:0:20:THR:HG22	1.97	0.47
1:A:573:PRO:HB3	1:A:720:ILE:HB	1.96	0.47
14:A:843:PQN:H272	13:J:1101:CLA:HBA1	1.95	0.47
2:B:259:THR:H	2:B:274:THR:HB	1.80	0.47
13:a:821:CLA:HBC3	13:a:827:CLA:H18	1.96	0.47
5:e:59:ASN:OD1	5:e:60:ASN:N	2.48	0.47
10:l:31:PHE:HB2	19:7:101:SQD:H81	1.96	0.47
2:2:91:ALA:HA	13:2:806:CLA:HED2	1.96	0.47
2:2:259:THR:H	2:2:274:THR:HB	1.80	0.47
13:2:834:CLA:H12	16:2:843:BCR:H352	1.95	0.47
2:B:175:GLU:HG3	2:B:294:TYR:HB3	1.96	0.47
5:E:59:ASN:OD1	5:E:60:ASN:N	2.48	0.47
13:b:806:CLA:HMB3	13:i:102:CLA:HHB	1.96	0.47
13:2:814:CLA:H192	13:2:822:CLA:HMA1	1.95	0.47
13:A:841:CLA:HMB3	2:B:689:HIS:HE1	1.79	0.47
2:B:53:HIS:ND1	13:B:810:CLA:OBD	2.46	0.47
2:B:597:LEU:HD22	13:B:833:CLA:HBB2	1.97	0.47
13:B:837:CLA:HBA1	16:B:845:BCR:H352	1.96	0.47
3:C:6:LYS:HD2	4:D:119:LYS:HE2	1.96	0.47
10:L:144:PHE:HZ	10:l:77:THR:HG23	1.75	0.47
13:a:811:CLA:H41	13:a:811:CLA:H61	1.74	0.47
13:a:841:CLA:HMB3	2:b:689:HIS:HE1	1.80	0.47
13:b:805:CLA:H112	13:b:805:CLA:H71	1.76	0.47
10:l:144:PHE:HE2	10:0:81:LEU:HG	1.80	0.47
13:1:818:CLA:HBA2	13:1:818:CLA:H3A	1.51	0.47
13:1:841:CLA:HMB3	2:2:689:HIS:HE1	1.80	0.47
2:2:59:ILE:HD11	16:z:101:BCR:HC7	1.95	0.47
2:2:392:VAL:HG22	2:2:541:LEU:HD11	1.96	0.47
2:2:464:GLU:OE2	2:2:469:GLN:NE2	2.36	0.47
13:2:814:CLA:H101	13:2:820:CLA:H41	1.96	0.47
1:A:546:VAL:HG21	13:A:838:CLA:HMA1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:804:CLA:HBD	13:B:804:CLA:H143	1.96	0.47
2:b:432:TRP:CE2	13:b:828:CLA:HAB	2.50	0.47
3:c:58:CYS:HB3	3:c:63:LEU:HD22	1.97	0.47
1:1:74:SER:OG	1:1:176:GLY:O	2.33	0.47
13:1:821:CLA:HBC3	13:1:827:CLA:H18	1.96	0.47
13:2:827:CLA:H51	16:6:205:BCR:H351	1.96	0.47
2:B:63:TRP:HA	13:I:101:CLA:HAB	1.97	0.47
3:C:58:CYS:HB3	3:C:63:LEU:HD22	1.97	0.47
13:1:806:CLA:H51	13:1:806:CLA:HMA2	1.96	0.47
13:1:833:CLA:HBB1	16:7:103:BCR:H282	1.96	0.47
13:2:836:CLA:HBA1	16:2:844:BCR:H352	1.95	0.47
2:B:531:ALA:O	2:B:535:HIS:ND1	2.37	0.47
13:L:203:CLA:CMD	10:l:95:SER:HB3	2.45	0.47
1:a:82:VAL:HG21	13:a:804:CLA:HBB1	1.97	0.47
13:a:806:CLA:H51	13:a:806:CLA:HMA2	1.96	0.47
2:b:53:HIS:ND1	13:b:810:CLA:OBD	2.46	0.47
13:A:802:CLA:H41	13:A:802:CLA:H62	1.60	0.46
13:A:821:CLA:HBC3	13:A:827:CLA:H18	1.96	0.46
10:L:132:LEU:HD21	10:0:53:MET:HE1	1.96	0.46
13:a:805:CLA:H8	16:a:851:BCR:H23C	1.97	0.46
3:c:6:LYS:HD2	4:d:119:LYS:HE2	1.96	0.46
10:l:7:VAL:HG13	10:l:20:THR:HG22	1.97	0.46
10:l:18:LEU:O	10:l:23:ASN:ND2	2.44	0.46
1:1:505:VAL:HG13	13:1:834:CLA:HED3	1.96	0.46
1:1:650:LEU:HD11	12:1:801:CL0:H42	1.97	0.46
2:2:214:ASN:HB3	2:2:218:VAL:HG23	1.97	0.46
2:B:405:ASP:OD1	4:D:133:LYS:NZ	2.41	0.46
13:B:815:CLA:H101	13:B:821:CLA:H41	1.96	0.46
10:L:41:GLY:HA3	10:l:121:LYS:HE2	1.98	0.46
2:2:432:TRP:CE2	13:2:827:CLA:HAB	2.50	0.46
2:2:600:TYR:HA	2:2:626:TRP:HH2	1.80	0.46
5:5:59:ASN:OD1	5:5:60:ASN:N	2.48	0.46
1:A:74:SER:OG	1:A:176:GLY:O	2.33	0.46
1:A:505:VAL:HG13	13:A:834:CLA:HED3	1.96	0.46
13:A:827:CLA:H2	13:A:827:CLA:H61	1.65	0.46
2:B:432:TRP:CE2	13:B:828:CLA:HAB	2.50	0.46
13:B:828:CLA:H51	16:F:205:BCR:H351	1.96	0.46
10:L:53:MET:HE1	10:l:132:LEU:HD21	1.98	0.46
2:2:53:HIS:ND1	13:2:809:CLA:OBD	2.46	0.46
13:L:203:CLA:HMD2	10:l:95:SER:HB3	1.98	0.46
1:a:539:ALA:O	1:a:543:HIS:ND1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:802:CLA:H41	13:1:802:CLA:H62	1.59	0.46
2:2:63:TRP:HA	13:7:102:CLA:HAB	1.97	0.46
2:2:73:TRP:NE1	7:7:6:ALA:O	2.33	0.46
13:A:825:CLA:H91	13:A:825:CLA:H111	1.80	0.46
10:L:7:VAL:HG13	10:L:20:THR:HG22	1.97	0.46
1:a:650:LEU:HD11	12:a:801:CL0:H42	1.97	0.46
1:1:546:VAL:HG21	13:1:838:CLA:HMA1	1.97	0.46
1:1:692:TYR:OH	13:1:802:CLA:OBD	2.27	0.46
13:1:806:CLA:HMA2	13:1:806:CLA:H11	1.98	0.46
13:1:824:CLA:H91	13:1:824:CLA:H111	1.77	0.46
2:2:28:ILE:HA	13:2:803:CLA:HMD3	1.98	0.46
1:A:204:LEU:HD11	13:A:813:CLA:H2	1.98	0.46
13:a:821:CLA:H61	16:a:846:BCR:H352	1.98	0.46
1:1:200:HIS:HB3	13:1:825:CLA:HED2	1.98	0.46
2:2:594:LEU:HD23	2:2:597:LEU:HD21	1.98	0.46
13:2:804:CLA:HBD	13:2:804:CLA:H143	1.96	0.46
1:A:82:VAL:HG21	13:A:804:CLA:HBB1	1.97	0.46
2:B:214:ASN:HB3	2:B:218:VAL:HG23	1.97	0.46
1:1:362:LEU:HD21	13:1:819:CLA:H72	1.98	0.46
13:2:806:CLA:HMB3	13:7:102:CLA:HHB	1.96	0.46
3:3:6:LYS:HD2	4:4:119:LYS:HE2	1.96	0.46
1:A:216:GLN:HA	1:A:220:SER:HB2	1.98	0.46
1:A:692:TYR:OH	13:A:802:CLA:OBD	2.27	0.46
13:A:806:CLA:HMA2	13:A:806:CLA:H11	1.98	0.46
2:B:600:TYR:HA	2:B:626:TRP:HH2	1.80	0.46
10:L:140:PHE:CE2	10:0:140:PHE:CE2	3.04	0.46
1:a:362:LEU:HD21	13:a:819:CLA:H72	1.98	0.46
1:a:577:PRO:HD3	2:b:568:GLY:HA2	1.98	0.46
13:a:806:CLA:HMA2	13:a:806:CLA:H11	1.98	0.46
1:1:288:LEU:HD13	13:1:818:CLA:HMA2	1.98	0.46
2:B:163:LYS:CE	10:0:4:ILE:HD13	2.46	0.46
2:B:594:LEU:HD23	2:B:597:LEU:HD21	1.98	0.46
13:B:810:CLA:H8	13:B:810:CLA:H122	1.71	0.46
2:b:259:THR:H	2:b:274:THR:HB	1.80	0.46
13:b:828:CLA:H51	16:f:205:BCR:H351	1.97	0.46
2:2:597:LEU:HD22	13:2:832:CLA:HBB2	1.97	0.46
10:0:136:CYS:HB3	16:0:201:BCR:C25	2.46	0.46
13:L:206:CLA:H112	13:L:206:CLA:H71	1.72	0.46
13:j:1103:CLA:H3A	13:j:1103:CLA:HBA2	1.59	0.46
10:0:46:ARG:NH2	13:0:205:CLA:OBD	2.49	0.46
1:a:204:LEU:HD11	13:a:813:CLA:H2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:25:ARG:NH1	10:l:104:LYS:O	2.34	0.45
1:1:473:ASP:OD1	1:1:479:GLN:NE2	2.49	0.45
1:1:539:ALA:O	1:1:543:HIS:ND1	2.49	0.45
13:1:805:CLA:H8	16:1:851:BCR:H23C	1.97	0.45
1:A:539:ALA:O	1:A:543:HIS:ND1	2.49	0.45
1:A:577:PRO:HD3	2:B:568:GLY:HA2	1.98	0.45
1:A:645:TRP:HB3	12:A:801:CL0:H48	1.98	0.45
13:A:805:CLA:H8	16:A:851:BCR:H23C	1.97	0.45
2:B:25:TRP:CG	2:B:711:GLN:HE22	2.34	0.45
1:a:695:GLU:OE1	2:b:551:SER:OG	2.24	0.45
2:b:214:ASN:HB3	2:b:218:VAL:HG23	1.97	0.45
1:1:645:TRP:HB3	12:1:801:CL0:H48	1.98	0.45
1:A:650:LEU:HD11	12:A:801:CL0:H42	1.97	0.45
1:a:546:VAL:HG21	13:a:838:CLA:HMA1	1.97	0.45
2:b:594:LEU:HD23	2:b:597:LEU:HD21	1.98	0.45
2:b:597:LEU:HD22	13:b:833:CLA:HBB2	1.97	0.45
2:b:600:TYR:HA	2:b:626:TRP:HH2	1.80	0.45
14:b:839:PQN:H141	14:b:839:PQN:H161	1.74	0.45
1:1:428:ARG:O	1:1:432:HIS:ND1	2.34	0.45
13:1:825:CLA:H91	13:1:825:CLA:H111	1.80	0.45
3:3:58:CYS:HB3	3:3:63:LEU:HD22	1.97	0.45
13:A:824:CLA:H41	13:A:824:CLA:H62	1.71	0.45
16:A:848:BCR:H361	16:A:848:BCR:H373	1.99	0.45
2:B:28:ILE:HA	13:B:803:CLA:HMD3	1.98	0.45
10:L:80:LEU:HD23	10:0:144:PHE:CE2	2.49	0.45
13:L:206:CLA:H3A	13:L:206:CLA:HBA2	1.70	0.45
1:a:200:HIS:HB3	13:a:825:CLA:HED2	1.98	0.45
1:a:576:GLY:HA2	2:b:569:PRO:HD3	1.99	0.45
13:b:829:CLA:H61	13:b:829:CLA:H101	1.74	0.45
1:1:577:PRO:HD3	2:2:568:GLY:HA2	1.98	0.45
2:2:349:LEU:O	2:2:353:THR:OG1	2.30	0.45
10:L:81:LEU:CD2	10:0:144:PHE:CD2	2.95	0.45
10:L:132:LEU:CD2	10:0:53:MET:HE1	2.47	0.45
1:a:473:ASP:OD1	1:a:479:GLN:NE2	2.49	0.45
2:b:25:TRP:CG	2:b:711:GLN:HE22	2.34	0.45
10:l:46:ARG:HG2	10:0:125:SER:HB3	1.98	0.45
13:l:207:CLA:H71	13:l:207:CLA:H112	1.72	0.45
1:1:82:VAL:HG21	13:1:804:CLA:HBB1	1.97	0.45
1:1:354:ILE:HD11	16:1:846:BCR:HC7	1.99	0.45
13:1:821:CLA:H61	16:1:846:BCR:H352	1.98	0.45
16:1:848:BCR:H361	16:1:848:BCR:H373	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:56:HIS:ND1	13:2:804:CLA:O1A	2.42	0.45
1:A:576:GLY:HA2	2:B:569:PRO:HD3	1.99	0.45
13:A:828:CLA:H141	13:A:828:CLA:H162	1.81	0.45
16:A:847:BCR:H20C	16:A:847:BCR:H361	1.82	0.45
2:B:129:THR:HG22	2:B:273:LEU:HD21	1.99	0.45
6:F:54:ASP:OD1	6:F:56:ARG:NH2	2.40	0.45
1:a:288:LEU:HD13	13:a:818:CLA:HMA2	1.98	0.45
1:a:685:PHE:HA	14:a:843:PQN:H9	1.99	0.45
13:f:201:CLA:H42	8:j:18:LEU:HD22	1.99	0.45
1:1:733:LEU:HD22	13:1:840:CLA:HMA1	1.99	0.45
13:1:805:CLA:H11	13:1:805:CLA:HBA2	1.72	0.45
3:3:32:ASP:OD1	3:3:32:ASP:N	2.47	0.45
1:A:35:ASP:HB2	1:A:38:LEU:HB2	1.99	0.45
1:A:362:LEU:HD21	13:A:819:CLA:H72	1.98	0.45
1:A:473:ASP:OD1	1:A:479:GLN:NE2	2.49	0.45
2:B:281:LEU:HD11	16:B:840:BCR:H342	1.99	0.45
1:a:90:MET:HE1	13:a:808:CLA:H2A	1.99	0.45
1:a:645:TRP:HB3	12:a:801:CL0:H48	1.98	0.45
13:a:818:CLA:HBA2	13:a:818:CLA:H3A	1.51	0.45
2:b:28:ILE:HA	13:b:803:CLA:HMD3	1.98	0.45
13:b:814:CLA:HBA2	13:b:814:CLA:H3A	1.48	0.45
1:1:12:ALA:HA	1:1:192:ASN:HD22	1.81	0.45
1:1:90:MET:HE1	13:1:808:CLA:H2A	1.99	0.45
1:1:204:LEU:HD11	13:1:813:CLA:H2	1.98	0.45
13:A:839:CLA:H171	6:F:81:GLY:HA2	1.99	0.45
10:L:144:PHE:HE2	10:l:81:LEU:HG	1.82	0.45
1:a:711:PRO:HG2	1:a:715:PRO:HD3	1.99	0.45
2:b:63:TRP:HA	13:i:102:CLA:HAB	1.97	0.45
2:b:132:MET:HE2	13:b:811:CLA:HMA2	1.99	0.45
5:5:8:LYS:HE3	5:5:22:VAL:HG12	1.99	0.45
1:A:90:MET:HE1	13:A:808:CLA:H2A	1.99	0.45
13:A:819:CLA:HHC	13:A:819:CLA:H92	1.99	0.45
10:L:46:ARG:NH2	13:L:203:CLA:OBD	2.49	0.45
10:L:148:THR:HG21	10:l:77:THR:HG22	1.93	0.45
16:a:845:BCR:H20C	16:a:845:BCR:H361	1.83	0.45
7:i:18:VAL:HG21	13:i:102:CLA:H11	1.99	0.45
1:1:216:GLN:HA	1:1:220:SER:HB2	1.98	0.45
1:1:579:ARG:NH2	4:4:64:GLU:OE2	2.46	0.45
13:1:852:CLA:HMB3	13:2:801:CLA:H201	1.99	0.45
2:2:432:TRP:HZ3	13:2:834:CLA:HBC2	1.82	0.45
10:0:18:LEU:O	10:0:23:ASN:ND2	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:HIS:HB3	13:A:825:CLA:HED2	1.98	0.45
10:L:46:ARG:NH1	10:L:50:GLU:OE1	2.38	0.45
10:L:95:SER:CB	13:O:205:CLA:HMD3	2.45	0.45
1:a:12:ALA:HA	1:a:192:ASN:HD22	1.81	0.45
2:b:281:LEU:HD11	16:b:840:BCR:H342	1.99	0.45
2:b:539:LEU:O	2:b:543:LYS:HB2	2.17	0.45
1:1:576:GLY:HA2	2:2:569:PRO:HD3	1.99	0.45
1:1:691:GLY:N	2:2:575:CYS:O	2.47	0.45
2:2:129:THR:HG22	2:2:273:LEU:HD21	1.99	0.45
16:8:1105:BCR:H20C	16:8:1105:BCR:H361	1.88	0.45
13:A:835:CLA:HMB1	16:A:847:BCR:H272	1.99	0.44
13:A:852:CLA:HMB3	13:B:801:CLA:H201	1.99	0.44
2:B:191:LEU:HD11	16:B:840:BCR:HC8	1.98	0.44
10:L:144:PHE:CD2	10:l:81:LEU:CD2	2.97	0.44
1:a:216:GLN:HA	1:a:220:SER:HB2	1.98	0.44
13:a:835:CLA:HMB1	16:a:847:BCR:H272	1.99	0.44
16:b:840:BCR:HC32	16:b:842:BCR:H333	1.99	0.44
1:1:561:LEU:O	4:4:62:ARG:NH1	2.46	0.44
2:2:191:LEU:HD11	16:2:839:BCR:HC8	1.98	0.44
2:2:281:LEU:HD11	16:2:839:BCR:H342	1.99	0.44
16:2:842:BCR:H24C	16:2:842:BCR:H371	1.80	0.44
7:7:18:VAL:HG21	13:7:102:CLA:H11	1.99	0.44
13:A:821:CLA:H61	16:A:846:BCR:H352	1.98	0.44
13:A:824:CLA:H3A	13:A:824:CLA:HBA2	1.57	0.44
16:a:848:BCR:H361	16:a:848:BCR:H373	1.99	0.44
2:b:56:HIS:ND1	13:b:804:CLA:O1A	2.42	0.44
2:b:129:THR:HG22	2:b:273:LEU:HD21	1.99	0.44
2:b:432:TRP:HZ3	13:b:835:CLA:HBC2	1.82	0.44
13:b:810:CLA:H122	13:b:810:CLA:H8	1.71	0.44
5:e:8:LYS:HE3	5:e:22:VAL:HG12	1.99	0.44
10:l:46:ARG:NH2	13:l:204:CLA:OBD	2.49	0.44
13:1:835:CLA:HMB1	16:1:847:BCR:H272	1.99	0.44
13:1:840:CLA:H8	13:1:840:CLA:H52	1.77	0.44
2:2:25:TRP:CG	2:2:711:GLN:HE22	2.34	0.44
1:A:12:ALA:HA	1:A:192:ASN:HD22	1.81	0.44
1:A:288:LEU:HD13	13:A:818:CLA:HMA2	1.98	0.44
1:A:354:ILE:HD11	16:A:846:BCR:HC7	1.99	0.44
1:A:733:LEU:HD22	13:A:840:CLA:HMA1	1.99	0.44
4:D:3:ILE:HG22	4:D:4:GLN:HG2	1.99	0.44
5:E:8:LYS:HE3	5:E:22:VAL:HG12	1.99	0.44
1:a:74:SER:OG	1:a:176:GLY:O	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:354:ILE:HD11	16:a:846:BCR:HC7	1.99	0.44
13:a:852:CLA:HMB3	13:b:801:CLA:H201	1.99	0.44
1:1:531:ASP:OD2	1:1:612:LYS:NZ	2.46	0.44
2:2:132:MET:HE2	13:2:810:CLA:HMA2	1.99	0.44
16:z:101:BCR:H24C	16:z:101:BCR:H371	1.81	0.44
13:A:811:CLA:H61	13:A:811:CLA:H41	1.74	0.44
2:B:539:LEU:O	2:B:543:LYS:HB2	2.17	0.44
13:a:819:CLA:HHC	13:a:819:CLA:H92	1.99	0.44
13:a:828:CLA:H143	13:a:828:CLA:H111	1.75	0.44
13:b:806:CLA:HBB	13:i:102:CLA:HBB	1.99	0.44
16:i:103:BCR:H20C	16:i:103:BCR:H361	1.80	0.44
16:j:1105:BCR:H15C	16:j:1105:BCR:H351	1.86	0.44
2:2:539:LEU:O	2:2:543:LYS:HB2	2.17	0.44
6:6:23:ASN:ND2	6:6:28:PRO:O	2.51	0.44
16:L:205:BCR:H15C	16:L:205:BCR:H351	1.85	0.44
1:a:35:ASP:HB2	1:a:38:LEU:HB2	1.99	0.44
1:a:561:LEU:O	4:d:62:ARG:NH1	2.46	0.44
1:a:733:LEU:HD22	13:a:840:CLA:HMA1	1.99	0.44
2:b:191:LEU:HD11	16:b:840:BCR:HC8	1.98	0.44
13:b:836:CLA:HAB	14:b:839:PQN:H141	2.00	0.44
1:1:35:ASP:HB2	1:1:38:LEU:HB2	1.99	0.44
13:1:828:CLA:H111	13:1:828:CLA:H143	1.75	0.44
2:2:313:PRO:HA	2:2:314:PRO:HD3	1.84	0.44
1:A:531:ASP:OD2	1:A:612:LYS:NZ	2.46	0.44
13:a:804:CLA:HBD	13:a:811:CLA:H2	1.99	0.44
13:a:839:CLA:H171	6:f:81:GLY:HA2	1.99	0.44
16:a:851:BCR:H20C	16:a:851:BCR:H361	1.85	0.44
2:B:432:TRP:HZ3	13:B:835:CLA:HBC2	1.82	0.44
16:B:841:BCR:H15C	16:B:841:BCR:H351	1.86	0.44
1:1:466:ARG:NH2	13:1:833:CLA:O1D	2.51	0.44
1:1:685:PHE:HA	14:1:843:PQN:H9	1.99	0.44
13:1:839:CLA:H171	6:6:81:GLY:HA2	1.99	0.44
2:2:83:ASP:HB3	2:2:87:VAL:HG23	2.00	0.44
13:2:820:CLA:H91	13:2:820:CLA:H111	1.85	0.44
13:2:835:CLA:HAB	14:2:838:PQN:H141	2.00	0.44
13:6:201:CLA:H42	8:8:18:LEU:HD22	1.99	0.44
4:D:25:ARG:NH1	10:L:104:LYS:O	2.34	0.44
6:F:23:ASN:ND2	6:F:28:PRO:O	2.51	0.44
10:L:144:PHE:CZ	10:l:77:THR:CG2	2.95	0.44
1:a:447:LEU:O	1:a:451:SER:OG	2.30	0.44
2:b:83:ASP:HB3	2:b:87:VAL:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:313:PRO:HA	2:b:314:PRO:HD3	1.84	0.44
13:b:808:CLA:H171	16:b:841:BCR:H14C	2.00	0.44
13:l:204:CLA:HMD3	10:0:95:SER:CB	2.48	0.44
2:2:662:LEU:O	2:2:666:THR:OG1	2.30	0.44
13:2:805:CLA:H112	13:2:805:CLA:H71	1.76	0.44
16:2:843:BCR:H20C	16:2:843:BCR:H361	1.80	0.44
16:8:1104:BCR:H351	16:8:1104:BCR:H15C	1.85	0.44
13:0:208:CLA:H162	13:0:208:CLA:H141	1.80	0.44
1:A:362:LEU:HD11	13:A:819:CLA:H72	2.00	0.44
1:A:579:ARG:NH2	4:D:64:GLU:OE2	2.46	0.44
2:B:345:ALA:HA	13:B:821:CLA:HAA1	2.00	0.44
13:B:836:CLA:HAB	14:B:839:PQN:H141	2.00	0.44
10:L:140:PHE:CZ	10:0:140:PHE:CZ	3.06	0.44
16:a:846:BCR:H20C	16:a:846:BCR:H361	1.87	0.44
2:b:430:LEU:HA	2:b:433:VAL:HG12	2.00	0.44
1:1:362:LEU:HD11	13:1:819:CLA:H72	2.00	0.44
2:2:366:TYR:OH	13:2:824:CLA:OBD	2.28	0.44
16:2:839:BCR:HC32	16:2:841:BCR:H333	1.99	0.44
13:B:829:CLA:HAB	13:B:830:CLA:HMB2	2.00	0.43
16:L:207:BCR:H24C	16:L:207:BCR:H371	1.87	0.43
2:b:180:HIS:HE1	13:b:809:CLA:HMA3	1.83	0.43
2:b:400:ILE:HD13	13:b:826:CLA:HED3	2.00	0.43
1:1:711:PRO:HG2	1:1:715:PRO:HD3	1.99	0.43
13:2:804:CLA:H141	13:2:804:CLA:H161	1.78	0.43
2:B:180:HIS:HE1	13:B:809:CLA:HMA3	1.83	0.43
13:B:805:CLA:H71	13:B:805:CLA:H112	1.76	0.43
10:L:84:ILE:HD12	16:L:207:BCR:H392	2.00	0.43
13:a:817:CLA:C1D	13:a:818:CLA:HBB2	2.49	0.43
13:a:824:CLA:H91	13:a:824:CLA:H111	1.77	0.43
2:b:359:HIS:ND1	13:b:814:CLA:OBD	2.40	0.43
2:2:180:HIS:HE1	13:2:808:CLA:HMA3	1.83	0.43
4:4:31:ILE:HG21	4:4:69:LEU:HD23	2.00	0.43
16:J:1104:BCR:H15C	16:J:1104:BCR:H351	1.85	0.43
13:1:817:CLA:C1D	13:1:818:CLA:HBB2	2.49	0.43
2:2:430:LEU:HA	2:2:433:VAL:HG12	2.00	0.43
13:2:814:CLA:HBA2	13:2:814:CLA:H3A	1.59	0.43
4:4:3:ILE:HG22	4:4:4:GLN:HG2	2.00	0.43
7:7:30:LEU:HD22	19:7:101:SQD:C28	2.44	0.43
1:A:505:VAL:HG21	13:A:834:CLA:HMA2	2.01	0.43
1:A:711:PRO:HG2	1:A:715:PRO:HD3	1.99	0.43
17:A:850:LHG:H142	17:A:850:LHG:H171	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:HIS:ND1	13:B:804:CLA:O1A	2.42	0.43
2:B:132:MET:HE2	13:B:811:CLA:HMA2	1.99	0.43
2:B:430:LEU:HA	2:B:433:VAL:HG12	2.00	0.43
7:I:26:VAL:HG13	19:I:103:SQD:H292	2.00	0.43
1:1:396:ILE:HD12	13:1:806:CLA:H143	2.00	0.43
13:1:802:CLA:HBA2	2:2:435:LEU:HD23	2.00	0.43
13:1:804:CLA:HBD	13:1:811:CLA:H2	1.99	0.43
13:1:840:CLA:H172	8:8:23:ALA:HB2	2.01	0.43
13:2:830:CLA:HMB3	13:2:832:CLA:HED2	2.00	0.43
13:2:835:CLA:H8	13:2:835:CLA:H51	1.81	0.43
1:A:685:PHE:HA	14:A:843:PQN:H9	1.99	0.43
13:A:804:CLA:HBD	13:A:811:CLA:H2	1.99	0.43
2:B:444:LEU:HD11	16:B:848:BCR:H342	2.01	0.43
13:B:827:CLA:HBA1	13:B:827:CLA:H3A	1.82	0.43
1:a:466:ARG:NH2	13:a:833:CLA:O1D	2.51	0.43
13:a:802:CLA:HBA2	2:b:435:LEU:HD23	2.00	0.43
13:a:837:CLA:H13	13:l:202:CLA:HAC2	2.00	0.43
14:a:843:PQN:H302	14:a:843:PQN:H262	1.83	0.43
2:b:345:ALA:HA	13:b:821:CLA:HAA1	2.00	0.43
2:b:594:LEU:O	2:b:598:THR:OG1	2.30	0.43
13:b:820:CLA:H61	13:b:820:CLA:H2	1.81	0.43
1:1:505:VAL:HG21	13:1:834:CLA:HMA2	2.01	0.43
13:1:819:CLA:H92	13:1:819:CLA:HHC	1.99	0.43
2:2:720:PHE:O	2:2:724:TYR:HB2	2.19	0.43
13:0:208:CLA:H112	13:0:208:CLA:H71	1.72	0.43
13:A:837:CLA:H8	13:A:837:CLA:H52	1.76	0.43
2:B:83:ASP:HB3	2:B:87:VAL:HG23	2.00	0.43
13:B:808:CLA:H171	16:B:841:BCR:H14C	2.00	0.43
14:B:839:PQN:H141	14:B:839:PQN:H161	1.74	0.43
9:K:7:VAL:HA	9:K:8:PRO:HD3	1.87	0.43
1:a:505:VAL:HG21	13:a:834:CLA:HMA2	2.01	0.43
2:b:193:TRP:HD1	2:b:280:HIS:CD2	2.37	0.43
16:b:844:BCR:H351	16:b:844:BCR:H15C	1.79	0.43
16:j:1104:BCR:H20C	16:j:1104:BCR:H361	1.87	0.43
2:2:300:ILE:HD11	13:2:816:CLA:HMA2	2.01	0.43
13:2:807:CLA:H171	16:2:840:BCR:H14C	2.00	0.43
13:A:817:CLA:C1D	13:A:818:CLA:HBB2	2.49	0.43
2:B:114:SER:HB2	7:I:3:GLY:HA2	2.01	0.43
2:B:300:ILE:HD11	13:B:817:CLA:HMA2	2.01	0.43
2:B:720:PHE:O	2:B:724:TYR:HB2	2.19	0.43
13:F:201:CLA:H42	8:J:18:LEU:HD22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:18:VAL:HA	7:I:22:MET:HG3	2.01	0.43
16:K:4004:BCR:H11C	16:K:4004:BCR:H341	1.91	0.43
1:a:362:LEU:HD11	13:a:819:CLA:H72	2.00	0.43
1:a:579:ARG:NH2	4:d:64:GLU:OE2	2.46	0.43
2:b:720:PHE:O	2:b:724:TYR:HB2	2.19	0.43
13:b:804:CLA:H143	13:b:804:CLA:H111	1.81	0.43
13:b:807:CLA:H92	13:b:807:CLA:H62	1.84	0.43
13:b:821:CLA:HBA2	13:b:821:CLA:HED3	2.00	0.43
16:b:848:BCR:H361	16:b:848:BCR:H20C	1.87	0.43
4:d:3:ILE:HG22	4:d:4:GLN:HG2	2.00	0.43
6:f:115:MET:HE2	6:f:118:LEU:CD1	2.21	0.43
8:j:15:ILE:HD12	8:j:15:ILE:HA	1.94	0.43
13:2:806:CLA:HHB	13:7:102:CLA:HHB	1.99	0.43
13:2:811:CLA:H3A	13:2:811:CLA:HBA1	1.79	0.43
16:0:204:BCR:H20C	16:0:204:BCR:H361	1.89	0.43
1:A:466:ARG:NH2	13:A:833:CLA:O1D	2.51	0.43
13:B:805:CLA:HMA2	13:B:805:CLA:H2	2.01	0.43
16:L:207:BCR:H313	13:0:202:CLA:H72	2.00	0.43
13:a:824:CLA:HBA2	13:a:824:CLA:H3A	1.57	0.43
4:d:31:ILE:HG21	4:d:69:LEU:HD23	2.00	0.43
10:l:136:CYS:HB3	16:l:201:BCR:C26	2.49	0.43
13:l:202:CLA:H72	16:0:201:BCR:H313	2.00	0.43
16:1:851:BCR:H20C	16:1:851:BCR:H361	1.85	0.43
2:2:114:SER:HB2	7:7:3:GLY:HA2	2.01	0.43
13:2:820:CLA:HBA2	13:2:820:CLA:HED3	2.00	0.43
1:A:298:LEU:HD22	13:A:815:CLA:HMC1	2.01	0.43
1:A:374:PRO:HA	1:A:375:PRO:HD3	1.83	0.43
1:A:691:GLY:N	2:B:575:CYS:O	2.47	0.43
13:A:802:CLA:HBA2	2:B:435:LEU:HD23	2.01	0.43
13:A:806:CLA:H51	13:A:806:CLA:H11	1.87	0.43
13:B:831:CLA:HMB3	13:B:833:CLA:HED2	2.00	0.43
16:B:840:BCR:HC32	16:B:842:BCR:H333	1.99	0.43
13:a:803:CLA:H91	13:b:802:CLA:H111	2.01	0.43
13:a:840:CLA:H172	8:j:23:ALA:HB2	2.01	0.43
10:l:144:PHE:CE2	10:0:80:LEU:HD23	2.49	0.43
13:2:828:CLA:H101	13:2:828:CLA:H61	1.74	0.43
13:2:828:CLA:HAB	13:2:829:CLA:HMB2	2.01	0.43
7:7:18:VAL:HA	7:7:22:MET:HG3	2.01	0.43
13:A:840:CLA:H172	8:J:23:ALA:HB2	2.01	0.43
13:J:1103:CLA:HBA2	13:J:1103:CLA:H3A	1.59	0.43
1:a:396:ILE:HD12	13:a:806:CLA:H143	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:396:ALA:HB1	13:b:826:CLA:HMD3	2.01	0.43
10:l:41:GLY:HA3	10:0:121:LYS:HE2	1.99	0.43
1:1:673:LEU:HD11	2:2:624:MET:HB2	2.01	0.43
2:2:677:TYR:OH	13:2:802:CLA:OBD	2.29	0.43
13:2:810:CLA:HMB1	13:2:824:CLA:H111	2.01	0.43
16:0:204:BCR:H15C	16:0:204:BCR:H351	1.91	0.43
2:B:400:ILE:HD13	13:B:826:CLA:HED3	2.00	0.42
3:C:34:CYS:SG	3:C:35:LYS:N	2.92	0.42
16:F:205:BCR:H20C	16:F:205:BCR:H361	1.85	0.42
9:K:80:LEU:HD22	2:b:216:LEU:HB3	2.01	0.42
13:a:821:CLA:H161	13:a:821:CLA:H122	1.81	0.42
2:b:104:VAL:HG11	7:i:1:ILE:HG13	2.01	0.42
2:b:300:ILE:HD11	13:b:817:CLA:HMA2	2.01	0.42
13:1:803:CLA:H91	13:2:802:CLA:H111	2.01	0.42
13:2:819:CLA:HED3	13:2:819:CLA:H2A	2.01	0.42
1:A:305:ILE:O	1:A:309:HIS:ND1	2.52	0.42
13:A:810:CLA:HBA1	13:A:810:CLA:H3A	1.93	0.42
10:L:95:SER:HB3	13:0:205:CLA:HMD2	2.00	0.42
13:b:829:CLA:HAB	13:b:830:CLA:HMB2	2.01	0.42
16:m:101:BCR:H24C	16:m:101:BCR:H371	1.81	0.42
2:2:63:TRP:NE1	13:2:823:CLA:OBD	2.51	0.42
16:2:847:BCR:H15C	16:2:847:BCR:H351	1.89	0.42
1:A:269:GLY:O	1:A:272:SER:HB3	2.19	0.42
1:A:412:MET:HE3	1:A:412:MET:HB3	1.91	0.42
13:A:837:CLA:H13	13:L:201:CLA:HAC2	2.00	0.42
2:B:180:HIS:CG	13:B:810:CLA:HMC2	2.55	0.42
4:D:31:ILE:HG21	4:D:69:LEU:HD23	2.00	0.42
1:a:305:ILE:O	1:a:309:HIS:ND1	2.52	0.42
13:b:831:CLA:HMB3	13:b:833:CLA:HED2	2.00	0.42
16:i:103:BCR:H15C	16:i:103:BCR:H351	1.90	0.42
10:l:140:PHE:HE2	10:0:140:PHE:CE2	2.34	0.42
1:1:298:LEU:HD22	13:1:815:CLA:HMC1	2.01	0.42
1:1:305:ILE:O	1:1:309:HIS:ND1	2.52	0.42
1:1:537:ILE:HD13	12:1:801:CL0:H59	2.02	0.42
1:1:589:ASP:HA	1:1:592:PHE:HB3	2.02	0.42
13:1:840:CLA:H202	13:1:840:CLA:H162	1.89	0.42
13:2:806:CLA:H141	13:2:806:CLA:H162	1.77	0.42
13:2:809:CLA:H122	13:2:809:CLA:H8	1.71	0.42
16:9:4001:BCR:H20C	16:9:4001:BCR:H361	1.86	0.42
13:A:832:CLA:HMD3	13:L:206:CLA:H193	2.02	0.42
16:A:846:BCR:H11C	16:A:846:BCR:H341	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:396:ALA:HB1	13:B:826:CLA:HMD3	2.01	0.42
13:B:805:CLA:H193	13:B:805:CLA:H161	1.84	0.42
13:B:806:CLA:HHB	13:I:101:CLA:HHB	1.99	0.42
7:I:18:VAL:HG21	13:I:101:CLA:H11	1.99	0.42
13:L:201:CLA:H72	16:l:201:BCR:H313	2.00	0.42
13:L:206:CLA:H141	13:L:206:CLA:H162	1.81	0.42
1:a:298:LEU:HD22	13:a:815:CLA:HMC1	2.01	0.42
13:a:802:CLA:H41	13:a:802:CLA:H62	1.60	0.42
13:a:825:CLA:H62	13:a:825:CLA:H92	1.81	0.42
13:a:832:CLA:HMD3	13:l:207:CLA:H193	2.02	0.42
2:b:114:SER:HB2	7:i:3:GLY:HA2	2.01	0.42
13:b:815:CLA:HBA2	13:b:815:CLA:H3A	1.59	0.42
3:c:34:CYS:SG	3:c:35:LYS:N	2.92	0.42
6:f:23:ASN:ND2	6:f:28:PRO:O	2.51	0.42
6:f:115:MET:HE3	6:f:118:LEU:CG	2.47	0.42
16:f:205:BCR:H331	16:f:205:BCR:H343	2.01	0.42
16:l:206:BCR:H11C	16:l:206:BCR:H341	1.92	0.42
1:1:367:ALA:HB2	1:1:393:HIS:HB2	2.02	0.42
13:1:828:CLA:H203	16:8:1104:BCR:H10C	2.01	0.42
13:1:837:CLA:H13	13:0:202:CLA:HAC2	2.00	0.42
2:2:396:ALA:HB1	13:2:825:CLA:HMD3	2.01	0.42
14:2:838:PQN:H141	14:2:838:PQN:H161	1.74	0.42
1:A:273:ASP:OD1	1:A:273:ASP:N	2.50	0.42
1:A:695:GLU:OE1	2:B:551:SER:OG	2.24	0.42
2:B:104:VAL:HG11	7:I:1:ILE:HG13	2.01	0.42
2:B:191:LEU:HD21	16:B:840:BCR:H321	2.02	0.42
10:L:132:LEU:CD2	13:0:205:CLA:HED2	2.36	0.42
2:b:444:LEU:HD11	16:b:848:BCR:H342	2.01	0.42
10:l:144:PHE:CD2	10:0:81:LEU:CD2	2.96	0.42
13:1:811:CLA:H41	13:1:811:CLA:H61	1.74	0.42
2:2:191:LEU:HD21	16:2:839:BCR:H321	2.02	0.42
2:2:345:ALA:HA	13:2:820:CLA:HAA1	2.00	0.42
2:2:444:LEU:HD11	16:2:847:BCR:H342	2.01	0.42
14:2:838:PQN:H193	14:2:838:PQN:H162	1.78	0.42
16:0:201:BCR:H24C	16:0:201:BCR:H371	1.87	0.42
2:B:53:HIS:HE1	13:B:804:CLA:H161	1.85	0.42
13:L:203:CLA:OBD	10:l:95:SER:OG	2.25	0.42
1:a:428:ARG:HB3	13:a:831:CLA:HED3	2.02	0.42
14:a:843:PQN:H141	14:a:843:PQN:H162	1.92	0.42
2:b:191:LEU:HD21	16:b:840:BCR:H321	2.02	0.42
13:b:811:CLA:HMB1	13:b:825:CLA:H111	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:b:820:CLA:H2A	13:b:820:CLA:HED3	2.01	0.42
16:b:848:BCR:H15C	16:b:848:BCR:H351	1.89	0.42
13:i:102:CLA:H71	13:i:102:CLA:H112	1.91	0.42
10:l:72:THR:HG22	10:l:74:TYR:H	1.85	0.42
1:l:661:TYR:HD2	2:2:452:VAL:HG12	1.84	0.42
13:l:833:CLA:H62	13:l:833:CLA:H2	1.83	0.42
2:2:180:HIS:CG	13:2:809:CLA:HMC2	2.55	0.42
2:2:400:ILE:HD13	13:2:825:CLA:HED3	2.00	0.42
16:2:842:BCR:H15C	16:2:842:BCR:H351	1.90	0.42
16:8:1104:BCR:H20C	16:8:1104:BCR:H361	1.87	0.42
1:A:396:ILE:HD12	13:A:806:CLA:H143	2.00	0.42
16:F:205:BCR:H331	16:F:205:BCR:H343	2.01	0.42
16:L:207:BCR:H11C	16:L:207:BCR:H341	1.93	0.42
1:a:367:ALA:HB2	1:a:393:HIS:HB2	2.02	0.42
13:b:825:CLA:H72	13:b:825:CLA:H112	1.85	0.42
4:d:15:SER:OG	4:d:16:THR:N	2.53	0.42
2:2:53:HIS:HE1	13:2:804:CLA:H161	1.85	0.42
2:2:381:THR:HG23	2:2:598:THR:HG21	2.02	0.42
10:0:72:THR:HG22	10:0:74:TYR:H	1.85	0.42
1:A:428:ARG:HB3	13:A:831:CLA:HED3	2.02	0.42
1:A:438:SER:HB2	2:B:688:ALA:HB2	2.02	0.42
1:A:661:TYR:HD2	2:B:452:VAL:HG12	1.85	0.42
13:A:828:CLA:H203	16:J:1104:BCR:H10C	2.01	0.42
2:B:181:HIS:HE1	13:B:804:CLA:H122	1.85	0.42
2:B:381:THR:HG23	2:B:598:THR:HG21	2.02	0.42
13:B:802:CLA:H141	13:B:802:CLA:H161	1.84	0.42
16:B:843:BCR:H371	16:B:843:BCR:H24C	1.80	0.42
10:L:84:ILE:HG21	10:0:141:PHE:CE1	2.55	0.42
1:a:537:ILE:HD13	12:a:801:CL0:H59	2.02	0.42
1:a:673:LEU:HD11	2:b:624:MET:HB2	2.01	0.42
16:a:848:BCR:H14C	13:a:852:CLA:H13	2.02	0.42
13:b:804:CLA:H161	13:b:804:CLA:H141	1.78	0.42
13:l:821:CLA:H161	13:l:821:CLA:H122	1.81	0.42
2:2:104:VAL:HG11	7:7:1:ILE:HG13	2.01	0.42
1:A:276:THR:HG21	1:A:278:LYS:HE3	2.02	0.42
1:A:367:ALA:HB2	1:A:393:HIS:HB2	2.02	0.42
16:A:851:BCR:H15C	16:A:851:BCR:H351	1.89	0.42
2:B:388:GLY:HA3	2:B:594:LEU:HD11	2.01	0.42
13:B:803:CLA:H92	13:B:803:CLA:H62	1.86	0.42
13:B:821:CLA:HBA2	13:B:821:CLA:HED3	2.00	0.42
16:B:844:BCR:H15C	16:B:844:BCR:H351	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:104:LYS:HA	10:L:105:PRO:HD3	1.94	0.42
1:a:438:SER:HB2	2:b:688:ALA:HB2	2.02	0.42
1:a:531:ASP:O	1:a:535:HIS:ND1	2.36	0.42
7:i:18:VAL:HA	7:i:22:MET:HG3	2.01	0.42
1:1:438:SER:HB2	2:2:688:ALA:HB2	2.02	0.42
13:1:827:CLA:H122	13:1:827:CLA:H161	1.80	0.42
1:A:537:ILE:HD13	12:A:801:CL0:H59	2.02	0.42
1:A:589:ASP:HA	1:A:592:PHE:HB3	2.02	0.42
13:A:821:CLA:H122	13:A:821:CLA:H161	1.81	0.42
2:B:72:ALA:HB2	2:B:138:LEU:HB2	2.02	0.42
7:I:30:LEU:HD22	19:I:103:SQD:C28	2.38	0.42
16:I:102:BCR:H15C	16:I:102:BCR:H351	1.90	0.42
10:L:121:LYS:HE2	10:0:41:GLY:HA3	2.01	0.42
1:a:273:ASP:OD1	1:a:273:ASP:N	2.50	0.42
3:c:25:VAL:HG13	3:c:45:THR:HA	2.02	0.42
10:l:141:PHE:CE1	10:0:84:ILE:HG21	2.55	0.42
13:l:204:CLA:OBD	10:0:95:SER:OG	2.33	0.42
16:1:848:BCR:H14C	13:1:852:CLA:H13	2.02	0.42
16:2:847:BCR:H20C	16:2:847:BCR:H361	1.87	0.42
6:6:114:PHE:CE2	6:6:115:MET:CG	2.90	0.42
1:A:293:THR:O	1:A:297:HIS:ND1	2.53	0.41
1:A:430:LEU:HD23	1:A:430:LEU:HA	1.90	0.41
1:A:613:MET:HE3	1:A:613:MET:HB3	1.97	0.41
1:A:691:GLY:O	1:A:695:GLU:HG2	2.20	0.41
2:B:193:TRP:HD1	2:B:280:HIS:CD2	2.37	0.41
10:L:140:PHE:CZ	10:l:140:PHE:CZ	3.07	0.41
1:a:293:THR:O	1:a:297:HIS:ND1	2.53	0.41
1:a:691:GLY:O	1:a:695:GLU:HG2	2.20	0.41
2:2:378:ALA:O	2:2:382:HIS:HB3	2.20	0.41
13:2:805:CLA:H2	13:2:805:CLA:HMA2	2.01	0.41
3:3:34:CYS:SG	3:3:35:LYS:N	2.92	0.41
13:A:809:CLA:HAB	13:B:830:CLA:HBC2	2.03	0.41
2:B:378:ALA:O	2:B:382:HIS:HB3	2.20	0.41
13:B:820:CLA:H2A	13:B:820:CLA:HED3	2.01	0.41
13:a:833:CLA:H62	13:a:833:CLA:H2	1.83	0.41
7:i:7:ALA:HB2	11:m:5:GLU:HG3	2.02	0.41
1:1:613:MET:HE3	1:1:613:MET:HB3	1.97	0.41
16:1:847:BCR:H20C	16:1:847:BCR:H361	1.82	0.41
16:2:843:BCR:H351	16:2:843:BCR:H15C	1.79	0.41
13:A:817:CLA:HMC2	13:A:817:CLA:H72	2.02	0.41
13:B:829:CLA:H101	13:B:829:CLA:H61	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:7:ALA:HB2	11:M:5:GLU:HG3	2.02	0.41
13:I:101:CLA:H71	13:I:101:CLA:H112	1.91	0.41
10:L:125:SER:HB3	10:0:46:ARG:HG2	2.03	0.41
1:a:66:GLU:HB2	1:a:187:LEU:HB2	2.02	0.41
13:a:824:CLA:H62	13:a:824:CLA:H41	1.71	0.41
2:b:53:HIS:HE1	13:b:804:CLA:H161	1.85	0.41
13:b:824:CLA:H3A	13:b:824:CLA:HBA2	1.44	0.41
13:b:847:CLA:H202	16:l:206:BCR:H311	2.02	0.41
1:1:269:GLY:O	1:1:272:SER:HB3	2.19	0.41
1:1:421:ASN:OD1	1:1:424:ASN:ND2	2.42	0.41
13:1:806:CLA:H51	13:1:806:CLA:H11	1.87	0.41
13:1:826:CLA:H41	13:1:826:CLA:H62	1.88	0.41
13:A:803:CLA:H91	13:B:802:CLA:H111	2.01	0.41
13:A:807:CLA:H2A	13:A:809:CLA:HED1	2.03	0.41
14:A:843:PQN:H302	14:A:843:PQN:H262	1.83	0.41
16:F:202:BCR:H15C	16:F:202:BCR:H351	1.92	0.41
16:M:101:BCR:H15C	16:M:101:BCR:H351	1.87	0.41
13:a:809:CLA:HAB	13:b:830:CLA:HBC2	2.03	0.41
13:a:827:CLA:H61	13:a:827:CLA:H2	1.65	0.41
2:b:388:GLY:HA3	2:b:594:LEU:HD11	2.01	0.41
13:b:805:CLA:HMA2	13:b:805:CLA:H2	2.01	0.41
13:f:201:CLA:H41	13:f:201:CLA:H62	1.91	0.41
13:l:207:CLA:H142	13:l:207:CLA:H111	1.86	0.41
1:1:293:THR:O	1:1:297:HIS:ND1	2.54	0.41
13:1:827:CLA:H2	13:1:827:CLA:H61	1.65	0.41
13:1:832:CLA:HMD3	13:0:208:CLA:H193	2.02	0.41
2:2:193:TRP:HD1	2:2:280:HIS:CD2	2.37	0.41
2:2:388:GLY:HA3	2:2:594:LEU:HD11	2.01	0.41
4:4:15:SER:OG	4:4:16:THR:N	2.53	0.41
10:0:5:ASP:OD1	10:0:5:ASP:N	2.44	0.41
16:A:845:BCR:H15C	16:A:845:BCR:H351	1.93	0.41
13:B:811:CLA:HMB1	13:B:825:CLA:H111	2.01	0.41
3:C:32:ASP:OD1	3:C:32:ASP:N	2.47	0.41
10:L:72:THR:HG22	10:L:74:TYR:H	1.85	0.41
16:L:202:BCR:H15C	16:L:202:BCR:H351	1.91	0.41
1:a:589:ASP:HA	1:a:592:PHE:HB3	2.02	0.41
2:b:181:HIS:HE1	13:b:804:CLA:H122	1.85	0.41
2:b:378:ALA:O	2:b:382:HIS:HB3	2.20	0.41
2:b:405:ASP:OD1	4:d:133:LYS:NZ	2.41	0.41
13:b:803:CLA:H92	13:b:803:CLA:H62	1.86	0.41
16:l:201:BCR:H15C	16:l:201:BCR:H351	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:840:BCR:H15C	16:2:840:BCR:H351	1.85	0.41
16:z:101:BCR:H15C	16:z:101:BCR:H351	1.87	0.41
1:A:673:LEU:HD11	2:B:624:MET:HB2	2.01	0.41
13:B:804:CLA:H161	13:B:804:CLA:H141	1.78	0.41
13:B:821:CLA:H91	13:B:821:CLA:H111	1.85	0.41
13:B:823:CLA:H141	13:B:823:CLA:H161	1.80	0.41
13:F:201:CLA:H11	13:F:201:CLA:H52	1.87	0.41
10:L:140:PHE:CE2	10:0:140:PHE:HE2	2.31	0.41
10:L:154:LEU:HD21	7:i:13:ILE:CG1	2.50	0.41
1:a:269:GLY:O	1:a:272:SER:HB3	2.19	0.41
1:a:276:THR:HG21	1:a:278:LYS:HE3	2.02	0.41
13:1:803:CLA:H193	13:1:803:CLA:H161	1.95	0.41
1:A:402:VAL:HG22	1:A:549:LEU:HD11	2.02	0.41
13:A:828:CLA:H143	13:A:828:CLA:H111	1.75	0.41
13:B:836:CLA:H8	13:B:836:CLA:H51	1.81	0.41
4:D:15:SER:OG	4:D:16:THR:N	2.53	0.41
13:a:839:CLA:H141	13:f:201:CLA:HBD	2.03	0.41
2:b:565:PRO:HB3	2:b:709:ILE:HB	2.03	0.41
16:b:843:BCR:H15C	16:b:843:BCR:H351	1.90	0.41
6:f:54:ASP:OD1	6:f:56:ARG:NH2	2.40	0.41
10:l:39:ARG:HB3	10:l:42:LEU:HD13	2.03	0.41
16:6:205:BCR:H20C	16:6:205:BCR:H361	1.85	0.41
13:0:203:CLA:H92	13:0:203:CLA:H62	1.84	0.41
2:B:426:ILE:HG23	13:B:835:CLA:HBB2	2.03	0.41
2:B:587:MET:HG3	2:B:717:LEU:HD21	2.03	0.41
16:L:205:BCR:H11C	16:L:205:BCR:H341	1.92	0.41
2:b:389:PHE:CE2	13:b:824:CLA:HMC1	2.56	0.41
1:1:66:GLU:HB2	1:1:187:LEU:HB2	2.02	0.41
2:2:583:PHE:O	2:2:587:MET:HG2	2.21	0.41
13:2:812:CLA:H2	13:2:812:CLA:H61	1.80	0.41
16:A:845:BCR:H11C	16:A:845:BCR:H341	1.96	0.41
16:A:848:BCR:H14C	13:A:852:CLA:H13	2.02	0.41
2:B:389:PHE:CE2	13:B:824:CLA:HMC1	2.56	0.41
2:B:514:SER:HA	2:B:517:LEU:HD21	2.03	0.41
2:B:565:PRO:HB3	2:B:709:ILE:HB	2.03	0.41
13:B:812:CLA:HBA1	13:B:812:CLA:H3A	1.79	0.41
13:B:816:CLA:H93	13:B:816:CLA:H111	1.93	0.41
13:F:201:CLA:H41	13:F:201:CLA:H62	1.91	0.41
10:L:62:PRO:HB3	13:L:204:CLA:HBB1	2.03	0.41
1:a:661:TYR:HD2	2:b:452:VAL:HG12	1.84	0.41
13:a:828:CLA:H203	16:j:1104:BCR:H10C	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:i:10:LEU:HD23	7:i:10:LEU:HA	1.95	0.41
10:l:53:MET:HE1	10:0:132:LEU:CD2	2.51	0.41
1:1:402:VAL:HG22	1:1:549:LEU:HD11	2.02	0.41
13:1:809:CLA:HAB	13:2:829:CLA:HBC2	2.03	0.41
13:1:824:CLA:H3A	13:1:824:CLA:HBA2	1.57	0.41
16:1:845:BCR:H392	16:9:4001:BCR:HC8	2.03	0.41
2:2:219:LYS:HA	2:2:220:PRO:HD3	1.98	0.41
2:2:356:VAL:HG21	13:2:824:CLA:HHD	2.03	0.41
2:2:565:PRO:HB3	2:2:709:ILE:HB	2.03	0.41
13:2:806:CLA:H2	13:2:806:CLA:H102	2.03	0.41
5:5:5:ARG:NH2	5:5:27:SER:OG	2.47	0.41
16:6:205:BCR:H331	16:6:205:BCR:H343	2.01	0.41
1:A:66:GLU:HB2	1:A:187:LEU:HB2	2.02	0.41
1:A:573:PRO:HG3	5:E:50:SER:HB3	2.03	0.41
16:A:846:BCR:H15C	16:A:846:BCR:H351	1.89	0.41
3:C:25:VAL:HG13	3:C:45:THR:HA	2.02	0.41
6:F:72:TYR:OH	6:F:114:PHE:O	2.36	0.41
13:F:203:CLA:HBA1	13:F:203:CLA:H3A	1.81	0.41
16:L:205:BCR:H20C	16:L:205:BCR:H361	1.83	0.41
1:a:332:PHE:HE1	10:l:21:PRO:HG2	1.86	0.41
1:a:374:PRO:HA	1:a:375:PRO:HD3	1.83	0.41
13:a:817:CLA:HMC2	13:a:817:CLA:H72	2.02	0.41
2:b:583:PHE:O	2:b:587:MET:HG2	2.21	0.41
16:k:4004:BCR:H20C	16:k:4004:BCR:H361	1.90	0.41
10:l:62:PRO:HB3	13:l:205:CLA:HBB1	2.03	0.41
1:1:428:ARG:HB3	13:1:831:CLA:HED3	2.02	0.41
1:1:573:PRO:HG3	5:5:50:SER:HB3	2.03	0.41
2:2:92:HIS:ND1	2:2:93:ALA:O	2.54	0.41
14:A:843:PQN:H141	14:A:843:PQN:H162	1.92	0.40
2:B:135:ASN:HD22	2:B:138:LEU:HD12	1.86	0.40
13:B:806:CLA:H102	13:B:806:CLA:H2	2.03	0.40
8:J:12:PRO:HB2	16:J:1105:BCR:H391	2.04	0.40
1:a:691:GLY:N	2:b:575:CYS:O	2.47	0.40
1:a:692:TYR:OH	13:a:802:CLA:OBD	2.27	0.40
13:a:826:CLA:H41	13:a:826:CLA:H62	1.88	0.40
2:b:180:HIS:CG	13:b:810:CLA:HMC2	2.55	0.40
2:b:381:THR:HG23	2:b:598:THR:HG21	2.02	0.40
13:b:831:CLA:H93	13:b:832:CLA:HBB1	2.04	0.40
16:b:843:BCR:H371	16:b:843:BCR:H24C	1.80	0.40
1:1:217:ILE:HD13	1:1:217:ILE:HA	1.93	0.40
13:1:817:CLA:H72	13:1:817:CLA:HMC2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1:847:BCR:H351	16:1:847:BCR:H15C	1.83	0.40
13:2:815:CLA:HMB2	13:2:820:CLA:HMA3	2.03	0.40
13:2:830:CLA:H93	13:2:831:CLA:HBB1	2.03	0.40
3:3:64:SER:OG	15:3:102:SF4:S3	2.79	0.40
7:7:7:ALA:HB2	11:z:5:GLU:HG3	2.02	0.40
1:A:564:ASP:OD1	1:A:564:ASP:N	2.46	0.40
1:A:588:TRP:CD1	13:A:830:CLA:HMD1	2.57	0.40
13:B:815:CLA:H143	13:B:815:CLA:H111	1.88	0.40
13:B:815:CLA:H3A	13:B:815:CLA:HBA2	1.59	0.40
13:B:847:CLA:H202	16:L:205:BCR:H311	2.02	0.40
10:L:84:ILE:CD1	16:L:207:BCR:H392	2.51	0.40
13:L:206:CLA:H93	13:L:206:CLA:H62	1.91	0.40
1:a:374:PRO:HG2	1:a:380:ALA:HB2	2.04	0.40
2:b:63:TRP:NE1	13:b:824:CLA:OBD	2.51	0.40
16:l:206:BCR:H15C	16:l:206:BCR:H351	1.85	0.40
1:1:588:TRP:CD1	13:1:830:CLA:HMD1	2.56	0.40
2:2:594:LEU:HD23	2:2:594:LEU:HA	1.97	0.40
16:9:4001:BCR:H11C	16:9:4001:BCR:H341	1.96	0.40
2:B:583:PHE:O	2:B:587:MET:HG2	2.21	0.40
2:B:662:LEU:O	2:B:666:THR:OG1	2.31	0.40
14:B:839:PQN:H162	14:B:839:PQN:H193	1.78	0.40
16:I:102:BCR:H361	16:I:102:BCR:H20C	1.80	0.40
10:L:39:ARG:HB3	10:L:42:LEU:HD13	2.03	0.40
1:a:588:TRP:CD1	13:a:830:CLA:HMD1	2.57	0.40
13:a:837:CLA:H52	13:a:837:CLA:H8	1.76	0.40
13:a:852:CLA:H62	13:a:852:CLA:H41	1.95	0.40
2:b:514:SER:HA	2:b:517:LEU:HD21	2.03	0.40
2:b:662:LEU:O	2:b:666:THR:OG1	2.31	0.40
13:f:203:CLA:HBA1	13:f:203:CLA:H3A	1.81	0.40
1:1:276:THR:HG21	1:1:278:LYS:HE3	2.02	0.40
2:2:72:ALA:HB2	2:2:138:LEU:HB2	2.02	0.40
2:2:389:PHE:CE2	13:2:823:CLA:HMC1	2.56	0.40
13:2:823:CLA:HBA2	13:2:823:CLA:H3A	1.44	0.40
1:A:332:PHE:HE1	10:L:21:PRO:HG2	1.87	0.40
1:A:561:LEU:O	4:D:62:ARG:NH1	2.46	0.40
2:B:694:LEU:HD11	10:L:35:LEU:HD13	2.04	0.40
13:B:831:CLA:H93	13:B:832:CLA:HBB1	2.03	0.40
1:a:196:MET:HB2	13:a:813:CLA:HBC2	2.03	0.40
1:a:391:THR:HG23	1:a:606:ILE:HG21	2.03	0.40
2:b:72:ALA:HB2	2:b:138:LEU:HB2	2.02	0.40
2:b:135:ASN:HD22	2:b:138:LEU:HD12	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:732:LEU:O	2:b:736:THR:HG22	2.21	0.40
13:b:806:CLA:H102	13:b:806:CLA:H2	2.03	0.40
13:b:825:CLA:H141	13:b:825:CLA:H162	1.90	0.40
13:b:827:CLA:HBA1	13:b:827:CLA:H3A	1.82	0.40
16:f:202:BCR:H11C	16:f:202:BCR:H341	1.93	0.40
16:j:1105:BCR:H24C	16:j:1105:BCR:H371	1.91	0.40
10:l:140:PHE:CE2	10:0:140:PHE:CE2	3.10	0.40
16:l:203:BCR:H20C	16:l:203:BCR:H361	1.89	0.40
1:1:666:SER:HB2	2:2:453:ALA:HB1	2.04	0.40
1:1:691:GLY:O	1:1:695:GLU:HG2	2.20	0.40
13:1:807:CLA:H2A	13:1:809:CLA:HED1	2.03	0.40
13:1:825:CLA:H62	13:1:825:CLA:H92	1.81	0.40
17:1:850:LHG:H142	17:1:850:LHG:H171	1.81	0.40
2:2:135:ASN:HD22	2:2:138:LEU:HD12	1.86	0.40
2:2:426:ILE:HG23	13:2:834:CLA:HBB2	2.03	0.40
2:2:514:SER:HA	2:2:517:LEU:HD21	2.02	0.40
13:2:846:CLA:H202	16:0:207:BCR:H311	2.02	0.40
6:6:27:ASP:HA	6:6:28:PRO:HD3	1.95	0.40
1:A:258:GLN:H	1:A:258:GLN:HG2	1.76	0.40
1:A:421:ASN:OD1	1:A:424:ASN:ND2	2.42	0.40
2:B:63:TRP:NE1	13:B:824:CLA:OBD	2.51	0.40
13:B:802:CLA:H142	13:B:802:CLA:H112	1.97	0.40
1:a:430:LEU:HD23	1:a:430:LEU:HA	1.90	0.40
2:b:73:TRP:NE1	7:i:6:ALA:O	2.33	0.40
13:b:805:CLA:HBB	13:b:826:CLA:HAB	2.04	0.40
13:b:813:CLA:H2	13:b:813:CLA:H61	1.79	0.40
13:b:816:CLA:HMB2	13:b:821:CLA:HMA3	2.03	0.40
1:1:374:PRO:HG2	1:1:380:ALA:HB2	2.04	0.40
13:1:805:CLA:H12	13:1:806:CLA:HBB1	2.03	0.40
13:2:802:CLA:H62	13:2:802:CLA:H92	1.88	0.40
3:3:25:VAL:HG13	3:3:45:THR:HA	2.02	0.40
8:8:12:PRO:HB2	16:8:1105:BCR:H391	2.04	0.40
13:9:4003:CLA:C1B	16:9:4004:BCR:H14C	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	739/741 (100%)	720 (97%)	19 (3%)	0	100	100
1	A	739/741 (100%)	719 (97%)	20 (3%)	0	100	100
1	a	739/741 (100%)	720 (97%)	19 (3%)	0	100	100
2	2	735/737 (100%)	712 (97%)	23 (3%)	0	100	100
2	B	735/737 (100%)	712 (97%)	23 (3%)	0	100	100
2	b	735/737 (100%)	712 (97%)	23 (3%)	0	100	100
3	3	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
3	C	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
3	c	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
4	4	137/139 (99%)	125 (91%)	12 (9%)	0	100	100
4	D	137/139 (99%)	125 (91%)	12 (9%)	0	100	100
4	d	137/139 (99%)	126 (92%)	11 (8%)	0	100	100
5	5	66/68 (97%)	64 (97%)	2 (3%)	0	100	100
5	E	66/68 (97%)	64 (97%)	2 (3%)	0	100	100
5	e	66/68 (97%)	64 (97%)	2 (3%)	0	100	100
6	6	139/141 (99%)	128 (92%)	11 (8%)	0	100	100
6	F	139/141 (99%)	128 (92%)	11 (8%)	0	100	100
6	f	139/141 (99%)	128 (92%)	11 (8%)	0	100	100
7	7	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
7	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
7	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	8	37/39 (95%)	37 (100%)	0	0	100	100
8	J	37/39 (95%)	37 (100%)	0	0	100	100
8	j	37/39 (95%)	37 (100%)	0	0	100	100
9	9	76/78 (97%)	69 (91%)	7 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	K	76/78 (97%)	69 (91%)	7 (9%)	0	100	100
9	k	76/78 (97%)	69 (91%)	7 (9%)	0	100	100
10	0	158/160 (99%)	144 (91%)	14 (9%)	0	100	100
10	L	158/160 (99%)	144 (91%)	14 (9%)	0	100	100
10	l	158/160 (99%)	145 (92%)	13 (8%)	0	100	100
11	M	28/30 (93%)	28 (100%)	0	0	100	100
11	m	28/30 (93%)	28 (100%)	0	0	100	100
11	z	28/30 (93%)	28 (100%)	0	0	100	100
All	All	6687/6753 (99%)	6412 (96%)	275 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	593/593 (100%)	593 (100%)	0	100	100
1	A	593/593 (100%)	593 (100%)	0	100	100
1	a	593/593 (100%)	593 (100%)	0	100	100
2	2	587/588 (100%)	587 (100%)	0	100	100
2	B	587/588 (100%)	587 (100%)	0	100	100
2	b	587/588 (100%)	587 (100%)	0	100	100
3	3	68/68 (100%)	68 (100%)	0	100	100
3	C	68/68 (100%)	68 (100%)	0	100	100
3	c	68/68 (100%)	68 (100%)	0	100	100
4	4	115/116 (99%)	115 (100%)	0	100	100
4	D	115/116 (99%)	115 (100%)	0	100	100
4	d	115/116 (99%)	115 (100%)	0	100	100
5	5	58/58 (100%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	58/58 (100%)	58 (100%)	0	100	100
5	e	58/58 (100%)	58 (100%)	0	100	100
6	6	117/118 (99%)	117 (100%)	0	100	100
6	F	117/118 (99%)	117 (100%)	0	100	100
6	f	117/118 (99%)	117 (100%)	0	100	100
7	7	29/29 (100%)	29 (100%)	0	100	100
7	I	29/29 (100%)	29 (100%)	0	100	100
7	i	29/29 (100%)	29 (100%)	0	100	100
8	8	34/34 (100%)	34 (100%)	0	100	100
8	J	34/34 (100%)	34 (100%)	0	100	100
8	j	34/34 (100%)	34 (100%)	0	100	100
9	9	53/55 (96%)	53 (100%)	0	100	100
9	K	53/55 (96%)	53 (100%)	0	100	100
9	k	53/55 (96%)	53 (100%)	0	100	100
10	0	124/124 (100%)	124 (100%)	0	100	100
10	L	124/124 (100%)	124 (100%)	0	100	100
10	l	124/124 (100%)	124 (100%)	0	100	100
11	M	25/25 (100%)	25 (100%)	0	100	100
11	m	25/25 (100%)	25 (100%)	0	100	100
11	z	25/25 (100%)	25 (100%)	0	100	100
All	All	5409/5424 (100%)	5409 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	240	HIS
1	A	441	ASN
1	A	637	GLN
2	B	74	GLN
2	B	101	GLN
2	B	135	ASN
2	B	238	GLN

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Mol	Chain	Res	Type
2	B	711	GLN
5	E	64	HIS
6	F	119	GLN
7	I	33	GLN
9	K	25	ASN
10	L	45	ASN
10	L	147	GLN
10	L	150	HIS
10	L	152	GLN
1	a	135	HIS
1	a	240	HIS
1	a	441	ASN
1	a	637	GLN
2	b	17	GLN
2	b	74	GLN
2	b	101	GLN
2	b	135	ASN
2	b	238	GLN
2	b	513	ASN
2	b	637	GLN
2	b	711	GLN
5	e	64	HIS
6	f	119	GLN
9	k	25	ASN
10	l	45	ASN
10	l	147	GLN
10	l	150	HIS
1	1	240	HIS
1	1	441	ASN
1	1	637	GLN
2	2	74	GLN
2	2	101	GLN
2	2	238	GLN
2	2	637	GLN
2	2	711	GLN
5	5	64	HIS
6	6	119	GLN
7	7	33	GLN
9	9	25	ASN
10	0	45	ASN
10	0	147	GLN
10	0	150	HIS

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 ⓘ

384 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
13	CLA	B	838	-	69,73,73	1.16	8 (11%)	82,113,113	1.22	5 (6%)
13	CLA	B	802	-	69,73,73	1.15	10 (14%)	82,113,113	1.40	7 (8%)
16	BCR	8	1105	-	41,41,41	1.11	2 (4%)	56,56,56	1.32	7 (12%)
16	BCR	9	4001	-	41,41,41	1.10	3 (7%)	56,56,56	1.33	6 (10%)
13	CLA	2	811	-	49,53,73	1.37	9 (18%)	58,89,113	1.35	6 (10%)
13	CLA	1	837	-	64,68,73	1.20	9 (14%)	76,107,113	1.26	6 (7%)
13	CLA	1	827	-	69,73,73	1.14	10 (14%)	82,113,113	1.20	6 (7%)
13	CLA	B	828	-	59,63,73	1.26	9 (15%)	70,101,113	1.37	5 (7%)
13	CLA	2	808	-	49,53,73	1.37	7 (14%)	58,89,113	1.41	6 (10%)
13	CLA	b	816	-	64,68,73	1.22	9 (14%)	76,107,113	1.38	5 (6%)
19	SQD	7	101	-	48,50,54	0.99	3 (6%)	58,61,65	1.46	10 (17%)
13	CLA	b	833	-	54,58,73	1.29	9 (16%)	64,95,113	1.50	11 (17%)
13	CLA	B	819	-	50,54,73	1.35	9 (18%)	59,90,113	1.38	4 (6%)
13	CLA	1	818	-	58,62,73	1.26	9 (15%)	68,99,113	1.45	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	831	-	69,73,73	1.16	8 (11%)	82,113,113	1.41	7 (8%)
13	CLA	b	835	-	54,58,73	1.29	8 (14%)	64,95,113	1.42	6 (9%)
16	BCR	9	4004	-	41,41,41	1.11	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	B	818	-	50,54,73	1.35	9 (18%)	59,90,113	1.42	6 (10%)
13	CLA	F	204	-	50,54,73	1.36	8 (16%)	59,90,113	1.26	3 (5%)
13	CLA	a	810	-	49,53,73	1.37	9 (18%)	58,89,113	1.43	5 (8%)
16	BCR	J	1104	-	41,41,41	1.05	2 (4%)	56,56,56	1.35	9 (16%)
13	CLA	2	827	-	59,63,73	1.26	8 (13%)	70,101,113	1.37	5 (7%)
16	BCR	b	842	-	41,41,41	1.10	2 (4%)	56,56,56	1.33	6 (10%)
13	CLA	j	1102	-	44,48,73	1.46	7 (15%)	51,82,113	1.47	5 (9%)
13	CLA	a	835	-	60,64,73	1.25	8 (13%)	71,102,113	1.26	6 (8%)
16	BCR	J	1105	-	41,41,41	1.12	2 (4%)	56,56,56	1.32	7 (12%)
13	CLA	a	821	-	69,73,73	1.16	9 (13%)	82,113,113	1.20	5 (6%)
13	CLA	6	204	-	50,54,73	1.36	7 (14%)	59,90,113	1.27	3 (5%)
13	CLA	L	204	-	50,54,73	1.34	9 (18%)	59,90,113	1.33	4 (6%)
13	CLA	A	835	-	60,64,73	1.25	8 (13%)	71,102,113	1.27	6 (8%)
16	BCR	A	846	-	41,41,41	1.15	3 (7%)	56,56,56	1.28	6 (10%)
13	CLA	8	1101	-	54,58,73	1.32	9 (16%)	64,95,113	1.31	7 (10%)
13	CLA	b	847	-	69,73,73	1.16	9 (13%)	82,113,113	1.34	7 (8%)
13	CLA	b	838	-	69,73,73	1.16	8 (11%)	82,113,113	1.22	5 (6%)
19	SQD	I	103	-	48,50,54	0.99	3 (6%)	58,61,65	1.45	10 (17%)
16	BCR	z	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.26	8 (14%)
13	CLA	1	817	-	59,63,73	1.25	9 (15%)	70,101,113	1.45	7 (10%)
13	CLA	0	206	-	50,54,73	1.34	9 (18%)	59,90,113	1.33	4 (6%)
17	LHG	a	849	-	35,35,48	0.76	1 (2%)	38,41,54	1.28	4 (10%)
16	BCR	1	846	-	41,41,41	1.15	3 (7%)	56,56,56	1.28	6 (10%)
13	CLA	2	814	-	69,73,73	1.16	9 (13%)	82,113,113	1.25	7 (8%)
13	CLA	2	803	-	64,68,73	1.18	8 (12%)	76,107,113	1.43	8 (10%)
16	BCR	a	846	-	41,41,41	1.15	3 (7%)	56,56,56	1.28	6 (10%)
13	CLA	B	816	-	64,68,73	1.22	9 (14%)	76,107,113	1.38	5 (6%)
13	CLA	A	824	-	64,68,73	1.21	9 (14%)	76,107,113	1.38	5 (6%)
13	CLA	B	823	-	69,73,73	1.17	9 (13%)	82,113,113	1.18	6 (7%)
13	CLA	B	829	-	66,70,73	1.17	9 (13%)	78,109,113	1.40	8 (10%)
13	CLA	A	830	-	69,73,73	1.17	9 (13%)	82,113,113	1.44	7 (8%)
13	CLA	2	806	-	69,73,73	1.17	8 (11%)	82,113,113	1.29	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCR	1	848	-	41,41,41	1.04	2 (4%)	56,56,56	1.26	7 (12%)
16	BCR	2	839	-	41,41,41	1.09	2 (4%)	56,56,56	1.25	6 (10%)
18	LMG	2	845	-	41,41,55	0.94	3 (7%)	49,49,63	1.19	3 (6%)
13	CLA	K	4003	-	50,54,73	1.37	9 (18%)	59,90,113	1.35	5 (8%)
13	CLA	1	822	-	54,58,73	1.30	8 (14%)	64,95,113	1.53	8 (12%)
12	CL0	1	801	-	69,73,73	1.19	9 (13%)	82,113,113	1.16	6 (7%)
13	CLA	f	204	-	50,54,73	1.36	8 (16%)	59,90,113	1.27	3 (5%)
16	BCR	k	4001	-	41,41,41	1.09	3 (7%)	56,56,56	1.33	6 (10%)
16	BCR	1	851	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	7 (12%)
13	CLA	b	834	-	64,68,73	1.21	9 (14%)	76,107,113	1.22	6 (7%)
13	CLA	A	822	-	54,58,73	1.30	9 (16%)	64,95,113	1.53	8 (12%)
13	CLA	A	831	-	54,58,73	1.30	9 (16%)	64,95,113	1.44	9 (14%)
13	CLA	1	812	-	50,54,73	1.34	8 (16%)	59,90,113	1.32	5 (8%)
13	CLA	A	816	-	50,54,73	1.36	8 (16%)	59,90,113	1.27	3 (5%)
13	CLA	f	201	-	59,63,73	1.26	9 (15%)	70,101,113	1.34	5 (7%)
13	CLA	b	814	-	54,58,73	1.32	9 (16%)	64,95,113	1.41	7 (10%)
13	CLA	2	804	-	69,73,73	1.15	9 (13%)	82,113,113	1.22	7 (8%)
13	CLA	b	817	-	45,49,73	1.40	8 (17%)	54,84,113	1.16	4 (7%)
15	SF4	3	102	3	0,12,12	-	-	-	-	-
16	BCR	i	103	-	41,41,41	1.08	2 (4%)	56,56,56	1.38	10 (17%)
16	BCR	A	851	-	41,41,41	1.13	3 (7%)	56,56,56	1.29	7 (12%)
13	CLA	1	805	-	59,63,73	1.26	9 (15%)	70,101,113	1.29	5 (7%)
13	CLA	1	828	-	69,73,73	1.15	8 (11%)	82,113,113	1.37	6 (7%)
13	CLA	B	833	-	54,58,73	1.29	9 (16%)	64,95,113	1.50	11 (17%)
13	CLA	A	802	-	64,68,73	1.20	11 (17%)	76,107,113	1.55	11 (14%)
13	CLA	A	807	-	59,63,73	1.25	9 (15%)	70,101,113	1.42	6 (8%)
13	CLA	A	812	-	50,54,73	1.34	8 (16%)	59,90,113	1.32	5 (8%)
13	CLA	a	831	-	54,58,73	1.30	9 (16%)	64,95,113	1.44	9 (14%)
16	BCR	a	851	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	7 (12%)
13	CLA	b	830	-	62,66,73	1.26	9 (14%)	73,104,113	1.43	5 (6%)
13	CLA	2	802	-	69,73,73	1.15	10 (14%)	82,113,113	1.40	6 (7%)
15	SF4	C	101	3	0,12,12	-	-	-	-	-
13	CLA	a	823	-	54,58,73	1.31	8 (14%)	64,95,113	1.43	4 (6%)
13	CLA	A	806	-	69,73,73	1.17	10 (14%)	82,113,113	1.34	7 (8%)
13	CLA	a	802	-	64,68,73	1.20	11 (17%)	76,107,113	1.55	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	i	102	-	69,73,73	1.15	8 (11%)	82,113,113	1.28	6 (7%)
13	CLA	L	203	-	54,58,73	1.30	9 (16%)	64,95,113	1.52	8 (12%)
13	CLA	a	828	-	69,73,73	1.15	8 (11%)	82,113,113	1.37	6 (7%)
14	PQN	1	843	-	34,34,34	0.39	0	43,45,45	1.08	2 (4%)
13	CLA	A	823	-	54,58,73	1.30	8 (14%)	64,95,113	1.42	4 (6%)
13	CLA	A	841	-	64,68,73	1.21	8 (12%)	76,107,113	1.26	7 (9%)
13	CLA	1	806	-	69,73,73	1.16	9 (13%)	82,113,113	1.33	7 (8%)
13	CLA	b	819	-	50,54,73	1.35	9 (18%)	59,90,113	1.39	4 (6%)
13	CLA	b	818	-	50,54,73	1.35	7 (14%)	59,90,113	1.41	6 (10%)
13	CLA	1	826	-	59,63,73	1.24	9 (15%)	70,101,113	1.22	6 (8%)
14	PQN	2	838	-	34,34,34	0.36	0	43,45,45	1.15	3 (6%)
13	CLA	a	826	-	59,63,73	1.25	9 (15%)	70,101,113	1.23	6 (8%)
16	BCR	0	201	-	41,41,41	1.06	2 (4%)	56,56,56	1.27	6 (10%)
16	BCR	A	845	-	41,41,41	1.10	2 (4%)	56,56,56	1.17	3 (5%)
13	CLA	a	816	-	50,54,73	1.36	8 (16%)	59,90,113	1.28	3 (5%)
19	SQD	i	101	-	48,50,54	0.99	3 (6%)	58,61,65	1.45	10 (17%)
13	CLA	a	815	-	49,53,73	1.37	9 (18%)	58,89,113	1.42	6 (10%)
13	CLA	a	825	-	66,70,73	1.20	9 (13%)	78,109,113	1.38	7 (8%)
16	BCR	j	1104	-	41,41,41	1.06	2 (4%)	56,56,56	1.34	9 (16%)
13	CLA	B	834	-	64,68,73	1.20	9 (14%)	76,107,113	1.22	5 (6%)
13	CLA	b	801	-	69,73,73	1.17	10 (14%)	82,113,113	1.56	10 (12%)
13	CLA	A	826	-	59,63,73	1.24	9 (15%)	70,101,113	1.23	6 (8%)
16	BCR	0	207	-	41,41,41	1.11	2 (4%)	56,56,56	1.30	6 (10%)
16	BCR	F	202	-	41,41,41	1.08	2 (4%)	56,56,56	1.27	6 (10%)
17	LHG	A	849	-	35,35,48	0.76	1 (2%)	38,41,54	1.28	4 (10%)
13	CLA	b	804	-	69,73,73	1.15	9 (13%)	82,113,113	1.21	7 (8%)
13	CLA	L	206	-	69,73,73	1.15	9 (13%)	82,113,113	1.36	5 (6%)
16	BCR	6	202	-	41,41,41	1.07	2 (4%)	56,56,56	1.27	7 (12%)
17	LHG	1	849	-	35,35,48	0.76	1 (2%)	38,41,54	1.28	4 (10%)
16	BCR	2	840	-	41,41,41	1.08	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	B	827	-	49,53,73	1.39	9 (18%)	58,89,113	1.30	6 (10%)
16	BCR	L	202	-	41,41,41	1.11	2 (4%)	56,56,56	1.28	9 (16%)
13	CLA	A	819	-	64,68,73	1.19	9 (14%)	76,107,113	1.52	7 (9%)
13	CLA	l	205	-	50,54,73	1.34	9 (18%)	59,90,113	1.33	4 (6%)
13	CLA	0	202	-	64,68,73	1.18	9 (14%)	76,107,113	1.31	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	7	102	-	69,73,73	1.14	8 (11%)	82,113,113	1.27	6 (7%)
13	CLA	9	4005	-	47,52,73	1.41	9 (19%)	55,88,113	1.48	6 (10%)
13	CLA	L	201	-	64,68,73	1.18	9 (14%)	76,107,113	1.31	8 (10%)
13	CLA	B	801	-	69,73,73	1.17	10 (14%)	82,113,113	1.55	10 (12%)
16	BCR	2	844	-	41,41,41	1.16	2 (4%)	56,56,56	1.19	6 (10%)
13	CLA	1	815	-	49,53,73	1.37	9 (18%)	58,89,113	1.41	5 (8%)
13	CLA	a	813	-	59,63,73	1.26	9 (15%)	70,101,113	1.29	8 (11%)
13	CLA	2	836	-	69,73,73	1.16	6 (8%)	82,113,113	1.21	6 (7%)
13	CLA	B	830	-	62,66,73	1.25	9 (14%)	73,104,113	1.41	5 (6%)
13	CLA	1	838	-	69,73,73	1.15	9 (13%)	82,113,113	1.34	6 (7%)
13	CLA	2	831	-	44,48,73	1.45	8 (18%)	51,82,113	1.41	5 (9%)
13	CLA	a	827	-	69,73,73	1.15	10 (14%)	82,113,113	1.20	5 (6%)
16	BCR	M	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	8 (14%)
16	BCR	2	847	-	41,41,41	1.16	3 (7%)	56,56,56	1.31	8 (14%)
13	CLA	A	813	-	59,63,73	1.26	9 (15%)	70,101,113	1.29	7 (10%)
13	CLA	B	837	-	69,73,73	1.16	6 (8%)	82,113,113	1.21	6 (7%)
13	CLA	B	817	-	45,49,73	1.40	7 (15%)	54,84,113	1.16	4 (7%)
13	CLA	B	820	-	59,63,73	1.27	9 (15%)	70,101,113	1.30	4 (5%)
13	CLA	A	809	-	54,58,73	1.31	8 (14%)	64,95,113	1.34	7 (10%)
13	CLA	2	810	-	50,54,73	1.33	9 (18%)	59,90,113	1.55	7 (11%)
13	CLA	a	838	-	69,73,73	1.16	9 (13%)	82,113,113	1.33	6 (7%)
13	CLA	6	203	-	49,53,73	1.39	8 (16%)	58,89,113	1.34	6 (10%)
16	BCR	b	844	-	41,41,41	1.13	2 (4%)	56,56,56	1.43	6 (10%)
13	CLA	B	822	-	54,58,73	1.30	9 (16%)	64,95,113	1.34	7 (10%)
16	BCR	0	204	-	41,41,41	1.12	2 (4%)	56,56,56	1.27	9 (16%)
13	CLA	b	811	-	50,54,73	1.34	9 (18%)	59,90,113	1.55	7 (11%)
13	CLA	b	822	-	54,58,73	1.31	9 (16%)	64,95,113	1.35	7 (10%)
13	CLA	2	813	-	54,58,73	1.32	9 (16%)	64,95,113	1.42	7 (10%)
13	CLA	B	807	-	69,73,73	1.16	9 (13%)	82,113,113	1.23	6 (7%)
16	BCR	l	201	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	6 (10%)
13	CLA	B	836	-	69,73,73	1.16	9 (13%)	82,113,113	1.23	6 (7%)
13	CLA	a	818	-	58,62,73	1.27	10 (17%)	68,99,113	1.45	7 (10%)
16	BCR	7	103	-	41,41,41	1.07	2 (4%)	56,56,56	1.38	10 (17%)
13	CLA	2	828	-	66,70,73	1.18	9 (13%)	78,109,113	1.40	9 (11%)
13	CLA	1	810	-	49,53,73	1.37	9 (18%)	58,89,113	1.43	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	b	805	-	69,73,73	1.17	9 (13%)	82,113,113	1.28	4 (4%)
13	CLA	b	828	-	59,63,73	1.27	9 (15%)	70,101,113	1.38	4 (5%)
13	CLA	A	836	-	55,59,73	1.29	8 (14%)	64,96,113	1.39	8 (12%)
13	CLA	a	834	-	69,73,73	1.17	9 (13%)	82,113,113	1.26	5 (6%)
13	CLA	1	835	-	60,64,73	1.25	8 (13%)	71,102,113	1.26	5 (7%)
13	CLA	A	808	-	54,58,73	1.29	9 (16%)	64,95,113	1.72	7 (10%)
13	CLA	b	823	-	69,73,73	1.16	9 (13%)	82,113,113	1.18	6 (7%)
13	CLA	1	821	-	69,73,73	1.15	9 (13%)	82,113,113	1.21	5 (6%)
13	CLA	1	813	-	59,63,73	1.25	9 (15%)	70,101,113	1.29	8 (11%)
16	BCR	b	841	-	41,41,41	1.07	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	k	4005	-	47,52,73	1.41	9 (19%)	55,88,113	1.48	6 (10%)
16	BCR	A	847	-	41,41,41	1.14	3 (7%)	56,56,56	1.42	9 (16%)
16	BCR	m	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	8 (14%)
13	CLA	a	830	-	69,73,73	1.17	9 (13%)	82,113,113	1.44	7 (8%)
13	CLA	9	4002	-	49,53,73	1.41	7 (14%)	58,89,113	1.36	4 (6%)
13	CLA	a	809	-	54,58,73	1.30	9 (16%)	64,95,113	1.34	7 (10%)
13	CLA	2	833	-	64,68,73	1.20	9 (14%)	76,107,113	1.22	5 (6%)
16	BCR	K	4004	-	41,41,41	1.11	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	9	4003	-	50,54,73	1.37	9 (18%)	59,90,113	1.35	5 (8%)
16	BCR	l	206	-	41,41,41	1.11	2 (4%)	56,56,56	1.30	6 (10%)
13	CLA	A	852	-	64,68,73	1.23	9 (14%)	76,107,113	1.24	6 (7%)
13	CLA	B	826	-	64,68,73	1.25	9 (14%)	76,107,113	1.48	8 (10%)
13	CLA	A	818	-	58,62,73	1.27	10 (17%)	68,99,113	1.45	7 (10%)
13	CLA	a	803	-	69,73,73	1.16	9 (13%)	82,113,113	1.23	8 (9%)
13	CLA	A	827	-	69,73,73	1.15	10 (14%)	82,113,113	1.20	5 (6%)
13	CLA	1	834	-	69,73,73	1.17	9 (13%)	82,113,113	1.27	4 (4%)
13	CLA	a	852	-	64,68,73	1.23	9 (14%)	76,107,113	1.25	6 (7%)
16	BCR	b	843	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	6 (10%)
13	CLA	1	842	-	49,53,73	1.37	9 (18%)	58,89,113	1.61	5 (8%)
16	BCR	8	1104	-	41,41,41	1.05	2 (4%)	56,56,56	1.35	9 (16%)
13	CLA	a	829	-	69,73,73	1.16	10 (14%)	82,113,113	1.46	7 (8%)
13	CLA	A	825	-	66,70,73	1.20	9 (13%)	78,109,113	1.38	7 (8%)
13	CLA	a	833	-	69,73,73	1.16	9 (13%)	82,113,113	1.42	6 (7%)
16	BCR	b	840	-	41,41,41	1.09	2 (4%)	56,56,56	1.26	6 (10%)
13	CLA	l	204	-	54,58,73	1.30	9 (16%)	64,95,113	1.52	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	824	-	59,63,73	1.26	10 (16%)	70,101,113	1.56	10 (14%)
13	CLA	1	852	-	64,68,73	1.23	9 (14%)	76,107,113	1.25	6 (7%)
13	CLA	a	822	-	54,58,73	1.30	9 (16%)	64,95,113	1.53	8 (12%)
13	CLA	I	101	-	69,73,73	1.14	9 (13%)	82,113,113	1.27	6 (7%)
12	CL0	a	801	-	69,73,73	1.18	9 (13%)	82,113,113	1.17	6 (7%)
13	CLA	1	830	-	69,73,73	1.17	9 (13%)	82,113,113	1.43	7 (8%)
16	BCR	F	205	-	41,41,41	1.07	2 (4%)	56,56,56	1.31	7 (12%)
13	CLA	1	809	-	54,58,73	1.30	8 (14%)	64,95,113	1.35	7 (10%)
16	BCR	2	842	-	41,41,41	1.09	2 (4%)	56,56,56	1.24	6 (10%)
13	CLA	a	837	-	64,68,73	1.21	9 (14%)	76,107,113	1.25	6 (7%)
13	CLA	A	838	-	69,73,73	1.15	9 (13%)	82,113,113	1.34	6 (7%)
16	BCR	1	845	-	41,41,41	1.10	2 (4%)	56,56,56	1.17	3 (5%)
13	CLA	2	825	-	64,68,73	1.24	9 (14%)	76,107,113	1.48	8 (10%)
13	CLA	A	839	-	69,73,73	1.15	9 (13%)	82,113,113	1.40	9 (10%)
13	CLA	B	832	-	44,48,73	1.45	8 (18%)	51,82,113	1.41	5 (9%)
13	CLA	2	826	-	49,53,73	1.40	9 (18%)	58,89,113	1.30	6 (10%)
13	CLA	b	807	-	69,73,73	1.16	9 (13%)	82,113,113	1.23	5 (6%)
13	CLA	2	846	-	69,73,73	1.17	9 (13%)	82,113,113	1.33	7 (8%)
16	BCR	a	845	-	41,41,41	1.09	2 (4%)	56,56,56	1.17	3 (5%)
14	PQN	A	843	-	34,34,34	0.39	0	43,45,45	1.08	2 (4%)
17	LHG	A	850	-	40,40,48	0.69	1 (2%)	43,46,54	1.29	6 (13%)
15	SF4	a	844	1,2	0,12,12	-	-	-	-	-
13	CLA	0	203	-	69,73,73	1.16	9 (13%)	82,113,113	1.24	5 (6%)
13	CLA	1	816	-	50,54,73	1.36	8 (16%)	59,90,113	1.28	3 (5%)
13	CLA	b	812	-	49,53,73	1.37	9 (18%)	58,89,113	1.35	6 (10%)
13	CLA	1	829	-	69,73,73	1.15	10 (14%)	82,113,113	1.46	7 (8%)
14	PQN	b	839	-	34,34,34	0.36	0	43,45,45	1.15	3 (6%)
13	CLA	B	805	-	69,73,73	1.17	9 (13%)	82,113,113	1.28	4 (4%)
13	CLA	a	839	-	69,73,73	1.15	9 (13%)	82,113,113	1.40	8 (9%)
13	CLA	b	803	-	64,68,73	1.18	9 (14%)	76,107,113	1.42	8 (10%)
13	CLA	J	1101	-	54,58,73	1.32	9 (16%)	64,95,113	1.31	7 (10%)
13	CLA	2	822	-	69,73,73	1.17	9 (13%)	82,113,113	1.17	6 (7%)
13	CLA	b	815	-	69,73,73	1.16	9 (13%)	82,113,113	1.25	7 (8%)
13	CLA	b	829	-	66,70,73	1.18	9 (13%)	78,109,113	1.40	8 (10%)
13	CLA	b	837	-	69,73,73	1.16	6 (8%)	82,113,113	1.21	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	812	-	49,53,73	1.37	9 (18%)	58,89,113	1.35	6 (10%)
13	CLA	b	802	-	69,73,73	1.15	10 (14%)	82,113,113	1.40	6 (7%)
13	CLA	1	823	-	54,58,73	1.30	8 (14%)	64,95,113	1.42	4 (6%)
13	CLA	1	839	-	69,73,73	1.15	10 (14%)	82,113,113	1.40	9 (10%)
13	CLA	2	823	-	59,63,73	1.26	10 (16%)	70,101,113	1.57	10 (14%)
13	CLA	a	807	-	59,63,73	1.24	9 (15%)	70,101,113	1.42	6 (8%)
13	CLA	8	1103	-	49,53,73	1.38	8 (16%)	58,89,113	1.35	5 (8%)
13	CLA	a	832	-	69,73,73	1.16	9 (13%)	82,113,113	1.32	7 (8%)
16	BCR	B	843	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	6 (10%)
13	CLA	B	811	-	50,54,73	1.34	9 (18%)	59,90,113	1.55	7 (11%)
13	CLA	k	4003	-	50,54,73	1.37	9 (18%)	59,90,113	1.35	5 (8%)
13	CLA	B	806	-	69,73,73	1.17	9 (13%)	82,113,113	1.30	5 (6%)
16	BCR	B	840	-	41,41,41	1.10	2 (4%)	56,56,56	1.25	6 (10%)
13	CLA	1	841	-	64,68,73	1.21	8 (12%)	76,107,113	1.26	7 (9%)
16	BCR	B	841	-	41,41,41	1.07	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	B	814	-	54,58,73	1.32	9 (16%)	64,95,113	1.41	7 (10%)
13	CLA	a	804	-	59,63,73	1.24	9 (15%)	70,101,113	1.32	6 (8%)
13	CLA	A	832	-	69,73,73	1.16	9 (13%)	82,113,113	1.32	7 (8%)
17	LHG	1	850	-	40,40,48	0.69	1 (2%)	43,46,54	1.29	6 (13%)
13	CLA	1	819	-	64,68,73	1.20	9 (14%)	76,107,113	1.53	7 (9%)
16	BCR	l	203	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	9 (16%)
13	CLA	A	829	-	69,73,73	1.16	10 (14%)	82,113,113	1.46	7 (8%)
13	CLA	a	819	-	64,68,73	1.20	9 (14%)	76,107,113	1.51	7 (9%)
13	CLA	b	813	-	69,73,73	1.17	8 (11%)	82,113,113	1.31	8 (9%)
13	CLA	F	201	-	59,63,73	1.26	9 (15%)	70,101,113	1.34	5 (7%)
13	CLA	1	825	-	66,70,73	1.20	9 (13%)	78,109,113	1.38	7 (8%)
16	BCR	B	842	-	41,41,41	1.10	2 (4%)	56,56,56	1.32	6 (10%)
12	CL0	A	801	-	69,73,73	1.19	9 (13%)	82,113,113	1.17	6 (7%)
13	CLA	a	841	-	64,68,73	1.21	8 (12%)	76,107,113	1.26	8 (10%)
16	BCR	6	205	-	41,41,41	1.06	2 (4%)	56,56,56	1.31	7 (12%)
13	CLA	A	834	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	4 (4%)
14	PQN	B	839	-	34,34,34	0.36	0	43,45,45	1.15	3 (6%)
13	CLA	a	820	-	50,54,73	1.35	6 (12%)	59,90,113	1.26	5 (8%)
13	CLA	B	803	-	64,68,73	1.18	8 (12%)	76,107,113	1.42	8 (10%)
13	CLA	2	834	-	54,58,73	1.29	8 (14%)	64,95,113	1.42	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCR	I	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.38	10 (17%)
13	CLA	B	835	-	54,58,73	1.29	8 (14%)	64,95,113	1.42	6 (9%)
13	CLA	2	819	-	59,63,73	1.27	9 (15%)	70,101,113	1.29	4 (5%)
13	CLA	B	815	-	69,73,73	1.16	9 (13%)	82,113,113	1.25	7 (8%)
13	CLA	B	847	-	69,73,73	1.17	9 (13%)	82,113,113	1.33	7 (8%)
13	CLA	B	821	-	69,73,73	1.19	9 (13%)	82,113,113	1.31	7 (8%)
13	CLA	2	817	-	50,54,73	1.35	9 (18%)	59,90,113	1.42	6 (10%)
13	CLA	a	805	-	59,63,73	1.26	9 (15%)	70,101,113	1.29	6 (8%)
13	CLA	2	837	-	69,73,73	1.17	8 (11%)	82,113,113	1.22	5 (6%)
16	BCR	1	847	-	41,41,41	1.13	3 (7%)	56,56,56	1.42	9 (16%)
13	CLA	2	830	-	69,73,73	1.15	9 (13%)	82,113,113	1.41	7 (8%)
15	SF4	C	102	3	0,12,12	-	-	-	-	-
13	CLA	A	803	-	69,73,73	1.16	9 (13%)	82,113,113	1.22	8 (9%)
13	CLA	B	808	-	69,73,73	1.15	9 (13%)	82,113,113	1.35	5 (6%)
13	CLA	1	824	-	64,68,73	1.20	9 (14%)	76,107,113	1.38	5 (6%)
16	BCR	a	847	-	41,41,41	1.13	3 (7%)	56,56,56	1.43	9 (16%)
13	CLA	b	836	-	69,73,73	1.17	9 (13%)	82,113,113	1.23	6 (7%)
13	CLA	2	821	-	54,58,73	1.31	9 (16%)	64,95,113	1.35	7 (10%)
13	CLA	b	820	-	59,63,73	1.27	9 (15%)	70,101,113	1.30	4 (5%)
13	CLA	a	824	-	64,68,73	1.20	9 (14%)	76,107,113	1.37	5 (6%)
13	CLA	2	809	-	69,73,73	1.16	10 (14%)	82,113,113	1.34	6 (7%)
13	CLA	A	810	-	49,53,73	1.37	9 (18%)	58,89,113	1.43	5 (8%)
13	CLA	2	818	-	50,54,73	1.36	9 (18%)	59,90,113	1.38	4 (6%)
13	CLA	A	840	-	69,73,73	1.16	9 (13%)	82,113,113	1.23	5 (6%)
13	CLA	A	814	-	54,58,73	1.31	9 (16%)	64,95,113	1.50	8 (12%)
13	CLA	B	804	-	69,73,73	1.15	9 (13%)	82,113,113	1.22	7 (8%)
13	CLA	K	4005	-	47,52,73	1.41	9 (19%)	55,88,113	1.48	6 (10%)
16	BCR	k	4004	-	41,41,41	1.11	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	b	827	-	49,53,73	1.39	9 (18%)	58,89,113	1.29	6 (10%)
13	CLA	J	1103	-	49,53,73	1.38	8 (16%)	58,89,113	1.34	5 (8%)
13	CLA	b	824	-	59,63,73	1.26	10 (16%)	70,101,113	1.56	9 (12%)
16	BCR	B	848	-	41,41,41	1.16	3 (7%)	56,56,56	1.31	8 (14%)
13	CLA	b	809	-	49,53,73	1.37	7 (14%)	58,89,113	1.41	5 (8%)
13	CLA	A	833	-	69,73,73	1.16	9 (13%)	82,113,113	1.41	6 (7%)
16	BCR	b	845	-	41,41,41	1.16	2 (4%)	56,56,56	1.19	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	a	814	-	54,58,73	1.31	9 (16%)	64,95,113	1.51	9 (14%)
13	CLA	b	821	-	69,73,73	1.19	9 (13%)	82,113,113	1.32	7 (8%)
13	CLA	l	207	-	69,73,73	1.15	8 (11%)	82,113,113	1.35	5 (6%)
13	CLA	B	810	-	69,73,73	1.16	10 (14%)	82,113,113	1.34	6 (7%)
13	CLA	a	817	-	59,63,73	1.25	9 (15%)	70,101,113	1.45	7 (10%)
13	CLA	a	836	-	55,59,73	1.28	8 (14%)	64,96,113	1.39	8 (12%)
16	BCR	f	205	-	41,41,41	1.07	2 (4%)	56,56,56	1.31	7 (12%)
15	SF4	3	101	3	0,12,12	-	-	-	-	-
16	BCR	f	202	-	41,41,41	1.08	2 (4%)	56,56,56	1.27	6 (10%)
13	CLA	b	808	-	69,73,73	1.15	9 (13%)	82,113,113	1.35	5 (6%)
13	CLA	A	811	-	60,64,73	1.25	9 (15%)	71,102,113	1.35	5 (7%)
18	LMG	b	846	-	41,41,55	0.94	3 (7%)	49,49,63	1.19	3 (6%)
13	CLA	1	803	-	69,73,73	1.16	9 (13%)	82,113,113	1.22	8 (9%)
13	CLA	a	812	-	50,54,73	1.34	8 (16%)	59,90,113	1.32	5 (8%)
13	CLA	1	833	-	69,73,73	1.16	9 (13%)	82,113,113	1.40	6 (7%)
16	BCR	L	207	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	7 (12%)
13	CLA	2	835	-	69,73,73	1.16	9 (13%)	82,113,113	1.23	6 (7%)
13	CLA	1	814	-	54,58,73	1.31	9 (16%)	64,95,113	1.50	9 (14%)
13	CLA	A	820	-	50,54,73	1.35	6 (12%)	59,90,113	1.26	5 (8%)
13	CLA	1	811	-	60,64,73	1.25	9 (15%)	71,102,113	1.36	4 (5%)
13	CLA	1	836	-	55,59,73	1.29	8 (14%)	64,96,113	1.39	8 (12%)
13	CLA	a	811	-	60,64,73	1.25	9 (15%)	71,102,113	1.36	5 (7%)
13	CLA	b	826	-	64,68,73	1.25	9 (14%)	76,107,113	1.48	8 (10%)
13	CLA	a	840	-	69,73,73	1.15	9 (13%)	82,113,113	1.23	5 (6%)
13	CLA	6	201	-	59,63,73	1.26	8 (13%)	70,101,113	1.34	5 (7%)
13	CLA	2	816	-	45,49,73	1.40	7 (15%)	54,84,113	1.16	4 (7%)
13	CLA	1	820	-	50,54,73	1.35	6 (12%)	59,90,113	1.25	4 (6%)
13	CLA	A	828	-	69,73,73	1.15	8 (11%)	82,113,113	1.37	6 (7%)
13	CLA	l	202	-	64,68,73	1.19	9 (14%)	76,107,113	1.31	8 (10%)
13	CLA	A	804	-	59,63,73	1.23	9 (15%)	70,101,113	1.33	6 (8%)
13	CLA	j	1101	-	54,58,73	1.32	9 (16%)	64,95,113	1.31	6 (9%)
13	CLA	a	808	-	54,58,73	1.29	9 (16%)	64,95,113	1.72	7 (10%)
16	BCR	B	845	-	41,41,41	1.16	2 (4%)	56,56,56	1.19	6 (10%)
13	CLA	1	831	-	54,58,73	1.29	9 (16%)	64,95,113	1.44	9 (14%)
16	BCR	A	848	-	41,41,41	1.04	2 (4%)	56,56,56	1.27	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCR	L	205	-	41,41,41	1.11	2 (4%)	56,56,56	1.30	6 (10%)
16	BCR	2	843	-	41,41,41	1.13	2 (4%)	56,56,56	1.43	6 (10%)
13	CLA	f	203	-	49,53,73	1.39	8 (16%)	58,89,113	1.34	6 (10%)
16	BCR	B	844	-	41,41,41	1.13	2 (4%)	56,56,56	1.43	6 (10%)
13	CLA	2	832	-	54,58,73	1.29	9 (16%)	64,95,113	1.50	11 (17%)
13	CLA	j	1103	-	49,53,73	1.39	8 (16%)	58,89,113	1.34	5 (8%)
13	CLA	1	840	-	69,73,73	1.15	9 (13%)	82,113,113	1.24	5 (6%)
13	CLA	1	832	-	69,73,73	1.16	9 (13%)	82,113,113	1.32	7 (8%)
13	CLA	2	805	-	69,73,73	1.17	9 (13%)	82,113,113	1.28	4 (4%)
13	CLA	2	829	-	62,66,73	1.25	9 (14%)	73,104,113	1.42	5 (6%)
13	CLA	1	802	-	64,68,73	1.20	11 (17%)	76,107,113	1.54	11 (14%)
15	SF4	A	844	1,2	0,12,12	-	-	-	-	-
14	PQN	a	843	-	34,34,34	0.39	0	43,45,45	1.08	2 (4%)
13	CLA	B	825	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	7 (8%)
13	CLA	A	842	-	49,53,73	1.37	9 (18%)	58,89,113	1.61	5 (8%)
13	CLA	F	203	-	49,53,73	1.39	8 (16%)	58,89,113	1.33	6 (10%)
13	CLA	A	815	-	49,53,73	1.37	9 (18%)	58,89,113	1.42	5 (8%)
13	CLA	0	205	-	54,58,73	1.30	9 (16%)	64,95,113	1.52	8 (12%)
16	BCR	a	848	-	41,41,41	1.04	2 (4%)	56,56,56	1.27	7 (12%)
13	CLA	b	825	-	69,73,73	1.16	10 (14%)	82,113,113	1.29	7 (8%)
13	CLA	b	806	-	69,73,73	1.17	8 (11%)	82,113,113	1.29	5 (6%)
15	SF4	c	101	3	0,12,12	-	-	-	-	-
16	BCR	K	4001	-	41,41,41	1.10	3 (7%)	56,56,56	1.33	6 (10%)
13	CLA	1	808	-	54,58,73	1.29	8 (14%)	64,95,113	1.73	6 (9%)
15	SF4	1	844	1,2	0,12,12	-	-	-	-	-
13	CLA	b	832	-	44,48,73	1.45	8 (18%)	51,82,113	1.41	5 (9%)
13	CLA	1	807	-	59,63,73	1.24	9 (15%)	70,101,113	1.42	6 (8%)
15	SF4	c	102	3	0,12,12	-	-	-	-	-
16	BCR	2	841	-	41,41,41	1.10	2 (4%)	56,56,56	1.32	6 (10%)
13	CLA	a	842	-	49,53,73	1.37	9 (18%)	58,89,113	1.61	5 (8%)
13	CLA	2	807	-	69,73,73	1.15	9 (13%)	82,113,113	1.35	5 (6%)
13	CLA	2	812	-	69,73,73	1.17	8 (11%)	82,113,113	1.31	8 (9%)
13	CLA	b	810	-	69,73,73	1.16	10 (14%)	82,113,113	1.34	6 (7%)
13	CLA	2	824	-	69,73,73	1.16	10 (14%)	82,113,113	1.29	7 (8%)
16	BCR	j	1105	-	41,41,41	1.12	2 (4%)	56,56,56	1.32	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	LHG	a	850	-	40,40,48	0.68	1 (2%)	43,46,54	1.29	6 (13%)
13	CLA	B	813	-	69,73,73	1.16	8 (11%)	82,113,113	1.31	8 (9%)
13	CLA	2	815	-	64,68,73	1.22	9 (14%)	76,107,113	1.38	5 (6%)
16	BCR	b	848	-	41,41,41	1.16	3 (7%)	56,56,56	1.31	8 (14%)
18	LMG	B	846	-	41,41,55	0.94	3 (7%)	49,49,63	1.19	3 (6%)
13	CLA	A	821	-	69,73,73	1.16	9 (13%)	82,113,113	1.20	5 (6%)
13	CLA	b	831	-	69,73,73	1.16	8 (11%)	82,113,113	1.41	7 (8%)
13	CLA	K	4002	-	49,53,73	1.41	7 (14%)	58,89,113	1.37	4 (6%)
13	CLA	a	806	-	69,73,73	1.17	10 (14%)	82,113,113	1.34	7 (8%)
13	CLA	2	820	-	69,73,73	1.20	9 (13%)	82,113,113	1.32	7 (8%)
13	CLA	A	805	-	59,63,73	1.26	9 (15%)	70,101,113	1.29	6 (8%)
13	CLA	A	817	-	59,63,73	1.25	9 (15%)	70,101,113	1.45	7 (10%)
13	CLA	J	1102	-	44,48,73	1.46	7 (15%)	51,82,113	1.48	5 (9%)
13	CLA	2	801	-	69,73,73	1.17	9 (13%)	82,113,113	1.56	11 (13%)
13	CLA	0	208	-	69,73,73	1.15	9 (13%)	82,113,113	1.36	5 (6%)
13	CLA	A	837	-	64,68,73	1.20	9 (14%)	76,107,113	1.25	6 (7%)
13	CLA	8	1102	-	44,48,73	1.45	7 (15%)	51,82,113	1.48	5 (9%)
13	CLA	1	804	-	59,63,73	1.23	9 (15%)	70,101,113	1.34	6 (8%)
13	CLA	k	4002	-	49,53,73	1.41	7 (14%)	58,89,113	1.37	4 (6%)
13	CLA	B	809	-	49,53,73	1.37	7 (14%)	58,89,113	1.41	5 (8%)

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
13	CLA	B	838	-	-	7/39/115/115	-
13	CLA	B	802	-	-	9/39/115/115	-
16	BCR	8	1105	-	-	11/29/63/63	0/2/2/2
16	BCR	9	4001	-	-	9/29/63/63	0/2/2/2
13	CLA	2	811	-	-	4/15/91/115	-
13	CLA	1	837	-	-	8/33/109/115	-
13	CLA	1	827	-	-	13/39/115/115	-
13	CLA	B	828	-	-	9/27/103/115	-
13	CLA	2	808	-	-	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	b	816	-	-	7/33/109/115	-
19	SQD	7	101	-	-	19/45/65/69	0/1/1/1
13	CLA	b	833	-	-	6/21/97/115	-
13	CLA	B	819	-	-	6/17/93/115	-
13	CLA	1	818	-	-	7/26/102/115	-
13	CLA	B	831	-	-	7/39/115/115	-
13	CLA	b	835	-	-	3/21/97/115	-
16	BCR	9	4004	-	-	11/29/63/63	0/2/2/2
13	CLA	B	818	-	-	10/17/93/115	-
13	CLA	F	204	-	-	8/17/93/115	-
13	CLA	a	810	-	-	8/15/91/115	-
16	BCR	J	1104	-	-	8/29/63/63	0/2/2/2
13	CLA	2	827	-	-	9/27/103/115	-
16	BCR	b	842	-	-	14/29/63/63	0/2/2/2
13	CLA	j	1102	-	-	6/10/82/115	-
13	CLA	a	835	-	-	14/29/105/115	-
16	BCR	J	1105	-	-	11/29/63/63	0/2/2/2
13	CLA	a	821	-	-	11/39/115/115	-
13	CLA	6	204	-	-	8/17/93/115	-
13	CLA	L	204	-	-	4/17/93/115	-
13	CLA	A	835	-	-	14/29/105/115	-
16	BCR	A	846	-	-	6/29/63/63	0/2/2/2
13	CLA	8	1101	-	-	9/21/97/115	-
13	CLA	b	847	-	-	9/39/115/115	-
13	CLA	b	838	-	-	7/39/115/115	-
19	SQD	I	103	-	-	19/45/65/69	0/1/1/1
16	BCR	z	101	-	-	7/29/63/63	0/2/2/2
13	CLA	1	817	-	-	8/27/103/115	-
13	CLA	0	206	-	-	4/17/93/115	-
17	LHG	a	849	-	-	16/40/40/53	-
16	BCR	1	846	-	-	6/29/63/63	0/2/2/2
13	CLA	2	814	-	-	12/39/115/115	-
13	CLA	2	803	-	-	11/33/109/115	-
16	BCR	a	846	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	816	-	-	7/33/109/115	-
13	CLA	A	824	-	-	16/33/109/115	-
13	CLA	B	823	-	-	12/39/115/115	-
13	CLA	B	829	-	-	17/36/112/115	-
13	CLA	A	830	-	-	13/39/115/115	-
13	CLA	2	806	-	-	17/39/115/115	-
16	BCR	1	848	-	-	15/29/63/63	0/2/2/2
16	BCR	2	839	-	-	11/29/63/63	0/2/2/2
18	LMG	2	845	-	-	17/36/56/70	0/1/1/1
13	CLA	K	4003	-	-	8/17/93/115	-
13	CLA	1	822	-	-	8/21/97/115	-
12	CL0	1	801	-	-	14/39/115/115	-
13	CLA	f	204	-	-	8/17/93/115	-
16	BCR	k	4001	-	-	8/29/63/63	0/2/2/2
16	BCR	1	851	-	-	13/29/63/63	0/2/2/2
13	CLA	b	834	-	-	6/33/109/115	-
13	CLA	A	822	-	-	8/21/97/115	-
13	CLA	A	831	-	-	8/21/97/115	-
13	CLA	1	812	-	-	6/17/93/115	-
13	CLA	A	816	-	-	8/17/93/115	-
13	CLA	f	201	-	-	6/27/103/115	-
13	CLA	b	814	-	-	8/21/97/115	-
13	CLA	2	804	-	-	17/39/115/115	-
13	CLA	b	817	-	-	2/10/86/115	-
16	BCR	i	103	-	-	8/29/63/63	0/2/2/2
15	SF4	3	102	3	-	-	0/6/5/5
16	BCR	A	851	-	-	13/29/63/63	0/2/2/2
13	CLA	1	805	-	-	12/27/103/115	-
13	CLA	1	828	-	-	9/39/115/115	-
13	CLA	B	833	-	-	6/21/97/115	-
13	CLA	A	802	-	-	10/33/109/115	-
13	CLA	A	807	-	-	4/27/103/115	-
13	CLA	A	812	-	-	6/17/93/115	-
13	CLA	a	831	-	-	8/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	a	851	-	-	13/29/63/63	0/2/2/2
13	CLA	b	830	-	-	10/31/107/115	-
13	CLA	2	802	-	-	9/39/115/115	-
15	SF4	C	101	3	-	-	0/6/5/5
13	CLA	a	823	-	-	7/21/97/115	-
13	CLA	A	806	-	-	12/39/115/115	-
13	CLA	a	802	-	-	10/33/109/115	-
13	CLA	i	102	-	-	14/39/115/115	-
13	CLA	L	203	-	-	7/21/97/115	-
13	CLA	a	828	-	-	9/39/115/115	-
14	PQN	1	843	-	-	10/23/43/43	0/2/2/2
13	CLA	A	823	-	-	7/21/97/115	-
13	CLA	A	841	-	-	12/33/109/115	-
13	CLA	1	806	-	-	12/39/115/115	-
13	CLA	b	819	-	-	6/17/93/115	-
13	CLA	b	818	-	-	10/17/93/115	-
13	CLA	1	826	-	-	7/27/103/115	-
14	PQN	2	838	-	-	10/23/43/43	0/2/2/2
13	CLA	a	826	-	-	7/27/103/115	-
16	BCR	0	201	-	-	7/29/63/63	0/2/2/2
16	BCR	A	845	-	-	8/29/63/63	0/2/2/2
13	CLA	a	816	-	-	8/17/93/115	-
19	SQD	i	101	-	-	19/45/65/69	0/1/1/1
13	CLA	a	815	-	-	3/15/91/115	-
13	CLA	a	825	-	-	15/36/112/115	-
16	BCR	j	1104	-	-	8/29/63/63	0/2/2/2
13	CLA	B	834	-	-	6/33/109/115	-
13	CLA	b	801	-	-	6/39/115/115	-
13	CLA	A	826	-	-	7/27/103/115	-
16	BCR	0	207	-	-	11/29/63/63	0/2/2/2
16	BCR	F	202	-	-	12/29/63/63	0/2/2/2
17	LHG	A	849	-	-	16/40/40/53	-
13	CLA	b	804	-	-	17/39/115/115	-
13	CLA	L	206	-	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	6	202	-	-	12/29/63/63	0/2/2/2
17	LHG	1	849	-	-	16/40/40/53	-
16	BCR	2	840	-	-	8/29/63/63	0/2/2/2
13	CLA	B	827	-	-	8/15/91/115	-
16	BCR	L	202	-	-	10/29/63/63	0/2/2/2
13	CLA	A	819	-	-	12/33/109/115	-
13	CLA	1	205	-	-	4/17/93/115	-
13	CLA	0	202	-	-	10/33/109/115	-
13	CLA	7	102	-	-	14/39/115/115	-
13	CLA	9	4005	-	-	6/13/89/115	-
13	CLA	L	201	-	-	10/33/109/115	-
13	CLA	B	801	-	-	6/39/115/115	-
16	BCR	2	844	-	-	15/29/63/63	0/2/2/2
13	CLA	1	815	-	-	3/15/91/115	-
13	CLA	a	813	-	-	10/27/103/115	-
13	CLA	2	836	-	-	14/39/115/115	-
13	CLA	B	830	-	-	10/31/107/115	-
13	CLA	1	838	-	-	10/39/115/115	-
13	CLA	2	831	-	-	4/10/82/115	-
13	CLA	a	827	-	-	13/39/115/115	-
16	BCR	M	101	-	-	7/29/63/63	0/2/2/2
16	BCR	2	847	-	-	10/29/63/63	0/2/2/2
13	CLA	A	813	-	-	10/27/103/115	-
13	CLA	B	837	-	-	14/39/115/115	-
13	CLA	B	817	-	-	2/10/86/115	-
13	CLA	B	820	-	-	8/27/103/115	-
13	CLA	A	809	-	-	9/21/97/115	-
13	CLA	2	810	-	-	8/17/93/115	-
13	CLA	a	838	-	-	10/39/115/115	-
13	CLA	6	203	-	-	1/15/91/115	-
16	BCR	b	844	-	-	6/29/63/63	0/2/2/2
13	CLA	B	822	-	-	2/21/97/115	-
16	BCR	0	204	-	-	10/29/63/63	0/2/2/2
13	CLA	b	811	-	-	8/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	b	822	-	-	2/21/97/115	-
13	CLA	2	813	-	-	8/21/97/115	-
13	CLA	B	807	-	-	15/39/115/115	-
16	BCR	l	201	-	-	7/29/63/63	0/2/2/2
13	CLA	B	836	-	-	5/39/115/115	-
13	CLA	a	818	-	-	7/26/102/115	-
16	BCR	7	103	-	-	8/29/63/63	0/2/2/2
13	CLA	2	828	-	-	17/36/112/115	-
13	CLA	1	810	-	-	8/15/91/115	-
13	CLA	b	805	-	-	13/39/115/115	-
13	CLA	b	828	-	-	9/27/103/115	-
13	CLA	A	836	-	-	6/23/99/115	-
13	CLA	a	834	-	-	12/39/115/115	-
13	CLA	1	835	-	-	14/29/105/115	-
13	CLA	A	808	-	-	5/21/97/115	-
13	CLA	b	823	-	-	12/39/115/115	-
13	CLA	1	821	-	-	11/39/115/115	-
13	CLA	1	813	-	-	10/27/103/115	-
16	BCR	b	841	-	-	8/29/63/63	0/2/2/2
13	CLA	k	4005	-	-	6/13/89/115	-
16	BCR	A	847	-	-	15/29/63/63	0/2/2/2
16	BCR	m	101	-	-	7/29/63/63	0/2/2/2
13	CLA	a	830	-	-	13/39/115/115	-
13	CLA	9	4002	-	-	7/15/91/115	-
13	CLA	a	809	-	-	9/21/97/115	-
13	CLA	2	833	-	-	6/33/109/115	-
16	BCR	K	4004	-	-	11/29/63/63	0/2/2/2
13	CLA	9	4003	-	-	8/17/93/115	-
16	BCR	l	206	-	-	11/29/63/63	0/2/2/2
13	CLA	A	852	-	-	13/33/109/115	-
13	CLA	B	826	-	-	14/33/109/115	-
13	CLA	A	818	-	-	7/26/102/115	-
13	CLA	a	803	-	-	11/39/115/115	-
13	CLA	A	827	-	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	1	834	-	-	12/39/115/115	-
13	CLA	a	852	-	-	13/33/109/115	-
16	BCR	b	843	-	-	9/29/63/63	0/2/2/2
13	CLA	1	842	-	-	7/15/91/115	-
16	BCR	8	1104	-	-	9/29/63/63	0/2/2/2
13	CLA	a	829	-	-	12/39/115/115	-
13	CLA	A	825	-	-	15/36/112/115	-
13	CLA	a	833	-	-	13/39/115/115	-
16	BCR	b	840	-	-	11/29/63/63	0/2/2/2
13	CLA	l	204	-	-	7/21/97/115	-
13	CLA	B	824	-	-	7/27/103/115	-
13	CLA	1	852	-	-	13/33/109/115	-
13	CLA	a	822	-	-	8/21/97/115	-
13	CLA	I	101	-	-	14/39/115/115	-
12	CL0	a	801	-	-	14/39/115/115	-
13	CLA	1	830	-	-	13/39/115/115	-
16	BCR	F	205	-	-	12/29/63/63	0/2/2/2
13	CLA	1	809	-	-	9/21/97/115	-
16	BCR	2	842	-	-	9/29/63/63	0/2/2/2
13	CLA	a	837	-	-	8/33/109/115	-
13	CLA	A	838	-	-	10/39/115/115	-
16	BCR	1	845	-	-	8/29/63/63	0/2/2/2
13	CLA	2	825	-	-	14/33/109/115	-
13	CLA	A	839	-	-	9/39/115/115	-
13	CLA	B	832	-	-	4/10/82/115	-
13	CLA	2	826	-	-	8/15/91/115	-
13	CLA	b	807	-	-	15/39/115/115	-
13	CLA	2	846	-	-	9/39/115/115	-
16	BCR	a	845	-	-	8/29/63/63	0/2/2/2
14	PQN	A	843	-	-	10/23/43/43	0/2/2/2
17	LHG	A	850	-	-	19/45/45/53	-
15	SF4	a	844	1,2	-	-	0/6/5/5
13	CLA	0	203	-	-	15/39/115/115	-
13	CLA	1	816	-	-	8/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	b	812	-	-	4/15/91/115	-
13	CLA	1	829	-	-	12/39/115/115	-
14	PQN	b	839	-	-	10/23/43/43	0/2/2/2
13	CLA	B	805	-	-	13/39/115/115	-
13	CLA	a	839	-	-	9/39/115/115	-
13	CLA	b	803	-	-	11/33/109/115	-
13	CLA	J	1101	-	-	9/21/97/115	-
13	CLA	2	822	-	-	12/39/115/115	-
13	CLA	b	815	-	-	12/39/115/115	-
13	CLA	b	829	-	-	17/36/112/115	-
13	CLA	b	837	-	-	14/39/115/115	-
13	CLA	B	812	-	-	4/15/91/115	-
13	CLA	b	802	-	-	9/39/115/115	-
13	CLA	1	823	-	-	7/21/97/115	-
13	CLA	1	839	-	-	9/39/115/115	-
13	CLA	2	823	-	-	7/27/103/115	-
13	CLA	a	807	-	-	4/27/103/115	-
13	CLA	8	1103	-	-	8/15/91/115	-
16	BCR	B	843	-	-	9/29/63/63	0/2/2/2
13	CLA	a	832	-	-	9/39/115/115	-
13	CLA	B	811	-	-	8/17/93/115	-
13	CLA	k	4003	-	-	8/17/93/115	-
13	CLA	B	806	-	-	16/39/115/115	-
16	BCR	B	840	-	-	11/29/63/63	0/2/2/2
13	CLA	1	841	-	-	12/33/109/115	-
16	BCR	B	841	-	-	8/29/63/63	0/2/2/2
13	CLA	B	814	-	-	8/21/97/115	-
13	CLA	a	804	-	-	3/27/103/115	-
13	CLA	A	832	-	-	9/39/115/115	-
17	LHG	1	850	-	-	20/45/45/53	-
13	CLA	1	819	-	-	12/33/109/115	-
16	BCR	l	203	-	-	10/29/63/63	0/2/2/2
13	CLA	A	829	-	-	12/39/115/115	-
13	CLA	a	819	-	-	12/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	b	813	-	-	15/39/115/115	-
13	CLA	F	201	-	-	6/27/103/115	-
13	CLA	1	825	-	-	15/36/112/115	-
16	BCR	B	842	-	-	14/29/63/63	0/2/2/2
12	CL0	A	801	-	-	14/39/115/115	-
13	CLA	a	841	-	-	12/33/109/115	-
16	BCR	6	205	-	-	12/29/63/63	0/2/2/2
13	CLA	A	834	-	-	12/39/115/115	-
14	PQN	B	839	-	-	10/23/43/43	0/2/2/2
13	CLA	a	820	-	-	5/17/93/115	-
13	CLA	B	803	-	-	11/33/109/115	-
13	CLA	2	834	-	-	3/21/97/115	-
16	BCR	I	102	-	-	8/29/63/63	0/2/2/2
13	CLA	B	835	-	-	3/21/97/115	-
13	CLA	2	819	-	-	8/27/103/115	-
13	CLA	B	815	-	-	12/39/115/115	-
13	CLA	B	847	-	-	9/39/115/115	-
13	CLA	B	821	-	-	19/39/115/115	-
13	CLA	2	817	-	-	10/17/93/115	-
13	CLA	a	805	-	-	12/27/103/115	-
13	CLA	2	837	-	-	7/39/115/115	-
16	BCR	1	847	-	-	15/29/63/63	0/2/2/2
13	CLA	2	830	-	-	7/39/115/115	-
15	SF4	C	102	3	-	-	0/6/5/5
13	CLA	A	803	-	-	11/39/115/115	-
13	CLA	B	808	-	-	14/39/115/115	-
13	CLA	1	824	-	-	16/33/109/115	-
16	BCR	a	847	-	-	15/29/63/63	0/2/2/2
13	CLA	b	836	-	-	5/39/115/115	-
13	CLA	2	821	-	-	2/21/97/115	-
13	CLA	b	820	-	-	8/27/103/115	-
13	CLA	a	824	-	-	16/33/109/115	-
13	CLA	2	809	-	-	15/39/115/115	-
13	CLA	A	810	-	-	8/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	2	818	-	-	6/17/93/115	-
13	CLA	A	840	-	-	13/39/115/115	-
13	CLA	A	814	-	-	4/21/97/115	-
13	CLA	B	804	-	-	17/39/115/115	-
13	CLA	K	4005	-	-	6/13/89/115	-
16	BCR	k	4004	-	-	11/29/63/63	0/2/2/2
13	CLA	b	827	-	-	8/15/91/115	-
13	CLA	J	1103	-	-	8/15/91/115	-
13	CLA	b	824	-	-	7/27/103/115	-
16	BCR	B	848	-	-	10/29/63/63	0/2/2/2
13	CLA	b	809	-	-	5/15/91/115	-
13	CLA	A	833	-	-	13/39/115/115	-
16	BCR	b	845	-	-	15/29/63/63	0/2/2/2
13	CLA	a	814	-	-	4/21/97/115	-
13	CLA	b	821	-	-	19/39/115/115	-
13	CLA	l	207	-	-	9/39/115/115	-
13	CLA	B	810	-	-	15/39/115/115	-
13	CLA	a	817	-	-	8/27/103/115	-
13	CLA	a	836	-	-	6/23/99/115	-
16	BCR	f	205	-	-	12/29/63/63	0/2/2/2
15	SF4	3	101	3	-	-	0/6/5/5
16	BCR	f	202	-	-	12/29/63/63	0/2/2/2
13	CLA	b	808	-	-	14/39/115/115	-
13	CLA	A	811	-	-	10/29/105/115	-
18	LMG	b	846	-	-	17/36/56/70	0/1/1/1
13	CLA	1	803	-	-	11/39/115/115	-
13	CLA	a	812	-	-	6/17/93/115	-
13	CLA	1	833	-	-	13/39/115/115	-
16	BCR	L	207	-	-	7/29/63/63	0/2/2/2
13	CLA	2	835	-	-	5/39/115/115	-
13	CLA	1	814	-	-	4/21/97/115	-
13	CLA	A	820	-	-	5/17/93/115	-
13	CLA	1	811	-	-	10/29/105/115	-
13	CLA	1	836	-	-	6/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	a	811	-	-	10/29/105/115	-
13	CLA	b	826	-	-	14/33/109/115	-
13	CLA	a	840	-	-	13/39/115/115	-
13	CLA	6	201	-	-	6/27/103/115	-
13	CLA	2	816	-	-	2/10/86/115	-
13	CLA	1	820	-	-	5/17/93/115	-
13	CLA	A	828	-	-	9/39/115/115	-
13	CLA	l	202	-	-	10/33/109/115	-
13	CLA	A	804	-	-	3/27/103/115	-
13	CLA	j	1101	-	-	9/21/97/115	-
13	CLA	a	808	-	-	5/21/97/115	-
16	BCR	B	845	-	-	15/29/63/63	0/2/2/2
13	CLA	1	831	-	-	8/21/97/115	-
16	BCR	A	848	-	-	15/29/63/63	0/2/2/2
16	BCR	L	205	-	-	11/29/63/63	0/2/2/2
16	BCR	2	843	-	-	6/29/63/63	0/2/2/2
13	CLA	f	203	-	-	1/15/91/115	-
16	BCR	B	844	-	-	6/29/63/63	0/2/2/2
13	CLA	2	832	-	-	6/21/97/115	-
13	CLA	j	1103	-	-	8/15/91/115	-
13	CLA	1	840	-	-	13/39/115/115	-
13	CLA	1	832	-	-	10/39/115/115	-
13	CLA	2	805	-	-	13/39/115/115	-
13	CLA	2	829	-	-	10/31/107/115	-
13	CLA	1	802	-	-	10/33/109/115	-
15	SF4	A	844	1,2	-	-	0/6/5/5
14	PQN	a	843	-	-	10/23/43/43	0/2/2/2
13	CLA	B	825	-	-	8/39/115/115	-
13	CLA	A	842	-	-	7/15/91/115	-
13	CLA	F	203	-	-	1/15/91/115	-
13	CLA	A	815	-	-	3/15/91/115	-
13	CLA	0	205	-	-	7/21/97/115	-
16	BCR	a	848	-	-	15/29/63/63	0/2/2/2
13	CLA	b	825	-	-	8/39/115/115	-
13	CLA	b	806	-	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	SF4	c	101	3	-	-	0/6/5/5
16	BCR	K	4001	-	-	8/29/63/63	0/2/2/2
13	CLA	1	808	-	-	5/21/97/115	-
15	SF4	1	844	1,2	-	-	0/6/5/5
13	CLA	b	832	-	-	4/10/82/115	-
13	CLA	1	807	-	-	4/27/103/115	-
16	BCR	2	841	-	-	14/29/63/63	0/2/2/2
15	SF4	c	102	3	-	-	0/6/5/5
13	CLA	a	842	-	-	7/15/91/115	-
13	CLA	2	807	-	-	14/39/115/115	-
13	CLA	2	812	-	-	16/39/115/115	-
13	CLA	b	810	-	-	15/39/115/115	-
13	CLA	2	824	-	-	8/39/115/115	-
16	BCR	j	1105	-	-	11/29/63/63	0/2/2/2
17	LHG	a	850	-	-	19/45/45/53	-
13	CLA	B	813	-	-	15/39/115/115	-
13	CLA	2	815	-	-	7/33/109/115	-
16	BCR	b	848	-	-	10/29/63/63	0/2/2/2
18	LMG	B	846	-	-	17/36/56/70	0/1/1/1
13	CLA	A	821	-	-	11/39/115/115	-
13	CLA	b	831	-	-	7/39/115/115	-
13	CLA	K	4002	-	-	7/15/91/115	-
13	CLA	a	806	-	-	12/39/115/115	-
13	CLA	2	820	-	-	19/39/115/115	-
13	CLA	A	805	-	-	12/27/103/115	-
13	CLA	A	817	-	-	8/27/103/115	-
13	CLA	J	1102	-	-	6/10/82/115	-
13	CLA	2	801	-	-	6/39/115/115	-
13	CLA	0	208	-	-	9/39/115/115	-
13	CLA	A	837	-	-	8/33/109/115	-
13	CLA	8	1102	-	-	6/10/82/115	-
13	CLA	1	804	-	-	3/27/103/115	-
13	CLA	k	4002	-	-	7/15/91/115	-
13	CLA	B	809	-	-	5/15/91/115	-

All (2696) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	842	BCR	C30-C25	-3.74	1.49	1.53
16	b	842	BCR	C30-C25	-3.73	1.49	1.53
16	2	841	BCR	C30-C25	-3.73	1.49	1.53
16	2	847	BCR	C1-C6	-3.64	1.49	1.53
16	B	848	BCR	C1-C6	-3.62	1.49	1.53
16	b	848	BCR	C1-C6	-3.57	1.49	1.53
13	k	4003	CLA	C1D-ND	3.57	1.42	1.37
16	2	844	BCR	C30-C25	-3.57	1.49	1.53
13	a	820	CLA	C1D-ND	3.56	1.42	1.37
13	B	817	CLA	C1D-ND	3.55	1.42	1.37
16	B	845	BCR	C30-C25	-3.55	1.49	1.53
13	2	816	CLA	C1D-ND	3.55	1.42	1.37
13	K	4003	CLA	C1D-ND	3.54	1.42	1.37
13	8	1101	CLA	C1D-ND	3.54	1.42	1.37
13	9	4003	CLA	C1D-ND	3.54	1.42	1.37
13	b	818	CLA	C1D-ND	3.54	1.42	1.37
16	b	845	BCR	C30-C25	-3.54	1.49	1.53
13	J	1102	CLA	C1D-ND	3.52	1.42	1.37
13	b	817	CLA	C1D-ND	3.52	1.42	1.37
13	a	835	CLA	C1D-ND	3.52	1.42	1.37
13	J	1101	CLA	C1D-ND	3.51	1.42	1.37
13	B	818	CLA	C1D-ND	3.50	1.42	1.37
13	A	820	CLA	C1D-ND	3.50	1.42	1.37
13	A	835	CLA	C1D-ND	3.50	1.42	1.37
13	1	820	CLA	C1D-ND	3.50	1.42	1.37
13	j	1102	CLA	C1D-ND	3.49	1.42	1.37
13	2	817	CLA	C1D-ND	3.49	1.42	1.37
13	a	852	CLA	C1D-ND	3.48	1.42	1.37
13	1	835	CLA	C1D-ND	3.48	1.42	1.37
13	8	1102	CLA	C1D-ND	3.48	1.42	1.37
13	j	1101	CLA	C1D-ND	3.47	1.42	1.37
16	K	4001	BCR	C1-C6	-3.46	1.49	1.53
13	2	836	CLA	C1D-ND	3.45	1.42	1.37
13	b	830	CLA	C1D-ND	3.45	1.42	1.37
13	2	818	CLA	C1D-ND	3.45	1.42	1.37
13	k	4002	CLA	C1D-ND	3.45	1.42	1.37
13	9	4002	CLA	C1D-ND	3.45	1.42	1.37
13	B	830	CLA	C1D-ND	3.44	1.42	1.37
13	K	4002	CLA	C1D-ND	3.44	1.42	1.37
13	b	837	CLA	C1D-ND	3.44	1.42	1.37
13	B	837	CLA	C1D-ND	3.44	1.42	1.37
13	1	852	CLA	C1D-ND	3.44	1.42	1.37
13	A	852	CLA	C1D-ND	3.43	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	6	203	CLA	C1D-ND	3.43	1.42	1.37
13	B	819	CLA	C1D-ND	3.43	1.42	1.37
13	j	1103	CLA	C1D-ND	3.43	1.42	1.37
13	2	829	CLA	C1D-ND	3.42	1.42	1.37
16	9	4001	BCR	C1-C6	-3.42	1.49	1.53
13	A	821	CLA	C1D-ND	3.42	1.42	1.37
16	k	4001	BCR	C1-C6	-3.41	1.49	1.53
13	a	816	CLA	C1D-ND	3.41	1.42	1.37
13	b	819	CLA	C1D-ND	3.41	1.42	1.37
13	1	825	CLA	C1D-ND	3.41	1.42	1.37
13	b	813	CLA	C1D-ND	3.41	1.42	1.37
13	1	810	CLA	C1D-ND	3.41	1.42	1.37
13	2	831	CLA	C1D-ND	3.41	1.42	1.37
13	a	821	CLA	C1D-ND	3.40	1.42	1.37
13	J	1103	CLA	C1D-ND	3.40	1.42	1.37
13	F	204	CLA	C1D-ND	3.39	1.42	1.37
13	A	825	CLA	C1D-ND	3.39	1.42	1.37
13	2	812	CLA	C1D-ND	3.39	1.42	1.37
13	b	834	CLA	C1D-ND	3.39	1.42	1.37
13	B	813	CLA	C1D-ND	3.38	1.42	1.37
13	F	203	CLA	C1D-ND	3.38	1.42	1.37
13	B	832	CLA	C1D-ND	3.38	1.42	1.37
13	K	4005	CLA	C1D-ND	3.38	1.42	1.37
13	2	833	CLA	C1D-ND	3.38	1.42	1.37
13	b	816	CLA	C1D-ND	3.37	1.42	1.37
13	2	815	CLA	C1D-ND	3.37	1.42	1.37
13	9	4005	CLA	C1D-ND	3.37	1.42	1.37
13	b	832	CLA	C1D-ND	3.36	1.42	1.37
13	0	206	CLA	C1D-ND	3.36	1.42	1.37
13	A	816	CLA	C1D-ND	3.36	1.42	1.37
13	a	812	CLA	C1D-ND	3.36	1.42	1.37
13	B	816	CLA	C1D-ND	3.36	1.42	1.37
16	j	1105	BCR	C1-C6	-3.36	1.49	1.53
13	A	815	CLA	C1D-ND	3.36	1.42	1.37
13	1	821	CLA	C1D-ND	3.36	1.42	1.37
13	1	839	CLA	C1D-ND	3.36	1.42	1.37
13	b	824	CLA	C1D-ND	3.36	1.42	1.37
13	a	815	CLA	C1D-ND	3.35	1.42	1.37
13	f	203	CLA	C1D-ND	3.35	1.42	1.37
13	l	205	CLA	C1D-ND	3.35	1.42	1.37
13	A	810	CLA	C1D-ND	3.35	1.42	1.37
13	L	204	CLA	C1D-ND	3.35	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	828	CLA	C1D-ND	3.34	1.42	1.37
13	A	839	CLA	C1D-ND	3.34	1.42	1.37
13	f	204	CLA	C1D-ND	3.34	1.42	1.37
13	1	816	CLA	C1D-ND	3.34	1.42	1.37
13	8	1103	CLA	C1D-ND	3.34	1.42	1.37
16	b	844	BCR	C1-C6	-3.34	1.49	1.53
16	A	847	BCR	C1-C6	-3.34	1.49	1.53
13	a	825	CLA	C1D-ND	3.34	1.42	1.37
13	a	834	CLA	C1D-ND	3.34	1.42	1.37
13	2	827	CLA	C1D-ND	3.34	1.42	1.37
13	b	821	CLA	C1D-ND	3.34	1.42	1.37
13	b	847	CLA	C1D-ND	3.34	1.42	1.37
13	B	834	CLA	C1D-ND	3.34	1.42	1.37
13	F	201	CLA	C1D-ND	3.33	1.42	1.37
13	b	812	CLA	C1D-ND	3.33	1.42	1.37
16	a	846	BCR	C1-C6	-3.33	1.49	1.53
13	6	204	CLA	C1D-ND	3.33	1.42	1.37
16	A	846	BCR	C1-C6	-3.33	1.49	1.53
13	1	815	CLA	C1D-ND	3.33	1.42	1.37
13	A	824	CLA	C1D-ND	3.33	1.42	1.37
13	1	808	CLA	C1D-ND	3.32	1.42	1.37
13	1	813	CLA	C1D-ND	3.32	1.42	1.37
13	B	828	CLA	C1D-ND	3.32	1.42	1.37
16	l	206	BCR	C1-C6	-3.32	1.49	1.53
16	1	846	BCR	C1-C6	-3.32	1.49	1.53
13	2	811	CLA	C1D-ND	3.32	1.42	1.37
16	0	201	BCR	C1-C6	-3.32	1.49	1.53
13	a	810	CLA	C1D-ND	3.32	1.42	1.37
13	1	812	CLA	C1D-ND	3.32	1.42	1.37
13	B	821	CLA	C1D-ND	3.31	1.42	1.37
13	a	824	CLA	C1D-ND	3.31	1.42	1.37
13	A	812	CLA	C1D-ND	3.31	1.42	1.37
13	k	4005	CLA	C1D-ND	3.31	1.42	1.37
13	2	820	CLA	C1D-ND	3.31	1.42	1.37
16	B	844	BCR	C1-C6	-3.31	1.49	1.53
16	9	4004	BCR	C1-C6	-3.31	1.49	1.53
16	J	1105	BCR	C1-C6	-3.31	1.49	1.53
13	B	838	CLA	C1D-ND	3.31	1.42	1.37
13	f	201	CLA	C1D-ND	3.31	1.42	1.37
13	2	823	CLA	C1D-ND	3.31	1.42	1.37
13	2	837	CLA	C1D-ND	3.31	1.42	1.37
13	A	813	CLA	C1D-ND	3.30	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	2	843	BCR	C1-C6	-3.30	1.49	1.53
13	A	808	CLA	C1D-ND	3.30	1.42	1.37
13	a	813	CLA	C1D-ND	3.30	1.42	1.37
16	K	4004	BCR	C1-C6	-3.30	1.49	1.53
16	1	847	BCR	C1-C6	-3.30	1.49	1.53
16	k	4004	BCR	C1-C6	-3.30	1.49	1.53
16	8	1105	BCR	C1-C6	-3.29	1.49	1.53
13	B	812	CLA	C1D-ND	3.29	1.42	1.37
16	a	847	BCR	C1-C6	-3.29	1.49	1.53
13	2	805	CLA	C1D-ND	3.29	1.42	1.37
16	l	201	BCR	C1-C6	-3.29	1.49	1.53
13	B	824	CLA	C1D-ND	3.29	1.42	1.37
13	b	805	CLA	C1D-ND	3.29	1.42	1.37
13	1	834	CLA	C1D-ND	3.29	1.42	1.37
16	L	205	BCR	C1-C6	-3.29	1.49	1.53
13	1	824	CLA	C1D-ND	3.29	1.42	1.37
16	1	845	BCR	C1-C6	-3.28	1.49	1.53
13	b	820	CLA	C1D-ND	3.28	1.42	1.37
13	a	839	CLA	C1D-ND	3.28	1.42	1.37
13	a	814	CLA	C1D-ND	3.28	1.42	1.37
13	2	819	CLA	C1D-ND	3.28	1.42	1.37
13	A	834	CLA	C1D-ND	3.28	1.42	1.37
13	B	820	CLA	C1D-ND	3.28	1.42	1.37
13	a	808	CLA	C1D-ND	3.28	1.42	1.37
13	b	838	CLA	C1D-ND	3.28	1.42	1.37
13	1	807	CLA	C1D-ND	3.28	1.42	1.37
13	6	201	CLA	C1D-ND	3.27	1.42	1.37
16	a	845	BCR	C1-C6	-3.27	1.49	1.53
13	a	817	CLA	C1D-ND	3.27	1.42	1.37
16	f	205	BCR	C1-C6	-3.27	1.49	1.53
13	A	817	CLA	C1D-ND	3.27	1.42	1.37
13	B	808	CLA	C1D-ND	3.27	1.42	1.37
13	B	847	CLA	C1D-ND	3.27	1.42	1.37
13	A	807	CLA	C1D-ND	3.27	1.42	1.37
13	L	201	CLA	C1D-ND	3.27	1.42	1.37
13	1	832	CLA	C1D-ND	3.27	1.42	1.37
13	a	807	CLA	C1D-ND	3.26	1.42	1.37
13	1	817	CLA	C1D-ND	3.26	1.42	1.37
13	B	805	CLA	C1D-ND	3.26	1.42	1.37
13	1	814	CLA	C1D-ND	3.26	1.42	1.37
13	2	834	CLA	C1D-ND	3.26	1.42	1.37
16	F	205	BCR	C1-C6	-3.26	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	2	807	CLA	C1D-ND	3.26	1.42	1.37
16	L	207	BCR	C1-C6	-3.26	1.49	1.53
13	l	202	CLA	C1D-ND	3.26	1.42	1.37
13	2	826	CLA	C1D-ND	3.26	1.42	1.37
13	B	827	CLA	C1D-ND	3.25	1.42	1.37
13	A	814	CLA	C1D-ND	3.25	1.42	1.37
13	b	815	CLA	C1D-ND	3.25	1.42	1.37
13	0	202	CLA	C1D-ND	3.25	1.42	1.37
13	2	813	CLA	C1D-ND	3.24	1.42	1.37
13	2	846	CLA	C1D-ND	3.24	1.42	1.37
13	2	806	CLA	C1D-ND	3.24	1.42	1.37
13	B	809	CLA	C1D-ND	3.24	1.42	1.37
13	2	814	CLA	C1D-ND	3.23	1.42	1.37
13	a	804	CLA	C1D-ND	3.23	1.42	1.37
16	z	101	BCR	C1-C6	-3.23	1.49	1.53
13	B	835	CLA	C1D-ND	3.23	1.42	1.37
16	0	207	BCR	C1-C6	-3.23	1.49	1.53
13	b	808	CLA	C1D-ND	3.23	1.42	1.37
13	b	831	CLA	C1D-ND	3.23	1.42	1.37
16	A	845	BCR	C1-C6	-3.23	1.49	1.53
13	b	827	CLA	C1D-ND	3.23	1.42	1.37
13	0	205	CLA	C1D-ND	3.23	1.42	1.37
16	2	839	BCR	C1-C6	-3.23	1.49	1.53
13	A	832	CLA	C1D-ND	3.22	1.42	1.37
13	B	806	CLA	C1D-ND	3.22	1.42	1.37
13	2	830	CLA	C1D-ND	3.22	1.42	1.37
13	b	806	CLA	C1D-ND	3.22	1.42	1.37
13	a	822	CLA	C1D-ND	3.22	1.42	1.37
16	M	101	BCR	C1-C6	-3.22	1.49	1.53
16	B	843	BCR	C30-C25	-3.22	1.49	1.53
16	6	205	BCR	C1-C6	-3.22	1.49	1.53
16	b	843	BCR	C30-C25	-3.22	1.49	1.53
13	1	811	CLA	C1D-ND	3.22	1.42	1.37
13	2	821	CLA	C1D-ND	3.21	1.42	1.37
13	2	822	CLA	C1D-ND	3.21	1.42	1.37
13	B	815	CLA	C1D-ND	3.21	1.42	1.37
13	2	808	CLA	C1D-ND	3.21	1.42	1.37
13	A	811	CLA	C1D-ND	3.21	1.42	1.37
13	a	806	CLA	C1D-ND	3.21	1.42	1.37
13	a	832	CLA	C1D-ND	3.21	1.42	1.37
16	b	843	BCR	C1-C6	-3.21	1.49	1.53
13	1	822	CLA	C1D-ND	3.21	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	m	101	BCR	C1-C6	-3.20	1.49	1.53
13	b	809	CLA	C1D-ND	3.20	1.42	1.37
13	B	831	CLA	C1D-ND	3.20	1.42	1.37
13	1	842	CLA	C1D-ND	3.20	1.42	1.37
16	2	842	BCR	C30-C25	-3.20	1.49	1.53
13	1	805	CLA	C1D-ND	3.20	1.42	1.37
13	b	835	CLA	C1D-ND	3.20	1.42	1.37
13	B	822	CLA	C1D-ND	3.20	1.42	1.37
16	B	840	BCR	C1-C6	-3.19	1.49	1.53
13	A	804	CLA	C1D-ND	3.19	1.42	1.37
13	B	823	CLA	C1D-ND	3.19	1.42	1.37
16	1	851	BCR	C1-C6	-3.19	1.49	1.53
13	a	819	CLA	C1D-ND	3.19	1.42	1.37
13	1	804	CLA	C1D-ND	3.19	1.42	1.37
13	7	102	CLA	C1D-ND	3.18	1.42	1.37
13	A	822	CLA	C1D-ND	3.18	1.42	1.37
16	A	851	BCR	C1-C6	-3.18	1.49	1.53
13	a	818	CLA	C1D-ND	3.18	1.42	1.37
16	b	840	BCR	C1-C6	-3.18	1.49	1.53
13	A	806	CLA	C1D-ND	3.18	1.42	1.37
13	B	814	CLA	C1D-ND	3.18	1.42	1.37
13	A	803	CLA	C1D-ND	3.18	1.42	1.37
13	b	823	CLA	C1D-ND	3.18	1.42	1.37
16	a	851	BCR	C1-C6	-3.18	1.49	1.53
13	b	822	CLA	C1D-ND	3.17	1.42	1.37
13	l	204	CLA	C1D-ND	3.17	1.42	1.37
16	B	841	BCR	C1-C6	-3.17	1.49	1.53
16	B	843	BCR	C1-C6	-3.17	1.49	1.53
13	A	818	CLA	C1D-ND	3.17	1.42	1.37
13	b	804	CLA	C1D-ND	3.17	1.42	1.37
13	A	830	CLA	C1D-ND	3.17	1.42	1.37
13	I	101	CLA	C1D-ND	3.17	1.42	1.37
13	1	818	CLA	C1D-ND	3.17	1.42	1.37
13	a	842	CLA	C1D-ND	3.17	1.42	1.37
13	1	809	CLA	C1D-ND	3.16	1.42	1.37
13	A	842	CLA	C1D-ND	3.16	1.42	1.37
13	A	805	CLA	C1D-ND	3.16	1.42	1.37
13	a	811	CLA	C1D-ND	3.16	1.42	1.37
13	i	102	CLA	C1D-ND	3.16	1.42	1.37
16	a	851	BCR	C30-C25	-3.16	1.49	1.53
16	A	851	BCR	C30-C25	-3.16	1.49	1.53
16	2	842	BCR	C1-C6	-3.16	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	814	CLA	C1D-ND	3.15	1.42	1.37
13	B	804	CLA	C1D-ND	3.15	1.42	1.37
16	1	851	BCR	C30-C25	-3.15	1.49	1.53
19	i	101	SQD	O48-C23	3.15	1.42	1.33
16	b	840	BCR	C30-C25	-3.15	1.49	1.53
16	0	204	BCR	C30-C25	-3.15	1.49	1.53
13	A	831	CLA	C1D-ND	3.15	1.42	1.37
13	a	830	CLA	C1D-ND	3.15	1.42	1.37
13	a	805	CLA	C1D-ND	3.15	1.42	1.37
13	a	831	CLA	C1D-ND	3.15	1.42	1.37
13	2	804	CLA	C1D-ND	3.15	1.42	1.37
16	B	840	BCR	C30-C25	-3.15	1.49	1.53
13	1	831	CLA	C1D-ND	3.15	1.42	1.37
13	A	809	CLA	C1D-ND	3.15	1.42	1.37
19	I	103	SQD	O48-C23	3.15	1.42	1.33
13	a	809	CLA	C1D-ND	3.14	1.42	1.37
19	7	101	SQD	O48-C23	3.14	1.42	1.33
13	a	803	CLA	C1D-ND	3.14	1.42	1.37
13	L	203	CLA	C1D-ND	3.14	1.42	1.37
12	a	801	CL0	C4B-NB	3.14	1.42	1.37
13	B	826	CLA	C1D-ND	3.14	1.42	1.37
16	a	846	BCR	C30-C25	-3.14	1.49	1.53
13	a	820	CLA	C4B-NB	3.14	1.42	1.37
13	1	806	CLA	C1D-ND	3.13	1.42	1.37
13	A	820	CLA	C4B-NB	3.13	1.42	1.37
16	A	846	BCR	C30-C25	-3.13	1.49	1.53
13	1	819	CLA	C1D-ND	3.13	1.42	1.37
13	1	830	CLA	C1D-ND	3.13	1.42	1.37
13	A	841	CLA	C1D-ND	3.12	1.42	1.37
13	A	819	CLA	C1D-ND	3.12	1.42	1.37
13	1	803	CLA	C1D-ND	3.11	1.42	1.37
16	b	845	BCR	C1-C6	-3.11	1.49	1.53
13	a	837	CLA	C1D-ND	3.11	1.41	1.37
13	1	841	CLA	C1D-ND	3.11	1.41	1.37
16	b	848	BCR	C30-C25	-3.10	1.49	1.53
13	2	835	CLA	C1D-ND	3.10	1.41	1.37
16	1	846	BCR	C30-C25	-3.10	1.49	1.53
12	A	801	CL0	C4B-NB	3.10	1.41	1.37
13	b	826	CLA	C1D-ND	3.10	1.41	1.37
13	1	838	CLA	C1D-ND	3.10	1.41	1.37
16	b	841	BCR	C1-C6	-3.10	1.49	1.53
13	A	838	CLA	C1D-ND	3.10	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	838	CLA	C1D-ND	3.10	1.41	1.37
16	B	845	BCR	C1-C6	-3.10	1.49	1.53
16	2	840	BCR	C1-C6	-3.10	1.49	1.53
13	A	836	CLA	C1D-ND	3.10	1.41	1.37
16	l	203	BCR	C30-C25	-3.09	1.49	1.53
13	a	841	CLA	C1D-ND	3.09	1.41	1.37
13	a	823	CLA	C1D-ND	3.09	1.41	1.37
12	1	801	CL0	C4B-NB	3.09	1.41	1.37
13	2	809	CLA	C1D-ND	3.09	1.41	1.37
16	f	202	BCR	C1-C6	-3.09	1.49	1.53
13	A	823	CLA	C1D-ND	3.08	1.41	1.37
16	2	839	BCR	C30-C25	-3.08	1.49	1.53
16	2	844	BCR	C1-C6	-3.08	1.49	1.53
16	A	845	BCR	C30-C25	-3.08	1.49	1.53
13	1	816	CLA	C4B-NB	3.08	1.41	1.37
13	2	825	CLA	C1D-ND	3.08	1.41	1.37
13	1	823	CLA	C1D-ND	3.08	1.41	1.37
13	1	820	CLA	C4B-NB	3.08	1.41	1.37
16	k	4004	BCR	C30-C25	-3.08	1.49	1.53
13	B	836	CLA	C1D-ND	3.07	1.41	1.37
16	a	845	BCR	C30-C25	-3.07	1.49	1.53
13	b	825	CLA	C1D-ND	3.07	1.41	1.37
13	B	810	CLA	C1D-ND	3.07	1.41	1.37
13	B	803	CLA	C1D-ND	3.07	1.41	1.37
13	j	1102	CLA	C4B-NB	3.07	1.41	1.37
13	2	816	CLA	C4B-NB	3.07	1.41	1.37
16	9	4004	BCR	C30-C25	-3.07	1.49	1.53
13	A	840	CLA	C1D-ND	3.07	1.41	1.37
13	b	817	CLA	C4B-NB	3.07	1.41	1.37
13	1	841	CLA	C4B-NB	3.07	1.41	1.37
13	1	833	CLA	C1D-ND	3.06	1.41	1.37
16	1	845	BCR	C30-C25	-3.06	1.49	1.53
13	A	816	CLA	C4B-NB	3.06	1.41	1.37
13	a	826	CLA	C1D-ND	3.06	1.41	1.37
13	b	836	CLA	C1D-ND	3.06	1.41	1.37
16	F	202	BCR	C1-C6	-3.06	1.49	1.53
13	A	837	CLA	C1D-ND	3.06	1.41	1.37
13	B	818	CLA	C4B-NB	3.06	1.41	1.37
16	L	202	BCR	C30-C25	-3.06	1.49	1.53
13	1	836	CLA	C1D-ND	3.06	1.41	1.37
13	b	818	CLA	C4B-NB	3.06	1.41	1.37
16	K	4004	BCR	C30-C25	-3.05	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	6	202	BCR	C1-C6	-3.05	1.49	1.53
13	a	816	CLA	C4B-NB	3.05	1.41	1.37
16	B	848	BCR	C30-C25	-3.04	1.49	1.53
13	A	826	CLA	C1D-ND	3.04	1.41	1.37
13	j	1103	CLA	C4B-NB	3.04	1.41	1.37
13	2	803	CLA	C1D-ND	3.04	1.41	1.37
13	a	836	CLA	C1D-ND	3.04	1.41	1.37
13	b	803	CLA	C1D-ND	3.04	1.41	1.37
13	B	817	CLA	C4B-NB	3.04	1.41	1.37
13	a	840	CLA	C1D-ND	3.04	1.41	1.37
13	a	833	CLA	C1D-ND	3.04	1.41	1.37
13	2	824	CLA	C1D-ND	3.04	1.41	1.37
13	J	1102	CLA	C4B-NB	3.03	1.41	1.37
13	9	4005	CLA	C4B-NB	3.03	1.41	1.37
13	A	833	CLA	C1D-ND	3.03	1.41	1.37
13	a	829	CLA	C1D-ND	3.03	1.41	1.37
13	1	837	CLA	C1D-ND	3.03	1.41	1.37
13	b	810	CLA	C1D-ND	3.02	1.41	1.37
13	8	1101	CLA	C4B-NB	3.02	1.41	1.37
13	0	203	CLA	C1D-ND	3.02	1.41	1.37
13	B	825	CLA	C1D-ND	3.02	1.41	1.37
13	2	817	CLA	C4B-NB	3.02	1.41	1.37
13	1	840	CLA	C1D-ND	3.02	1.41	1.37
13	A	841	CLA	C4B-NB	3.01	1.41	1.37
13	k	4005	CLA	C4B-NB	3.01	1.41	1.37
16	2	847	BCR	C30-C25	-3.01	1.49	1.53
13	J	1103	CLA	C4B-NB	3.01	1.41	1.37
13	2	828	CLA	C1D-ND	3.00	1.41	1.37
13	8	1102	CLA	C4B-NB	3.00	1.41	1.37
13	K	4005	CLA	C4B-NB	2.99	1.41	1.37
13	1	828	CLA	C1D-ND	2.99	1.41	1.37
13	j	1101	CLA	C4B-NB	2.99	1.41	1.37
13	1	826	CLA	C1D-ND	2.99	1.41	1.37
13	A	828	CLA	C1D-ND	2.99	1.41	1.37
13	2	829	CLA	C4B-NB	2.99	1.41	1.37
13	A	829	CLA	C1D-ND	2.98	1.41	1.37
13	b	829	CLA	C1D-ND	2.98	1.41	1.37
13	l	207	CLA	C1D-ND	2.98	1.41	1.37
13	J	1101	CLA	C4B-NB	2.98	1.41	1.37
13	B	809	CLA	C4B-NB	2.98	1.41	1.37
13	B	826	CLA	CMB-C2B	-2.98	1.44	1.50
16	j	1104	BCR	C1-C6	-2.97	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	J	1104	BCR	C1-C6	-2.97	1.50	1.53
13	B	829	CLA	C1D-ND	2.97	1.41	1.37
13	a	841	CLA	C4B-NB	2.97	1.41	1.37
13	2	808	CLA	C4B-NB	2.97	1.41	1.37
13	B	807	CLA	C1D-ND	2.97	1.41	1.37
13	b	830	CLA	C4B-NB	2.97	1.41	1.37
13	2	826	CLA	C4B-NB	2.97	1.41	1.37
13	B	832	CLA	C4B-NB	2.96	1.41	1.37
13	L	206	CLA	C1D-ND	2.96	1.41	1.37
13	1	812	CLA	C4B-NB	2.96	1.41	1.37
13	b	826	CLA	CMB-C2B	-2.96	1.44	1.50
13	B	830	CLA	C4B-NB	2.96	1.41	1.37
16	8	1104	BCR	C1-C6	-2.96	1.50	1.53
13	a	828	CLA	C1D-ND	2.96	1.41	1.37
13	B	833	CLA	C1D-ND	2.95	1.41	1.37
13	1	829	CLA	C1D-ND	2.95	1.41	1.37
13	6	204	CLA	C4B-NB	2.95	1.41	1.37
13	b	827	CLA	C4B-NB	2.95	1.41	1.37
13	2	825	CLA	CMB-C2B	-2.95	1.44	1.50
13	a	827	CLA	C1D-ND	2.95	1.41	1.37
13	B	827	CLA	C4B-NB	2.94	1.41	1.37
13	b	807	CLA	C1D-ND	2.94	1.41	1.37
13	F	204	CLA	C4B-NB	2.94	1.41	1.37
13	b	833	CLA	C1D-ND	2.94	1.41	1.37
13	8	1103	CLA	C4B-NB	2.94	1.41	1.37
13	2	831	CLA	C4B-NB	2.94	1.41	1.37
13	2	832	CLA	C1D-ND	2.94	1.41	1.37
13	1	825	CLA	C4B-NB	2.94	1.41	1.37
13	b	813	CLA	C4B-NB	2.94	1.41	1.37
13	0	208	CLA	C1D-ND	2.94	1.41	1.37
13	a	825	CLA	C4B-NB	2.93	1.41	1.37
13	A	840	CLA	C4B-NB	2.93	1.41	1.37
13	b	809	CLA	C4B-NB	2.93	1.41	1.37
13	1	822	CLA	C4B-NB	2.93	1.41	1.37
13	A	822	CLA	C4B-NB	2.93	1.41	1.37
13	f	203	CLA	C4B-NB	2.93	1.41	1.37
13	1	827	CLA	C1D-ND	2.93	1.41	1.37
13	A	827	CLA	C1D-ND	2.92	1.41	1.37
13	F	203	CLA	C4B-NB	2.92	1.41	1.37
13	1	840	CLA	C4B-NB	2.92	1.41	1.37
13	2	812	CLA	C4B-NB	2.92	1.41	1.37
13	b	832	CLA	C4B-NB	2.92	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	813	CLA	C4B-NB	2.92	1.41	1.37
13	b	814	CLA	C4B-NB	2.91	1.41	1.37
13	2	801	CLA	C1D-ND	2.91	1.41	1.37
13	A	812	CLA	C4B-NB	2.91	1.41	1.37
13	b	802	CLA	C1D-ND	2.91	1.41	1.37
13	a	822	CLA	C4B-NB	2.91	1.41	1.37
13	2	837	CLA	C4B-NB	2.90	1.41	1.37
13	a	812	CLA	C4B-NB	2.90	1.41	1.37
13	6	203	CLA	C4B-NB	2.90	1.41	1.37
13	b	821	CLA	C4B-NB	2.90	1.41	1.37
13	A	809	CLA	C4B-NB	2.90	1.41	1.37
13	A	825	CLA	C4B-NB	2.89	1.41	1.37
13	L	204	CLA	C4B-NB	2.89	1.41	1.37
13	f	201	CLA	C4B-NB	2.89	1.41	1.37
13	b	801	CLA	C1D-ND	2.89	1.41	1.37
13	B	801	CLA	C1D-ND	2.89	1.41	1.37
13	6	201	CLA	C4B-NB	2.89	1.41	1.37
13	2	820	CLA	C4B-NB	2.88	1.41	1.37
13	b	801	CLA	C1B-C2B	2.88	1.49	1.43
13	a	840	CLA	C4B-NB	2.88	1.41	1.37
13	K	4003	CLA	C4B-NB	2.88	1.41	1.37
13	l	205	CLA	C4B-NB	2.88	1.41	1.37
12	1	801	CL0	C1D-ND	2.88	1.41	1.37
13	F	201	CLA	C4B-NB	2.88	1.41	1.37
13	f	204	CLA	C4B-NB	2.88	1.41	1.37
13	9	4002	CLA	C4B-NB	2.88	1.41	1.37
13	b	837	CLA	C4B-NB	2.87	1.41	1.37
13	k	4003	CLA	C4B-NB	2.87	1.41	1.37
13	a	842	CLA	C4B-NB	2.87	1.41	1.37
13	a	805	CLA	C4B-NB	2.87	1.41	1.37
13	a	837	CLA	C4B-NB	2.87	1.41	1.37
13	b	811	CLA	C1D-ND	2.86	1.41	1.37
13	2	846	CLA	C4B-NB	2.86	1.41	1.37
13	L	206	CLA	C4B-NB	2.86	1.41	1.37
13	1	809	CLA	C4B-NB	2.86	1.41	1.37
16	j	1105	BCR	C30-C25	-2.85	1.50	1.53
13	0	203	CLA	C4B-NB	2.85	1.41	1.37
13	0	206	CLA	C4B-NB	2.85	1.41	1.37
13	B	802	CLA	C1D-ND	2.85	1.41	1.37
13	B	811	CLA	C1D-ND	2.85	1.41	1.37
13	B	838	CLA	C4B-NB	2.85	1.41	1.37
13	9	4003	CLA	C4B-NB	2.85	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	2	801	CLA	C1B-C2B	2.85	1.49	1.43
13	2	821	CLA	C4B-NB	2.85	1.41	1.37
13	A	842	CLA	C4B-NB	2.84	1.41	1.37
13	B	801	CLA	C1B-C2B	2.84	1.49	1.43
13	A	837	CLA	C4B-NB	2.84	1.41	1.37
12	A	801	CL0	C1D-ND	2.84	1.41	1.37
13	A	805	CLA	C4B-NB	2.84	1.41	1.37
13	B	821	CLA	C4B-NB	2.84	1.41	1.37
13	1	805	CLA	C4B-NB	2.84	1.41	1.37
13	A	814	CLA	C4B-NB	2.84	1.41	1.37
13	a	809	CLA	C4B-NB	2.84	1.41	1.37
13	0	208	CLA	C4B-NB	2.84	1.41	1.37
13	B	837	CLA	C4B-NB	2.84	1.41	1.37
13	K	4002	CLA	C4B-NB	2.83	1.41	1.37
13	2	813	CLA	C4B-NB	2.83	1.41	1.37
13	B	814	CLA	C4B-NB	2.83	1.41	1.37
13	2	822	CLA	C4B-NB	2.83	1.41	1.37
13	B	823	CLA	C4B-NB	2.83	1.41	1.37
13	b	838	CLA	C4B-NB	2.83	1.41	1.37
13	1	837	CLA	C4B-NB	2.83	1.41	1.37
13	A	810	CLA	C4B-NB	2.83	1.41	1.37
13	2	802	CLA	C1D-ND	2.83	1.41	1.37
13	a	814	CLA	C4B-NB	2.83	1.41	1.37
13	a	810	CLA	C4B-NB	2.82	1.41	1.37
13	2	828	CLA	C4B-NB	2.82	1.41	1.37
13	b	828	CLA	C4B-NB	2.82	1.41	1.37
13	1	810	CLA	C4B-NB	2.82	1.41	1.37
13	b	807	CLA	C4B-NB	2.82	1.41	1.37
13	a	827	CLA	C4B-NB	2.82	1.41	1.37
13	B	807	CLA	C4B-NB	2.82	1.41	1.37
16	J	1105	BCR	C30-C25	-2.81	1.50	1.53
13	b	823	CLA	C4B-NB	2.81	1.41	1.37
13	1	839	CLA	C4B-NB	2.81	1.41	1.37
13	1	842	CLA	C4B-NB	2.81	1.41	1.37
12	a	801	CL0	C1D-ND	2.81	1.41	1.37
13	1	803	CLA	C4B-NB	2.81	1.41	1.37
13	1	814	CLA	C4B-NB	2.81	1.41	1.37
13	2	810	CLA	C1D-ND	2.81	1.41	1.37
13	1	852	CLA	C4B-NB	2.81	1.41	1.37
13	b	829	CLA	C4B-NB	2.80	1.41	1.37
13	b	822	CLA	C4B-NB	2.80	1.41	1.37
13	k	4002	CLA	C4B-NB	2.80	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	828	CLA	C4B-NB	2.79	1.41	1.37
13	B	829	CLA	C4B-NB	2.79	1.41	1.37
13	b	804	CLA	C4B-NB	2.79	1.41	1.37
13	2	822	CLA	C1B-C2B	2.79	1.49	1.43
13	K	4002	CLA	C1B-C2B	2.79	1.49	1.43
13	j	1102	CLA	C1B-C2B	2.79	1.49	1.43
13	A	852	CLA	C4B-NB	2.79	1.41	1.37
13	B	816	CLA	C4B-NB	2.79	1.41	1.37
13	B	822	CLA	C4B-NB	2.79	1.41	1.37
13	B	847	CLA	C4B-NB	2.79	1.41	1.37
19	7	101	SQD	O47-C7	2.79	1.42	1.34
13	A	827	CLA	C4B-NB	2.79	1.41	1.37
16	8	1105	BCR	C30-C25	-2.79	1.50	1.53
13	B	831	CLA	C4B-NB	2.79	1.41	1.37
13	b	816	CLA	C4B-NB	2.79	1.41	1.37
13	a	834	CLA	C4B-NB	2.79	1.41	1.37
13	B	804	CLA	C4B-NB	2.78	1.41	1.37
13	l	207	CLA	C4B-NB	2.78	1.41	1.37
13	a	830	CLA	CMB-C2B	-2.78	1.45	1.50
13	B	803	CLA	C4B-NB	2.78	1.41	1.37
13	2	836	CLA	C4B-NB	2.78	1.41	1.37
13	k	4002	CLA	C1B-C2B	2.78	1.49	1.43
13	2	810	CLA	C4B-NB	2.78	1.41	1.37
13	b	823	CLA	C1B-C2B	2.78	1.49	1.43
13	2	818	CLA	C4B-NB	2.78	1.41	1.37
13	2	824	CLA	CMD-C2D	-2.78	1.45	1.50
19	i	101	SQD	O47-C7	2.78	1.42	1.34
13	B	808	CLA	C4B-NB	2.78	1.41	1.37
13	A	803	CLA	C4B-NB	2.78	1.41	1.37
13	A	817	CLA	C4B-NB	2.78	1.41	1.37
13	a	821	CLA	C4B-NB	2.78	1.41	1.37
13	b	831	CLA	C4B-NB	2.78	1.41	1.37
13	2	803	CLA	C4B-NB	2.78	1.41	1.37
13	1	802	CLA	C4B-NB	2.77	1.41	1.37
13	2	815	CLA	C4B-NB	2.77	1.41	1.37
13	B	819	CLA	C4B-NB	2.77	1.41	1.37
13	2	804	CLA	C4B-NB	2.77	1.41	1.37
19	I	103	SQD	O47-C7	2.77	1.42	1.34
13	8	1102	CLA	C1B-C2B	2.77	1.49	1.43
13	a	852	CLA	C4B-NB	2.77	1.41	1.37
13	A	821	CLA	C4B-NB	2.77	1.41	1.37
13	1	835	CLA	C4B-NB	2.77	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	834	CLA	C4B-NB	2.77	1.41	1.37
13	2	827	CLA	C4B-NB	2.77	1.41	1.37
13	J	1102	CLA	C1B-C2B	2.77	1.49	1.43
16	f	202	BCR	C30-C25	-2.77	1.50	1.53
13	a	813	CLA	C4B-NB	2.77	1.41	1.37
13	1	817	CLA	C4B-NB	2.77	1.41	1.37
13	A	813	CLA	C4B-NB	2.77	1.41	1.37
13	b	820	CLA	C4B-NB	2.76	1.41	1.37
16	6	202	BCR	C30-C25	-2.76	1.50	1.53
13	9	4002	CLA	C1B-C2B	2.76	1.49	1.43
13	a	803	CLA	C4B-NB	2.76	1.41	1.37
13	a	818	CLA	C4B-NB	2.76	1.41	1.37
13	b	819	CLA	C4B-NB	2.76	1.41	1.37
16	7	103	BCR	C30-C25	-2.76	1.50	1.53
13	b	803	CLA	C4B-NB	2.76	1.41	1.37
13	b	808	CLA	C4B-NB	2.76	1.41	1.37
13	2	807	CLA	C4B-NB	2.76	1.41	1.37
13	b	811	CLA	C4B-NB	2.76	1.41	1.37
13	2	830	CLA	C4B-NB	2.76	1.41	1.37
13	A	818	CLA	C4B-NB	2.76	1.41	1.37
16	2	843	BCR	C30-C25	-2.76	1.50	1.53
13	a	817	CLA	C4B-NB	2.76	1.41	1.37
13	a	809	CLA	C1B-C2B	2.76	1.49	1.43
13	1	834	CLA	C4B-NB	2.76	1.41	1.37
13	B	823	CLA	C1B-C2B	2.75	1.49	1.43
13	2	802	CLA	CMC-C2C	-2.75	1.45	1.50
13	A	839	CLA	C4B-NB	2.75	1.41	1.37
13	1	827	CLA	C4B-NB	2.75	1.41	1.37
16	B	844	BCR	C30-C25	-2.75	1.50	1.53
13	A	830	CLA	CMB-C2B	-2.75	1.45	1.50
13	B	811	CLA	C4B-NB	2.75	1.41	1.37
13	B	825	CLA	CMD-C2D	-2.75	1.45	1.50
13	1	830	CLA	CMB-C2B	-2.75	1.45	1.50
13	2	837	CLA	C1B-C2B	2.75	1.49	1.43
16	F	202	BCR	C30-C25	-2.75	1.50	1.53
13	2	817	CLA	C1B-C2B	2.75	1.49	1.43
13	a	831	CLA	C4B-NB	2.75	1.41	1.37
16	b	844	BCR	C30-C25	-2.74	1.50	1.53
13	b	835	CLA	C4B-NB	2.74	1.41	1.37
16	I	102	BCR	C30-C25	-2.74	1.50	1.53
13	b	825	CLA	CMD-C2D	-2.74	1.45	1.50
13	B	802	CLA	CMC-C2C	-2.74	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	835	CLA	C4B-NB	2.74	1.41	1.37
13	B	820	CLA	C4B-NB	2.74	1.41	1.37
13	a	839	CLA	C4B-NB	2.74	1.41	1.37
13	A	802	CLA	C4B-NB	2.74	1.41	1.37
13	2	818	CLA	C1B-C2B	2.73	1.49	1.43
13	b	802	CLA	CMC-C2C	-2.73	1.45	1.50
13	B	818	CLA	C1B-C2B	2.73	1.49	1.43
13	1	821	CLA	C1B-C2B	2.73	1.49	1.43
13	A	824	CLA	C4B-NB	2.73	1.41	1.37
13	b	847	CLA	C4B-NB	2.73	1.41	1.37
13	B	819	CLA	C1B-C2B	2.73	1.49	1.43
13	b	836	CLA	C4B-NB	2.73	1.41	1.37
13	a	835	CLA	C4B-NB	2.73	1.41	1.37
13	1	809	CLA	C1B-C2B	2.73	1.49	1.43
13	B	835	CLA	C4B-NB	2.72	1.41	1.37
13	A	831	CLA	C4B-NB	2.72	1.41	1.37
13	A	806	CLA	C4B-NB	2.72	1.41	1.37
13	b	818	CLA	C1B-C2B	2.72	1.49	1.43
13	f	201	CLA	C1B-C2B	2.72	1.49	1.43
13	A	809	CLA	C1B-C2B	2.72	1.49	1.43
16	i	103	BCR	C30-C25	-2.72	1.50	1.53
13	1	821	CLA	C4B-NB	2.72	1.41	1.37
13	2	816	CLA	C1B-C2B	2.72	1.49	1.43
13	2	811	CLA	C1B-C2B	2.71	1.49	1.43
13	B	817	CLA	C1B-C2B	2.71	1.49	1.43
13	A	807	CLA	C4B-NB	2.71	1.41	1.37
13	1	806	CLA	C4B-NB	2.71	1.41	1.37
13	2	825	CLA	C4B-NB	2.71	1.41	1.37
13	B	838	CLA	C1B-C2B	2.71	1.49	1.43
13	2	830	CLA	C1B-C2B	2.71	1.49	1.43
13	a	824	CLA	C4B-NB	2.71	1.41	1.37
13	1	818	CLA	C4B-NB	2.71	1.41	1.37
13	B	812	CLA	C1B-C2B	2.71	1.49	1.43
16	i	103	BCR	C1-C6	-2.71	1.50	1.53
13	K	4005	CLA	C1B-C2B	2.71	1.49	1.43
13	F	201	CLA	C1B-C2B	2.71	1.49	1.43
13	B	831	CLA	C1B-C2B	2.71	1.49	1.43
13	a	808	CLA	C4B-NB	2.71	1.41	1.37
13	b	806	CLA	C4B-NB	2.71	1.41	1.37
13	1	813	CLA	C4B-NB	2.71	1.41	1.37
13	b	826	CLA	C4B-NB	2.71	1.41	1.37
13	A	821	CLA	C1B-C2B	2.71	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	806	CLA	C1B-C2B	2.70	1.49	1.43
13	2	815	CLA	C1B-C2B	2.70	1.49	1.43
13	2	819	CLA	C4B-NB	2.70	1.41	1.37
13	k	4005	CLA	C1B-C2B	2.70	1.49	1.43
13	B	826	CLA	C4B-NB	2.70	1.41	1.37
13	b	834	CLA	C4B-NB	2.70	1.41	1.37
13	f	203	CLA	C1B-C2B	2.70	1.49	1.43
13	a	804	CLA	C4B-NB	2.70	1.41	1.37
13	B	816	CLA	C1B-C2B	2.70	1.49	1.43
13	a	821	CLA	C1B-C2B	2.70	1.49	1.43
13	a	806	CLA	C4B-NB	2.70	1.41	1.37
13	2	811	CLA	C4B-NB	2.70	1.41	1.37
13	b	819	CLA	C1B-C2B	2.70	1.49	1.43
13	a	842	CLA	C1B-C2B	2.70	1.49	1.43
13	b	838	CLA	C1B-C2B	2.70	1.49	1.43
13	b	817	CLA	C1B-C2B	2.70	1.49	1.43
13	a	826	CLA	C4B-NB	2.70	1.41	1.37
13	1	830	CLA	C4B-NB	2.70	1.41	1.37
13	A	842	CLA	C1B-C2B	2.69	1.49	1.43
16	l	203	BCR	C1-C6	-2.69	1.50	1.53
13	A	804	CLA	C4B-NB	2.69	1.41	1.37
13	1	807	CLA	C4B-NB	2.69	1.41	1.37
13	2	806	CLA	C1B-C2B	2.69	1.49	1.43
13	b	812	CLA	C1B-C2B	2.69	1.49	1.43
13	9	4005	CLA	C1B-C2B	2.69	1.49	1.43
13	B	806	CLA	C4B-NB	2.69	1.41	1.37
13	2	821	CLA	C1B-C2B	2.69	1.49	1.43
13	1	808	CLA	C4B-NB	2.69	1.41	1.37
13	J	1101	CLA	C1B-C2B	2.69	1.49	1.43
13	1	831	CLA	C4B-NB	2.69	1.41	1.37
13	b	816	CLA	C1B-C2B	2.69	1.49	1.43
13	a	802	CLA	C4B-NB	2.69	1.41	1.37
13	F	204	CLA	C1B-C2B	2.69	1.49	1.43
13	b	831	CLA	C1B-C2B	2.69	1.49	1.43
13	1	842	CLA	C1B-C2B	2.69	1.49	1.43
16	a	847	BCR	C30-C25	-2.68	1.50	1.53
13	6	203	CLA	C1B-C2B	2.68	1.49	1.43
16	A	847	BCR	C30-C25	-2.68	1.50	1.53
16	1	847	BCR	C30-C25	-2.68	1.50	1.53
13	2	834	CLA	C4B-NB	2.68	1.41	1.37
13	1	826	CLA	C4B-NB	2.68	1.41	1.37
13	6	204	CLA	C1B-C2B	2.68	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	807	CLA	C4B-NB	2.68	1.41	1.37
13	1	824	CLA	C4B-NB	2.68	1.41	1.37
13	f	204	CLA	C1B-C2B	2.68	1.49	1.43
13	F	203	CLA	C1B-C2B	2.68	1.49	1.43
13	J	1103	CLA	C1B-C2B	2.68	1.49	1.43
13	b	822	CLA	C1B-C2B	2.68	1.49	1.43
13	A	830	CLA	C4B-NB	2.68	1.41	1.37
13	A	808	CLA	C4B-NB	2.68	1.41	1.37
13	2	835	CLA	C4B-NB	2.68	1.41	1.37
13	B	809	CLA	C1B-C2B	2.68	1.49	1.43
13	b	837	CLA	C1B-C2B	2.68	1.49	1.43
13	L	206	CLA	C1B-C2B	2.68	1.49	1.43
13	j	1103	CLA	C1B-C2B	2.68	1.49	1.43
16	2	840	BCR	C30-C25	-2.68	1.50	1.53
16	I	102	BCR	C1-C6	-2.67	1.50	1.53
16	7	103	BCR	C1-C6	-2.67	1.50	1.53
13	a	810	CLA	C1B-C2B	2.67	1.49	1.43
13	j	1101	CLA	C1B-C2B	2.67	1.49	1.43
13	1	810	CLA	C1B-C2B	2.67	1.49	1.43
13	8	1101	CLA	C1B-C2B	2.67	1.49	1.43
13	b	825	CLA	C4B-NB	2.67	1.41	1.37
13	1	806	CLA	C1B-C2B	2.67	1.49	1.43
13	2	808	CLA	C1B-C2B	2.67	1.49	1.43
13	A	810	CLA	C1B-C2B	2.67	1.49	1.43
13	A	826	CLA	C4B-NB	2.67	1.41	1.37
13	2	824	CLA	C4B-NB	2.67	1.41	1.37
13	K	4003	CLA	C1B-C2B	2.67	1.49	1.43
13	l	207	CLA	C1B-C2B	2.67	1.49	1.43
13	k	4003	CLA	C1B-C2B	2.67	1.49	1.43
13	B	834	CLA	C4B-NB	2.67	1.41	1.37
13	b	809	CLA	C1B-C2B	2.67	1.49	1.43
13	0	208	CLA	C1B-C2B	2.67	1.49	1.43
13	6	201	CLA	C1B-C2B	2.67	1.49	1.43
13	B	836	CLA	C4B-NB	2.66	1.41	1.37
13	2	806	CLA	C4B-NB	2.66	1.41	1.37
13	0	202	CLA	C4B-NB	2.66	1.41	1.37
13	b	824	CLA	C1B-C2B	2.66	1.49	1.43
13	9	4003	CLA	C1B-C2B	2.66	1.49	1.43
13	B	806	CLA	C1B-C2B	2.66	1.49	1.43
13	B	822	CLA	C1B-C2B	2.66	1.49	1.43
13	a	832	CLA	C4B-NB	2.66	1.41	1.37
13	B	825	CLA	C4B-NB	2.66	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	8	1103	CLA	C1B-C2B	2.66	1.49	1.43
16	L	202	BCR	C1-C6	-2.66	1.50	1.53
13	1	804	CLA	C4B-NB	2.66	1.41	1.37
13	A	806	CLA	C1B-C2B	2.66	1.49	1.43
13	A	823	CLA	C4B-NB	2.66	1.41	1.37
13	A	811	CLA	C4B-NB	2.66	1.41	1.37
13	a	830	CLA	C4B-NB	2.66	1.41	1.37
13	l	202	CLA	C4B-NB	2.66	1.41	1.37
16	l	206	BCR	C30-C25	-2.66	1.50	1.53
13	1	824	CLA	C1B-C2B	2.65	1.49	1.43
13	A	824	CLA	C1B-C2B	2.65	1.49	1.43
13	a	823	CLA	C4B-NB	2.65	1.41	1.37
13	A	823	CLA	C1B-C2B	2.65	1.49	1.43
13	2	828	CLA	C1B-C2B	2.65	1.49	1.43
16	0	204	BCR	C1-C6	-2.65	1.50	1.53
13	A	819	CLA	C1B-C2B	2.65	1.49	1.43
13	L	201	CLA	C4B-NB	2.65	1.41	1.37
13	1	829	CLA	C4B-NB	2.65	1.41	1.37
13	a	811	CLA	C4B-NB	2.64	1.41	1.37
13	A	815	CLA	C1B-C2B	2.64	1.49	1.43
13	B	805	CLA	C1B-C2B	2.64	1.49	1.43
13	a	824	CLA	C1B-C2B	2.64	1.49	1.43
13	1	823	CLA	C1B-C2B	2.64	1.49	1.43
13	a	823	CLA	C1B-C2B	2.64	1.49	1.43
13	B	837	CLA	C1B-C2B	2.64	1.49	1.43
13	a	819	CLA	C1B-C2B	2.64	1.49	1.43
13	2	805	CLA	C1B-C2B	2.64	1.49	1.43
13	a	806	CLA	C1B-C2B	2.64	1.49	1.43
13	L	203	CLA	C1B-C2B	2.64	1.49	1.43
13	A	829	CLA	C4B-NB	2.63	1.41	1.37
13	2	833	CLA	C4B-NB	2.63	1.41	1.37
13	B	829	CLA	C1B-C2B	2.63	1.49	1.43
13	1	813	CLA	C1B-C2B	2.63	1.49	1.43
13	1	823	CLA	C4B-NB	2.63	1.41	1.37
13	l	204	CLA	C1B-C2B	2.63	1.49	1.43
16	L	205	BCR	C30-C25	-2.63	1.50	1.53
13	A	811	CLA	C1B-C2B	2.63	1.49	1.43
13	1	815	CLA	C1B-C2B	2.63	1.49	1.43
13	0	205	CLA	C1B-C2B	2.63	1.49	1.43
13	1	826	CLA	C1B-C2B	2.63	1.49	1.43
13	A	832	CLA	C4B-NB	2.63	1.41	1.37
13	A	826	CLA	C1B-C2B	2.63	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	807	CLA	C1B-C2B	2.63	1.49	1.43
13	1	819	CLA	C1B-C2B	2.63	1.49	1.43
13	B	824	CLA	C1B-C2B	2.63	1.49	1.43
13	B	812	CLA	C4B-NB	2.63	1.41	1.37
13	1	802	CLA	MG-NB	-2.63	2.00	2.05
13	1	811	CLA	C4B-NB	2.62	1.41	1.37
13	2	836	CLA	C1B-C2B	2.62	1.49	1.43
13	1	832	CLA	C4B-NB	2.62	1.41	1.37
16	a	848	BCR	C1-C6	-2.62	1.50	1.53
13	2	814	CLA	C4B-NB	2.62	1.41	1.37
13	L	204	CLA	C1B-C2B	2.62	1.49	1.43
13	a	826	CLA	C1B-C2B	2.62	1.49	1.43
13	a	802	CLA	CMB-C2B	-2.62	1.45	1.50
13	a	829	CLA	C1B-C2B	2.62	1.49	1.43
13	A	838	CLA	C4B-NB	2.62	1.41	1.37
13	1	833	CLA	C1B-C2B	2.61	1.49	1.43
13	b	805	CLA	C1B-C2B	2.61	1.49	1.43
13	1	829	CLA	C1B-C2B	2.61	1.49	1.43
13	2	823	CLA	C1B-C2B	2.61	1.49	1.43
13	2	809	CLA	C4B-NB	2.61	1.41	1.37
13	a	814	CLA	C1B-C2B	2.61	1.49	1.43
13	1	809	CLA	CMD-C2D	-2.61	1.45	1.50
13	2	829	CLA	C1B-C2B	2.61	1.49	1.43
13	a	815	CLA	C1B-C2B	2.61	1.49	1.43
13	1	811	CLA	C1B-C2B	2.61	1.49	1.43
13	a	829	CLA	C4B-NB	2.61	1.41	1.37
13	l	204	CLA	C4B-NB	2.61	1.41	1.37
13	b	835	CLA	C1B-C2B	2.61	1.49	1.43
13	A	802	CLA	MG-NB	-2.61	2.00	2.05
13	B	810	CLA	C1B-C2B	2.61	1.49	1.43
13	A	809	CLA	CMD-C2D	-2.61	1.45	1.50
13	A	814	CLA	C1B-C2B	2.60	1.49	1.43
13	1	805	CLA	C1B-C2B	2.60	1.49	1.43
13	A	813	CLA	C1B-C2B	2.60	1.49	1.43
13	B	835	CLA	C1B-C2B	2.60	1.49	1.43
13	b	829	CLA	C1B-C2B	2.60	1.49	1.43
13	l	205	CLA	C1B-C2B	2.60	1.49	1.43
13	a	811	CLA	C1B-C2B	2.60	1.49	1.43
13	a	828	CLA	C4B-NB	2.60	1.41	1.37
13	0	203	CLA	C1B-C2B	2.60	1.49	1.43
13	L	203	CLA	C4B-NB	2.60	1.41	1.37
13	a	838	CLA	C4B-NB	2.60	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	829	CLA	C1B-C2B	2.60	1.49	1.43
13	a	833	CLA	C1B-C2B	2.60	1.49	1.43
13	a	820	CLA	C1B-C2B	2.60	1.49	1.43
16	A	848	BCR	C1-C6	-2.60	1.50	1.53
13	B	815	CLA	C1B-C2B	2.60	1.49	1.43
13	b	815	CLA	C1B-C2B	2.60	1.49	1.43
16	0	207	BCR	C30-C25	-2.60	1.50	1.53
13	1	814	CLA	C1B-C2B	2.60	1.49	1.43
13	B	807	CLA	C1B-C2B	2.59	1.49	1.43
16	B	841	BCR	C30-C25	-2.59	1.50	1.53
13	1	802	CLA	CMB-C2B	-2.59	1.45	1.50
13	2	825	CLA	CMD-C2D	-2.59	1.45	1.50
13	1	838	CLA	C4B-NB	2.59	1.41	1.37
13	0	206	CLA	C1B-C2B	2.59	1.49	1.43
13	b	810	CLA	C4B-NB	2.59	1.41	1.37
13	1	827	CLA	C1B-C2B	2.59	1.49	1.43
13	1	828	CLA	C4B-NB	2.59	1.41	1.37
13	a	813	CLA	C1B-C2B	2.59	1.49	1.43
13	B	830	CLA	C1B-C2B	2.59	1.49	1.43
13	a	832	CLA	C1B-C2B	2.59	1.49	1.43
13	B	820	CLA	C1B-C2B	2.59	1.49	1.43
13	A	820	CLA	C1B-C2B	2.59	1.49	1.43
13	k	4002	CLA	CMD-C2D	-2.59	1.45	1.50
13	B	815	CLA	C4B-NB	2.59	1.41	1.37
13	0	205	CLA	C4B-NB	2.59	1.41	1.37
16	b	841	BCR	C30-C25	-2.58	1.50	1.53
13	K	4002	CLA	CMD-C2D	-2.58	1.45	1.50
13	A	807	CLA	C1B-C2B	2.58	1.49	1.43
13	A	833	CLA	C1B-C2B	2.58	1.49	1.43
13	b	812	CLA	C4B-NB	2.58	1.41	1.37
13	2	809	CLA	C1B-C2B	2.58	1.49	1.43
13	2	834	CLA	C1B-C2B	2.58	1.49	1.43
13	A	802	CLA	CMB-C2B	-2.58	1.45	1.50
13	a	827	CLA	C1B-C2B	2.58	1.49	1.43
13	a	809	CLA	CMD-C2D	-2.58	1.45	1.50
13	A	805	CLA	C1B-C2B	2.58	1.49	1.43
13	2	814	CLA	C1B-C2B	2.58	1.49	1.43
13	b	820	CLA	C1B-C2B	2.58	1.49	1.43
13	a	816	CLA	C1B-C2B	2.58	1.49	1.43
13	b	830	CLA	C1B-C2B	2.58	1.49	1.43
13	a	807	CLA	C1B-C2B	2.57	1.49	1.43
13	2	807	CLA	C1B-C2B	2.57	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	808	CLA	C1B-C2B	2.57	1.49	1.43
13	2	819	CLA	C1B-C2B	2.57	1.49	1.43
13	a	802	CLA	MG-NB	-2.57	2.00	2.05
13	a	812	CLA	C1B-C2B	2.57	1.49	1.43
13	B	802	CLA	C1B-C2B	2.57	1.49	1.43
13	b	810	CLA	C1B-C2B	2.57	1.49	1.43
13	B	810	CLA	C4B-NB	2.57	1.41	1.37
13	b	803	CLA	C1B-C2B	2.57	1.49	1.43
13	2	802	CLA	C1B-C2B	2.57	1.49	1.43
13	A	827	CLA	C1B-C2B	2.57	1.49	1.43
13	B	803	CLA	C1B-C2B	2.57	1.49	1.43
13	2	803	CLA	C1B-C2B	2.57	1.49	1.43
13	b	826	CLA	CMD-C2D	-2.57	1.45	1.50
13	b	802	CLA	C1B-C2B	2.57	1.49	1.43
13	B	826	CLA	CMD-C2D	-2.57	1.45	1.50
13	B	804	CLA	C1B-C2B	2.56	1.49	1.43
13	2	833	CLA	C1B-C2B	2.56	1.49	1.43
13	B	808	CLA	C1B-C2B	2.56	1.49	1.43
13	A	828	CLA	C4B-NB	2.56	1.41	1.37
13	B	834	CLA	C1B-C2B	2.56	1.49	1.43
13	1	832	CLA	C1B-C2B	2.56	1.49	1.43
13	A	816	CLA	C1B-C2B	2.56	1.49	1.43
13	i	102	CLA	C1B-C2B	2.56	1.49	1.43
16	j	1104	BCR	C30-C25	-2.56	1.50	1.53
13	A	832	CLA	C1B-C2B	2.56	1.49	1.43
13	1	822	CLA	C1B-C2B	2.56	1.49	1.43
13	b	833	CLA	C4B-NB	2.56	1.41	1.37
13	b	804	CLA	C1B-C2B	2.56	1.49	1.43
13	a	805	CLA	C1B-C2B	2.56	1.49	1.43
13	2	832	CLA	C4B-NB	2.56	1.41	1.37
13	2	812	CLA	C1B-C2B	2.55	1.49	1.43
13	1	812	CLA	C1B-C2B	2.55	1.49	1.43
13	1	820	CLA	C1B-C2B	2.55	1.49	1.43
13	1	807	CLA	C1B-C2B	2.55	1.49	1.43
13	A	812	CLA	C1B-C2B	2.55	1.49	1.43
13	I	101	CLA	C1B-C2B	2.55	1.49	1.43
13	9	4002	CLA	CMD-C2D	-2.55	1.45	1.50
13	B	813	CLA	C1B-C2B	2.55	1.49	1.43
16	1	848	BCR	C1-C6	-2.55	1.50	1.53
13	1	816	CLA	C1B-C2B	2.55	1.49	1.43
13	a	817	CLA	C1B-C2B	2.54	1.49	1.43
13	1	817	CLA	C1B-C2B	2.54	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	834	CLA	C1B-C2B	2.54	1.49	1.43
13	I	101	CLA	C4B-NB	2.54	1.41	1.37
13	a	815	CLA	C4B-NB	2.54	1.41	1.37
13	b	815	CLA	C4B-NB	2.54	1.41	1.37
13	A	817	CLA	C1B-C2B	2.54	1.49	1.43
13	b	814	CLA	CMB-C2B	-2.54	1.45	1.50
13	i	102	CLA	C4B-NB	2.54	1.41	1.37
13	2	804	CLA	C1B-C2B	2.54	1.49	1.43
13	b	813	CLA	C1B-C2B	2.54	1.49	1.43
13	A	822	CLA	C1B-C2B	2.54	1.49	1.43
13	B	833	CLA	C4B-NB	2.53	1.41	1.37
13	1	834	CLA	C1B-C2B	2.53	1.49	1.43
13	2	827	CLA	C1B-C2B	2.53	1.49	1.43
16	9	4001	BCR	C30-C25	-2.53	1.50	1.53
13	7	102	CLA	C4B-NB	2.53	1.41	1.37
13	A	834	CLA	C1B-C2B	2.53	1.49	1.43
13	7	102	CLA	C1B-C2B	2.53	1.49	1.43
13	a	838	CLA	C1B-C2B	2.53	1.49	1.43
13	2	846	CLA	CMB-C2B	-2.53	1.45	1.50
13	A	838	CLA	C1B-C2B	2.53	1.49	1.43
13	a	834	CLA	C1B-C2B	2.52	1.49	1.43
13	1	836	CLA	C4B-NB	2.52	1.41	1.37
13	A	841	CLA	C1B-C2B	2.52	1.49	1.43
13	1	838	CLA	C1B-C2B	2.52	1.49	1.43
13	b	826	CLA	MG-NB	-2.52	2.00	2.05
13	b	824	CLA	MG-NB	-2.52	2.00	2.05
16	K	4001	BCR	C30-C25	-2.52	1.50	1.53
13	B	828	CLA	C1B-C2B	2.52	1.49	1.43
13	A	835	CLA	C1B-C2B	2.52	1.49	1.43
13	2	823	CLA	MG-NB	-2.52	2.00	2.05
13	1	836	CLA	C1B-C2B	2.52	1.49	1.43
13	A	840	CLA	C1B-C2B	2.51	1.49	1.43
13	1	841	CLA	C1B-C2B	2.51	1.49	1.43
13	a	822	CLA	C1B-C2B	2.51	1.49	1.43
13	a	841	CLA	C1B-C2B	2.51	1.49	1.43
13	B	847	CLA	CMB-C2B	-2.51	1.45	1.50
16	b	842	BCR	C1-C6	-2.51	1.50	1.53
13	A	815	CLA	C4B-NB	2.51	1.41	1.37
13	a	840	CLA	C1B-C2B	2.51	1.49	1.43
13	1	828	CLA	C1B-C2B	2.51	1.49	1.43
13	A	828	CLA	C1B-C2B	2.51	1.49	1.43
13	a	825	CLA	C1B-C2B	2.51	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	814	CLA	CMB-C2B	-2.51	1.45	1.50
13	b	847	CLA	CMB-C2B	-2.51	1.45	1.50
13	1	815	CLA	C4B-NB	2.51	1.41	1.37
16	1	848	BCR	C30-C25	-2.50	1.50	1.53
13	A	836	CLA	C1B-C2B	2.50	1.49	1.43
13	A	836	CLA	C4B-NB	2.50	1.41	1.37
13	A	833	CLA	C4B-NB	2.50	1.41	1.37
13	A	825	CLA	C1B-C2B	2.50	1.49	1.43
13	1	840	CLA	C1B-C2B	2.50	1.49	1.43
13	1	836	CLA	CMD-C2D	-2.50	1.45	1.50
13	1	808	CLA	CHC-C1C	2.50	1.43	1.38
13	2	825	CLA	MG-NB	-2.50	2.00	2.05
16	B	842	BCR	C1-C6	-2.50	1.50	1.53
13	a	804	CLA	C1B-C2B	2.49	1.49	1.43
13	2	801	CLA	CMD-C2D	-2.49	1.45	1.50
16	k	4001	BCR	C30-C25	-2.49	1.50	1.53
13	b	832	CLA	C1B-C2B	2.49	1.49	1.43
13	B	801	CLA	CMD-C2D	-2.49	1.45	1.50
13	a	835	CLA	C1B-C2B	2.49	1.49	1.43
13	1	835	CLA	C1B-C2B	2.49	1.49	1.43
18	2	845	LMG	C4-C5	2.49	1.58	1.53
13	2	831	CLA	C1B-C2B	2.49	1.49	1.43
13	b	828	CLA	C1B-C2B	2.49	1.49	1.43
12	a	801	CL0	CMD-C2D	-2.49	1.45	1.50
13	2	823	CLA	CMC-C2C	-2.49	1.45	1.50
13	b	801	CLA	CMD-C2D	-2.49	1.45	1.50
13	B	824	CLA	MG-NB	-2.49	2.00	2.05
13	B	826	CLA	MG-NB	-2.49	2.00	2.05
16	8	1104	BCR	C30-C25	-2.49	1.50	1.53
13	1	823	CLA	CMD-C2D	-2.49	1.45	1.50
13	2	813	CLA	CMB-C2B	-2.49	1.45	1.50
16	A	848	BCR	C30-C25	-2.48	1.50	1.53
16	a	848	BCR	C30-C25	-2.48	1.50	1.53
13	1	833	CLA	C4B-NB	2.48	1.41	1.37
13	A	818	CLA	C1B-C2B	2.48	1.49	1.43
16	z	101	BCR	C30-C25	-2.48	1.50	1.53
16	J	1104	BCR	C30-C25	-2.48	1.50	1.53
18	B	846	LMG	C4-C5	2.48	1.58	1.53
18	b	846	LMG	C4-C5	2.48	1.58	1.53
13	B	827	CLA	C1B-C2B	2.48	1.48	1.43
13	a	823	CLA	CMD-C2D	-2.48	1.45	1.50
13	1	818	CLA	C1B-C2B	2.48	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	828	CLA	C1B-C2B	2.48	1.48	1.43
16	2	841	BCR	C1-C6	-2.48	1.50	1.53
16	f	205	BCR	C30-C25	-2.48	1.50	1.53
13	B	832	CLA	C1B-C2B	2.48	1.48	1.43
12	a	801	CL0	C3B-C4B	2.48	1.49	1.42
13	a	836	CLA	C1B-C2B	2.47	1.48	1.43
13	B	811	CLA	C1B-C2B	2.47	1.48	1.43
13	A	808	CLA	C1B-C2B	2.47	1.48	1.43
12	A	801	CL0	C3B-C4B	2.47	1.49	1.42
13	A	804	CLA	C1B-C2B	2.47	1.48	1.43
12	1	801	CL0	CMD-C2D	-2.47	1.45	1.50
13	b	806	CLA	MG-NB	-2.47	2.00	2.05
12	A	801	CL0	CMD-C2D	-2.47	1.45	1.50
13	A	831	CLA	CMD-C2D	-2.47	1.45	1.50
13	b	827	CLA	C1B-C2B	2.47	1.48	1.43
13	B	836	CLA	C1B-C2B	2.47	1.48	1.43
13	a	818	CLA	C1B-C2B	2.47	1.48	1.43
13	a	831	CLA	CMD-C2D	-2.46	1.45	1.50
13	a	808	CLA	C1B-C2B	2.46	1.48	1.43
13	a	808	CLA	CHC-C1C	2.46	1.43	1.38
13	1	831	CLA	CMD-C2D	-2.46	1.45	1.50
13	1	804	CLA	C1B-C2B	2.46	1.48	1.43
13	2	824	CLA	C1B-C2B	2.46	1.48	1.43
13	2	810	CLA	C1B-C2B	2.45	1.48	1.43
13	b	811	CLA	C1B-C2B	2.45	1.48	1.43
13	A	836	CLA	CMD-C2D	-2.45	1.45	1.50
13	1	834	CLA	CMB-C2B	-2.45	1.45	1.50
13	2	826	CLA	C1B-C2B	2.45	1.48	1.43
13	2	835	CLA	C1B-C2B	2.45	1.48	1.43
16	6	205	BCR	C30-C25	-2.45	1.50	1.53
13	1	825	CLA	C1B-C2B	2.45	1.48	1.43
13	A	808	CLA	CHC-C1C	2.45	1.43	1.38
13	A	828	CLA	CHC-C1C	2.45	1.43	1.38
13	1	828	CLA	CHC-C1C	2.45	1.43	1.38
13	a	833	CLA	C4B-NB	2.45	1.41	1.37
13	a	828	CLA	CHC-C1C	2.45	1.43	1.38
13	a	836	CLA	C4B-NB	2.45	1.41	1.37
13	b	836	CLA	C1B-C2B	2.45	1.48	1.43
13	0	205	CLA	MG-NB	-2.45	2.00	2.05
13	A	834	CLA	CMB-C2B	-2.45	1.45	1.50
13	B	824	CLA	CMC-C2C	-2.45	1.45	1.50
12	1	801	CL0	C3B-C4B	2.45	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	837	CLA	C1B-C2B	2.44	1.48	1.43
16	F	205	BCR	C30-C25	-2.44	1.50	1.53
13	A	841	CLA	CMB-C2B	-2.44	1.45	1.50
13	1	808	CLA	C1B-C2B	2.44	1.48	1.43
13	L	203	CLA	MG-NB	-2.44	2.00	2.05
13	A	823	CLA	CMD-C2D	-2.44	1.45	1.50
13	a	834	CLA	CMB-C2B	-2.44	1.45	1.50
13	B	806	CLA	MG-NB	-2.44	2.01	2.05
13	1	841	CLA	CMB-C2B	-2.44	1.45	1.50
13	2	802	CLA	C4B-NB	2.44	1.41	1.37
13	1	833	CLA	MG-NB	-2.44	2.01	2.05
13	a	829	CLA	MG-NB	-2.43	2.01	2.05
13	l	202	CLA	C1B-C2B	2.43	1.48	1.43
13	b	825	CLA	C1B-C2B	2.43	1.48	1.43
13	A	837	CLA	C1B-C2B	2.43	1.48	1.43
13	a	819	CLA	MG-NB	-2.43	2.01	2.05
13	b	820	CLA	CMD-C2D	-2.43	1.45	1.50
13	L	201	CLA	C1B-C2B	2.43	1.48	1.43
13	b	824	CLA	CMC-C2C	-2.43	1.45	1.50
13	l	204	CLA	MG-NB	-2.43	2.01	2.05
13	A	836	CLA	MG-NB	-2.43	2.01	2.05
13	1	837	CLA	C1B-C2B	2.43	1.48	1.43
13	B	820	CLA	CMD-C2D	-2.43	1.45	1.50
13	a	817	CLA	C3B-C4B	2.42	1.49	1.42
13	B	825	CLA	C1B-C2B	2.42	1.48	1.43
12	A	801	CL0	C1B-C2B	2.42	1.48	1.43
13	B	802	CLA	C4B-NB	2.42	1.41	1.37
13	1	836	CLA	MG-NB	-2.42	2.01	2.05
16	M	101	BCR	C30-C25	-2.42	1.50	1.53
13	A	829	CLA	MG-NB	-2.42	2.01	2.05
13	2	819	CLA	CMD-C2D	-2.42	1.45	1.50
13	2	806	CLA	MG-NB	-2.42	2.01	2.05
13	0	202	CLA	C1B-C2B	2.42	1.48	1.43
13	B	811	CLA	CHC-C1C	2.42	1.43	1.38
13	b	811	CLA	CHC-C1C	2.42	1.43	1.38
13	b	801	CLA	MG-NB	-2.42	2.01	2.05
18	b	846	LMG	C7-C8	2.42	1.58	1.50
18	2	845	LMG	C7-C8	2.42	1.58	1.50
13	2	819	CLA	CMC-C2C	-2.41	1.45	1.50
13	1	819	CLA	MG-NB	-2.41	2.01	2.05
13	a	841	CLA	CMB-C2B	-2.41	1.45	1.50
13	a	836	CLA	CMD-C2D	-2.41	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	2	820	CLA	CMD-C2D	-2.41	1.45	1.50
13	2	801	CLA	MG-NB	-2.41	2.01	2.05
13	b	821	CLA	CHC-C1C	2.41	1.43	1.38
13	A	828	CLA	CMC-C2C	-2.41	1.45	1.50
12	1	801	CL0	C1B-C2B	2.41	1.48	1.43
13	b	837	CLA	CMB-C2B	-2.41	1.45	1.50
13	A	817	CLA	C3B-C4B	2.41	1.49	1.42
13	B	825	CLA	MG-NB	-2.41	2.01	2.05
13	1	819	CLA	C4B-NB	2.41	1.41	1.37
13	B	801	CLA	MG-NB	-2.41	2.01	2.05
13	A	819	CLA	MG-NB	-2.41	2.01	2.05
13	b	814	CLA	C1B-C2B	2.41	1.48	1.43
13	2	835	CLA	CMD-C2D	-2.41	1.45	1.50
12	a	801	CL0	C1B-C2B	2.41	1.48	1.43
18	B	846	LMG	C7-C8	2.41	1.58	1.50
13	2	820	CLA	C1B-C2B	2.41	1.48	1.43
13	B	821	CLA	C1B-C2B	2.41	1.48	1.43
17	1	849	LHG	O7-C5	-2.41	1.40	1.46
13	1	817	CLA	C3B-C4B	2.40	1.49	1.42
13	a	803	CLA	C1B-C2B	2.40	1.48	1.43
13	2	836	CLA	CMB-C2B	-2.40	1.45	1.50
13	A	833	CLA	MG-NB	-2.40	2.01	2.05
13	a	839	CLA	C1B-C2B	2.40	1.48	1.43
13	1	803	CLA	CMB-C2B	-2.40	1.45	1.50
13	b	821	CLA	CMD-C2D	-2.40	1.45	1.50
13	b	825	CLA	MG-NB	-2.40	2.01	2.05
13	A	852	CLA	CMB-C2B	-2.40	1.45	1.50
13	9	4002	CLA	CHC-C1C	2.40	1.43	1.38
13	2	805	CLA	C4B-NB	2.40	1.41	1.37
13	B	814	CLA	C1B-C2B	2.40	1.48	1.43
13	2	810	CLA	CHC-C1C	2.40	1.43	1.38
13	A	803	CLA	C1B-C2B	2.40	1.48	1.43
13	1	829	CLA	MG-NB	-2.40	2.01	2.05
13	a	802	CLA	C1D-ND	2.40	1.41	1.37
13	B	821	CLA	CHC-C1C	2.40	1.43	1.38
16	m	101	BCR	C30-C25	-2.39	1.50	1.53
13	B	821	CLA	CMD-C2D	-2.39	1.45	1.50
13	2	802	CLA	MG-NB	-2.39	2.01	2.05
13	a	852	CLA	CMB-C2B	-2.39	1.45	1.50
13	2	814	CLA	MG-NB	-2.39	2.01	2.05
13	2	813	CLA	C1B-C2B	2.39	1.48	1.43
13	B	837	CLA	CMB-C2B	-2.39	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	832	CLA	CMB-C2B	-2.39	1.45	1.50
13	1	852	CLA	CMB-C2B	-2.39	1.45	1.50
13	2	824	CLA	MG-NB	-2.39	2.01	2.05
13	K	4003	CLA	C3B-C4B	2.39	1.49	1.42
13	a	828	CLA	CMC-C2C	-2.39	1.45	1.50
17	A	849	LHG	O7-C5	-2.39	1.41	1.46
13	1	839	CLA	C1B-C2B	2.39	1.48	1.43
13	A	803	CLA	CMB-C2B	-2.39	1.45	1.50
17	a	849	LHG	O7-C5	-2.39	1.41	1.46
13	A	818	CLA	MG-NB	-2.39	2.01	2.05
13	a	836	CLA	MG-NB	-2.39	2.01	2.05
13	B	836	CLA	CMD-C2D	-2.39	1.45	1.50
13	b	805	CLA	C4B-NB	2.38	1.41	1.37
13	B	832	CLA	CMB-C2B	-2.38	1.45	1.50
13	A	828	CLA	C3B-C4B	2.38	1.49	1.42
13	a	833	CLA	MG-NB	-2.38	2.01	2.05
13	9	4003	CLA	C3B-C4B	2.38	1.49	1.42
13	B	805	CLA	C4B-NB	2.38	1.41	1.37
13	b	821	CLA	C1B-C2B	2.38	1.48	1.43
13	b	802	CLA	C4B-NB	2.38	1.41	1.37
13	b	801	CLA	MG-ND	-2.38	2.01	2.05
13	B	802	CLA	CMD-C2D	-2.38	1.45	1.50
13	a	803	CLA	CMB-C2B	-2.38	1.45	1.50
13	b	836	CLA	CMD-C2D	-2.38	1.45	1.50
13	B	820	CLA	CMC-C2C	-2.38	1.45	1.50
13	b	830	CLA	C3B-C4B	2.38	1.49	1.42
13	k	4002	CLA	CHC-C1C	2.38	1.43	1.38
13	2	831	CLA	C3B-C4B	2.38	1.49	1.42
13	b	801	CLA	C4B-NB	2.38	1.41	1.37
13	B	827	CLA	CMB-C2B	-2.38	1.45	1.50
13	b	820	CLA	CMC-C2C	-2.38	1.45	1.50
13	1	811	CLA	MG-NB	-2.38	2.01	2.05
13	1	818	CLA	MG-NB	-2.37	2.01	2.05
13	1	803	CLA	C1B-C2B	2.37	1.48	1.43
13	b	827	CLA	CMB-C2B	-2.37	1.45	1.50
13	1	828	CLA	CMC-C2C	-2.37	1.45	1.50
13	a	828	CLA	C3B-C4B	2.37	1.49	1.42
13	a	818	CLA	MG-NB	-2.37	2.01	2.05
13	1	816	CLA	C3B-C4B	2.37	1.49	1.42
13	A	839	CLA	C1B-C2B	2.37	1.48	1.43
13	2	820	CLA	CHC-C1C	2.37	1.43	1.38
13	2	820	CLA	C3B-C4B	2.37	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	829	CLA	CHC-C1C	2.37	1.43	1.38
13	A	816	CLA	C3B-C4B	2.37	1.49	1.42
13	B	801	CLA	MG-ND	-2.37	2.01	2.05
13	a	811	CLA	MG-NB	-2.37	2.01	2.05
13	K	4002	CLA	CHC-C1C	2.37	1.43	1.38
13	2	826	CLA	CMB-C2B	-2.37	1.45	1.50
13	1	838	CLA	MG-NB	-2.37	2.01	2.05
13	2	846	CLA	MG-NB	-2.37	2.01	2.05
13	k	4003	CLA	C3B-C4B	2.37	1.49	1.42
13	2	802	CLA	CMD-C2D	-2.37	1.45	1.50
13	2	828	CLA	MG-NB	-2.37	2.01	2.05
13	a	814	CLA	C3B-C4B	2.37	1.49	1.42
13	a	816	CLA	C3B-C4B	2.37	1.49	1.42
13	A	835	CLA	C3B-C4B	2.37	1.49	1.42
13	A	802	CLA	CMC-C2C	-2.37	1.45	1.50
13	b	802	CLA	CMD-C2D	-2.37	1.45	1.50
13	1	835	CLA	C3B-C4B	2.37	1.49	1.42
13	b	829	CLA	CHC-C1C	2.37	1.43	1.38
13	1	841	CLA	CMD-C2D	-2.37	1.45	1.50
13	A	802	CLA	C1D-ND	2.37	1.41	1.37
13	b	815	CLA	MG-NB	-2.36	2.01	2.05
13	B	802	CLA	MG-NB	-2.36	2.01	2.05
13	A	838	CLA	MG-NB	-2.36	2.01	2.05
13	B	813	CLA	C3B-C4B	2.36	1.49	1.42
13	B	832	CLA	C3B-C4B	2.36	1.49	1.42
13	a	828	CLA	MG-NB	-2.36	2.01	2.05
13	b	810	CLA	MG-NB	-2.36	2.01	2.05
13	B	830	CLA	C3B-C4B	2.36	1.49	1.42
13	1	802	CLA	CMC-C2C	-2.36	1.45	1.50
13	2	831	CLA	CMB-C2B	-2.36	1.45	1.50
13	b	832	CLA	C3B-C4B	2.36	1.49	1.42
13	j	1103	CLA	C3B-C4B	2.36	1.49	1.42
13	2	828	CLA	CHC-C1C	2.36	1.43	1.38
13	a	825	CLA	CMD-C2D	-2.36	1.45	1.50
13	f	203	CLA	C3B-C4B	2.36	1.49	1.42
13	1	828	CLA	C3B-C4B	2.36	1.49	1.42
13	B	847	CLA	MG-NB	-2.36	2.01	2.05
13	2	801	CLA	MG-ND	-2.36	2.01	2.05
13	B	821	CLA	C3B-C4B	2.36	1.49	1.42
13	1	804	CLA	CHC-C1C	2.36	1.43	1.38
13	6	204	CLA	C3B-C4B	2.36	1.49	1.42
13	a	838	CLA	MG-NB	-2.36	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	814	CLA	C3B-C4B	2.36	1.49	1.42
13	1	829	CLA	CMD-C2D	-2.35	1.45	1.50
13	B	833	CLA	MG-NB	-2.35	2.01	2.05
13	2	832	CLA	CHC-C1C	2.35	1.43	1.38
13	A	805	CLA	CMC-C2C	-2.35	1.45	1.50
13	2	801	CLA	C4B-NB	2.35	1.41	1.37
13	B	806	CLA	CMD-C2D	-2.35	1.45	1.50
13	a	825	CLA	CMB-C2B	-2.35	1.45	1.50
13	2	806	CLA	CMD-C2D	-2.35	1.45	1.50
13	A	819	CLA	C4B-NB	2.35	1.41	1.37
13	F	204	CLA	C3B-C4B	2.35	1.49	1.42
13	b	833	CLA	C1B-C2B	2.35	1.48	1.43
13	f	204	CLA	C3B-C4B	2.35	1.49	1.42
13	2	812	CLA	C3B-C4B	2.35	1.49	1.42
13	A	811	CLA	MG-NB	-2.35	2.01	2.05
13	B	801	CLA	C4B-NB	2.35	1.40	1.37
13	b	813	CLA	C3B-C4B	2.35	1.49	1.42
13	b	821	CLA	C3B-C4B	2.35	1.49	1.42
13	A	825	CLA	CMD-C2D	-2.35	1.46	1.50
13	B	811	CLA	CMD-C2D	-2.35	1.46	1.50
13	a	819	CLA	C4B-NB	2.35	1.40	1.37
13	B	847	CLA	C1B-C2B	2.35	1.48	1.43
13	1	814	CLA	C3B-C4B	2.35	1.49	1.42
13	a	837	CLA	CMB-C2B	-2.35	1.46	1.50
13	1	826	CLA	CHC-C1C	2.35	1.43	1.38
13	b	811	CLA	C3B-C4B	2.35	1.49	1.42
13	J	1101	CLA	C3B-C4B	2.35	1.49	1.42
13	j	1101	CLA	C3B-C4B	2.35	1.49	1.42
13	8	1103	CLA	C3B-C4B	2.35	1.49	1.42
13	2	809	CLA	MG-NB	-2.35	2.01	2.05
13	B	817	CLA	C3B-C4B	2.35	1.49	1.42
13	a	835	CLA	C3B-C4B	2.35	1.49	1.42
13	A	812	CLA	C3B-C4B	2.34	1.49	1.42
13	B	811	CLA	C3B-C4B	2.34	1.49	1.42
13	1	805	CLA	CMC-C2C	-2.34	1.46	1.50
13	1	825	CLA	CMD-C2D	-2.34	1.46	1.50
13	2	816	CLA	C3B-C4B	2.34	1.49	1.42
13	2	804	CLA	CHC-C1C	2.34	1.43	1.38
13	A	829	CLA	CMD-C2D	-2.34	1.46	1.50
13	A	804	CLA	C3B-C4B	2.34	1.49	1.42
13	2	829	CLA	C3B-C4B	2.34	1.49	1.42
13	b	847	CLA	MG-NB	-2.34	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	J	1103	CLA	C3B-C4B	2.34	1.49	1.42
13	a	826	CLA	C3B-C4B	2.34	1.49	1.42
13	1	828	CLA	MG-NB	-2.34	2.01	2.05
13	F	203	CLA	C3B-C4B	2.34	1.49	1.42
13	B	810	CLA	MG-NB	-2.34	2.01	2.05
13	2	832	CLA	C1B-C2B	2.34	1.48	1.43
13	B	815	CLA	MG-NB	-2.34	2.01	2.05
13	k	4002	CLA	C3B-C4B	2.34	1.49	1.42
13	a	829	CLA	CMD-C2D	-2.34	1.46	1.50
13	b	810	CLA	CHC-C1C	2.34	1.43	1.38
13	J	1102	CLA	C3B-C4B	2.34	1.49	1.42
13	A	837	CLA	CMB-C2B	-2.34	1.46	1.50
13	B	833	CLA	C1B-C2B	2.34	1.48	1.43
13	a	852	CLA	CHC-C1C	2.34	1.43	1.38
13	b	802	CLA	MG-NB	-2.34	2.01	2.05
13	1	804	CLA	C3B-C4B	2.34	1.49	1.42
13	1	802	CLA	C1D-ND	2.34	1.40	1.37
13	b	829	CLA	MG-NB	-2.34	2.01	2.05
13	a	805	CLA	CMC-C2C	-2.33	1.46	1.50
13	2	802	CLA	CHC-C1C	2.33	1.43	1.38
13	2	832	CLA	MG-NB	-2.33	2.01	2.05
13	a	812	CLA	C3B-C4B	2.33	1.49	1.42
13	a	837	CLA	C3B-C4B	2.33	1.49	1.42
13	b	823	CLA	CMC-C2C	-2.33	1.46	1.50
13	b	811	CLA	MG-NB	-2.33	2.01	2.05
13	A	852	CLA	CHC-C1C	2.33	1.43	1.38
13	b	833	CLA	CHC-C1C	2.33	1.43	1.38
13	b	805	CLA	MG-NB	-2.33	2.01	2.05
13	1	811	CLA	C3B-C4B	2.33	1.49	1.42
13	b	847	CLA	C1B-C2B	2.33	1.48	1.43
13	8	1102	CLA	C3B-C4B	2.33	1.49	1.42
13	K	4002	CLA	C3B-C4B	2.33	1.49	1.42
13	A	804	CLA	CHC-C1C	2.33	1.43	1.38
13	1	837	CLA	CMB-C2B	-2.33	1.46	1.50
13	b	810	CLA	C3B-C4B	2.33	1.49	1.42
13	a	808	CLA	MG-NB	-2.33	2.01	2.05
13	1	822	CLA	C3B-C4B	2.33	1.49	1.42
13	2	826	CLA	C3B-C4B	2.33	1.49	1.42
13	a	837	CLA	MG-NB	-2.33	2.01	2.05
13	2	810	CLA	MG-NB	-2.33	2.01	2.05
13	1	812	CLA	C3B-C4B	2.33	1.49	1.42
13	A	841	CLA	CMD-C2D	-2.33	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	835	CLA	MG-NB	-2.33	2.01	2.05
13	2	833	CLA	MG-NB	-2.33	2.01	2.05
13	B	833	CLA	CHC-C1C	2.33	1.43	1.38
13	a	826	CLA	MG-NB	-2.33	2.01	2.05
13	2	810	CLA	C3B-C4B	2.33	1.49	1.42
13	B	829	CLA	MG-NB	-2.33	2.01	2.05
13	6	203	CLA	C3B-C4B	2.33	1.49	1.42
13	a	817	CLA	CHC-C1C	2.33	1.43	1.38
13	2	846	CLA	C1B-C2B	2.33	1.48	1.43
13	a	804	CLA	CHC-C1C	2.33	1.43	1.38
13	b	806	CLA	CMC-C2C	-2.33	1.46	1.50
13	a	804	CLA	C3B-C4B	2.33	1.49	1.42
13	B	804	CLA	CHC-C1C	2.33	1.43	1.38
13	A	825	CLA	CMB-C2B	-2.33	1.46	1.50
13	B	820	CLA	MG-NB	-2.33	2.01	2.05
13	8	1101	CLA	C3B-C4B	2.32	1.49	1.42
13	a	841	CLA	CMD-C2D	-2.32	1.46	1.50
13	B	827	CLA	C3B-C4B	2.32	1.49	1.42
13	1	837	CLA	C3B-C4B	2.32	1.49	1.42
13	A	828	CLA	MG-NB	-2.32	2.01	2.05
13	b	834	CLA	MG-NB	-2.32	2.01	2.05
13	2	832	CLA	C3B-C4B	2.32	1.49	1.42
13	9	4002	CLA	C3B-C4B	2.32	1.49	1.42
13	B	834	CLA	MG-NB	-2.32	2.01	2.05
13	1	826	CLA	MG-NB	-2.32	2.01	2.05
13	2	819	CLA	MG-NB	-2.32	2.01	2.05
13	A	817	CLA	CHC-C1C	2.32	1.43	1.38
13	B	802	CLA	CHC-C1C	2.32	1.43	1.38
16	l	201	BCR	C30-C25	-2.32	1.50	1.53
13	b	820	CLA	MG-NB	-2.32	2.01	2.05
13	b	817	CLA	C3B-C4B	2.32	1.49	1.42
13	b	804	CLA	CHC-C1C	2.32	1.43	1.38
13	A	826	CLA	C3B-C4B	2.32	1.49	1.42
13	b	811	CLA	CMD-C2D	-2.32	1.46	1.50
13	b	807	CLA	C3B-C4B	2.32	1.49	1.42
13	B	811	CLA	MG-NB	-2.32	2.01	2.05
13	a	830	CLA	C1B-C2B	2.32	1.48	1.43
13	A	814	CLA	CHC-C1C	2.32	1.43	1.38
13	B	823	CLA	CMC-C2C	-2.32	1.46	1.50
13	A	826	CLA	CHC-C1C	2.32	1.43	1.38
13	2	809	CLA	C3B-C4B	2.32	1.49	1.42
13	b	833	CLA	MG-NB	-2.32	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	806	CLA	CMD-C2D	-2.32	1.46	1.50
13	B	810	CLA	CHC-C1C	2.32	1.43	1.38
13	2	806	CLA	CMC-C2C	-2.32	1.46	1.50
13	b	822	CLA	C3B-C4B	2.32	1.49	1.42
13	1	817	CLA	CHC-C1C	2.32	1.43	1.38
13	A	831	CLA	MG-NB	-2.31	2.01	2.05
13	a	802	CLA	CMD-C2D	-2.31	1.46	1.50
13	a	802	CLA	CMC-C2C	-2.31	1.46	1.50
13	A	806	CLA	MG-NB	-2.31	2.01	2.05
13	1	806	CLA	MG-NB	-2.31	2.01	2.05
13	b	803	CLA	C3B-C4B	2.31	1.49	1.42
13	b	827	CLA	C3B-C4B	2.31	1.49	1.42
13	A	837	CLA	C3B-C4B	2.31	1.49	1.42
13	B	810	CLA	C3B-C4B	2.31	1.49	1.42
13	b	833	CLA	C3B-C4B	2.31	1.49	1.42
13	j	1102	CLA	C3B-C4B	2.31	1.49	1.42
13	A	802	CLA	CMD-C2D	-2.31	1.46	1.50
13	a	814	CLA	CHC-C1C	2.31	1.43	1.38
13	1	808	CLA	MG-NB	-2.31	2.01	2.05
13	B	822	CLA	CHC-C1C	2.31	1.43	1.38
13	2	821	CLA	CHC-C1C	2.31	1.43	1.38
16	0	201	BCR	C30-C25	-2.31	1.50	1.53
13	2	812	CLA	CHC-C1C	2.31	1.43	1.38
13	a	823	CLA	MG-NB	-2.31	2.01	2.05
13	2	810	CLA	CMD-C2D	-2.31	1.46	1.50
13	B	833	CLA	C3B-C4B	2.31	1.49	1.42
13	A	808	CLA	MG-NB	-2.31	2.01	2.05
13	2	809	CLA	CHC-C1C	2.31	1.43	1.38
16	L	207	BCR	C30-C25	-2.31	1.50	1.53
13	1	852	CLA	MG-NB	-2.31	2.01	2.05
13	2	808	CLA	C3B-C4B	2.31	1.49	1.42
13	B	809	CLA	C3B-C4B	2.31	1.49	1.42
13	A	822	CLA	C3B-C4B	2.31	1.49	1.42
13	b	815	CLA	C3B-C4B	2.31	1.49	1.42
13	B	803	CLA	C3B-C4B	2.30	1.49	1.42
13	a	835	CLA	MG-NB	-2.30	2.01	2.05
13	1	814	CLA	CHC-C1C	2.30	1.43	1.38
13	A	811	CLA	C3B-C4B	2.30	1.49	1.42
13	B	822	CLA	C3B-C4B	2.30	1.49	1.42
13	b	815	CLA	CHC-C1C	2.30	1.43	1.38
13	1	825	CLA	CMB-C2B	-2.30	1.46	1.50
13	1	802	CLA	C1B-C2B	2.30	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	1	831	CLA	CMB-C2B	-2.30	1.46	1.50
13	2	814	CLA	CHC-C1C	2.30	1.43	1.38
13	A	831	CLA	CMB-C2B	-2.30	1.46	1.50
13	B	815	CLA	CHC-C1C	2.30	1.43	1.38
13	2	820	CLA	MG-NB	-2.30	2.01	2.05
13	b	809	CLA	C3B-C4B	2.30	1.49	1.42
13	B	807	CLA	C3B-C4B	2.30	1.49	1.42
13	1	808	CLA	C3B-C4B	2.30	1.49	1.42
13	A	837	CLA	MG-NB	-2.30	2.01	2.05
13	1	837	CLA	MG-NB	-2.30	2.01	2.05
13	b	821	CLA	MG-NB	-2.30	2.01	2.05
13	b	822	CLA	CHC-C1C	2.30	1.43	1.38
13	B	806	CLA	CMC-C2C	-2.30	1.46	1.50
13	A	830	CLA	C1B-C2B	2.30	1.48	1.43
13	A	852	CLA	MG-NB	-2.30	2.01	2.05
13	2	837	CLA	C3B-C4B	2.30	1.49	1.42
13	B	821	CLA	MG-NB	-2.30	2.01	2.05
13	b	830	CLA	MG-NB	-2.30	2.01	2.05
13	B	815	CLA	C3B-C4B	2.30	1.49	1.42
13	1	852	CLA	CHC-C1C	2.30	1.43	1.38
13	b	836	CLA	MG-NB	-2.30	2.01	2.05
13	2	815	CLA	CMB-C2B	-2.29	1.46	1.50
13	2	822	CLA	CMC-C2C	-2.29	1.46	1.50
13	a	822	CLA	C3B-C4B	2.29	1.49	1.42
13	a	826	CLA	CHC-C1C	2.29	1.43	1.38
13	a	828	CLA	CMD-C2D	-2.29	1.46	1.50
13	2	821	CLA	C3B-C4B	2.29	1.49	1.42
13	1	828	CLA	CMD-C2D	-2.29	1.46	1.50
13	a	819	CLA	CMB-C2B	-2.29	1.46	1.50
13	1	811	CLA	CHC-C1C	2.29	1.43	1.38
13	8	1102	CLA	CHC-C1C	2.29	1.43	1.38
13	B	835	CLA	MG-NB	-2.29	2.01	2.05
13	b	827	CLA	MG-NB	-2.29	2.01	2.05
13	a	813	CLA	C3B-C4B	2.29	1.49	1.42
13	2	809	CLA	CMC-C2C	-2.29	1.46	1.50
13	B	838	CLA	C3B-C4B	2.29	1.49	1.42
13	1	815	CLA	C3B-C4B	2.29	1.49	1.42
13	b	802	CLA	CHC-C1C	2.29	1.43	1.38
13	A	830	CLA	MG-NB	-2.29	2.01	2.05
13	A	815	CLA	C3B-C4B	2.29	1.49	1.42
13	B	814	CLA	MG-NB	-2.29	2.01	2.05
13	1	826	CLA	C3B-C4B	2.29	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	831	CLA	CMB-C2B	-2.29	1.46	1.50
13	a	806	CLA	MG-NB	-2.29	2.01	2.05
13	B	805	CLA	MG-NB	-2.29	2.01	2.05
13	A	826	CLA	MG-NB	-2.29	2.01	2.05
13	A	835	CLA	MG-NB	-2.29	2.01	2.05
13	1	802	CLA	CMD-C2D	-2.29	1.46	1.50
13	A	808	CLA	C3B-C4B	2.29	1.49	1.42
13	1	831	CLA	C3B-C4B	2.29	1.49	1.42
13	2	834	CLA	MG-NB	-2.28	2.01	2.05
13	1	831	CLA	MG-NB	-2.28	2.01	2.05
13	J	1102	CLA	CHC-C1C	2.28	1.43	1.38
13	B	834	CLA	CMB-C2B	-2.28	1.46	1.50
13	b	836	CLA	CMB-C2B	-2.28	1.46	1.50
13	a	811	CLA	C3B-C4B	2.28	1.49	1.42
13	a	802	CLA	C1B-C2B	2.28	1.48	1.43
13	b	803	CLA	CHC-C1C	2.28	1.43	1.38
13	2	833	CLA	CMB-C2B	-2.28	1.46	1.50
13	b	829	CLA	C3B-C4B	2.28	1.49	1.42
13	1	830	CLA	MG-NB	-2.28	2.01	2.05
13	a	831	CLA	MG-NB	-2.28	2.01	2.05
13	2	814	CLA	C3B-C4B	2.28	1.49	1.42
13	2	813	CLA	C3B-C4B	2.28	1.49	1.42
13	b	808	CLA	C3B-C4B	2.28	1.49	1.42
13	1	803	CLA	MG-NB	-2.28	2.01	2.05
13	A	831	CLA	C1B-C2B	2.28	1.48	1.43
13	A	802	CLA	C1B-C2B	2.28	1.48	1.43
13	a	852	CLA	MG-NB	-2.28	2.01	2.05
13	A	819	CLA	CMB-C2B	-2.28	1.46	1.50
13	A	818	CLA	CHC-C1C	2.28	1.43	1.38
13	a	831	CLA	C1B-C2B	2.28	1.48	1.43
13	A	823	CLA	MG-NB	-2.28	2.01	2.05
13	2	805	CLA	MG-NB	-2.28	2.01	2.05
13	2	826	CLA	MG-NB	-2.28	2.01	2.05
13	2	803	CLA	C3B-C4B	2.27	1.49	1.42
13	B	836	CLA	CMB-C2B	-2.27	1.46	1.50
13	B	813	CLA	CHC-C1C	2.27	1.43	1.38
13	a	840	CLA	CMD-C2D	-2.27	1.46	1.50
13	a	808	CLA	C3B-C4B	2.27	1.49	1.42
13	a	834	CLA	C3B-C4B	2.27	1.49	1.42
13	B	804	CLA	C3B-C4B	2.27	1.49	1.42
13	2	804	CLA	MG-NB	-2.27	2.01	2.05
13	1	202	CLA	CHC-C1C	2.27	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	828	CLA	CMD-C2D	-2.27	1.46	1.50
13	B	810	CLA	CMC-C2C	-2.27	1.46	1.50
13	a	830	CLA	MG-NB	-2.27	2.01	2.05
13	b	810	CLA	CMC-C2C	-2.27	1.46	1.50
13	2	805	CLA	CMB-C2B	-2.27	1.46	1.50
13	A	831	CLA	C3B-C4B	2.27	1.49	1.42
13	1	835	CLA	MG-NB	-2.27	2.01	2.05
13	0	203	CLA	C3B-C4B	2.27	1.49	1.42
13	B	836	CLA	MG-NB	-2.27	2.01	2.05
13	A	834	CLA	C3B-C4B	2.27	1.49	1.42
13	1	813	CLA	C3B-C4B	2.27	1.49	1.42
13	1	833	CLA	C3B-C4B	2.27	1.49	1.42
13	a	818	CLA	CHC-C1C	2.27	1.43	1.38
13	1	818	CLA	CHC-C1C	2.27	1.43	1.38
13	F	204	CLA	CHC-C1C	2.27	1.43	1.38
13	A	818	CLA	CMB-C2B	-2.27	1.46	1.50
13	A	813	CLA	C3B-C4B	2.27	1.49	1.42
13	B	808	CLA	C3B-C4B	2.27	1.49	1.42
13	a	833	CLA	C3B-C4B	2.27	1.49	1.42
13	b	814	CLA	MG-NB	-2.27	2.01	2.05
13	A	811	CLA	CHC-C1C	2.27	1.43	1.38
13	f	204	CLA	CHC-C1C	2.27	1.43	1.38
13	A	833	CLA	C3B-C4B	2.27	1.49	1.42
13	1	830	CLA	C1B-C2B	2.27	1.48	1.43
13	b	813	CLA	CHC-C1C	2.27	1.43	1.38
13	2	807	CLA	C3B-C4B	2.27	1.49	1.42
13	B	805	CLA	CMB-C2B	-2.27	1.46	1.50
13	b	806	CLA	CMB-C2B	-2.26	1.46	1.50
13	1	820	CLA	CMB-C2B	-2.26	1.46	1.50
13	b	805	CLA	CMB-C2B	-2.26	1.46	1.50
13	B	827	CLA	MG-NB	-2.26	2.01	2.05
13	2	811	CLA	MG-NB	-2.26	2.01	2.05
13	a	839	CLA	C3B-C4B	2.26	1.49	1.42
13	1	834	CLA	C3B-C4B	2.26	1.49	1.42
13	2	834	CLA	CMD-C2D	-2.26	1.46	1.50
13	a	811	CLA	CHC-C1C	2.26	1.43	1.38
13	2	818	CLA	CMD-C2D	-2.26	1.46	1.50
13	a	842	CLA	C3B-C4B	2.26	1.49	1.42
13	1	840	CLA	CMD-C2D	-2.26	1.46	1.50
13	2	813	CLA	MG-NB	-2.26	2.01	2.05
13	a	818	CLA	CMB-C2B	-2.26	1.46	1.50
13	b	804	CLA	C3B-C4B	2.26	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	815	CLA	C3B-C4B	2.26	1.49	1.42
13	b	816	CLA	CMB-C2B	-2.26	1.46	1.50
13	A	839	CLA	C3B-C4B	2.26	1.49	1.42
13	a	815	CLA	MG-NB	-2.26	2.01	2.05
13	a	825	CLA	MG-NB	-2.26	2.01	2.05
13	b	825	CLA	CHC-C1C	2.26	1.43	1.38
13	A	825	CLA	MG-NB	-2.26	2.01	2.05
13	2	828	CLA	C3B-C4B	2.26	1.49	1.42
13	2	806	CLA	CMB-C2B	-2.26	1.46	1.50
13	1	833	CLA	CHC-C1C	2.26	1.43	1.38
13	A	820	CLA	CMD-C2D	-2.26	1.46	1.50
13	A	803	CLA	MG-NB	-2.26	2.01	2.05
13	2	803	CLA	CHC-C1C	2.26	1.43	1.38
13	2	837	CLA	CHC-C1C	2.26	1.43	1.38
13	K	4005	CLA	C3B-C4B	2.26	1.49	1.42
13	B	806	CLA	CMB-C2B	-2.26	1.46	1.50
13	1	202	CLA	C3B-C4B	2.25	1.49	1.42
13	2	835	CLA	MG-NB	-2.25	2.01	2.05
13	B	803	CLA	CHC-C1C	2.25	1.43	1.38
13	1	831	CLA	C1B-C2B	2.25	1.48	1.43
13	b	819	CLA	CMD-C2D	-2.25	1.46	1.50
13	a	813	CLA	MG-NB	-2.25	2.01	2.05
13	A	833	CLA	CHC-C1C	2.25	1.43	1.38
13	B	814	CLA	C3B-C4B	2.25	1.49	1.42
13	b	828	CLA	C3B-C4B	2.25	1.49	1.42
13	B	829	CLA	C3B-C4B	2.25	1.49	1.42
13	a	831	CLA	C3B-C4B	2.25	1.49	1.42
13	2	804	CLA	C3B-C4B	2.25	1.49	1.42
13	A	840	CLA	CMD-C2D	-2.25	1.46	1.50
13	2	823	CLA	CMD-C2D	-2.25	1.46	1.50
13	1	839	CLA	C3B-C4B	2.25	1.49	1.42
13	B	830	CLA	MG-NB	-2.25	2.01	2.05
13	0	203	CLA	MG-NB	-2.25	2.01	2.05
13	2	827	CLA	C3B-C4B	2.25	1.49	1.42
13	B	819	CLA	CMD-C2D	-2.25	1.46	1.50
13	6	204	CLA	CHC-C1C	2.25	1.43	1.38
13	L	201	CLA	C3B-C4B	2.25	1.49	1.42
12	1	801	CL0	MG-NB	-2.25	2.01	2.05
13	2	829	CLA	MG-NB	-2.25	2.01	2.05
13	B	816	CLA	CMB-C2B	-2.25	1.46	1.50
13	a	832	CLA	CMB-C2B	-2.25	1.46	1.50
13	1	818	CLA	CMB-C2B	-2.25	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	j	1102	CLA	CHC-C1C	2.25	1.43	1.38
13	l	207	CLA	MG-NB	-2.25	2.01	2.05
13	a	826	CLA	CMD-C2D	-2.25	1.46	1.50
13	1	842	CLA	C3B-C4B	2.25	1.49	1.42
13	L	206	CLA	MG-NB	-2.25	2.01	2.05
13	A	842	CLA	C3B-C4B	2.25	1.49	1.42
13	b	824	CLA	C4B-NB	2.25	1.40	1.37
13	B	804	CLA	MG-NB	-2.25	2.01	2.05
13	1	824	CLA	MG-NB	-2.25	2.01	2.05
13	B	828	CLA	C3B-C4B	2.25	1.49	1.42
13	k	4005	CLA	C3B-C4B	2.25	1.49	1.42
13	B	838	CLA	CHC-C1C	2.25	1.43	1.38
13	1	840	CLA	C3B-C4B	2.25	1.49	1.42
13	0	202	CLA	CHC-C1C	2.25	1.43	1.38
13	b	838	CLA	C3B-C4B	2.25	1.49	1.42
13	k	4005	CLA	CHC-C1C	2.25	1.43	1.38
13	2	835	CLA	CMB-C2B	-2.25	1.46	1.50
13	b	820	CLA	CHC-C1C	2.24	1.43	1.38
13	1	819	CLA	CMB-C2B	-2.24	1.46	1.50
13	0	202	CLA	C3B-C4B	2.24	1.49	1.42
13	2	826	CLA	CHC-C1C	2.24	1.43	1.38
12	A	801	CL0	MG-NB	-2.24	2.01	2.05
13	9	4005	CLA	C3B-C4B	2.24	1.49	1.42
12	A	801	CL0	CMB-C2B	-2.24	1.46	1.50
13	A	822	CLA	CHC-C1C	2.24	1.43	1.38
13	L	201	CLA	CHC-C1C	2.24	1.43	1.38
13	b	834	CLA	CMB-C2B	-2.24	1.46	1.50
13	K	4003	CLA	MG-NB	-2.24	2.01	2.05
12	a	801	CL0	MG-NB	-2.24	2.01	2.05
13	a	832	CLA	MG-NB	-2.24	2.01	2.05
13	K	4005	CLA	CHC-C1C	2.24	1.43	1.38
13	a	827	CLA	CHC-C1C	2.24	1.43	1.38
13	A	805	CLA	CMD-C2D	-2.24	1.46	1.50
13	A	817	CLA	CMC-C2C	-2.24	1.46	1.50
13	j	1101	CLA	CMC-C2C	-2.24	1.46	1.50
13	a	803	CLA	MG-NB	-2.24	2.01	2.05
13	A	820	CLA	CMB-C2B	-2.24	1.46	1.50
13	2	827	CLA	MG-NB	-2.24	2.01	2.05
13	b	812	CLA	C3B-C4B	2.24	1.49	1.42
13	b	820	CLA	C3B-C4B	2.24	1.49	1.42
13	1	817	CLA	CMC-C2C	-2.24	1.46	1.50
13	1	832	CLA	CMB-C2B	-2.24	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	802	CLA	C3B-C4B	2.24	1.49	1.42
13	2	824	CLA	C3B-C4B	2.24	1.49	1.42
13	a	833	CLA	CHC-C1C	2.24	1.43	1.38
13	b	822	CLA	MG-NB	-2.24	2.01	2.05
13	i	102	CLA	CHC-C1C	2.24	1.43	1.38
13	B	824	CLA	C4B-NB	2.24	1.40	1.37
13	b	816	CLA	MG-NB	-2.24	2.01	2.05
13	1	823	CLA	MG-NB	-2.24	2.01	2.05
13	B	824	CLA	CMD-C2D	-2.24	1.46	1.50
13	b	801	CLA	CMC-C2C	-2.24	1.46	1.50
13	A	840	CLA	C3B-C4B	2.24	1.49	1.42
13	B	812	CLA	CMC-C2C	-2.24	1.46	1.50
13	b	827	CLA	CHC-C1C	2.24	1.43	1.38
13	2	823	CLA	C4B-NB	2.24	1.40	1.37
13	a	820	CLA	CMB-C2B	-2.24	1.46	1.50
13	A	852	CLA	C3B-C4B	2.24	1.49	1.42
13	b	804	CLA	MG-NB	-2.24	2.01	2.05
13	B	825	CLA	CHC-C1C	2.24	1.43	1.38
13	1	822	CLA	CHC-C1C	2.24	1.43	1.38
13	A	839	CLA	MG-NB	-2.24	2.01	2.05
13	1	852	CLA	C3B-C4B	2.24	1.49	1.42
13	a	813	CLA	CMD-C2D	-2.23	1.46	1.50
13	B	820	CLA	C3B-C4B	2.23	1.49	1.42
13	2	815	CLA	C3B-C4B	2.23	1.49	1.42
13	b	831	CLA	MG-NB	-2.23	2.01	2.05
13	B	825	CLA	C3B-C4B	2.23	1.49	1.42
13	2	819	CLA	C3B-C4B	2.23	1.49	1.42
13	b	825	CLA	C3B-C4B	2.23	1.49	1.42
13	B	812	CLA	C3B-C4B	2.23	1.49	1.42
13	b	814	CLA	C3B-C4B	2.23	1.49	1.42
13	2	802	CLA	C3B-C4B	2.23	1.49	1.42
13	b	807	CLA	MG-NB	-2.23	2.01	2.05
13	a	817	CLA	CMC-C2C	-2.23	1.46	1.50
13	1	813	CLA	CHC-C1C	2.23	1.43	1.38
13	L	204	CLA	C3B-C4B	2.23	1.49	1.42
13	1	825	CLA	MG-NB	-2.23	2.01	2.05
12	1	801	CL0	CMB-C2B	-2.23	1.46	1.50
13	b	830	CLA	CHC-C1C	2.23	1.43	1.38
13	2	815	CLA	MG-NB	-2.23	2.01	2.05
13	2	822	CLA	CMD-C2D	-2.23	1.46	1.50
13	b	838	CLA	CHC-C1C	2.23	1.43	1.38
13	B	802	CLA	C3B-C4B	2.23	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	840	CLA	MG-NB	-2.23	2.01	2.05
13	1	827	CLA	CMD-C2D	-2.23	1.46	1.50
13	B	820	CLA	CHC-C1C	2.23	1.43	1.38
13	9	4003	CLA	MG-NB	-2.23	2.01	2.05
12	a	801	CL0	CMB-C2B	-2.23	1.46	1.50
13	A	824	CLA	MG-NB	-2.23	2.01	2.05
13	B	816	CLA	MG-NB	-2.23	2.01	2.05
13	1	815	CLA	MG-NB	-2.23	2.01	2.05
13	a	822	CLA	CHC-C1C	2.23	1.43	1.38
13	2	834	CLA	CHC-C1C	2.23	1.43	1.38
13	A	815	CLA	MG-NB	-2.23	2.01	2.05
13	1	814	CLA	MG-NB	-2.23	2.01	2.05
13	B	822	CLA	CMD-C2D	-2.23	1.46	1.50
13	B	824	CLA	CMB-C2B	-2.23	1.46	1.50
13	a	839	CLA	MG-NB	-2.23	2.01	2.05
13	b	826	CLA	C1B-C2B	2.23	1.48	1.43
13	a	832	CLA	CMD-C2D	-2.23	1.46	1.50
12	A	801	CL0	CHC-C1C	2.23	1.43	1.38
13	A	827	CLA	CMD-C2D	-2.23	1.46	1.50
13	B	835	CLA	CMD-C2D	-2.23	1.46	1.50
13	b	822	CLA	CMD-C2D	-2.23	1.46	1.50
13	a	842	CLA	MG-NB	-2.23	2.01	2.05
13	A	813	CLA	CMD-C2D	-2.23	1.46	1.50
13	9	4005	CLA	CHC-C1C	2.23	1.43	1.38
13	A	813	CLA	CHC-C1C	2.23	1.42	1.38
13	1	829	CLA	CHC-C1C	2.23	1.42	1.38
13	a	840	CLA	C3B-C4B	2.23	1.49	1.42
13	A	826	CLA	CMD-C2D	-2.23	1.46	1.50
13	A	830	CLA	CMD-C2D	-2.23	1.46	1.50
13	a	820	CLA	CMD-C2D	-2.23	1.46	1.50
13	B	812	CLA	MG-NB	-2.23	2.01	2.05
13	k	4003	CLA	MG-NB	-2.23	2.01	2.05
13	a	852	CLA	C1B-C2B	2.23	1.48	1.43
13	1	802	CLA	C3B-C4B	2.23	1.49	1.42
13	a	824	CLA	MG-NB	-2.23	2.01	2.05
13	2	829	CLA	CHC-C1C	2.23	1.42	1.38
13	B	826	CLA	C1B-C2B	2.23	1.48	1.43
13	b	824	CLA	CMB-C2B	-2.23	1.46	1.50
12	1	801	CL0	CHC-C1C	2.23	1.42	1.38
13	a	802	CLA	C3B-C4B	2.23	1.49	1.42
13	2	817	CLA	C3B-C4B	2.23	1.49	1.42
13	b	828	CLA	CHC-C1C	2.22	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	j	1101	CLA	CHC-C1C	2.22	1.42	1.38
13	1	815	CLA	CHC-C1C	2.22	1.42	1.38
13	8	1101	CLA	CHC-C1C	2.22	1.42	1.38
13	A	832	CLA	CMB-C2B	-2.22	1.46	1.50
13	1	813	CLA	CMD-C2D	-2.22	1.46	1.50
13	B	832	CLA	MG-NB	-2.22	2.01	2.05
13	B	828	CLA	MG-NB	-2.22	2.01	2.05
13	2	830	CLA	MG-NB	-2.22	2.01	2.05
13	a	823	CLA	C3B-C4B	2.22	1.49	1.42
13	a	852	CLA	C3B-C4B	2.22	1.49	1.42
13	a	813	CLA	CHC-C1C	2.22	1.42	1.38
13	2	819	CLA	CHC-C1C	2.22	1.42	1.38
13	b	812	CLA	CHC-C1C	2.22	1.42	1.38
13	a	805	CLA	CMD-C2D	-2.22	1.46	1.50
13	A	820	CLA	C3B-C4B	2.22	1.49	1.42
13	b	847	CLA	CMD-C2D	-2.22	1.46	1.50
13	a	821	CLA	C3B-C4B	2.22	1.49	1.42
13	a	840	CLA	MG-NB	-2.22	2.01	2.05
13	7	102	CLA	MG-NB	-2.22	2.01	2.05
13	B	830	CLA	CHC-C1C	2.22	1.42	1.38
13	J	1101	CLA	CHC-C1C	2.22	1.42	1.38
13	B	831	CLA	MG-NB	-2.22	2.01	2.05
13	b	832	CLA	MG-NB	-2.22	2.01	2.05
13	B	804	CLA	CMC-C2C	-2.22	1.46	1.50
13	a	830	CLA	CMD-C2D	-2.22	1.46	1.50
13	A	852	CLA	C1B-C2B	2.22	1.48	1.43
13	9	4003	CLA	CHC-C1C	2.22	1.42	1.38
13	A	802	CLA	C3B-C4B	2.22	1.49	1.42
13	2	811	CLA	C3B-C4B	2.22	1.49	1.42
13	0	208	CLA	MG-NB	-2.22	2.01	2.05
13	a	827	CLA	CMD-C2D	-2.22	1.46	1.50
13	a	819	CLA	CHC-C1C	2.22	1.42	1.38
13	A	842	CLA	CHC-C1C	2.22	1.42	1.38
13	1	835	CLA	CHC-C1C	2.22	1.42	1.38
13	a	820	CLA	C3B-C4B	2.22	1.49	1.42
13	b	828	CLA	MG-NB	-2.22	2.01	2.05
13	2	801	CLA	CMC-C2C	-2.22	1.46	1.50
13	b	824	CLA	CMD-C2D	-2.22	1.46	1.50
13	2	822	CLA	C3B-C4B	2.22	1.49	1.42
13	B	801	CLA	CMC-C2C	-2.22	1.46	1.50
13	a	810	CLA	C3B-C4B	2.22	1.49	1.42
13	B	827	CLA	CHC-C1C	2.22	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	K	4003	CLA	CHC-C1C	2.22	1.42	1.38
13	a	807	CLA	CHC-C1C	2.22	1.42	1.38
13	1	810	CLA	CHC-C1C	2.22	1.42	1.38
13	2	827	CLA	CHC-C1C	2.22	1.42	1.38
13	a	811	CLA	CMD-C2D	-2.22	1.46	1.50
13	l	205	CLA	C3B-C4B	2.21	1.49	1.42
13	A	807	CLA	CHC-C1C	2.21	1.42	1.38
13	1	839	CLA	MG-NB	-2.21	2.01	2.05
13	B	847	CLA	CMD-C2D	-2.21	1.46	1.50
13	b	812	CLA	MG-NB	-2.21	2.01	2.05
13	b	835	CLA	CHC-C1C	2.21	1.42	1.38
13	1	807	CLA	CHC-C1C	2.21	1.42	1.38
13	B	816	CLA	C3B-C4B	2.21	1.49	1.42
13	b	835	CLA	CMD-C2D	-2.21	1.46	1.50
13	2	821	CLA	MG-NB	-2.21	2.01	2.05
13	a	829	CLA	CHC-C1C	2.21	1.42	1.38
13	A	841	CLA	C3B-C4B	2.21	1.49	1.42
13	J	1101	CLA	CMC-C2C	-2.21	1.46	1.50
13	B	822	CLA	MG-NB	-2.21	2.01	2.05
13	a	827	CLA	C3B-C4B	2.21	1.49	1.42
13	b	816	CLA	C3B-C4B	2.21	1.49	1.42
13	1	809	CLA	CMC-C2C	-2.21	1.46	1.50
13	2	811	CLA	CMC-C2C	-2.21	1.46	1.50
13	A	815	CLA	CHC-C1C	2.21	1.42	1.38
13	B	828	CLA	CHC-C1C	2.21	1.42	1.38
13	J	1101	CLA	CMD-C2D	-2.21	1.46	1.50
13	1	827	CLA	C3B-C4B	2.21	1.49	1.42
13	1	805	CLA	CMD-C2D	-2.21	1.46	1.50
13	a	827	CLA	MG-NB	-2.21	2.01	2.05
13	B	818	CLA	C3B-C4B	2.21	1.49	1.42
13	1	820	CLA	CMD-C2D	-2.21	1.46	1.50
13	a	805	CLA	C3B-C4B	2.21	1.49	1.42
13	2	825	CLA	C1B-C2B	2.21	1.48	1.43
13	A	813	CLA	MG-NB	-2.21	2.01	2.05
13	A	827	CLA	MG-NB	-2.21	2.01	2.05
13	0	206	CLA	C3B-C4B	2.21	1.49	1.42
13	B	823	CLA	CMD-C2D	-2.21	1.46	1.50
13	8	1101	CLA	CMD-C2D	-2.21	1.46	1.50
13	a	841	CLA	C3B-C4B	2.21	1.49	1.42
13	A	835	CLA	CHC-C1C	2.21	1.42	1.38
13	b	831	CLA	CHC-C1C	2.21	1.42	1.38
13	b	823	CLA	CMD-C2D	-2.21	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	2	804	CLA	CMC-C2C	-2.21	1.46	1.50
13	2	813	CLA	CMD-C2D	-2.21	1.46	1.50
13	1	827	CLA	MG-NB	-2.21	2.01	2.05
12	a	801	CL0	CHC-C1C	2.21	1.42	1.38
13	A	821	CLA	C3B-C4B	2.21	1.49	1.42
13	A	814	CLA	MG-NB	-2.21	2.01	2.05
13	B	832	CLA	CHC-C1C	2.21	1.42	1.38
13	B	835	CLA	CHC-C1C	2.21	1.42	1.38
13	1	822	CLA	CMD-C2D	-2.21	1.46	1.50
13	1	826	CLA	CMD-C2D	-2.21	1.46	1.50
13	1	810	CLA	C3B-C4B	2.21	1.49	1.42
13	2	831	CLA	MG-NB	-2.21	2.01	2.05
13	A	827	CLA	CHC-C1C	2.21	1.42	1.38
13	A	829	CLA	CHC-C1C	2.21	1.42	1.38
13	a	803	CLA	CMC-C2C	-2.21	1.46	1.50
13	A	805	CLA	C3B-C4B	2.21	1.49	1.42
13	k	4003	CLA	CHC-C1C	2.21	1.42	1.38
13	B	807	CLA	MG-NB	-2.21	2.01	2.05
13	1	842	CLA	CHC-C1C	2.21	1.42	1.38
13	1	805	CLA	C3B-C4B	2.20	1.49	1.42
13	A	827	CLA	C3B-C4B	2.20	1.49	1.42
13	a	835	CLA	CHC-C1C	2.20	1.42	1.38
13	B	807	CLA	CMD-C2D	-2.20	1.46	1.50
13	1	821	CLA	C3B-C4B	2.20	1.49	1.42
13	b	832	CLA	CHC-C1C	2.20	1.42	1.38
13	A	803	CLA	CMD-C2D	-2.20	1.46	1.50
13	A	809	CLA	CMC-C2C	-2.20	1.46	1.50
13	1	830	CLA	CMD-C2D	-2.20	1.46	1.50
13	2	821	CLA	CMD-C2D	-2.20	1.46	1.50
13	b	804	CLA	CMC-C2C	-2.20	1.46	1.50
13	2	823	CLA	CMB-C2B	-2.20	1.46	1.50
13	0	208	CLA	C3B-C4B	2.20	1.49	1.42
13	1	813	CLA	MG-NB	-2.20	2.01	2.05
13	B	812	CLA	CHC-C1C	2.20	1.42	1.38
13	8	1103	CLA	CHC-C1C	2.20	1.42	1.38
13	A	840	CLA	CMB-C2B	-2.20	1.46	1.50
13	B	830	CLA	CMB-C2B	-2.20	1.46	1.50
13	1	805	CLA	MG-NB	-2.20	2.01	2.05
13	L	203	CLA	CMB-C2B	-2.20	1.46	1.50
13	b	804	CLA	CMD-C2D	-2.20	1.46	1.50
13	b	833	CLA	CMD-C2D	-2.20	1.46	1.50
13	l	204	CLA	CMB-C2B	-2.20	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	1	819	CLA	C3B-C4B	2.20	1.49	1.42
13	A	832	CLA	MG-NB	-2.20	2.01	2.05
13	2	824	CLA	CHC-C1C	2.20	1.42	1.38
13	a	803	CLA	CMD-C2D	-2.20	1.46	1.50
13	a	830	CLA	CMC-C2C	-2.20	1.46	1.50
13	B	823	CLA	C3B-C4B	2.20	1.49	1.42
13	b	818	CLA	C3B-C4B	2.20	1.49	1.42
13	2	811	CLA	CHC-C1C	2.20	1.42	1.38
13	A	811	CLA	CMD-C2D	-2.20	1.46	1.50
13	1	852	CLA	C1B-C2B	2.20	1.48	1.43
13	1	835	CLA	CMB-C2B	-2.20	1.46	1.50
13	A	806	CLA	C3B-C4B	2.20	1.49	1.42
13	b	830	CLA	CMB-C2B	-2.20	1.46	1.50
13	A	810	CLA	C3B-C4B	2.20	1.49	1.42
13	1	817	CLA	CMD-C2D	-2.20	1.46	1.50
13	1	820	CLA	C3B-C4B	2.20	1.49	1.42
13	A	810	CLA	CHC-C1C	2.20	1.42	1.38
13	1	830	CLA	C3B-C4B	2.20	1.49	1.42
13	A	832	CLA	CMD-C2D	-2.20	1.46	1.50
13	A	835	CLA	CMB-C2B	-2.20	1.46	1.50
13	1	803	CLA	CMC-C2C	-2.20	1.46	1.50
13	b	807	CLA	CMD-C2D	-2.20	1.46	1.50
13	1	822	CLA	MG-NB	-2.20	2.01	2.05
13	1	840	CLA	MG-NB	-2.20	2.01	2.05
13	F	201	CLA	CMD-C2D	-2.20	1.46	1.50
13	b	828	CLA	CMD-C2D	-2.20	1.46	1.50
13	2	829	CLA	CMB-C2B	-2.20	1.46	1.50
13	8	1101	CLA	CMC-C2C	-2.20	1.46	1.50
13	I	101	CLA	CHC-C1C	2.20	1.42	1.38
13	A	834	CLA	CMD-C2D	-2.20	1.46	1.50
13	A	819	CLA	C3B-C4B	2.20	1.49	1.42
13	a	819	CLA	C3B-C4B	2.20	1.49	1.42
13	1	832	CLA	MG-NB	-2.20	2.01	2.05
13	1	825	CLA	C3B-C4B	2.20	1.49	1.42
13	6	201	CLA	CMD-C2D	-2.20	1.46	1.50
13	B	814	CLA	CMD-C2D	-2.20	1.46	1.50
13	a	824	CLA	CHC-C1C	2.20	1.42	1.38
13	F	201	CLA	C3B-C4B	2.20	1.49	1.42
13	b	823	CLA	C3B-C4B	2.19	1.49	1.42
13	1	808	CLA	CMD-C2D	-2.19	1.46	1.50
13	b	819	CLA	C3B-C4B	2.19	1.49	1.42
13	J	1103	CLA	CHC-C1C	2.19	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	814	CLA	MG-NB	-2.19	2.01	2.05
13	a	842	CLA	CHC-C1C	2.19	1.42	1.38
13	A	824	CLA	C3B-C4B	2.19	1.49	1.42
13	1	803	CLA	CMD-C2D	-2.19	1.46	1.50
13	A	819	CLA	CHC-C1C	2.19	1.42	1.38
13	2	818	CLA	C3B-C4B	2.19	1.49	1.42
13	a	822	CLA	CMD-C2D	-2.19	1.46	1.50
13	a	806	CLA	C3B-C4B	2.19	1.49	1.42
13	A	813	CLA	CMC-C2C	-2.19	1.46	1.50
13	A	805	CLA	MG-NB	-2.19	2.01	2.05
13	A	803	CLA	CMC-C2C	-2.19	1.46	1.50
13	1	806	CLA	C3B-C4B	2.19	1.49	1.42
13	A	825	CLA	C3B-C4B	2.19	1.49	1.42
13	B	819	CLA	C3B-C4B	2.19	1.49	1.42
13	b	830	CLA	CMD-C2D	-2.19	1.46	1.50
13	B	837	CLA	CMD-C2D	-2.19	1.46	1.50
13	1	819	CLA	CMC-C2C	-2.19	1.46	1.50
13	A	823	CLA	C3B-C4B	2.19	1.49	1.42
13	f	201	CLA	C3B-C4B	2.19	1.49	1.42
13	A	821	CLA	CMC-C2C	-2.19	1.46	1.50
13	B	834	CLA	CMD-C2D	-2.19	1.46	1.50
13	1	807	CLA	C3B-C4B	2.19	1.49	1.42
13	1	811	CLA	CMD-C2D	-2.19	1.46	1.50
13	1	821	CLA	CMC-C2C	-2.19	1.46	1.50
13	l	207	CLA	C3B-C4B	2.19	1.49	1.42
13	1	823	CLA	C3B-C4B	2.19	1.49	1.42
13	A	830	CLA	C3B-C4B	2.19	1.49	1.42
13	a	807	CLA	C3B-C4B	2.19	1.49	1.42
13	a	830	CLA	C3B-C4B	2.19	1.49	1.42
13	b	837	CLA	CMD-C2D	-2.19	1.46	1.50
13	1	832	CLA	CMD-C2D	-2.19	1.46	1.50
13	2	830	CLA	CHC-C1C	2.19	1.42	1.38
13	a	815	CLA	CHC-C1C	2.19	1.42	1.38
13	1	824	CLA	C3B-C4B	2.19	1.49	1.42
13	a	818	CLA	C3B-C4B	2.19	1.49	1.42
13	b	812	CLA	CMC-C2C	-2.19	1.46	1.50
13	2	829	CLA	CMC-C2C	-2.19	1.46	1.50
13	0	203	CLA	CMD-C2D	-2.19	1.46	1.50
13	1	841	CLA	C3B-C4B	2.19	1.49	1.42
13	a	806	CLA	CHC-C1C	2.19	1.42	1.38
13	L	206	CLA	C3B-C4B	2.19	1.49	1.42
13	b	805	CLA	CMD-C2D	-2.19	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	817	CLA	CHC-C1C	2.19	1.42	1.38
13	j	1103	CLA	CHC-C1C	2.19	1.42	1.38
13	A	822	CLA	MG-NB	-2.19	2.01	2.05
13	a	834	CLA	CMD-C2D	-2.19	1.46	1.50
13	a	832	CLA	C3B-C4B	2.19	1.49	1.42
13	A	832	CLA	C3B-C4B	2.19	1.49	1.42
13	A	842	CLA	MG-NB	-2.19	2.01	2.05
13	B	830	CLA	CMD-C2D	-2.19	1.46	1.50
13	2	846	CLA	CMD-C2D	-2.19	1.46	1.50
13	a	825	CLA	C3B-C4B	2.19	1.49	1.42
13	a	812	CLA	CMD-C2D	-2.19	1.46	1.50
13	a	833	CLA	CMC-C2C	-2.19	1.46	1.50
13	b	830	CLA	CMC-C2C	-2.19	1.46	1.50
13	b	834	CLA	CMD-C2D	-2.19	1.46	1.50
13	B	826	CLA	MG-ND	-2.18	2.01	2.05
13	a	831	CLA	CHC-C1C	2.18	1.42	1.38
13	2	831	CLA	CHC-C1C	2.18	1.42	1.38
13	A	817	CLA	CMD-C2D	-2.18	1.46	1.50
13	a	810	CLA	CHC-C1C	2.18	1.42	1.38
13	1	806	CLA	CHC-C1C	2.18	1.42	1.38
13	a	840	CLA	CMB-C2B	-2.18	1.46	1.50
13	1	841	CLA	CMC-C2C	-2.18	1.46	1.50
13	a	802	CLA	MG-ND	-2.18	2.01	2.05
13	b	831	CLA	C3B-C4B	2.18	1.49	1.42
13	a	816	CLA	CMB-C2B	-2.18	1.46	1.50
13	2	836	CLA	CMD-C2D	-2.18	1.46	1.50
13	b	838	CLA	CMD-C2D	-2.18	1.46	1.50
13	0	205	CLA	CMB-C2B	-2.18	1.46	1.50
13	A	807	CLA	C3B-C4B	2.18	1.49	1.42
13	b	814	CLA	CHC-C1C	2.18	1.42	1.38
13	a	805	CLA	MG-NB	-2.18	2.01	2.05
13	7	102	CLA	CHC-C1C	2.18	1.42	1.38
13	a	831	CLA	CMC-C2C	-2.18	1.46	1.50
13	0	208	CLA	CMD-C2D	-2.18	1.46	1.50
13	A	810	CLA	MG-NB	-2.18	2.01	2.05
13	I	101	CLA	MG-NB	-2.18	2.01	2.05
13	a	824	CLA	C3B-C4B	2.18	1.49	1.42
13	L	201	CLA	MG-NB	-2.18	2.01	2.05
13	A	806	CLA	CHC-C1C	2.18	1.42	1.38
13	1	827	CLA	CHC-C1C	2.18	1.42	1.38
13	A	822	CLA	CMD-C2D	-2.18	1.46	1.50
13	b	836	CLA	C3B-C4B	2.18	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	2	847	BCR	C33-C5	-2.18	1.47	1.50
13	A	816	CLA	CMB-C2B	-2.18	1.46	1.50
13	1	832	CLA	C3B-C4B	2.18	1.49	1.42
13	6	201	CLA	C3B-C4B	2.18	1.49	1.42
13	A	824	CLA	CMD-C2D	-2.18	1.46	1.50
13	B	833	CLA	CMD-C2D	-2.18	1.46	1.50
13	a	807	CLA	CMD-C2D	-2.18	1.46	1.50
13	a	821	CLA	CMC-C2C	-2.18	1.46	1.50
13	1	813	CLA	CMC-C2C	-2.18	1.46	1.50
13	2	827	CLA	CMD-C2D	-2.18	1.46	1.50
13	a	821	CLA	MG-NB	-2.18	2.01	2.05
13	F	201	CLA	MG-NB	-2.18	2.01	2.05
13	l	202	CLA	MG-NB	-2.18	2.01	2.05
13	B	831	CLA	C3B-C4B	2.18	1.49	1.42
13	a	806	CLA	CMD-C2D	-2.18	1.46	1.50
13	2	815	CLA	CMD-C2D	-2.18	1.46	1.50
13	a	841	CLA	CMC-C2C	-2.18	1.46	1.50
13	l	204	CLA	C3B-C4B	2.18	1.49	1.42
13	1	824	CLA	CMD-C2D	-2.17	1.46	1.50
13	2	803	CLA	CMD-C2D	-2.17	1.46	1.50
13	B	814	CLA	CHC-C1C	2.17	1.42	1.38
13	1	810	CLA	MG-NB	-2.17	2.01	2.05
13	a	805	CLA	CMB-C2B	-2.17	1.46	1.50
13	2	833	CLA	CMD-C2D	-2.17	1.46	1.50
13	a	808	CLA	CMC-C2C	-2.17	1.46	1.50
13	a	813	CLA	CMC-C2C	-2.17	1.46	1.50
13	a	842	CLA	CMB-C2B	-2.17	1.46	1.50
13	a	839	CLA	CHC-C1C	2.17	1.42	1.38
13	a	821	CLA	CMB-C2B	-2.17	1.46	1.50
13	j	1101	CLA	CMD-C2D	-2.17	1.46	1.50
13	a	829	CLA	C3B-C4B	2.17	1.49	1.42
13	B	831	CLA	CHC-C1C	2.17	1.42	1.38
13	B	804	CLA	CMD-C2D	-2.17	1.46	1.50
13	f	201	CLA	CMD-C2D	-2.17	1.46	1.50
13	1	829	CLA	C3B-C4B	2.17	1.49	1.42
13	B	813	CLA	MG-NB	-2.17	2.01	2.05
13	f	204	CLA	MG-NB	-2.17	2.01	2.05
13	L	206	CLA	CMD-C2D	-2.17	1.46	1.50
13	b	814	CLA	CMD-C2D	-2.17	1.46	1.50
13	A	816	CLA	CHC-C1C	2.17	1.42	1.38
13	A	831	CLA	CHC-C1C	2.17	1.42	1.38
13	f	201	CLA	MG-NB	-2.17	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	821	CLA	MG-NB	-2.17	2.01	2.05
13	A	839	CLA	CHC-C1C	2.17	1.42	1.38
13	2	813	CLA	CHC-C1C	2.17	1.42	1.38
13	A	818	CLA	C3B-C4B	2.17	1.49	1.42
13	B	830	CLA	CMC-C2C	-2.17	1.46	1.50
13	1	842	CLA	MG-NB	-2.17	2.01	2.05
13	i	102	CLA	C3B-C4B	2.17	1.49	1.42
13	2	830	CLA	C3B-C4B	2.17	1.49	1.42
13	a	809	CLA	CMC-C2C	-2.17	1.46	1.50
13	A	841	CLA	CMC-C2C	-2.17	1.46	1.50
13	I	101	CLA	C3B-C4B	2.17	1.49	1.42
13	b	803	CLA	CMD-C2D	-2.17	1.46	1.50
13	a	807	CLA	MG-NB	-2.17	2.01	2.05
13	B	836	CLA	C3B-C4B	2.17	1.49	1.42
13	2	835	CLA	C3B-C4B	2.17	1.49	1.42
13	1	840	CLA	CMB-C2B	-2.17	1.46	1.50
13	A	842	CLA	CMB-C2B	-2.17	1.46	1.50
13	0	206	CLA	MG-NB	-2.17	2.01	2.05
13	A	819	CLA	CMC-C2C	-2.17	1.46	1.50
13	b	829	CLA	CMD-C2D	-2.17	1.46	1.50
13	1	834	CLA	CMD-C2D	-2.17	1.46	1.50
13	2	832	CLA	CMB-C2B	-2.17	1.46	1.50
13	a	837	CLA	CHC-C1C	2.17	1.42	1.38
13	A	824	CLA	CHC-C1C	2.16	1.42	1.38
13	b	847	CLA	CMC-C2C	-2.16	1.46	1.50
13	F	203	CLA	CMB-C2B	-2.16	1.46	1.50
13	b	833	CLA	CMB-C2B	-2.16	1.46	1.50
13	0	206	CLA	CMD-C2D	-2.16	1.46	1.50
13	2	806	CLA	C3B-C4B	2.16	1.49	1.42
13	a	817	CLA	CMD-C2D	-2.16	1.46	1.50
13	2	812	CLA	MG-NB	-2.16	2.01	2.05
13	2	830	CLA	CMB-C2B	-2.16	1.46	1.50
13	a	816	CLA	CHC-C1C	2.16	1.42	1.38
13	A	830	CLA	CMC-C2C	-2.16	1.46	1.50
13	a	819	CLA	CMD-C2D	-2.16	1.46	1.50
13	l	205	CLA	CMD-C2D	-2.16	1.46	1.50
13	1	842	CLA	CMB-C2B	-2.16	1.46	1.50
13	a	810	CLA	MG-NB	-2.16	2.01	2.05
13	b	813	CLA	MG-NB	-2.16	2.01	2.05
13	k	4002	CLA	MG-NB	-2.16	2.01	2.05
13	1	821	CLA	MG-NB	-2.16	2.01	2.05
13	B	803	CLA	CMD-C2D	-2.16	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	1	806	CLA	CMD-C2D	-2.16	1.46	1.50
13	A	819	CLA	CMD-C2D	-2.16	1.46	1.50
13	a	833	CLA	CMB-C2B	-2.16	1.46	1.50
13	6	204	CLA	MG-NB	-2.16	2.01	2.05
13	1	819	CLA	CHC-C1C	2.16	1.42	1.38
13	B	833	CLA	CMB-C2B	-2.16	1.46	1.50
13	2	804	CLA	CMD-C2D	-2.16	1.46	1.50
13	1	826	CLA	CMC-C2C	-2.16	1.46	1.50
13	L	204	CLA	MG-NB	-2.16	2.01	2.05
13	a	835	CLA	CMB-C2B	-2.16	1.46	1.50
13	A	805	CLA	CMB-C2B	-2.16	1.46	1.50
13	l	207	CLA	CMD-C2D	-2.16	1.46	1.50
13	1	830	CLA	CMC-C2C	-2.16	1.46	1.50
13	0	205	CLA	CMD-C2D	-2.16	1.46	1.50
13	A	829	CLA	C3B-C4B	2.16	1.49	1.42
13	b	809	CLA	CHC-C1C	2.16	1.42	1.38
13	a	809	CLA	CMB-C2B	-2.16	1.46	1.50
16	B	848	BCR	C33-C5	-2.16	1.47	1.50
13	A	833	CLA	CMC-C2C	-2.16	1.46	1.50
13	B	835	CLA	CMB-C2B	-2.16	1.46	1.50
13	b	816	CLA	CMD-C2D	-2.16	1.46	1.50
13	1	824	CLA	CHC-C1C	2.16	1.42	1.38
13	1	837	CLA	CHC-C1C	2.16	1.42	1.38
13	A	802	CLA	MG-ND	-2.16	2.01	2.05
13	a	824	CLA	CMB-C2B	-2.16	1.46	1.50
13	B	809	CLA	CHC-C1C	2.16	1.42	1.38
13	B	817	CLA	CHC-C1C	2.16	1.42	1.38
13	a	821	CLA	CHC-C1C	2.16	1.42	1.38
13	1	802	CLA	MG-ND	-2.16	2.01	2.05
13	B	805	CLA	CMD-C2D	-2.16	1.46	1.50
13	a	819	CLA	CMC-C2C	-2.16	1.46	1.50
13	2	823	CLA	MG-ND	-2.16	2.01	2.05
13	2	832	CLA	CMD-C2D	-2.16	1.46	1.50
13	F	204	CLA	MG-NB	-2.16	2.01	2.05
13	b	824	CLA	MG-ND	-2.16	2.01	2.05
13	A	826	CLA	CMC-C2C	-2.16	1.46	1.50
13	B	807	CLA	CHC-C1C	2.16	1.42	1.38
13	2	816	CLA	CHC-C1C	2.16	1.42	1.38
13	7	102	CLA	C3B-C4B	2.16	1.49	1.42
16	b	848	BCR	C33-C5	-2.16	1.47	1.50
13	A	808	CLA	CMD-C2D	-2.16	1.46	1.50
13	a	838	CLA	CMD-C2D	-2.16	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	808	CLA	CMD-C2D	-2.15	1.46	1.50
13	1	805	CLA	CMB-C2B	-2.15	1.46	1.50
13	1	821	CLA	CMB-C2B	-2.15	1.46	1.50
13	B	831	CLA	CMB-C2B	-2.15	1.46	1.50
13	6	203	CLA	CMB-C2B	-2.15	1.46	1.50
13	K	4002	CLA	MG-NB	-2.15	2.01	2.05
13	A	823	CLA	CHC-C1C	2.15	1.42	1.38
13	B	806	CLA	C3B-C4B	2.15	1.49	1.42
13	1	818	CLA	C3B-C4B	2.15	1.49	1.42
13	l	202	CLA	CMC-C2C	-2.15	1.46	1.50
13	1	818	CLA	CMD-C2D	-2.15	1.46	1.50
13	1	816	CLA	CHC-C1C	2.15	1.42	1.38
13	B	828	CLA	CMD-C2D	-2.15	1.46	1.50
13	J	1101	CLA	MG-NB	-2.15	2.01	2.05
13	A	805	CLA	CHC-C1C	2.15	1.42	1.38
16	1	846	BCR	C33-C5	-2.15	1.47	1.50
13	B	838	CLA	CMD-C2D	-2.15	1.46	1.50
13	B	824	CLA	MG-ND	-2.15	2.01	2.05
13	0	202	CLA	MG-NB	-2.15	2.01	2.05
13	0	205	CLA	C3B-C4B	2.15	1.49	1.42
13	A	824	CLA	CMB-C2B	-2.15	1.46	1.50
13	B	829	CLA	CMD-C2D	-2.15	1.46	1.50
13	a	829	CLA	CMB-C2B	-2.15	1.46	1.50
13	2	815	CLA	CHC-C1C	2.15	1.42	1.38
13	2	834	CLA	C3B-C4B	2.15	1.49	1.42
13	j	1101	CLA	MG-NB	-2.15	2.01	2.05
13	a	823	CLA	CHC-C1C	2.15	1.42	1.38
13	a	817	CLA	MG-NB	-2.15	2.01	2.05
13	0	205	CLA	CHC-C1C	2.15	1.42	1.38
13	A	806	CLA	CMD-C2D	-2.15	1.46	1.50
13	a	822	CLA	MG-NB	-2.15	2.01	2.05
13	A	808	CLA	CMC-C2C	-2.15	1.46	1.50
13	1	808	CLA	CMC-C2C	-2.15	1.46	1.50
13	1	812	CLA	CMD-C2D	-2.15	1.46	1.50
13	L	203	CLA	C3B-C4B	2.15	1.49	1.42
13	1	817	CLA	MG-NB	-2.15	2.01	2.05
13	b	807	CLA	CHC-C1C	2.15	1.42	1.38
13	1	816	CLA	CMB-C2B	-2.15	1.46	1.50
13	b	806	CLA	C3B-C4B	2.15	1.49	1.42
13	1	840	CLA	CHC-C1C	2.15	1.42	1.38
13	A	821	CLA	CMB-C2B	-2.15	1.46	1.50
13	b	812	CLA	CMD-C2D	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	2	822	CLA	CMB-C2B	-2.15	1.46	1.50
13	1	207	CLA	CHC-C1C	2.15	1.42	1.38
13	1	839	CLA	CHC-C1C	2.15	1.42	1.38
13	2	822	CLA	CHC-C1C	2.15	1.42	1.38
13	L	203	CLA	CMD-C2D	-2.15	1.46	1.50
13	2	805	CLA	CMD-C2D	-2.15	1.46	1.50
13	1	205	CLA	CHC-C1C	2.15	1.42	1.38
13	1	831	CLA	CHC-C1C	2.15	1.42	1.38
13	i	102	CLA	MG-NB	-2.15	2.01	2.05
13	a	815	CLA	CMC-C2C	-2.15	1.46	1.50
13	2	818	CLA	CHC-C1C	2.15	1.42	1.38
13	f	201	CLA	CMB-C2B	-2.15	1.46	1.50
13	6	201	CLA	MG-NB	-2.15	2.01	2.05
13	1	819	CLA	CMD-C2D	-2.15	1.46	1.50
13	2	810	CLA	CMC-C2C	-2.15	1.46	1.50
13	1	821	CLA	CHC-C1C	2.14	1.42	1.38
13	A	809	CLA	MG-NB	-2.14	2.01	2.05
13	B	816	CLA	CMD-C2D	-2.14	1.46	1.50
13	a	842	CLA	CMC-C2C	-2.14	1.46	1.50
13	1	810	CLA	CMD-C2D	-2.14	1.46	1.50
13	1	831	CLA	CMC-C2C	-2.14	1.46	1.50
17	1	850	LHG	O7-C5	-2.14	1.41	1.46
13	2	833	CLA	C3B-C4B	2.14	1.49	1.42
13	L	206	CLA	CHC-C1C	2.14	1.42	1.38
13	a	805	CLA	CHC-C1C	2.14	1.42	1.38
13	2	825	CLA	MG-ND	-2.14	2.01	2.05
13	A	818	CLA	CMD-C2D	-2.14	1.46	1.50
13	B	834	CLA	C3B-C4B	2.14	1.49	1.42
13	1	205	CLA	MG-NB	-2.14	2.01	2.05
13	L	204	CLA	CMD-C2D	-2.14	1.46	1.50
13	b	808	CLA	CMB-C2B	-2.14	1.46	1.50
13	B	811	CLA	CMC-C2C	-2.14	1.46	1.50
13	a	811	CLA	CMB-C2B	-2.14	1.46	1.50
13	1	833	CLA	CMC-C2C	-2.14	1.46	1.50
13	9	4002	CLA	MG-NB	-2.14	2.01	2.05
13	A	834	CLA	MG-NB	-2.14	2.01	2.05
13	A	831	CLA	CMC-C2C	-2.14	1.46	1.50
13	B	835	CLA	C3B-C4B	2.14	1.49	1.42
13	2	820	CLA	CMB-C2B	-2.14	1.46	1.50
13	1	806	CLA	CMB-C2B	-2.14	1.46	1.50
13	8	1101	CLA	MG-NB	-2.14	2.01	2.05
13	1	802	CLA	CHC-C1C	2.14	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	809	CLA	CMB-C2B	-2.14	1.46	1.50
13	b	831	CLA	CMB-C2B	-2.14	1.46	1.50
13	b	835	CLA	C3B-C4B	2.14	1.49	1.42
13	L	203	CLA	CHC-C1C	2.14	1.42	1.38
13	b	818	CLA	CHC-C1C	2.14	1.42	1.38
13	B	808	CLA	MG-NB	-2.14	2.01	2.05
13	a	817	CLA	CMB-C2B	-2.14	1.46	1.50
13	A	837	CLA	CHC-C1C	2.14	1.42	1.38
13	B	847	CLA	CMC-C2C	-2.14	1.46	1.50
13	b	811	CLA	CMC-C2C	-2.14	1.46	1.50
13	b	808	CLA	MG-NB	-2.14	2.01	2.05
13	A	806	CLA	CMB-C2B	-2.14	1.46	1.50
13	2	828	CLA	CMD-C2D	-2.14	1.46	1.50
13	2	834	CLA	CMB-C2B	-2.14	1.46	1.50
13	b	819	CLA	CHC-C1C	2.14	1.42	1.38
13	A	833	CLA	CMB-C2B	-2.14	1.46	1.50
13	a	833	CLA	CMD-C2D	-2.14	1.46	1.50
13	1	824	CLA	CMB-C2B	-2.14	1.46	1.50
13	l	204	CLA	CHC-C1C	2.14	1.42	1.38
13	B	808	CLA	CMB-C2B	-2.14	1.46	1.50
13	A	817	CLA	MG-NB	-2.14	2.01	2.05
13	A	815	CLA	CMC-C2C	-2.13	1.46	1.50
13	2	829	CLA	CMD-C2D	-2.13	1.46	1.50
13	a	809	CLA	MG-NB	-2.13	2.01	2.05
13	1	834	CLA	MG-NB	-2.13	2.01	2.05
13	A	829	CLA	CMB-C2B	-2.13	1.46	1.50
13	a	806	CLA	CMB-C2B	-2.13	1.46	1.50
13	f	203	CLA	CMB-C2B	-2.13	1.46	1.50
13	2	808	CLA	CHC-C1C	2.13	1.42	1.38
13	0	203	CLA	CHC-C1C	2.13	1.42	1.38
13	a	834	CLA	MG-NB	-2.13	2.01	2.05
13	A	842	CLA	CMC-C2C	-2.13	1.46	1.50
13	A	802	CLA	CHC-C1C	2.13	1.42	1.38
13	b	826	CLA	MG-ND	-2.13	2.01	2.05
13	1	838	CLA	CMD-C2D	-2.13	1.46	1.50
13	0	202	CLA	CMC-C2C	-2.13	1.46	1.50
13	f	201	CLA	CHC-C1C	2.13	1.42	1.38
13	B	821	CLA	CMB-C2B	-2.13	1.46	1.50
13	B	847	CLA	C3B-C4B	2.13	1.49	1.42
13	a	824	CLA	CMD-C2D	-2.13	1.46	1.50
13	A	838	CLA	CMD-C2D	-2.13	1.46	1.50
13	0	208	CLA	CHC-C1C	2.13	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	812	CLA	CMD-C2D	-2.13	1.46	1.50
13	a	818	CLA	CMD-C2D	-2.13	1.46	1.50
13	1	834	CLA	CHC-C1C	2.13	1.42	1.38
13	A	807	CLA	MG-NB	-2.13	2.01	2.05
13	a	839	CLA	CMD-C2D	-2.13	1.46	1.50
13	2	807	CLA	CMB-C2B	-2.13	1.46	1.50
13	L	204	CLA	CMB-C2B	-2.13	1.46	1.50
13	B	816	CLA	CHC-C1C	2.13	1.42	1.38
13	B	818	CLA	CHC-C1C	2.13	1.42	1.38
13	A	814	CLA	CMD-C2D	-2.13	1.46	1.50
13	A	815	CLA	CMD-C2D	-2.13	1.46	1.50
13	F	201	CLA	CMB-C2B	-2.13	1.46	1.50
13	A	821	CLA	CHC-C1C	2.13	1.42	1.38
13	L	204	CLA	CHC-C1C	2.13	1.42	1.38
13	a	802	CLA	CHC-C1C	2.13	1.42	1.38
13	K	4005	CLA	MG-NB	-2.13	2.01	2.05
13	k	4005	CLA	MG-NB	-2.13	2.01	2.05
13	A	837	CLA	CMD-C2D	-2.13	1.46	1.50
13	b	801	CLA	CMB-C2B	-2.13	1.46	1.50
13	l	204	CLA	CMD-C2D	-2.13	1.46	1.50
13	a	836	CLA	MG-ND	-2.13	2.01	2.05
13	b	813	CLA	CMD-C2D	-2.13	1.46	1.50
13	b	847	CLA	C3B-C4B	2.13	1.48	1.42
13	1	815	CLA	CMC-C2C	-2.13	1.46	1.50
13	B	808	CLA	CHC-C1C	2.13	1.42	1.38
13	B	823	CLA	CMB-C2B	-2.13	1.46	1.50
13	b	805	CLA	CMC-C2C	-2.13	1.46	1.50
13	2	837	CLA	CMD-C2D	-2.13	1.46	1.50
13	2	807	CLA	CHC-C1C	2.13	1.42	1.38
13	6	201	CLA	CHC-C1C	2.13	1.42	1.38
13	A	811	CLA	CMB-C2B	-2.13	1.46	1.50
13	L	201	CLA	CMC-C2C	-2.13	1.46	1.50
13	1	811	CLA	CMB-C2B	-2.13	1.46	1.50
13	2	824	CLA	CMC-C2C	-2.13	1.46	1.50
13	A	841	CLA	MG-NB	-2.13	2.01	2.05
13	A	807	CLA	CMD-C2D	-2.12	1.46	1.50
13	2	811	CLA	CMD-C2D	-2.12	1.46	1.50
13	0	206	CLA	CMB-C2B	-2.12	1.46	1.50
13	A	838	CLA	CMB-C2B	-2.12	1.46	1.50
13	1	833	CLA	CMD-C2D	-2.12	1.46	1.50
13	0	206	CLA	CHC-C1C	2.12	1.42	1.38
13	B	804	CLA	CMB-C2B	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	839	CLA	CMB-C2B	-2.12	1.46	1.50
13	b	823	CLA	CMB-C2B	-2.12	1.46	1.50
13	b	826	CLA	C3B-C4B	2.12	1.48	1.42
13	2	818	CLA	MG-NB	-2.12	2.01	2.05
13	b	809	CLA	CMD-C2D	-2.12	1.46	1.50
13	1	852	CLA	CMD-C2D	-2.12	1.46	1.50
13	9	4005	CLA	MG-NB	-2.12	2.01	2.05
13	B	805	CLA	CMC-C2C	-2.12	1.46	1.50
13	A	810	CLA	CMD-C2D	-2.12	1.46	1.50
13	B	820	CLA	CMB-C2B	-2.12	1.46	1.50
13	0	202	CLA	CMD-C2D	-2.12	1.46	1.50
13	a	834	CLA	CHC-C1C	2.12	1.42	1.38
13	a	837	CLA	CMD-C2D	-2.12	1.46	1.50
17	A	850	LHG	O7-C5	-2.12	1.41	1.46
13	A	810	CLA	CMB-C2B	-2.12	1.46	1.50
13	L	206	CLA	CMB-C2B	-2.12	1.46	1.50
13	2	804	CLA	CMB-C2B	-2.12	1.46	1.50
13	1	823	CLA	CHC-C1C	2.12	1.42	1.38
13	B	813	CLA	CMD-C2D	-2.12	1.46	1.50
13	a	838	CLA	CMB-C2B	-2.12	1.46	1.50
13	2	807	CLA	MG-NB	-2.12	2.01	2.05
13	b	809	CLA	CMB-C2B	-2.12	1.46	1.50
13	2	808	CLA	CMD-C2D	-2.12	1.46	1.50
13	B	819	CLA	CHC-C1C	2.12	1.42	1.38
13	A	839	CLA	CMD-C2D	-2.12	1.46	1.50
13	B	801	CLA	CMB-C2B	-2.12	1.46	1.50
13	8	1103	CLA	CMD-C2D	-2.12	1.46	1.50
13	a	812	CLA	CHC-C1C	2.12	1.42	1.38
13	a	814	CLA	CMD-C2D	-2.12	1.46	1.50
13	a	826	CLA	CMC-C2C	-2.12	1.46	1.50
13	1	815	CLA	CMD-C2D	-2.12	1.46	1.50
13	1	817	CLA	CMB-C2B	-2.12	1.46	1.50
13	2	828	CLA	CMC-C2C	-2.12	1.46	1.50
13	F	201	CLA	CHC-C1C	2.12	1.42	1.38
13	a	840	CLA	CHC-C1C	2.12	1.42	1.38
13	a	810	CLA	CMB-C2B	-2.12	1.46	1.50
13	1	807	CLA	CMD-C2D	-2.12	1.46	1.50
13	1	809	CLA	CMB-C2B	-2.12	1.46	1.50
13	2	811	CLA	CMB-C2B	-2.12	1.46	1.50
13	2	836	CLA	C3B-C4B	2.12	1.48	1.42
13	A	840	CLA	CHC-C1C	2.12	1.42	1.38
13	b	808	CLA	CHC-C1C	2.12	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	819	CLA	MG-NB	-2.12	2.01	2.05
13	j	1103	CLA	MG-NB	-2.12	2.01	2.05
16	A	846	BCR	C33-C5	-2.12	1.47	1.50
13	K	4005	CLA	CMD-C2D	-2.12	1.46	1.50
13	a	815	CLA	CMD-C2D	-2.12	1.46	1.50
13	2	814	CLA	CMB-C2B	-2.11	1.46	1.50
13	6	201	CLA	CMB-C2B	-2.11	1.46	1.50
13	A	834	CLA	CHC-C1C	2.11	1.42	1.38
13	1	841	CLA	MG-NB	-2.11	2.01	2.05
13	B	837	CLA	C3B-C4B	2.11	1.48	1.42
13	1	829	CLA	CMB-C2B	-2.11	1.46	1.50
13	1	805	CLA	CHC-C1C	2.11	1.42	1.38
13	1	812	CLA	CHC-C1C	2.11	1.42	1.38
13	B	809	CLA	CMB-C2B	-2.11	1.46	1.50
13	B	809	CLA	CMD-C2D	-2.11	1.46	1.50
13	2	846	CLA	C3B-C4B	2.11	1.48	1.42
13	B	812	CLA	CMB-C2B	-2.11	1.46	1.50
13	a	804	CLA	CMD-C2D	-2.11	1.46	1.50
13	1	814	CLA	CMD-C2D	-2.11	1.46	1.50
13	2	814	CLA	CMC-C2C	-2.11	1.46	1.50
13	b	805	CLA	C3B-C4B	2.11	1.48	1.42
13	A	840	CLA	CMC-C2C	-2.11	1.46	1.50
13	B	827	CLA	CMD-C2D	-2.11	1.46	1.50
13	B	826	CLA	C3B-C4B	2.11	1.48	1.42
13	B	825	CLA	CMC-C2C	-2.11	1.46	1.50
13	2	819	CLA	CMB-C2B	-2.11	1.46	1.50
13	9	4005	CLA	CMD-C2D	-2.11	1.46	1.50
13	0	208	CLA	CMB-C2B	-2.11	1.46	1.50
13	b	834	CLA	C3B-C4B	2.11	1.48	1.42
19	7	101	SQD	O2-C2	-2.11	1.37	1.43
13	A	852	CLA	CMD-C2D	-2.11	1.46	1.50
13	K	4003	CLA	CMD-C2D	-2.11	1.46	1.50
13	b	815	CLA	CMD-C2D	-2.11	1.46	1.50
13	B	812	CLA	CMD-C2D	-2.11	1.46	1.50
13	B	823	CLA	CHC-C1C	2.11	1.42	1.38
13	B	819	CLA	MG-NB	-2.11	2.01	2.05
13	a	852	CLA	CMD-C2D	-2.11	1.46	1.50
13	l	202	CLA	CMD-C2D	-2.11	1.46	1.50
13	1	839	CLA	CMD-C2D	-2.11	1.46	1.50
13	b	815	CLA	CMB-C2B	-2.11	1.46	1.50
13	j	1101	CLA	CMB-C2B	-2.11	1.46	1.50
13	1	833	CLA	CMB-C2B	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	1	810	CLA	CMB-C2B	-2.11	1.46	1.50
13	B	838	CLA	MG-NB	-2.11	2.01	2.05
13	L	201	CLA	CMD-C2D	-2.11	1.46	1.50
13	2	846	CLA	CMC-C2C	-2.11	1.46	1.50
13	1	842	CLA	CMC-C2C	-2.11	1.46	1.50
13	b	807	CLA	CMB-C2B	-2.11	1.46	1.50
13	A	833	CLA	CMD-C2D	-2.11	1.46	1.50
13	b	835	CLA	CMB-C2B	-2.11	1.46	1.50
13	8	1101	CLA	CMB-C2B	-2.11	1.46	1.50
13	a	841	CLA	MG-NB	-2.11	2.01	2.05
13	b	836	CLA	CHC-C1C	2.11	1.42	1.38
13	B	815	CLA	CMC-C2C	-2.11	1.46	1.50
13	b	808	CLA	CMD-C2D	-2.11	1.46	1.50
16	a	846	BCR	C33-C5	-2.10	1.47	1.50
13	B	815	CLA	CMD-C2D	-2.10	1.46	1.50
13	B	818	CLA	CMD-C2D	-2.10	1.46	1.50
13	1	207	CLA	CMB-C2B	-2.10	1.46	1.50
13	2	825	CLA	C3B-C4B	2.10	1.48	1.42
13	J	1101	CLA	CMB-C2B	-2.10	1.46	1.50
13	b	828	CLA	CMB-C2B	-2.10	1.46	1.50
13	2	807	CLA	CMD-C2D	-2.10	1.46	1.50
13	B	836	CLA	CHC-C1C	2.10	1.42	1.38
13	B	808	CLA	CMD-C2D	-2.10	1.46	1.50
13	a	840	CLA	CMC-C2C	-2.10	1.46	1.50
13	8	1103	CLA	CMB-C2B	-2.10	1.46	1.50
13	1	205	CLA	CMB-C2B	-2.10	1.46	1.50
13	1	812	CLA	CMB-C2B	-2.10	1.46	1.50
13	b	837	CLA	C3B-C4B	2.10	1.48	1.42
13	A	817	CLA	CMB-C2B	-2.10	1.46	1.50
13	A	839	CLA	CMB-C2B	-2.10	1.46	1.50
13	f	203	CLA	CMD-C2D	-2.10	1.46	1.50
13	b	804	CLA	CMB-C2B	-2.10	1.46	1.50
13	1	840	CLA	CMC-C2C	-2.10	1.46	1.50
13	B	815	CLA	CMB-C2B	-2.10	1.46	1.50
13	2	805	CLA	CMC-C2C	-2.10	1.46	1.50
13	B	817	CLA	CMD-C2D	-2.10	1.46	1.50
13	a	826	CLA	CMB-C2B	-2.10	1.46	1.50
13	1	839	CLA	CMB-C2B	-2.10	1.46	1.50
13	b	815	CLA	CMC-C2C	-2.10	1.46	1.50
13	1	836	CLA	CMB-C2B	-2.10	1.46	1.50
13	b	818	CLA	CMD-C2D	-2.10	1.46	1.50
13	2	814	CLA	CMD-C2D	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	2	817	CLA	CMD-C2D	-2.10	1.46	1.50
19	i	101	SQD	O2-C2	-2.10	1.37	1.43
13	1	809	CLA	MG-NB	-2.10	2.01	2.05
13	B	831	CLA	CMD-C2D	-2.10	1.46	1.50
13	a	814	CLA	CMB-C2B	-2.10	1.46	1.50
13	1	838	CLA	CMB-C2B	-2.09	1.46	1.50
13	B	805	CLA	C3B-C4B	2.09	1.48	1.42
13	b	820	CLA	CMB-C2B	-2.09	1.46	1.50
13	2	812	CLA	CMD-C2D	-2.09	1.46	1.50
13	b	838	CLA	MG-NB	-2.09	2.01	2.05
13	B	828	CLA	CMB-C2B	-2.09	1.46	1.50
13	b	827	CLA	CMD-C2D	-2.09	1.46	1.50
13	6	203	CLA	CMD-C2D	-2.09	1.46	1.50
13	b	816	CLA	CHC-C1C	2.09	1.42	1.38
13	1	803	CLA	CHC-C1C	2.09	1.42	1.38
13	A	836	CLA	MG-ND	-2.09	2.01	2.05
13	A	826	CLA	CMB-C2B	-2.09	1.46	1.50
13	F	203	CLA	CMD-C2D	-2.09	1.46	1.50
13	B	822	CLA	CMC-C2C	-2.09	1.46	1.50
13	b	807	CLA	CMC-C2C	-2.09	1.46	1.50
13	k	4003	CLA	CMB-C2B	-2.09	1.46	1.50
13	1	804	CLA	CMB-C2B	-2.09	1.46	1.50
13	b	825	CLA	CMC-C2C	-2.09	1.46	1.50
13	1	837	CLA	CMD-C2D	-2.09	1.46	1.50
13	A	812	CLA	CHC-C1C	2.09	1.42	1.38
13	2	817	CLA	CHC-C1C	2.09	1.42	1.38
13	b	802	CLA	MG-ND	-2.09	2.01	2.05
13	2	808	CLA	CMB-C2B	-2.09	1.46	1.50
13	2	815	CLA	CMC-C2C	-2.09	1.46	1.50
13	A	835	CLA	CMD-C2D	-2.09	1.46	1.50
13	b	831	CLA	CMD-C2D	-2.09	1.46	1.50
13	A	816	CLA	MG-NB	-2.09	2.01	2.05
19	I	103	SQD	O2-C2	-2.09	1.37	1.43
13	k	4005	CLA	CMB-C2B	-2.09	1.46	1.50
13	b	821	CLA	CMB-C2B	-2.09	1.46	1.50
13	1	823	CLA	CMB-C2B	-2.09	1.46	1.50
17	a	850	LHG	O7-C5	-2.09	1.41	1.46
13	2	805	CLA	C3B-C4B	2.09	1.48	1.42
13	1	807	CLA	MG-NB	-2.09	2.01	2.05
13	1	839	CLA	CMC-C2C	-2.09	1.46	1.50
13	9	4003	CLA	CMD-C2D	-2.09	1.46	1.50
13	a	830	CLA	CHC-C1C	2.09	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	807	CLA	CMB-C2B	-2.09	1.46	1.50
13	B	826	CLA	CMC-C2C	-2.09	1.46	1.50
13	k	4005	CLA	CMD-C2D	-2.09	1.46	1.50
13	j	1102	CLA	MG-NB	-2.09	2.01	2.05
13	l	832	CLA	CMC-C2C	-2.09	1.46	1.50
13	K	4005	CLA	CMB-C2B	-2.09	1.46	1.50
13	a	832	CLA	CMC-C2C	-2.09	1.46	1.50
13	1	826	CLA	CMB-C2B	-2.09	1.46	1.50
13	2	833	CLA	CHC-C1C	2.09	1.42	1.38
13	9	4005	CLA	CMB-C2B	-2.09	1.46	1.50
13	J	1103	CLA	MG-NB	-2.09	2.01	2.05
13	2	816	CLA	CMD-C2D	-2.09	1.46	1.50
13	2	837	CLA	MG-NB	-2.09	2.01	2.05
13	A	804	CLA	MG-NB	-2.09	2.01	2.05
13	1	804	CLA	MG-NB	-2.09	2.01	2.05
13	a	804	CLA	MG-NB	-2.08	2.01	2.05
13	A	823	CLA	CMB-C2B	-2.08	1.46	1.50
13	A	852	CLA	CMC-C2C	-2.08	1.46	1.50
13	B	807	CLA	CMC-C2C	-2.08	1.46	1.50
13	1	842	CLA	CMD-C2D	-2.08	1.46	1.50
13	2	825	CLA	CMC-C2C	-2.08	1.46	1.50
13	i	102	CLA	CMD-C2D	-2.08	1.46	1.50
13	b	812	CLA	CMB-C2B	-2.08	1.46	1.50
13	2	826	CLA	CMD-C2D	-2.08	1.46	1.50
13	J	1102	CLA	MG-NB	-2.08	2.01	2.05
13	1	836	CLA	MG-ND	-2.08	2.01	2.05
13	2	801	CLA	CMB-C2B	-2.08	1.46	1.50
13	B	824	CLA	CHC-C1C	2.08	1.42	1.38
13	B	834	CLA	CHC-C1C	2.08	1.42	1.38
13	a	810	CLA	CMD-C2D	-2.08	1.46	1.50
13	0	205	CLA	CMC-C2C	-2.08	1.46	1.50
13	a	812	CLA	CMB-C2B	-2.08	1.46	1.50
13	j	1103	CLA	CMD-C2D	-2.08	1.46	1.50
13	1	814	CLA	CMC-C2C	-2.08	1.46	1.50
13	b	832	CLA	CMD-C2D	-2.08	1.46	1.50
13	A	804	CLA	CMD-C2D	-2.08	1.46	1.50
13	b	817	CLA	CMD-C2D	-2.08	1.46	1.50
13	B	827	CLA	CMC-C2C	-2.08	1.46	1.50
13	2	835	CLA	CHC-C1C	2.08	1.42	1.38
13	1	837	CLA	CMC-C2C	-2.08	1.46	1.50
13	A	804	CLA	CMB-C2B	-2.08	1.46	1.50
13	I	101	CLA	CMD-C2D	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	829	CLA	CMC-C2C	-2.08	1.46	1.50
13	0	203	CLA	CMC-C2C	-2.08	1.46	1.50
13	1	838	CLA	C3B-C4B	2.08	1.48	1.42
13	a	803	CLA	CHC-C1C	2.08	1.42	1.38
13	b	814	CLA	CMC-C2C	-2.08	1.46	1.50
13	2	831	CLA	CMD-C2D	-2.08	1.46	1.50
13	b	827	CLA	CMC-C2C	-2.08	1.46	1.50
13	9	4003	CLA	CMB-C2B	-2.08	1.46	1.50
13	A	830	CLA	CHC-C1C	2.08	1.42	1.38
13	f	203	CLA	MG-NB	-2.08	2.01	2.05
13	a	804	CLA	CMB-C2B	-2.08	1.46	1.50
13	b	823	CLA	CHC-C1C	2.08	1.42	1.38
13	a	838	CLA	C3B-C4B	2.08	1.48	1.42
13	F	203	CLA	MG-NB	-2.08	2.01	2.05
13	L	204	CLA	CMC-C2C	-2.08	1.46	1.50
13	1	827	CLA	CMC-C2C	-2.08	1.46	1.50
13	2	826	CLA	CMC-C2C	-2.08	1.46	1.50
13	a	835	CLA	CMD-C2D	-2.08	1.46	1.50
13	K	4003	CLA	CMB-C2B	-2.08	1.46	1.50
13	2	816	CLA	CMB-C2B	-2.08	1.46	1.50
13	2	827	CLA	CMB-C2B	-2.08	1.46	1.50
13	A	812	CLA	CMB-C2B	-2.07	1.46	1.50
13	A	814	CLA	CMB-C2B	-2.07	1.46	1.50
13	A	836	CLA	CMC-C2C	-2.07	1.46	1.50
13	J	1103	CLA	CMB-C2B	-2.07	1.46	1.50
13	2	830	CLA	CMD-C2D	-2.07	1.46	1.50
13	a	852	CLA	CMC-C2C	-2.07	1.46	1.50
13	2	822	CLA	MG-NB	-2.07	2.01	2.05
13	J	1103	CLA	CMD-C2D	-2.07	1.46	1.50
13	1	824	CLA	CMC-C2C	-2.07	1.46	1.50
13	a	838	CLA	CHC-C1C	2.07	1.42	1.38
13	1	802	CLA	C1B-NB	-2.07	1.35	1.37
13	a	811	CLA	CMC-C2C	-2.07	1.46	1.50
13	1	804	CLA	CMC-C2C	-2.07	1.46	1.50
13	A	824	CLA	CMC-C2C	-2.07	1.46	1.50
13	B	829	CLA	CMC-C2C	-2.07	1.46	1.50
13	B	816	CLA	CMC-C2C	-2.07	1.46	1.50
13	1	836	CLA	CMC-C2C	-2.07	1.46	1.50
13	A	807	CLA	CMB-C2B	-2.07	1.46	1.50
13	b	802	CLA	CMB-C2B	-2.07	1.46	1.50
13	b	817	CLA	CMB-C2B	-2.07	1.46	1.50
13	A	814	CLA	CMC-C2C	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	842	CLA	CMD-C2D	-2.07	1.46	1.50
13	f	204	CLA	CMB-C2B	-2.07	1.46	1.50
13	1	835	CLA	CMD-C2D	-2.07	1.46	1.50
13	A	838	CLA	C3B-C4B	2.07	1.48	1.42
13	a	803	CLA	C3B-C4B	2.07	1.48	1.42
13	A	832	CLA	CMC-C2C	-2.07	1.46	1.50
13	2	809	CLA	CMD-C2D	-2.07	1.46	1.50
13	b	816	CLA	CMC-C2C	-2.07	1.46	1.50
13	1	809	CLA	C3B-C4B	2.07	1.48	1.42
13	2	818	CLA	CMB-C2B	-2.07	1.46	1.50
13	6	204	CLA	CMB-C2B	-2.07	1.46	1.50
13	1	852	CLA	CMC-C2C	-2.07	1.46	1.50
13	b	834	CLA	CHC-C1C	2.06	1.42	1.38
13	k	4003	CLA	CMD-C2D	-2.06	1.46	1.50
13	1	803	CLA	C3B-C4B	2.06	1.48	1.42
13	2	823	CLA	CHC-C1C	2.06	1.42	1.38
13	B	814	CLA	CMC-C2C	-2.06	1.46	1.50
13	b	822	CLA	CMC-C2C	-2.06	1.46	1.50
13	2	817	CLA	CMC-C2C	-2.06	1.46	1.50
13	a	836	CLA	CMC-C2C	-2.06	1.46	1.50
13	a	839	CLA	CMC-C2C	-2.06	1.46	1.50
13	2	821	CLA	CMC-C2C	-2.06	1.46	1.50
13	8	1102	CLA	MG-NB	-2.06	2.01	2.05
13	B	832	CLA	CMD-C2D	-2.06	1.46	1.50
13	A	827	CLA	CMC-C2C	-2.06	1.46	1.50
13	B	810	CLA	CMD-C2D	-2.06	1.46	1.50
13	a	823	CLA	CMB-C2B	-2.06	1.46	1.50
13	a	827	CLA	CMC-C2C	-2.06	1.46	1.50
13	a	837	CLA	CMC-C2C	-2.06	1.46	1.50
13	a	821	CLA	CMD-C2D	-2.06	1.46	1.50
13	2	802	CLA	CMB-C2B	-2.06	1.46	1.50
13	2	823	CLA	C3B-C4B	2.06	1.48	1.42
13	L	203	CLA	CMC-C2C	-2.06	1.46	1.50
13	b	826	CLA	CMC-C2C	-2.06	1.46	1.50
13	1	827	CLA	CMB-C2B	-2.06	1.46	1.50
13	b	818	CLA	MG-NB	-2.06	2.01	2.05
13	F	203	CLA	CHC-C1C	2.06	1.42	1.38
13	A	822	CLA	CMB-C2B	-2.06	1.46	1.50
13	F	204	CLA	CMB-C2B	-2.06	1.46	1.50
13	6	203	CLA	CHC-C1C	2.06	1.42	1.38
13	b	833	CLA	CMC-C2C	-2.06	1.46	1.50
13	a	816	CLA	MG-NB	-2.06	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	b	824	CLA	CHC-C1C	2.06	1.42	1.38
13	b	822	CLA	CMB-C2B	-2.06	1.46	1.50
13	B	823	CLA	MG-NB	-2.06	2.01	2.05
13	A	803	CLA	C3B-C4B	2.06	1.48	1.42
13	A	803	CLA	CHC-C1C	2.06	1.42	1.38
13	a	804	CLA	CMC-C2C	-2.06	1.46	1.50
13	A	837	CLA	CMC-C2C	-2.06	1.46	1.50
13	B	819	CLA	CMB-C2B	-2.06	1.46	1.50
13	A	821	CLA	CMD-C2D	-2.06	1.46	1.50
13	9	4003	CLA	CMC-C2C	-2.06	1.46	1.50
13	A	811	CLA	CMC-C2C	-2.06	1.46	1.50
13	A	836	CLA	CMB-C2B	-2.06	1.46	1.50
13	1	814	CLA	CMB-C2B	-2.06	1.46	1.50
13	A	827	CLA	CMB-C2B	-2.06	1.46	1.50
13	B	833	CLA	CMC-C2C	-2.06	1.46	1.50
13	1	804	CLA	CMD-C2D	-2.06	1.46	1.50
13	7	102	CLA	CMD-C2D	-2.06	1.46	1.50
13	1	829	CLA	MG-ND	-2.06	2.01	2.05
13	2	817	CLA	MG-NB	-2.06	2.01	2.05
13	B	810	CLA	CMB-C2B	-2.06	1.46	1.50
13	a	807	CLA	CMB-C2B	-2.06	1.46	1.50
13	2	813	CLA	CMC-C2C	-2.06	1.46	1.50
13	8	1102	CLA	CMD-C2D	-2.06	1.46	1.50
13	0	206	CLA	CMC-C2C	-2.05	1.46	1.50
13	a	832	CLA	CHC-C1C	2.05	1.42	1.38
13	1	832	CLA	CHC-C1C	2.05	1.42	1.38
13	a	802	CLA	C1B-NB	-2.05	1.35	1.37
13	A	806	CLA	CMC-C2C	-2.05	1.46	1.50
13	J	1102	CLA	CMD-C2D	-2.05	1.46	1.50
13	l	205	CLA	CMC-C2C	-2.05	1.46	1.50
13	1	812	CLA	MG-NB	-2.05	2.01	2.05
13	b	829	CLA	CMB-C2B	-2.05	1.46	1.50
13	2	832	CLA	CMC-C2C	-2.05	1.46	1.50
13	0	203	CLA	CMB-C2B	-2.05	1.46	1.50
13	A	804	CLA	CMC-C2C	-2.05	1.46	1.50
13	a	818	CLA	MG-ND	-2.05	2.01	2.05
13	j	1103	CLA	CMB-C2B	-2.05	1.46	1.50
13	B	802	CLA	MG-ND	-2.05	2.01	2.05
13	b	824	CLA	C3B-C4B	2.05	1.48	1.42
13	1	816	CLA	MG-NB	-2.05	2.01	2.05
13	l	204	CLA	CMC-C2C	-2.05	1.46	1.50
13	a	813	CLA	CMB-C2B	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	2	821	CLA	CMB-C2B	-2.05	1.46	1.50
13	B	824	CLA	C3B-C4B	2.05	1.48	1.42
13	1	827	CLA	MG-ND	-2.05	2.01	2.05
13	A	838	CLA	CHC-C1C	2.05	1.42	1.38
13	j	1102	CLA	CMD-C2D	-2.05	1.46	1.50
13	2	824	CLA	CMB-C2B	-2.05	1.46	1.50
13	1	822	CLA	CMB-C2B	-2.05	1.46	1.50
13	A	809	CLA	C3B-C4B	2.05	1.48	1.42
13	A	825	CLA	CHC-C1C	2.05	1.42	1.38
13	K	4005	CLA	CMC-C2C	-2.04	1.46	1.50
13	a	809	CLA	C3B-C4B	2.04	1.48	1.42
13	8	1103	CLA	MG-NB	-2.04	2.01	2.05
13	1	807	CLA	CMB-C2B	-2.04	1.46	1.50
13	A	829	CLA	CMC-C2C	-2.04	1.46	1.50
13	B	817	CLA	CMB-C2B	-2.04	1.46	1.50
13	a	822	CLA	CMB-C2B	-2.04	1.46	1.50
13	a	824	CLA	CMC-C2C	-2.04	1.46	1.50
13	1	816	CLA	CMD-C2D	-2.04	1.46	1.50
13	1	830	CLA	CHC-C1C	2.04	1.42	1.38
13	A	829	CLA	MG-ND	-2.04	2.01	2.05
13	B	818	CLA	MG-NB	-2.04	2.01	2.05
13	6	203	CLA	MG-NB	-2.04	2.01	2.05
13	A	839	CLA	CMC-C2C	-2.04	1.46	1.50
13	A	816	CLA	CMD-C2D	-2.04	1.46	1.50
13	b	828	CLA	CMC-C2C	-2.04	1.46	1.50
13	B	825	CLA	CMB-C2B	-2.04	1.46	1.50
13	1	838	CLA	MG-ND	-2.04	2.01	2.05
13	B	829	CLA	CMB-C2B	-2.04	1.46	1.50
13	a	806	CLA	CMC-C2C	-2.04	1.46	1.50
13	9	4005	CLA	CMC-C2C	-2.04	1.46	1.50
13	a	829	CLA	MG-ND	-2.04	2.01	2.05
12	A	801	CL0	CMC-C2C	-2.04	1.46	1.50
13	b	801	CLA	CHC-C1C	2.04	1.42	1.38
13	A	813	CLA	CMB-C2B	-2.04	1.46	1.50
13	A	832	CLA	CHC-C1C	2.04	1.42	1.38
13	A	838	CLA	MG-ND	-2.04	2.01	2.05
16	A	847	BCR	C33-C5	-2.04	1.47	1.50
18	b	846	LMG	C3-C2	2.04	1.57	1.52
13	a	842	CLA	CMD-C2D	-2.04	1.46	1.50
12	1	801	CL0	CMC-C2C	-2.04	1.46	1.50
13	B	802	CLA	CMB-C2B	-2.04	1.46	1.50
13	a	814	CLA	CMC-C2C	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	2	830	CLA	CMC-C2C	-2.04	1.46	1.50
13	b	805	CLA	CHC-C1C	2.04	1.42	1.38
13	b	810	CLA	CMD-C2D	-2.03	1.46	1.50
13	b	825	CLA	CMB-C2B	-2.03	1.46	1.50
13	i	102	CLA	CMB-C2B	-2.03	1.46	1.50
13	1	811	CLA	CMC-C2C	-2.03	1.46	1.50
13	a	827	CLA	CMB-C2B	-2.03	1.46	1.50
13	2	818	CLA	CMC-C2C	-2.03	1.46	1.50
13	B	847	CLA	CHC-C1C	2.03	1.42	1.38
13	1	825	CLA	CHC-C1C	2.03	1.42	1.38
16	a	847	BCR	C33-C5	-2.03	1.47	1.50
16	1	847	BCR	C33-C5	-2.03	1.47	1.50
13	1	815	CLA	CMB-C2B	-2.03	1.46	1.50
13	2	809	CLA	CMB-C2B	-2.03	1.46	1.50
13	B	801	CLA	CHC-C1C	2.03	1.42	1.38
13	b	823	CLA	MG-NB	-2.03	2.01	2.05
13	2	802	CLA	MG-ND	-2.03	2.01	2.05
13	2	828	CLA	CMB-C2B	-2.03	1.46	1.50
13	a	825	CLA	CHC-C1C	2.03	1.42	1.38
13	b	810	CLA	CMB-C2B	-2.03	1.46	1.50
13	A	802	CLA	C1B-NB	-2.03	1.35	1.37
13	b	834	CLA	CMC-C2C	-2.03	1.46	1.50
13	b	819	CLA	CMC-C2C	-2.03	1.46	1.50
13	k	4003	CLA	CMC-C2C	-2.03	1.46	1.50
18	B	846	LMG	C3-C2	2.03	1.57	1.52
13	a	807	CLA	CMC-C2C	-2.03	1.46	1.50
13	B	803	CLA	CMB-C2B	-2.03	1.46	1.50
13	f	201	CLA	CMC-C2C	-2.03	1.46	1.50
13	2	824	CLA	MG-ND	-2.03	2.01	2.05
13	b	803	CLA	CMB-C2B	-2.03	1.46	1.50
13	2	846	CLA	CHC-C1C	2.03	1.42	1.38
13	F	204	CLA	CMD-C2D	-2.03	1.46	1.50
13	K	4003	CLA	CMC-C2C	-2.03	1.46	1.50
13	A	815	CLA	CMB-C2B	-2.03	1.46	1.50
13	a	809	CLA	CHC-C1C	2.03	1.42	1.38
13	f	203	CLA	CHC-C1C	2.03	1.42	1.38
13	f	204	CLA	CMD-C2D	-2.02	1.46	1.50
13	2	801	CLA	CHC-C1C	2.02	1.42	1.38
13	B	818	CLA	CMC-C2C	-2.02	1.46	1.50
13	b	819	CLA	CMB-C2B	-2.02	1.46	1.50
13	A	818	CLA	MG-ND	-2.02	2.01	2.05
13	A	810	CLA	CMC-C2C	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	2	817	CLA	CMB-C2B	-2.02	1.46	1.50
13	B	813	CLA	CMC-C2C	-2.02	1.46	1.50
13	B	834	CLA	CMC-C2C	-2.02	1.46	1.50
16	K	4001	BCR	C33-C5	-2.02	1.47	1.50
13	a	822	CLA	CMC-C2C	-2.02	1.46	1.50
13	a	836	CLA	CMB-C2B	-2.02	1.46	1.50
12	a	801	CL0	CMC-C2C	-2.02	1.46	1.50
13	B	822	CLA	CMB-C2B	-2.02	1.46	1.50
13	2	820	CLA	CMC-C2C	-2.02	1.46	1.50
13	2	807	CLA	CMC-C2C	-2.02	1.46	1.50
13	A	807	CLA	CMC-C2C	-2.02	1.46	1.50
13	a	810	CLA	CMC-C2C	-2.02	1.46	1.50
13	B	836	CLA	CMC-C2C	-2.02	1.46	1.50
13	a	815	CLA	CMB-C2B	-2.02	1.46	1.50
13	b	813	CLA	CMC-C2C	-2.02	1.46	1.50
13	a	834	CLA	CMC-C2C	-2.02	1.46	1.50
13	1	829	CLA	CMC-C2C	-2.02	1.46	1.50
13	7	102	CLA	CMB-C2B	-2.02	1.46	1.50
13	I	101	CLA	CMB-C2B	-2.02	1.46	1.50
13	B	811	CLA	CMB-C2B	-2.02	1.46	1.50
13	F	201	CLA	CMC-C2C	-2.02	1.46	1.50
13	2	809	CLA	MG-ND	-2.02	2.01	2.05
13	a	829	CLA	CMC-C2C	-2.02	1.46	1.50
13	l	202	CLA	CMB-C2B	-2.02	1.46	1.50
13	B	801	CLA	C3B-C4B	2.02	1.48	1.42
13	B	805	CLA	CHC-C1C	2.02	1.42	1.38
13	k	4005	CLA	CMC-C2C	-2.02	1.46	1.50
13	2	805	CLA	CHC-C1C	2.02	1.42	1.38
13	a	808	CLA	CMB-C2B	-2.02	1.46	1.50
13	1	818	CLA	MG-ND	-2.02	2.01	2.05
13	A	818	CLA	CMC-C2C	-2.01	1.46	1.50
13	B	821	CLA	CMC-C2C	-2.01	1.46	1.50
13	2	833	CLA	CMC-C2C	-2.01	1.46	1.50
13	1	810	CLA	CMC-C2C	-2.01	1.46	1.50
13	0	208	CLA	CMC-C2C	-2.01	1.46	1.50
13	1	825	CLA	CMC-C2C	-2.01	1.46	1.50
13	b	821	CLA	CMC-C2C	-2.01	1.46	1.50
13	1	821	CLA	CMD-C2D	-2.01	1.46	1.50
13	2	803	CLA	CMC-C2C	-2.01	1.46	1.50
13	B	819	CLA	CMC-C2C	-2.01	1.46	1.50
13	B	828	CLA	CMC-C2C	-2.01	1.46	1.50
13	1	806	CLA	CMC-C2C	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	838	CLA	MG-ND	-2.01	2.01	2.05
13	L	201	CLA	CMB-C2B	-2.01	1.46	1.50
13	1	839	CLA	MG-ND	-2.01	2.01	2.05
13	L	206	CLA	CMC-C2C	-2.01	1.46	1.50
13	b	811	CLA	CMB-C2B	-2.01	1.46	1.50
13	2	835	CLA	CMC-C2C	-2.01	1.46	1.50
13	b	825	CLA	MG-ND	-2.01	2.01	2.05
13	B	808	CLA	CMC-C2C	-2.01	1.46	1.50
13	b	836	CLA	CMC-C2C	-2.01	1.46	1.50
16	k	4001	BCR	C33-C5	-2.01	1.47	1.50
13	B	818	CLA	CMB-C2B	-2.01	1.46	1.50
13	1	834	CLA	CMC-C2C	-2.01	1.46	1.50
13	2	803	CLA	CMB-C2B	-2.01	1.46	1.50
13	1	838	CLA	CHC-C1C	2.01	1.42	1.38
13	A	827	CLA	MG-ND	-2.01	2.01	2.05
13	1	807	CLA	CMC-C2C	-2.01	1.46	1.50
13	A	806	CLA	MG-ND	-2.01	2.01	2.05
13	A	834	CLA	CMC-C2C	-2.01	1.46	1.50
13	a	825	CLA	CMC-C2C	-2.01	1.46	1.50
13	B	806	CLA	CHC-C1C	2.01	1.42	1.38
16	9	4001	BCR	C33-C5	-2.01	1.47	1.50
16	A	851	BCR	C38-C26	-2.01	1.47	1.50
13	b	808	CLA	CMC-C2C	-2.01	1.46	1.50
13	A	822	CLA	CMC-C2C	-2.01	1.46	1.50
13	B	810	CLA	MG-ND	-2.01	2.01	2.05
13	a	806	CLA	MG-ND	-2.01	2.01	2.05
13	b	810	CLA	MG-ND	-2.01	2.01	2.05
13	b	801	CLA	C3B-C4B	2.01	1.48	1.42
13	b	838	CLA	CMB-C2B	-2.01	1.46	1.50
13	b	803	CLA	MG-NB	-2.00	2.01	2.05
13	b	803	CLA	CMC-C2C	-2.00	1.46	1.50
13	I	101	CLA	CMC-C2C	-2.00	1.46	1.50
13	1	813	CLA	CMB-C2B	-2.00	1.46	1.50
18	2	845	LMG	C3-C2	2.00	1.57	1.52
13	A	825	CLA	CMC-C2C	-2.00	1.46	1.50
13	B	803	CLA	CMC-C2C	-2.00	1.46	1.50
13	a	827	CLA	MG-ND	-2.00	2.01	2.05
13	a	812	CLA	CMC-C2C	-2.00	1.46	1.50
13	b	817	CLA	CMC-C2C	-2.00	1.46	1.50
13	2	837	CLA	CMB-C2B	-2.00	1.46	1.50
13	A	812	CLA	MG-NB	-2.00	2.01	2.05
13	2	810	CLA	CMB-C2B	-2.00	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	838	CLA	CMB-C2B	-2.00	1.46	1.50
13	a	818	CLA	CMC-C2C	-2.00	1.46	1.50
13	0	202	CLA	CMB-C2B	-2.00	1.46	1.50
13	b	847	CLA	CHC-C1C	2.00	1.42	1.38
13	a	816	CLA	CMC-C2C	-2.00	1.46	1.50
13	2	812	CLA	CMB-C2B	-2.00	1.46	1.50
13	A	808	CLA	CMB-C2B	-2.00	1.46	1.50

All (2345) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	808	CLA	C4A-NA-C1A	9.75	111.13	106.68
13	A	808	CLA	C4A-NA-C1A	9.65	111.08	106.68
13	a	808	CLA	C4A-NA-C1A	9.64	111.08	106.68
13	b	801	CLA	C4A-NA-C1A	8.88	110.73	106.68
13	1	819	CLA	C4A-NA-C1A	8.76	110.67	106.68
13	2	801	CLA	C4A-NA-C1A	8.73	110.66	106.68
13	B	801	CLA	C4A-NA-C1A	8.73	110.66	106.68
13	A	819	CLA	C4A-NA-C1A	8.60	110.60	106.68
13	a	819	CLA	C4A-NA-C1A	8.51	110.56	106.68
13	A	829	CLA	C4A-NA-C1A	8.35	110.49	106.68
13	a	829	CLA	C4A-NA-C1A	8.35	110.49	106.68
13	1	829	CLA	C4A-NA-C1A	8.29	110.46	106.68
13	1	842	CLA	C4A-NA-C1A	8.16	110.40	106.68
13	a	842	CLA	C4A-NA-C1A	8.16	110.40	106.68
13	A	842	CLA	C4A-NA-C1A	8.13	110.39	106.68
13	2	823	CLA	C4A-NA-C1A	8.11	110.38	106.68
13	b	824	CLA	C4A-NA-C1A	8.05	110.35	106.68
13	B	824	CLA	C4A-NA-C1A	8.04	110.35	106.68
13	L	206	CLA	C4A-NA-C1A	7.92	110.29	106.68
13	0	208	CLA	C4A-NA-C1A	7.88	110.28	106.68
13	1	207	CLA	C4A-NA-C1A	7.80	110.24	106.68
13	a	814	CLA	C4A-NA-C1A	7.77	110.22	106.68
13	B	831	CLA	C4A-NA-C1A	7.77	110.22	106.68
13	2	830	CLA	C4A-NA-C1A	7.77	110.22	106.68
13	A	814	CLA	C4A-NA-C1A	7.76	110.22	106.68
13	b	831	CLA	C4A-NA-C1A	7.75	110.22	106.68
13	a	822	CLA	C4A-NA-C1A	7.75	110.21	106.68
13	1	822	CLA	C4A-NA-C1A	7.75	110.21	106.68
13	A	822	CLA	C4A-NA-C1A	7.72	110.20	106.68
13	1	814	CLA	C4A-NA-C1A	7.71	110.20	106.68
13	a	806	CLA	C4A-NA-C1A	7.67	110.18	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	833	CLA	C4A-NA-C1A	7.67	110.18	106.68
13	1	825	CLA	C4A-NA-C1A	7.62	110.15	106.68
13	A	825	CLA	C4A-NA-C1A	7.61	110.15	106.68
13	a	825	CLA	C4A-NA-C1A	7.60	110.15	106.68
13	A	806	CLA	C4A-NA-C1A	7.60	110.15	106.68
13	b	830	CLA	C4A-NA-C1A	7.60	110.15	106.68
13	B	811	CLA	C4A-NA-C1A	7.60	110.14	106.68
13	b	811	CLA	C4A-NA-C1A	7.59	110.14	106.68
13	A	833	CLA	C4A-NA-C1A	7.58	110.14	106.68
13	1	806	CLA	C4A-NA-C1A	7.57	110.13	106.68
13	2	810	CLA	C4A-NA-C1A	7.57	110.13	106.68
13	2	829	CLA	C4A-NA-C1A	7.53	110.11	106.68
13	1	833	CLA	C4A-NA-C1A	7.52	110.11	106.68
13	1	824	CLA	C4A-NA-C1A	7.52	110.11	106.68
13	2	803	CLA	C4A-NA-C1A	7.48	110.09	106.68
13	B	830	CLA	C4A-NA-C1A	7.45	110.08	106.68
13	A	824	CLA	C4A-NA-C1A	7.44	110.08	106.68
13	a	824	CLA	C4A-NA-C1A	7.41	110.06	106.68
13	B	803	CLA	C4A-NA-C1A	7.40	110.06	106.68
13	b	816	CLA	C4A-NA-C1A	7.40	110.05	106.68
13	B	816	CLA	C4A-NA-C1A	7.38	110.05	106.68
13	2	815	CLA	C4A-NA-C1A	7.35	110.03	106.68
13	b	803	CLA	C4A-NA-C1A	7.35	110.03	106.68
13	B	808	CLA	C4A-NA-C1A	7.29	110.00	106.68
13	1	834	CLA	C4A-NA-C1A	7.27	110.00	106.68
13	b	808	CLA	C4A-NA-C1A	7.25	109.98	106.68
13	A	834	CLA	C4A-NA-C1A	7.24	109.98	106.68
13	a	834	CLA	C4A-NA-C1A	7.19	109.96	106.68
13	2	807	CLA	C4A-NA-C1A	7.18	109.95	106.68
13	a	823	CLA	C4A-NA-C1A	7.16	109.95	106.68
13	A	823	CLA	C4A-NA-C1A	7.14	109.94	106.68
13	L	203	CLA	C4A-NA-C1A	7.11	109.92	106.68
13	0	205	CLA	C4A-NA-C1A	7.11	109.92	106.68
13	1	823	CLA	C4A-NA-C1A	7.07	109.90	106.68
13	l	204	CLA	C4A-NA-C1A	7.06	109.90	106.68
13	b	828	CLA	C4A-NA-C1A	7.05	109.89	106.68
13	A	830	CLA	C4A-NA-C1A	7.03	109.88	106.68
13	2	828	CLA	C4A-NA-C1A	7.02	109.88	106.68
13	2	825	CLA	C4A-NA-C1A	7.01	109.88	106.68
13	a	830	CLA	C4A-NA-C1A	7.01	109.88	106.68
13	b	826	CLA	C4A-NA-C1A	7.01	109.88	106.68
13	B	826	CLA	C4A-NA-C1A	6.99	109.87	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	829	CLA	C4A-NA-C1A	6.98	109.86	106.68
13	b	829	CLA	C4A-NA-C1A	6.96	109.86	106.68
13	a	828	CLA	C4A-NA-C1A	6.96	109.85	106.68
13	1	830	CLA	C4A-NA-C1A	6.95	109.85	106.68
13	2	809	CLA	C4A-NA-C1A	6.95	109.85	106.68
13	b	810	CLA	C4A-NA-C1A	6.95	109.85	106.68
13	B	828	CLA	C4A-NA-C1A	6.94	109.84	106.68
13	a	807	CLA	C4A-NA-C1A	6.93	109.84	106.68
13	A	807	CLA	C4A-NA-C1A	6.90	109.83	106.68
13	1	807	CLA	C4A-NA-C1A	6.89	109.82	106.68
13	1	817	CLA	C4A-NA-C1A	6.89	109.82	106.68
13	2	827	CLA	C4A-NA-C1A	6.88	109.82	106.68
13	B	810	CLA	C4A-NA-C1A	6.88	109.82	106.68
13	A	817	CLA	C4A-NA-C1A	6.88	109.82	106.68
13	A	828	CLA	C4A-NA-C1A	6.88	109.82	106.68
13	a	817	CLA	C4A-NA-C1A	6.86	109.81	106.68
13	1	828	CLA	C4A-NA-C1A	6.85	109.80	106.68
13	K	4005	CLA	C4A-NA-C1A	6.83	109.80	106.68
13	k	4005	CLA	C4A-NA-C1A	6.83	109.80	106.68
13	a	839	CLA	C4A-NA-C1A	6.74	109.75	106.68
13	9	4005	CLA	C4A-NA-C1A	6.72	109.75	106.68
13	A	839	CLA	C4A-NA-C1A	6.65	109.71	106.68
13	1	838	CLA	C4A-NA-C1A	6.64	109.71	106.68
13	b	806	CLA	C4A-NA-C1A	6.64	109.71	106.68
13	1	839	CLA	C4A-NA-C1A	6.64	109.71	106.68
13	A	838	CLA	C4A-NA-C1A	6.63	109.71	106.68
13	B	806	CLA	C4A-NA-C1A	6.63	109.70	106.68
13	2	806	CLA	C4A-NA-C1A	6.60	109.69	106.68
13	a	838	CLA	C4A-NA-C1A	6.60	109.69	106.68
13	1	818	CLA	C4A-NA-C1A	6.56	109.67	106.68
13	a	818	CLA	C4A-NA-C1A	6.55	109.67	106.68
13	a	811	CLA	C4A-NA-C1A	6.53	109.66	106.68
13	A	818	CLA	C4A-NA-C1A	6.50	109.64	106.68
13	i	102	CLA	C4A-NA-C1A	6.50	109.64	106.68
13	A	802	CLA	C4A-NA-C1A	6.49	109.64	106.68
13	f	201	CLA	C4A-NA-C1A	6.45	109.62	106.68
13	2	820	CLA	C4A-NA-C1A	6.44	109.62	106.68
13	1	802	CLA	C4A-NA-C1A	6.44	109.62	106.68
13	F	201	CLA	C4A-NA-C1A	6.44	109.61	106.68
13	a	802	CLA	C4A-NA-C1A	6.43	109.61	106.68
13	b	847	CLA	C4A-NA-C1A	6.43	109.61	106.68
13	6	201	CLA	C4A-NA-C1A	6.43	109.61	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	821	CLA	C4A-NA-C1A	6.42	109.61	106.68
13	0	203	CLA	C4A-NA-C1A	6.41	109.61	106.68
13	I	101	CLA	C4A-NA-C1A	6.40	109.60	106.68
13	B	847	CLA	C4A-NA-C1A	6.39	109.59	106.68
13	1	811	CLA	C4A-NA-C1A	6.38	109.59	106.68
13	B	821	CLA	C4A-NA-C1A	6.38	109.59	106.68
13	A	811	CLA	C4A-NA-C1A	6.37	109.58	106.68
13	b	807	CLA	C4A-NA-C1A	6.36	109.58	106.68
13	B	807	CLA	C4A-NA-C1A	6.35	109.58	106.68
13	2	817	CLA	C4A-NA-C1A	6.35	109.58	106.68
13	7	102	CLA	C4A-NA-C1A	6.33	109.57	106.68
13	2	846	CLA	C4A-NA-C1A	6.33	109.57	106.68
13	B	818	CLA	C4A-NA-C1A	6.29	109.55	106.68
13	1	804	CLA	C4A-NA-C1A	6.24	109.52	106.68
13	b	818	CLA	C4A-NA-C1A	6.20	109.51	106.68
13	2	808	CLA	C4A-NA-C1A	6.12	109.47	106.68
13	b	819	CLA	C4A-NA-C1A	6.11	109.47	106.68
13	b	805	CLA	C4A-NA-C1A	6.10	109.46	106.68
13	A	815	CLA	C4A-NA-C1A	6.09	109.46	106.68
13	A	804	CLA	C4A-NA-C1A	6.09	109.46	106.68
13	0	202	CLA	C4A-NA-C1A	6.09	109.46	106.68
13	2	805	CLA	C4A-NA-C1A	6.08	109.45	106.68
13	B	809	CLA	C4A-NA-C1A	6.08	109.45	106.68
13	a	815	CLA	C4A-NA-C1A	6.07	109.45	106.68
13	B	805	CLA	C4A-NA-C1A	6.07	109.45	106.68
13	l	202	CLA	C4A-NA-C1A	6.05	109.44	106.68
13	L	201	CLA	C4A-NA-C1A	6.05	109.44	106.68
13	2	834	CLA	C4A-NA-C1A	6.05	109.44	106.68
13	b	813	CLA	C4A-NA-C1A	6.04	109.44	106.68
13	1	815	CLA	C4A-NA-C1A	6.04	109.44	106.68
13	b	809	CLA	C4A-NA-C1A	6.04	109.43	106.68
13	B	819	CLA	C4A-NA-C1A	6.02	109.43	106.68
13	a	804	CLA	C4A-NA-C1A	6.02	109.42	106.68
13	B	813	CLA	C4A-NA-C1A	5.99	109.41	106.68
13	2	818	CLA	C4A-NA-C1A	5.99	109.41	106.68
13	f	203	CLA	C4A-NA-C1A	5.98	109.41	106.68
13	6	203	CLA	C4A-NA-C1A	5.98	109.41	106.68
13	2	812	CLA	C4A-NA-C1A	5.95	109.39	106.68
13	B	835	CLA	C4A-NA-C1A	5.94	109.39	106.68
13	F	203	CLA	C4A-NA-C1A	5.94	109.39	106.68
13	b	835	CLA	C4A-NA-C1A	5.93	109.38	106.68
13	A	810	CLA	C4A-NA-C1A	5.90	109.37	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	J	1102	CLA	C4A-NA-C1A	5.87	109.36	106.68
13	a	810	CLA	C4A-NA-C1A	5.83	109.34	106.68
13	b	825	CLA	C4A-NA-C1A	5.82	109.33	106.68
13	0	206	CLA	C4A-NA-C1A	5.81	109.33	106.68
13	K	4002	CLA	C4A-NA-C1A	5.80	109.33	106.68
13	j	1102	CLA	C4A-NA-C1A	5.80	109.33	106.68
13	B	825	CLA	C4A-NA-C1A	5.80	109.33	106.68
13	k	4002	CLA	C4A-NA-C1A	5.80	109.32	106.68
13	2	824	CLA	C4A-NA-C1A	5.78	109.31	106.68
13	8	1102	CLA	C4A-NA-C1A	5.77	109.31	106.68
13	l	205	CLA	C4A-NA-C1A	5.77	109.31	106.68
13	1	810	CLA	C4A-NA-C1A	5.77	109.31	106.68
13	L	204	CLA	C4A-NA-C1A	5.77	109.31	106.68
13	a	831	CLA	C4A-NA-C1A	5.76	109.31	106.68
13	A	831	CLA	C4A-NA-C1A	5.76	109.31	106.68
13	k	4003	CLA	C4A-NA-C1A	5.75	109.30	106.68
13	9	4002	CLA	C4A-NA-C1A	5.75	109.30	106.68
13	1	809	CLA	C4A-NA-C1A	5.74	109.30	106.68
13	K	4003	CLA	C4A-NA-C1A	5.74	109.30	106.68
13	9	4003	CLA	C4A-NA-C1A	5.73	109.30	106.68
13	8	1103	CLA	C4A-NA-C1A	5.73	109.29	106.68
13	1	840	CLA	C4A-NA-C1A	5.72	109.29	106.68
13	2	811	CLA	C4A-NA-C1A	5.71	109.28	106.68
13	B	812	CLA	C4A-NA-C1A	5.69	109.28	106.68
13	A	809	CLA	C4A-NA-C1A	5.69	109.27	106.68
13	j	1103	CLA	C4A-NA-C1A	5.69	109.27	106.68
13	b	820	CLA	C4A-NA-C1A	5.68	109.27	106.68
13	1	831	CLA	C4A-NA-C1A	5.68	109.27	106.68
13	J	1103	CLA	C4A-NA-C1A	5.67	109.27	106.68
13	a	841	CLA	C4A-NA-C1A	5.65	109.26	106.68
13	B	838	CLA	C4A-NA-C1A	5.64	109.25	106.68
13	b	812	CLA	C4A-NA-C1A	5.64	109.25	106.68
13	a	809	CLA	C4A-NA-C1A	5.63	109.25	106.68
13	B	820	CLA	C4A-NA-C1A	5.62	109.24	106.68
13	b	838	CLA	C4A-NA-C1A	5.61	109.24	106.68
13	2	814	CLA	C4A-NA-C1A	5.61	109.24	106.68
13	A	832	CLA	C4A-NA-C1A	5.61	109.24	106.68
13	A	840	CLA	C4A-NA-C1A	5.61	109.24	106.68
13	1	832	CLA	C4A-NA-C1A	5.61	109.24	106.68
13	b	836	CLA	C4A-NA-C1A	5.60	109.23	106.68
13	2	835	CLA	C4A-NA-C1A	5.60	109.23	106.68
13	a	832	CLA	C4A-NA-C1A	5.60	109.23	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	836	CLA	C4A-NA-C1A	5.59	109.23	106.68
13	1	841	CLA	C4A-NA-C1A	5.59	109.23	106.68
13	a	840	CLA	C4A-NA-C1A	5.58	109.22	106.68
13	2	819	CLA	C4A-NA-C1A	5.58	109.22	106.68
13	2	837	CLA	C4A-NA-C1A	5.58	109.22	106.68
13	b	837	CLA	C4A-NA-C1A	5.58	109.22	106.68
13	A	841	CLA	C4A-NA-C1A	5.57	109.22	106.68
13	B	815	CLA	C4A-NA-C1A	5.54	109.21	106.68
13	1	821	CLA	C4A-NA-C1A	5.54	109.21	106.68
13	b	815	CLA	C4A-NA-C1A	5.54	109.20	106.68
13	B	837	CLA	C4A-NA-C1A	5.53	109.20	106.68
13	a	821	CLA	C4A-NA-C1A	5.53	109.20	106.68
13	1	812	CLA	C4A-NA-C1A	5.52	109.20	106.68
13	2	804	CLA	C4A-NA-C1A	5.51	109.19	106.68
13	B	804	CLA	C4A-NA-C1A	5.50	109.19	106.68
13	1	837	CLA	C4A-NA-C1A	5.50	109.19	106.68
13	A	821	CLA	C4A-NA-C1A	5.49	109.18	106.68
13	A	812	CLA	C4A-NA-C1A	5.47	109.17	106.68
13	a	816	CLA	C4A-NA-C1A	5.47	109.17	106.68
13	a	812	CLA	C4A-NA-C1A	5.45	109.16	106.68
13	A	837	CLA	C4A-NA-C1A	5.44	109.16	106.68
13	a	837	CLA	C4A-NA-C1A	5.44	109.16	106.68
13	2	836	CLA	C4A-NA-C1A	5.44	109.16	106.68
13	1	816	CLA	C4A-NA-C1A	5.44	109.16	106.68
13	b	804	CLA	C4A-NA-C1A	5.44	109.16	106.68
13	a	827	CLA	C4A-NA-C1A	5.41	109.15	106.68
13	6	204	CLA	C4A-NA-C1A	5.40	109.14	106.68
13	A	816	CLA	C4A-NA-C1A	5.40	109.14	106.68
13	f	204	CLA	C4A-NA-C1A	5.40	109.14	106.68
13	F	204	CLA	C4A-NA-C1A	5.37	109.13	106.68
13	B	802	CLA	C4A-NA-C1A	5.37	109.13	106.68
13	A	827	CLA	C4A-NA-C1A	5.37	109.13	106.68
13	8	1101	CLA	C4A-NA-C1A	5.36	109.12	106.68
13	J	1101	CLA	C4A-NA-C1A	5.35	109.12	106.68
13	j	1101	CLA	C4A-NA-C1A	5.34	109.11	106.68
13	1	827	CLA	C4A-NA-C1A	5.33	109.11	106.68
13	2	802	CLA	C4A-NA-C1A	5.31	109.10	106.68
13	b	802	CLA	C4A-NA-C1A	5.28	109.09	106.68
13	1	836	CLA	C4A-NA-C1A	5.25	109.07	106.68
13	b	832	CLA	C4A-NA-C1A	5.24	109.07	106.68
13	B	832	CLA	C4A-NA-C1A	5.23	109.06	106.68
13	A	805	CLA	C4A-NA-C1A	5.23	109.06	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	823	CLA	C4A-NA-C1A	5.23	109.06	106.68
13	A	836	CLA	C4A-NA-C1A	5.19	109.05	106.68
13	2	822	CLA	C4A-NA-C1A	5.19	109.05	106.68
13	b	823	CLA	C4A-NA-C1A	5.18	109.04	106.68
13	2	813	CLA	C4A-NA-C1A	5.17	109.04	106.68
13	1	805	CLA	C4A-NA-C1A	5.17	109.04	106.68
13	2	831	CLA	C4A-NA-C1A	5.17	109.04	106.68
13	a	805	CLA	C4A-NA-C1A	5.16	109.03	106.68
13	a	836	CLA	C4A-NA-C1A	5.16	109.03	106.68
13	B	814	CLA	C4A-NA-C1A	5.15	109.03	106.68
13	b	814	CLA	C4A-NA-C1A	5.13	109.02	106.68
13	a	820	CLA	C4A-NA-C1A	5.09	109.00	106.68
13	2	821	CLA	C4A-NA-C1A	5.07	108.99	106.68
13	A	820	CLA	C4A-NA-C1A	5.06	108.99	106.68
13	b	822	CLA	C4A-NA-C1A	5.06	108.99	106.68
13	a	826	CLA	C4A-NA-C1A	5.02	108.97	106.68
13	1	820	CLA	C4A-NA-C1A	5.00	108.96	106.68
13	A	826	CLA	C4A-NA-C1A	5.00	108.96	106.68
13	B	822	CLA	C4A-NA-C1A	4.99	108.96	106.68
13	1	826	CLA	C4A-NA-C1A	4.97	108.95	106.68
13	1	817	CLA	C3B-C4B-NB	-4.94	106.12	110.53
13	a	817	CLA	C3B-C4B-NB	-4.94	106.12	110.53
13	A	817	CLA	C3B-C4B-NB	-4.91	106.14	110.53
13	b	802	CLA	C3B-C4B-NB	-4.87	106.18	110.53
13	B	802	CLA	C3B-C4B-NB	-4.87	106.18	110.53
13	a	813	CLA	C4A-NA-C1A	4.82	108.88	106.68
13	2	802	CLA	C3B-C4B-NB	-4.82	106.23	110.53
13	A	813	CLA	C4A-NA-C1A	4.81	108.87	106.68
13	1	813	CLA	C4A-NA-C1A	4.81	108.87	106.68
13	B	833	CLA	CMB-C2B-C1B	-4.77	118.16	125.42
13	b	833	CLA	CMB-C2B-C1B	-4.77	118.16	125.42
13	2	832	CLA	CMB-C2B-C1B	-4.77	118.16	125.42
13	b	833	CLA	C3B-C4B-NB	-4.71	106.32	110.53
13	2	832	CLA	C3B-C4B-NB	-4.71	106.32	110.53
13	a	803	CLA	C4A-NA-C1A	4.71	108.83	106.68
13	B	833	CLA	C3B-C4B-NB	-4.68	106.35	110.53
13	A	835	CLA	C4A-NA-C1A	4.64	108.80	106.68
13	a	830	CLA	CMB-C2B-C1B	-4.61	118.40	125.42
13	A	830	CLA	CMB-C2B-C1B	-4.58	118.44	125.42
13	1	830	CLA	CMB-C2B-C1B	-4.57	118.47	125.42
13	A	803	CLA	C4A-NA-C1A	4.56	108.76	106.68
13	1	835	CLA	C4A-NA-C1A	4.55	108.75	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	801	CL0	C4A-NA-C1A	4.54	108.75	106.68
12	a	801	CL0	C4A-NA-C1A	4.53	108.75	106.68
13	a	835	CLA	C4A-NA-C1A	4.50	108.73	106.68
13	1	803	CLA	C4A-NA-C1A	4.45	108.71	106.68
13	2	805	CLA	C3B-C4B-NB	-4.44	106.56	110.53
12	1	801	CL0	C4A-NA-C1A	4.42	108.70	106.68
17	a	849	LHG	O4-P-O5	4.42	133.00	112.44
13	1	832	CLA	C3B-C4B-NB	-4.41	106.59	110.53
17	A	849	LHG	O4-P-O5	4.41	132.96	112.44
17	1	849	LHG	O4-P-O5	4.41	132.94	112.44
13	B	805	CLA	C3B-C4B-NB	-4.40	106.60	110.53
13	b	805	CLA	C3B-C4B-NB	-4.40	106.60	110.53
17	a	850	LHG	O4-P-O5	4.39	132.88	112.44
17	A	850	LHG	O4-P-O5	4.39	132.87	112.44
17	1	850	LHG	O4-P-O5	4.39	132.87	112.44
13	A	832	CLA	C3B-C4B-NB	-4.38	106.62	110.53
13	a	832	CLA	C3B-C4B-NB	-4.36	106.64	110.53
13	1	835	CLA	C3B-C4B-NB	-4.35	106.65	110.53
13	A	835	CLA	C3B-C4B-NB	-4.33	106.66	110.53
13	1	829	CLA	C3B-C4B-NB	-4.33	106.67	110.53
13	a	829	CLA	C3B-C4B-NB	-4.30	106.69	110.53
13	A	829	CLA	C3B-C4B-NB	-4.29	106.70	110.53
13	B	813	CLA	C3B-C4B-NB	-4.28	106.71	110.53
13	a	835	CLA	C3B-C4B-NB	-4.28	106.71	110.53
13	b	813	CLA	C3B-C4B-NB	-4.27	106.72	110.53
13	2	812	CLA	C3B-C4B-NB	-4.26	106.73	110.53
13	A	828	CLA	C3B-C4B-NB	-4.16	106.81	110.53
13	2	826	CLA	C4A-NA-C1A	4.16	108.58	106.68
13	A	819	CLA	C3B-C4B-NB	-4.16	106.82	110.53
13	1	819	CLA	C3B-C4B-NB	-4.15	106.82	110.53
13	a	828	CLA	C3B-C4B-NB	-4.15	106.82	110.53
13	1	828	CLA	C3B-C4B-NB	-4.14	106.83	110.53
13	a	819	CLA	C3B-C4B-NB	-4.14	106.84	110.53
13	b	827	CLA	C4A-NA-C1A	4.10	108.55	106.68
13	B	827	CLA	C4A-NA-C1A	4.09	108.54	106.68
13	a	836	CLA	C3B-C4B-NB	-4.01	106.95	110.53
13	1	836	CLA	C3B-C4B-NB	-4.01	106.95	110.53
13	a	852	CLA	C4A-NA-C1A	4.00	108.50	106.68
13	a	818	CLA	C3B-C4B-NB	-3.99	106.97	110.53
13	A	836	CLA	C3B-C4B-NB	-3.98	106.97	110.53
13	l	204	CLA	C3B-C4B-NB	-3.97	106.98	110.53
13	A	818	CLA	C3B-C4B-NB	-3.96	106.99	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	0	205	CLA	C3B-C4B-NB	-3.96	107.00	110.53
13	L	203	CLA	C3B-C4B-NB	-3.96	107.00	110.53
13	1	818	CLA	C3B-C4B-NB	-3.94	107.01	110.53
13	1	852	CLA	C3B-C4B-NB	-3.94	107.01	110.53
16	b	842	BCR	C24-C23-C22	-3.94	120.41	126.23
16	2	841	BCR	C24-C23-C22	-3.94	120.41	126.23
13	b	831	CLA	C3B-C4B-NB	-3.94	107.01	110.53
13	B	831	CLA	C3B-C4B-NB	-3.93	107.02	110.53
13	2	830	CLA	C3B-C4B-NB	-3.93	107.02	110.53
13	B	834	CLA	C3B-C4B-NB	-3.93	107.02	110.53
13	A	852	CLA	C4A-NA-C1A	3.93	108.47	106.68
13	a	802	CLA	C3B-C4B-NB	-3.92	107.03	110.53
16	B	842	BCR	C24-C23-C22	-3.92	120.44	126.23
13	1	852	CLA	C4A-NA-C1A	3.92	108.47	106.68
16	b	844	BCR	C15-C16-C17	-3.92	115.50	123.52
13	b	811	CLA	C3B-C4B-NB	-3.91	107.04	110.53
13	b	834	CLA	C3B-C4B-NB	-3.90	107.05	110.53
19	i	101	SQD	O9-S-O7	-3.90	101.13	113.82
19	7	101	SQD	O9-S-O7	-3.90	101.14	113.82
13	B	811	CLA	C3B-C4B-NB	-3.90	107.05	110.53
13	1	810	CLA	C3B-C4B-NB	-3.90	107.05	110.53
19	I	103	SQD	O9-S-O7	-3.90	101.14	113.82
16	B	844	BCR	C15-C16-C17	-3.90	115.54	123.52
13	A	852	CLA	C3B-C4B-NB	-3.90	107.05	110.53
13	A	810	CLA	C3B-C4B-NB	-3.89	107.05	110.53
13	A	802	CLA	C3B-C4B-NB	-3.89	107.06	110.53
13	2	833	CLA	C3B-C4B-NB	-3.88	107.07	110.53
13	a	810	CLA	C3B-C4B-NB	-3.88	107.07	110.53
13	2	810	CLA	C3B-C4B-NB	-3.88	107.07	110.53
16	2	843	BCR	C15-C16-C17	-3.88	115.59	123.52
13	a	852	CLA	C3B-C4B-NB	-3.87	107.07	110.53
13	1	802	CLA	C3B-C4B-NB	-3.87	107.08	110.53
13	2	825	CLA	CMB-C2B-C1B	-3.84	119.57	125.42
13	b	826	CLA	CMB-C2B-C1B	-3.83	119.59	125.42
13	B	826	CLA	CMB-C2B-C1B	-3.82	119.60	125.42
13	a	833	CLA	C3B-C4B-NB	-3.81	107.13	110.53
13	a	808	CLA	C3B-C4B-NB	-3.80	107.13	110.53
13	A	808	CLA	C3B-C4B-NB	-3.80	107.14	110.53
13	A	833	CLA	C3B-C4B-NB	-3.80	107.14	110.53
13	1	808	CLA	C3B-C4B-NB	-3.79	107.14	110.53
13	b	830	CLA	C3B-C4B-NB	-3.78	107.15	110.53
13	B	808	CLA	C3B-C4B-NB	-3.78	107.16	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	839	CLA	CMB-C2B-C1B	-3.78	119.67	125.42
13	1	833	CLA	C3B-C4B-NB	-3.77	107.16	110.53
13	b	808	CLA	C3B-C4B-NB	-3.77	107.16	110.53
13	2	829	CLA	C3B-C4B-NB	-3.77	107.16	110.53
13	a	839	CLA	CMB-C2B-C1B	-3.76	119.69	125.42
13	A	839	CLA	CMB-C2B-C1B	-3.76	119.70	125.42
13	B	830	CLA	C3B-C4B-NB	-3.75	107.19	110.53
13	b	834	CLA	C4A-NA-C1A	3.74	108.38	106.68
13	2	807	CLA	C3B-C4B-NB	-3.73	107.20	110.53
16	J	1104	BCR	C2-C1-C6	3.73	115.85	110.44
16	j	1104	BCR	C2-C1-C6	3.71	115.83	110.44
16	8	1104	BCR	C2-C1-C6	3.71	115.83	110.44
13	A	811	CLA	C3B-C4B-NB	-3.71	107.22	110.53
13	1	811	CLA	C3B-C4B-NB	-3.69	107.23	110.53
13	a	811	CLA	C3B-C4B-NB	-3.69	107.24	110.53
13	a	807	CLA	C3B-C4B-NB	-3.69	107.24	110.53
13	b	829	CLA	C3B-C4B-NB	-3.68	107.24	110.53
13	B	829	CLA	C3B-C4B-NB	-3.68	107.25	110.53
13	1	807	CLA	C3B-C4B-NB	-3.67	107.25	110.53
13	B	834	CLA	C4A-NA-C1A	3.67	108.35	106.68
13	A	807	CLA	C3B-C4B-NB	-3.66	107.26	110.53
13	2	801	CLA	C3B-C4B-NB	-3.66	107.27	110.53
13	2	828	CLA	C3B-C4B-NB	-3.65	107.27	110.53
13	B	827	CLA	C3B-C4B-NB	-3.65	107.27	110.53
13	2	826	CLA	C3B-C4B-NB	-3.64	107.28	110.53
13	B	801	CLA	C3B-C4B-NB	-3.63	107.29	110.53
13	B	847	CLA	CMB-C2B-C1B	-3.62	119.91	125.42
13	2	833	CLA	C4A-NA-C1A	3.62	108.33	106.68
13	b	801	CLA	C3B-C4B-NB	-3.61	107.30	110.53
13	b	847	CLA	CMB-C2B-C1B	-3.61	119.92	125.42
13	2	846	CLA	CMB-C2B-C1B	-3.60	119.93	125.42
13	1	802	CLA	CMB-C2B-C1B	-3.60	119.94	125.42
13	A	802	CLA	CMB-C2B-C1B	-3.60	119.94	125.42
13	b	827	CLA	C3B-C4B-NB	-3.60	107.32	110.53
13	2	813	CLA	C3B-C4B-NB	-3.60	107.32	110.53
13	B	818	CLA	C3B-C4B-NB	-3.60	107.32	110.53
13	A	838	CLA	C3B-C4B-NB	-3.60	107.32	110.53
13	a	802	CLA	CMB-C2B-C1B	-3.60	119.94	125.42
19	I	103	SQD	O47-C7-C8	3.59	119.26	111.48
13	b	814	CLA	C3B-C4B-NB	-3.59	107.32	110.53
13	a	831	CLA	C3B-C4B-NB	-3.59	107.33	110.53
13	a	838	CLA	C3B-C4B-NB	-3.59	107.33	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	822	CLA	C3B-C4B-NB	-3.58	107.33	110.53
19	i	101	SQD	O47-C7-C8	3.58	119.22	111.48
13	1	831	CLA	C3B-C4B-NB	-3.57	107.34	110.53
13	b	822	CLA	C3B-C4B-NB	-3.57	107.34	110.53
13	1	822	CLA	C3B-C4B-NB	-3.57	107.34	110.53
13	1	838	CLA	C3B-C4B-NB	-3.57	107.34	110.53
13	2	817	CLA	C3B-C4B-NB	-3.57	107.35	110.53
13	A	822	CLA	C3B-C4B-NB	-3.57	107.35	110.53
19	7	101	SQD	O47-C7-C8	3.56	119.19	111.48
13	A	831	CLA	C3B-C4B-NB	-3.56	107.35	110.53
13	b	818	CLA	C3B-C4B-NB	-3.55	107.36	110.53
13	2	809	CLA	C3B-C4B-NB	-3.55	107.36	110.53
13	b	835	CLA	C3B-C4B-NB	-3.55	107.36	110.53
13	B	833	CLA	C4A-NA-C1A	3.55	108.30	106.68
13	B	835	CLA	C3B-C4B-NB	-3.54	107.37	110.53
13	B	814	CLA	C3B-C4B-NB	-3.54	107.37	110.53
13	B	810	CLA	C3B-C4B-NB	-3.54	107.37	110.53
13	2	821	CLA	C3B-C4B-NB	-3.54	107.37	110.53
13	B	804	CLA	C3B-C4B-NB	-3.53	107.38	110.53
13	b	804	CLA	C3B-C4B-NB	-3.53	107.38	110.53
13	A	839	CLA	C3B-C4B-NB	-3.53	107.38	110.53
13	a	839	CLA	C3B-C4B-NB	-3.53	107.38	110.53
13	b	810	CLA	C3B-C4B-NB	-3.53	107.38	110.53
16	a	847	BCR	C24-C23-C22	-3.52	121.02	126.23
13	B	822	CLA	C3B-C4B-NB	-3.52	107.39	110.53
13	2	804	CLA	C3B-C4B-NB	-3.52	107.39	110.53
13	2	832	CLA	C4A-NA-C1A	3.51	108.28	106.68
13	1	839	CLA	C3B-C4B-NB	-3.51	107.40	110.53
13	2	834	CLA	C3B-C4B-NB	-3.51	107.40	110.53
13	a	813	CLA	C3B-C4B-NB	-3.51	107.40	110.53
16	1	847	BCR	C24-C23-C22	-3.51	121.05	126.23
14	B	839	PQN	C14-C13-C15	3.50	121.31	115.23
13	A	813	CLA	C3B-C4B-NB	-3.50	107.40	110.53
13	b	825	CLA	C3B-C4B-NB	-3.50	107.41	110.53
16	A	847	BCR	C24-C23-C22	-3.50	121.06	126.23
14	2	838	PQN	C14-C13-C15	3.49	121.29	115.23
13	B	809	CLA	C3B-C4B-NB	-3.49	107.41	110.53
12	a	801	CL0	C3B-C4B-NB	-3.49	107.41	110.53
14	b	839	PQN	C14-C13-C15	3.49	121.28	115.23
13	1	809	CLA	C3B-C4B-NB	-3.49	107.42	110.53
13	1	813	CLA	C3B-C4B-NB	-3.49	107.42	110.53
13	2	824	CLA	C3B-C4B-NB	-3.48	107.42	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	809	CLA	C3B-C4B-NB	-3.48	107.42	110.53
12	A	801	CL0	C3B-C4B-NB	-3.48	107.42	110.53
13	a	802	CLA	O2D-CGD-O1D	-3.48	117.07	123.85
13	B	825	CLA	C3B-C4B-NB	-3.48	107.42	110.53
13	a	804	CLA	C3B-C4B-NB	-3.47	107.43	110.53
13	2	808	CLA	C3B-C4B-NB	-3.47	107.43	110.53
13	J	1101	CLA	C3B-C4B-NB	-3.47	107.43	110.53
13	j	1101	CLA	C3B-C4B-NB	-3.47	107.43	110.53
13	2	827	CLA	C3B-C4B-NB	-3.47	107.44	110.53
13	b	833	CLA	C4A-NA-C1A	3.47	108.26	106.68
13	A	802	CLA	O2D-CGD-O1D	-3.47	117.10	123.85
13	1	802	CLA	O2D-CGD-O1D	-3.46	117.11	123.85
13	A	809	CLA	C3B-C4B-NB	-3.46	107.44	110.53
13	1	804	CLA	C3B-C4B-NB	-3.46	107.44	110.53
13	8	1101	CLA	C3B-C4B-NB	-3.46	107.44	110.53
13	a	826	CLA	C3B-C4B-NB	-3.46	107.44	110.53
13	A	804	CLA	C3B-C4B-NB	-3.45	107.45	110.53
13	2	825	CLA	O2D-CGD-O1D	-3.45	117.14	123.85
13	a	809	CLA	C3B-C4B-NB	-3.45	107.45	110.53
13	b	819	CLA	C3B-C4B-NB	-3.44	107.45	110.53
13	b	828	CLA	C3B-C4B-NB	-3.44	107.46	110.53
13	A	826	CLA	C3B-C4B-NB	-3.44	107.46	110.53
13	B	828	CLA	C3B-C4B-NB	-3.44	107.46	110.53
13	B	819	CLA	C3B-C4B-NB	-3.44	107.46	110.53
12	1	801	CL0	C3B-C4B-NB	-3.43	107.46	110.53
13	b	826	CLA	O2D-CGD-O1D	-3.43	117.16	123.85
13	B	826	CLA	O2D-CGD-O1D	-3.43	117.17	123.85
13	2	818	CLA	C3B-C4B-NB	-3.43	107.47	110.53
13	b	821	CLA	C3B-C4B-NB	-3.42	107.47	110.53
13	2	835	CLA	CMB-C2B-C1B	-3.42	120.21	125.42
13	2	806	CLA	C3B-C4B-NB	-3.42	107.48	110.53
13	2	801	CLA	O2D-CGD-O1D	-3.42	117.20	123.85
13	B	806	CLA	C3B-C4B-NB	-3.41	107.48	110.53
13	1	826	CLA	C3B-C4B-NB	-3.41	107.48	110.53
13	1	830	CLA	C3B-C4B-NB	-3.41	107.48	110.53
13	b	806	CLA	C3B-C4B-NB	-3.40	107.49	110.53
13	b	803	CLA	C3B-C4B-NB	-3.40	107.49	110.53
13	B	801	CLA	O2D-CGD-O1D	-3.40	117.23	123.85
13	B	836	CLA	CMB-C2B-C1B	-3.40	120.25	125.42
13	b	814	CLA	CMB-C2B-C1B	-3.40	120.25	125.42
13	2	835	CLA	C3B-C4B-NB	-3.40	107.50	110.53
13	B	824	CLA	C3B-C4B-NB	-3.39	107.50	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	830	CLA	C3B-C4B-NB	-3.39	107.50	110.53
13	b	836	CLA	CMB-C2B-C1B	-3.39	120.25	125.42
13	b	836	CLA	C3B-C4B-NB	-3.39	107.51	110.53
13	2	813	CLA	CMB-C2B-C1B	-3.39	120.26	125.42
13	A	815	CLA	C3B-C4B-NB	-3.39	107.51	110.53
13	B	803	CLA	C3B-C4B-NB	-3.38	107.51	110.53
13	2	803	CLA	C3B-C4B-NB	-3.38	107.51	110.53
13	B	814	CLA	CMB-C2B-C1B	-3.38	120.27	125.42
13	B	817	CLA	C4A-NA-C1A	3.38	108.22	106.68
13	A	830	CLA	C3B-C4B-NB	-3.38	107.52	110.53
13	b	801	CLA	O2D-CGD-O1D	-3.38	117.28	123.85
13	2	823	CLA	C3B-C4B-NB	-3.37	107.52	110.53
13	B	836	CLA	C3B-C4B-NB	-3.37	107.52	110.53
13	2	816	CLA	C4A-NA-C1A	3.36	108.21	106.68
13	b	810	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
13	B	821	CLA	C3B-C4B-NB	-3.36	107.53	110.53
13	1	815	CLA	C3B-C4B-NB	-3.36	107.53	110.53
13	2	837	CLA	C3B-C4B-NB	-3.36	107.53	110.53
13	a	815	CLA	C3B-C4B-NB	-3.36	107.53	110.53
13	B	810	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
13	b	824	CLA	C3B-C4B-NB	-3.35	107.54	110.53
13	2	820	CLA	C3B-C4B-NB	-3.35	107.54	110.53
16	2	843	BCR	C15-C14-C13	-3.35	122.58	127.28
13	6	201	CLA	O2D-CGD-O1D	-3.34	117.34	123.85
13	2	809	CLA	O2D-CGD-O1D	-3.34	117.35	123.85
13	f	201	CLA	O2D-CGD-O1D	-3.34	117.35	123.85
16	B	844	BCR	C15-C14-C13	-3.34	122.60	127.28
13	F	201	CLA	O2D-CGD-O1D	-3.33	117.37	123.85
16	b	844	BCR	C15-C14-C13	-3.33	122.61	127.28
13	1	803	CLA	O2D-CGD-O1D	-3.32	117.38	123.85
13	b	817	CLA	C4A-NA-C1A	3.31	108.19	106.68
13	B	838	CLA	C3B-C4B-NB	-3.31	107.58	110.53
13	1	838	CLA	O2D-CGD-O1D	-3.29	117.45	123.85
16	B	844	BCR	C24-C23-C22	-3.29	121.37	126.23
13	2	819	CLA	C3B-C4B-NB	-3.28	107.60	110.53
13	B	820	CLA	C3B-C4B-NB	-3.28	107.60	110.53
13	A	803	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
13	a	814	CLA	C3B-C4B-NB	-3.28	107.60	110.53
13	A	838	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
16	2	843	BCR	C24-C23-C22	-3.28	121.39	126.23
13	0	202	CLA	C3B-C4B-NB	-3.27	107.61	110.53
13	b	838	CLA	C3B-C4B-NB	-3.27	107.61	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	7	103	BCR	C24-C23-C22	-3.26	121.41	126.23
13	a	838	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
13	2	824	CLA	CMB-C2B-C1B	-3.26	120.46	125.42
16	b	844	BCR	C24-C23-C22	-3.26	121.42	126.23
13	l	202	CLA	C3B-C4B-NB	-3.26	107.62	110.53
13	a	803	CLA	O2D-CGD-O1D	-3.26	117.51	123.85
16	i	103	BCR	C24-C23-C22	-3.25	121.42	126.23
13	b	802	CLA	O2D-CGD-O1D	-3.25	117.51	123.85
16	I	102	BCR	C24-C23-C22	-3.25	121.42	126.23
13	b	820	CLA	C3B-C4B-NB	-3.25	107.63	110.53
13	A	814	CLA	C3B-C4B-NB	-3.25	107.63	110.53
13	a	803	CLA	C3B-C4B-NB	-3.25	107.63	110.53
13	A	832	CLA	O2D-CGD-O1D	-3.25	117.53	123.85
13	2	802	CLA	O2D-CGD-O1D	-3.25	117.53	123.85
13	j	1103	CLA	C3B-C4B-NB	-3.24	107.64	110.53
13	B	802	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
13	a	812	CLA	C3B-C4B-NB	-3.24	107.64	110.53
13	1	832	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
13	a	832	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
13	b	825	CLA	CMB-C2B-C1B	-3.23	120.49	125.42
13	A	812	CLA	C3B-C4B-NB	-3.23	107.64	110.53
13	J	1103	CLA	C3B-C4B-NB	-3.23	107.65	110.53
13	L	201	CLA	C3B-C4B-NB	-3.23	107.65	110.53
13	f	201	CLA	C3B-C4B-NB	-3.23	107.65	110.53
13	1	818	CLA	CMB-C2B-C1B	-3.22	120.51	125.42
13	A	818	CLA	CMB-C2B-C1B	-3.22	120.51	125.42
13	1	812	CLA	C3B-C4B-NB	-3.22	107.66	110.53
13	1	805	CLA	C3B-C4B-NB	-3.22	107.66	110.53
13	8	1103	CLA	C3B-C4B-NB	-3.22	107.66	110.53
13	a	819	CLA	O2D-CGD-O1D	-3.22	117.59	123.85
13	F	201	CLA	C3B-C4B-NB	-3.21	107.66	110.53
13	a	805	CLA	C3B-C4B-NB	-3.21	107.66	110.53
13	B	825	CLA	CMB-C2B-C1B	-3.21	120.52	125.42
13	1	814	CLA	C3B-C4B-NB	-3.21	107.66	110.53
13	a	837	CLA	C3B-C4B-NB	-3.21	107.66	110.53
13	j	1102	CLA	C3B-C4B-NB	-3.21	107.66	110.53
13	a	818	CLA	CMB-C2B-C1B	-3.21	120.53	125.42
13	A	805	CLA	C3B-C4B-NB	-3.21	107.66	110.53
16	1	847	BCR	C11-C10-C9	-3.21	122.78	127.28
13	1	837	CLA	C3B-C4B-NB	-3.21	107.67	110.53
13	0	208	CLA	C3B-C4B-NB	-3.21	107.67	110.53
16	a	846	BCR	C11-C10-C9	-3.21	122.78	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	819	CLA	O2D-CGD-O1D	-3.21	117.61	123.85
13	A	803	CLA	C3B-C4B-NB	-3.20	107.67	110.53
13	J	1102	CLA	C3B-C4B-NB	-3.20	107.67	110.53
13	6	201	CLA	C3B-C4B-NB	-3.20	107.67	110.53
16	A	846	BCR	C11-C10-C9	-3.20	122.79	127.28
13	2	802	CLA	CMB-C2B-C1B	-3.19	120.56	125.42
13	A	837	CLA	C3B-C4B-NB	-3.19	107.68	110.53
13	1	803	CLA	C3B-C4B-NB	-3.19	107.68	110.53
13	A	819	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
13	B	829	CLA	O2D-CGD-O1D	-3.19	117.65	123.85
13	8	1102	CLA	C3B-C4B-NB	-3.18	107.69	110.53
13	B	835	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
13	2	828	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
16	1	846	BCR	C11-C10-C9	-3.18	122.82	127.28
13	b	829	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
13	A	824	CLA	C3B-C4B-NB	-3.18	107.69	110.53
13	B	802	CLA	CMB-C2B-C1B	-3.18	120.58	125.42
13	1	831	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
13	B	806	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
13	b	835	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
13	a	831	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
13	b	802	CLA	CMB-C2B-C1B	-3.17	120.59	125.42
13	b	806	CLA	O2D-CGD-O1D	-3.17	117.69	123.85
13	L	206	CLA	C3B-C4B-NB	-3.17	107.70	110.53
13	2	834	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
13	A	831	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
13	b	815	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
13	l	207	CLA	C3B-C4B-NB	-3.16	107.71	110.53
13	2	814	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
13	j	1102	CLA	C3A-C2A-C1A	-3.15	103.08	106.30
13	a	824	CLA	C3B-C4B-NB	-3.15	107.72	110.53
13	8	1102	CLA	C3A-C2A-C1A	-3.15	103.08	106.30
13	2	806	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
16	A	847	BCR	C11-C10-C9	-3.15	122.86	127.28
13	B	815	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
13	l	205	CLA	C3B-C4B-NB	-3.14	107.72	110.53
16	a	851	BCR	C27-C26-C25	3.14	126.95	122.70
13	L	204	CLA	C3B-C4B-NB	-3.14	107.73	110.53
16	a	847	BCR	C11-C10-C9	-3.13	122.89	127.28
13	1	823	CLA	C3B-C4B-NB	-3.13	107.73	110.53
13	J	1102	CLA	C3A-C2A-C1A	-3.13	103.10	106.30
16	A	851	BCR	C27-C26-C25	3.13	126.93	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	824	CLA	C3B-C4B-NB	-3.13	107.74	110.53
16	1	851	BCR	C27-C26-C25	3.13	126.93	122.70
13	1	833	CLA	O2D-CGD-O1D	-3.13	117.77	123.85
13	A	823	CLA	C3B-C4B-NB	-3.12	107.75	110.53
16	b	840	BCR	C15-C16-C17	-3.12	117.14	123.52
16	2	839	BCR	C15-C16-C17	-3.11	117.15	123.52
13	a	803	CLA	CMB-C2B-C1B	-3.11	120.68	125.42
19	I	103	SQD	O7-S-C6	3.11	111.40	106.76
13	A	833	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
16	a	846	BCR	C15-C16-C17	-3.11	117.16	123.52
16	B	840	BCR	C15-C16-C17	-3.11	117.16	123.52
13	b	808	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
19	i	101	SQD	O7-S-C6	3.10	111.39	106.76
19	7	101	SQD	O7-S-C6	3.10	111.39	106.76
13	A	821	CLA	C3B-C4B-NB	-3.10	107.76	110.53
13	0	206	CLA	C3B-C4B-NB	-3.10	107.76	110.53
13	b	825	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
13	a	821	CLA	C3B-C4B-NB	-3.10	107.77	110.53
13	a	833	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
13	2	807	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
16	b	844	BCR	C28-C27-C26	-3.09	108.55	114.06
16	A	846	BCR	C15-C16-C17	-3.09	117.20	123.52
13	B	808	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
13	B	825	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
13	a	823	CLA	C3B-C4B-NB	-3.09	107.77	110.53
13	a	835	CLA	O2D-CGD-O1D	-3.08	117.84	123.85
13	A	803	CLA	CMB-C2B-C1B	-3.08	120.72	125.42
13	b	832	CLA	C3A-C2A-C1A	-3.08	103.15	106.30
13	1	803	CLA	CMB-C2B-C1B	-3.08	120.73	125.42
13	a	828	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
13	1	821	CLA	C3B-C4B-NB	-3.08	107.78	110.53
13	A	828	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
13	1	828	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
16	B	844	BCR	C28-C27-C26	-3.07	108.57	114.06
16	1	846	BCR	C15-C16-C17	-3.07	117.24	123.52
13	a	806	CLA	C3B-C4B-NB	-3.07	107.79	110.53
13	A	806	CLA	C3B-C4B-NB	-3.07	107.79	110.53
13	b	812	CLA	O2D-CGD-O1D	-3.06	117.88	123.85
13	A	835	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
13	2	824	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
13	B	832	CLA	C3A-C2A-C1A	-3.06	103.17	106.30
13	B	812	CLA	O2D-CGD-O1D	-3.06	117.89	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	842	CLA	C3B-C4B-NB	-3.06	107.80	110.53
13	A	824	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
13	i	102	CLA	C3B-C4B-NB	-3.06	107.80	110.53
13	1	835	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
16	2	843	BCR	C28-C27-C26	-3.05	108.61	114.06
13	a	842	CLA	C3B-C4B-NB	-3.05	107.81	110.53
13	2	831	CLA	C3A-C2A-C1A	-3.05	103.18	106.30
13	1	824	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
13	2	811	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
13	9	4005	CLA	C3B-C4B-NB	-3.05	107.81	110.53
13	a	824	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
13	1	806	CLA	C3B-C4B-NB	-3.05	107.81	110.53
13	j	1101	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
13	b	826	CLA	C3B-C4B-NB	-3.04	107.81	110.53
13	J	1101	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
13	8	1101	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
16	B	843	BCR	C15-C16-C17	-3.04	117.30	123.52
16	a	847	BCR	C15-C16-C17	-3.04	117.30	123.52
13	1	813	CLA	CMB-C2B-C1B	-3.03	120.80	125.42
13	1	842	CLA	C3B-C4B-NB	-3.03	107.82	110.53
16	k	4001	BCR	C15-C14-C13	-3.03	123.03	127.28
16	b	843	BCR	C15-C16-C17	-3.03	117.32	123.52
13	a	811	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
16	1	847	BCR	C15-C16-C17	-3.03	117.32	123.52
16	A	847	BCR	C15-C16-C17	-3.03	117.32	123.52
13	A	813	CLA	CMB-C2B-C1B	-3.03	120.81	125.42
13	a	840	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
16	2	842	BCR	C15-C16-C17	-3.03	117.33	123.52
16	k	4001	BCR	C15-C16-C17	-3.02	117.34	123.52
13	a	802	CLA	C2B-C1B-NB	-3.02	107.19	110.33
13	1	811	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
13	b	824	CLA	CMB-C2B-C1B	-3.02	120.82	125.42
13	2	825	CLA	C3B-C4B-NB	-3.02	107.84	110.53
13	A	802	CLA	C2B-C1B-NB	-3.02	107.20	110.33
13	k	4005	CLA	C3B-C4B-NB	-3.02	107.84	110.53
16	K	4001	BCR	C15-C14-C13	-3.02	123.05	127.28
13	B	826	CLA	C3B-C4B-NB	-3.01	107.84	110.53
13	1	840	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
13	9	4002	CLA	C3B-C4B-NB	-3.01	107.84	110.53
13	A	810	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
13	a	813	CLA	CMB-C2B-C1B	-3.01	120.83	125.42
13	a	810	CLA	O2D-CGD-O1D	-3.01	117.98	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	K	4001	BCR	C15-C16-C17	-3.01	117.36	123.52
16	9	4001	BCR	C15-C14-C13	-3.01	123.06	127.28
13	I	101	CLA	C3B-C4B-NB	-3.01	107.84	110.53
13	K	4002	CLA	C3B-C4B-NB	-3.01	107.84	110.53
16	F	202	BCR	C15-C14-C13	-3.01	123.06	127.28
16	0	207	BCR	C15-C16-C17	-3.01	117.36	123.52
16	L	205	BCR	C15-C16-C17	-3.01	117.37	123.52
13	1	810	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
13	A	811	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
13	1	830	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
13	A	830	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
16	l	206	BCR	C15-C16-C17	-3.00	117.38	123.52
13	B	824	CLA	CMB-C2B-C1B	-3.00	120.85	125.42
13	A	840	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
16	9	4001	BCR	C15-C16-C17	-3.00	117.38	123.52
13	2	815	CLA	C3B-C4B-NB	-3.00	107.85	110.53
13	b	811	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
13	K	4005	CLA	C3B-C4B-NB	-3.00	107.85	110.53
13	k	4002	CLA	C3B-C4B-NB	-3.00	107.86	110.53
13	2	823	CLA	CMB-C2B-C1B	-3.00	120.86	125.42
13	b	834	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
13	2	833	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
19	7	101	SQD	O9-S-C6	2.99	111.22	106.76
13	0	206	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
13	L	204	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
13	B	834	CLA	O2D-CGD-O1D	-2.99	118.04	123.85
13	B	811	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
16	f	202	BCR	C15-C14-C13	-2.98	123.10	127.28
13	7	102	CLA	C3B-C4B-NB	-2.98	107.87	110.53
13	2	804	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
13	2	810	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
13	l	205	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
16	6	202	BCR	C15-C14-C13	-2.98	123.10	127.28
13	2	837	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
13	B	804	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
13	B	815	CLA	C3B-C4B-NB	-2.98	107.87	110.53
13	a	830	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
13	1	802	CLA	C2B-C1B-NB	-2.97	107.24	110.33
13	f	204	CLA	C3B-C4B-NB	-2.97	107.88	110.53
13	l	202	CLA	CMB-C2B-C1B	-2.97	120.90	125.42
13	b	804	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
13	B	838	CLA	O2D-CGD-O1D	-2.96	118.08	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	a	847	BCR	C15-C14-C13	-2.96	123.12	127.28
13	F	204	CLA	C3B-C4B-NB	-2.96	107.89	110.53
13	1	827	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
13	B	824	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
13	L	201	CLA	CMB-C2B-C1B	-2.96	120.92	125.42
13	2	823	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
13	b	824	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
19	i	101	SQD	O9-S-C6	2.96	111.17	106.76
13	b	838	CLA	O2D-CGD-O1D	-2.96	118.10	123.85
19	I	103	SQD	O9-S-C6	2.95	111.17	106.76
13	a	816	CLA	C3B-C4B-NB	-2.95	107.89	110.53
13	b	803	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
13	B	816	CLA	C3B-C4B-NB	-2.95	107.90	110.53
16	j	1104	BCR	C3-C4-C5	-2.95	108.80	114.06
13	A	827	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
13	0	203	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
13	B	807	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
13	b	816	CLA	C3B-C4B-NB	-2.94	107.90	110.53
13	a	841	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
13	0	202	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
13	0	202	CLA	CMB-C2B-C1B	-2.94	120.94	125.42
13	B	847	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
13	2	846	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
16	1	847	BCR	C15-C14-C13	-2.94	123.16	127.28
13	b	809	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
13	2	812	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
13	1	813	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
13	B	809	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
16	A	847	BCR	C15-C14-C13	-2.94	123.16	127.28
16	8	1104	BCR	C3-C4-C5	-2.93	108.82	114.06
13	a	827	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
13	2	808	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
13	6	204	CLA	C3B-C4B-NB	-2.93	107.91	110.53
13	A	813	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
16	J	1104	BCR	C3-C4-C5	-2.93	108.83	114.06
13	L	201	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
13	b	847	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
13	B	813	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
13	b	813	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
13	1	807	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
13	1	841	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
16	b	848	BCR	C33-C5-C6	-2.93	121.29	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	l	202	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
13	b	821	CLA	CMB-C2B-C1B	-2.93	120.96	125.42
13	A	807	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
13	b	807	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
16	b	840	BCR	C15-C14-C13	-2.92	123.18	127.28
13	A	841	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
13	b	815	CLA	C3B-C4B-NB	-2.92	107.92	110.53
13	1	816	CLA	C3B-C4B-NB	-2.92	107.92	110.53
13	B	833	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
13	2	846	CLA	C3B-C4B-NB	-2.92	107.92	110.53
13	0	208	CLA	CHD-C1D-ND	-2.92	120.69	124.80
13	a	813	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
13	2	811	CLA	C3B-C4B-NB	-2.92	107.92	110.53
13	a	807	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
13	B	821	CLA	CMB-C2B-C1B	-2.92	120.98	125.42
16	B	848	BCR	C33-C5-C6	-2.92	121.30	124.48
13	b	833	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
13	2	820	CLA	CMB-C2B-C1B	-2.92	120.98	125.42
13	A	804	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
13	a	825	CLA	O2D-CGD-O1D	-2.91	118.17	123.85
13	B	803	CLA	O2D-CGD-O1D	-2.91	118.17	123.85
16	2	847	BCR	C33-C5-C6	-2.91	121.30	124.48
13	2	814	CLA	C3B-C4B-NB	-2.91	107.93	110.53
13	1	804	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
13	a	814	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
13	b	822	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
13	B	831	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
13	b	831	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
13	1	814	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
13	L	203	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
13	B	847	CLA	C3B-C4B-NB	-2.91	107.94	110.53
16	B	840	BCR	C15-C14-C13	-2.91	123.20	127.28
13	2	830	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
13	l	207	CLA	CHD-C1D-ND	-2.91	120.71	124.80
13	A	816	CLA	C3B-C4B-NB	-2.91	107.94	110.53
13	B	812	CLA	C3B-C4B-NB	-2.91	107.94	110.53
13	a	804	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
13	b	812	CLA	C3B-C4B-NB	-2.90	107.94	110.53
13	A	814	CLA	O2D-CGD-O1D	-2.90	118.19	123.85
13	B	822	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
13	0	205	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
13	a	805	CLA	O2D-CGD-O1D	-2.90	118.20	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	2	803	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
13	2	815	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
13	L	206	CLA	CHD-C1D-ND	-2.90	120.72	124.80
13	A	818	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
17	a	849	LHG	O8-C23-C24	2.90	120.67	111.83
13	a	818	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
16	2	839	BCR	C15-C14-C13	-2.90	123.21	127.28
13	2	832	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
13	A	840	CLA	C3B-C4B-NB	-2.90	107.94	110.53
13	1	840	CLA	C3B-C4B-NB	-2.90	107.94	110.53
16	J	1104	BCR	C15-C14-C13	-2.90	123.22	127.28
13	A	825	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
17	A	849	LHG	O8-C23-C24	2.89	120.66	111.83
13	a	821	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
13	A	821	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
13	a	827	CLA	C3B-C4B-NB	-2.89	107.95	110.53
13	b	847	CLA	C3B-C4B-NB	-2.89	107.95	110.53
13	A	805	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
13	1	825	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
13	b	816	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
13	1	837	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
13	A	808	CLA	CMB-C2B-C1B	-2.89	121.02	125.42
17	1	849	LHG	O8-C23-C24	2.89	120.64	111.83
13	1	818	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
13	1	805	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
16	j	1104	BCR	C15-C14-C13	-2.88	123.23	127.28
16	j	1105	BCR	C15-C16-C17	-2.88	117.62	123.52
13	B	837	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
16	8	1105	BCR	C15-C16-C17	-2.88	117.62	123.52
13	A	837	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
13	2	821	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
13	2	827	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
13	1	808	CLA	CMB-C2B-C1B	-2.88	121.03	125.42
13	l	204	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
16	a	847	BCR	C28-C27-C26	-2.88	108.92	114.06
16	A	847	BCR	C28-C27-C26	-2.88	108.92	114.06
13	A	808	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
13	2	836	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
13	k	4003	CLA	C3B-C4B-NB	-2.88	107.96	110.53
13	1	821	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
13	b	837	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
13	1	808	CLA	O2D-CGD-O1D	-2.88	118.25	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	J	1105	BCR	C15-C16-C17	-2.87	117.64	123.52
16	1	847	BCR	C28-C27-C26	-2.87	108.93	114.06
13	b	830	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
13	a	808	CLA	CMB-C2B-C1B	-2.87	121.05	125.42
13	B	816	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
13	a	808	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
13	A	820	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
13	1	827	CLA	C3B-C4B-NB	-2.87	107.97	110.53
13	B	828	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
13	B	830	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
13	a	837	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
13	1	820	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
13	1	822	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
13	A	827	CLA	C3B-C4B-NB	-2.86	107.97	110.53
13	b	819	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
13	B	819	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
13	A	822	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
13	2	829	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
16	8	1104	BCR	C15-C14-C13	-2.86	123.27	127.28
13	2	805	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
13	K	4003	CLA	C3B-C4B-NB	-2.86	107.98	110.53
13	a	822	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
13	2	818	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
13	b	828	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
16	F	205	BCR	C15-C16-C17	-2.85	117.68	123.52
13	B	805	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
13	8	1102	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
13	b	823	CLA	C3B-C4B-NB	-2.85	107.99	110.53
13	9	4003	CLA	C3B-C4B-NB	-2.85	107.99	110.53
13	a	820	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
13	6	204	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
13	A	804	CLA	CMB-C2B-C1B	-2.85	121.08	125.42
13	a	804	CLA	CMB-C2B-C1B	-2.85	121.08	125.42
13	a	840	CLA	C3B-C4B-NB	-2.84	107.99	110.53
13	2	828	CLA	CHD-C1D-ND	-2.84	120.80	124.80
16	f	205	BCR	C15-C16-C17	-2.84	117.71	123.52
13	B	829	CLA	CHD-C1D-ND	-2.84	120.81	124.80
16	B	843	BCR	C27-C26-C25	2.84	126.54	122.70
16	6	205	BCR	C15-C14-C13	-2.84	123.30	127.28
13	1	809	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
13	9	4003	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
13	b	805	CLA	O2D-CGD-O1D	-2.84	118.33	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	k	4003	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
13	B	823	CLA	C3B-C4B-NB	-2.84	108.00	110.53
13	A	809	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
16	b	843	BCR	C27-C26-C25	2.83	126.53	122.70
13	A	836	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
13	J	1102	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
13	J	1103	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
13	1	836	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
13	K	4003	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
13	2	822	CLA	C3B-C4B-NB	-2.83	108.01	110.53
16	6	205	BCR	C15-C16-C17	-2.83	117.73	123.52
13	1	842	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
16	F	205	BCR	C15-C14-C13	-2.83	123.32	127.28
13	a	809	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
13	1	804	CLA	CMB-C2B-C1B	-2.82	121.12	125.42
16	2	842	BCR	C27-C26-C25	2.82	126.52	122.70
13	1	852	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
13	j	1103	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
13	B	832	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
13	b	829	CLA	CHD-C1D-ND	-2.82	120.83	124.80
13	a	836	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
13	a	852	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
16	f	205	BCR	C15-C14-C13	-2.82	123.32	127.28
13	f	204	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
13	2	831	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
13	A	842	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
13	L	206	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
13	A	852	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
13	b	832	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
16	k	4004	BCR	C15-C16-C17	-2.81	117.77	123.52
13	b	815	CLA	CMB-C2B-C1B	-2.81	121.14	125.42
16	2	841	BCR	C27-C26-C25	2.81	126.50	122.70
16	9	4004	BCR	C15-C16-C17	-2.81	117.77	123.52
13	F	204	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
16	K	4004	BCR	C15-C16-C17	-2.81	117.78	123.52
13	2	814	CLA	CMB-C2B-C1B	-2.81	121.14	125.42
13	j	1102	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
13	1	817	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
13	8	1103	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
16	8	1105	BCR	C28-C27-C26	-2.81	109.05	114.06
13	2	828	CLA	CMB-C2B-C1B	-2.80	121.15	125.42
13	2	826	CLA	O2D-CGD-O1D	-2.80	118.39	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	842	BCR	C27-C26-C25	2.80	126.49	122.70
13	i	102	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
13	B	815	CLA	CMB-C2B-C1B	-2.80	121.15	125.42
16	j	1105	BCR	C28-C27-C26	-2.80	109.06	114.06
13	l	207	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
13	I	101	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
14	a	843	PQN	C14-C13-C15	2.80	120.09	115.23
13	1	834	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
14	A	843	PQN	C14-C13-C15	2.80	120.08	115.23
13	B	829	CLA	CMB-C2B-C1B	-2.80	121.16	125.42
13	7	102	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
13	A	817	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
13	A	807	CLA	CMB-C2B-C1B	-2.79	121.17	125.42
13	1	823	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
16	J	1105	BCR	C28-C27-C26	-2.79	109.08	114.06
13	b	827	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
13	B	827	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
13	a	829	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
13	0	208	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
13	a	807	CLA	CMB-C2B-C1B	-2.79	121.17	125.42
16	b	842	BCR	C27-C26-C25	2.79	126.47	122.70
13	a	842	CLA	O2D-CGD-O1D	-2.79	118.43	123.85
13	1	807	CLA	CMB-C2B-C1B	-2.78	121.18	125.42
13	2	819	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
13	a	834	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
13	a	834	CLA	C3B-C4B-NB	-2.78	108.05	110.53
13	A	829	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
14	1	843	PQN	C14-C13-C15	2.78	120.05	115.23
13	a	823	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
13	A	834	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
13	a	817	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
13	A	823	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
13	B	821	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
13	l	204	CLA	CMB-C2B-C1B	-2.78	121.19	125.42
13	b	824	CLA	C2D-C1D-ND	-2.77	107.38	110.13
16	l	206	BCR	C15-C14-C13	-2.77	123.39	127.28
13	B	820	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
13	2	820	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
13	1	834	CLA	C3B-C4B-NB	-2.77	108.06	110.53
13	1	829	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
13	A	834	CLA	C3B-C4B-NB	-2.76	108.07	110.53
13	a	815	CLA	O2D-CGD-O1D	-2.76	118.48	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	829	CLA	CMB-C2B-C1B	-2.76	121.22	125.42
16	B	848	BCR	C15-C16-C17	-2.76	117.88	123.52
13	b	821	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
13	A	812	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
13	a	812	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
13	b	817	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
16	2	847	BCR	C15-C16-C17	-2.75	117.89	123.52
13	B	824	CLA	C2D-C1D-ND	-2.75	107.40	110.13
13	0	205	CLA	CMB-C2B-C1B	-2.75	121.23	125.42
13	b	820	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
13	L	203	CLA	CMB-C2B-C1B	-2.75	121.23	125.42
13	a	828	CLA	CMB-C2B-C1B	-2.75	121.23	125.42
13	B	817	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
13	2	816	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
13	A	828	CLA	CMB-C2B-C1B	-2.75	121.24	125.42
13	A	815	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
16	b	848	BCR	C15-C16-C17	-2.75	117.90	123.52
16	0	201	BCR	C15-C16-C17	-2.74	117.91	123.52
16	L	205	BCR	C15-C14-C13	-2.74	123.44	127.28
13	a	839	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
16	l	201	BCR	C15-C16-C17	-2.74	117.92	123.52
13	2	817	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
16	m	101	BCR	C15-C16-C17	-2.73	117.93	123.52
13	l	812	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
16	M	101	BCR	C15-C16-C17	-2.73	117.94	123.52
16	z	101	BCR	C15-C16-C17	-2.73	117.94	123.52
12	a	801	CL0	O2D-CGD-O1D	-2.73	118.54	123.85
13	B	802	CLA	C3C-C4C-NC	-2.73	106.94	110.43
13	a	835	CLA	CMB-C2B-C1B	-2.73	121.27	125.42
16	b	842	BCR	C2-C1-C6	2.73	114.40	110.44
16	0	207	BCR	C15-C14-C13	-2.73	123.45	127.28
16	2	839	BCR	C27-C26-C25	2.73	126.39	122.70
13	1	815	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
16	L	207	BCR	C15-C16-C17	-2.72	117.95	123.52
13	1	828	CLA	CMB-C2B-C1B	-2.72	121.27	125.42
12	1	801	CL0	O2D-CGD-O1D	-2.72	118.55	123.85
12	A	801	CL0	O2D-CGD-O1D	-2.72	118.55	123.85
16	b	840	BCR	C27-C26-C25	2.72	126.38	122.70
13	A	835	CLA	CMB-C2B-C1B	-2.71	121.28	125.42
16	B	842	BCR	C2-C1-C6	2.71	114.38	110.44
16	B	840	BCR	C27-C26-C25	2.71	126.37	122.70
13	B	818	CLA	O2D-CGD-O1D	-2.71	118.57	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	2	823	CLA	C2D-C1D-ND	-2.71	107.44	110.13
13	A	839	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
19	i	101	SQD	C44-O6-C1	2.71	119.60	113.80
13	B	823	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
13	b	818	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
13	1	839	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
13	1	835	CLA	CMB-C2B-C1B	-2.70	121.30	125.42
16	b	841	BCR	C15-C16-C17	-2.70	117.99	123.52
19	7	101	SQD	C44-O6-C1	2.70	119.58	113.80
13	2	802	CLA	C3C-C4C-NC	-2.70	106.97	110.43
13	b	823	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
16	B	841	BCR	C15-C16-C17	-2.70	118.00	123.52
16	2	840	BCR	C15-C16-C17	-2.70	118.00	123.52
16	2	841	BCR	C2-C1-C6	2.69	114.35	110.44
13	b	802	CLA	C3C-C4C-NC	-2.69	106.98	110.43
19	I	103	SQD	C44-O6-C1	2.69	119.57	113.80
16	0	207	BCR	C28-C27-C26	-2.69	109.26	114.06
16	1	846	BCR	C27-C26-C25	2.69	126.33	122.70
16	1	203	BCR	C2-C1-C6	2.69	114.34	110.44
13	1	840	CLA	C2D-C1D-ND	-2.68	107.47	110.13
13	a	831	CLA	C2B-C1B-NB	-2.68	107.54	110.33
13	A	840	CLA	C2D-C1D-ND	-2.68	107.47	110.13
13	2	822	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
13	2	813	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
16	B	848	BCR	C27-C26-C25	2.67	126.32	122.70
16	2	847	BCR	C27-C26-C25	2.67	126.32	122.70
13	b	814	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
16	L	205	BCR	C28-C27-C26	-2.67	109.29	114.06
13	B	814	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
16	b	848	BCR	C27-C26-C25	2.67	126.31	122.70
13	a	806	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
13	A	825	CLA	CMB-C2B-C1B	-2.67	121.36	125.42
13	a	840	CLA	C2D-C1D-ND	-2.67	107.49	110.13
13	A	806	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
13	1	806	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
16	a	845	BCR	C27-C26-C25	2.66	126.30	122.70
13	1	836	CLA	CMB-C2B-C1B	-2.66	121.36	125.42
13	A	831	CLA	C2B-C1B-NB	-2.66	107.56	110.33
16	2	839	BCR	C24-C23-C22	-2.66	122.30	126.23
16	A	845	BCR	C27-C26-C25	2.66	126.30	122.70
13	A	836	CLA	CMB-C2B-C1B	-2.66	121.37	125.42
13	a	825	CLA	CMB-C2B-C1B	-2.66	121.37	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	825	CLA	CMB-C2B-C1B	-2.66	121.37	125.42
13	f	203	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
13	1	831	CLA	C2B-C1B-NB	-2.66	107.57	110.33
16	L	205	BCR	C29-C30-C25	2.66	114.30	110.44
16	B	840	BCR	C24-C23-C22	-2.66	122.30	126.23
13	a	816	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
13	a	836	CLA	CMB-C2B-C1B	-2.66	121.37	125.42
13	A	816	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
13	a	802	CLA	CHD-C1D-ND	-2.66	121.07	124.80
16	L	202	BCR	C2-C1-C6	2.65	114.30	110.44
13	6	203	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
13	2	820	CLA	C3C-C4C-NC	-2.65	107.03	110.43
13	K	4005	CLA	O2D-CGD-O1D	-2.65	118.07	124.08
13	k	4005	CLA	O2D-CGD-O1D	-2.65	118.07	124.08
13	F	203	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
16	A	848	BCR	C31-C1-C6	2.65	114.40	110.24
16	l	206	BCR	C28-C27-C26	-2.65	109.33	114.06
16	A	846	BCR	C27-C26-C25	2.65	126.28	122.70
13	B	821	CLA	C3C-C4C-NC	-2.65	107.04	110.43
13	1	816	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
16	1	845	BCR	C27-C26-C25	2.64	126.28	122.70
13	2	831	CLA	C3B-C4B-NB	-2.64	108.17	110.53
16	l	206	BCR	C29-C30-C25	2.64	114.28	110.44
16	0	207	BCR	C29-C30-C25	2.64	114.28	110.44
16	B	845	BCR	C27-C26-C25	2.64	126.28	122.70
16	b	840	BCR	C24-C23-C22	-2.64	122.33	126.23
16	b	845	BCR	C27-C26-C25	2.64	126.27	122.70
13	9	4005	CLA	O2D-CGD-O1D	-2.64	118.09	124.08
16	a	846	BCR	C27-C26-C25	2.64	126.27	122.70
16	0	204	BCR	C2-C1-C6	2.64	114.27	110.44
16	9	4004	BCR	C27-C26-C25	2.63	126.26	122.70
13	1	802	CLA	CHD-C1D-ND	-2.63	121.10	124.80
16	1	848	BCR	C31-C1-C6	2.63	114.36	110.24
13	b	821	CLA	C3C-C4C-NC	-2.63	107.07	110.43
16	k	4004	BCR	C27-C26-C25	2.62	126.25	122.70
13	B	832	CLA	C3B-C4B-NB	-2.62	108.19	110.53
16	a	848	BCR	C31-C1-C6	2.62	114.36	110.24
13	A	802	CLA	CHD-C1D-ND	-2.62	121.11	124.80
13	b	817	CLA	C3B-C4B-NB	-2.62	108.19	110.53
13	b	832	CLA	C3B-C4B-NB	-2.62	108.19	110.53
16	K	4004	BCR	C27-C26-C25	2.62	126.24	122.70
13	b	835	CLA	C3C-C4C-NC	-2.61	107.09	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	2	844	BCR	C27-C26-C25	2.61	126.23	122.70
16	b	848	BCR	C11-C10-C9	-2.60	123.62	127.28
16	B	848	BCR	C11-C10-C9	-2.60	123.63	127.28
13	1	825	CLA	C3B-C4B-NB	-2.60	108.21	110.53
13	A	821	CLA	CHA-C1A-NA	-2.60	120.51	126.39
13	a	821	CLA	CHA-C1A-NA	-2.60	120.51	126.39
19	7	101	SQD	C1-O5-C5	2.60	118.79	113.72
16	2	847	BCR	C11-C10-C9	-2.59	123.64	127.28
13	B	817	CLA	C3B-C4B-NB	-2.59	108.22	110.53
13	2	834	CLA	C3C-C4C-NC	-2.59	107.11	110.43
13	B	835	CLA	C3C-C4C-NC	-2.59	107.12	110.43
13	1	821	CLA	CHA-C1A-NA	-2.59	120.53	126.39
16	b	848	BCR	C7-C8-C9	-2.59	122.41	126.23
16	l	203	BCR	C24-C23-C22	-2.59	122.41	126.23
13	f	203	CLA	C3B-C4B-NB	-2.58	108.23	110.53
16	j	1105	BCR	C29-C30-C25	2.58	114.19	110.44
16	b	840	BCR	C11-C10-C9	-2.58	123.66	127.28
17	1	849	LHG	C11-C10-C9	-2.58	101.33	114.37
19	I	103	SQD	C1-O5-C5	2.58	118.75	113.72
16	8	1105	BCR	C29-C30-C25	2.58	114.18	110.44
17	A	849	LHG	C11-C10-C9	-2.58	101.35	114.37
19	i	101	SQD	C1-O5-C5	2.58	118.75	113.72
17	a	849	LHG	C11-C10-C9	-2.57	101.37	114.37
13	2	837	CLA	CMB-C2B-C1B	-2.57	121.50	125.42
19	7	101	SQD	O5-C5-C4	2.57	114.33	109.70
16	J	1105	BCR	C29-C30-C25	2.57	114.17	110.44
13	b	819	CLA	CMB-C2B-C1B	-2.57	121.51	125.42
16	L	202	BCR	C24-C23-C22	-2.57	122.44	126.23
13	A	841	CLA	C3B-C4B-NB	-2.57	108.24	110.53
16	K	4001	BCR	C24-C23-C22	-2.56	122.44	126.23
13	1	826	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
13	f	201	CLA	CHB-C4A-NA	2.56	128.10	124.40
13	F	203	CLA	C3B-C4B-NB	-2.56	108.24	110.53
13	a	839	CLA	C1-C2-C3	-2.56	122.00	126.20
13	6	201	CLA	CHB-C4A-NA	2.56	128.09	124.40
13	A	839	CLA	C1-C2-C3	-2.56	122.01	126.20
13	A	826	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
13	2	816	CLA	C3B-C4B-NB	-2.56	108.25	110.53
13	F	201	CLA	CHB-C4A-NA	2.56	128.09	124.40
19	i	101	SQD	O5-C5-C4	2.56	114.30	109.70
16	B	848	BCR	C7-C8-C9	-2.56	122.45	126.23
17	A	850	LHG	O8-C23-C24	2.55	119.62	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	850	LHG	O8-C23-C24	2.55	119.62	111.83
13	6	203	CLA	C3B-C4B-NB	-2.55	108.25	110.53
16	k	4001	BCR	C24-C23-C22	-2.55	122.46	126.23
16	2	847	BCR	C7-C8-C9	-2.55	122.46	126.23
13	B	838	CLA	CMB-C2B-C1B	-2.55	121.53	125.42
16	2	844	BCR	C15-C16-C17	-2.55	118.30	123.52
13	1	839	CLA	C1-C2-C3	-2.55	122.02	126.20
13	2	813	CLA	C2D-C1D-ND	-2.55	107.61	110.13
13	A	825	CLA	C3B-C4B-NB	-2.55	108.26	110.53
13	1	841	CLA	C3B-C4B-NB	-2.55	108.26	110.53
13	a	826	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
16	0	204	BCR	C24-C23-C22	-2.54	122.47	126.23
16	b	844	BCR	C11-C10-C9	-2.54	123.71	127.28
13	1	831	CLA	O2D-CGD-CBD	2.54	115.67	111.23
17	a	850	LHG	O8-C23-C24	2.54	119.58	111.83
13	L	204	CLA	CMB-C2B-C1B	-2.54	121.55	125.42
16	2	843	BCR	C11-C10-C9	-2.54	123.72	127.28
16	B	845	BCR	C15-C16-C17	-2.54	118.33	123.52
16	b	845	BCR	C15-C16-C17	-2.54	118.33	123.52
16	B	840	BCR	C11-C10-C9	-2.54	123.72	127.28
16	9	4001	BCR	C24-C23-C22	-2.54	122.48	126.23
13	a	820	CLA	C3B-C4B-NB	-2.54	108.27	110.53
16	b	843	BCR	C24-C23-C22	-2.54	122.48	126.23
19	I	103	SQD	O5-C5-C4	2.53	114.27	109.70
13	A	831	CLA	O2D-CGD-CBD	2.53	115.66	111.23
13	B	819	CLA	CMB-C2B-C1B	-2.53	121.56	125.42
13	A	820	CLA	C3B-C4B-NB	-2.53	108.27	110.53
13	1	842	CLA	CMB-C2B-C1B	-2.53	121.56	125.42
13	a	833	CLA	CHB-C4A-NA	2.53	128.05	124.40
13	A	831	CLA	CMB-C2B-C1B	-2.53	121.57	125.42
13	a	826	CLA	CMB-C2B-C1B	-2.53	121.57	125.42
13	B	814	CLA	C2D-C1D-ND	-2.53	107.62	110.13
13	a	831	CLA	O2D-CGD-CBD	2.53	115.65	111.23
16	a	846	BCR	C7-C8-C9	-2.53	122.50	126.23
13	A	826	CLA	CMB-C2B-C1B	-2.53	121.57	125.42
13	b	838	CLA	CMB-C2B-C1B	-2.53	121.57	125.42
13	b	837	CLA	CHD-C1D-ND	-2.53	121.25	124.80
13	1	826	CLA	CMB-C2B-C1B	-2.53	121.57	125.42
13	b	814	CLA	C2D-C1D-ND	-2.52	107.63	110.13
16	B	844	BCR	C11-C10-C9	-2.52	123.74	127.28
16	B	843	BCR	C24-C23-C22	-2.52	122.50	126.23
16	2	842	BCR	C24-C23-C22	-2.52	122.50	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	831	CLA	CMB-C2B-C1B	-2.52	121.58	125.42
13	1	205	CLA	CMB-C2B-C1B	-2.52	121.58	125.42
13	2	836	CLA	CHD-C1D-ND	-2.52	121.26	124.80
13	2	818	CLA	CMB-C2B-C1B	-2.52	121.58	125.42
13	a	842	CLA	CMB-C2B-C1B	-2.52	121.58	125.42
13	1	831	CLA	CMB-C2B-C1B	-2.52	121.59	125.42
13	0	206	CLA	CMB-C2B-C1B	-2.51	121.59	125.42
13	a	825	CLA	C3B-C4B-NB	-2.51	108.29	110.53
13	L	203	CLA	CHB-C4A-NA	2.51	128.03	124.40
13	1	832	CLA	CHB-C4A-NA	2.51	128.03	124.40
13	B	837	CLA	CHD-C1D-ND	-2.51	121.27	124.80
13	A	842	CLA	CMB-C2B-C1B	-2.51	121.60	125.42
16	F	205	BCR	C11-C10-C9	-2.51	123.76	127.28
16	2	839	BCR	C11-C10-C9	-2.51	123.76	127.28
13	0	205	CLA	CHB-C4A-NA	2.51	128.02	124.40
16	A	846	BCR	C7-C8-C9	-2.51	122.53	126.23
16	6	205	BCR	C11-C10-C9	-2.51	123.76	127.28
16	f	205	BCR	C11-C10-C9	-2.50	123.77	127.28
13	A	832	CLA	CHB-C4A-NA	2.50	128.01	124.40
13	2	803	CLA	CMB-C2B-C1B	-2.50	121.61	125.42
13	a	841	CLA	C3B-C4B-NB	-2.50	108.30	110.53
13	1	824	CLA	CHD-C1D-ND	-2.50	121.28	124.80
13	A	833	CLA	CHB-C4A-NA	2.50	128.00	124.40
13	B	836	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
16	1	846	BCR	C7-C8-C9	-2.49	122.55	126.23
13	1	820	CLA	C3B-C4B-NB	-2.49	108.31	110.53
14	1	843	PQN	C11-C12-C13	-2.49	122.54	126.83
13	b	803	CLA	CMB-C2B-C1B	-2.49	121.63	125.42
13	b	836	CLA	O2D-CGD-O1D	-2.49	119.01	123.85
13	B	827	CLA	CHD-C1D-ND	-2.49	121.30	124.80
13	1	204	CLA	CHB-C4A-NA	2.48	127.99	124.40
13	1	802	CLA	CMD-C2D-C1D	-2.48	120.36	124.73
13	2	835	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
13	a	832	CLA	CHB-C4A-NA	2.48	127.98	124.40
14	A	843	PQN	C11-C12-C13	-2.48	122.56	126.83
16	7	103	BCR	C31-C1-C6	2.48	114.13	110.24
13	B	803	CLA	CMB-C2B-C1B	-2.48	121.65	125.42
13	b	827	CLA	CHD-C1D-ND	-2.48	121.32	124.80
16	1	206	BCR	C11-C10-C9	-2.48	123.80	127.28
13	2	824	CLA	CHA-C1A-NA	-2.48	120.78	126.39
16	0	207	BCR	C11-C10-C9	-2.47	123.81	127.28
13	2	826	CLA	CHD-C1D-ND	-2.47	121.32	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	824	CLA	CHD-C1D-ND	-2.47	121.32	124.80
14	a	843	PQN	C11-C12-C13	-2.47	122.58	126.83
13	B	825	CLA	CHA-C1A-NA	-2.47	120.80	126.39
13	B	836	CLA	CHA-C1A-NA	-2.47	120.81	126.39
16	2	842	BCR	C15-C14-C13	-2.47	123.82	127.28
13	a	825	CLA	O2A-CGA-O1A	-2.47	117.46	123.63
16	j	1105	BCR	C15-C14-C13	-2.46	123.83	127.28
13	1	833	CLA	CHB-C4A-NA	2.46	127.95	124.40
13	a	828	CLA	CHD-C1D-ND	-2.46	121.34	124.80
16	l	201	BCR	C11-C10-C9	-2.46	123.83	127.28
13	b	836	CLA	CHA-C1A-NA	-2.46	120.82	126.39
13	a	824	CLA	CHD-C1D-ND	-2.46	121.34	124.80
16	i	103	BCR	C31-C1-C6	2.46	114.10	110.24
16	B	843	BCR	C15-C14-C13	-2.46	123.83	127.28
13	A	802	CLA	CMD-C2D-C1D	-2.46	120.40	124.73
16	k	4004	BCR	C7-C8-C9	-2.46	122.60	126.23
13	2	835	CLA	CHA-C1A-NA	-2.46	120.83	126.39
13	A	805	CLA	O2A-CGA-O1A	-2.46	117.49	123.63
13	a	802	CLA	CMD-C2D-C1D	-2.45	120.41	124.73
16	L	205	BCR	C11-C10-C9	-2.45	123.84	127.28
16	L	202	BCR	C15-C16-C17	-2.45	118.50	123.52
13	1	805	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
13	a	805	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
13	A	825	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
16	l	203	BCR	C15-C16-C17	-2.45	118.51	123.52
13	1	825	CLA	O2A-CGA-O1A	-2.45	117.51	123.63
13	1	841	CLA	CHB-C4A-NA	2.45	127.93	124.40
16	K	4004	BCR	C7-C8-C9	-2.45	122.62	126.23
16	I	102	BCR	C31-C1-C6	2.45	114.08	110.24
16	b	843	BCR	C15-C14-C13	-2.45	123.85	127.28
13	b	825	CLA	CHA-C1A-NA	-2.45	120.85	126.39
16	j	1105	BCR	C24-C23-C22	-2.44	122.62	126.23
17	1	850	LHG	C11-C10-C9	-2.44	102.02	114.37
16	b	842	BCR	C15-C16-C17	-2.44	118.52	123.52
16	0	204	BCR	C15-C16-C17	-2.44	118.52	123.52
16	A	846	BCR	C15-C14-C13	-2.44	123.86	127.28
16	L	207	BCR	C11-C10-C9	-2.44	123.86	127.28
16	2	841	BCR	C15-C16-C17	-2.44	118.53	123.52
16	0	201	BCR	C11-C10-C9	-2.44	123.86	127.28
16	J	1105	BCR	C24-C23-C22	-2.44	122.63	126.23
16	b	844	BCR	C29-C30-C25	2.44	113.98	110.44
16	1	847	BCR	C29-C30-C25	2.44	113.98	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	850	LHG	C11-C10-C9	-2.44	102.06	114.37
17	a	850	LHG	C11-C10-C9	-2.44	102.06	114.37
16	A	847	BCR	C29-C30-C25	2.43	113.98	110.44
13	B	807	CLA	C3B-C4B-NB	-2.43	108.36	110.53
16	B	842	BCR	C15-C16-C17	-2.43	118.54	123.52
16	B	844	BCR	C29-C30-C25	2.43	113.97	110.44
16	a	847	BCR	C29-C30-C25	2.43	113.97	110.44
16	f	202	BCR	C15-C16-C17	-2.43	118.55	123.52
16	9	4004	BCR	C7-C8-C9	-2.43	122.64	126.23
16	F	202	BCR	C24-C23-C22	-2.43	122.64	126.23
16	1	846	BCR	C15-C14-C13	-2.43	123.87	127.28
16	6	202	BCR	C24-C23-C22	-2.42	122.65	126.23
16	a	846	BCR	C15-C14-C13	-2.42	123.88	127.28
13	b	834	CLA	CMB-C2B-C1B	-2.42	121.73	125.42
13	A	841	CLA	CHB-C4A-NA	2.42	127.90	124.40
16	J	1105	BCR	C15-C14-C13	-2.42	123.88	127.28
16	F	202	BCR	C15-C16-C17	-2.42	118.56	123.52
13	b	801	CLA	CHB-C4A-NA	2.42	127.89	124.40
13	A	828	CLA	CHD-C1D-ND	-2.42	121.40	124.80
13	a	841	CLA	CHB-C4A-NA	2.42	127.89	124.40
13	A	822	CLA	CMB-C2B-C1B	-2.42	121.74	125.42
13	2	833	CLA	CMB-C2B-C1B	-2.42	121.74	125.42
16	b	843	BCR	C11-C10-C9	-2.42	123.89	127.28
16	0	201	BCR	C7-C8-C9	-2.42	122.66	126.23
16	8	1105	BCR	C24-C23-C22	-2.42	122.66	126.23
16	2	843	BCR	C29-C30-C25	2.42	113.95	110.44
13	K	4005	CLA	CHB-C4A-NA	2.42	127.89	124.40
13	b	807	CLA	C3B-C4B-NB	-2.42	108.37	110.53
16	l	201	BCR	C7-C8-C9	-2.42	122.66	126.23
13	2	817	CLA	C3C-C4C-NC	-2.41	107.34	110.43
13	b	801	CLA	C1D-ND-C4D	2.41	108.01	106.31
16	0	201	BCR	C27-C26-C25	2.41	125.97	122.70
13	a	822	CLA	CMB-C2B-C1B	-2.41	121.74	125.42
13	1	828	CLA	CHD-C1D-ND	-2.41	121.41	124.80
13	1	822	CLA	CMB-C2B-C1B	-2.41	121.75	125.42
16	f	202	BCR	C24-C23-C22	-2.41	122.67	126.23
16	6	202	BCR	C15-C16-C17	-2.41	118.59	123.52
13	B	834	CLA	CMB-C2B-C1B	-2.41	121.76	125.42
13	b	801	CLA	C3A-C2A-C1A	2.40	104.94	101.34
13	K	4002	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
13	B	804	CLA	CHD-C1D-ND	-2.40	121.42	124.80
16	8	1105	BCR	C15-C14-C13	-2.40	123.91	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	k	4005	CLA	CHB-C4A-NA	2.40	127.87	124.40
13	9	4005	CLA	CHB-C4A-NA	2.40	127.87	124.40
16	F	205	BCR	C27-C26-C25	2.40	125.95	122.70
13	0	203	CLA	C3B-C4B-NB	-2.40	108.39	110.53
13	9	4002	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
13	1	836	CLA	C1-C2-C3	-2.40	122.27	126.20
16	2	842	BCR	C11-C10-C9	-2.40	123.92	127.28
16	6	205	BCR	C27-C26-C25	2.40	125.94	122.70
13	2	804	CLA	CHD-C1D-ND	-2.40	121.43	124.80
13	b	833	CLA	C2D-C1D-ND	-2.39	107.76	110.13
13	b	804	CLA	CHD-C1D-ND	-2.39	121.43	124.80
16	L	207	BCR	C7-C8-C9	-2.39	122.69	126.23
16	B	843	BCR	C11-C10-C9	-2.39	123.92	127.28
13	B	818	CLA	C3C-C4C-NC	-2.39	107.36	110.43
13	2	801	CLA	C1D-ND-C4D	2.39	107.99	106.31
13	B	813	CLA	CHD-C1D-ND	-2.39	121.44	124.80
13	k	4003	CLA	CHB-C4A-NA	2.39	127.85	124.40
16	z	101	BCR	C24-C23-C22	-2.39	122.70	126.23
13	b	818	CLA	C3C-C4C-NC	-2.39	107.37	110.43
13	b	813	CLA	CHD-C1D-ND	-2.39	121.44	124.80
16	m	101	BCR	C24-C23-C22	-2.39	122.70	126.23
13	k	4002	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
13	2	801	CLA	CHB-C4A-NA	2.39	127.84	124.40
16	l	201	BCR	C27-C26-C25	2.39	125.93	122.70
16	a	851	BCR	C15-C16-C17	-2.38	118.64	123.52
13	1	813	CLA	CHB-C4A-NA	2.38	127.84	124.40
13	a	802	CLA	CMB-C2B-C3B	2.38	132.15	126.55
16	b	841	BCR	C28-C27-C26	-2.38	109.81	114.06
13	a	836	CLA	C1-C2-C3	-2.38	122.30	126.20
13	1	802	CLA	CMB-C2B-C3B	2.38	132.15	126.55
13	B	801	CLA	C1D-ND-C4D	2.38	107.98	106.31
16	M	101	BCR	C24-C23-C22	-2.38	122.72	126.23
13	A	836	CLA	C1-C2-C3	-2.38	122.30	126.20
13	B	801	CLA	CHB-C4A-NA	2.38	127.83	124.40
16	1	851	BCR	C15-C16-C17	-2.38	118.66	123.52
13	B	833	CLA	C2D-C1D-ND	-2.38	107.77	110.13
16	L	207	BCR	C27-C26-C25	2.37	125.91	122.70
16	B	841	BCR	C28-C27-C26	-2.37	109.82	114.06
16	0	204	BCR	C16-C15-C14	-2.37	118.66	123.52
13	9	4003	CLA	CHB-C4A-NA	2.37	127.83	124.40
17	A	850	LHG	C20-C19-C18	-2.37	102.37	114.37
17	1	850	LHG	C20-C19-C18	-2.37	102.37	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	K	4003	CLA	CHB-C4A-NA	2.37	127.83	124.40
13	B	801	CLA	C3A-C2A-C1A	2.37	104.89	101.34
17	a	850	LHG	C20-C19-C18	-2.37	102.38	114.37
13	2	812	CLA	CHD-C1D-ND	-2.37	121.47	124.80
13	A	838	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
16	l	203	BCR	C16-C15-C14	-2.37	118.67	123.52
13	A	802	CLA	CMB-C2B-C3B	2.37	132.12	126.55
13	a	838	CLA	O2A-CGA-O1A	-2.37	117.71	123.63
16	A	851	BCR	C15-C16-C17	-2.37	118.68	123.52
16	L	202	BCR	C16-C15-C14	-2.37	118.68	123.52
16	2	840	BCR	C28-C27-C26	-2.37	109.84	114.06
16	f	205	BCR	C27-C26-C25	2.36	125.90	122.70
13	A	813	CLA	CHB-C4A-NA	2.36	127.81	124.40
13	2	832	CLA	C2D-C1D-ND	-2.36	107.79	110.13
13	2	801	CLA	C3A-C2A-C1A	2.36	104.87	101.34
13	2	832	CLA	C1-C2-C3	-2.36	122.94	126.76
13	a	806	CLA	C3C-C4C-NC	-2.36	107.41	110.43
16	a	848	BCR	C2-C1-C6	2.36	113.86	110.44
13	1	838	CLA	O2A-CGA-O1A	-2.36	117.74	123.63
16	a	847	BCR	C7-C8-C9	-2.35	122.76	126.23
16	l	203	BCR	C27-C26-C25	2.35	125.88	122.70
13	B	833	CLA	C1-C2-C3	-2.35	122.96	126.76
13	b	808	CLA	CMB-C2B-C1B	-2.35	121.84	125.42
13	a	837	CLA	CHD-C1D-ND	-2.35	121.50	124.80
16	0	201	BCR	C15-C14-C13	-2.35	123.98	127.28
12	1	801	CL0	O2A-CGA-O1A	-2.35	117.75	123.63
13	a	813	CLA	CHB-C4A-NA	2.34	127.78	124.40
16	8	1104	BCR	C15-C16-C17	-2.34	118.72	123.52
13	A	836	CLA	CHA-C1A-NA	-2.34	121.09	126.39
13	a	836	CLA	CHA-C1A-NA	-2.34	121.09	126.39
16	A	847	BCR	C7-C8-C9	-2.34	122.78	126.23
16	1	847	BCR	C7-C8-C9	-2.34	122.78	126.23
13	1	836	CLA	CHA-C1A-NA	-2.34	121.10	126.39
16	j	1104	BCR	C15-C16-C17	-2.34	118.74	123.52
16	b	841	BCR	C15-C14-C13	-2.34	124.00	127.28
16	2	840	BCR	C15-C14-C13	-2.34	124.00	127.28
16	J	1104	BCR	C15-C16-C17	-2.34	118.74	123.52
16	l	201	BCR	C15-C14-C13	-2.34	124.00	127.28
13	B	808	CLA	CMB-C2B-C1B	-2.33	121.86	125.42
13	1	829	CLA	CMB-C2B-C1B	-2.33	121.87	125.42
13	a	802	CLA	C4-C3-C5	2.33	119.28	115.23
13	B	824	CLA	CHA-C1A-NA	-2.33	121.11	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	9	4004	BCR	C11-C10-C9	-2.33	124.01	127.28
13	2	807	CLA	CMB-C2B-C1B	-2.33	121.87	125.42
16	1	848	BCR	C2-C1-C6	2.33	113.83	110.44
13	b	824	CLA	CHA-C1A-NA	-2.33	121.11	126.39
13	A	829	CLA	CMB-C2B-C1B	-2.33	121.87	125.42
12	a	801	CL0	O2A-CGA-O1A	-2.33	117.80	123.63
16	A	848	BCR	C2-C1-C6	2.33	113.82	110.44
16	L	207	BCR	C15-C14-C13	-2.33	124.01	127.28
13	A	818	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
13	a	804	CLA	CHD-C1D-ND	-2.33	121.53	124.80
16	B	841	BCR	C15-C14-C13	-2.33	124.02	127.28
13	1	818	CLA	O2A-CGA-O1A	-2.33	117.81	123.63
13	a	818	CLA	O2A-CGA-O1A	-2.32	117.81	123.63
12	A	801	CL0	O2A-CGA-O1A	-2.32	117.82	123.63
13	A	806	CLA	C3C-C4C-NC	-2.32	107.45	110.43
13	b	833	CLA	C1-C2-C3	-2.32	123.01	126.76
13	a	829	CLA	CMB-C2B-C1B	-2.32	121.88	125.42
13	1	804	CLA	CHD-C1D-ND	-2.32	121.54	124.80
16	j	1104	BCR	C7-C8-C9	-2.32	122.80	126.23
16	L	202	BCR	C27-C26-C25	2.32	125.84	122.70
13	b	826	CLA	C2D-C1D-ND	-2.32	107.83	110.13
13	1	827	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
13	A	804	CLA	CHD-C1D-ND	-2.32	121.54	124.80
13	A	837	CLA	CHD-C1D-ND	-2.32	121.54	124.80
16	z	101	BCR	C15-C14-C13	-2.32	124.03	127.28
13	A	818	CLA	C4D-C3D-CAD	-2.31	105.59	108.11
13	B	811	CLA	CMB-C2B-C1B	-2.31	121.89	125.42
13	a	831	CLA	C1-C2-C3	-2.31	123.02	126.76
19	7	101	SQD	O48-C23-C24	2.31	118.89	111.83
13	a	818	CLA	C4D-C3D-CAD	-2.31	105.59	108.11
13	A	802	CLA	C4-C3-C5	2.31	119.24	115.23
13	A	827	CLA	CMB-C2B-C1B	-2.31	121.90	125.42
13	2	810	CLA	CMB-C2B-C1B	-2.31	121.90	125.42
13	1	831	CLA	C1-C2-C3	-2.31	123.02	126.76
13	2	823	CLA	CHA-C1A-NA	-2.31	121.15	126.39
13	1	806	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
13	1	837	CLA	CHD-C1D-ND	-2.31	121.55	124.80
16	M	101	BCR	C15-C14-C13	-2.31	124.04	127.28
13	B	829	CLA	CHA-C1A-NA	-2.31	121.17	126.39
13	1	806	CLA	C3C-C4C-NC	-2.31	107.47	110.43
13	2	846	CLA	CHA-C1A-NA	-2.31	121.17	126.39
13	a	806	CLA	O2A-CGA-O1A	-2.31	117.86	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	I	103	SQD	O48-C23-C24	2.30	118.86	111.83
13	A	831	CLA	C1-C2-C3	-2.30	123.03	126.76
13	B	822	CLA	CMB-C2B-C1B	-2.30	121.91	125.42
13	2	821	CLA	CMB-C2B-C1B	-2.30	121.91	125.42
16	K	4004	BCR	C11-C10-C9	-2.30	124.05	127.28
16	6	202	BCR	C29-C30-C25	2.30	113.78	110.44
16	a	848	BCR	C24-C23-C22	-2.30	122.83	126.23
19	i	101	SQD	O48-C23-C24	2.30	118.85	111.83
13	b	830	CLA	CHB-C4A-NA	2.30	127.72	124.40
16	0	204	BCR	C15-C14-C13	-2.30	124.05	127.28
13	1	802	CLA	C4-C3-C5	2.30	119.22	115.23
16	9	4001	BCR	C27-C26-C25	2.30	125.81	122.70
13	1	817	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
13	a	827	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
16	J	1104	BCR	C7-C8-C9	-2.30	122.83	126.23
13	b	811	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
13	b	847	CLA	CHA-C1A-NA	-2.30	121.19	126.39
13	A	806	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
13	b	821	CLA	O1D-CGD-CBD	2.30	129.05	124.52
13	2	806	CLA	O2A-CGA-O1A	-2.30	117.89	123.63
13	B	838	CLA	CHB-C4A-NA	2.30	127.71	124.40
13	2	828	CLA	CHA-C1A-NA	-2.30	121.19	126.39
13	b	829	CLA	CHA-C1A-NA	-2.30	121.19	126.39
13	a	808	CLA	CHA-C1A-NA	-2.29	121.19	126.39
13	A	808	CLA	CHA-C1A-NA	-2.29	121.20	126.39
13	b	847	CLA	CHB-C4A-NA	2.29	127.71	124.40
13	a	817	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
16	f	202	BCR	C29-C30-C25	2.29	113.77	110.44
13	B	847	CLA	CHA-C1A-NA	-2.29	121.20	126.39
13	1	808	CLA	CHA-C1A-NA	-2.29	121.20	126.39
13	B	821	CLA	O1D-CGD-CBD	2.29	129.04	124.52
13	1	813	CLA	CHD-C1D-ND	-2.29	121.58	124.80
13	A	817	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
13	2	820	CLA	O1D-CGD-CBD	2.29	129.03	124.52
16	F	202	BCR	C29-C30-C25	2.29	113.76	110.44
13	b	822	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
16	8	1104	BCR	C7-C8-C9	-2.29	122.85	126.23
16	K	4001	BCR	C27-C26-C25	2.29	125.80	122.70
13	1	841	CLA	CHA-C1A-NA	-2.29	121.21	126.39
16	A	848	BCR	C24-C23-C22	-2.29	122.85	126.23
13	1	818	CLA	C4D-C3D-CAD	-2.29	105.62	108.11
13	B	806	CLA	O2A-CGA-O1A	-2.29	117.91	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	a	845	BCR	C24-C23-C22	-2.28	122.86	126.23
19	7	101	SQD	C4-C3-C2	2.28	114.84	110.83
13	A	836	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
13	B	807	CLA	C2D-C1D-ND	-2.28	107.87	110.13
13	2	829	CLA	CHB-C4A-NA	2.28	127.69	124.40
16	k	4001	BCR	C27-C26-C25	2.28	125.79	122.70
16	0	204	BCR	C27-C26-C25	2.28	125.79	122.70
13	b	838	CLA	CHB-C4A-NA	2.28	127.69	124.40
16	m	101	BCR	C15-C14-C13	-2.28	124.08	127.28
16	k	4004	BCR	C11-C10-C9	-2.28	124.08	127.28
13	2	832	CLA	C2B-C1B-NB	-2.28	107.96	110.33
13	A	841	CLA	CHA-C1A-NA	-2.28	121.23	126.39
16	A	845	BCR	C24-C23-C22	-2.28	122.86	126.23
13	A	815	CLA	CMB-C2B-C1B	-2.28	121.95	125.42
13	a	841	CLA	CHA-C1A-NA	-2.28	121.23	126.39
13	2	837	CLA	CHB-C4A-NA	2.28	127.69	124.40
13	1	836	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
13	0	203	CLA	C2D-C1D-ND	-2.28	107.87	110.13
16	1	848	BCR	C24-C23-C22	-2.28	122.87	126.23
13	B	847	CLA	CHB-C4A-NA	2.27	127.68	124.40
16	6	202	BCR	C27-C26-C25	2.27	125.78	122.70
13	i	102	CLA	C3C-C4C-NC	-2.27	107.52	110.43
13	a	808	CLA	CHD-C1D-ND	-2.27	121.60	124.80
13	b	811	CLA	C2D-C1D-ND	-2.27	107.88	110.13
16	B	848	BCR	C15-C14-C13	-2.27	124.09	127.28
13	1	852	CLA	CHA-C1A-NA	-2.27	121.25	126.39
13	b	823	CLA	CHB-C4A-NA	2.27	127.68	124.40
19	I	103	SQD	C4-C3-C2	2.27	114.81	110.83
19	i	101	SQD	C4-C3-C2	2.27	114.81	110.83
13	a	836	CLA	O2A-CGA-O1A	-2.27	117.96	123.63
16	F	202	BCR	C27-C26-C25	2.27	125.77	122.70
13	b	807	CLA	C2D-C1D-ND	-2.27	107.88	110.13
13	A	833	CLA	CHA-C1A-NA	-2.27	121.26	126.39
16	L	202	BCR	C15-C14-C13	-2.26	124.10	127.28
13	b	806	CLA	O2A-CGA-O1A	-2.26	117.96	123.63
13	2	830	CLA	CHB-C4A-NA	2.26	127.67	124.40
13	a	833	CLA	CHA-C1A-NA	-2.26	121.27	126.39
13	B	823	CLA	CHB-C4A-NA	2.26	127.67	124.40
13	a	825	CLA	CHA-C1A-NA	-2.26	121.27	126.39
13	1	825	CLA	CHA-C1A-NA	-2.26	121.27	126.39
16	j	1104	BCR	C24-C23-C22	-2.26	122.89	126.23
13	1	833	CLA	CHA-C1A-NA	-2.26	121.27	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	2	847	BCR	C15-C14-C13	-2.26	124.11	127.28
16	f	202	BCR	C27-C26-C25	2.26	125.76	122.70
16	2	841	BCR	C31-C1-C6	2.26	113.79	110.24
13	2	822	CLA	CHB-C4A-NA	2.26	127.66	124.40
13	A	825	CLA	CHA-C1A-NA	-2.26	121.28	126.39
13	A	852	CLA	CHA-C1A-NA	-2.26	121.28	126.39
13	1	808	CLA	CHD-C1D-ND	-2.26	121.62	124.80
13	1	815	CLA	CMB-C2B-C1B	-2.26	121.98	125.42
13	2	810	CLA	C2D-C1D-ND	-2.26	107.89	110.13
13	a	852	CLA	CHA-C1A-NA	-2.26	121.28	126.39
16	1	845	BCR	C24-C23-C22	-2.26	122.90	126.23
16	k	4001	BCR	C11-C10-C9	-2.26	124.11	127.28
13	2	817	CLA	CHB-C4A-NA	2.26	127.66	124.40
13	1	803	CLA	CAA-CBA-CGA	-2.26	106.81	113.21
13	B	837	CLA	C3B-C4B-NB	-2.25	108.52	110.53
13	B	830	CLA	CHB-C4A-NA	2.25	127.65	124.40
13	B	830	CLA	CHA-C1A-NA	-2.25	121.28	126.39
13	a	852	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
16	J	1104	BCR	C24-C23-C22	-2.25	122.90	126.23
13	A	808	CLA	CHD-C1D-ND	-2.25	121.63	124.80
13	B	811	CLA	C2D-C1D-ND	-2.25	107.90	110.13
18	b	846	LMG	O3-C3-C2	-2.25	105.06	110.38
13	B	826	CLA	C2D-C1D-ND	-2.25	107.90	110.13
16	A	845	BCR	C16-C15-C14	-2.25	118.91	123.52
18	B	846	LMG	O3-C3-C2	-2.25	105.07	110.38
16	K	4001	BCR	C11-C10-C9	-2.25	124.12	127.28
13	A	813	CLA	CHD-C1D-ND	-2.25	121.64	124.80
13	1	852	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
13	2	826	CLA	CHB-C4A-NA	2.25	127.64	124.40
13	I	101	CLA	C3C-C4C-NC	-2.25	107.55	110.43
13	2	846	CLA	CHB-C4A-NA	2.25	127.64	124.40
13	A	809	CLA	CHB-C4A-NA	2.25	127.64	124.40
16	B	842	BCR	C31-C1-C6	2.25	113.77	110.24
16	8	1104	BCR	C24-C23-C22	-2.25	122.91	126.23
13	2	814	CLA	C2D-C1D-ND	-2.25	107.90	110.13
13	B	831	CLA	CHB-C4A-NA	2.25	127.64	124.40
13	a	814	CLA	CHB-C4A-NA	2.25	127.64	124.40
13	B	833	CLA	C2B-C1B-NB	-2.25	108.00	110.33
16	b	848	BCR	C15-C14-C13	-2.25	124.13	127.28
16	a	845	BCR	C16-C15-C14	-2.25	118.92	123.52
13	a	803	CLA	CAA-CBA-CGA	-2.25	106.83	113.21
13	2	809	CLA	CMB-C2B-C1B	-2.24	122.00	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	2	829	CLA	CHA-C1A-NA	-2.24	121.31	126.39
13	A	803	CLA	CAA-CBA-CGA	-2.24	106.83	113.21
16	1	845	BCR	C16-C15-C14	-2.24	118.93	123.52
13	b	837	CLA	C3B-C4B-NB	-2.24	108.53	110.53
13	I	101	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
16	b	842	BCR	C31-C1-C6	2.24	113.76	110.24
16	9	4001	BCR	C11-C10-C9	-2.24	124.13	127.28
13	A	852	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
13	B	818	CLA	CHB-C4A-NA	2.24	127.63	124.40
13	a	815	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
13	1	809	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
16	b	841	BCR	C7-C8-C9	-2.24	122.92	126.23
13	7	102	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
13	b	810	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
13	b	830	CLA	CHA-C1A-NA	-2.24	121.32	126.39
13	b	815	CLA	O2D-CGD-CBD	2.24	115.14	111.23
13	2	831	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
13	7	102	CLA	C3C-C4C-NC	-2.24	107.56	110.43
13	2	804	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
13	A	814	CLA	CHB-C4A-NA	2.24	127.63	124.40
16	8	1104	BCR	C27-C26-C25	2.24	125.73	122.70
13	A	828	CLA	CMB-C2B-C3B	2.24	131.81	126.55
13	a	809	CLA	CHB-C4A-NA	2.23	127.62	124.40
13	2	825	CLA	C2D-C1D-ND	-2.23	107.92	110.13
13	2	836	CLA	C3B-C4B-NB	-2.23	108.54	110.53
13	2	814	CLA	O2D-CGD-CBD	2.23	115.13	111.23
18	2	845	LMG	O3-C3-C2	-2.23	105.11	110.38
13	b	804	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
13	b	831	CLA	CHB-C4A-NA	2.23	127.62	124.40
19	i	101	SQD	O8-S-C6	2.23	110.28	105.97
13	1	809	CLA	CHB-C4A-NA	2.23	127.62	124.40
13	B	804	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
16	B	841	BCR	C7-C8-C9	-2.23	122.94	126.23
13	B	810	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
13	B	814	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
16	l	203	BCR	C15-C14-C13	-2.23	124.15	127.28
13	B	815	CLA	C2D-C1D-ND	-2.23	107.92	110.13
13	1	828	CLA	CMB-C2B-C3B	2.23	131.79	126.55
14	b	839	PQN	C11-C12-C13	-2.23	123.00	126.83
16	f	205	BCR	C33-C5-C6	-2.23	122.06	124.48
13	b	818	CLA	CHB-C4A-NA	2.23	127.61	124.40
13	i	102	CLA	O2A-CGA-O1A	-2.23	118.06	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	832	CLA	CMB-C2B-C1B	-2.23	122.03	125.42
19	7	101	SQD	O8-S-C6	2.22	110.27	105.97
19	I	103	SQD	O8-S-C6	2.22	110.27	105.97
13	2	810	CLA	C3C-C4C-NC	-2.22	107.58	110.43
16	2	840	BCR	C7-C8-C9	-2.22	122.95	126.23
13	B	810	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
13	a	832	CLA	C1-C2-C3	-2.22	122.56	126.20
16	f	202	BCR	C11-C10-C9	-2.22	124.16	127.28
13	b	814	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
13	b	837	CLA	CHB-C4A-NA	2.22	127.60	124.40
13	8	1103	CLA	CHB-C4A-NA	2.22	127.60	124.40
16	J	1104	BCR	C27-C26-C25	2.22	125.70	122.70
13	A	803	CLA	C3C-C4C-NC	-2.22	107.59	110.43
16	b	845	BCR	C10-C11-C12	-2.22	116.77	123.20
16	7	103	BCR	C27-C26-C25	2.22	125.70	122.70
16	2	844	BCR	C10-C11-C12	-2.22	116.77	123.20
13	B	811	CLA	C3C-C4C-NC	-2.22	107.59	110.43
13	1	822	CLA	C3C-C4C-NC	-2.22	107.59	110.43
13	a	828	CLA	CMB-C2B-C3B	2.22	131.77	126.55
13	1	814	CLA	CHB-C4A-NA	2.22	127.60	124.40
16	B	845	BCR	C10-C11-C12	-2.22	116.78	123.20
13	b	833	CLA	C2B-C1B-NB	-2.22	108.03	110.33
13	b	832	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
13	1	832	CLA	C1-C2-C3	-2.22	122.57	126.20
16	a	847	BCR	C33-C5-C6	-2.22	122.07	124.48
13	2	815	CLA	CHA-C1A-NA	-2.22	121.37	126.39
13	b	810	CLA	CMB-C2B-C1B	-2.22	122.05	125.42
13	B	815	CLA	O2D-CGD-CBD	2.22	115.10	111.23
13	2	823	CLA	CHD-C1D-ND	-2.22	121.69	124.80
13	A	809	CLA	CMB-C2B-C1B	-2.22	122.05	125.42
16	6	205	BCR	C33-C5-C6	-2.22	122.07	124.48
14	B	839	PQN	C11-C12-C13	-2.21	123.02	126.83
13	2	813	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
13	J	1103	CLA	CHB-C4A-NA	2.21	127.59	124.40
13	A	832	CLA	C1-C2-C3	-2.21	122.57	126.20
13	A	822	CLA	C3C-C4C-NC	-2.21	107.60	110.43
13	a	809	CLA	CMB-C2B-C1B	-2.21	122.05	125.42
16	F	205	BCR	C33-C5-C6	-2.21	122.07	124.48
13	2	801	CLA	CMB-C2B-C1B	-2.21	122.06	125.42
16	a	851	BCR	C20-C21-C22	-2.21	124.18	127.28
16	I	102	BCR	C27-C26-C25	2.21	125.69	122.70
13	B	816	CLA	CHA-C1A-NA	-2.21	121.39	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	2	809	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
16	A	847	BCR	C33-C5-C6	-2.21	122.08	124.48
13	a	813	CLA	CHD-C1D-ND	-2.21	121.70	124.80
13	b	811	CLA	C3C-C4C-NC	-2.21	107.60	110.43
13	j	1103	CLA	CHB-C4A-NA	2.21	127.58	124.40
16	i	103	BCR	C2-C1-C6	2.21	113.64	110.44
13	1	836	CLA	CHB-C4A-NA	2.21	127.58	124.40
13	a	822	CLA	C3C-C4C-NC	-2.20	107.61	110.43
13	1	832	CLA	CMB-C2B-C1B	-2.20	122.06	125.42
13	1	803	CLA	C3C-C4C-NC	-2.20	107.61	110.43
13	A	836	CLA	CHB-C4A-NA	2.20	127.58	124.40
13	B	827	CLA	CHB-C4A-NA	2.20	127.58	124.40
16	j	1104	BCR	C11-C10-C9	-2.20	124.19	127.28
16	2	844	BCR	C15-C14-C13	-2.20	124.19	127.28
13	1	822	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
13	a	803	CLA	C3C-C4C-NC	-2.20	107.61	110.43
13	a	810	CLA	CMB-C2B-C1B	-2.20	122.07	125.42
16	1	851	BCR	C20-C21-C22	-2.20	124.19	127.28
13	b	829	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
13	b	827	CLA	CHB-C4A-NA	2.20	127.58	124.40
13	B	837	CLA	CHB-C4A-NA	2.20	127.58	124.40
16	7	103	BCR	C15-C16-C17	-2.20	119.02	123.52
16	6	202	BCR	C11-C10-C9	-2.20	124.19	127.28
14	2	838	PQN	C11-C12-C13	-2.20	123.04	126.83
16	I	102	BCR	C15-C16-C17	-2.20	119.02	123.52
13	1	810	CLA	CMB-C2B-C1B	-2.20	122.07	125.42
16	2	840	BCR	C29-C30-C25	2.20	113.63	110.44
13	1	830	CLA	CHA-C1A-NA	-2.20	121.41	126.39
13	b	816	CLA	CHA-C1A-NA	-2.20	121.42	126.39
16	i	103	BCR	C27-C26-C25	2.20	125.67	122.70
13	2	830	CLA	CHA-C1A-NA	-2.20	121.42	126.39
13	2	832	CLA	CHA-C1A-NA	-2.20	121.42	126.39
13	1	814	CLA	O2A-CGA-O1A	-2.20	118.14	123.63
16	i	103	BCR	C15-C16-C17	-2.19	119.03	123.52
16	b	841	BCR	C29-C30-C25	2.19	113.62	110.44
13	B	815	CLA	CHB-C4A-NA	2.19	127.56	124.40
13	A	822	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
13	b	801	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
16	A	851	BCR	C20-C21-C22	-2.19	124.20	127.28
13	b	815	CLA	CHB-C4A-NA	2.19	127.56	124.40
13	L	201	CLA	CHA-C1A-NA	-2.19	121.43	126.39
16	F	202	BCR	C11-C10-C9	-2.19	124.20	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	806	CLA	C1-C2-C3	-2.19	122.61	126.20
13	b	831	CLA	CHA-C1A-NA	-2.19	121.43	126.39
13	B	801	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
13	B	833	CLA	CHA-C1A-NA	-2.19	121.43	126.39
13	a	822	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
16	B	845	BCR	C15-C14-C13	-2.19	124.20	127.28
16	8	1104	BCR	C11-C10-C9	-2.19	124.20	127.28
13	2	814	CLA	CHB-C4A-NA	2.19	127.56	124.40
13	2	824	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
13	A	832	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
16	B	841	BCR	C29-C30-C25	2.19	113.62	110.44
13	a	817	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
13	B	831	CLA	CHA-C1A-NA	-2.19	121.43	126.39
13	0	205	CLA	CHA-C1A-NA	-2.19	121.43	126.39
13	B	825	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
13	1	825	CLA	C2A-C1A-CHA	2.19	127.67	123.87
13	l	202	CLA	CHA-C1A-NA	-2.19	121.43	126.39
13	a	814	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
13	2	832	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
13	B	801	CLA	CHA-C1A-NA	-2.19	121.44	126.39
13	B	820	CLA	CHA-C1A-NA	-2.19	121.44	126.39
13	2	819	CLA	CHA-C1A-NA	-2.19	121.44	126.39
13	0	202	CLA	CHA-C1A-NA	-2.19	121.44	126.39
16	0	207	BCR	C33-C5-C6	-2.19	122.10	124.48
13	L	203	CLA	CHA-C1A-NA	-2.19	121.44	126.39
13	j	1103	CLA	CHD-C1D-ND	-2.19	121.72	124.80
13	A	817	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
13	2	803	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
13	B	829	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
13	l	204	CLA	CHA-C1A-NA	-2.19	121.44	126.39
13	B	806	CLA	C1-C2-C3	-2.19	122.62	126.20
13	2	806	CLA	C1-C2-C3	-2.19	122.62	126.20
13	A	825	CLA	C2A-C1A-CHA	2.18	127.66	123.87
13	f	201	CLA	O2D-CGD-CBD	2.18	115.05	111.23
16	J	1104	BCR	C11-C10-C9	-2.18	124.22	127.28
13	a	830	CLA	C2B-C1B-NB	-2.18	108.06	110.33
13	A	830	CLA	CHA-C1A-NA	-2.18	121.45	126.39
13	A	814	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
13	a	822	CLA	C1-C2-C3	-2.18	123.23	126.76
16	1	847	BCR	C33-C5-C6	-2.18	122.10	124.48
13	1	829	CLA	CHA-C1A-NA	-2.18	121.45	126.39
13	a	832	CLA	CMB-C2B-C1B	-2.18	122.10	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	823	CLA	CMB-C2B-C1B	-2.18	122.10	125.42
13	2	825	CLA	O2D-CGD-CBD	2.18	115.04	111.23
13	2	836	CLA	CHB-C4A-NA	2.18	127.55	124.40
13	b	824	CLA	CHD-C1D-ND	-2.18	121.74	124.80
13	b	833	CLA	CHA-C1A-NA	-2.18	121.46	126.39
13	2	801	CLA	CHA-C1A-NA	-2.18	121.46	126.39
13	B	803	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
13	A	810	CLA	CMB-C2B-C1B	-2.18	122.10	125.42
13	b	826	CLA	O2D-CGD-CBD	2.18	115.04	111.23
13	a	825	CLA	C2A-C1A-CHA	2.18	127.65	123.87
13	1	824	CLA	CHB-C4A-NA	2.18	127.54	124.40
13	1	817	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
13	6	201	CLA	O2D-CGD-CBD	2.18	115.04	111.23
13	a	836	CLA	CHB-C4A-NA	2.18	127.54	124.40
16	9	4004	BCR	C24-C23-C22	-2.18	123.02	126.23
16	A	851	BCR	C33-C5-C6	-2.18	122.11	124.48
16	I	102	BCR	C2-C1-C6	2.18	113.60	110.44
13	b	801	CLA	CHA-C1A-NA	-2.18	121.47	126.39
13	1	806	CLA	CMB-C2B-C1B	-2.18	122.11	125.42
13	a	830	CLA	CHA-C1A-NA	-2.17	121.47	126.39
16	7	103	BCR	C2-C1-C6	2.17	113.60	110.44
13	2	811	CLA	CHB-C4A-NA	2.17	127.54	124.40
12	a	801	CL0	C2B-C1B-NB	-2.17	108.07	110.33
13	b	825	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
13	2	803	CLA	C2D-C1D-ND	-2.17	107.97	110.13
13	b	803	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
13	1	803	CLA	O1D-CGD-CBD	2.17	128.80	124.52
13	B	824	CLA	CHD-C1D-ND	-2.17	121.75	124.80
13	B	812	CLA	CHB-C4A-NA	2.17	127.53	124.40
13	b	815	CLA	C2D-C1D-ND	-2.17	107.98	110.13
13	B	826	CLA	O2D-CGD-CBD	2.17	115.03	111.23
13	1	802	CLA	O2D-CGD-CBD	2.17	115.02	111.23
13	B	833	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
16	K	4004	BCR	C24-C23-C22	-2.17	123.03	126.23
13	a	837	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
13	a	802	CLA	O2D-CGD-CBD	2.17	115.02	111.23
13	A	830	CLA	C2B-C1B-NB	-2.17	108.08	110.33
13	B	816	CLA	CHB-C4A-NA	2.17	127.53	124.40
13	b	820	CLA	CHA-C1A-NA	-2.17	121.48	126.39
16	k	4004	BCR	C24-C23-C22	-2.17	123.03	126.23
13	A	829	CLA	CHA-C1A-NA	-2.17	121.48	126.39
13	1	830	CLA	C2B-C1B-NB	-2.17	108.08	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	b	845	BCR	C15-C14-C13	-2.17	124.24	127.28
13	f	203	CLA	O2A-CGA-O1A	-2.17	117.76	123.33
13	B	810	CLA	O2D-CGD-CBD	2.17	115.02	111.23
13	A	829	CLA	C1-C2-C3	-2.16	122.65	126.20
13	B	813	CLA	O2A-CGA-O1A	-2.16	118.21	123.63
13	F	201	CLA	O2D-CGD-CBD	2.16	115.01	111.23
13	A	822	CLA	C1-C2-C3	-2.16	123.26	126.76
13	2	828	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
13	A	803	CLA	O1D-CGD-CBD	2.16	128.79	124.52
16	a	851	BCR	C33-C5-C6	-2.16	122.12	124.48
13	a	829	CLA	CHA-C1A-NA	-2.16	121.49	126.39
13	1	822	CLA	C1-C2-C3	-2.16	123.26	126.76
13	J	1103	CLA	CHD-C1D-ND	-2.16	121.76	124.80
13	k	4003	CLA	CHA-C1A-NA	-2.16	121.50	126.39
13	1	819	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
13	1	837	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
13	B	823	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
16	j	1104	BCR	C27-C26-C25	2.16	125.62	122.70
13	a	823	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
13	A	819	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
13	1	807	CLA	CHD-C1D-ND	-2.16	121.76	124.80
16	a	851	BCR	C16-C15-C14	-2.16	119.10	123.52
13	b	816	CLA	CHB-C4A-NA	2.16	127.52	124.40
13	2	811	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
13	A	802	CLA	O2D-CGD-CBD	2.16	115.00	111.23
13	A	804	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
13	A	837	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
13	A	806	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
13	9	4003	CLA	CHA-C1A-NA	-2.16	121.51	126.39
17	A	850	LHG	C27-C26-C25	-2.16	103.47	114.37
13	B	801	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
13	I	101	CLA	CMB-C2B-C1B	-2.16	122.14	125.42
13	2	809	CLA	O2D-CGD-CBD	2.16	115.00	111.23
13	2	815	CLA	CHB-C4A-NA	2.16	127.51	124.40
13	a	806	CLA	CMB-C2B-C1B	-2.16	122.14	125.42
17	a	850	LHG	C27-C26-C25	-2.16	103.47	114.37
13	a	803	CLA	O1D-CGD-CBD	2.15	128.77	124.52
16	K	4001	BCR	C33-C5-C6	-2.15	122.13	124.48
13	6	203	CLA	O2A-CGA-O1A	-2.15	117.79	123.33
13	b	812	CLA	CHB-C4A-NA	2.15	127.51	124.40
13	a	819	CLA	CMB-C2B-C1B	-2.15	122.14	125.42
13	K	4003	CLA	CHA-C1A-NA	-2.15	121.52	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	823	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
16	2	844	BCR	C16-C15-C14	-2.15	119.11	123.52
13	2	801	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
13	F	203	CLA	CHD-C1D-ND	-2.15	121.77	124.80
13	a	804	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
13	b	833	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
13	a	831	CLA	CHB-C4A-NA	2.15	127.50	124.40
13	1	804	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
13	1	835	CLA	CHA-C1A-NA	-2.15	121.52	126.39
13	A	807	CLA	CHD-C1D-ND	-2.15	121.78	124.80
13	1	807	CLA	CHA-C1A-NA	-2.15	121.52	126.39
17	1	850	LHG	C27-C26-C25	-2.15	103.50	114.37
13	1	837	CLA	CMB-C2B-C1B	-2.15	122.14	125.42
12	a	801	CL0	C1-C2-C3	-2.15	122.67	126.20
13	a	812	CLA	CMB-C2B-C1B	-2.15	122.15	125.42
12	A	801	CL0	C2B-C1B-NB	-2.15	108.10	110.33
13	b	803	CLA	C2D-C1D-ND	-2.15	108.00	110.13
16	L	207	BCR	C40-C30-C25	2.15	113.61	110.24
13	2	822	CLA	CMB-C2B-C1B	-2.15	122.15	125.42
13	b	810	CLA	O2D-CGD-CBD	2.15	114.99	111.23
13	6	203	CLA	CHD-C1D-ND	-2.15	121.78	124.80
13	A	807	CLA	CHA-C1A-NA	-2.15	121.53	126.39
16	k	4001	BCR	C33-C5-C6	-2.15	122.14	124.48
16	z	101	BCR	C28-C27-C26	-2.15	110.22	114.06
13	J	1102	CLA	CHB-C4A-NA	2.15	127.50	124.40
13	2	804	CLA	O2D-CGD-CBD	2.15	114.98	111.23
13	a	824	CLA	CHB-C4A-NA	2.15	127.50	124.40
13	2	812	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
13	a	807	CLA	CHA-C1A-NA	-2.15	121.53	126.39
13	a	835	CLA	CHA-C1A-NA	-2.15	121.53	126.39
13	7	102	CLA	CMB-C2B-C1B	-2.15	122.15	125.42
13	A	824	CLA	CHB-C4A-NA	2.15	127.50	124.40
13	B	812	CLA	CMB-C2B-C1B	-2.14	122.15	125.42
13	A	818	CLA	C1-C2-C3	-2.14	122.69	126.20
16	K	4004	BCR	C15-C14-C13	-2.14	124.27	127.28
16	L	205	BCR	C33-C5-C6	-2.14	122.15	124.48
13	A	831	CLA	CHB-C4A-NA	2.14	127.49	124.40
13	1	823	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
13	B	813	CLA	CHA-C1A-NA	-2.14	121.54	126.39
13	b	812	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
13	1	809	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
16	1	851	BCR	C16-C15-C14	-2.14	119.14	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	1	801	CL0	C1-C2-C3	-2.14	122.69	126.20
13	1	829	CLA	C1-C2-C3	-2.14	122.69	126.20
13	a	802	CLA	C4-C3-C2	-2.14	118.13	123.63
16	0	201	BCR	C40-C30-C25	2.14	113.60	110.24
16	B	845	BCR	C16-C15-C14	-2.14	119.14	123.52
12	A	801	CL0	C1-C2-C3	-2.14	122.69	126.20
13	b	813	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
16	9	4001	BCR	C33-C5-C6	-2.14	122.15	124.48
16	f	205	BCR	C24-C23-C22	-2.14	123.07	126.23
16	l	201	BCR	C40-C30-C25	2.14	113.60	110.24
13	1	822	CLA	CHA-C1A-NA	-2.14	121.55	126.39
16	1	851	BCR	C33-C5-C6	-2.14	122.15	124.48
13	a	829	CLA	C1-C2-C3	-2.14	122.69	126.20
13	A	809	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
13	B	803	CLA	C2D-C1D-ND	-2.14	108.01	110.13
17	a	850	LHG	C18-C17-C16	-2.14	103.57	114.37
13	F	203	CLA	CHB-C4A-NA	2.14	127.48	124.40
13	8	1102	CLA	CHB-C4A-NA	2.14	127.48	124.40
13	6	203	CLA	CHB-C4A-NA	2.14	127.48	124.40
17	A	850	LHG	C18-C17-C16	-2.14	103.57	114.37
13	F	203	CLA	O2A-CGA-O1A	-2.14	117.84	123.33
13	B	847	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
13	a	806	CLA	CHD-C1D-ND	-2.13	121.80	124.80
13	a	819	CLA	O2D-CGD-CBD	2.13	114.96	111.23
16	k	4004	BCR	C15-C14-C13	-2.13	124.28	127.28
13	A	822	CLA	CHA-C1A-NA	-2.13	121.56	126.39
17	1	850	LHG	C18-C17-C16	-2.13	103.58	114.37
13	A	814	CLA	CHD-C1D-ND	-2.13	121.80	124.80
13	b	801	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
13	a	822	CLA	CHA-C1A-NA	-2.13	121.56	126.39
16	M	101	BCR	C28-C27-C26	-2.13	110.25	114.06
13	2	812	CLA	CHA-C1A-NA	-2.13	121.56	126.39
16	z	101	BCR	C27-C26-C25	2.13	125.58	122.70
13	2	801	CLA	CAA-CBA-CGA	-2.13	107.16	113.21
13	a	809	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
13	B	801	CLA	CAA-CBA-CGA	-2.13	107.16	113.21
13	b	826	CLA	C3C-C4C-NC	-2.13	107.70	110.43
13	B	804	CLA	O2D-CGD-CBD	2.13	114.95	111.23
13	2	846	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
13	1	814	CLA	CHD-C1D-ND	-2.13	121.81	124.80
13	b	813	CLA	CHA-C1A-NA	-2.13	121.57	126.39
13	b	804	CLA	O2D-CGD-CBD	2.13	114.95	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	847	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
13	1	820	CLA	CHD-C1D-ND	-2.13	121.81	124.80
16	F	205	BCR	C24-C23-C22	-2.13	123.08	126.23
13	a	830	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
13	f	203	CLA	CHB-C4A-NA	2.13	127.47	124.40
16	6	205	BCR	C24-C23-C22	-2.13	123.09	126.23
16	m	101	BCR	C28-C27-C26	-2.13	110.26	114.06
13	8	1103	CLA	CHD-C1D-ND	-2.13	121.81	124.80
16	M	101	BCR	C27-C26-C25	2.13	125.58	122.70
16	b	845	BCR	C16-C15-C14	-2.13	119.17	123.52
13	1	831	CLA	CHB-C4A-NA	2.13	127.47	124.40
13	2	823	CLA	CHB-C4A-NA	2.13	127.47	124.40
12	1	801	CL0	C2B-C1B-NB	-2.13	108.12	110.33
13	2	820	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
13	i	102	CLA	CMB-C2B-C1B	-2.13	122.18	125.42
13	A	802	CLA	C4-C3-C2	-2.13	118.16	123.63
13	0	208	CLA	CHB-C4A-NA	2.13	127.47	124.40
13	1	830	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
16	A	851	BCR	C16-C15-C14	-2.13	119.17	123.52
13	0	203	CLA	CHB-C4A-NA	2.13	127.47	124.40
13	A	812	CLA	CMB-C2B-C1B	-2.13	122.18	125.42
13	B	821	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
13	j	1102	CLA	CHB-C4A-NA	2.12	127.46	124.40
13	b	801	CLA	CAA-CBA-CGA	-2.12	107.18	113.21
13	A	835	CLA	CHA-C1A-NA	-2.12	121.58	126.39
13	B	807	CLA	CHB-C4A-NA	2.12	127.46	124.40
13	1	818	CLA	C1-C2-C3	-2.12	122.72	126.20
16	9	4004	BCR	C15-C14-C13	-2.12	124.30	127.28
13	a	814	CLA	CHD-C1D-ND	-2.12	121.82	124.80
13	b	824	CLA	CHB-C4A-NA	2.12	127.46	124.40
13	A	820	CLA	CHD-C1D-ND	-2.12	121.82	124.80
13	b	807	CLA	CHB-C4A-NA	2.12	127.46	124.40
13	a	807	CLA	CHD-C1D-ND	-2.12	121.82	124.80
13	A	819	CLA	O2D-CGD-CBD	2.12	114.94	111.23
13	B	811	CLA	CMB-C2B-C3B	2.12	131.53	126.55
13	1	802	CLA	C4-C3-C2	-2.12	118.19	123.63
13	A	837	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
13	A	806	CLA	CHD-C1D-ND	-2.12	121.82	124.80
13	1	841	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
13	1	827	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
13	A	830	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
13	2	821	CLA	C2D-C1D-ND	-2.12	108.03	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	837	CLA	CMB-C2B-C1B	-2.12	122.20	125.42
13	b	834	CLA	C3C-C4C-NC	-2.12	107.72	110.43
13	a	827	CLA	O2A-CGA-O1A	-2.12	118.34	123.63
13	a	832	CLA	O2A-CGA-O1A	-2.12	118.34	123.63
13	b	821	CLA	O2A-CGA-O1A	-2.12	118.34	123.63
13	B	824	CLA	CHB-C4A-NA	2.11	127.45	124.40
13	1	812	CLA	CMB-C2B-C1B	-2.11	122.20	125.42
13	b	824	CLA	C1-C2-C3	-2.11	122.73	126.20
13	1	817	CLA	CHA-C1A-NA	-2.11	121.61	126.39
16	b	843	BCR	C33-C5-C6	-2.11	122.18	124.48
13	A	827	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
16	2	842	BCR	C33-C5-C6	-2.11	122.18	124.48
16	i	103	BCR	C20-C21-C22	-2.11	124.32	127.28
13	b	822	CLA	C2D-C1D-ND	-2.11	108.04	110.13
13	1	819	CLA	O2D-CGD-CBD	2.11	114.92	111.23
13	2	810	CLA	CMB-C2B-C3B	2.11	131.51	126.55
13	L	206	CLA	CHB-C4A-NA	2.11	127.44	124.40
13	2	830	CLA	C2D-C1D-ND	-2.11	108.04	110.13
13	K	4002	CLA	CHB-C4A-NA	2.11	127.44	124.40
13	A	817	CLA	CHA-C1A-NA	-2.11	121.62	126.39
13	a	829	CLA	CHD-C1D-ND	-2.11	121.84	124.80
13	9	4002	CLA	CHB-C4A-NA	2.11	127.44	124.40
13	b	811	CLA	CMB-C2B-C3B	2.11	131.50	126.55
13	A	841	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
13	a	818	CLA	C1-C2-C3	-2.11	122.75	126.20
17	1	849	LHG	C27-C26-C25	-2.11	103.72	114.37
13	l	202	CLA	C1-C2-C3	-2.11	122.75	126.20
17	a	849	LHG	C27-C26-C25	-2.11	103.73	114.37
13	2	803	CLA	CHB-C4A-NA	2.11	127.44	124.40
13	0	202	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
18	2	845	LMG	O2-C2-C1	-2.10	105.06	110.08
13	b	835	CLA	C1-C2-C3	-2.10	123.36	126.76
17	A	849	LHG	C27-C26-C25	-2.10	103.73	114.37
13	a	820	CLA	CHD-C1D-ND	-2.10	121.84	124.80
13	9	4005	CLA	CHA-C1A-NA	-2.10	121.63	126.39
13	a	841	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
13	f	203	CLA	CHD-C1D-ND	-2.10	121.84	124.80
13	2	833	CLA	C3C-C4C-NC	-2.10	107.74	110.43
13	a	831	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
16	m	101	BCR	C27-C26-C25	2.10	125.55	122.70
13	b	833	CLA	CMB-C2B-C3B	2.10	131.50	126.55
13	L	201	CLA	O2A-CGA-O1A	-2.10	118.37	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	z	101	BCR	C29-C30-C25	2.10	113.49	110.44
13	1	831	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
13	2	816	CLA	CHD-C1D-ND	-2.10	121.85	124.80
13	a	817	CLA	CHD-C1D-ND	-2.10	121.85	124.80
18	B	846	LMG	O2-C2-C1	-2.10	105.08	110.08
16	8	1104	BCR	C29-C30-C25	2.10	113.48	110.44
16	J	1105	BCR	C33-C5-C6	-2.10	122.20	124.48
13	1	832	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
13	1	814	CLA	C1-C2-C3	-2.10	123.37	126.76
13	l	207	CLA	CHB-C4A-NA	2.10	127.42	124.40
16	l	206	BCR	C33-C5-C6	-2.10	122.20	124.48
16	A	848	BCR	C27-C26-C25	2.10	125.53	122.70
13	a	811	CLA	C3C-C4C-NC	-2.09	107.75	110.43
13	B	809	CLA	CMB-C2B-C1B	-2.09	122.23	125.42
13	A	832	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
13	b	823	CLA	C3C-C4C-NC	-2.09	107.75	110.43
13	1	803	CLA	CHA-C1A-NA	-2.09	121.65	126.39
13	1	806	CLA	CHD-C1D-ND	-2.09	121.86	124.80
13	B	833	CLA	CMB-C2B-C3B	2.09	131.47	126.55
16	a	848	BCR	C27-C26-C25	2.09	125.53	122.70
18	b	846	LMG	O2-C2-C1	-2.09	105.09	110.08
13	B	831	CLA	C2D-C1D-ND	-2.09	108.06	110.13
13	A	803	CLA	CHA-C1A-NA	-2.09	121.66	126.39
16	j	1105	BCR	C33-C5-C6	-2.09	122.20	124.48
13	A	819	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
13	B	834	CLA	C3C-C4C-NC	-2.09	107.75	110.43
13	A	817	CLA	CHD-C1D-ND	-2.09	121.86	124.80
13	a	817	CLA	CHA-C1A-NA	-2.09	121.66	126.39
16	b	845	BCR	C30-C25-C26	-2.09	119.78	122.64
16	B	843	BCR	C33-C5-C6	-2.09	122.20	124.48
14	2	838	PQN	C11-C3-C4	-2.09	116.38	118.58
16	a	848	BCR	C10-C11-C12	-2.09	117.15	123.20
13	b	803	CLA	CHB-C4A-NA	2.09	127.41	124.40
13	2	807	CLA	CHA-C1A-NA	-2.09	121.66	126.39
13	2	812	CLA	CMB-C2B-C3B	2.09	131.46	126.55
13	k	4002	CLA	CHB-C4A-NA	2.09	127.41	124.40
13	b	831	CLA	C2D-C1D-ND	-2.09	108.06	110.13
16	B	845	BCR	C30-C25-C26	-2.09	119.78	122.64
16	A	848	BCR	C7-C8-C9	-2.09	123.15	126.23
13	8	1101	CLA	CHB-C4A-NA	2.09	127.41	124.40
13	A	831	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
16	A	848	BCR	C10-C11-C12	-2.09	117.16	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	j	1104	BCR	C29-C30-C25	2.09	113.47	110.44
13	A	842	CLA	CHA-C1A-NA	-2.09	121.67	126.39
13	A	829	CLA	CHD-C1D-ND	-2.09	121.87	124.80
13	B	826	CLA	C3C-C4C-NC	-2.09	107.76	110.43
13	a	819	CLA	O2A-CGA-O1A	-2.08	118.41	123.63
13	2	808	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
16	b	848	BCR	C24-C23-C22	-2.08	123.15	126.23
13	B	822	CLA	CHD-C1D-ND	-2.08	121.87	124.80
13	J	1101	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
16	m	101	BCR	C33-C5-C6	-2.08	122.21	124.48
13	K	4005	CLA	CHA-C1A-NA	-2.08	121.68	126.39
16	j	1105	BCR	C11-C10-C9	-2.08	124.36	127.28
13	j	1101	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
13	2	834	CLA	C1-C2-C3	-2.08	123.39	126.76
13	1	813	CLA	CHA-C1A-NA	-2.08	121.68	126.39
13	B	823	CLA	C3C-C4C-NC	-2.08	107.76	110.43
13	2	822	CLA	C3C-C4C-NC	-2.08	107.76	110.43
14	B	839	PQN	C11-C3-C4	-2.08	116.39	118.58
13	l	202	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
13	0	205	CLA	C1-C2-C3	-2.08	123.40	126.76
13	B	813	CLA	CMB-C2B-C3B	2.08	131.44	126.55
13	B	803	CLA	CHB-C4A-NA	2.08	127.40	124.40
13	B	824	CLA	C1-C2-C3	-2.08	122.79	126.20
13	A	810	CLA	C3C-C4C-NC	-2.08	107.77	110.43
16	B	848	BCR	C24-C23-C22	-2.08	123.16	126.23
16	8	1105	BCR	C33-C5-C6	-2.08	122.22	124.48
13	B	822	CLA	C2D-C1D-ND	-2.08	108.07	110.13
13	1	829	CLA	CHD-C1D-ND	-2.08	121.88	124.80
13	A	839	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
13	b	817	CLA	CHD-C1D-ND	-2.08	121.88	124.80
13	B	817	CLA	CHD-C1D-ND	-2.08	121.88	124.80
13	1	842	CLA	CHA-C1A-NA	-2.08	121.69	126.39
16	1	848	BCR	C10-C11-C12	-2.08	117.19	123.20
13	J	1101	CLA	CHB-C4A-NA	2.08	127.39	124.40
13	A	813	CLA	CHA-C1A-NA	-2.08	121.69	126.39
13	L	203	CLA	C1-C2-C3	-2.08	123.41	126.76
16	I	102	BCR	C20-C21-C22	-2.07	124.37	127.28
16	J	1104	BCR	C29-C30-C25	2.07	113.45	110.44
13	1	817	CLA	CHD-C1D-ND	-2.07	121.88	124.80
13	L	201	CLA	C1-C2-C3	-2.07	122.80	126.20
13	a	839	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
13	l	204	CLA	C1-C2-C3	-2.07	123.41	126.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	809	CLA	CMB-C2B-C1B	-2.07	122.26	125.42
16	2	847	BCR	C24-C23-C22	-2.07	123.17	126.23
13	B	835	CLA	C1-C2-C3	-2.07	123.41	126.76
13	b	833	CLA	CHB-C1B-C2B	-2.07	121.41	127.43
13	a	814	CLA	C1-C2-C3	-2.07	123.41	126.76
13	2	825	CLA	C3C-C4C-NC	-2.07	107.78	110.43
13	2	832	CLA	CMB-C2B-C3B	2.07	131.42	126.55
16	7	103	BCR	C37-C22-C21	-2.07	119.46	122.82
13	1	839	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
13	k	4005	CLA	CHA-C1A-NA	-2.07	121.70	126.39
13	A	814	CLA	C1-C2-C3	-2.07	123.41	126.76
13	b	822	CLA	C1-C2-C3	-2.07	123.41	126.76
13	j	1101	CLA	CHB-C4A-NA	2.07	127.39	124.40
13	a	813	CLA	CHA-C1A-NA	-2.07	121.70	126.39
14	b	839	PQN	C11-C3-C4	-2.07	116.40	118.58
13	B	827	CLA	CHA-C1A-NA	-2.07	121.70	126.39
16	M	101	BCR	C33-C5-C6	-2.07	122.23	124.48
16	1	848	BCR	C27-C26-C25	2.07	125.50	122.70
16	A	851	BCR	C24-C23-C22	-2.07	123.17	126.23
13	2	823	CLA	C1-C2-C3	-2.07	122.81	126.20
13	B	814	CLA	CHB-C1B-C2B	-2.07	121.42	127.43
13	B	833	CLA	CHB-C1B-C2B	-2.07	121.42	127.43
18	b	846	LMG	O7-C10-O9	-2.07	118.87	123.70
13	a	842	CLA	CHA-C1A-NA	-2.07	121.71	126.39
16	J	1105	BCR	C11-C10-C9	-2.07	124.38	127.28
16	1	851	BCR	C24-C23-C22	-2.07	123.18	126.23
13	B	812	CLA	O2A-CGA-O1A	-2.07	118.02	123.33
13	B	837	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
13	2	826	CLA	CHA-C1A-NA	-2.07	121.71	126.39
13	b	812	CLA	O2A-CGA-O1A	-2.07	118.02	123.33
13	2	832	CLA	CHB-C1B-C2B	-2.06	121.43	127.43
13	a	803	CLA	CHA-C1A-NA	-2.06	121.72	126.39
13	b	808	CLA	CHA-C1A-NA	-2.06	121.72	126.39
13	B	831	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
13	b	814	CLA	CHB-C1B-C2B	-2.06	121.44	127.43
13	2	813	CLA	CHB-C1B-C2B	-2.06	121.44	127.43
16	6	205	BCR	C40-C30-C25	2.06	113.48	110.24
13	1	819	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
16	I	102	BCR	C16-C15-C14	-2.06	119.30	123.52
13	B	808	CLA	CHA-C1A-NA	-2.06	121.72	126.39
16	l	203	BCR	C10-C11-C12	-2.06	117.22	123.20
13	b	828	CLA	O2A-CGA-O1A	-2.06	118.47	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	826	CLA	CHB-C4A-NA	2.06	127.38	124.40
16	I	102	BCR	C37-C22-C21	-2.06	119.48	122.82
13	b	827	CLA	CHA-C1A-NA	-2.06	121.72	126.39
16	7	103	BCR	C16-C15-C14	-2.06	119.30	123.52
13	l	202	CLA	CMB-C2B-C3B	2.06	131.40	126.55
13	8	1101	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
18	2	845	LMG	O7-C10-O9	-2.06	118.89	123.70
16	M	101	BCR	C29-C30-C25	2.06	113.43	110.44
16	a	848	BCR	C7-C8-C9	-2.06	123.19	126.23
16	a	851	BCR	C24-C23-C22	-2.06	123.19	126.23
13	2	811	CLA	O2A-CGA-O1A	-2.06	118.04	123.33
18	B	846	LMG	O7-C10-O9	-2.06	118.89	123.70
13	A	811	CLA	C3C-C4C-NC	-2.06	107.79	110.43
13	2	836	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
16	l	203	BCR	C1-C6-C5	-2.06	119.82	122.64
16	2	844	BCR	C30-C25-C26	-2.06	119.82	122.64
13	b	803	CLA	C1-C2-C3	-2.06	122.83	126.20
13	b	835	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
13	2	830	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
13	1	810	CLA	C3C-C4C-NC	-2.06	107.80	110.43
13	2	827	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
13	1	821	CLA	O2A-CGA-O1A	-2.06	118.49	123.63
16	1	846	BCR	C24-C23-C22	-2.06	123.19	126.23
16	L	202	BCR	C10-C11-C12	-2.06	117.25	123.20
13	b	813	CLA	CMB-C2B-C3B	2.06	131.38	126.55
13	B	803	CLA	C1-C2-C3	-2.06	122.83	126.20
16	7	103	BCR	C20-C21-C22	-2.05	124.40	127.28
13	a	814	CLA	CHA-C1A-NA	-2.05	121.74	126.39
16	i	103	BCR	C16-C15-C14	-2.05	119.32	123.52
13	B	828	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
13	2	821	CLA	C1-C2-C3	-2.05	123.44	126.76
16	8	1105	BCR	C11-C10-C9	-2.05	124.40	127.28
13	B	822	CLA	C1-C2-C3	-2.05	123.44	126.76
13	2	821	CLA	CHD-C1D-ND	-2.05	121.91	124.80
16	1	848	BCR	C7-C8-C9	-2.05	123.20	126.23
13	9	4005	CLA	C2D-C1D-ND	-2.05	108.09	110.13
16	f	205	BCR	C40-C30-C25	2.05	113.46	110.24
16	i	103	BCR	C1-C6-C5	-2.05	119.83	122.64
13	A	821	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
13	A	839	CLA	C3C-C4C-NC	-2.05	107.80	110.43
13	a	810	CLA	C3C-C4C-NC	-2.05	107.80	110.43
16	7	103	BCR	C28-C27-C26	-2.05	110.40	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	F	205	BCR	C40-C30-C25	2.05	113.46	110.24
16	A	848	BCR	C29-C30-C25	2.05	113.42	110.44
13	b	822	CLA	CHD-C1D-ND	-2.05	121.92	124.80
13	b	831	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
16	i	103	BCR	C28-C27-C26	-2.05	110.40	114.06
13	A	812	CLA	CHA-C1A-NA	-2.05	121.75	126.39
16	0	204	BCR	C10-C11-C12	-2.05	117.27	123.20
16	b	842	BCR	C3-C4-C5	-2.05	110.41	114.06
13	1	852	CLA	CHD-C1D-ND	-2.05	121.92	124.80
16	B	842	BCR	C3-C4-C5	-2.05	110.41	114.06
16	2	841	BCR	C3-C4-C5	-2.05	110.41	114.06
13	B	835	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
13	1	812	CLA	CHA-C1A-NA	-2.05	121.76	126.39
13	2	803	CLA	C1-C2-C3	-2.05	122.85	126.20
13	a	821	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
13	A	833	CLA	C3C-C4C-NC	-2.05	107.81	110.43
16	L	202	BCR	C1-C6-C5	-2.05	119.84	122.64
13	k	4005	CLA	C2D-C1D-ND	-2.05	108.10	110.13
13	1	839	CLA	C2D-C1D-ND	-2.05	108.10	110.13
16	I	102	BCR	C28-C27-C26	-2.04	110.41	114.06
13	b	804	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
13	A	814	CLA	CHA-C1A-NA	-2.04	121.76	126.39
13	L	201	CLA	CMB-C2B-C3B	2.04	131.36	126.55
16	L	202	BCR	C20-C21-C22	-2.04	124.41	127.28
13	a	826	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
13	1	841	CLA	C1-C2-C3	-2.04	122.85	126.20
16	2	840	BCR	C33-C5-C6	-2.04	122.25	124.48
13	1	811	CLA	C3C-C4C-NC	-2.04	107.81	110.43
13	b	837	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
13	A	826	CLA	CHB-C4A-NA	2.04	127.34	124.40
16	l	203	BCR	C20-C21-C22	-2.04	124.42	127.28
16	a	846	BCR	C24-C23-C22	-2.04	123.22	126.23
13	a	812	CLA	CHA-C1A-NA	-2.04	121.77	126.39
16	1	848	BCR	C29-C30-C25	2.04	113.40	110.44
13	2	825	CLA	CHA-C1A-NA	-2.04	121.77	126.39
13	a	805	CLA	CHB-C4A-NA	2.04	127.34	124.40
13	a	852	CLA	CHD-C1D-ND	-2.04	121.93	124.80
13	8	1101	CLA	CHD-C1D-ND	-2.04	121.93	124.80
13	A	838	CLA	C1-C2-C3	-2.04	122.86	126.20
13	0	202	CLA	C1-C2-C3	-2.04	122.86	126.20
13	2	824	CLA	CMB-C2B-C3B	2.04	131.34	126.55
16	A	846	BCR	C24-C23-C22	-2.04	123.22	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	833	CLA	C3C-C4C-NC	-2.04	107.82	110.43
13	b	825	CLA	CMB-C2B-C3B	2.04	131.34	126.55
13	B	836	CLA	CHB-C4A-NA	2.04	127.34	124.40
13	a	808	CLA	C3C-C4C-NC	-2.04	107.82	110.43
13	A	840	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
13	1	839	CLA	C3C-C4C-NC	-2.04	107.82	110.43
16	a	851	BCR	C15-C14-C13	-2.04	124.42	127.28
16	1	851	BCR	C15-C14-C13	-2.04	124.42	127.28
13	B	802	CLA	CMB-C2B-C3B	2.04	131.34	126.55
16	2	847	BCR	C31-C1-C6	2.04	113.44	110.24
13	2	834	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
13	B	804	CLA	CMB-C2B-C1B	-2.04	122.32	125.42
16	I	102	BCR	C1-C6-C5	-2.03	119.86	122.64
13	a	834	CLA	CMB-C2B-C1B	-2.03	122.32	125.42
13	1	805	CLA	CMB-C2B-C1B	-2.03	122.32	125.42
16	i	103	BCR	C37-C22-C21	-2.03	119.52	122.82
13	2	802	CLA	CMB-C2B-C3B	2.03	131.34	126.55
13	2	812	CLA	CHB-C4A-NA	2.03	127.33	124.40
13	1	809	CLA	C1-C2-C3	-2.03	123.47	126.76
13	1	838	CLA	C1-C2-C3	-2.03	122.87	126.20
13	2	828	CLA	O1D-CGD-CBD	2.03	128.53	124.52
13	b	802	CLA	CMB-C2B-C3B	2.03	131.33	126.55
16	B	848	BCR	C31-C1-C6	2.03	113.43	110.24
16	m	101	BCR	C29-C30-C25	2.03	113.39	110.44
13	1	838	CLA	O2D-CGD-CBD	2.03	114.78	111.23
16	b	840	BCR	C7-C8-C9	-2.03	123.23	126.23
16	2	839	BCR	C7-C8-C9	-2.03	123.23	126.23
13	a	811	CLA	CHB-C4A-NA	2.03	127.33	124.40
13	1	814	CLA	CHA-C1A-NA	-2.03	121.79	126.39
13	a	841	CLA	CHD-C1D-ND	-2.03	121.94	124.80
13	a	819	CLA	CHA-C1A-NA	-2.03	121.79	126.39
13	1	840	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
13	A	819	CLA	CHA-C1A-NA	-2.03	121.80	126.39
13	B	805	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
13	A	839	CLA	C2D-C1D-ND	-2.03	108.12	110.13
13	A	826	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
13	2	805	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
13	b	836	CLA	CHB-C4A-NA	2.03	127.33	124.40
13	b	826	CLA	CHA-C1A-NA	-2.03	121.80	126.39
13	K	4005	CLA	C2D-C1D-ND	-2.03	108.12	110.13
16	a	848	BCR	C29-C30-C25	2.03	113.38	110.44
13	a	839	CLA	C3C-C4C-NC	-2.03	107.83	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	0	202	CLA	CMB-C2B-C3B	2.03	131.32	126.55
13	1	819	CLA	CHA-C1A-NA	-2.03	121.80	126.39
13	a	838	CLA	C1-C2-C3	-2.03	122.88	126.20
13	1	833	CLA	C3C-C4C-NC	-2.03	107.83	110.43
13	L	203	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
13	A	815	CLA	CHD-C1D-ND	-2.03	121.95	124.80
13	B	813	CLA	CHB-C4A-NA	2.02	127.32	124.40
13	A	852	CLA	CHD-C1D-ND	-2.02	121.95	124.80
13	2	808	CLA	CHD-C1D-ND	-2.02	121.95	124.80
16	B	841	BCR	C33-C5-C6	-2.02	122.28	124.48
13	A	838	CLA	O2D-CGD-CBD	2.02	114.77	111.23
13	A	808	CLA	C3C-C4C-NC	-2.02	107.84	110.43
13	A	841	CLA	C1-C2-C3	-2.02	122.88	126.20
16	z	101	BCR	C33-C5-C6	-2.02	122.28	124.48
13	2	804	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
16	b	848	BCR	C31-C1-C6	2.02	113.42	110.24
13	b	805	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
13	b	829	CLA	O1D-CGD-CBD	2.02	128.51	124.52
13	2	817	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
13	B	809	CLA	CHD-C1D-ND	-2.02	121.96	124.80
13	a	839	CLA	CHD-C1D-ND	-2.02	121.96	124.80
13	1	815	CLA	CHD-C1D-ND	-2.02	121.96	124.80
13	B	829	CLA	O1D-CGD-CBD	2.02	128.51	124.52
16	B	840	BCR	C7-C8-C9	-2.02	123.24	126.23
13	a	840	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
16	7	103	BCR	C1-C6-C5	-2.02	119.87	122.64
16	A	847	BCR	C20-C21-C22	-2.02	124.44	127.28
13	A	834	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
13	2	835	CLA	CHB-C4A-NA	2.02	127.32	124.40
13	b	834	CLA	CHD-C1D-ND	-2.02	121.96	124.80
13	0	205	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
13	a	835	CLA	O2D-CGD-CBD	2.02	114.76	111.23
13	B	826	CLA	CHA-C1A-NA	-2.02	121.81	126.39
13	A	839	CLA	CHD-C1D-ND	-2.02	121.96	124.80
13	l	204	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
13	1	834	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
16	A	851	BCR	C15-C14-C13	-2.02	124.45	127.28
13	B	818	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
13	A	805	CLA	CHB-C4A-NA	2.02	127.31	124.40
13	A	809	CLA	C1-C2-C3	-2.02	123.50	126.76
13	B	825	CLA	CMB-C2B-C3B	2.02	131.29	126.55
16	0	204	BCR	C20-C21-C22	-2.02	124.45	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	b	841	BCR	C33-C5-C6	-2.02	122.28	124.48
13	a	841	CLA	C1-C2-C3	-2.02	122.89	126.20
13	2	828	CLA	CHB-C4A-NA	2.02	127.31	124.40
16	1	847	BCR	C20-C21-C22	-2.02	124.45	127.28
13	b	813	CLA	CHB-C4A-NA	2.02	127.31	124.40
13	1	826	CLA	CHB-C4A-NA	2.02	127.31	124.40
13	b	809	CLA	CHD-C1D-ND	-2.02	121.97	124.80
13	1	826	CLA	O2A-CGA-O1A	-2.02	118.59	123.63
16	M	101	BCR	C10-C11-C12	-2.01	117.36	123.20
16	z	101	BCR	C10-C11-C12	-2.01	117.36	123.20
13	2	823	CLA	O2D-CGD-CBD	2.01	114.75	111.23
13	a	815	CLA	C2D-C1D-ND	-2.01	108.13	110.13
13	a	814	CLA	C3A-C2A-C1A	2.01	104.35	101.34
13	A	820	CLA	CMB-C2B-C1B	-2.01	122.35	125.42
13	B	828	CLA	CMB-C2B-C1B	-2.01	122.35	125.42
13	2	827	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
16	m	101	BCR	C10-C11-C12	-2.01	117.37	123.20
13	A	805	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
13	1	814	CLA	C3A-C2A-C1A	2.01	104.35	101.34
13	a	813	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
16	a	847	BCR	C20-C21-C22	-2.01	124.46	127.28
13	a	838	CLA	O2D-CGD-CBD	2.01	114.75	111.23
13	a	805	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
13	8	1101	CLA	O2D-CGD-CBD	2.01	114.74	111.23
13	2	808	CLA	CHB-C4A-NA	2.01	127.30	124.40
13	1	839	CLA	CHD-C1D-ND	-2.01	121.98	124.80
13	2	801	CLA	O1D-CGD-CBD	2.01	128.48	124.52
13	a	815	CLA	CHD-C1D-ND	-2.01	121.98	124.80
13	b	818	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
13	B	802	CLA	CHB-C4A-NA	2.01	127.30	124.40
13	B	824	CLA	O2D-CGD-CBD	2.01	114.74	111.23
13	j	1101	CLA	O2D-CGD-CBD	2.01	114.74	111.23
13	1	827	CLA	CHD-C1D-ND	-2.01	121.98	124.80
16	L	207	BCR	C33-C5-C6	-2.01	122.30	124.48
13	1	813	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
16	0	204	BCR	C1-C6-C5	-2.01	119.89	122.64
13	a	834	CLA	CHA-C1A-NA	-2.01	121.85	126.39
13	a	809	CLA	C1-C2-C3	-2.01	123.52	126.76
13	A	835	CLA	O2D-CGD-CBD	2.00	114.73	111.23
13	J	1101	CLA	O2D-CGD-CBD	2.00	114.73	111.23
13	a	820	CLA	CMB-C2B-C1B	-2.00	122.37	125.42
13	A	811	CLA	CHB-C4A-NA	2.00	127.29	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	J	1101	CLA	CHD-C1D-ND	-2.00	121.99	124.80
16	6	202	BCR	C28-C27-C26	-2.00	110.49	114.06
13	l	204	CLA	O2D-CGD-CBD	2.00	114.73	111.23
13	B	807	CLA	O2A-CGA-O1A	-2.00	118.62	123.63

There are no chirality outliers.

All (3615) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	805	CLA	CBA-CGA-O2A-C1
13	A	805	CLA	O1A-CGA-O2A-C1
13	A	806	CLA	C1A-C2A-CAA-CBA
13	A	807	CLA	CBD-CGD-O2D-CED
13	A	808	CLA	CHA-CBD-CGD-O1D
13	A	808	CLA	CHA-CBD-CGD-O2D
13	A	809	CLA	C1A-C2A-CAA-CBA
13	A	810	CLA	C1A-C2A-CAA-CBA
13	A	810	CLA	C3A-C2A-CAA-CBA
13	A	811	CLA	C4B-C3B-CAB-CBB
13	A	816	CLA	C4B-C3B-CAB-CBB
13	A	818	CLA	C3A-C2A-CAA-CBA
13	A	818	CLA	CBD-CGD-O2D-CED
13	A	820	CLA	CBA-CGA-O2A-C1
13	A	820	CLA	C4B-C3B-CAB-CBB
13	A	824	CLA	C1A-C2A-CAA-CBA
13	A	824	CLA	C3A-C2A-CAA-CBA
13	A	824	CLA	C4B-C3B-CAB-CBB
13	A	828	CLA	CBD-CGD-O2D-CED
13	A	831	CLA	CHA-CBD-CGD-O1D
13	A	831	CLA	CHA-CBD-CGD-O2D
13	A	833	CLA	C4B-C3B-CAB-CBB
13	A	834	CLA	C4B-C3B-CAB-CBB
13	A	836	CLA	C1A-C2A-CAA-CBA
13	A	837	CLA	C4B-C3B-CAB-CBB
13	A	838	CLA	C1A-C2A-CAA-CBA
13	A	840	CLA	C1A-C2A-CAA-CBA
13	A	840	CLA	C4B-C3B-CAB-CBB
13	A	841	CLA	C1A-C2A-CAA-CBA
13	A	841	CLA	C3A-C2A-CAA-CBA
13	A	841	CLA	C4B-C3B-CAB-CBB
13	A	842	CLA	C1A-C2A-CAA-CBA
13	A	852	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	A	852	CLA	CAD-CBD-CGD-O1D
13	A	852	CLA	CAD-CBD-CGD-O2D
13	B	802	CLA	CBD-CGD-O2D-CED
13	B	803	CLA	CHA-CBD-CGD-O1D
13	B	803	CLA	CHA-CBD-CGD-O2D
13	B	804	CLA	C3A-C2A-CAA-CBA
13	B	804	CLA	CAD-CBD-CGD-O1D
13	B	804	CLA	CAD-CBD-CGD-O2D
13	B	805	CLA	C6-C7-C8-C9
13	B	807	CLA	C4B-C3B-CAB-CBB
13	B	810	CLA	C1A-C2A-CAA-CBA
13	B	811	CLA	CBD-CGD-O2D-CED
13	B	813	CLA	C1A-C2A-CAA-CBA
13	B	814	CLA	C3A-C2A-CAA-CBA
13	B	814	CLA	C4B-C3B-CAB-CBB
13	B	815	CLA	C1A-C2A-CAA-CBA
13	B	815	CLA	C3A-C2A-CAA-CBA
13	B	816	CLA	C2B-C3B-CAB-CBB
13	B	816	CLA	C4B-C3B-CAB-CBB
13	B	817	CLA	C4B-C3B-CAB-CBB
13	B	819	CLA	CBD-CGD-O2D-CED
13	B	820	CLA	CBD-CGD-O2D-CED
13	B	821	CLA	CBD-CGD-O2D-CED
13	B	822	CLA	CHA-CBD-CGD-O1D
13	B	822	CLA	CHA-CBD-CGD-O2D
13	B	824	CLA	C1A-C2A-CAA-CBA
13	B	824	CLA	C3A-C2A-CAA-CBA
13	B	827	CLA	C2B-C3B-CAB-CBB
13	B	827	CLA	C4B-C3B-CAB-CBB
13	B	829	CLA	CAD-CBD-CGD-O1D
13	B	829	CLA	CAD-CBD-CGD-O2D
13	B	830	CLA	C1A-C2A-CAA-CBA
13	B	830	CLA	C3A-C2A-CAA-CBA
13	B	832	CLA	C4B-C3B-CAB-CBB
13	B	833	CLA	C3A-C2A-CAA-CBA
13	B	834	CLA	C4B-C3B-CAB-CBB
13	B	835	CLA	C4B-C3B-CAB-CBB
13	B	837	CLA	C2B-C3B-CAB-CBB
13	B	837	CLA	C4B-C3B-CAB-CBB
13	F	203	CLA	C4B-C3B-CAB-CBB
13	F	204	CLA	C4B-C3B-CAB-CBB
13	I	101	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
13	J	1101	CLA	C4B-C3B-CAB-CBB
13	J	1101	CLA	CHA-CBD-CGD-O1D
13	J	1101	CLA	CHA-CBD-CGD-O2D
13	J	1102	CLA	CAD-CBD-CGD-O1D
13	J	1102	CLA	CAD-CBD-CGD-O2D
13	J	1103	CLA	C1A-C2A-CAA-CBA
13	J	1103	CLA	C3A-C2A-CAA-CBA
13	J	1103	CLA	C4B-C3B-CAB-CBB
13	J	1103	CLA	CBD-CGD-O2D-CED
13	K	4002	CLA	C4B-C3B-CAB-CBB
13	K	4002	CLA	CHA-CBD-CGD-O1D
13	K	4002	CLA	CHA-CBD-CGD-O2D
13	K	4003	CLA	C4B-C3B-CAB-CBB
13	K	4005	CLA	C4B-C3B-CAB-CBB
13	L	201	CLA	C1A-C2A-CAA-CBA
13	L	201	CLA	O1A-CGA-O2A-C1
13	L	203	CLA	C4B-C3B-CAB-CBB
13	L	206	CLA	C1A-C2A-CAA-CBA
13	a	805	CLA	CBA-CGA-O2A-C1
13	a	805	CLA	O1A-CGA-O2A-C1
13	a	806	CLA	C1A-C2A-CAA-CBA
13	a	807	CLA	CBD-CGD-O2D-CED
13	a	808	CLA	CHA-CBD-CGD-O1D
13	a	808	CLA	CHA-CBD-CGD-O2D
13	a	809	CLA	C1A-C2A-CAA-CBA
13	a	810	CLA	C1A-C2A-CAA-CBA
13	a	810	CLA	C3A-C2A-CAA-CBA
13	a	811	CLA	C4B-C3B-CAB-CBB
13	a	816	CLA	C4B-C3B-CAB-CBB
13	a	818	CLA	C3A-C2A-CAA-CBA
13	a	818	CLA	CBD-CGD-O2D-CED
13	a	820	CLA	CBA-CGA-O2A-C1
13	a	820	CLA	C4B-C3B-CAB-CBB
13	a	824	CLA	C1A-C2A-CAA-CBA
13	a	824	CLA	C3A-C2A-CAA-CBA
13	a	824	CLA	C4B-C3B-CAB-CBB
13	a	828	CLA	CBD-CGD-O2D-CED
13	a	831	CLA	CHA-CBD-CGD-O1D
13	a	831	CLA	CHA-CBD-CGD-O2D
13	a	833	CLA	C4B-C3B-CAB-CBB
13	a	834	CLA	C4B-C3B-CAB-CBB
13	a	836	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	a	837	CLA	C4B-C3B-CAB-CBB
13	a	838	CLA	C1A-C2A-CAA-CBA
13	a	840	CLA	C1A-C2A-CAA-CBA
13	a	840	CLA	C4B-C3B-CAB-CBB
13	a	841	CLA	C1A-C2A-CAA-CBA
13	a	841	CLA	C3A-C2A-CAA-CBA
13	a	841	CLA	C4B-C3B-CAB-CBB
13	a	842	CLA	C1A-C2A-CAA-CBA
13	a	852	CLA	C2B-C3B-CAB-CBB
13	a	852	CLA	CAD-CBD-CGD-O1D
13	a	852	CLA	CAD-CBD-CGD-O2D
13	b	802	CLA	CBD-CGD-O2D-CED
13	b	803	CLA	CHA-CBD-CGD-O1D
13	b	803	CLA	CHA-CBD-CGD-O2D
13	b	804	CLA	C3A-C2A-CAA-CBA
13	b	804	CLA	CAD-CBD-CGD-O1D
13	b	804	CLA	CAD-CBD-CGD-O2D
13	b	805	CLA	C6-C7-C8-C9
13	b	807	CLA	C4B-C3B-CAB-CBB
13	b	810	CLA	C1A-C2A-CAA-CBA
13	b	811	CLA	CBD-CGD-O2D-CED
13	b	813	CLA	C1A-C2A-CAA-CBA
13	b	814	CLA	C3A-C2A-CAA-CBA
13	b	814	CLA	C4B-C3B-CAB-CBB
13	b	815	CLA	C1A-C2A-CAA-CBA
13	b	815	CLA	C3A-C2A-CAA-CBA
13	b	816	CLA	C2B-C3B-CAB-CBB
13	b	816	CLA	C4B-C3B-CAB-CBB
13	b	817	CLA	C4B-C3B-CAB-CBB
13	b	819	CLA	CBD-CGD-O2D-CED
13	b	820	CLA	CBD-CGD-O2D-CED
13	b	821	CLA	CBD-CGD-O2D-CED
13	b	822	CLA	CHA-CBD-CGD-O1D
13	b	822	CLA	CHA-CBD-CGD-O2D
13	b	824	CLA	C1A-C2A-CAA-CBA
13	b	824	CLA	C3A-C2A-CAA-CBA
13	b	827	CLA	C2B-C3B-CAB-CBB
13	b	827	CLA	C4B-C3B-CAB-CBB
13	b	829	CLA	CAD-CBD-CGD-O1D
13	b	829	CLA	CAD-CBD-CGD-O2D
13	b	830	CLA	C1A-C2A-CAA-CBA
13	b	830	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	b	832	CLA	C4B-C3B-CAB-CBB
13	b	833	CLA	C3A-C2A-CAA-CBA
13	b	834	CLA	C4B-C3B-CAB-CBB
13	b	835	CLA	C4B-C3B-CAB-CBB
13	b	837	CLA	C2B-C3B-CAB-CBB
13	b	837	CLA	C4B-C3B-CAB-CBB
13	f	203	CLA	C4B-C3B-CAB-CBB
13	f	204	CLA	C4B-C3B-CAB-CBB
13	i	102	CLA	C11-C10-C8-C7
13	j	1101	CLA	C4B-C3B-CAB-CBB
13	j	1101	CLA	CHA-CBD-CGD-O1D
13	j	1101	CLA	CHA-CBD-CGD-O2D
13	j	1102	CLA	CAD-CBD-CGD-O1D
13	j	1102	CLA	CAD-CBD-CGD-O2D
13	j	1103	CLA	C1A-C2A-CAA-CBA
13	j	1103	CLA	C3A-C2A-CAA-CBA
13	j	1103	CLA	C4B-C3B-CAB-CBB
13	j	1103	CLA	CBD-CGD-O2D-CED
13	k	4002	CLA	C4B-C3B-CAB-CBB
13	k	4002	CLA	CHA-CBD-CGD-O1D
13	k	4002	CLA	CHA-CBD-CGD-O2D
13	k	4003	CLA	C4B-C3B-CAB-CBB
13	k	4005	CLA	C4B-C3B-CAB-CBB
13	l	202	CLA	C1A-C2A-CAA-CBA
13	l	202	CLA	O1A-CGA-O2A-C1
13	l	204	CLA	C4B-C3B-CAB-CBB
13	l	207	CLA	C1A-C2A-CAA-CBA
13	1	805	CLA	CBA-CGA-O2A-C1
13	1	805	CLA	O1A-CGA-O2A-C1
13	1	806	CLA	C1A-C2A-CAA-CBA
13	1	807	CLA	CBD-CGD-O2D-CED
13	1	808	CLA	CHA-CBD-CGD-O1D
13	1	808	CLA	CHA-CBD-CGD-O2D
13	1	809	CLA	C1A-C2A-CAA-CBA
13	1	810	CLA	C1A-C2A-CAA-CBA
13	1	810	CLA	C3A-C2A-CAA-CBA
13	1	811	CLA	C4B-C3B-CAB-CBB
13	1	816	CLA	C4B-C3B-CAB-CBB
13	1	818	CLA	C3A-C2A-CAA-CBA
13	1	818	CLA	CBD-CGD-O2D-CED
13	1	820	CLA	CBA-CGA-O2A-C1
13	1	820	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	1	824	CLA	C1A-C2A-CAA-CBA
13	1	824	CLA	C3A-C2A-CAA-CBA
13	1	824	CLA	C4B-C3B-CAB-CBB
13	1	828	CLA	CBD-CGD-O2D-CED
13	1	831	CLA	CHA-CBD-CGD-O1D
13	1	831	CLA	CHA-CBD-CGD-O2D
13	1	833	CLA	C4B-C3B-CAB-CBB
13	1	834	CLA	C4B-C3B-CAB-CBB
13	1	836	CLA	C1A-C2A-CAA-CBA
13	1	837	CLA	C4B-C3B-CAB-CBB
13	1	838	CLA	C1A-C2A-CAA-CBA
13	1	840	CLA	C1A-C2A-CAA-CBA
13	1	840	CLA	C4B-C3B-CAB-CBB
13	1	841	CLA	C1A-C2A-CAA-CBA
13	1	841	CLA	C3A-C2A-CAA-CBA
13	1	841	CLA	C4B-C3B-CAB-CBB
13	1	842	CLA	C1A-C2A-CAA-CBA
13	1	852	CLA	C2B-C3B-CAB-CBB
13	1	852	CLA	CAD-CBD-CGD-O1D
13	1	852	CLA	CAD-CBD-CGD-O2D
13	2	802	CLA	CBD-CGD-O2D-CED
13	2	803	CLA	CHA-CBD-CGD-O1D
13	2	803	CLA	CHA-CBD-CGD-O2D
13	2	804	CLA	C3A-C2A-CAA-CBA
13	2	804	CLA	CAD-CBD-CGD-O1D
13	2	804	CLA	CAD-CBD-CGD-O2D
13	2	805	CLA	C6-C7-C8-C9
13	2	809	CLA	C1A-C2A-CAA-CBA
13	2	810	CLA	CBD-CGD-O2D-CED
13	2	812	CLA	C1A-C2A-CAA-CBA
13	2	813	CLA	C3A-C2A-CAA-CBA
13	2	813	CLA	C4B-C3B-CAB-CBB
13	2	814	CLA	C1A-C2A-CAA-CBA
13	2	814	CLA	C3A-C2A-CAA-CBA
13	2	815	CLA	C2B-C3B-CAB-CBB
13	2	815	CLA	C4B-C3B-CAB-CBB
13	2	816	CLA	C4B-C3B-CAB-CBB
13	2	818	CLA	CBD-CGD-O2D-CED
13	2	819	CLA	CBD-CGD-O2D-CED
13	2	820	CLA	CBD-CGD-O2D-CED
13	2	821	CLA	CHA-CBD-CGD-O1D
13	2	821	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
13	2	823	CLA	C1A-C2A-CAA-CBA
13	2	823	CLA	C3A-C2A-CAA-CBA
13	2	826	CLA	C2B-C3B-CAB-CBB
13	2	826	CLA	C4B-C3B-CAB-CBB
13	2	828	CLA	CAD-CBD-CGD-O1D
13	2	828	CLA	CAD-CBD-CGD-O2D
13	2	829	CLA	C1A-C2A-CAA-CBA
13	2	829	CLA	C3A-C2A-CAA-CBA
13	2	831	CLA	C4B-C3B-CAB-CBB
13	2	832	CLA	C3A-C2A-CAA-CBA
13	2	833	CLA	C4B-C3B-CAB-CBB
13	2	834	CLA	C4B-C3B-CAB-CBB
13	2	836	CLA	C2B-C3B-CAB-CBB
13	2	836	CLA	C4B-C3B-CAB-CBB
13	6	203	CLA	C4B-C3B-CAB-CBB
13	6	204	CLA	C4B-C3B-CAB-CBB
13	7	102	CLA	C11-C10-C8-C7
13	8	1101	CLA	C4B-C3B-CAB-CBB
13	8	1101	CLA	CHA-CBD-CGD-O1D
13	8	1101	CLA	CHA-CBD-CGD-O2D
13	8	1102	CLA	CAD-CBD-CGD-O1D
13	8	1102	CLA	CAD-CBD-CGD-O2D
13	8	1103	CLA	C1A-C2A-CAA-CBA
13	8	1103	CLA	C3A-C2A-CAA-CBA
13	8	1103	CLA	C4B-C3B-CAB-CBB
13	8	1103	CLA	CBD-CGD-O2D-CED
13	9	4002	CLA	C4B-C3B-CAB-CBB
13	9	4002	CLA	CHA-CBD-CGD-O1D
13	9	4002	CLA	CHA-CBD-CGD-O2D
13	9	4003	CLA	C4B-C3B-CAB-CBB
13	9	4005	CLA	C4B-C3B-CAB-CBB
13	0	202	CLA	C1A-C2A-CAA-CBA
13	0	202	CLA	O1A-CGA-O2A-C1
13	0	203	CLA	C4B-C3B-CAB-CBB
13	0	205	CLA	C4B-C3B-CAB-CBB
13	0	208	CLA	C1A-C2A-CAA-CBA
16	A	845	BCR	C20-C21-C22-C37
16	A	847	BCR	C6-C7-C8-C9
16	A	847	BCR	C15-C16-C17-C18
16	A	847	BCR	C37-C22-C23-C24
16	A	847	BCR	C22-C23-C24-C25
16	A	848	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
16	A	848	BCR	C19-C20-C21-C22
16	A	848	BCR	C21-C22-C23-C24
16	A	851	BCR	C22-C23-C24-C25
16	B	840	BCR	C7-C8-C9-C10
16	B	840	BCR	C7-C8-C9-C34
16	B	840	BCR	C37-C22-C23-C24
16	B	840	BCR	C22-C23-C24-C25
16	B	841	BCR	C20-C21-C22-C37
16	B	841	BCR	C22-C23-C24-C25
16	B	842	BCR	C18-C19-C20-C21
16	B	844	BCR	C21-C22-C23-C24
16	B	844	BCR	C22-C23-C24-C25
16	B	845	BCR	C11-C10-C9-C34
16	B	845	BCR	C10-C11-C12-C13
16	B	845	BCR	C11-C12-C13-C14
16	B	845	BCR	C22-C23-C24-C25
16	B	848	BCR	C6-C7-C8-C9
16	B	848	BCR	C7-C8-C9-C10
16	B	848	BCR	C11-C12-C13-C35
16	F	202	BCR	C14-C15-C16-C17
16	F	205	BCR	C6-C7-C8-C9
16	F	205	BCR	C10-C11-C12-C13
16	F	205	BCR	C11-C12-C13-C14
16	I	102	BCR	C6-C7-C8-C9
16	I	102	BCR	C7-C8-C9-C34
16	I	102	BCR	C21-C22-C23-C24
16	I	102	BCR	C37-C22-C23-C24
16	J	1104	BCR	C6-C7-C8-C9
16	J	1104	BCR	C14-C15-C16-C17
16	J	1105	BCR	C6-C7-C8-C9
16	J	1105	BCR	C21-C22-C23-C24
16	K	4001	BCR	C7-C8-C9-C10
16	K	4001	BCR	C7-C8-C9-C34
16	K	4004	BCR	C14-C15-C16-C17
16	K	4004	BCR	C16-C17-C18-C19
16	K	4004	BCR	C16-C17-C18-C36
16	K	4004	BCR	C22-C23-C24-C25
16	L	202	BCR	C6-C7-C8-C9
16	L	202	BCR	C7-C8-C9-C34
16	L	205	BCR	C20-C21-C22-C23
16	L	205	BCR	C37-C22-C23-C24
16	L	205	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
16	M	101	BCR	C7-C8-C9-C10
16	a	845	BCR	C20-C21-C22-C37
16	a	847	BCR	C6-C7-C8-C9
16	a	847	BCR	C15-C16-C17-C18
16	a	847	BCR	C37-C22-C23-C24
16	a	847	BCR	C22-C23-C24-C25
16	a	848	BCR	C18-C19-C20-C21
16	a	848	BCR	C19-C20-C21-C22
16	a	848	BCR	C21-C22-C23-C24
16	a	851	BCR	C22-C23-C24-C25
16	b	840	BCR	C7-C8-C9-C10
16	b	840	BCR	C7-C8-C9-C34
16	b	840	BCR	C37-C22-C23-C24
16	b	840	BCR	C22-C23-C24-C25
16	b	841	BCR	C20-C21-C22-C37
16	b	841	BCR	C22-C23-C24-C25
16	b	842	BCR	C18-C19-C20-C21
16	b	844	BCR	C21-C22-C23-C24
16	b	844	BCR	C22-C23-C24-C25
16	b	845	BCR	C11-C10-C9-C34
16	b	845	BCR	C10-C11-C12-C13
16	b	845	BCR	C11-C12-C13-C14
16	b	845	BCR	C22-C23-C24-C25
16	b	848	BCR	C6-C7-C8-C9
16	b	848	BCR	C7-C8-C9-C10
16	b	848	BCR	C11-C12-C13-C35
16	f	202	BCR	C14-C15-C16-C17
16	f	205	BCR	C6-C7-C8-C9
16	f	205	BCR	C10-C11-C12-C13
16	f	205	BCR	C11-C12-C13-C14
16	i	103	BCR	C6-C7-C8-C9
16	i	103	BCR	C7-C8-C9-C34
16	i	103	BCR	C21-C22-C23-C24
16	i	103	BCR	C37-C22-C23-C24
16	j	1104	BCR	C6-C7-C8-C9
16	j	1104	BCR	C14-C15-C16-C17
16	j	1105	BCR	C6-C7-C8-C9
16	j	1105	BCR	C21-C22-C23-C24
16	k	4001	BCR	C7-C8-C9-C10
16	k	4001	BCR	C7-C8-C9-C34
16	k	4004	BCR	C14-C15-C16-C17
16	k	4004	BCR	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
16	k	4004	BCR	C16-C17-C18-C36
16	k	4004	BCR	C22-C23-C24-C25
16	l	203	BCR	C6-C7-C8-C9
16	l	203	BCR	C7-C8-C9-C34
16	l	206	BCR	C20-C21-C22-C23
16	l	206	BCR	C37-C22-C23-C24
16	m	101	BCR	C7-C8-C9-C10
16	1	845	BCR	C20-C21-C22-C37
16	1	847	BCR	C6-C7-C8-C9
16	1	847	BCR	C15-C16-C17-C18
16	1	847	BCR	C37-C22-C23-C24
16	1	847	BCR	C22-C23-C24-C25
16	1	848	BCR	C18-C19-C20-C21
16	1	848	BCR	C19-C20-C21-C22
16	1	848	BCR	C21-C22-C23-C24
16	1	851	BCR	C22-C23-C24-C25
16	2	839	BCR	C7-C8-C9-C10
16	2	839	BCR	C7-C8-C9-C34
16	2	839	BCR	C37-C22-C23-C24
16	2	839	BCR	C22-C23-C24-C25
16	2	840	BCR	C20-C21-C22-C37
16	2	840	BCR	C22-C23-C24-C25
16	2	841	BCR	C18-C19-C20-C21
16	2	843	BCR	C21-C22-C23-C24
16	2	843	BCR	C22-C23-C24-C25
16	2	844	BCR	C11-C10-C9-C34
16	2	844	BCR	C10-C11-C12-C13
16	2	844	BCR	C11-C12-C13-C14
16	2	844	BCR	C22-C23-C24-C25
16	2	847	BCR	C6-C7-C8-C9
16	2	847	BCR	C7-C8-C9-C10
16	2	847	BCR	C11-C12-C13-C35
16	6	202	BCR	C14-C15-C16-C17
16	6	205	BCR	C6-C7-C8-C9
16	6	205	BCR	C10-C11-C12-C13
16	6	205	BCR	C11-C12-C13-C14
16	7	103	BCR	C6-C7-C8-C9
16	7	103	BCR	C7-C8-C9-C34
16	7	103	BCR	C21-C22-C23-C24
16	7	103	BCR	C37-C22-C23-C24
16	8	1104	BCR	C6-C7-C8-C9
16	8	1104	BCR	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
16	8	1105	BCR	C6-C7-C8-C9
16	8	1105	BCR	C21-C22-C23-C24
16	9	4001	BCR	C7-C8-C9-C10
16	9	4001	BCR	C7-C8-C9-C34
16	9	4004	BCR	C14-C15-C16-C17
16	9	4004	BCR	C16-C17-C18-C19
16	9	4004	BCR	C16-C17-C18-C36
16	9	4004	BCR	C22-C23-C24-C25
16	0	204	BCR	C6-C7-C8-C9
16	0	204	BCR	C7-C8-C9-C34
16	0	207	BCR	C20-C21-C22-C23
16	0	207	BCR	C37-C22-C23-C24
16	0	207	BCR	C23-C24-C25-C26
16	z	101	BCR	C7-C8-C9-C10
17	A	849	LHG	C3-O3-P-O4
17	A	849	LHG	C3-O3-P-O6
17	A	849	LHG	C4-O6-P-O3
17	A	849	LHG	C4-O6-P-O5
17	A	850	LHG	C3-O3-P-O5
17	a	849	LHG	C3-O3-P-O4
17	a	849	LHG	C3-O3-P-O6
17	a	849	LHG	C4-O6-P-O3
17	a	849	LHG	C4-O6-P-O5
17	a	850	LHG	C3-O3-P-O5
17	1	849	LHG	C3-O3-P-O4
17	1	849	LHG	C3-O3-P-O6
17	1	849	LHG	C4-O6-P-O3
17	1	849	LHG	C4-O6-P-O5
17	1	850	LHG	C3-O3-P-O5
19	I	103	SQD	C5-C6-S-O8
19	I	103	SQD	C5-C6-S-O9
19	i	101	SQD	C5-C6-S-O8
19	i	101	SQD	C5-C6-S-O9
19	7	101	SQD	C5-C6-S-O8
19	7	101	SQD	C5-C6-S-O9
13	A	832	CLA	O1D-CGD-O2D-CED
13	B	802	CLA	O1D-CGD-O2D-CED
13	B	820	CLA	O1D-CGD-O2D-CED
13	B	821	CLA	O1D-CGD-O2D-CED
13	a	832	CLA	O1D-CGD-O2D-CED
13	b	802	CLA	O1D-CGD-O2D-CED
13	b	820	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	b	821	CLA	O1D-CGD-O2D-CED
13	1	832	CLA	O1D-CGD-O2D-CED
13	2	802	CLA	O1D-CGD-O2D-CED
13	2	819	CLA	O1D-CGD-O2D-CED
13	2	820	CLA	O1D-CGD-O2D-CED
13	A	810	CLA	O1D-CGD-O2D-CED
13	A	811	CLA	O1D-CGD-O2D-CED
13	A	828	CLA	O1D-CGD-O2D-CED
13	a	810	CLA	O1D-CGD-O2D-CED
13	a	811	CLA	O1D-CGD-O2D-CED
13	a	828	CLA	O1D-CGD-O2D-CED
13	1	810	CLA	O1D-CGD-O2D-CED
13	1	811	CLA	O1D-CGD-O2D-CED
13	1	828	CLA	O1D-CGD-O2D-CED
13	A	802	CLA	CBD-CGD-O2D-CED
13	A	805	CLA	CBD-CGD-O2D-CED
13	A	810	CLA	CBD-CGD-O2D-CED
13	A	811	CLA	CBD-CGD-O2D-CED
13	A	814	CLA	CBD-CGD-O2D-CED
13	A	824	CLA	CBD-CGD-O2D-CED
13	A	832	CLA	CBD-CGD-O2D-CED
13	A	838	CLA	CBD-CGD-O2D-CED
13	B	807	CLA	CBD-CGD-O2D-CED
13	B	808	CLA	CBD-CGD-O2D-CED
13	B	809	CLA	CBD-CGD-O2D-CED
13	B	829	CLA	CBD-CGD-O2D-CED
13	B	831	CLA	CBD-CGD-O2D-CED
13	B	837	CLA	CBD-CGD-O2D-CED
13	B	838	CLA	CBD-CGD-O2D-CED
13	F	204	CLA	CBD-CGD-O2D-CED
13	L	203	CLA	CBD-CGD-O2D-CED
13	a	802	CLA	CBD-CGD-O2D-CED
13	a	805	CLA	CBD-CGD-O2D-CED
13	a	810	CLA	CBD-CGD-O2D-CED
13	a	811	CLA	CBD-CGD-O2D-CED
13	a	814	CLA	CBD-CGD-O2D-CED
13	a	824	CLA	CBD-CGD-O2D-CED
13	a	832	CLA	CBD-CGD-O2D-CED
13	a	838	CLA	CBD-CGD-O2D-CED
13	b	807	CLA	CBD-CGD-O2D-CED
13	b	808	CLA	CBD-CGD-O2D-CED
13	b	809	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	b	829	CLA	CBD-CGD-O2D-CED
13	b	831	CLA	CBD-CGD-O2D-CED
13	b	837	CLA	CBD-CGD-O2D-CED
13	b	838	CLA	CBD-CGD-O2D-CED
13	f	204	CLA	CBD-CGD-O2D-CED
13	l	204	CLA	CBD-CGD-O2D-CED
13	1	802	CLA	CBD-CGD-O2D-CED
13	1	805	CLA	CBD-CGD-O2D-CED
13	1	810	CLA	CBD-CGD-O2D-CED
13	1	811	CLA	CBD-CGD-O2D-CED
13	1	814	CLA	CBD-CGD-O2D-CED
13	1	824	CLA	CBD-CGD-O2D-CED
13	1	832	CLA	CBD-CGD-O2D-CED
13	1	838	CLA	CBD-CGD-O2D-CED
13	2	807	CLA	CBD-CGD-O2D-CED
13	2	808	CLA	CBD-CGD-O2D-CED
13	2	828	CLA	CBD-CGD-O2D-CED
13	2	830	CLA	CBD-CGD-O2D-CED
13	2	836	CLA	CBD-CGD-O2D-CED
13	2	837	CLA	CBD-CGD-O2D-CED
13	6	204	CLA	CBD-CGD-O2D-CED
13	0	203	CLA	CBD-CGD-O2D-CED
13	0	205	CLA	CBD-CGD-O2D-CED
13	B	825	CLA	O1A-CGA-O2A-C1
13	b	825	CLA	O1A-CGA-O2A-C1
13	2	824	CLA	O1A-CGA-O2A-C1
13	A	812	CLA	O1A-CGA-O2A-C1
13	a	812	CLA	O1A-CGA-O2A-C1
13	1	812	CLA	O1A-CGA-O2A-C1
13	A	812	CLA	CBA-CGA-O2A-C1
13	a	812	CLA	CBA-CGA-O2A-C1
13	1	812	CLA	CBA-CGA-O2A-C1
13	A	824	CLA	O1D-CGD-O2D-CED
13	B	831	CLA	O1D-CGD-O2D-CED
13	B	837	CLA	O1D-CGD-O2D-CED
13	F	204	CLA	O1D-CGD-O2D-CED
13	a	824	CLA	O1D-CGD-O2D-CED
13	b	831	CLA	O1D-CGD-O2D-CED
13	b	837	CLA	O1D-CGD-O2D-CED
13	f	204	CLA	O1D-CGD-O2D-CED
13	1	824	CLA	O1D-CGD-O2D-CED
13	2	830	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	2	836	CLA	O1D-CGD-O2D-CED
13	6	204	CLA	O1D-CGD-O2D-CED
13	B	825	CLA	CBA-CGA-O2A-C1
13	b	825	CLA	CBA-CGA-O2A-C1
13	2	824	CLA	CBA-CGA-O2A-C1
13	A	803	CLA	CBD-CGD-O2D-CED
13	F	201	CLA	CBD-CGD-O2D-CED
13	a	803	CLA	CBD-CGD-O2D-CED
13	f	201	CLA	CBD-CGD-O2D-CED
13	1	803	CLA	CBD-CGD-O2D-CED
13	6	201	CLA	CBD-CGD-O2D-CED
13	A	817	CLA	O1A-CGA-O2A-C1
13	A	822	CLA	O1A-CGA-O2A-C1
13	A	823	CLA	O1A-CGA-O2A-C1
13	A	831	CLA	O1A-CGA-O2A-C1
13	A	835	CLA	O1A-CGA-O2A-C1
13	B	801	CLA	O1A-CGA-O2A-C1
13	B	807	CLA	O1A-CGA-O2A-C1
13	B	826	CLA	O1A-CGA-O2A-C1
13	B	838	CLA	O1A-CGA-O2A-C1
13	I	101	CLA	O1A-CGA-O2A-C1
13	a	817	CLA	O1A-CGA-O2A-C1
13	a	822	CLA	O1A-CGA-O2A-C1
13	a	823	CLA	O1A-CGA-O2A-C1
13	a	831	CLA	O1A-CGA-O2A-C1
13	a	835	CLA	O1A-CGA-O2A-C1
13	b	801	CLA	O1A-CGA-O2A-C1
13	b	807	CLA	O1A-CGA-O2A-C1
13	b	826	CLA	O1A-CGA-O2A-C1
13	b	838	CLA	O1A-CGA-O2A-C1
13	i	102	CLA	O1A-CGA-O2A-C1
13	1	817	CLA	O1A-CGA-O2A-C1
13	1	822	CLA	O1A-CGA-O2A-C1
13	1	823	CLA	O1A-CGA-O2A-C1
13	1	831	CLA	O1A-CGA-O2A-C1
13	1	835	CLA	O1A-CGA-O2A-C1
13	2	801	CLA	O1A-CGA-O2A-C1
13	2	825	CLA	O1A-CGA-O2A-C1
13	2	837	CLA	O1A-CGA-O2A-C1
13	7	102	CLA	O1A-CGA-O2A-C1
13	0	203	CLA	O1A-CGA-O2A-C1
13	A	820	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	a	820	CLA	O1A-CGA-O2A-C1
13	1	820	CLA	O1A-CGA-O2A-C1
13	A	818	CLA	O1D-CGD-O2D-CED
13	B	819	CLA	O1D-CGD-O2D-CED
13	a	818	CLA	O1D-CGD-O2D-CED
13	b	819	CLA	O1D-CGD-O2D-CED
13	1	818	CLA	O1D-CGD-O2D-CED
13	2	818	CLA	O1D-CGD-O2D-CED
13	A	807	CLA	O1D-CGD-O2D-CED
13	J	1103	CLA	O1D-CGD-O2D-CED
13	a	807	CLA	O1D-CGD-O2D-CED
13	j	1103	CLA	O1D-CGD-O2D-CED
13	1	807	CLA	O1D-CGD-O2D-CED
13	8	1103	CLA	O1D-CGD-O2D-CED
13	A	821	CLA	CBD-CGD-O2D-CED
13	a	821	CLA	CBD-CGD-O2D-CED
13	1	821	CLA	CBD-CGD-O2D-CED
18	B	846	LMG	O9-C10-O7-C8
18	b	846	LMG	O9-C10-O7-C8
18	2	845	LMG	O9-C10-O7-C8
13	B	819	CLA	CBA-CGA-O2A-C1
13	b	819	CLA	CBA-CGA-O2A-C1
13	2	818	CLA	CBA-CGA-O2A-C1
12	A	801	CL0	C3-C5-C6-C7
12	a	801	CL0	C3-C5-C6-C7
12	1	801	CL0	C3-C5-C6-C7
13	A	834	CLA	C3-C5-C6-C7
13	A	837	CLA	C3-C5-C6-C7
13	A	838	CLA	C3-C5-C6-C7
13	B	806	CLA	C3-C5-C6-C7
13	B	813	CLA	C3-C5-C6-C7
13	B	829	CLA	C3-C5-C6-C7
13	B	847	CLA	C3-C5-C6-C7
13	L	201	CLA	C3-C5-C6-C7
13	a	834	CLA	C3-C5-C6-C7
13	a	837	CLA	C3-C5-C6-C7
13	a	838	CLA	C3-C5-C6-C7
13	b	806	CLA	C3-C5-C6-C7
13	b	813	CLA	C3-C5-C6-C7
13	b	829	CLA	C3-C5-C6-C7
13	b	847	CLA	C3-C5-C6-C7
13	l	202	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
13	1	834	CLA	C3-C5-C6-C7
13	1	837	CLA	C3-C5-C6-C7
13	1	838	CLA	C3-C5-C6-C7
13	2	806	CLA	C3-C5-C6-C7
13	2	812	CLA	C3-C5-C6-C7
13	2	828	CLA	C3-C5-C6-C7
13	2	846	CLA	C3-C5-C6-C7
13	0	202	CLA	C3-C5-C6-C7
13	A	822	CLA	CBA-CGA-O2A-C1
13	A	823	CLA	CBA-CGA-O2A-C1
13	A	835	CLA	CBA-CGA-O2A-C1
13	B	807	CLA	CBA-CGA-O2A-C1
13	I	101	CLA	CBA-CGA-O2A-C1
13	L	201	CLA	CBA-CGA-O2A-C1
13	a	822	CLA	CBA-CGA-O2A-C1
13	a	823	CLA	CBA-CGA-O2A-C1
13	a	835	CLA	CBA-CGA-O2A-C1
13	b	807	CLA	CBA-CGA-O2A-C1
13	i	102	CLA	CBA-CGA-O2A-C1
13	l	202	CLA	CBA-CGA-O2A-C1
13	1	822	CLA	CBA-CGA-O2A-C1
13	1	823	CLA	CBA-CGA-O2A-C1
13	1	835	CLA	CBA-CGA-O2A-C1
13	7	102	CLA	CBA-CGA-O2A-C1
13	0	202	CLA	CBA-CGA-O2A-C1
13	0	203	CLA	CBA-CGA-O2A-C1
13	A	813	CLA	CBD-CGD-O2D-CED
13	A	819	CLA	CBD-CGD-O2D-CED
13	A	825	CLA	CBD-CGD-O2D-CED
13	A	833	CLA	CBD-CGD-O2D-CED
13	A	841	CLA	CBD-CGD-O2D-CED
13	A	842	CLA	CBD-CGD-O2D-CED
13	B	803	CLA	CBD-CGD-O2D-CED
13	B	805	CLA	CBD-CGD-O2D-CED
13	B	812	CLA	CBD-CGD-O2D-CED
13	B	816	CLA	CBD-CGD-O2D-CED
13	B	824	CLA	CBD-CGD-O2D-CED
13	B	830	CLA	CBD-CGD-O2D-CED
13	B	834	CLA	CBD-CGD-O2D-CED
13	L	204	CLA	CBD-CGD-O2D-CED
13	a	813	CLA	CBD-CGD-O2D-CED
13	a	819	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	a	825	CLA	CBD-CGD-O2D-CED
13	a	833	CLA	CBD-CGD-O2D-CED
13	a	841	CLA	CBD-CGD-O2D-CED
13	a	842	CLA	CBD-CGD-O2D-CED
13	b	803	CLA	CBD-CGD-O2D-CED
13	b	805	CLA	CBD-CGD-O2D-CED
13	b	812	CLA	CBD-CGD-O2D-CED
13	b	816	CLA	CBD-CGD-O2D-CED
13	b	824	CLA	CBD-CGD-O2D-CED
13	b	830	CLA	CBD-CGD-O2D-CED
13	b	834	CLA	CBD-CGD-O2D-CED
13	l	205	CLA	CBD-CGD-O2D-CED
13	1	813	CLA	CBD-CGD-O2D-CED
13	1	819	CLA	CBD-CGD-O2D-CED
13	1	825	CLA	CBD-CGD-O2D-CED
13	1	833	CLA	CBD-CGD-O2D-CED
13	1	841	CLA	CBD-CGD-O2D-CED
13	1	842	CLA	CBD-CGD-O2D-CED
13	2	803	CLA	CBD-CGD-O2D-CED
13	2	805	CLA	CBD-CGD-O2D-CED
13	2	811	CLA	CBD-CGD-O2D-CED
13	2	815	CLA	CBD-CGD-O2D-CED
13	2	823	CLA	CBD-CGD-O2D-CED
13	2	829	CLA	CBD-CGD-O2D-CED
13	2	833	CLA	CBD-CGD-O2D-CED
13	0	206	CLA	CBD-CGD-O2D-CED
13	B	818	CLA	O1A-CGA-O2A-C1
13	B	819	CLA	O1A-CGA-O2A-C1
13	b	818	CLA	O1A-CGA-O2A-C1
13	b	819	CLA	O1A-CGA-O2A-C1
13	2	817	CLA	O1A-CGA-O2A-C1
13	2	818	CLA	O1A-CGA-O2A-C1
13	B	811	CLA	O1D-CGD-O2D-CED
13	b	811	CLA	O1D-CGD-O2D-CED
13	2	810	CLA	O1D-CGD-O2D-CED
13	A	811	CLA	C4-C3-C5-C6
13	A	828	CLA	C4-C3-C5-C6
13	a	811	CLA	C4-C3-C5-C6
13	a	828	CLA	C4-C3-C5-C6
13	1	811	CLA	C4-C3-C5-C6
13	1	828	CLA	C4-C3-C5-C6
13	A	811	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	a	811	CLA	C2-C3-C5-C6
13	1	811	CLA	C2-C3-C5-C6
13	B	818	CLA	CBA-CGA-O2A-C1
13	b	818	CLA	CBA-CGA-O2A-C1
13	2	817	CLA	CBA-CGA-O2A-C1
13	A	838	CLA	O1D-CGD-O2D-CED
13	a	838	CLA	O1D-CGD-O2D-CED
13	1	838	CLA	O1D-CGD-O2D-CED
18	B	846	LMG	O6-C5-C6-O5
18	b	846	LMG	O6-C5-C6-O5
18	2	845	LMG	O6-C5-C6-O5
13	A	827	CLA	C2A-CAA-CBA-CGA
13	B	803	CLA	C2A-CAA-CBA-CGA
13	B	813	CLA	C2A-CAA-CBA-CGA
13	a	827	CLA	C2A-CAA-CBA-CGA
13	b	803	CLA	C2A-CAA-CBA-CGA
13	b	813	CLA	C2A-CAA-CBA-CGA
13	1	827	CLA	C2A-CAA-CBA-CGA
13	2	803	CLA	C2A-CAA-CBA-CGA
13	2	812	CLA	C2A-CAA-CBA-CGA
13	A	817	CLA	C3-C5-C6-C7
13	A	829	CLA	C3-C5-C6-C7
13	B	824	CLA	C3-C5-C6-C7
13	a	817	CLA	C3-C5-C6-C7
13	a	829	CLA	C3-C5-C6-C7
13	b	824	CLA	C3-C5-C6-C7
13	1	817	CLA	C3-C5-C6-C7
13	1	829	CLA	C3-C5-C6-C7
13	2	823	CLA	C3-C5-C6-C7
13	A	811	CLA	CBA-CGA-O2A-C1
13	A	817	CLA	CBA-CGA-O2A-C1
13	A	831	CLA	CBA-CGA-O2A-C1
13	B	801	CLA	CBA-CGA-O2A-C1
13	B	813	CLA	CBA-CGA-O2A-C1
13	B	826	CLA	CBA-CGA-O2A-C1
13	B	838	CLA	CBA-CGA-O2A-C1
13	a	811	CLA	CBA-CGA-O2A-C1
13	a	817	CLA	CBA-CGA-O2A-C1
13	a	831	CLA	CBA-CGA-O2A-C1
13	b	801	CLA	CBA-CGA-O2A-C1
13	b	813	CLA	CBA-CGA-O2A-C1
13	b	826	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	b	838	CLA	CBA-CGA-O2A-C1
13	1	811	CLA	CBA-CGA-O2A-C1
13	1	817	CLA	CBA-CGA-O2A-C1
13	1	831	CLA	CBA-CGA-O2A-C1
13	2	801	CLA	CBA-CGA-O2A-C1
13	2	812	CLA	CBA-CGA-O2A-C1
13	2	825	CLA	CBA-CGA-O2A-C1
13	2	837	CLA	CBA-CGA-O2A-C1
16	A	851	BCR	C19-C20-C21-C22
16	B	842	BCR	C15-C16-C17-C18
16	a	851	BCR	C19-C20-C21-C22
16	b	842	BCR	C15-C16-C17-C18
16	1	851	BCR	C19-C20-C21-C22
16	2	841	BCR	C15-C16-C17-C18
13	A	802	CLA	O1A-CGA-O2A-C1
13	A	811	CLA	O1A-CGA-O2A-C1
13	A	821	CLA	O1A-CGA-O2A-C1
13	B	813	CLA	O1A-CGA-O2A-C1
13	B	823	CLA	O1A-CGA-O2A-C1
13	a	802	CLA	O1A-CGA-O2A-C1
13	a	811	CLA	O1A-CGA-O2A-C1
13	a	821	CLA	O1A-CGA-O2A-C1
13	b	813	CLA	O1A-CGA-O2A-C1
13	b	823	CLA	O1A-CGA-O2A-C1
13	1	802	CLA	O1A-CGA-O2A-C1
13	1	811	CLA	O1A-CGA-O2A-C1
13	1	821	CLA	O1A-CGA-O2A-C1
13	2	812	CLA	O1A-CGA-O2A-C1
13	2	822	CLA	O1A-CGA-O2A-C1
13	B	809	CLA	O1D-CGD-O2D-CED
13	B	829	CLA	O1D-CGD-O2D-CED
13	2	808	CLA	O1D-CGD-O2D-CED
13	b	809	CLA	O1D-CGD-O2D-CED
13	b	829	CLA	O1D-CGD-O2D-CED
13	2	828	CLA	O1D-CGD-O2D-CED
13	A	809	CLA	CBD-CGD-O2D-CED
13	A	835	CLA	CBD-CGD-O2D-CED
13	a	809	CLA	CBD-CGD-O2D-CED
13	a	835	CLA	CBD-CGD-O2D-CED
13	1	809	CLA	CBD-CGD-O2D-CED
13	1	835	CLA	CBD-CGD-O2D-CED
13	B	807	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	b	807	CLA	O1D-CGD-O2D-CED
13	0	203	CLA	O1D-CGD-O2D-CED
13	A	806	CLA	CBA-CGA-O2A-C1
13	A	840	CLA	CBA-CGA-O2A-C1
13	B	821	CLA	CBA-CGA-O2A-C1
13	B	823	CLA	CBA-CGA-O2A-C1
13	B	837	CLA	CBA-CGA-O2A-C1
13	a	806	CLA	CBA-CGA-O2A-C1
13	a	840	CLA	CBA-CGA-O2A-C1
13	b	821	CLA	CBA-CGA-O2A-C1
13	b	823	CLA	CBA-CGA-O2A-C1
13	b	837	CLA	CBA-CGA-O2A-C1
13	1	806	CLA	CBA-CGA-O2A-C1
13	1	840	CLA	CBA-CGA-O2A-C1
13	2	820	CLA	CBA-CGA-O2A-C1
13	2	822	CLA	CBA-CGA-O2A-C1
13	2	836	CLA	CBA-CGA-O2A-C1
13	L	203	CLA	O1D-CGD-O2D-CED
13	l	204	CLA	O1D-CGD-O2D-CED
13	0	205	CLA	O1D-CGD-O2D-CED
13	A	802	CLA	O1D-CGD-O2D-CED
13	B	838	CLA	O1D-CGD-O2D-CED
13	a	802	CLA	O1D-CGD-O2D-CED
13	b	838	CLA	O1D-CGD-O2D-CED
13	1	802	CLA	O1D-CGD-O2D-CED
13	2	837	CLA	O1D-CGD-O2D-CED
13	A	840	CLA	C3-C5-C6-C7
13	a	840	CLA	C3-C5-C6-C7
13	1	840	CLA	C3-C5-C6-C7
14	B	839	PQN	C13-C15-C16-C17
14	b	839	PQN	C13-C15-C16-C17
14	2	838	PQN	C13-C15-C16-C17
13	A	822	CLA	CBD-CGD-O2D-CED
13	a	822	CLA	CBD-CGD-O2D-CED
13	1	822	CLA	CBD-CGD-O2D-CED
13	2	825	CLA	CBD-CGD-O2D-CED
13	B	808	CLA	O1D-CGD-O2D-CED
13	b	808	CLA	O1D-CGD-O2D-CED
13	2	807	CLA	O1D-CGD-O2D-CED
13	A	802	CLA	CBA-CGA-O2A-C1
13	A	821	CLA	CBA-CGA-O2A-C1
13	a	802	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	a	821	CLA	CBA-CGA-O2A-C1
13	1	802	CLA	CBA-CGA-O2A-C1
13	1	821	CLA	CBA-CGA-O2A-C1
13	A	802	CLA	C4-C3-C5-C6
13	A	824	CLA	C4-C3-C5-C6
13	a	802	CLA	C4-C3-C5-C6
13	a	824	CLA	C4-C3-C5-C6
13	1	802	CLA	C4-C3-C5-C6
13	1	824	CLA	C4-C3-C5-C6
13	A	802	CLA	C2-C3-C5-C6
13	A	828	CLA	C2-C3-C5-C6
13	a	802	CLA	C2-C3-C5-C6
13	a	828	CLA	C2-C3-C5-C6
13	1	802	CLA	C2-C3-C5-C6
13	1	828	CLA	C2-C3-C5-C6
13	B	821	CLA	O1A-CGA-O2A-C1
13	b	821	CLA	O1A-CGA-O2A-C1
13	2	820	CLA	O1A-CGA-O2A-C1
18	B	846	LMG	C4-C5-C6-O5
18	b	846	LMG	C4-C5-C6-O5
18	2	845	LMG	C4-C5-C6-O5
13	a	816	CLA	CBA-CGA-O2A-C1
13	B	826	CLA	CBD-CGD-O2D-CED
13	b	826	CLA	CBD-CGD-O2D-CED
13	A	824	CLA	C2A-CAA-CBA-CGA
13	A	829	CLA	C2A-CAA-CBA-CGA
13	a	824	CLA	C2A-CAA-CBA-CGA
13	a	829	CLA	C2A-CAA-CBA-CGA
13	1	824	CLA	C2A-CAA-CBA-CGA
13	1	829	CLA	C2A-CAA-CBA-CGA
13	A	805	CLA	O1D-CGD-O2D-CED
13	A	814	CLA	O1D-CGD-O2D-CED
13	a	805	CLA	O1D-CGD-O2D-CED
13	1	805	CLA	O1D-CGD-O2D-CED
13	A	806	CLA	O1A-CGA-O2A-C1
13	B	837	CLA	O1A-CGA-O2A-C1
13	a	806	CLA	O1A-CGA-O2A-C1
13	b	837	CLA	O1A-CGA-O2A-C1
13	1	806	CLA	O1A-CGA-O2A-C1
13	2	836	CLA	O1A-CGA-O2A-C1
13	a	814	CLA	O1D-CGD-O2D-CED
13	1	814	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	A	804	CLA	CBA-CGA-O2A-C1
13	B	828	CLA	CBA-CGA-O2A-C1
13	a	804	CLA	CBA-CGA-O2A-C1
13	1	804	CLA	CBA-CGA-O2A-C1
13	A	831	CLA	CBD-CGD-O2D-CED
13	A	840	CLA	CBD-CGD-O2D-CED
13	B	801	CLA	CBD-CGD-O2D-CED
13	B	825	CLA	CBD-CGD-O2D-CED
13	B	828	CLA	CBD-CGD-O2D-CED
13	B	847	CLA	CBD-CGD-O2D-CED
13	a	831	CLA	CBD-CGD-O2D-CED
13	a	840	CLA	CBD-CGD-O2D-CED
13	b	801	CLA	CBD-CGD-O2D-CED
13	b	825	CLA	CBD-CGD-O2D-CED
13	b	828	CLA	CBD-CGD-O2D-CED
13	b	847	CLA	CBD-CGD-O2D-CED
13	1	831	CLA	CBD-CGD-O2D-CED
13	1	840	CLA	CBD-CGD-O2D-CED
13	2	801	CLA	CBD-CGD-O2D-CED
13	2	824	CLA	CBD-CGD-O2D-CED
13	2	827	CLA	CBD-CGD-O2D-CED
13	2	846	CLA	CBD-CGD-O2D-CED
13	A	816	CLA	CBA-CGA-O2A-C1
13	1	816	CLA	CBA-CGA-O2A-C1
13	A	840	CLA	O1A-CGA-O2A-C1
13	a	840	CLA	O1A-CGA-O2A-C1
13	1	840	CLA	O1A-CGA-O2A-C1
13	A	804	CLA	O1A-CGA-O2A-C1
13	a	804	CLA	O1A-CGA-O2A-C1
13	1	804	CLA	O1A-CGA-O2A-C1
17	A	850	LHG	C1-C2-C3-O3
17	a	850	LHG	C1-C2-C3-O3
17	1	850	LHG	C1-C2-C3-O3
13	A	803	CLA	O1D-CGD-O2D-CED
13	a	803	CLA	O1D-CGD-O2D-CED
13	1	803	CLA	O1D-CGD-O2D-CED
12	A	801	CL0	CBA-CGA-O2A-C1
12	a	801	CL0	CBA-CGA-O2A-C1
12	1	801	CL0	CBA-CGA-O2A-C1
13	A	830	CLA	CBA-CGA-O2A-C1
13	J	1101	CLA	CBA-CGA-O2A-C1
13	a	830	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	b	828	CLA	CBA-CGA-O2A-C1
13	j	1101	CLA	CBA-CGA-O2A-C1
13	1	830	CLA	CBA-CGA-O2A-C1
13	2	827	CLA	CBA-CGA-O2A-C1
13	8	1101	CLA	CBA-CGA-O2A-C1
13	A	806	CLA	CBD-CGD-O2D-CED
13	B	832	CLA	CBD-CGD-O2D-CED
13	a	806	CLA	CBD-CGD-O2D-CED
13	b	832	CLA	CBD-CGD-O2D-CED
13	1	806	CLA	CBD-CGD-O2D-CED
13	2	831	CLA	CBD-CGD-O2D-CED
13	A	821	CLA	O1D-CGD-O2D-CED
13	B	812	CLA	O1D-CGD-O2D-CED
13	B	824	CLA	O1D-CGD-O2D-CED
13	F	201	CLA	O1D-CGD-O2D-CED
13	a	821	CLA	O1D-CGD-O2D-CED
13	b	824	CLA	O1D-CGD-O2D-CED
13	f	201	CLA	O1D-CGD-O2D-CED
13	1	821	CLA	O1D-CGD-O2D-CED
13	2	823	CLA	O1D-CGD-O2D-CED
13	6	201	CLA	O1D-CGD-O2D-CED
13	L	204	CLA	O1D-CGD-O2D-CED
13	a	833	CLA	O1D-CGD-O2D-CED
13	b	812	CLA	O1D-CGD-O2D-CED
13	l	205	CLA	O1D-CGD-O2D-CED
13	1	833	CLA	O1D-CGD-O2D-CED
13	2	811	CLA	O1D-CGD-O2D-CED
13	A	824	CLA	C2-C3-C5-C6
13	a	824	CLA	C2-C3-C5-C6
13	1	824	CLA	C2-C3-C5-C6
12	A	801	CL0	C11-C12-C13-C14
12	a	801	CL0	C11-C12-C13-C14
12	1	801	CL0	C11-C12-C13-C14
13	B	804	CLA	C11-C12-C13-C14
13	b	804	CLA	C11-C12-C13-C14
13	2	804	CLA	C11-C12-C13-C14
13	A	819	CLA	O1D-CGD-O2D-CED
13	A	833	CLA	O1D-CGD-O2D-CED
13	A	841	CLA	O1D-CGD-O2D-CED
13	B	803	CLA	O1D-CGD-O2D-CED
13	B	805	CLA	O1D-CGD-O2D-CED
13	a	819	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	a	841	CLA	O1D-CGD-O2D-CED
13	b	803	CLA	O1D-CGD-O2D-CED
13	b	805	CLA	O1D-CGD-O2D-CED
13	1	819	CLA	O1D-CGD-O2D-CED
13	1	841	CLA	O1D-CGD-O2D-CED
13	2	803	CLA	O1D-CGD-O2D-CED
13	2	805	CLA	O1D-CGD-O2D-CED
13	0	206	CLA	O1D-CGD-O2D-CED
13	F	204	CLA	CBA-CGA-O2A-C1
13	f	204	CLA	CBA-CGA-O2A-C1
13	6	204	CLA	CBA-CGA-O2A-C1
13	B	830	CLA	O1D-CGD-O2D-CED
16	A	847	BCR	C7-C8-C9-C34
16	A	848	BCR	C37-C22-C23-C24
16	A	851	BCR	C7-C8-C9-C34
16	A	851	BCR	C37-C22-C23-C24
16	B	843	BCR	C36-C18-C19-C20
16	B	845	BCR	C11-C12-C13-C35
16	F	202	BCR	C7-C8-C9-C34
16	F	202	BCR	C37-C22-C23-C24
16	F	205	BCR	C11-C12-C13-C35
16	J	1105	BCR	C7-C8-C9-C34
16	L	202	BCR	C11-C12-C13-C35
16	L	205	BCR	C7-C8-C9-C34
16	L	207	BCR	C7-C8-C9-C34
16	M	101	BCR	C7-C8-C9-C34
16	a	847	BCR	C7-C8-C9-C34
16	a	848	BCR	C37-C22-C23-C24
16	a	851	BCR	C7-C8-C9-C34
16	a	851	BCR	C37-C22-C23-C24
16	b	843	BCR	C36-C18-C19-C20
16	b	845	BCR	C11-C12-C13-C35
16	f	202	BCR	C7-C8-C9-C34
16	f	202	BCR	C37-C22-C23-C24
16	f	205	BCR	C11-C12-C13-C35
16	j	1105	BCR	C7-C8-C9-C34
16	l	201	BCR	C7-C8-C9-C34
16	l	203	BCR	C11-C12-C13-C35
16	l	206	BCR	C7-C8-C9-C34
16	m	101	BCR	C7-C8-C9-C34
16	1	847	BCR	C7-C8-C9-C34
16	1	848	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
16	1	851	BCR	C7-C8-C9-C34
16	1	851	BCR	C37-C22-C23-C24
16	2	842	BCR	C36-C18-C19-C20
16	2	844	BCR	C11-C12-C13-C35
16	6	202	BCR	C7-C8-C9-C34
16	6	202	BCR	C37-C22-C23-C24
16	6	205	BCR	C11-C12-C13-C35
16	8	1105	BCR	C7-C8-C9-C34
16	0	201	BCR	C7-C8-C9-C34
16	0	204	BCR	C11-C12-C13-C35
16	0	207	BCR	C7-C8-C9-C34
16	z	101	BCR	C7-C8-C9-C34
16	A	847	BCR	C7-C8-C9-C10
16	A	847	BCR	C21-C22-C23-C24
16	B	840	BCR	C21-C22-C23-C24
16	B	848	BCR	C11-C12-C13-C14
16	L	205	BCR	C7-C8-C9-C10
16	a	847	BCR	C7-C8-C9-C10
16	a	847	BCR	C21-C22-C23-C24
16	b	840	BCR	C21-C22-C23-C24
16	b	848	BCR	C11-C12-C13-C14
16	l	206	BCR	C7-C8-C9-C10
16	1	847	BCR	C7-C8-C9-C10
16	1	847	BCR	C21-C22-C23-C24
16	2	839	BCR	C21-C22-C23-C24
16	2	847	BCR	C11-C12-C13-C14
16	0	207	BCR	C7-C8-C9-C10
13	b	830	CLA	O1D-CGD-O2D-CED
13	2	829	CLA	O1D-CGD-O2D-CED
17	A	849	LHG	O6-C4-C5-O7
17	a	849	LHG	O6-C4-C5-O7
17	1	849	LHG	O6-C4-C5-O7
13	B	801	CLA	C5-C6-C7-C8
13	I	101	CLA	C8-C10-C11-C12
13	b	801	CLA	C5-C6-C7-C8
13	i	102	CLA	C8-C10-C11-C12
13	2	801	CLA	C5-C6-C7-C8
13	7	102	CLA	C8-C10-C11-C12
13	B	834	CLA	O1D-CGD-O2D-CED
13	b	834	CLA	O1D-CGD-O2D-CED
13	2	833	CLA	O1D-CGD-O2D-CED
13	A	806	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
13	A	824	CLA	C10-C11-C12-C13
13	B	806	CLA	C15-C16-C17-C18
13	B	813	CLA	C10-C11-C12-C13
13	B	825	CLA	C8-C10-C11-C12
13	a	806	CLA	C15-C16-C17-C18
13	a	824	CLA	C10-C11-C12-C13
13	b	806	CLA	C15-C16-C17-C18
13	b	813	CLA	C10-C11-C12-C13
13	b	825	CLA	C8-C10-C11-C12
13	1	806	CLA	C15-C16-C17-C18
13	1	824	CLA	C10-C11-C12-C13
13	2	806	CLA	C15-C16-C17-C18
13	2	812	CLA	C10-C11-C12-C13
13	2	824	CLA	C8-C10-C11-C12
13	B	801	CLA	C3-C5-C6-C7
13	b	801	CLA	C3-C5-C6-C7
13	2	801	CLA	C3-C5-C6-C7
13	A	825	CLA	O1D-CGD-O2D-CED
13	B	816	CLA	O1D-CGD-O2D-CED
13	a	825	CLA	O1D-CGD-O2D-CED
13	b	816	CLA	O1D-CGD-O2D-CED
13	1	825	CLA	O1D-CGD-O2D-CED
13	2	815	CLA	O1D-CGD-O2D-CED
13	J	1101	CLA	O1A-CGA-O2A-C1
13	j	1101	CLA	O1A-CGA-O2A-C1
13	8	1101	CLA	O1A-CGA-O2A-C1
13	B	829	CLA	C5-C6-C7-C8
13	b	829	CLA	C5-C6-C7-C8
13	2	828	CLA	C5-C6-C7-C8
13	B	813	CLA	CBD-CGD-O2D-CED
13	b	813	CLA	CBD-CGD-O2D-CED
13	2	812	CLA	CBD-CGD-O2D-CED
13	A	825	CLA	CBA-CGA-O2A-C1
13	a	825	CLA	CBA-CGA-O2A-C1
13	1	825	CLA	CBA-CGA-O2A-C1
16	B	841	BCR	C19-C20-C21-C22
16	B	848	BCR	C9-C10-C11-C12
16	b	841	BCR	C19-C20-C21-C22
16	b	848	BCR	C9-C10-C11-C12
16	2	840	BCR	C19-C20-C21-C22
16	2	847	BCR	C9-C10-C11-C12
13	A	826	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
13	a	826	CLA	C5-C6-C7-C8
13	1	826	CLA	C5-C6-C7-C8
17	A	850	LHG	C7-C8-C9-C10
17	A	850	LHG	C23-C24-C25-C26
17	a	850	LHG	C7-C8-C9-C10
17	a	850	LHG	C23-C24-C25-C26
17	1	850	LHG	C7-C8-C9-C10
17	1	850	LHG	C23-C24-C25-C26
12	A	801	CL0	O1A-CGA-O2A-C1
12	a	801	CL0	O1A-CGA-O2A-C1
12	1	801	CL0	O1A-CGA-O2A-C1
13	1	830	CLA	O1A-CGA-O2A-C1
13	B	806	CLA	CBD-CGD-O2D-CED
13	b	806	CLA	CBD-CGD-O2D-CED
13	2	806	CLA	CBD-CGD-O2D-CED
13	A	813	CLA	O1D-CGD-O2D-CED
13	a	813	CLA	O1D-CGD-O2D-CED
13	1	813	CLA	O1D-CGD-O2D-CED
13	B	805	CLA	CBA-CGA-O2A-C1
13	b	805	CLA	CBA-CGA-O2A-C1
13	2	805	CLA	CBA-CGA-O2A-C1
13	B	805	CLA	C10-C11-C12-C13
13	B	813	CLA	C5-C6-C7-C8
13	B	838	CLA	C10-C11-C12-C13
13	L	206	CLA	C5-C6-C7-C8
13	b	805	CLA	C10-C11-C12-C13
13	b	813	CLA	C5-C6-C7-C8
13	b	838	CLA	C10-C11-C12-C13
13	1	207	CLA	C5-C6-C7-C8
13	2	805	CLA	C10-C11-C12-C13
13	2	812	CLA	C5-C6-C7-C8
13	2	837	CLA	C10-C11-C12-C13
13	0	208	CLA	C5-C6-C7-C8
14	B	839	PQN	C15-C16-C17-C18
14	b	839	PQN	C15-C16-C17-C18
14	2	838	PQN	C15-C16-C17-C18
13	A	841	CLA	C2A-CAA-CBA-CGA
13	A	852	CLA	C2A-CAA-CBA-CGA
13	B	807	CLA	C2A-CAA-CBA-CGA
13	B	814	CLA	C2A-CAA-CBA-CGA
13	B	836	CLA	C2A-CAA-CBA-CGA
13	a	841	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
13	a	852	CLA	C2A-CAA-CBA-CGA
13	b	807	CLA	C2A-CAA-CBA-CGA
13	b	814	CLA	C2A-CAA-CBA-CGA
13	b	836	CLA	C2A-CAA-CBA-CGA
13	1	841	CLA	C2A-CAA-CBA-CGA
13	1	852	CLA	C2A-CAA-CBA-CGA
13	2	813	CLA	C2A-CAA-CBA-CGA
13	2	835	CLA	C2A-CAA-CBA-CGA
13	0	203	CLA	C2A-CAA-CBA-CGA
16	B	840	BCR	C18-C19-C20-C21
16	B	845	BCR	C18-C19-C20-C21
16	b	840	BCR	C18-C19-C20-C21
16	b	845	BCR	C18-C19-C20-C21
16	2	839	BCR	C18-C19-C20-C21
16	2	844	BCR	C18-C19-C20-C21
13	B	810	CLA	C15-C16-C17-C18
13	B	823	CLA	C5-C6-C7-C8
13	B	834	CLA	C5-C6-C7-C8
13	b	810	CLA	C15-C16-C17-C18
13	b	823	CLA	C5-C6-C7-C8
13	b	834	CLA	C5-C6-C7-C8
13	2	809	CLA	C15-C16-C17-C18
13	2	822	CLA	C5-C6-C7-C8
13	2	833	CLA	C5-C6-C7-C8
13	A	830	CLA	O1A-CGA-O2A-C1
13	a	830	CLA	O1A-CGA-O2A-C1
13	A	802	CLA	C3-C5-C6-C7
13	B	831	CLA	C3-C5-C6-C7
13	a	802	CLA	C3-C5-C6-C7
13	b	831	CLA	C3-C5-C6-C7
13	1	802	CLA	C3-C5-C6-C7
13	2	830	CLA	C3-C5-C6-C7
13	A	825	CLA	C10-C11-C12-C13
13	A	841	CLA	C5-C6-C7-C8
13	B	802	CLA	C15-C16-C17-C18
13	B	804	CLA	C10-C11-C12-C13
13	B	806	CLA	C5-C6-C7-C8
13	I	101	CLA	C10-C11-C12-C13
13	a	825	CLA	C10-C11-C12-C13
13	a	841	CLA	C5-C6-C7-C8
13	b	802	CLA	C15-C16-C17-C18
13	b	804	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
13	b	806	CLA	C5-C6-C7-C8
13	i	102	CLA	C10-C11-C12-C13
13	1	825	CLA	C10-C11-C12-C13
13	1	841	CLA	C5-C6-C7-C8
13	2	802	CLA	C15-C16-C17-C18
13	2	804	CLA	C10-C11-C12-C13
13	2	806	CLA	C5-C6-C7-C8
13	7	102	CLA	C10-C11-C12-C13
17	A	850	LHG	O2-C2-C3-O3
17	a	850	LHG	O2-C2-C3-O3
17	1	850	LHG	O2-C2-C3-O3
13	B	828	CLA	O1A-CGA-O2A-C1
13	b	828	CLA	O1A-CGA-O2A-C1
13	2	827	CLA	O1A-CGA-O2A-C1
13	A	842	CLA	O1D-CGD-O2D-CED
13	a	842	CLA	O1D-CGD-O2D-CED
13	1	842	CLA	O1D-CGD-O2D-CED
13	A	803	CLA	C10-C11-C12-C13
13	A	828	CLA	C13-C15-C16-C17
13	B	808	CLA	C8-C10-C11-C12
13	a	803	CLA	C10-C11-C12-C13
13	a	828	CLA	C13-C15-C16-C17
13	b	808	CLA	C8-C10-C11-C12
13	1	803	CLA	C10-C11-C12-C13
13	1	828	CLA	C13-C15-C16-C17
13	2	807	CLA	C8-C10-C11-C12
13	J	1101	CLA	CBD-CGD-O2D-CED
13	j	1101	CLA	CBD-CGD-O2D-CED
13	8	1101	CLA	CBD-CGD-O2D-CED
13	0	202	CLA	CBD-CGD-O2D-CED
14	B	839	PQN	C12-C13-C15-C16
14	b	839	PQN	C12-C13-C15-C16
14	2	838	PQN	C12-C13-C15-C16
13	A	835	CLA	O1D-CGD-O2D-CED
13	a	835	CLA	O1D-CGD-O2D-CED
13	1	835	CLA	O1D-CGD-O2D-CED
13	A	806	CLA	C10-C11-C12-C13
13	a	806	CLA	C10-C11-C12-C13
13	1	806	CLA	C10-C11-C12-C13
13	A	833	CLA	CBA-CGA-O2A-C1
13	A	841	CLA	CBA-CGA-O2A-C1
13	B	808	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	B	833	CLA	CBA-CGA-O2A-C1
13	a	827	CLA	CBA-CGA-O2A-C1
13	a	833	CLA	CBA-CGA-O2A-C1
13	a	841	CLA	CBA-CGA-O2A-C1
13	b	808	CLA	CBA-CGA-O2A-C1
13	b	833	CLA	CBA-CGA-O2A-C1
13	1	833	CLA	CBA-CGA-O2A-C1
13	2	807	CLA	CBA-CGA-O2A-C1
13	2	832	CLA	CBA-CGA-O2A-C1
17	A	850	LHG	C24-C23-O8-C6
17	a	850	LHG	C24-C23-O8-C6
17	1	850	LHG	C24-C23-O8-C6
13	L	201	CLA	CBD-CGD-O2D-CED
13	l	202	CLA	CBD-CGD-O2D-CED
18	B	846	LMG	C11-C10-O7-C8
18	b	846	LMG	C11-C10-O7-C8
18	2	845	LMG	C11-C10-O7-C8
19	I	103	SQD	C8-C7-O47-C45
19	i	101	SQD	C8-C7-O47-C45
19	7	101	SQD	C8-C7-O47-C45
13	A	809	CLA	O1D-CGD-O2D-CED
13	1	809	CLA	O1D-CGD-O2D-CED
13	B	826	CLA	C2A-CAA-CBA-CGA
13	b	826	CLA	C2A-CAA-CBA-CGA
13	2	825	CLA	C2A-CAA-CBA-CGA
13	a	809	CLA	O1D-CGD-O2D-CED
13	A	827	CLA	CBA-CGA-O2A-C1
13	B	804	CLA	CBA-CGA-O2A-C1
13	b	804	CLA	CBA-CGA-O2A-C1
13	1	827	CLA	CBA-CGA-O2A-C1
13	1	841	CLA	CBA-CGA-O2A-C1
13	2	804	CLA	CBA-CGA-O2A-C1
16	A	848	BCR	C14-C15-C16-C17
16	a	848	BCR	C14-C15-C16-C17
16	1	848	BCR	C14-C15-C16-C17
13	A	821	CLA	C8-C10-C11-C12
13	A	825	CLA	C8-C10-C11-C12
13	B	821	CLA	C8-C10-C11-C12
13	B	821	CLA	C13-C15-C16-C17
13	a	821	CLA	C8-C10-C11-C12
13	a	825	CLA	C8-C10-C11-C12
13	b	821	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
13	b	821	CLA	C13-C15-C16-C17
13	1	821	CLA	C8-C10-C11-C12
13	1	825	CLA	C8-C10-C11-C12
13	2	820	CLA	C8-C10-C11-C12
13	2	820	CLA	C13-C15-C16-C17
13	A	830	CLA	C8-C10-C11-C12
13	A	852	CLA	C5-C6-C7-C8
13	a	830	CLA	C8-C10-C11-C12
13	a	852	CLA	C5-C6-C7-C8
13	1	830	CLA	C8-C10-C11-C12
13	1	852	CLA	C5-C6-C7-C8
14	B	839	PQN	C18-C20-C21-C22
14	b	839	PQN	C18-C20-C21-C22
14	2	838	PQN	C18-C20-C21-C22
13	A	840	CLA	C15-C16-C17-C18
13	a	840	CLA	C15-C16-C17-C18
13	1	840	CLA	C15-C16-C17-C18
14	A	843	PQN	C15-C16-C17-C18
14	a	843	PQN	C15-C16-C17-C18
14	1	843	PQN	C15-C16-C17-C18
17	A	849	LHG	C7-C8-C9-C10
17	a	849	LHG	C7-C8-C9-C10
17	1	849	LHG	C7-C8-C9-C10
14	B	839	PQN	C14-C13-C15-C16
14	b	839	PQN	C14-C13-C15-C16
14	2	838	PQN	C14-C13-C15-C16
13	B	826	CLA	O1D-CGD-O2D-CED
13	A	816	CLA	O1A-CGA-O2A-C1
13	a	816	CLA	O1A-CGA-O2A-C1
13	1	816	CLA	O1A-CGA-O2A-C1
13	A	824	CLA	C8-C10-C11-C12
13	a	824	CLA	C8-C10-C11-C12
13	1	824	CLA	C8-C10-C11-C12
13	A	827	CLA	C3-C5-C6-C7
13	a	827	CLA	C3-C5-C6-C7
13	1	827	CLA	C3-C5-C6-C7
13	b	826	CLA	O1D-CGD-O2D-CED
13	2	825	CLA	O1D-CGD-O2D-CED
13	A	833	CLA	C5-C6-C7-C8
13	a	833	CLA	C5-C6-C7-C8
13	1	833	CLA	C5-C6-C7-C8
13	B	810	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
13	b	810	CLA	C16-C17-C18-C19
13	2	809	CLA	C16-C17-C18-C19
16	A	848	BCR	C35-C13-C14-C15
16	A	848	BCR	C16-C17-C18-C36
16	A	851	BCR	C20-C21-C22-C37
16	B	842	BCR	C16-C17-C18-C36
16	B	845	BCR	C20-C21-C22-C37
16	F	202	BCR	C16-C17-C18-C36
16	F	205	BCR	C35-C13-C14-C15
16	F	205	BCR	C20-C21-C22-C37
16	I	102	BCR	C20-C21-C22-C37
16	J	1104	BCR	C16-C17-C18-C36
16	a	848	BCR	C35-C13-C14-C15
16	a	848	BCR	C16-C17-C18-C36
16	a	851	BCR	C20-C21-C22-C37
16	b	842	BCR	C16-C17-C18-C36
16	b	845	BCR	C20-C21-C22-C37
16	f	202	BCR	C16-C17-C18-C36
16	f	205	BCR	C35-C13-C14-C15
16	f	205	BCR	C20-C21-C22-C37
16	i	103	BCR	C20-C21-C22-C37
16	j	1104	BCR	C16-C17-C18-C36
16	1	848	BCR	C35-C13-C14-C15
16	1	848	BCR	C16-C17-C18-C36
16	1	851	BCR	C20-C21-C22-C37
16	2	841	BCR	C16-C17-C18-C36
16	2	844	BCR	C20-C21-C22-C37
16	6	202	BCR	C16-C17-C18-C36
16	6	205	BCR	C35-C13-C14-C15
16	6	205	BCR	C20-C21-C22-C37
16	7	103	BCR	C20-C21-C22-C37
16	8	1104	BCR	C16-C17-C18-C36
16	A	848	BCR	C7-C8-C9-C34
16	A	851	BCR	C11-C12-C13-C35
16	B	848	BCR	C7-C8-C9-C34
16	a	848	BCR	C7-C8-C9-C34
16	a	851	BCR	C11-C12-C13-C35
16	b	848	BCR	C7-C8-C9-C34
16	1	848	BCR	C7-C8-C9-C34
16	1	851	BCR	C11-C12-C13-C35
16	2	847	BCR	C7-C8-C9-C34
16	B	842	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
16	B	843	BCR	C7-C8-C9-C10
16	L	205	BCR	C21-C22-C23-C24
16	L	207	BCR	C7-C8-C9-C10
16	b	842	BCR	C21-C22-C23-C24
16	b	843	BCR	C7-C8-C9-C10
16	l	201	BCR	C7-C8-C9-C10
16	l	206	BCR	C21-C22-C23-C24
16	2	841	BCR	C21-C22-C23-C24
16	2	842	BCR	C7-C8-C9-C10
16	0	201	BCR	C7-C8-C9-C10
16	0	207	BCR	C21-C22-C23-C24
13	A	825	CLA	O1A-CGA-O2A-C1
13	B	808	CLA	O1A-CGA-O2A-C1
13	a	825	CLA	O1A-CGA-O2A-C1
13	b	808	CLA	O1A-CGA-O2A-C1
13	1	825	CLA	O1A-CGA-O2A-C1
13	2	807	CLA	O1A-CGA-O2A-C1
13	A	803	CLA	C2A-CAA-CBA-CGA
13	A	811	CLA	C2A-CAA-CBA-CGA
13	A	812	CLA	C2A-CAA-CBA-CGA
13	A	813	CLA	C2A-CAA-CBA-CGA
13	A	818	CLA	C2A-CAA-CBA-CGA
13	B	809	CLA	C2A-CAA-CBA-CGA
13	B	815	CLA	C2A-CAA-CBA-CGA
13	B	824	CLA	C2A-CAA-CBA-CGA
13	a	803	CLA	C2A-CAA-CBA-CGA
13	a	811	CLA	C2A-CAA-CBA-CGA
13	a	812	CLA	C2A-CAA-CBA-CGA
13	a	813	CLA	C2A-CAA-CBA-CGA
13	a	818	CLA	C2A-CAA-CBA-CGA
13	b	809	CLA	C2A-CAA-CBA-CGA
13	b	815	CLA	C2A-CAA-CBA-CGA
13	b	824	CLA	C2A-CAA-CBA-CGA
13	1	803	CLA	C2A-CAA-CBA-CGA
13	1	811	CLA	C2A-CAA-CBA-CGA
13	1	812	CLA	C2A-CAA-CBA-CGA
13	1	813	CLA	C2A-CAA-CBA-CGA
13	1	818	CLA	C2A-CAA-CBA-CGA
13	2	808	CLA	C2A-CAA-CBA-CGA
13	2	814	CLA	C2A-CAA-CBA-CGA
13	2	823	CLA	C2A-CAA-CBA-CGA
13	K	4003	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	k	4003	CLA	CBA-CGA-O2A-C1
13	9	4003	CLA	CBA-CGA-O2A-C1
13	A	824	CLA	C11-C12-C13-C14
13	A	839	CLA	C16-C17-C18-C19
13	B	821	CLA	C16-C17-C18-C19
13	B	823	CLA	C16-C17-C18-C20
13	a	824	CLA	C11-C12-C13-C14
13	a	839	CLA	C16-C17-C18-C19
13	b	821	CLA	C16-C17-C18-C19
13	b	823	CLA	C16-C17-C18-C20
13	1	824	CLA	C11-C12-C13-C14
13	1	839	CLA	C16-C17-C18-C19
13	2	820	CLA	C16-C17-C18-C19
13	2	822	CLA	C16-C17-C18-C20
13	A	833	CLA	O1A-CGA-O2A-C1
13	B	805	CLA	O1A-CGA-O2A-C1
13	B	833	CLA	O1A-CGA-O2A-C1
13	a	833	CLA	O1A-CGA-O2A-C1
13	b	805	CLA	O1A-CGA-O2A-C1
13	b	833	CLA	O1A-CGA-O2A-C1
13	1	833	CLA	O1A-CGA-O2A-C1
13	2	805	CLA	O1A-CGA-O2A-C1
13	2	832	CLA	O1A-CGA-O2A-C1
16	A	848	BCR	C11-C10-C9-C8
16	A	851	BCR	C16-C17-C18-C19
16	B	841	BCR	C20-C21-C22-C23
16	I	102	BCR	C11-C10-C9-C8
16	J	1104	BCR	C16-C17-C18-C19
16	L	202	BCR	C11-C10-C9-C8
16	M	101	BCR	C11-C10-C9-C8
16	a	848	BCR	C11-C10-C9-C8
16	a	851	BCR	C16-C17-C18-C19
16	b	841	BCR	C20-C21-C22-C23
16	i	103	BCR	C11-C10-C9-C8
16	j	1104	BCR	C16-C17-C18-C19
16	l	203	BCR	C11-C10-C9-C8
16	m	101	BCR	C11-C10-C9-C8
16	1	848	BCR	C11-C10-C9-C8
16	1	851	BCR	C16-C17-C18-C19
16	2	840	BCR	C20-C21-C22-C23
16	7	103	BCR	C11-C10-C9-C8
16	8	1104	BCR	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
16	0	204	BCR	C11-C10-C9-C8
16	z	101	BCR	C11-C10-C9-C8
13	A	822	CLA	O1D-CGD-O2D-CED
13	a	822	CLA	O1D-CGD-O2D-CED
13	1	822	CLA	O1D-CGD-O2D-CED
13	B	829	CLA	CBA-CGA-O2A-C1
13	b	829	CLA	CBA-CGA-O2A-C1
13	2	828	CLA	CBA-CGA-O2A-C1
13	A	803	CLA	C13-C15-C16-C17
13	B	808	CLA	C10-C11-C12-C13
13	a	803	CLA	C13-C15-C16-C17
13	b	808	CLA	C10-C11-C12-C13
13	1	803	CLA	C13-C15-C16-C17
13	2	807	CLA	C10-C11-C12-C13
14	B	839	PQN	C20-C21-C22-C23
14	b	839	PQN	C20-C21-C22-C23
14	2	838	PQN	C20-C21-C22-C23
13	A	803	CLA	C3-C5-C6-C7
13	a	803	CLA	C3-C5-C6-C7
13	1	803	CLA	C3-C5-C6-C7
13	A	835	CLA	C2-C1-O2A-CGA
13	B	826	CLA	C2-C1-O2A-CGA
13	B	828	CLA	C2-C1-O2A-CGA
13	a	835	CLA	C2-C1-O2A-CGA
13	b	826	CLA	C2-C1-O2A-CGA
13	b	828	CLA	C2-C1-O2A-CGA
13	1	835	CLA	C2-C1-O2A-CGA
13	2	825	CLA	C2-C1-O2A-CGA
13	2	827	CLA	C2-C1-O2A-CGA
12	A	801	CL0	C16-C17-C18-C20
12	a	801	CL0	C16-C17-C18-C20
12	1	801	CL0	C16-C17-C18-C20
13	A	819	CLA	C11-C12-C13-C15
13	A	828	CLA	C16-C17-C18-C19
13	A	839	CLA	C16-C17-C18-C20
13	B	821	CLA	C16-C17-C18-C20
13	B	823	CLA	C16-C17-C18-C19
13	B	826	CLA	C11-C12-C13-C14
13	B	836	CLA	C16-C17-C18-C19
13	a	819	CLA	C11-C12-C13-C15
13	a	828	CLA	C16-C17-C18-C19
13	a	839	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
13	b	821	CLA	C16-C17-C18-C20
13	b	823	CLA	C16-C17-C18-C19
13	b	826	CLA	C11-C12-C13-C14
13	b	836	CLA	C16-C17-C18-C19
13	1	819	CLA	C11-C12-C13-C15
13	1	828	CLA	C16-C17-C18-C19
13	1	839	CLA	C16-C17-C18-C20
13	2	820	CLA	C16-C17-C18-C20
13	2	822	CLA	C16-C17-C18-C19
13	2	825	CLA	C11-C12-C13-C14
13	2	835	CLA	C16-C17-C18-C19
13	A	827	CLA	O1A-CGA-O2A-C1
13	A	841	CLA	O1A-CGA-O2A-C1
13	a	827	CLA	O1A-CGA-O2A-C1
13	a	841	CLA	O1A-CGA-O2A-C1
13	1	827	CLA	O1A-CGA-O2A-C1
13	1	841	CLA	O1A-CGA-O2A-C1
13	B	847	CLA	O1D-CGD-O2D-CED
13	2	846	CLA	O1D-CGD-O2D-CED
13	b	847	CLA	O1D-CGD-O2D-CED
17	A	850	LHG	C11-C12-C13-C14
17	a	850	LHG	C11-C12-C13-C14
17	1	850	LHG	C11-C12-C13-C14
13	B	816	CLA	C5-C6-C7-C8
13	b	816	CLA	C5-C6-C7-C8
13	2	815	CLA	C5-C6-C7-C8
13	A	806	CLA	C4B-C3B-CAB-CBB
13	A	812	CLA	C4B-C3B-CAB-CBB
13	A	814	CLA	C4B-C3B-CAB-CBB
13	A	831	CLA	C4B-C3B-CAB-CBB
13	A	852	CLA	C4B-C3B-CAB-CBB
13	B	805	CLA	C4B-C3B-CAB-CBB
13	B	806	CLA	C4B-C3B-CAB-CBB
13	B	820	CLA	C4B-C3B-CAB-CBB
13	B	828	CLA	C4B-C3B-CAB-CBB
13	B	830	CLA	C4B-C3B-CAB-CBB
13	B	831	CLA	C4B-C3B-CAB-CBB
13	I	101	CLA	C4B-C3B-CAB-CBB
13	L	206	CLA	C4B-C3B-CAB-CBB
13	a	806	CLA	C4B-C3B-CAB-CBB
13	a	812	CLA	C4B-C3B-CAB-CBB
13	a	814	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	a	831	CLA	C4B-C3B-CAB-CBB
13	a	852	CLA	C4B-C3B-CAB-CBB
13	b	805	CLA	C4B-C3B-CAB-CBB
13	b	806	CLA	C4B-C3B-CAB-CBB
13	b	820	CLA	C4B-C3B-CAB-CBB
13	b	828	CLA	C4B-C3B-CAB-CBB
13	b	830	CLA	C4B-C3B-CAB-CBB
13	b	831	CLA	C4B-C3B-CAB-CBB
13	i	102	CLA	C4B-C3B-CAB-CBB
13	l	207	CLA	C4B-C3B-CAB-CBB
13	1	806	CLA	C4B-C3B-CAB-CBB
13	1	812	CLA	C4B-C3B-CAB-CBB
13	1	814	CLA	C4B-C3B-CAB-CBB
13	1	831	CLA	C4B-C3B-CAB-CBB
13	1	852	CLA	C4B-C3B-CAB-CBB
13	2	805	CLA	C4B-C3B-CAB-CBB
13	2	806	CLA	C4B-C3B-CAB-CBB
13	2	819	CLA	C4B-C3B-CAB-CBB
13	2	827	CLA	C4B-C3B-CAB-CBB
13	2	829	CLA	C4B-C3B-CAB-CBB
13	2	830	CLA	C4B-C3B-CAB-CBB
13	7	102	CLA	C4B-C3B-CAB-CBB
13	0	208	CLA	C4B-C3B-CAB-CBB
13	A	828	CLA	C16-C17-C18-C20
13	B	804	CLA	C16-C17-C18-C19
13	a	828	CLA	C16-C17-C18-C20
13	b	804	CLA	C16-C17-C18-C19
13	1	828	CLA	C16-C17-C18-C20
13	2	804	CLA	C16-C17-C18-C19
13	2	804	CLA	C16-C17-C18-C20
13	A	823	CLA	C2A-CAA-CBA-CGA
13	L	203	CLA	C2A-CAA-CBA-CGA
13	L	206	CLA	C2A-CAA-CBA-CGA
13	a	823	CLA	C2A-CAA-CBA-CGA
13	l	204	CLA	C2A-CAA-CBA-CGA
13	l	207	CLA	C2A-CAA-CBA-CGA
13	1	823	CLA	C2A-CAA-CBA-CGA
13	0	205	CLA	C2A-CAA-CBA-CGA
13	0	208	CLA	C2A-CAA-CBA-CGA
13	a	839	CLA	C15-C16-C17-C18
13	1	830	CLA	C10-C11-C12-C13
13	B	815	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
13	b	815	CLA	C6-C7-C8-C10
13	2	814	CLA	C6-C7-C8-C10
13	A	827	CLA	C5-C6-C7-C8
13	A	830	CLA	C10-C11-C12-C13
13	A	839	CLA	C15-C16-C17-C18
13	a	827	CLA	C5-C6-C7-C8
13	a	830	CLA	C10-C11-C12-C13
13	1	827	CLA	C5-C6-C7-C8
13	1	839	CLA	C15-C16-C17-C18
13	b	804	CLA	O1A-CGA-O2A-C1
13	2	804	CLA	O1A-CGA-O2A-C1
13	A	805	CLA	C3A-C2A-CAA-CBA
13	A	806	CLA	C3A-C2A-CAA-CBA
13	A	809	CLA	C3A-C2A-CAA-CBA
13	A	815	CLA	C3A-C2A-CAA-CBA
13	A	816	CLA	C3A-C2A-CAA-CBA
13	A	827	CLA	C3A-C2A-CAA-CBA
13	A	835	CLA	C3A-C2A-CAA-CBA
13	A	836	CLA	C3A-C2A-CAA-CBA
13	A	838	CLA	C3A-C2A-CAA-CBA
13	A	840	CLA	C3A-C2A-CAA-CBA
13	A	842	CLA	C3A-C2A-CAA-CBA
13	B	810	CLA	C3A-C2A-CAA-CBA
13	B	813	CLA	C3A-C2A-CAA-CBA
13	B	821	CLA	C3A-C2A-CAA-CBA
13	J	1101	CLA	C3A-C2A-CAA-CBA
13	K	4002	CLA	C3A-C2A-CAA-CBA
13	L	201	CLA	C3A-C2A-CAA-CBA
13	L	206	CLA	C3A-C2A-CAA-CBA
13	a	805	CLA	C3A-C2A-CAA-CBA
13	a	806	CLA	C3A-C2A-CAA-CBA
13	a	809	CLA	C3A-C2A-CAA-CBA
13	a	815	CLA	C3A-C2A-CAA-CBA
13	a	816	CLA	C3A-C2A-CAA-CBA
13	a	827	CLA	C3A-C2A-CAA-CBA
13	a	835	CLA	C3A-C2A-CAA-CBA
13	a	836	CLA	C3A-C2A-CAA-CBA
13	a	838	CLA	C3A-C2A-CAA-CBA
13	a	840	CLA	C3A-C2A-CAA-CBA
13	a	842	CLA	C3A-C2A-CAA-CBA
13	b	810	CLA	C3A-C2A-CAA-CBA
13	b	813	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	b	821	CLA	C3A-C2A-CAA-CBA
13	j	1101	CLA	C3A-C2A-CAA-CBA
13	k	4002	CLA	C3A-C2A-CAA-CBA
13	l	202	CLA	C3A-C2A-CAA-CBA
13	l	207	CLA	C3A-C2A-CAA-CBA
13	1	805	CLA	C3A-C2A-CAA-CBA
13	1	806	CLA	C3A-C2A-CAA-CBA
13	1	809	CLA	C3A-C2A-CAA-CBA
13	1	815	CLA	C3A-C2A-CAA-CBA
13	1	816	CLA	C3A-C2A-CAA-CBA
13	1	827	CLA	C3A-C2A-CAA-CBA
13	1	835	CLA	C3A-C2A-CAA-CBA
13	1	836	CLA	C3A-C2A-CAA-CBA
13	1	838	CLA	C3A-C2A-CAA-CBA
13	1	840	CLA	C3A-C2A-CAA-CBA
13	1	842	CLA	C3A-C2A-CAA-CBA
13	2	809	CLA	C3A-C2A-CAA-CBA
13	2	812	CLA	C3A-C2A-CAA-CBA
13	2	820	CLA	C3A-C2A-CAA-CBA
13	8	1101	CLA	C3A-C2A-CAA-CBA
13	9	4002	CLA	C3A-C2A-CAA-CBA
13	0	202	CLA	C3A-C2A-CAA-CBA
13	0	208	CLA	C3A-C2A-CAA-CBA
13	B	825	CLA	O1D-CGD-O2D-CED
13	b	825	CLA	O1D-CGD-O2D-CED
13	2	824	CLA	O1D-CGD-O2D-CED
13	A	835	CLA	C5-C6-C7-C8
13	a	835	CLA	C5-C6-C7-C8
13	A	831	CLA	O1D-CGD-O2D-CED
13	a	831	CLA	O1D-CGD-O2D-CED
13	1	831	CLA	O1D-CGD-O2D-CED
13	B	804	CLA	C16-C17-C18-C20
13	B	826	CLA	C11-C12-C13-C15
13	b	804	CLA	C16-C17-C18-C20
13	b	826	CLA	C11-C12-C13-C15
13	2	825	CLA	C11-C12-C13-C15
13	B	804	CLA	O1A-CGA-O2A-C1
13	A	837	CLA	C5-C6-C7-C8
13	a	837	CLA	C5-C6-C7-C8
13	1	835	CLA	C5-C6-C7-C8
13	1	837	CLA	C5-C6-C7-C8
13	J	1102	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	j	1102	CLA	CBD-CGD-O2D-CED
13	8	1102	CLA	CBD-CGD-O2D-CED
19	I	103	SQD	C7-C8-C9-C10
19	i	101	SQD	C7-C8-C9-C10
19	7	101	SQD	C7-C8-C9-C10
17	A	850	LHG	C25-C26-C27-C28
17	a	850	LHG	C25-C26-C27-C28
17	1	850	LHG	C25-C26-C27-C28
13	1	840	CLA	O1D-CGD-O2D-CED
13	L	201	CLA	C5-C6-C7-C8
13	l	202	CLA	C5-C6-C7-C8
13	0	202	CLA	C5-C6-C7-C8
13	A	840	CLA	O1D-CGD-O2D-CED
13	B	801	CLA	O1D-CGD-O2D-CED
13	B	828	CLA	O1D-CGD-O2D-CED
13	a	840	CLA	O1D-CGD-O2D-CED
13	b	828	CLA	O1D-CGD-O2D-CED
13	2	801	CLA	O1D-CGD-O2D-CED
13	2	827	CLA	O1D-CGD-O2D-CED
13	A	817	CLA	C6-C7-C8-C9
13	a	817	CLA	C6-C7-C8-C9
13	1	817	CLA	C6-C7-C8-C9
13	B	829	CLA	O1A-CGA-O2A-C1
13	b	829	CLA	O1A-CGA-O2A-C1
13	2	828	CLA	O1A-CGA-O2A-C1
13	F	201	CLA	C2B-C3B-CAB-CBB
13	f	201	CLA	C2B-C3B-CAB-CBB
13	6	201	CLA	C2B-C3B-CAB-CBB
16	A	847	BCR	C23-C24-C25-C30
16	A	851	BCR	C23-C24-C25-C26
16	A	851	BCR	C23-C24-C25-C30
16	B	843	BCR	C23-C24-C25-C30
16	B	844	BCR	C23-C24-C25-C26
16	B	844	BCR	C23-C24-C25-C30
16	B	848	BCR	C1-C6-C7-C8
16	B	848	BCR	C5-C6-C7-C8
16	J	1105	BCR	C23-C24-C25-C30
16	L	205	BCR	C23-C24-C25-C30
16	a	847	BCR	C23-C24-C25-C30
16	a	851	BCR	C23-C24-C25-C26
16	a	851	BCR	C23-C24-C25-C30
16	b	843	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
16	b	844	BCR	C23-C24-C25-C26
16	b	844	BCR	C23-C24-C25-C30
16	b	848	BCR	C1-C6-C7-C8
16	b	848	BCR	C5-C6-C7-C8
16	j	1105	BCR	C23-C24-C25-C30
16	l	206	BCR	C23-C24-C25-C26
16	l	206	BCR	C23-C24-C25-C30
16	1	847	BCR	C23-C24-C25-C30
16	1	851	BCR	C23-C24-C25-C26
16	1	851	BCR	C23-C24-C25-C30
16	2	842	BCR	C23-C24-C25-C30
16	2	843	BCR	C23-C24-C25-C26
16	2	843	BCR	C23-C24-C25-C30
16	2	847	BCR	C1-C6-C7-C8
16	2	847	BCR	C5-C6-C7-C8
16	8	1105	BCR	C23-C24-C25-C30
16	0	207	BCR	C23-C24-C25-C30
13	b	801	CLA	O1D-CGD-O2D-CED
13	A	817	CLA	C2A-CAA-CBA-CGA
13	a	817	CLA	C2A-CAA-CBA-CGA
13	1	817	CLA	C2A-CAA-CBA-CGA
19	I	103	SQD	C9-C10-C11-C12
19	i	101	SQD	C9-C10-C11-C12
19	7	101	SQD	C9-C10-C11-C12
16	F	202	BCR	C18-C19-C20-C21
16	L	207	BCR	C18-C19-C20-C21
16	f	202	BCR	C18-C19-C20-C21
16	l	201	BCR	C18-C19-C20-C21
16	6	202	BCR	C18-C19-C20-C21
16	0	201	BCR	C18-C19-C20-C21
13	F	204	CLA	O1A-CGA-O2A-C1
13	f	204	CLA	O1A-CGA-O2A-C1
13	6	204	CLA	O1A-CGA-O2A-C1
18	B	846	LMG	C31-C32-C33-C34
18	b	846	LMG	C31-C32-C33-C34
18	2	845	LMG	C31-C32-C33-C34
16	A	847	BCR	C9-C10-C11-C12
16	a	847	BCR	C9-C10-C11-C12
16	1	847	BCR	C9-C10-C11-C12
13	A	819	CLA	C11-C12-C13-C14
13	B	836	CLA	C16-C17-C18-C20
13	b	836	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
13	2	835	CLA	C16-C17-C18-C20
16	B	842	BCR	C37-C22-C23-C24
16	b	842	BCR	C37-C22-C23-C24
16	2	841	BCR	C37-C22-C23-C24
13	A	809	CLA	C2A-CAA-CBA-CGA
13	a	809	CLA	C2A-CAA-CBA-CGA
13	1	809	CLA	C2A-CAA-CBA-CGA
13	A	835	CLA	C11-C10-C8-C9
13	a	835	CLA	C11-C10-C8-C9
13	1	835	CLA	C11-C10-C8-C9
13	A	817	CLA	C6-C7-C8-C10
13	a	817	CLA	C6-C7-C8-C10
13	a	819	CLA	C11-C12-C13-C14
13	1	817	CLA	C6-C7-C8-C10
13	1	819	CLA	C11-C12-C13-C14
14	A	843	PQN	C18-C20-C21-C22
14	a	843	PQN	C18-C20-C21-C22
14	1	843	PQN	C18-C20-C21-C22
13	A	837	CLA	C10-C11-C12-C13
13	a	837	CLA	C10-C11-C12-C13
13	1	837	CLA	C10-C11-C12-C13
13	A	806	CLA	O1D-CGD-O2D-CED
13	a	806	CLA	O1D-CGD-O2D-CED
13	1	806	CLA	O1D-CGD-O2D-CED
13	B	810	CLA	C16-C17-C18-C20
13	b	810	CLA	C16-C17-C18-C20
13	2	809	CLA	C16-C17-C18-C20
13	B	834	CLA	C10-C11-C12-C13
13	B	813	CLA	C4-C3-C5-C6
13	b	813	CLA	C4-C3-C5-C6
13	2	812	CLA	C4-C3-C5-C6
12	A	801	CL0	C2-C3-C5-C6
12	a	801	CL0	C2-C3-C5-C6
12	1	801	CL0	C2-C3-C5-C6
19	I	103	SQD	O49-C7-O47-C45
19	i	101	SQD	O49-C7-O47-C45
19	7	101	SQD	O49-C7-O47-C45
13	b	834	CLA	C10-C11-C12-C13
13	2	833	CLA	C10-C11-C12-C13
13	A	802	CLA	C2A-CAA-CBA-CGA
13	A	835	CLA	C2A-CAA-CBA-CGA
13	B	802	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
13	I	101	CLA	C2A-CAA-CBA-CGA
13	a	802	CLA	C2A-CAA-CBA-CGA
13	a	835	CLA	C2A-CAA-CBA-CGA
13	b	802	CLA	C2A-CAA-CBA-CGA
13	i	102	CLA	C2A-CAA-CBA-CGA
13	1	802	CLA	C2A-CAA-CBA-CGA
13	2	802	CLA	C2A-CAA-CBA-CGA
13	7	102	CLA	C2A-CAA-CBA-CGA
13	B	832	CLA	O1D-CGD-O2D-CED
13	b	832	CLA	O1D-CGD-O2D-CED
13	2	831	CLA	O1D-CGD-O2D-CED
13	A	805	CLA	C1A-C2A-CAA-CBA
13	A	815	CLA	C1A-C2A-CAA-CBA
13	A	816	CLA	C1A-C2A-CAA-CBA
13	A	818	CLA	C1A-C2A-CAA-CBA
13	A	820	CLA	C1A-C2A-CAA-CBA
13	A	821	CLA	C1A-C2A-CAA-CBA
13	A	827	CLA	C1A-C2A-CAA-CBA
13	A	830	CLA	C1A-C2A-CAA-CBA
13	A	833	CLA	C1A-C2A-CAA-CBA
13	A	835	CLA	C1A-C2A-CAA-CBA
13	B	804	CLA	C1A-C2A-CAA-CBA
13	B	809	CLA	C1A-C2A-CAA-CBA
13	B	811	CLA	C1A-C2A-CAA-CBA
13	B	814	CLA	C1A-C2A-CAA-CBA
13	B	821	CLA	C1A-C2A-CAA-CBA
13	B	825	CLA	C1A-C2A-CAA-CBA
13	B	826	CLA	C1A-C2A-CAA-CBA
13	B	829	CLA	C1A-C2A-CAA-CBA
13	B	833	CLA	C1A-C2A-CAA-CBA
13	B	835	CLA	C1A-C2A-CAA-CBA
13	B	837	CLA	C1A-C2A-CAA-CBA
13	I	101	CLA	C1A-C2A-CAA-CBA
13	J	1101	CLA	C1A-C2A-CAA-CBA
13	K	4002	CLA	C1A-C2A-CAA-CBA
13	L	203	CLA	C1A-C2A-CAA-CBA
13	a	805	CLA	C1A-C2A-CAA-CBA
13	a	815	CLA	C1A-C2A-CAA-CBA
13	a	816	CLA	C1A-C2A-CAA-CBA
13	a	818	CLA	C1A-C2A-CAA-CBA
13	a	820	CLA	C1A-C2A-CAA-CBA
13	a	821	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	a	827	CLA	C1A-C2A-CAA-CBA
13	a	830	CLA	C1A-C2A-CAA-CBA
13	a	833	CLA	C1A-C2A-CAA-CBA
13	a	835	CLA	C1A-C2A-CAA-CBA
13	b	804	CLA	C1A-C2A-CAA-CBA
13	b	809	CLA	C1A-C2A-CAA-CBA
13	b	811	CLA	C1A-C2A-CAA-CBA
13	b	814	CLA	C1A-C2A-CAA-CBA
13	b	821	CLA	C1A-C2A-CAA-CBA
13	b	825	CLA	C1A-C2A-CAA-CBA
13	b	826	CLA	C1A-C2A-CAA-CBA
13	b	829	CLA	C1A-C2A-CAA-CBA
13	b	833	CLA	C1A-C2A-CAA-CBA
13	b	835	CLA	C1A-C2A-CAA-CBA
13	b	837	CLA	C1A-C2A-CAA-CBA
13	i	102	CLA	C1A-C2A-CAA-CBA
13	j	1101	CLA	C1A-C2A-CAA-CBA
13	k	4002	CLA	C1A-C2A-CAA-CBA
13	l	204	CLA	C1A-C2A-CAA-CBA
13	1	805	CLA	C1A-C2A-CAA-CBA
13	1	815	CLA	C1A-C2A-CAA-CBA
13	1	816	CLA	C1A-C2A-CAA-CBA
13	1	818	CLA	C1A-C2A-CAA-CBA
13	1	820	CLA	C1A-C2A-CAA-CBA
13	1	821	CLA	C1A-C2A-CAA-CBA
13	1	827	CLA	C1A-C2A-CAA-CBA
13	1	830	CLA	C1A-C2A-CAA-CBA
13	1	833	CLA	C1A-C2A-CAA-CBA
13	1	835	CLA	C1A-C2A-CAA-CBA
13	2	804	CLA	C1A-C2A-CAA-CBA
13	2	808	CLA	C1A-C2A-CAA-CBA
13	2	810	CLA	C1A-C2A-CAA-CBA
13	2	813	CLA	C1A-C2A-CAA-CBA
13	2	820	CLA	C1A-C2A-CAA-CBA
13	2	824	CLA	C1A-C2A-CAA-CBA
13	2	825	CLA	C1A-C2A-CAA-CBA
13	2	828	CLA	C1A-C2A-CAA-CBA
13	2	832	CLA	C1A-C2A-CAA-CBA
13	2	834	CLA	C1A-C2A-CAA-CBA
13	2	836	CLA	C1A-C2A-CAA-CBA
13	7	102	CLA	C1A-C2A-CAA-CBA
13	8	1101	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	9	4002	CLA	C1A-C2A-CAA-CBA
13	0	205	CLA	C1A-C2A-CAA-CBA
12	A	801	CL0	C11-C10-C8-C7
12	a	801	CL0	C11-C10-C8-C7
12	1	801	CL0	C11-C10-C8-C7
13	A	829	CLA	C11-C10-C8-C7
13	A	830	CLA	C6-C7-C8-C10
13	A	834	CLA	C6-C7-C8-C10
13	A	834	CLA	C11-C10-C8-C7
13	B	830	CLA	C6-C7-C8-C10
13	B	838	CLA	C11-C12-C13-C15
13	a	829	CLA	C11-C10-C8-C7
13	a	830	CLA	C6-C7-C8-C10
13	a	834	CLA	C6-C7-C8-C10
13	a	834	CLA	C11-C10-C8-C7
13	b	830	CLA	C6-C7-C8-C10
13	b	838	CLA	C11-C12-C13-C15
13	1	829	CLA	C11-C10-C8-C7
13	1	830	CLA	C6-C7-C8-C10
13	1	834	CLA	C6-C7-C8-C10
13	1	834	CLA	C11-C10-C8-C7
13	2	829	CLA	C6-C7-C8-C10
13	2	837	CLA	C11-C12-C13-C15
13	a	824	CLA	C11-C12-C13-C15
19	I	103	SQD	C16-C17-C18-C19
19	i	101	SQD	C16-C17-C18-C19
19	7	101	SQD	C16-C17-C18-C19
13	1	835	CLA	C2A-CAA-CBA-CGA
13	A	819	CLA	C6-C7-C8-C9
13	A	829	CLA	C11-C10-C8-C9
13	A	830	CLA	C6-C7-C8-C9
13	B	815	CLA	C6-C7-C8-C9
13	B	815	CLA	C11-C10-C8-C9
13	B	825	CLA	C11-C12-C13-C14
13	B	831	CLA	C6-C7-C8-C9
13	B	838	CLA	C11-C12-C13-C14
13	a	819	CLA	C6-C7-C8-C9
13	a	829	CLA	C11-C10-C8-C9
13	a	830	CLA	C6-C7-C8-C9
13	b	815	CLA	C6-C7-C8-C9
13	b	815	CLA	C11-C10-C8-C9
13	b	825	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
13	b	831	CLA	C6-C7-C8-C9
13	b	838	CLA	C11-C12-C13-C14
13	1	819	CLA	C6-C7-C8-C9
13	1	829	CLA	C11-C10-C8-C9
13	1	830	CLA	C6-C7-C8-C9
13	2	814	CLA	C6-C7-C8-C9
13	2	814	CLA	C11-C10-C8-C9
13	2	824	CLA	C11-C12-C13-C14
13	2	830	CLA	C6-C7-C8-C9
13	2	837	CLA	C11-C12-C13-C14
14	B	839	PQN	C21-C22-C23-C24
14	b	839	PQN	C21-C22-C23-C24
14	2	838	PQN	C21-C22-C23-C24
13	A	824	CLA	C11-C12-C13-C15
13	1	824	CLA	C11-C12-C13-C15
13	B	806	CLA	C13-C15-C16-C17
13	b	806	CLA	C13-C15-C16-C17
13	2	806	CLA	C13-C15-C16-C17
19	I	103	SQD	C44-C45-C46-O48
19	i	101	SQD	C44-C45-C46-O48
19	7	101	SQD	C44-C45-C46-O48
13	2	802	CLA	C8-C10-C11-C12
13	B	813	CLA	O1D-CGD-O2D-CED
13	b	813	CLA	O1D-CGD-O2D-CED
13	2	812	CLA	O1D-CGD-O2D-CED
16	B	840	BCR	C11-C10-C9-C34
16	B	843	BCR	C16-C17-C18-C36
16	F	202	BCR	C20-C21-C22-C37
16	J	1105	BCR	C16-C17-C18-C36
16	b	840	BCR	C11-C10-C9-C34
16	b	843	BCR	C16-C17-C18-C36
16	f	202	BCR	C20-C21-C22-C37
16	j	1105	BCR	C16-C17-C18-C36
16	2	839	BCR	C11-C10-C9-C34
16	2	842	BCR	C16-C17-C18-C36
16	6	202	BCR	C20-C21-C22-C37
16	8	1105	BCR	C16-C17-C18-C36
13	B	802	CLA	C8-C10-C11-C12
13	b	802	CLA	C8-C10-C11-C12
12	A	801	CL0	C4-C3-C5-C6
12	a	801	CL0	C4-C3-C5-C6
12	1	801	CL0	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	B	813	CLA	C2-C3-C5-C6
13	b	813	CLA	C2-C3-C5-C6
13	2	812	CLA	C2-C3-C5-C6
13	B	811	CLA	CBA-CGA-O2A-C1
13	b	811	CLA	CBA-CGA-O2A-C1
13	2	810	CLA	CBA-CGA-O2A-C1
13	B	806	CLA	O1D-CGD-O2D-CED
13	b	806	CLA	O1D-CGD-O2D-CED
13	2	806	CLA	O1D-CGD-O2D-CED
13	B	810	CLA	CBA-CGA-O2A-C1
13	b	810	CLA	CBA-CGA-O2A-C1
13	2	809	CLA	CBA-CGA-O2A-C1
18	B	846	LMG	C9-C8-O7-C10
18	b	846	LMG	C9-C8-O7-C10
18	2	845	LMG	C9-C8-O7-C10
16	A	847	BCR	C10-C11-C12-C13
16	a	847	BCR	C10-C11-C12-C13
13	A	839	CLA	C13-C15-C16-C17
13	1	839	CLA	C13-C15-C16-C17
19	I	103	SQD	C11-C12-C13-C14
16	K	4004	BCR	C13-C14-C15-C16
16	k	4004	BCR	C13-C14-C15-C16
16	9	4004	BCR	C13-C14-C15-C16
19	i	101	SQD	C11-C12-C13-C14
19	7	101	SQD	C11-C12-C13-C14
13	a	839	CLA	C13-C15-C16-C17
17	1	850	LHG	C15-C16-C17-C18
17	A	850	LHG	C15-C16-C17-C18
17	a	850	LHG	C15-C16-C17-C18
19	I	103	SQD	C30-C31-C32-C33
17	A	849	LHG	C27-C28-C29-C30
17	a	849	LHG	C27-C28-C29-C30
19	i	101	SQD	C30-C31-C32-C33
19	7	101	SQD	C30-C31-C32-C33
17	1	849	LHG	C27-C28-C29-C30
13	A	822	CLA	C2A-CAA-CBA-CGA
13	1	822	CLA	C2A-CAA-CBA-CGA
17	A	850	LHG	C24-C25-C26-C27
17	a	850	LHG	C24-C25-C26-C27
17	1	850	LHG	C24-C25-C26-C27
13	l	202	CLA	O1D-CGD-O2D-CED
13	L	201	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	0	202	CLA	O1D-CGD-O2D-CED
13	A	805	CLA	C2C-C3C-CAC-CBC
13	K	4003	CLA	O1A-CGA-O2A-C1
13	k	4003	CLA	O1A-CGA-O2A-C1
13	9	4003	CLA	O1A-CGA-O2A-C1
12	A	801	CL0	C11-C10-C8-C9
12	a	801	CL0	C11-C10-C8-C9
12	1	801	CL0	C11-C10-C8-C9
13	A	803	CLA	C14-C13-C15-C16
13	A	834	CLA	C11-C10-C8-C9
13	A	839	CLA	C11-C12-C13-C14
13	B	805	CLA	C14-C13-C15-C16
13	B	808	CLA	C6-C7-C8-C9
13	B	821	CLA	C11-C12-C13-C14
13	B	829	CLA	C14-C13-C15-C16
13	B	830	CLA	C6-C7-C8-C9
13	B	837	CLA	C14-C13-C15-C16
13	a	803	CLA	C14-C13-C15-C16
13	a	834	CLA	C11-C10-C8-C9
13	a	839	CLA	C11-C12-C13-C14
13	b	805	CLA	C14-C13-C15-C16
13	b	808	CLA	C6-C7-C8-C9
13	b	821	CLA	C11-C12-C13-C14
13	b	829	CLA	C14-C13-C15-C16
13	b	830	CLA	C6-C7-C8-C9
13	b	837	CLA	C14-C13-C15-C16
13	1	803	CLA	C14-C13-C15-C16
13	1	834	CLA	C11-C10-C8-C9
13	1	839	CLA	C11-C12-C13-C14
13	2	805	CLA	C14-C13-C15-C16
13	2	807	CLA	C6-C7-C8-C9
13	2	820	CLA	C11-C12-C13-C14
13	2	828	CLA	C14-C13-C15-C16
13	2	829	CLA	C6-C7-C8-C9
13	2	836	CLA	C14-C13-C15-C16
12	A	801	CL0	C4B-C3B-CAB-CBB
12	a	801	CL0	C4B-C3B-CAB-CBB
12	1	801	CL0	C4B-C3B-CAB-CBB
13	A	809	CLA	C4B-C3B-CAB-CBB
13	A	823	CLA	C4B-C3B-CAB-CBB
13	A	832	CLA	C4B-C3B-CAB-CBB
13	A	842	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	B	809	CLA	C4B-C3B-CAB-CBB
13	B	810	CLA	C4B-C3B-CAB-CBB
13	B	813	CLA	C4B-C3B-CAB-CBB
13	F	201	CLA	C4B-C3B-CAB-CBB
13	a	809	CLA	C4B-C3B-CAB-CBB
13	a	823	CLA	C4B-C3B-CAB-CBB
13	a	832	CLA	C4B-C3B-CAB-CBB
13	a	842	CLA	C4B-C3B-CAB-CBB
13	b	809	CLA	C4B-C3B-CAB-CBB
13	b	810	CLA	C4B-C3B-CAB-CBB
13	b	813	CLA	C4B-C3B-CAB-CBB
13	f	201	CLA	C4B-C3B-CAB-CBB
13	1	809	CLA	C4B-C3B-CAB-CBB
13	1	823	CLA	C4B-C3B-CAB-CBB
13	1	832	CLA	C4B-C3B-CAB-CBB
13	1	842	CLA	C4B-C3B-CAB-CBB
13	2	808	CLA	C4B-C3B-CAB-CBB
13	2	809	CLA	C4B-C3B-CAB-CBB
13	2	812	CLA	C4B-C3B-CAB-CBB
13	6	201	CLA	C4B-C3B-CAB-CBB
13	a	805	CLA	C2C-C3C-CAC-CBC
13	B	821	CLA	C2A-CAA-CBA-CGA
13	a	822	CLA	C2A-CAA-CBA-CGA
13	b	821	CLA	C2A-CAA-CBA-CGA
13	2	820	CLA	C2A-CAA-CBA-CGA
17	A	850	LHG	C9-C10-C11-C12
17	a	850	LHG	C9-C10-C11-C12
17	1	850	LHG	C9-C10-C11-C12
17	A	849	LHG	O6-C4-C5-C6
17	A	850	LHG	O6-C4-C5-C6
17	a	849	LHG	O6-C4-C5-C6
17	a	850	LHG	O6-C4-C5-C6
17	1	849	LHG	O6-C4-C5-C6
17	1	850	LHG	O6-C4-C5-C6
13	1	805	CLA	C2C-C3C-CAC-CBC
13	A	803	CLA	C12-C13-C15-C16
13	A	819	CLA	C6-C7-C8-C10
13	A	829	CLA	C6-C7-C8-C10
13	A	832	CLA	C12-C13-C15-C16
13	A	839	CLA	C11-C12-C13-C15
13	B	805	CLA	C6-C7-C8-C10
13	B	805	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
13	B	808	CLA	C6-C7-C8-C10
13	B	808	CLA	C11-C12-C13-C15
13	B	815	CLA	C11-C10-C8-C7
13	B	821	CLA	C11-C12-C13-C15
13	B	825	CLA	C11-C12-C13-C15
13	B	829	CLA	C12-C13-C15-C16
13	B	831	CLA	C6-C7-C8-C10
13	B	837	CLA	C12-C13-C15-C16
13	a	803	CLA	C12-C13-C15-C16
13	a	819	CLA	C6-C7-C8-C10
13	a	829	CLA	C6-C7-C8-C10
13	a	832	CLA	C12-C13-C15-C16
13	a	839	CLA	C11-C12-C13-C15
13	b	805	CLA	C6-C7-C8-C10
13	b	805	CLA	C12-C13-C15-C16
13	b	808	CLA	C6-C7-C8-C10
13	b	808	CLA	C11-C12-C13-C15
13	b	815	CLA	C11-C10-C8-C7
13	b	821	CLA	C11-C12-C13-C15
13	b	825	CLA	C11-C12-C13-C15
13	b	829	CLA	C12-C13-C15-C16
13	b	831	CLA	C6-C7-C8-C10
13	b	837	CLA	C12-C13-C15-C16
13	1	803	CLA	C12-C13-C15-C16
13	1	819	CLA	C6-C7-C8-C10
13	1	829	CLA	C6-C7-C8-C10
13	1	832	CLA	C12-C13-C15-C16
13	1	839	CLA	C11-C12-C13-C15
13	2	805	CLA	C6-C7-C8-C10
13	2	805	CLA	C12-C13-C15-C16
13	2	807	CLA	C6-C7-C8-C10
13	2	807	CLA	C11-C12-C13-C15
13	2	814	CLA	C11-C10-C8-C7
13	2	820	CLA	C11-C12-C13-C15
13	2	824	CLA	C11-C12-C13-C15
13	2	828	CLA	C12-C13-C15-C16
13	2	830	CLA	C6-C7-C8-C10
13	2	836	CLA	C12-C13-C15-C16
14	B	839	PQN	C21-C22-C23-C25
14	b	839	PQN	C21-C22-C23-C25
14	2	838	PQN	C21-C22-C23-C25
14	A	843	PQN	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
14	a	843	PQN	C20-C21-C22-C23
14	1	843	PQN	C20-C21-C22-C23
13	A	813	CLA	C3A-C2A-CAA-CBA
13	A	821	CLA	C4-C3-C5-C6
13	B	806	CLA	C4-C3-C5-C6
13	a	813	CLA	C3A-C2A-CAA-CBA
13	a	821	CLA	C4-C3-C5-C6
13	b	806	CLA	C4-C3-C5-C6
13	1	813	CLA	C3A-C2A-CAA-CBA
13	1	821	CLA	C4-C3-C5-C6
13	2	806	CLA	C4-C3-C5-C6
13	B	823	CLA	C10-C11-C12-C13
13	b	823	CLA	C10-C11-C12-C13
17	a	850	LHG	C10-C11-C12-C13
13	A	825	CLA	CAA-CBA-CGA-O2A
13	a	825	CLA	CAA-CBA-CGA-O2A
13	1	825	CLA	CAA-CBA-CGA-O2A
13	A	821	CLA	C2-C3-C5-C6
13	a	821	CLA	C2-C3-C5-C6
17	A	850	LHG	C10-C11-C12-C13
17	1	850	LHG	C10-C11-C12-C13
18	B	846	LMG	C34-C35-C36-C37
18	b	846	LMG	C34-C35-C36-C37
18	2	845	LMG	C34-C35-C36-C37
13	2	822	CLA	C10-C11-C12-C13
19	I	103	SQD	C12-C13-C14-C15
19	i	101	SQD	C12-C13-C14-C15
19	7	101	SQD	C12-C13-C14-C15
13	j	1101	CLA	O1D-CGD-O2D-CED
13	A	837	CLA	CBA-CGA-O2A-C1
13	a	837	CLA	CBA-CGA-O2A-C1
13	1	837	CLA	CBA-CGA-O2A-C1
17	A	849	LHG	C4-C5-C6-O8
17	a	849	LHG	C4-C5-C6-O8
17	1	849	LHG	C4-C5-C6-O8
18	B	846	LMG	C7-C8-C9-O8
18	b	846	LMG	C7-C8-C9-O8
18	2	845	LMG	C7-C8-C9-O8
13	J	1101	CLA	O1D-CGD-O2D-CED
13	A	825	CLA	C4-C3-C5-C6
13	a	825	CLA	C4-C3-C5-C6
13	1	825	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	1	821	CLA	C2-C3-C5-C6
13	8	1101	CLA	O1D-CGD-O2D-CED
13	B	820	CLA	C6-C7-C8-C9
13	b	820	CLA	C6-C7-C8-C9
13	2	819	CLA	C6-C7-C8-C9
16	A	845	BCR	C1-C6-C7-C8
16	A	846	BCR	C23-C24-C25-C30
16	A	847	BCR	C1-C6-C7-C8
16	A	848	BCR	C23-C24-C25-C30
16	A	851	BCR	C1-C6-C7-C8
16	B	840	BCR	C1-C6-C7-C8
16	B	840	BCR	C23-C24-C25-C30
16	B	841	BCR	C1-C6-C7-C8
16	B	843	BCR	C1-C6-C7-C8
16	B	844	BCR	C1-C6-C7-C8
16	B	845	BCR	C1-C6-C7-C8
16	B	848	BCR	C23-C24-C25-C30
16	F	202	BCR	C1-C6-C7-C8
16	F	205	BCR	C1-C6-C7-C8
16	F	205	BCR	C5-C6-C7-C8
16	J	1104	BCR	C1-C6-C7-C8
16	J	1105	BCR	C1-C6-C7-C8
16	K	4001	BCR	C1-C6-C7-C8
16	K	4004	BCR	C23-C24-C25-C30
16	L	202	BCR	C23-C24-C25-C30
16	L	205	BCR	C1-C6-C7-C8
16	L	207	BCR	C1-C6-C7-C8
16	M	101	BCR	C1-C6-C7-C8
16	M	101	BCR	C23-C24-C25-C30
16	a	845	BCR	C1-C6-C7-C8
16	a	846	BCR	C23-C24-C25-C30
16	a	847	BCR	C1-C6-C7-C8
16	a	848	BCR	C23-C24-C25-C30
16	a	851	BCR	C1-C6-C7-C8
16	b	840	BCR	C1-C6-C7-C8
16	b	840	BCR	C23-C24-C25-C30
16	b	841	BCR	C1-C6-C7-C8
16	b	843	BCR	C1-C6-C7-C8
16	b	844	BCR	C1-C6-C7-C8
16	b	845	BCR	C1-C6-C7-C8
16	b	848	BCR	C23-C24-C25-C30
16	f	202	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
16	f	205	BCR	C1-C6-C7-C8
16	f	205	BCR	C5-C6-C7-C8
16	j	1104	BCR	C1-C6-C7-C8
16	j	1105	BCR	C1-C6-C7-C8
16	k	4001	BCR	C1-C6-C7-C8
16	k	4004	BCR	C1-C6-C7-C8
16	k	4004	BCR	C23-C24-C25-C30
16	l	201	BCR	C1-C6-C7-C8
16	l	203	BCR	C23-C24-C25-C30
16	l	206	BCR	C1-C6-C7-C8
16	m	101	BCR	C1-C6-C7-C8
16	m	101	BCR	C23-C24-C25-C30
16	1	845	BCR	C1-C6-C7-C8
16	1	846	BCR	C23-C24-C25-C30
16	1	847	BCR	C1-C6-C7-C8
16	1	848	BCR	C23-C24-C25-C30
16	1	851	BCR	C1-C6-C7-C8
16	2	839	BCR	C1-C6-C7-C8
16	2	839	BCR	C23-C24-C25-C30
16	2	840	BCR	C1-C6-C7-C8
16	2	842	BCR	C1-C6-C7-C8
16	2	843	BCR	C1-C6-C7-C8
16	2	844	BCR	C1-C6-C7-C8
16	2	847	BCR	C23-C24-C25-C30
16	6	202	BCR	C1-C6-C7-C8
16	6	205	BCR	C1-C6-C7-C8
16	8	1104	BCR	C1-C6-C7-C8
16	8	1105	BCR	C1-C6-C7-C8
16	9	4001	BCR	C1-C6-C7-C8
16	9	4004	BCR	C1-C6-C7-C8
16	9	4004	BCR	C23-C24-C25-C30
16	0	201	BCR	C1-C6-C7-C8
16	0	204	BCR	C23-C24-C25-C30
16	0	207	BCR	C1-C6-C7-C8
16	z	101	BCR	C1-C6-C7-C8
16	z	101	BCR	C23-C24-C25-C30
13	A	803	CLA	C8-C10-C11-C12
13	a	803	CLA	C8-C10-C11-C12
13	1	803	CLA	C8-C10-C11-C12
13	B	816	CLA	C3-C5-C6-C7
13	b	816	CLA	C3-C5-C6-C7
13	2	815	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
13	B	804	CLA	C15-C16-C17-C18
13	b	804	CLA	C15-C16-C17-C18
13	2	804	CLA	C15-C16-C17-C18
18	B	846	LMG	O7-C8-C9-O8
18	b	846	LMG	O7-C8-C9-O8
18	2	845	LMG	O7-C8-C9-O8
13	B	810	CLA	O1A-CGA-O2A-C1
13	2	809	CLA	O1A-CGA-O2A-C1
18	B	846	LMG	C12-C13-C14-C15
18	b	846	LMG	C12-C13-C14-C15
18	2	845	LMG	C12-C13-C14-C15
16	J	1105	BCR	C10-C11-C12-C13
16	J	1105	BCR	C18-C19-C20-C21
16	j	1105	BCR	C10-C11-C12-C13
16	j	1105	BCR	C18-C19-C20-C21
16	1	847	BCR	C10-C11-C12-C13
16	8	1105	BCR	C10-C11-C12-C13
16	8	1105	BCR	C18-C19-C20-C21
13	A	825	CLA	C5-C6-C7-C8
13	B	802	CLA	C13-C15-C16-C17
13	a	825	CLA	C5-C6-C7-C8
13	b	802	CLA	C13-C15-C16-C17
13	2	802	CLA	C13-C15-C16-C17
13	8	1102	CLA	O1D-CGD-O2D-CED
12	A	801	CL0	C16-C17-C18-C19
12	a	801	CL0	C16-C17-C18-C19
12	1	801	CL0	C16-C17-C18-C19
13	1	825	CLA	C5-C6-C7-C8
13	1	834	CLA	C10-C11-C12-C13
17	A	849	LHG	C23-C24-C25-C26
17	a	849	LHG	C23-C24-C25-C26
17	1	849	LHG	C23-C24-C25-C26
13	J	1102	CLA	O1D-CGD-O2D-CED
13	b	810	CLA	O1A-CGA-O2A-C1
13	A	834	CLA	C6-C7-C8-C9
13	A	837	CLA	C11-C10-C8-C9
13	I	101	CLA	C11-C10-C8-C9
13	I	101	CLA	C14-C13-C15-C16
13	a	834	CLA	C6-C7-C8-C9
13	a	837	CLA	C11-C10-C8-C9
13	i	102	CLA	C11-C10-C8-C9
13	i	102	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
13	1	834	CLA	C6-C7-C8-C9
13	1	837	CLA	C11-C10-C8-C9
13	7	102	CLA	C11-C10-C8-C9
13	7	102	CLA	C14-C13-C15-C16
14	B	839	PQN	C19-C18-C20-C21
14	b	839	PQN	C19-C18-C20-C21
14	2	838	PQN	C19-C18-C20-C21
13	A	834	CLA	C10-C11-C12-C13
13	a	834	CLA	C10-C11-C12-C13
13	j	1102	CLA	O1D-CGD-O2D-CED
16	A	846	BCR	C6-C7-C8-C9
16	B	842	BCR	C22-C23-C24-C25
16	K	4001	BCR	C22-C23-C24-C25
16	a	846	BCR	C6-C7-C8-C9
16	b	842	BCR	C22-C23-C24-C25
16	k	4001	BCR	C22-C23-C24-C25
16	1	846	BCR	C6-C7-C8-C9
16	2	841	BCR	C22-C23-C24-C25
16	9	4001	BCR	C22-C23-C24-C25
16	B	842	BCR	C14-C15-C16-C17
16	b	842	BCR	C14-C15-C16-C17
16	2	841	BCR	C14-C15-C16-C17
18	B	846	LMG	C2-C1-O1-C7
18	b	846	LMG	C2-C1-O1-C7
18	2	845	LMG	C2-C1-O1-C7
13	A	840	CLA	C2A-CAA-CBA-CGA
13	a	840	CLA	C2A-CAA-CBA-CGA
13	1	840	CLA	C2A-CAA-CBA-CGA
13	A	825	CLA	C2-C3-C5-C6
13	a	825	CLA	C2-C3-C5-C6
13	1	825	CLA	C2-C3-C5-C6
13	B	820	CLA	C6-C7-C8-C10
13	b	820	CLA	C6-C7-C8-C10
13	2	819	CLA	C6-C7-C8-C10
16	A	847	BCR	C16-C17-C18-C36
16	B	842	BCR	C20-C21-C22-C37
16	J	1105	BCR	C20-C21-C22-C37
16	a	847	BCR	C16-C17-C18-C36
16	b	842	BCR	C20-C21-C22-C37
16	j	1105	BCR	C20-C21-C22-C37
16	1	847	BCR	C16-C17-C18-C36
16	2	841	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
16	8	1105	BCR	C20-C21-C22-C37
13	b	802	CLA	C5-C6-C7-C8
13	B	802	CLA	C5-C6-C7-C8
13	2	802	CLA	C5-C6-C7-C8
16	B	843	BCR	C7-C8-C9-C34
16	b	843	BCR	C7-C8-C9-C34
16	2	842	BCR	C7-C8-C9-C34
13	A	830	CLA	C11-C10-C8-C7
13	A	834	CLA	C11-C12-C13-C15
13	B	837	CLA	C11-C12-C13-C15
13	B	847	CLA	C11-C10-C8-C7
13	I	101	CLA	C12-C13-C15-C16
13	a	830	CLA	C11-C10-C8-C7
13	a	834	CLA	C11-C12-C13-C15
13	b	837	CLA	C11-C12-C13-C15
13	b	847	CLA	C11-C10-C8-C7
13	i	102	CLA	C12-C13-C15-C16
13	1	830	CLA	C11-C10-C8-C7
13	1	834	CLA	C11-C12-C13-C15
13	2	836	CLA	C11-C12-C13-C15
13	2	846	CLA	C11-C10-C8-C7
13	7	102	CLA	C12-C13-C15-C16
14	B	839	PQN	C17-C18-C20-C21
14	b	839	PQN	C17-C18-C20-C21
14	2	838	PQN	C17-C18-C20-C21
13	B	823	CLA	C13-C15-C16-C17
13	b	823	CLA	C13-C15-C16-C17
13	2	822	CLA	C13-C15-C16-C17
16	A	851	BCR	C7-C8-C9-C10
16	L	202	BCR	C7-C8-C9-C10
16	L	202	BCR	C11-C12-C13-C14
16	a	851	BCR	C7-C8-C9-C10
16	l	203	BCR	C7-C8-C9-C10
16	l	203	BCR	C11-C12-C13-C14
16	1	851	BCR	C7-C8-C9-C10
16	0	204	BCR	C7-C8-C9-C10
16	0	204	BCR	C11-C12-C13-C14
13	A	824	CLA	CBA-CGA-O2A-C1
13	A	838	CLA	CBA-CGA-O2A-C1
13	A	852	CLA	CBA-CGA-O2A-C1
13	a	824	CLA	CBA-CGA-O2A-C1
13	a	838	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	a	852	CLA	CBA-CGA-O2A-C1
13	1	824	CLA	CBA-CGA-O2A-C1
13	1	838	CLA	CBA-CGA-O2A-C1
13	1	852	CLA	CBA-CGA-O2A-C1
13	B	806	CLA	C2-C3-C5-C6
13	b	806	CLA	C2-C3-C5-C6
13	2	806	CLA	C2-C3-C5-C6
13	l	207	CLA	C8-C10-C11-C12
17	A	850	LHG	C27-C28-C29-C30
17	a	850	LHG	C27-C28-C29-C30
17	1	850	LHG	C27-C28-C29-C30
13	A	805	CLA	C5-C6-C7-C8
13	L	206	CLA	C8-C10-C11-C12
13	a	805	CLA	C5-C6-C7-C8
13	0	208	CLA	C8-C10-C11-C12
16	B	845	BCR	C20-C21-C22-C23
16	K	4004	BCR	C12-C13-C14-C15
16	b	845	BCR	C20-C21-C22-C23
16	k	4004	BCR	C12-C13-C14-C15
16	2	844	BCR	C20-C21-C22-C23
16	9	4004	BCR	C12-C13-C14-C15
13	1	805	CLA	C5-C6-C7-C8
18	B	846	LMG	O1-C7-C8-C9
18	b	846	LMG	O1-C7-C8-C9
18	2	845	LMG	O1-C7-C8-C9
13	K	4002	CLA	C2C-C3C-CAC-CBC
13	A	837	CLA	O1A-CGA-O2A-C1
13	a	837	CLA	O1A-CGA-O2A-C1
19	I	103	SQD	C26-C27-C28-C29
19	i	101	SQD	C26-C27-C28-C29
19	7	101	SQD	C26-C27-C28-C29
13	k	4002	CLA	C2C-C3C-CAC-CBC
13	1	837	CLA	O1A-CGA-O2A-C1
17	A	849	LHG	O7-C5-C6-O8
17	a	849	LHG	O7-C5-C6-O8
17	1	849	LHG	O7-C5-C6-O8
13	A	834	CLA	C11-C12-C13-C14
13	B	837	CLA	C11-C12-C13-C14
13	B	847	CLA	C11-C10-C8-C9
13	a	834	CLA	C11-C12-C13-C14
13	b	837	CLA	C11-C12-C13-C14
13	b	847	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
13	1	834	CLA	C11-C12-C13-C14
13	2	836	CLA	C11-C12-C13-C14
13	2	846	CLA	C11-C10-C8-C9
13	9	4002	CLA	C2C-C3C-CAC-CBC
17	A	849	LHG	C11-C10-C9-C8
17	A	849	LHG	C24-C25-C26-C27
17	a	849	LHG	C11-C10-C9-C8
17	a	849	LHG	C24-C25-C26-C27
17	1	849	LHG	C11-C10-C9-C8
17	1	849	LHG	C24-C25-C26-C27
13	A	827	CLA	C10-C11-C12-C13
13	a	827	CLA	C10-C11-C12-C13
13	1	827	CLA	C10-C11-C12-C13
13	B	829	CLA	C2-C1-O2A-CGA
13	b	829	CLA	C2-C1-O2A-CGA
13	2	828	CLA	C2-C1-O2A-CGA
16	K	4001	BCR	C13-C14-C15-C16
16	k	4001	BCR	C13-C14-C15-C16
16	9	4001	BCR	C13-C14-C15-C16
13	B	837	CLA	C5-C6-C7-C8
13	b	837	CLA	C5-C6-C7-C8
13	B	805	CLA	C4-C3-C5-C6
13	B	810	CLA	C4-C3-C5-C6
13	b	805	CLA	C4-C3-C5-C6
13	b	810	CLA	C4-C3-C5-C6
13	2	805	CLA	C4-C3-C5-C6
13	2	809	CLA	C4-C3-C5-C6
13	A	819	CLA	C8-C10-C11-C12
13	B	847	CLA	C13-C15-C16-C17
13	a	819	CLA	C8-C10-C11-C12
13	1	819	CLA	C8-C10-C11-C12
13	2	836	CLA	C5-C6-C7-C8
13	2	846	CLA	C13-C15-C16-C17
13	A	826	CLA	CBA-CGA-O2A-C1
13	1	826	CLA	CBA-CGA-O2A-C1
13	b	847	CLA	C13-C15-C16-C17
13	A	824	CLA	C3-C5-C6-C7
13	a	824	CLA	C3-C5-C6-C7
13	1	824	CLA	C3-C5-C6-C7
13	a	826	CLA	CBA-CGA-O2A-C1
13	A	803	CLA	C1A-C2A-CAA-CBA
13	A	813	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	A	831	CLA	C1A-C2A-CAA-CBA
13	A	835	CLA	C4B-C3B-CAB-CBB
13	B	808	CLA	C1A-C2A-CAA-CBA
13	B	847	CLA	C1A-C2A-CAA-CBA
13	K	4003	CLA	C1A-C2A-CAA-CBA
13	K	4005	CLA	C1A-C2A-CAA-CBA
13	a	803	CLA	C1A-C2A-CAA-CBA
13	a	813	CLA	C1A-C2A-CAA-CBA
13	a	831	CLA	C1A-C2A-CAA-CBA
13	a	835	CLA	C4B-C3B-CAB-CBB
13	b	808	CLA	C1A-C2A-CAA-CBA
13	b	847	CLA	C1A-C2A-CAA-CBA
13	k	4003	CLA	C1A-C2A-CAA-CBA
13	k	4005	CLA	C1A-C2A-CAA-CBA
13	1	803	CLA	C1A-C2A-CAA-CBA
13	1	813	CLA	C1A-C2A-CAA-CBA
13	1	831	CLA	C1A-C2A-CAA-CBA
13	1	835	CLA	C4B-C3B-CAB-CBB
13	2	807	CLA	C1A-C2A-CAA-CBA
13	2	846	CLA	C1A-C2A-CAA-CBA
13	9	4003	CLA	C1A-C2A-CAA-CBA
13	9	4005	CLA	C1A-C2A-CAA-CBA
13	B	803	CLA	CBA-CGA-O2A-C1
13	B	815	CLA	CBA-CGA-O2A-C1
13	b	803	CLA	CBA-CGA-O2A-C1
13	b	815	CLA	CBA-CGA-O2A-C1
13	2	803	CLA	CBA-CGA-O2A-C1
13	2	814	CLA	CBA-CGA-O2A-C1
16	L	205	BCR	C22-C23-C24-C25
16	l	206	BCR	C22-C23-C24-C25
16	0	207	BCR	C22-C23-C24-C25
13	1	828	CLA	C10-C11-C12-C13
13	A	824	CLA	O1A-CGA-O2A-C1
13	A	838	CLA	O1A-CGA-O2A-C1
13	A	852	CLA	O1A-CGA-O2A-C1
13	a	838	CLA	O1A-CGA-O2A-C1
13	a	852	CLA	O1A-CGA-O2A-C1
13	1	824	CLA	O1A-CGA-O2A-C1
13	1	838	CLA	O1A-CGA-O2A-C1
13	1	852	CLA	O1A-CGA-O2A-C1
13	a	824	CLA	O1A-CGA-O2A-C1
12	A	801	CL0	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
12	a	801	CL0	C11-C12-C13-C15
12	1	801	CL0	C11-C12-C13-C15
13	A	840	CLA	C11-C10-C8-C7
13	A	852	CLA	C6-C7-C8-C10
13	B	806	CLA	C11-C10-C8-C7
13	B	810	CLA	C11-C10-C8-C7
13	B	821	CLA	C12-C13-C15-C16
13	B	826	CLA	C11-C10-C8-C7
13	B	836	CLA	C6-C7-C8-C10
13	a	840	CLA	C11-C10-C8-C7
13	a	852	CLA	C6-C7-C8-C10
13	b	806	CLA	C11-C10-C8-C7
13	b	810	CLA	C11-C10-C8-C7
13	b	821	CLA	C12-C13-C15-C16
13	b	826	CLA	C11-C10-C8-C7
13	b	836	CLA	C6-C7-C8-C10
13	1	840	CLA	C11-C10-C8-C7
13	1	852	CLA	C6-C7-C8-C10
13	2	806	CLA	C11-C10-C8-C7
13	2	809	CLA	C11-C10-C8-C7
13	2	820	CLA	C12-C13-C15-C16
13	2	825	CLA	C11-C10-C8-C7
13	2	835	CLA	C6-C7-C8-C10
14	A	843	PQN	C22-C23-C25-C26
14	a	843	PQN	C22-C23-C25-C26
14	1	843	PQN	C22-C23-C25-C26
13	A	828	CLA	C10-C11-C12-C13
13	A	834	CLA	CBA-CGA-O2A-C1
13	a	834	CLA	CBA-CGA-O2A-C1
13	1	834	CLA	CBA-CGA-O2A-C1
17	a	850	LHG	O10-C23-O8-C6
13	a	828	CLA	C10-C11-C12-C13
17	A	850	LHG	O10-C23-O8-C6
17	1	850	LHG	O10-C23-O8-C6
17	A	850	LHG	O6-C4-C5-O7
17	a	850	LHG	O6-C4-C5-O7
17	1	850	LHG	O6-C4-C5-O7
13	A	829	CLA	C6-C7-C8-C9
13	A	830	CLA	C11-C10-C8-C9
13	B	836	CLA	C6-C7-C8-C9
13	a	829	CLA	C6-C7-C8-C9
13	a	830	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
13	b	836	CLA	C6-C7-C8-C9
13	1	829	CLA	C6-C7-C8-C9
13	1	830	CLA	C11-C10-C8-C9
13	2	835	CLA	C6-C7-C8-C9
13	b	815	CLA	O1A-CGA-O2A-C1
18	B	846	LMG	C32-C33-C34-C35
18	b	846	LMG	C32-C33-C34-C35
13	B	830	CLA	C3-C5-C6-C7
13	b	830	CLA	C3-C5-C6-C7
13	2	829	CLA	C3-C5-C6-C7
18	2	845	LMG	C32-C33-C34-C35
13	B	815	CLA	O1A-CGA-O2A-C1
13	2	814	CLA	O1A-CGA-O2A-C1
18	B	846	LMG	O1-C7-C8-O7
18	b	846	LMG	O1-C7-C8-O7
18	2	845	LMG	O1-C7-C8-O7
17	A	850	LHG	C4-C5-C6-O8
17	a	850	LHG	C4-C5-C6-O8
17	1	850	LHG	C4-C5-C6-O8
13	B	805	CLA	C2-C3-C5-C6
13	B	810	CLA	C2-C3-C5-C6
13	b	805	CLA	C2-C3-C5-C6
13	b	810	CLA	C2-C3-C5-C6
13	2	805	CLA	C2-C3-C5-C6
13	2	809	CLA	C2-C3-C5-C6
18	b	846	LMG	C35-C36-C37-C38
18	2	845	LMG	C35-C36-C37-C38
13	A	805	CLA	CAD-CBD-CGD-O2D
13	A	813	CLA	CAD-CBD-CGD-O2D
13	A	822	CLA	CAD-CBD-CGD-O2D
13	A	827	CLA	CAD-CBD-CGD-O2D
13	B	827	CLA	CAD-CBD-CGD-O2D
13	F	204	CLA	CAD-CBD-CGD-O2D
13	a	805	CLA	CAD-CBD-CGD-O2D
13	a	813	CLA	CAD-CBD-CGD-O2D
13	a	822	CLA	CAD-CBD-CGD-O2D
13	a	827	CLA	CAD-CBD-CGD-O2D
13	b	827	CLA	CAD-CBD-CGD-O2D
13	f	204	CLA	CAD-CBD-CGD-O2D
13	1	805	CLA	CAD-CBD-CGD-O2D
13	1	813	CLA	CAD-CBD-CGD-O2D
13	1	822	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
13	1	827	CLA	CAD-CBD-CGD-O2D
13	2	826	CLA	CAD-CBD-CGD-O2D
13	6	204	CLA	CAD-CBD-CGD-O2D
17	1	850	LHG	C13-C14-C15-C16
18	B	846	LMG	C35-C36-C37-C38
13	A	834	CLA	O1A-CGA-O2A-C1
13	B	803	CLA	O1A-CGA-O2A-C1
13	a	834	CLA	O1A-CGA-O2A-C1
19	I	103	SQD	C24-C23-O48-C46
17	A	850	LHG	C13-C14-C15-C16
17	a	850	LHG	C13-C14-C15-C16
13	B	823	CLA	C2A-CAA-CBA-CGA
13	b	823	CLA	C2A-CAA-CBA-CGA
13	2	822	CLA	C2A-CAA-CBA-CGA
13	a	826	CLA	O1A-CGA-O2A-C1
13	b	803	CLA	O1A-CGA-O2A-C1
13	1	826	CLA	O1A-CGA-O2A-C1
13	1	834	CLA	O1A-CGA-O2A-C1
13	2	803	CLA	O1A-CGA-O2A-C1
19	i	101	SQD	C24-C23-O48-C46
13	A	826	CLA	O1A-CGA-O2A-C1
13	A	805	CLA	CAD-CBD-CGD-O1D
13	A	813	CLA	CAD-CBD-CGD-O1D
13	A	819	CLA	CHA-CBD-CGD-O1D
13	A	819	CLA	CHA-CBD-CGD-O2D
13	A	822	CLA	CAD-CBD-CGD-O1D
13	A	827	CLA	CAD-CBD-CGD-O1D
13	A	838	CLA	CHA-CBD-CGD-O1D
13	B	811	CLA	CHA-CBD-CGD-O1D
13	B	811	CLA	CHA-CBD-CGD-O2D
13	B	818	CLA	CHA-CBD-CGD-O1D
13	B	818	CLA	CHA-CBD-CGD-O2D
13	B	827	CLA	CAD-CBD-CGD-O1D
13	F	204	CLA	CAD-CBD-CGD-O1D
13	a	805	CLA	CAD-CBD-CGD-O1D
13	a	813	CLA	CAD-CBD-CGD-O1D
13	a	819	CLA	CHA-CBD-CGD-O1D
13	a	819	CLA	CHA-CBD-CGD-O2D
13	a	822	CLA	CAD-CBD-CGD-O1D
13	a	827	CLA	CAD-CBD-CGD-O1D
13	a	838	CLA	CHA-CBD-CGD-O1D
13	b	811	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
13	b	811	CLA	CHA-CBD-CGD-O2D
13	b	818	CLA	CHA-CBD-CGD-O1D
13	b	818	CLA	CHA-CBD-CGD-O2D
13	b	827	CLA	CAD-CBD-CGD-O1D
13	f	204	CLA	CAD-CBD-CGD-O1D
13	1	805	CLA	CAD-CBD-CGD-O1D
13	1	813	CLA	CAD-CBD-CGD-O1D
13	1	819	CLA	CHA-CBD-CGD-O1D
13	1	819	CLA	CHA-CBD-CGD-O2D
13	1	822	CLA	CAD-CBD-CGD-O1D
13	1	827	CLA	CAD-CBD-CGD-O1D
13	1	832	CLA	CAD-CBD-CGD-O1D
13	1	838	CLA	CHA-CBD-CGD-O1D
13	2	806	CLA	CAD-CBD-CGD-O1D
13	2	810	CLA	CHA-CBD-CGD-O1D
13	2	810	CLA	CHA-CBD-CGD-O2D
13	2	817	CLA	CHA-CBD-CGD-O1D
13	2	817	CLA	CHA-CBD-CGD-O2D
13	2	826	CLA	CAD-CBD-CGD-O1D
13	6	204	CLA	CAD-CBD-CGD-O1D
17	A	849	LHG	C4-O6-P-O4
17	a	849	LHG	C4-O6-P-O4
17	1	849	LHG	C4-O6-P-O4
17	1	850	LHG	C4-O6-P-O5
13	A	805	CLA	C2B-C3B-CAB-CBB
13	A	809	CLA	C2B-C3B-CAB-CBB
13	A	811	CLA	C2B-C3B-CAB-CBB
13	A	814	CLA	C2B-C3B-CAB-CBB
13	A	823	CLA	C2B-C3B-CAB-CBB
13	A	838	CLA	C2B-C3B-CAB-CBB
13	B	804	CLA	C2B-C3B-CAB-CBB
13	B	818	CLA	C2B-C3B-CAB-CBB
13	B	823	CLA	C2B-C3B-CAB-CBB
13	K	4005	CLA	C2B-C3B-CAB-CBB
13	a	805	CLA	C2B-C3B-CAB-CBB
13	a	809	CLA	C2B-C3B-CAB-CBB
13	a	811	CLA	C2B-C3B-CAB-CBB
13	a	814	CLA	C2B-C3B-CAB-CBB
13	a	823	CLA	C2B-C3B-CAB-CBB
13	a	838	CLA	C2B-C3B-CAB-CBB
13	b	804	CLA	C2B-C3B-CAB-CBB
13	b	818	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	b	823	CLA	C2B-C3B-CAB-CBB
13	k	4005	CLA	C2B-C3B-CAB-CBB
13	1	805	CLA	C2B-C3B-CAB-CBB
13	1	809	CLA	C2B-C3B-CAB-CBB
13	1	811	CLA	C2B-C3B-CAB-CBB
13	1	814	CLA	C2B-C3B-CAB-CBB
13	1	823	CLA	C2B-C3B-CAB-CBB
13	1	838	CLA	C2B-C3B-CAB-CBB
13	2	804	CLA	C2B-C3B-CAB-CBB
13	2	817	CLA	C2B-C3B-CAB-CBB
13	2	822	CLA	C2B-C3B-CAB-CBB
13	9	4005	CLA	C2B-C3B-CAB-CBB
16	A	845	BCR	C23-C24-C25-C30
16	A	846	BCR	C1-C6-C7-C8
16	A	851	BCR	C5-C6-C7-C8
16	J	1105	BCR	C23-C24-C25-C26
16	K	4004	BCR	C1-C6-C7-C8
16	a	846	BCR	C1-C6-C7-C8
16	a	851	BCR	C5-C6-C7-C8
16	1	845	BCR	C23-C24-C25-C30
16	1	846	BCR	C1-C6-C7-C8
16	1	851	BCR	C5-C6-C7-C8
16	6	205	BCR	C5-C6-C7-C8
16	8	1105	BCR	C23-C24-C25-C26
13	B	802	CLA	C2C-C3C-CAC-CBC
13	b	802	CLA	C2C-C3C-CAC-CBC
13	2	802	CLA	C2C-C3C-CAC-CBC
19	7	101	SQD	C24-C23-O48-C46
13	B	804	CLA	C13-C15-C16-C17
13	b	804	CLA	C13-C15-C16-C17
13	2	804	CLA	C13-C15-C16-C17
13	b	811	CLA	O1A-CGA-O2A-C1
16	A	847	BCR	C19-C20-C21-C22
16	a	847	BCR	C19-C20-C21-C22
16	1	847	BCR	C19-C20-C21-C22
13	B	811	CLA	O1A-CGA-O2A-C1
13	2	810	CLA	O1A-CGA-O2A-C1
13	A	825	CLA	C11-C10-C8-C9
13	A	825	CLA	C14-C13-C15-C16
13	A	830	CLA	C11-C12-C13-C14
13	A	832	CLA	C14-C13-C15-C16
13	A	852	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
13	B	807	CLA	C11-C12-C13-C14
13	B	808	CLA	C11-C12-C13-C14
13	B	830	CLA	C11-C10-C8-C9
13	a	825	CLA	C11-C10-C8-C9
13	a	825	CLA	C14-C13-C15-C16
13	a	830	CLA	C11-C12-C13-C14
13	a	832	CLA	C14-C13-C15-C16
13	a	852	CLA	C6-C7-C8-C9
13	b	807	CLA	C11-C12-C13-C14
13	b	808	CLA	C11-C12-C13-C14
13	b	830	CLA	C11-C10-C8-C9
13	1	825	CLA	C11-C10-C8-C9
13	1	825	CLA	C14-C13-C15-C16
13	1	830	CLA	C11-C12-C13-C14
13	1	832	CLA	C14-C13-C15-C16
13	1	852	CLA	C6-C7-C8-C9
13	2	807	CLA	C11-C12-C13-C14
13	2	829	CLA	C11-C10-C8-C9
13	0	203	CLA	C11-C12-C13-C14
14	A	843	PQN	C21-C22-C23-C24
14	A	843	PQN	C24-C23-C25-C26
14	a	843	PQN	C21-C22-C23-C24
14	a	843	PQN	C24-C23-C25-C26
14	1	843	PQN	C21-C22-C23-C24
14	1	843	PQN	C24-C23-C25-C26
19	i	101	SQD	C14-C15-C16-C17
13	A	830	CLA	C11-C12-C13-C15
13	A	833	CLA	C12-C13-C15-C16
13	B	807	CLA	C11-C12-C13-C15
13	B	823	CLA	C11-C12-C13-C15
13	B	830	CLA	C11-C10-C8-C7
13	a	830	CLA	C11-C12-C13-C15
13	a	833	CLA	C12-C13-C15-C16
13	b	807	CLA	C11-C12-C13-C15
13	b	823	CLA	C11-C12-C13-C15
13	b	830	CLA	C11-C10-C8-C7
13	1	830	CLA	C11-C12-C13-C15
13	1	833	CLA	C12-C13-C15-C16
13	2	822	CLA	C11-C12-C13-C15
13	2	829	CLA	C11-C10-C8-C7
13	0	203	CLA	C11-C12-C13-C15
14	A	843	PQN	C21-C22-C23-C25

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Mol	Chain	Res	Type	Atoms
14	a	843	PQN	C21-C22-C23-C25
14	1	843	PQN	C21-C22-C23-C25
19	7	101	SQD	C14-C15-C16-C17
16	A	848	BCR	C16-C17-C18-C19
16	a	848	BCR	C16-C17-C18-C19
16	1	848	BCR	C16-C17-C18-C19
19	I	103	SQD	C14-C15-C16-C17
13	l	207	CLA	C16-C17-C18-C20
13	0	208	CLA	C16-C17-C18-C20
13	B	847	CLA	CAA-CBA-CGA-O2A
13	b	847	CLA	CAA-CBA-CGA-O2A
13	2	846	CLA	CAA-CBA-CGA-O2A
13	B	803	CLA	C4C-C3C-CAC-CBC
13	b	803	CLA	C4C-C3C-CAC-CBC
13	2	803	CLA	C4C-C3C-CAC-CBC
13	L	206	CLA	C16-C17-C18-C20
17	A	850	LHG	O7-C5-C6-O8
17	a	850	LHG	O7-C5-C6-O8
17	1	850	LHG	O7-C5-C6-O8
16	A	848	BCR	C15-C16-C17-C18
16	a	848	BCR	C15-C16-C17-C18
16	1	848	BCR	C15-C16-C17-C18
13	A	841	CLA	C2-C1-O2A-CGA
13	a	841	CLA	C2-C1-O2A-CGA
13	1	841	CLA	C2-C1-O2A-CGA
13	L	206	CLA	C16-C17-C18-C19
13	l	207	CLA	C16-C17-C18-C19
13	0	208	CLA	C16-C17-C18-C19
13	b	829	CLA	C2C-C3C-CAC-CBC
13	A	830	CLA	CBD-CGD-O2D-CED
13	B	829	CLA	C2C-C3C-CAC-CBC
13	2	828	CLA	C2C-C3C-CAC-CBC
13	A	816	CLA	CAA-CBA-CGA-O2A
13	B	829	CLA	CAA-CBA-CGA-O2A
13	a	816	CLA	CAA-CBA-CGA-O2A
13	b	829	CLA	CAA-CBA-CGA-O2A
13	1	816	CLA	CAA-CBA-CGA-O2A
13	2	828	CLA	CAA-CBA-CGA-O2A
13	1	830	CLA	CBD-CGD-O2D-CED
13	l	207	CLA	C10-C11-C12-C13
13	L	206	CLA	C10-C11-C12-C13
13	0	208	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
17	A	849	LHG	C29-C30-C31-C32
17	a	849	LHG	C29-C30-C31-C32
13	A	839	CLA	C2A-CAA-CBA-CGA
13	a	839	CLA	C2A-CAA-CBA-CGA
13	1	839	CLA	C2A-CAA-CBA-CGA
17	1	849	LHG	C29-C30-C31-C32
13	b	808	CLA	C4-C3-C5-C6
13	2	807	CLA	C4-C3-C5-C6
13	A	829	CLA	C14-C13-C15-C16
13	A	840	CLA	C11-C10-C8-C9
13	B	821	CLA	C14-C13-C15-C16
13	a	829	CLA	C14-C13-C15-C16
13	a	840	CLA	C11-C10-C8-C9
13	b	821	CLA	C14-C13-C15-C16
13	1	829	CLA	C14-C13-C15-C16
13	1	840	CLA	C11-C10-C8-C9
13	2	820	CLA	C14-C13-C15-C16
13	A	830	CLA	O1D-CGD-O2D-CED
13	A	810	CLA	C4B-C3B-CAB-CBB
13	B	823	CLA	C4B-C3B-CAB-CBB
13	a	810	CLA	C4B-C3B-CAB-CBB
13	b	823	CLA	C4B-C3B-CAB-CBB
13	1	810	CLA	C4B-C3B-CAB-CBB
13	2	822	CLA	C4B-C3B-CAB-CBB
13	a	830	CLA	CBD-CGD-O2D-CED
13	a	830	CLA	O1D-CGD-O2D-CED
13	A	839	CLA	C10-C11-C12-C13
13	B	824	CLA	C2C-C3C-CAC-CBC
13	2	823	CLA	C2C-C3C-CAC-CBC
13	2	806	CLA	CBA-CGA-O2A-C1
13	A	811	CLA	C5-C6-C7-C8
13	a	811	CLA	C5-C6-C7-C8
13	a	839	CLA	C10-C11-C12-C13
13	1	811	CLA	C5-C6-C7-C8
13	1	839	CLA	C10-C11-C12-C13
13	B	808	CLA	C4-C3-C5-C6
13	b	824	CLA	C2C-C3C-CAC-CBC
13	B	806	CLA	CBA-CGA-O2A-C1
13	b	806	CLA	CBA-CGA-O2A-C1
13	1	830	CLA	O1D-CGD-O2D-CED
13	A	806	CLA	C11-C10-C8-C7
13	A	829	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
13	B	807	CLA	C12-C13-C15-C16
13	a	806	CLA	C11-C10-C8-C7
13	a	829	CLA	C12-C13-C15-C16
13	b	807	CLA	C12-C13-C15-C16
13	1	806	CLA	C11-C10-C8-C7
13	1	829	CLA	C12-C13-C15-C16
13	0	203	CLA	C12-C13-C15-C16
13	B	814	CLA	CBA-CGA-O2A-C1
13	b	814	CLA	CBA-CGA-O2A-C1
13	2	813	CLA	CBA-CGA-O2A-C1
12	A	801	CL0	C5-C6-C7-C8
12	a	801	CL0	C5-C6-C7-C8
12	1	801	CL0	C5-C6-C7-C8
18	2	845	LMG	C17-C18-C19-C20
13	A	803	CLA	C3A-C2A-CAA-CBA
13	A	832	CLA	C4-C3-C5-C6
13	B	820	CLA	C3A-C2A-CAA-CBA
13	B	827	CLA	C3A-C2A-CAA-CBA
13	a	803	CLA	C3A-C2A-CAA-CBA
13	a	832	CLA	C4-C3-C5-C6
13	b	820	CLA	C3A-C2A-CAA-CBA
13	b	827	CLA	C3A-C2A-CAA-CBA
13	1	803	CLA	C3A-C2A-CAA-CBA
13	1	832	CLA	C4-C3-C5-C6
13	2	819	CLA	C3A-C2A-CAA-CBA
13	2	826	CLA	C3A-C2A-CAA-CBA
18	B	846	LMG	C17-C18-C19-C20
18	b	846	LMG	C17-C18-C19-C20
16	B	842	BCR	C11-C10-C9-C34
16	L	202	BCR	C20-C21-C22-C37
16	b	842	BCR	C11-C10-C9-C34
16	1	203	BCR	C20-C21-C22-C37
16	2	841	BCR	C11-C10-C9-C34
16	0	204	BCR	C20-C21-C22-C37
13	B	820	CLA	C2-C1-O2A-CGA
13	b	820	CLA	C2-C1-O2A-CGA
13	2	819	CLA	C2-C1-O2A-CGA
16	8	1104	BCR	C7-C8-C9-C34
16	9	4004	BCR	C7-C8-C9-C10
13	B	806	CLA	C16-C17-C18-C19
13	I	101	CLA	C16-C17-C18-C19
13	b	806	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
13	i	102	CLA	C16-C17-C18-C19
13	2	806	CLA	C16-C17-C18-C19
13	7	102	CLA	C16-C17-C18-C19
13	B	807	CLA	C10-C11-C12-C13
13	b	807	CLA	C10-C11-C12-C13
13	0	203	CLA	C10-C11-C12-C13
13	B	818	CLA	C2A-CAA-CBA-CGA
13	b	818	CLA	C2A-CAA-CBA-CGA
13	2	817	CLA	C2A-CAA-CBA-CGA
13	b	826	CLA	C3-C5-C6-C7
13	1	833	CLA	C8-C10-C11-C12
13	K	4005	CLA	CAA-CBA-CGA-O1A
13	k	4005	CLA	CAA-CBA-CGA-O1A
13	9	4005	CLA	CAA-CBA-CGA-O1A
13	A	838	CLA	C11-C10-C8-C9
13	B	807	CLA	C14-C13-C15-C16
13	B	821	CLA	C6-C7-C8-C9
13	B	823	CLA	C14-C13-C15-C16
13	B	826	CLA	C11-C10-C8-C9
13	a	838	CLA	C11-C10-C8-C9
13	b	807	CLA	C14-C13-C15-C16
13	b	821	CLA	C6-C7-C8-C9
13	b	823	CLA	C14-C13-C15-C16
13	b	826	CLA	C11-C10-C8-C9
13	1	838	CLA	C11-C10-C8-C9
13	2	820	CLA	C6-C7-C8-C9
13	2	822	CLA	C14-C13-C15-C16
13	2	825	CLA	C11-C10-C8-C9
13	0	203	CLA	C14-C13-C15-C16
12	1	801	CL0	CAA-CBA-CGA-O2A
13	B	828	CLA	CAA-CBA-CGA-O2A
13	b	828	CLA	CAA-CBA-CGA-O2A
13	2	827	CLA	CAA-CBA-CGA-O2A
13	A	833	CLA	C8-C10-C11-C12
13	a	833	CLA	C8-C10-C11-C12
13	A	818	CLA	C3-C5-C6-C7
13	B	826	CLA	C3-C5-C6-C7
13	2	825	CLA	C3-C5-C6-C7
13	k	4005	CLA	CAA-CBA-CGA-O2A
12	A	801	CL0	CAA-CBA-CGA-O2A
12	a	801	CL0	CAA-CBA-CGA-O2A
13	a	818	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
13	1	818	CLA	C3-C5-C6-C7
13	K	4005	CLA	CAA-CBA-CGA-O2A
13	9	4005	CLA	CAA-CBA-CGA-O2A
13	b	815	CLA	CBD-CGD-O2D-CED
13	1	828	CLA	C2A-CAA-CBA-CGA
13	A	812	CLA	C1A-C2A-CAA-CBA
13	B	816	CLA	C1A-C2A-CAA-CBA
13	B	818	CLA	C1A-C2A-CAA-CBA
13	B	827	CLA	C1A-C2A-CAA-CBA
13	F	201	CLA	C1A-C2A-CAA-CBA
13	a	812	CLA	C1A-C2A-CAA-CBA
13	b	816	CLA	C1A-C2A-CAA-CBA
13	b	818	CLA	C1A-C2A-CAA-CBA
13	b	827	CLA	C1A-C2A-CAA-CBA
13	f	201	CLA	C1A-C2A-CAA-CBA
13	1	812	CLA	C1A-C2A-CAA-CBA
13	2	815	CLA	C1A-C2A-CAA-CBA
13	2	817	CLA	C1A-C2A-CAA-CBA
13	2	826	CLA	C1A-C2A-CAA-CBA
13	6	201	CLA	C1A-C2A-CAA-CBA
16	a	845	BCR	C20-C21-C22-C23
16	1	845	BCR	C20-C21-C22-C23
13	A	852	CLA	C11-C12-C13-C15
13	a	852	CLA	C11-C12-C13-C15
13	1	852	CLA	C11-C12-C13-C15
13	2	814	CLA	CBD-CGD-O2D-CED
13	A	804	CLA	C2B-C3B-CAB-CBB
13	A	810	CLA	C2B-C3B-CAB-CBB
13	A	812	CLA	C2B-C3B-CAB-CBB
13	A	815	CLA	C2B-C3B-CAB-CBB
13	A	816	CLA	C2B-C3B-CAB-CBB
13	A	819	CLA	C2B-C3B-CAB-CBB
13	A	820	CLA	C2B-C3B-CAB-CBB
13	A	822	CLA	C2B-C3B-CAB-CBB
13	A	833	CLA	C2B-C3B-CAB-CBB
13	A	834	CLA	C2B-C3B-CAB-CBB
13	A	836	CLA	C2B-C3B-CAB-CBB
13	A	841	CLA	C2B-C3B-CAB-CBB
13	B	810	CLA	C2B-C3B-CAB-CBB
13	B	811	CLA	C2B-C3B-CAB-CBB
13	B	812	CLA	C2B-C3B-CAB-CBB
13	B	817	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	B	831	CLA	C2B-C3B-CAB-CBB
13	B	832	CLA	C2B-C3B-CAB-CBB
13	B	834	CLA	C2B-C3B-CAB-CBB
13	F	204	CLA	C2B-C3B-CAB-CBB
13	J	1102	CLA	C2B-C3B-CAB-CBB
13	K	4002	CLA	C2B-C3B-CAB-CBB
13	K	4003	CLA	C2B-C3B-CAB-CBB
13	a	804	CLA	C2B-C3B-CAB-CBB
13	a	810	CLA	C2B-C3B-CAB-CBB
13	a	812	CLA	C2B-C3B-CAB-CBB
13	a	815	CLA	C2B-C3B-CAB-CBB
13	a	816	CLA	C2B-C3B-CAB-CBB
13	a	819	CLA	C2B-C3B-CAB-CBB
13	a	820	CLA	C2B-C3B-CAB-CBB
13	a	822	CLA	C2B-C3B-CAB-CBB
13	a	833	CLA	C2B-C3B-CAB-CBB
13	a	834	CLA	C2B-C3B-CAB-CBB
13	a	836	CLA	C2B-C3B-CAB-CBB
13	a	841	CLA	C2B-C3B-CAB-CBB
13	b	810	CLA	C2B-C3B-CAB-CBB
13	b	811	CLA	C2B-C3B-CAB-CBB
13	b	812	CLA	C2B-C3B-CAB-CBB
13	b	817	CLA	C2B-C3B-CAB-CBB
13	b	831	CLA	C2B-C3B-CAB-CBB
13	b	832	CLA	C2B-C3B-CAB-CBB
13	b	834	CLA	C2B-C3B-CAB-CBB
13	f	204	CLA	C2B-C3B-CAB-CBB
13	j	1102	CLA	C2B-C3B-CAB-CBB
13	k	4002	CLA	C2B-C3B-CAB-CBB
13	k	4003	CLA	C2B-C3B-CAB-CBB
13	1	804	CLA	C2B-C3B-CAB-CBB
13	1	810	CLA	C2B-C3B-CAB-CBB
13	1	812	CLA	C2B-C3B-CAB-CBB
13	1	815	CLA	C2B-C3B-CAB-CBB
13	1	816	CLA	C2B-C3B-CAB-CBB
13	1	819	CLA	C2B-C3B-CAB-CBB
13	1	820	CLA	C2B-C3B-CAB-CBB
13	1	822	CLA	C2B-C3B-CAB-CBB
13	1	833	CLA	C2B-C3B-CAB-CBB
13	1	834	CLA	C2B-C3B-CAB-CBB
13	1	836	CLA	C2B-C3B-CAB-CBB
13	1	841	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	2	809	CLA	C2B-C3B-CAB-CBB
13	2	810	CLA	C2B-C3B-CAB-CBB
13	2	811	CLA	C2B-C3B-CAB-CBB
13	2	816	CLA	C2B-C3B-CAB-CBB
13	2	830	CLA	C2B-C3B-CAB-CBB
13	2	831	CLA	C2B-C3B-CAB-CBB
13	2	833	CLA	C2B-C3B-CAB-CBB
13	6	204	CLA	C2B-C3B-CAB-CBB
13	8	1102	CLA	C2B-C3B-CAB-CBB
13	9	4002	CLA	C2B-C3B-CAB-CBB
13	9	4003	CLA	C2B-C3B-CAB-CBB
16	A	845	BCR	C5-C6-C7-C8
16	A	846	BCR	C5-C6-C7-C8
16	A	846	BCR	C23-C24-C25-C26
16	A	847	BCR	C5-C6-C7-C8
16	A	847	BCR	C23-C24-C25-C26
16	A	848	BCR	C23-C24-C25-C26
16	B	840	BCR	C5-C6-C7-C8
16	B	840	BCR	C23-C24-C25-C26
16	B	841	BCR	C5-C6-C7-C8
16	B	842	BCR	C23-C24-C25-C30
16	B	843	BCR	C5-C6-C7-C8
16	B	843	BCR	C23-C24-C25-C26
16	B	844	BCR	C5-C6-C7-C8
16	B	845	BCR	C5-C6-C7-C8
16	B	845	BCR	C23-C24-C25-C30
16	B	848	BCR	C23-C24-C25-C26
16	F	202	BCR	C5-C6-C7-C8
16	F	202	BCR	C23-C24-C25-C30
16	I	102	BCR	C23-C24-C25-C30
16	J	1104	BCR	C5-C6-C7-C8
16	J	1104	BCR	C23-C24-C25-C30
16	J	1105	BCR	C5-C6-C7-C8
16	K	4001	BCR	C5-C6-C7-C8
16	K	4001	BCR	C23-C24-C25-C30
16	K	4004	BCR	C5-C6-C7-C8
16	K	4004	BCR	C23-C24-C25-C26
16	L	202	BCR	C23-C24-C25-C26
16	L	205	BCR	C5-C6-C7-C8
16	L	207	BCR	C5-C6-C7-C8
16	L	207	BCR	C23-C24-C25-C30
16	M	101	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
16	M	101	BCR	C23-C24-C25-C26
16	a	845	BCR	C5-C6-C7-C8
16	a	845	BCR	C23-C24-C25-C30
16	a	846	BCR	C5-C6-C7-C8
16	a	846	BCR	C23-C24-C25-C26
16	a	847	BCR	C5-C6-C7-C8
16	a	847	BCR	C23-C24-C25-C26
16	a	848	BCR	C23-C24-C25-C26
16	b	840	BCR	C5-C6-C7-C8
16	b	840	BCR	C23-C24-C25-C26
16	b	841	BCR	C5-C6-C7-C8
16	b	842	BCR	C23-C24-C25-C30
16	b	843	BCR	C5-C6-C7-C8
16	b	843	BCR	C23-C24-C25-C26
16	b	844	BCR	C5-C6-C7-C8
16	b	845	BCR	C5-C6-C7-C8
16	b	845	BCR	C23-C24-C25-C30
16	b	848	BCR	C23-C24-C25-C26
16	f	202	BCR	C5-C6-C7-C8
16	f	202	BCR	C23-C24-C25-C30
16	i	103	BCR	C23-C24-C25-C30
16	j	1104	BCR	C5-C6-C7-C8
16	j	1104	BCR	C23-C24-C25-C30
16	j	1105	BCR	C5-C6-C7-C8
16	j	1105	BCR	C23-C24-C25-C26
16	k	4001	BCR	C5-C6-C7-C8
16	k	4001	BCR	C23-C24-C25-C30
16	k	4004	BCR	C5-C6-C7-C8
16	k	4004	BCR	C23-C24-C25-C26
16	l	201	BCR	C5-C6-C7-C8
16	l	201	BCR	C23-C24-C25-C30
16	l	203	BCR	C23-C24-C25-C26
16	l	206	BCR	C5-C6-C7-C8
16	m	101	BCR	C5-C6-C7-C8
16	m	101	BCR	C23-C24-C25-C26
16	1	845	BCR	C5-C6-C7-C8
16	1	846	BCR	C5-C6-C7-C8
16	1	846	BCR	C23-C24-C25-C26
16	1	847	BCR	C5-C6-C7-C8
16	1	847	BCR	C23-C24-C25-C26
16	1	848	BCR	C23-C24-C25-C26
16	2	839	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
16	2	839	BCR	C23-C24-C25-C26
16	2	840	BCR	C5-C6-C7-C8
16	2	841	BCR	C23-C24-C25-C30
16	2	842	BCR	C5-C6-C7-C8
16	2	842	BCR	C23-C24-C25-C26
16	2	843	BCR	C5-C6-C7-C8
16	2	844	BCR	C5-C6-C7-C8
16	2	844	BCR	C23-C24-C25-C30
16	2	847	BCR	C23-C24-C25-C26
16	6	202	BCR	C5-C6-C7-C8
16	6	202	BCR	C23-C24-C25-C30
16	7	103	BCR	C23-C24-C25-C30
16	8	1104	BCR	C5-C6-C7-C8
16	8	1104	BCR	C23-C24-C25-C30
16	8	1105	BCR	C5-C6-C7-C8
16	9	4001	BCR	C5-C6-C7-C8
16	9	4001	BCR	C23-C24-C25-C30
16	9	4004	BCR	C5-C6-C7-C8
16	9	4004	BCR	C23-C24-C25-C26
16	0	201	BCR	C5-C6-C7-C8
16	0	201	BCR	C23-C24-C25-C30
16	0	204	BCR	C23-C24-C25-C26
16	0	207	BCR	C5-C6-C7-C8
16	z	101	BCR	C5-C6-C7-C8
16	z	101	BCR	C23-C24-C25-C26
13	B	814	CLA	O1A-CGA-O2A-C1
13	B	815	CLA	CBD-CGD-O2D-CED
17	A	849	LHG	C30-C31-C32-C33
17	a	849	LHG	C30-C31-C32-C33
17	1	849	LHG	C30-C31-C32-C33
13	b	814	CLA	O1A-CGA-O2A-C1
13	2	806	CLA	O1A-CGA-O2A-C1
13	b	806	CLA	O1A-CGA-O2A-C1
13	B	821	CLA	C6-C7-C8-C10
13	B	837	CLA	C6-C7-C8-C10
13	b	821	CLA	C6-C7-C8-C10
13	b	837	CLA	C6-C7-C8-C10
13	2	820	CLA	C6-C7-C8-C10
13	2	836	CLA	C6-C7-C8-C10
14	A	843	PQN	C16-C17-C18-C20
14	a	843	PQN	C16-C17-C18-C20
14	1	843	PQN	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
13	A	819	CLA	C2A-CAA-CBA-CGA
13	A	828	CLA	C2A-CAA-CBA-CGA
13	A	837	CLA	C2A-CAA-CBA-CGA
13	B	806	CLA	C2A-CAA-CBA-CGA
13	a	819	CLA	C2A-CAA-CBA-CGA
13	a	828	CLA	C2A-CAA-CBA-CGA
13	a	837	CLA	C2A-CAA-CBA-CGA
13	b	806	CLA	C2A-CAA-CBA-CGA
13	1	819	CLA	C2A-CAA-CBA-CGA
13	1	837	CLA	C2A-CAA-CBA-CGA
13	2	806	CLA	C2A-CAA-CBA-CGA
19	7	101	SQD	O47-C45-C46-O48
19	I	103	SQD	C27-C28-C29-C30
13	2	813	CLA	O1A-CGA-O2A-C1
19	i	101	SQD	C27-C28-C29-C30
19	7	101	SQD	C27-C28-C29-C30
13	A	835	CLA	C11-C10-C8-C7
13	a	835	CLA	C11-C10-C8-C7
13	1	835	CLA	C11-C10-C8-C7
16	F	205	BCR	C37-C22-C23-C24
16	J	1104	BCR	C7-C8-C9-C34
16	f	205	BCR	C37-C22-C23-C24
16	j	1104	BCR	C7-C8-C9-C34
16	6	205	BCR	C37-C22-C23-C24
13	B	806	CLA	O1A-CGA-O2A-C1
13	A	832	CLA	C2-C3-C5-C6
13	1	832	CLA	C2-C3-C5-C6
19	7	101	SQD	C17-C18-C19-C20
13	A	826	CLA	C2-C1-O2A-CGA
13	B	833	CLA	C2-C1-O2A-CGA
13	a	826	CLA	C2-C1-O2A-CGA
13	b	833	CLA	C2-C1-O2A-CGA
13	1	826	CLA	C2-C1-O2A-CGA
13	2	832	CLA	C2-C1-O2A-CGA
16	K	4004	BCR	C7-C8-C9-C10
16	k	4004	BCR	C7-C8-C9-C10
16	1	845	BCR	C21-C22-C23-C24
19	i	101	SQD	C17-C18-C19-C20
19	I	103	SQD	C17-C18-C19-C20
16	A	846	BCR	C19-C20-C21-C22
16	F	202	BCR	C13-C14-C15-C16
16	a	846	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
16	f	202	BCR	C13-C14-C15-C16
16	1	846	BCR	C19-C20-C21-C22
16	6	202	BCR	C13-C14-C15-C16
13	A	825	CLA	CAA-CBA-CGA-O1A
13	a	825	CLA	CAA-CBA-CGA-O1A
13	1	825	CLA	CAA-CBA-CGA-O1A
13	B	808	CLA	C2-C3-C5-C6
13	a	832	CLA	C2-C3-C5-C6
13	b	808	CLA	C2-C3-C5-C6
13	2	807	CLA	C2-C3-C5-C6
13	2	806	CLA	C16-C17-C18-C20
13	J	1103	CLA	C2A-CAA-CBA-CGA
13	j	1103	CLA	C2A-CAA-CBA-CGA
13	8	1103	CLA	C2A-CAA-CBA-CGA
13	B	806	CLA	C16-C17-C18-C20
13	b	806	CLA	C16-C17-C18-C20
13	B	827	CLA	CAA-CBA-CGA-O2A
13	b	827	CLA	CAA-CBA-CGA-O2A
13	2	826	CLA	CAA-CBA-CGA-O2A
13	A	805	CLA	C4B-C3B-CAB-CBB
13	A	807	CLA	C4B-C3B-CAB-CBB
13	A	808	CLA	C4B-C3B-CAB-CBB
13	B	808	CLA	C4B-C3B-CAB-CBB
13	B	821	CLA	C4B-C3B-CAB-CBB
13	a	805	CLA	C4B-C3B-CAB-CBB
13	a	807	CLA	C4B-C3B-CAB-CBB
13	a	808	CLA	C4B-C3B-CAB-CBB
13	b	808	CLA	C4B-C3B-CAB-CBB
13	b	821	CLA	C4B-C3B-CAB-CBB
13	1	805	CLA	C4B-C3B-CAB-CBB
13	1	807	CLA	C4B-C3B-CAB-CBB
13	1	808	CLA	C4B-C3B-CAB-CBB
13	2	807	CLA	C4B-C3B-CAB-CBB
13	2	820	CLA	C4B-C3B-CAB-CBB
13	a	852	CLA	C8-C10-C11-C12
13	1	852	CLA	C8-C10-C11-C12
13	A	852	CLA	C8-C10-C11-C12
16	A	848	BCR	C11-C10-C9-C34
16	B	841	BCR	C11-C10-C9-C34
16	L	205	BCR	C20-C21-C22-C37
16	a	848	BCR	C11-C10-C9-C34
16	b	841	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
16	l	206	BCR	C20-C21-C22-C37
16	1	848	BCR	C11-C10-C9-C34
16	2	840	BCR	C11-C10-C9-C34
16	0	207	BCR	C20-C21-C22-C37
13	B	814	CLA	CAA-CBA-CGA-O2A
13	b	814	CLA	CAA-CBA-CGA-O2A
13	2	813	CLA	CAA-CBA-CGA-O2A
19	I	103	SQD	O47-C45-C46-O48
19	i	101	SQD	O47-C45-C46-O48
13	K	4003	CLA	CAA-CBA-CGA-O2A
13	k	4003	CLA	CAA-CBA-CGA-O2A
13	9	4003	CLA	CAA-CBA-CGA-O2A
13	B	807	CLA	C5-C6-C7-C8
16	A	845	BCR	C21-C22-C23-C24
16	a	845	BCR	C21-C22-C23-C24
13	B	803	CLA	C11-C10-C8-C9
13	B	806	CLA	C11-C10-C8-C9
13	L	201	CLA	C6-C7-C8-C9
13	b	803	CLA	C11-C10-C8-C9
13	b	806	CLA	C11-C10-C8-C9
13	l	202	CLA	C6-C7-C8-C9
13	2	803	CLA	C11-C10-C8-C9
13	2	806	CLA	C11-C10-C8-C9
13	0	202	CLA	C6-C7-C8-C9
13	A	810	CLA	CAA-CBA-CGA-O2A
13	a	810	CLA	CAA-CBA-CGA-O2A
13	1	810	CLA	CAA-CBA-CGA-O2A
13	A	813	CLA	C2-C1-O2A-CGA
13	B	804	CLA	C2-C1-O2A-CGA
13	a	813	CLA	C2-C1-O2A-CGA
13	b	804	CLA	C2-C1-O2A-CGA
13	1	813	CLA	C2-C1-O2A-CGA
13	2	804	CLA	C2-C1-O2A-CGA
13	I	101	CLA	C16-C17-C18-C20
13	i	102	CLA	C16-C17-C18-C20
13	7	102	CLA	C16-C17-C18-C20
13	b	807	CLA	C5-C6-C7-C8
13	0	203	CLA	C5-C6-C7-C8
13	A	808	CLA	C3A-C2A-CAA-CBA
13	B	818	CLA	C3A-C2A-CAA-CBA
13	B	847	CLA	C3A-C2A-CAA-CBA
13	a	808	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	b	818	CLA	C3A-C2A-CAA-CBA
13	b	847	CLA	C3A-C2A-CAA-CBA
13	1	808	CLA	C3A-C2A-CAA-CBA
13	2	817	CLA	C3A-C2A-CAA-CBA
13	2	846	CLA	C3A-C2A-CAA-CBA
13	a	818	CLA	CAA-CBA-CGA-O2A
13	A	818	CLA	CAA-CBA-CGA-O2A
13	9	4003	CLA	O1D-CGD-O2D-CED
13	1	818	CLA	CAA-CBA-CGA-O2A
18	B	846	LMG	C29-C30-C31-C32
18	2	845	LMG	C29-C30-C31-C32
13	B	827	CLA	CAA-CBA-CGA-O1A
13	b	827	CLA	CAA-CBA-CGA-O1A
13	2	826	CLA	CAA-CBA-CGA-O1A
18	b	846	LMG	C29-C30-C31-C32
16	A	845	BCR	C20-C21-C22-C23
16	B	841	BCR	C11-C10-C9-C8
16	B	842	BCR	C11-C10-C9-C8
16	F	202	BCR	C16-C17-C18-C19
16	F	205	BCR	C12-C13-C14-C15
16	L	202	BCR	C20-C21-C22-C23
16	b	841	BCR	C11-C10-C9-C8
16	b	842	BCR	C11-C10-C9-C8
16	f	202	BCR	C16-C17-C18-C19
16	f	205	BCR	C12-C13-C14-C15
16	l	203	BCR	C20-C21-C22-C23
16	2	840	BCR	C11-C10-C9-C8
16	2	841	BCR	C11-C10-C9-C8
16	6	202	BCR	C16-C17-C18-C19
16	6	205	BCR	C12-C13-C14-C15
16	0	204	BCR	C20-C21-C22-C23
13	k	4003	CLA	O1D-CGD-O2D-CED
13	K	4003	CLA	O1D-CGD-O2D-CED
13	b	815	CLA	O1D-CGD-O2D-CED
13	B	815	CLA	O1D-CGD-O2D-CED
13	A	821	CLA	C2A-CAA-CBA-CGA
13	a	821	CLA	C2A-CAA-CBA-CGA
13	1	821	CLA	C2A-CAA-CBA-CGA
13	A	810	CLA	CAA-CBA-CGA-O1A
13	a	810	CLA	CAA-CBA-CGA-O1A
13	1	810	CLA	CAA-CBA-CGA-O1A
13	a	835	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
13	B	810	CLA	C11-C10-C8-C9
13	B	829	CLA	C11-C10-C8-C9
13	b	810	CLA	C11-C10-C8-C9
13	b	829	CLA	C11-C10-C8-C9
13	2	809	CLA	C11-C10-C8-C9
13	2	828	CLA	C11-C10-C8-C9
13	A	835	CLA	CAA-CBA-CGA-O2A
16	F	202	BCR	C7-C8-C9-C10
16	f	202	BCR	C7-C8-C9-C10
16	6	202	BCR	C7-C8-C9-C10
13	1	835	CLA	CAA-CBA-CGA-O2A
13	2	814	CLA	O1D-CGD-O2D-CED
13	A	841	CLA	C11-C10-C8-C7
13	B	803	CLA	C11-C10-C8-C7
13	B	804	CLA	C11-C12-C13-C15
13	B	813	CLA	C11-C12-C13-C15
13	L	201	CLA	C6-C7-C8-C10
13	a	841	CLA	C11-C10-C8-C7
13	b	803	CLA	C11-C10-C8-C7
13	b	804	CLA	C11-C12-C13-C15
13	b	813	CLA	C11-C12-C13-C15
13	l	202	CLA	C6-C7-C8-C10
13	1	841	CLA	C11-C10-C8-C7
13	2	803	CLA	C11-C10-C8-C7
13	2	804	CLA	C11-C12-C13-C15
13	2	812	CLA	C11-C12-C13-C15
13	0	202	CLA	C6-C7-C8-C10
13	A	808	CLA	C2B-C3B-CAB-CBB
13	A	824	CLA	C2B-C3B-CAB-CBB
13	A	825	CLA	C2B-C3B-CAB-CBB
13	A	826	CLA	C2B-C3B-CAB-CBB
13	A	827	CLA	C2B-C3B-CAB-CBB
13	A	829	CLA	C2B-C3B-CAB-CBB
13	A	832	CLA	C2B-C3B-CAB-CBB
13	A	840	CLA	C2B-C3B-CAB-CBB
13	B	805	CLA	C2B-C3B-CAB-CBB
13	B	814	CLA	C2B-C3B-CAB-CBB
13	B	820	CLA	C2B-C3B-CAB-CBB
13	B	826	CLA	C2B-C3B-CAB-CBB
13	B	833	CLA	C2B-C3B-CAB-CBB
13	B	835	CLA	C2B-C3B-CAB-CBB
13	L	204	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	a	808	CLA	C2B-C3B-CAB-CBB
13	a	824	CLA	C2B-C3B-CAB-CBB
13	a	825	CLA	C2B-C3B-CAB-CBB
13	a	826	CLA	C2B-C3B-CAB-CBB
13	a	827	CLA	C2B-C3B-CAB-CBB
13	a	829	CLA	C2B-C3B-CAB-CBB
13	a	832	CLA	C2B-C3B-CAB-CBB
13	a	840	CLA	C2B-C3B-CAB-CBB
13	b	805	CLA	C2B-C3B-CAB-CBB
13	b	814	CLA	C2B-C3B-CAB-CBB
13	b	820	CLA	C2B-C3B-CAB-CBB
13	b	826	CLA	C2B-C3B-CAB-CBB
13	b	833	CLA	C2B-C3B-CAB-CBB
13	b	835	CLA	C2B-C3B-CAB-CBB
13	l	205	CLA	C2B-C3B-CAB-CBB
13	1	808	CLA	C2B-C3B-CAB-CBB
13	1	824	CLA	C2B-C3B-CAB-CBB
13	1	825	CLA	C2B-C3B-CAB-CBB
13	1	826	CLA	C2B-C3B-CAB-CBB
13	1	827	CLA	C2B-C3B-CAB-CBB
13	1	829	CLA	C2B-C3B-CAB-CBB
13	1	832	CLA	C2B-C3B-CAB-CBB
13	1	840	CLA	C2B-C3B-CAB-CBB
13	2	805	CLA	C2B-C3B-CAB-CBB
13	2	813	CLA	C2B-C3B-CAB-CBB
13	2	819	CLA	C2B-C3B-CAB-CBB
13	2	825	CLA	C2B-C3B-CAB-CBB
13	2	832	CLA	C2B-C3B-CAB-CBB
13	2	834	CLA	C2B-C3B-CAB-CBB
13	0	206	CLA	C2B-C3B-CAB-CBB
16	A	845	BCR	C23-C24-C25-C26
16	A	848	BCR	C5-C6-C7-C8
16	B	842	BCR	C1-C6-C7-C8
16	B	842	BCR	C5-C6-C7-C8
16	B	842	BCR	C23-C24-C25-C26
16	B	845	BCR	C23-C24-C25-C26
16	F	205	BCR	C23-C24-C25-C26
16	F	205	BCR	C23-C24-C25-C30
16	I	102	BCR	C5-C6-C7-C8
16	L	207	BCR	C23-C24-C25-C26
16	a	845	BCR	C23-C24-C25-C26
16	a	848	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
16	b	842	BCR	C1-C6-C7-C8
16	b	842	BCR	C5-C6-C7-C8
16	b	842	BCR	C23-C24-C25-C26
16	b	845	BCR	C23-C24-C25-C26
16	f	205	BCR	C23-C24-C25-C26
16	f	205	BCR	C23-C24-C25-C30
16	i	103	BCR	C5-C6-C7-C8
16	l	201	BCR	C23-C24-C25-C26
16	1	845	BCR	C23-C24-C25-C26
16	1	848	BCR	C5-C6-C7-C8
16	2	841	BCR	C1-C6-C7-C8
16	2	841	BCR	C5-C6-C7-C8
16	2	841	BCR	C23-C24-C25-C26
16	2	844	BCR	C23-C24-C25-C26
16	6	205	BCR	C23-C24-C25-C26
16	6	205	BCR	C23-C24-C25-C30
16	7	103	BCR	C5-C6-C7-C8
16	8	1104	BCR	C23-C24-C25-C26
16	9	4001	BCR	C23-C24-C25-C26
16	0	201	BCR	C23-C24-C25-C26
13	b	819	CLA	CAA-CBA-CGA-O2A
13	B	807	CLA	C2-C1-O2A-CGA
13	b	807	CLA	C2-C1-O2A-CGA
13	0	203	CLA	C2-C1-O2A-CGA
13	A	806	CLA	CAA-CBA-CGA-O2A
13	B	804	CLA	CAA-CBA-CGA-O2A
13	B	819	CLA	CAA-CBA-CGA-O2A
13	a	806	CLA	CAA-CBA-CGA-O2A
13	a	821	CLA	CAA-CBA-CGA-O2A
13	b	804	CLA	CAA-CBA-CGA-O2A
13	2	804	CLA	CAA-CBA-CGA-O2A
13	2	818	CLA	CAA-CBA-CGA-O2A
13	B	829	CLA	C10-C11-C12-C13
13	b	829	CLA	C10-C11-C12-C13
13	2	828	CLA	C10-C11-C12-C13
13	A	821	CLA	CAA-CBA-CGA-O2A
13	1	806	CLA	CAA-CBA-CGA-O2A
13	1	821	CLA	CAA-CBA-CGA-O2A
13	A	829	CLA	C15-C16-C17-C18
13	1	829	CLA	C15-C16-C17-C18
13	2	828	CLA	C8-C10-C11-C12
13	B	828	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
13	b	828	CLA	C2A-CAA-CBA-CGA
13	2	827	CLA	C2A-CAA-CBA-CGA
13	a	829	CLA	C15-C16-C17-C18
13	b	829	CLA	C8-C10-C11-C12
13	A	842	CLA	CAA-CBA-CGA-O2A
13	J	1103	CLA	CAA-CBA-CGA-O2A
13	a	842	CLA	CAA-CBA-CGA-O2A
13	j	1103	CLA	CAA-CBA-CGA-O2A
13	1	842	CLA	CAA-CBA-CGA-O2A
13	8	1103	CLA	CAA-CBA-CGA-O2A
13	A	827	CLA	CAA-CBA-CGA-O2A
13	a	827	CLA	CAA-CBA-CGA-O2A
13	1	827	CLA	CAA-CBA-CGA-O2A
13	B	829	CLA	C8-C10-C11-C12
13	B	810	CLA	CAA-CBA-CGA-O2A
13	a	813	CLA	CAA-CBA-CGA-O2A
13	b	810	CLA	CAA-CBA-CGA-O2A
13	1	813	CLA	CAA-CBA-CGA-O2A
13	2	809	CLA	CAA-CBA-CGA-O2A
13	A	813	CLA	CAA-CBA-CGA-O2A
13	1	852	CLA	C11-C12-C13-C14
13	A	817	CLA	C4B-C3B-CAB-CBB
13	A	829	CLA	C4B-C3B-CAB-CBB
13	B	804	CLA	C4B-C3B-CAB-CBB
13	B	812	CLA	C4B-C3B-CAB-CBB
13	J	1102	CLA	C4B-C3B-CAB-CBB
13	L	204	CLA	C1A-C2A-CAA-CBA
13	a	817	CLA	C4B-C3B-CAB-CBB
13	a	829	CLA	C4B-C3B-CAB-CBB
13	b	804	CLA	C4B-C3B-CAB-CBB
13	b	812	CLA	C4B-C3B-CAB-CBB
13	j	1102	CLA	C4B-C3B-CAB-CBB
13	l	205	CLA	C1A-C2A-CAA-CBA
13	1	817	CLA	C4B-C3B-CAB-CBB
13	1	829	CLA	C4B-C3B-CAB-CBB
13	2	804	CLA	C4B-C3B-CAB-CBB
13	2	811	CLA	C4B-C3B-CAB-CBB
13	8	1102	CLA	C4B-C3B-CAB-CBB
13	0	206	CLA	C1A-C2A-CAA-CBA
16	A	851	BCR	C21-C22-C23-C24
16	K	4001	BCR	C21-C22-C23-C24
16	a	851	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
16	k	4001	BCR	C21-C22-C23-C24
16	1	851	BCR	C21-C22-C23-C24
16	9	4001	BCR	C21-C22-C23-C24
16	B	843	BCR	C9-C10-C11-C12
16	b	843	BCR	C9-C10-C11-C12
16	2	842	BCR	C9-C10-C11-C12
13	k	4003	CLA	CBD-CGD-O2D-CED
13	A	852	CLA	C11-C12-C13-C14
13	a	852	CLA	C11-C12-C13-C14
13	a	829	CLA	C5-C6-C7-C8
13	b	803	CLA	C5-C6-C7-C8
13	2	803	CLA	C5-C6-C7-C8
13	A	833	CLA	CAA-CBA-CGA-O2A
13	B	818	CLA	CAA-CBA-CGA-O2A
13	a	833	CLA	CAA-CBA-CGA-O2A
13	b	818	CLA	CAA-CBA-CGA-O2A
13	1	833	CLA	CAA-CBA-CGA-O2A
13	K	4003	CLA	CBD-CGD-O2D-CED
13	9	4003	CLA	CBD-CGD-O2D-CED
13	1	809	CLA	O1A-CGA-O2A-C1
13	B	803	CLA	C5-C6-C7-C8
13	A	829	CLA	C5-C6-C7-C8
13	1	829	CLA	C5-C6-C7-C8
13	A	809	CLA	O1A-CGA-O2A-C1
13	L	203	CLA	CAA-CBA-CGA-O2A
13	l	204	CLA	CAA-CBA-CGA-O2A
13	2	817	CLA	CAA-CBA-CGA-O2A
13	0	205	CLA	CAA-CBA-CGA-O2A
13	j	1103	CLA	CAA-CBA-CGA-O1A
19	I	103	SQD	C5-C6-S-O7
19	i	101	SQD	C5-C6-S-O7
19	7	101	SQD	C5-C6-S-O7
14	A	843	PQN	C25-C26-C27-C28
14	a	843	PQN	C25-C26-C27-C28
14	1	843	PQN	C25-C26-C27-C28
13	A	802	CLA	C11-C12-C13-C14
13	a	802	CLA	C11-C12-C13-C14
13	1	802	CLA	C11-C12-C13-C14
13	a	809	CLA	O1A-CGA-O2A-C1
13	J	1103	CLA	CAA-CBA-CGA-O1A
13	A	817	CLA	CAA-CBA-CGA-O2A
13	B	807	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
13	a	817	CLA	CAA-CBA-CGA-O2A
13	b	807	CLA	CAA-CBA-CGA-O2A
13	0	203	CLA	CAA-CBA-CGA-O2A
19	I	103	SQD	C10-C11-C12-C13
13	8	1103	CLA	CAA-CBA-CGA-O1A
19	i	101	SQD	C10-C11-C12-C13
19	7	101	SQD	C10-C11-C12-C13
13	1	817	CLA	CAA-CBA-CGA-O2A
13	A	836	CLA	CBA-CGA-O2A-C1
13	1	839	CLA	CBA-CGA-O2A-C1
13	A	826	CLA	C4-C3-C5-C6
13	F	201	CLA	C3A-C2A-CAA-CBA
13	K	4005	CLA	CHA-CBD-CGD-O1D
13	a	826	CLA	C4-C3-C5-C6
13	f	201	CLA	C3A-C2A-CAA-CBA
13	k	4005	CLA	CHA-CBD-CGD-O1D
13	1	826	CLA	C4-C3-C5-C6
13	6	201	CLA	C3A-C2A-CAA-CBA
13	9	4005	CLA	CHA-CBD-CGD-O1D
13	A	806	CLA	CAA-CBA-CGA-O1A
13	B	810	CLA	CAA-CBA-CGA-O1A
13	a	806	CLA	CAA-CBA-CGA-O1A
13	b	810	CLA	CAA-CBA-CGA-O1A
13	1	806	CLA	CAA-CBA-CGA-O1A
13	2	809	CLA	CAA-CBA-CGA-O1A
16	B	845	BCR	C11-C10-C9-C8
16	B	845	BCR	C12-C13-C14-C15
16	b	845	BCR	C11-C10-C9-C8
16	b	845	BCR	C12-C13-C14-C15
16	2	844	BCR	C11-C10-C9-C8
16	2	844	BCR	C12-C13-C14-C15
13	A	842	CLA	CAA-CBA-CGA-O1A
13	a	842	CLA	CAA-CBA-CGA-O1A
13	1	842	CLA	CAA-CBA-CGA-O1A
13	A	809	CLA	CBA-CGA-O2A-C1
13	A	839	CLA	CBA-CGA-O2A-C1
13	a	809	CLA	CBA-CGA-O2A-C1
13	a	836	CLA	CBA-CGA-O2A-C1
13	a	839	CLA	CBA-CGA-O2A-C1
13	1	836	CLA	CBA-CGA-O2A-C1
13	A	821	CLA	CAA-CBA-CGA-O1A
13	a	821	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
13	1	821	CLA	CAA-CBA-CGA-O1A
13	a	832	CLA	C13-C15-C16-C17
13	A	825	CLA	C2A-CAA-CBA-CGA
13	a	825	CLA	C2A-CAA-CBA-CGA
13	1	825	CLA	C2A-CAA-CBA-CGA
13	1	809	CLA	CBA-CGA-O2A-C1
13	A	833	CLA	C14-C13-C15-C16
13	B	813	CLA	C11-C12-C13-C14
13	B	837	CLA	C6-C7-C8-C9
13	a	833	CLA	C14-C13-C15-C16
13	b	813	CLA	C11-C12-C13-C14
13	b	837	CLA	C6-C7-C8-C9
13	1	833	CLA	C14-C13-C15-C16
13	2	812	CLA	C11-C12-C13-C14
13	2	836	CLA	C6-C7-C8-C9
14	A	843	PQN	C16-C17-C18-C19
14	a	843	PQN	C16-C17-C18-C19
14	1	843	PQN	C16-C17-C18-C19
13	B	819	CLA	CAA-CBA-CGA-O1A
13	b	819	CLA	CAA-CBA-CGA-O1A
13	2	818	CLA	CAA-CBA-CGA-O1A
13	A	832	CLA	C13-C15-C16-C17
13	1	832	CLA	C13-C15-C16-C17
13	A	819	CLA	C4-C3-C5-C6
13	a	819	CLA	C4-C3-C5-C6
13	A	813	CLA	CAA-CBA-CGA-O1A
13	A	827	CLA	CAA-CBA-CGA-O1A
13	L	203	CLA	CAA-CBA-CGA-O1A
13	a	827	CLA	CAA-CBA-CGA-O1A
13	1	827	CLA	CAA-CBA-CGA-O1A
13	0	205	CLA	CAA-CBA-CGA-O1A
13	b	815	CLA	CAA-CBA-CGA-O2A
13	A	836	CLA	O1A-CGA-O2A-C1
13	a	836	CLA	O1A-CGA-O2A-C1
13	1	836	CLA	O1A-CGA-O2A-C1
13	1	813	CLA	CAA-CBA-CGA-O1A
13	b	828	CLA	C5-C6-C7-C8
13	B	828	CLA	C5-C6-C7-C8
13	2	827	CLA	C5-C6-C7-C8
13	B	807	CLA	CAA-CBA-CGA-O1A
13	a	813	CLA	CAA-CBA-CGA-O1A
13	1	204	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
13	A	835	CLA	CAA-CBA-CGA-O1A
13	b	807	CLA	CAA-CBA-CGA-O1A
13	1	835	CLA	CAA-CBA-CGA-O1A
13	0	203	CLA	CAA-CBA-CGA-O1A
13	B	815	CLA	CAA-CBA-CGA-O2A
13	2	814	CLA	CAA-CBA-CGA-O2A
13	A	802	CLA	C2C-C3C-CAC-CBC
13	a	802	CLA	C2C-C3C-CAC-CBC
13	a	835	CLA	CAA-CBA-CGA-O1A
13	B	821	CLA	CAA-CBA-CGA-O2A
13	b	821	CLA	CAA-CBA-CGA-O2A
13	2	820	CLA	CAA-CBA-CGA-O2A
13	B	818	CLA	CAA-CBA-CGA-O1A
13	b	818	CLA	CAA-CBA-CGA-O1A
13	1	802	CLA	C2C-C3C-CAC-CBC
13	A	807	CLA	CAD-CBD-CGD-O2D
13	A	816	CLA	CAD-CBD-CGD-O2D
13	A	826	CLA	CAD-CBD-CGD-O2D
13	B	826	CLA	CAD-CBD-CGD-O2D
13	a	807	CLA	CAD-CBD-CGD-O2D
13	a	816	CLA	CAD-CBD-CGD-O2D
13	a	826	CLA	CAD-CBD-CGD-O2D
13	b	826	CLA	CAD-CBD-CGD-O2D
13	1	807	CLA	CAD-CBD-CGD-O2D
13	1	816	CLA	CAD-CBD-CGD-O2D
13	1	826	CLA	CAD-CBD-CGD-O2D
13	2	825	CLA	CAD-CBD-CGD-O2D
13	A	833	CLA	CAA-CBA-CGA-O1A
13	a	833	CLA	CAA-CBA-CGA-O1A
13	1	833	CLA	CAA-CBA-CGA-O1A
13	2	817	CLA	CAA-CBA-CGA-O1A
16	A	845	BCR	C6-C7-C8-C9
16	B	845	BCR	C6-C7-C8-C9
16	a	845	BCR	C6-C7-C8-C9
16	b	845	BCR	C6-C7-C8-C9
16	1	845	BCR	C6-C7-C8-C9
16	2	844	BCR	C6-C7-C8-C9
13	I	101	CLA	CAA-CBA-CGA-O2A
13	A	836	CLA	C2A-CAA-CBA-CGA
13	a	836	CLA	C2A-CAA-CBA-CGA
13	1	836	CLA	C2A-CAA-CBA-CGA
13	B	802	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
13	1	819	CLA	C4-C3-C5-C6
13	2	812	CLA	C6-C7-C8-C10
13	A	823	CLA	CAA-CBA-CGA-O2A
13	a	823	CLA	CAA-CBA-CGA-O2A
13	i	102	CLA	CAA-CBA-CGA-O2A
13	1	823	CLA	CAA-CBA-CGA-O2A
13	7	102	CLA	CAA-CBA-CGA-O2A
13	2	802	CLA	C10-C11-C12-C13
13	a	823	CLA	CAA-CBA-CGA-O1A
13	b	802	CLA	C10-C11-C12-C13
13	A	823	CLA	CAA-CBA-CGA-O1A
13	1	823	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

336 monomers are involved in 858 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	838	CLA	1	0
13	B	802	CLA	5	0
16	8	1105	BCR	2	0
16	9	4001	BCR	4	0
13	2	811	CLA	1	0
13	1	837	CLA	3	0
13	1	827	CLA	3	0
13	B	828	CLA	2	0
13	2	808	CLA	1	0
13	b	816	CLA	1	0
19	7	101	SQD	12	0
13	b	833	CLA	2	0
13	1	818	CLA	4	0
13	B	831	CLA	2	0
13	b	835	CLA	2	0
16	9	4004	BCR	1	0
13	B	818	CLA	1	0
13	a	810	CLA	1	0
16	J	1104	BCR	2	0
13	2	827	CLA	2	0
16	b	842	BCR	1	0
13	a	835	CLA	1	0
16	J	1105	BCR	1	0
13	a	821	CLA	6	0
13	L	204	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	835	CLA	1	0
16	A	846	BCR	5	0
13	8	1101	CLA	1	0
13	b	847	CLA	2	0
13	b	838	CLA	1	0
19	I	103	SQD	13	0
16	z	101	BCR	3	0
13	1	817	CLA	3	0
16	1	846	BCR	3	0
13	2	814	CLA	4	0
13	2	803	CLA	1	0
16	a	846	BCR	4	0
13	B	816	CLA	1	0
13	A	824	CLA	3	0
13	B	823	CLA	4	0
13	B	829	CLA	4	0
13	A	830	CLA	4	0
13	2	806	CLA	9	0
16	1	848	BCR	6	0
16	2	839	BCR	4	0
18	2	845	LMG	3	0
13	1	822	CLA	1	0
12	1	801	CL0	5	0
16	k	4001	BCR	1	0
16	1	851	BCR	2	0
13	A	822	CLA	1	0
13	A	831	CLA	4	0
13	f	201	CLA	5	0
13	b	814	CLA	3	0
13	2	804	CLA	5	0
13	b	817	CLA	1	0
15	3	102	SF4	1	0
16	i	103	BCR	5	0
16	A	851	BCR	2	0
13	1	805	CLA	4	0
13	1	828	CLA	9	0
13	B	833	CLA	2	0
13	A	802	CLA	5	0
13	A	807	CLA	1	0
13	a	831	CLA	4	0
16	a	851	BCR	2	0
13	b	830	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	2	802	CLA	4	0
13	a	823	CLA	2	0
13	A	806	CLA	6	0
13	a	802	CLA	5	0
13	i	102	CLA	9	0
13	L	203	CLA	9	0
13	a	828	CLA	9	0
14	1	843	PQN	2	0
13	A	823	CLA	2	0
13	A	841	CLA	5	0
13	1	806	CLA	7	0
13	b	818	CLA	1	0
13	1	826	CLA	4	0
14	2	838	PQN	7	0
13	a	826	CLA	4	0
16	0	201	BCR	6	0
16	A	845	BCR	3	0
19	i	101	SQD	12	0
13	a	815	CLA	2	0
13	a	825	CLA	4	0
16	j	1104	BCR	2	0
13	b	801	CLA	1	0
13	A	826	CLA	3	0
16	0	207	BCR	1	0
16	F	202	BCR	2	0
13	b	804	CLA	7	0
13	L	206	CLA	7	0
16	6	202	BCR	1	0
16	2	840	BCR	5	0
13	B	827	CLA	2	0
16	L	202	BCR	2	0
13	A	819	CLA	5	0
13	l	205	CLA	1	0
13	0	202	CLA	2	0
13	7	102	CLA	8	0
13	L	201	CLA	2	0
13	B	801	CLA	1	0
16	2	844	BCR	3	0
13	1	815	CLA	2	0
13	a	813	CLA	4	0
13	2	836	CLA	3	0
13	B	830	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	1	838	CLA	5	0
13	2	831	CLA	1	0
13	a	827	CLA	2	0
16	M	101	BCR	2	0
16	2	847	BCR	4	0
13	A	813	CLA	3	0
13	B	837	CLA	3	0
13	B	817	CLA	1	0
13	B	820	CLA	2	0
13	A	809	CLA	2	0
13	2	810	CLA	2	0
13	a	838	CLA	5	0
16	b	844	BCR	4	0
16	0	204	BCR	3	0
13	b	811	CLA	2	0
13	2	813	CLA	2	0
16	l	201	BCR	7	0
13	B	836	CLA	4	0
13	a	818	CLA	4	0
16	7	103	BCR	3	0
13	2	828	CLA	4	0
13	1	810	CLA	1	0
13	b	805	CLA	6	0
13	b	828	CLA	2	0
13	A	836	CLA	1	0
13	a	834	CLA	4	0
13	1	835	CLA	1	0
13	A	808	CLA	4	0
13	b	823	CLA	3	0
13	1	821	CLA	6	0
13	1	813	CLA	3	0
16	b	841	BCR	4	0
16	A	847	BCR	4	0
16	m	101	BCR	2	0
13	a	830	CLA	4	0
13	a	809	CLA	1	0
16	K	4004	BCR	1	0
13	9	4003	CLA	1	0
16	l	206	BCR	3	0
13	A	852	CLA	8	0
13	B	826	CLA	3	0
13	A	818	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	a	803	CLA	2	0
13	A	827	CLA	2	0
13	1	834	CLA	4	0
13	a	852	CLA	9	0
16	b	843	BCR	2	0
13	1	842	CLA	1	0
16	8	1104	BCR	3	0
13	a	829	CLA	3	0
13	A	825	CLA	4	0
13	a	833	CLA	3	0
16	b	840	BCR	4	0
13	l	204	CLA	7	0
13	B	824	CLA	6	0
13	1	852	CLA	8	0
13	a	822	CLA	1	0
13	I	101	CLA	9	0
12	a	801	CL0	5	0
13	1	830	CLA	4	0
16	F	205	BCR	3	0
13	1	809	CLA	2	0
16	2	842	BCR	2	0
13	a	837	CLA	4	0
13	A	838	CLA	5	0
16	1	845	BCR	2	0
13	2	825	CLA	3	0
13	A	839	CLA	3	0
13	B	832	CLA	1	0
13	2	826	CLA	1	0
13	b	807	CLA	1	0
13	2	846	CLA	2	0
16	a	845	BCR	2	0
14	A	843	PQN	4	0
17	A	850	LHG	2	0
13	0	203	CLA	1	0
13	1	829	CLA	3	0
14	b	839	PQN	6	0
13	B	805	CLA	6	0
13	a	839	CLA	4	0
13	b	803	CLA	2	0
13	J	1101	CLA	1	0
13	2	822	CLA	3	0
13	b	815	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	b	829	CLA	4	0
13	b	837	CLA	3	0
13	B	812	CLA	1	0
13	b	802	CLA	3	0
13	1	823	CLA	2	0
13	1	839	CLA	3	0
13	2	823	CLA	7	0
13	8	1103	CLA	2	0
13	a	832	CLA	3	0
16	B	843	BCR	1	0
13	B	811	CLA	2	0
13	B	806	CLA	8	0
16	B	840	BCR	4	0
13	1	841	CLA	5	0
16	B	841	BCR	5	0
13	B	814	CLA	2	0
13	a	804	CLA	3	0
13	A	832	CLA	3	0
17	1	850	LHG	2	0
13	1	819	CLA	5	0
16	l	203	BCR	2	0
13	A	829	CLA	3	0
13	a	819	CLA	5	0
13	b	813	CLA	2	0
13	F	201	CLA	5	0
13	1	825	CLA	5	0
16	B	842	BCR	1	0
12	A	801	CL0	5	0
13	a	841	CLA	5	0
16	6	205	BCR	3	0
13	A	834	CLA	4	0
14	B	839	PQN	7	0
13	a	820	CLA	1	0
13	B	803	CLA	2	0
13	2	834	CLA	3	0
16	I	102	BCR	5	0
13	B	835	CLA	3	0
13	2	819	CLA	2	0
13	B	815	CLA	5	0
13	B	847	CLA	2	0
13	B	821	CLA	6	0
13	2	817	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	a	805	CLA	2	0
13	2	837	CLA	1	0
16	1	847	BCR	5	0
13	2	830	CLA	2	0
13	A	803	CLA	2	0
13	B	808	CLA	3	0
13	1	824	CLA	3	0
16	a	847	BCR	3	0
13	b	836	CLA	3	0
13	b	820	CLA	3	0
13	a	824	CLA	4	0
13	2	809	CLA	7	0
13	A	810	CLA	2	0
13	A	840	CLA	3	0
13	B	804	CLA	6	0
16	k	4004	BCR	1	0
13	b	827	CLA	2	0
13	J	1103	CLA	2	0
13	b	824	CLA	7	0
16	B	848	BCR	2	0
13	b	809	CLA	1	0
13	A	833	CLA	2	0
16	b	845	BCR	3	0
13	b	821	CLA	6	0
13	l	207	CLA	5	0
13	B	810	CLA	7	0
13	a	817	CLA	3	0
13	a	836	CLA	1	0
16	f	205	BCR	2	0
16	f	202	BCR	2	0
13	b	808	CLA	3	0
13	A	811	CLA	2	0
18	b	846	LMG	3	0
13	1	803	CLA	3	0
13	1	833	CLA	3	0
16	L	207	BCR	10	0
13	2	835	CLA	4	0
13	A	820	CLA	1	0
13	1	811	CLA	2	0
13	1	836	CLA	1	0
13	a	811	CLA	2	0
13	b	826	CLA	4	0

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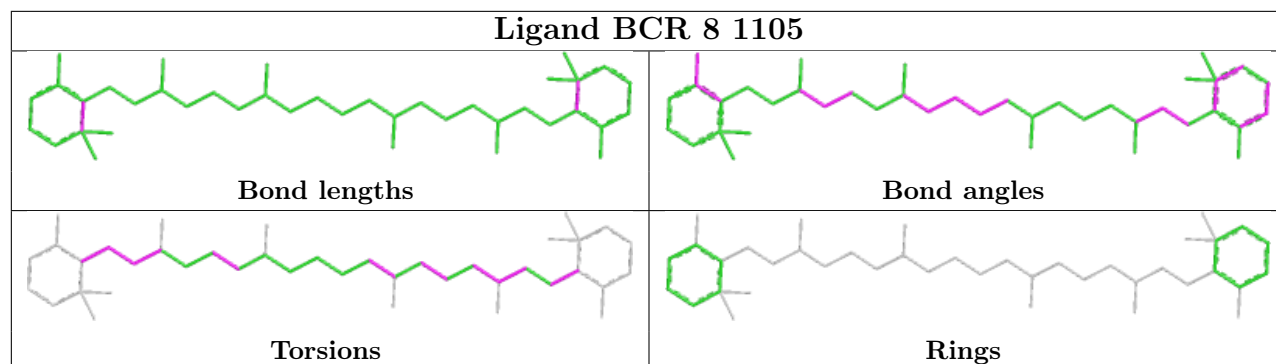
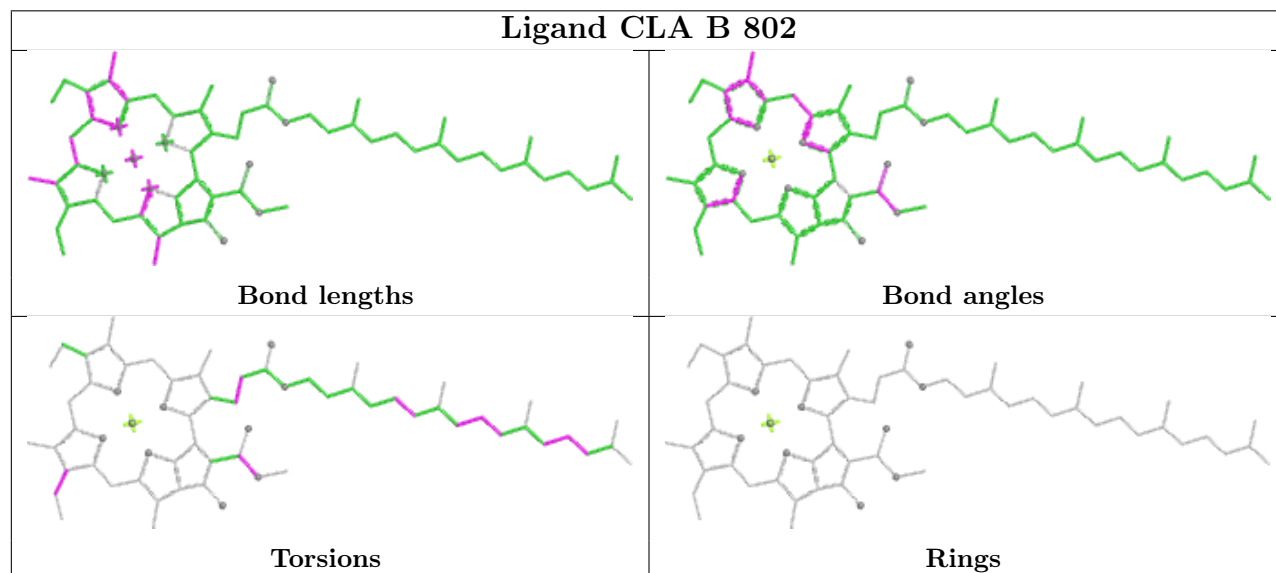
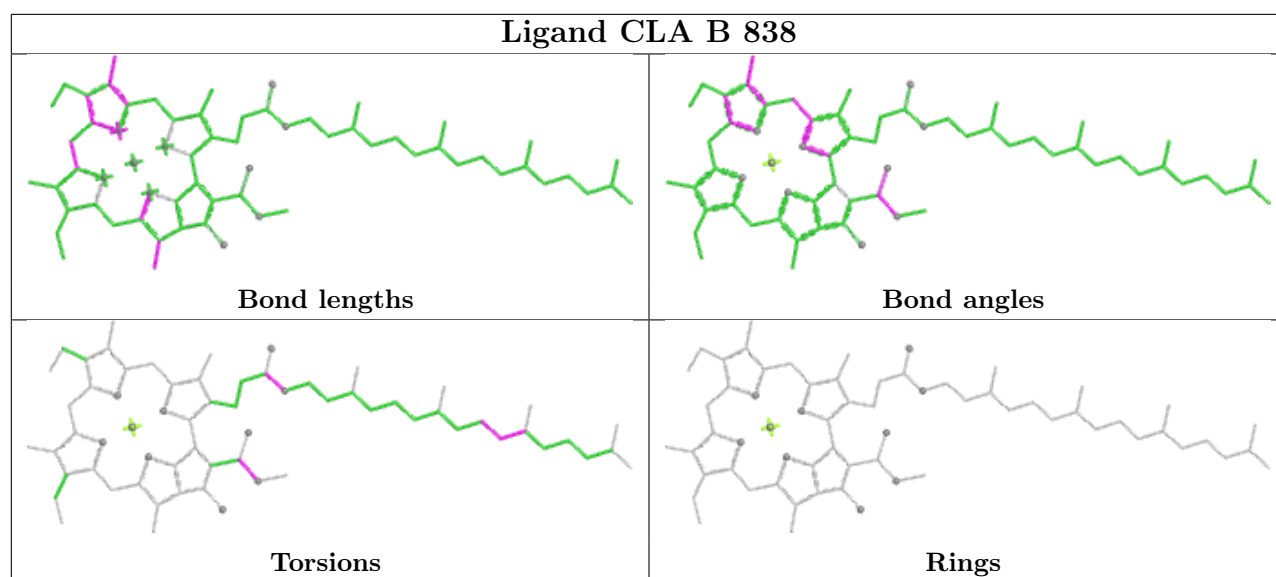
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	a	840	CLA	3	0
13	6	201	CLA	3	0
13	2	816	CLA	1	0
13	1	820	CLA	1	0
13	A	828	CLA	10	0
13	l	202	CLA	2	0
13	A	804	CLA	3	0
13	j	1101	CLA	1	0
13	a	808	CLA	4	0
16	B	845	BCR	3	0
13	1	831	CLA	4	0
16	A	848	BCR	6	0
16	L	205	BCR	4	0
16	2	843	BCR	5	0
13	f	203	CLA	1	0
16	B	844	BCR	4	0
13	2	832	CLA	2	0
13	j	1103	CLA	2	0
13	1	840	CLA	5	0
13	1	832	CLA	3	0
13	2	805	CLA	5	0
13	2	829	CLA	2	0
13	1	802	CLA	5	0
14	a	843	PQN	4	0
13	B	825	CLA	2	0
13	A	842	CLA	1	0
13	F	203	CLA	1	0
13	A	815	CLA	2	0
13	0	205	CLA	8	0
16	a	848	BCR	6	0
13	b	825	CLA	4	0
13	b	806	CLA	8	0
16	K	4001	BCR	1	0
13	1	808	CLA	4	0
13	b	832	CLA	1	0
13	1	807	CLA	1	0
16	2	841	BCR	1	0
13	a	842	CLA	1	0
13	2	807	CLA	3	0
13	2	812	CLA	2	0
13	b	810	CLA	7	0
13	2	824	CLA	4	0

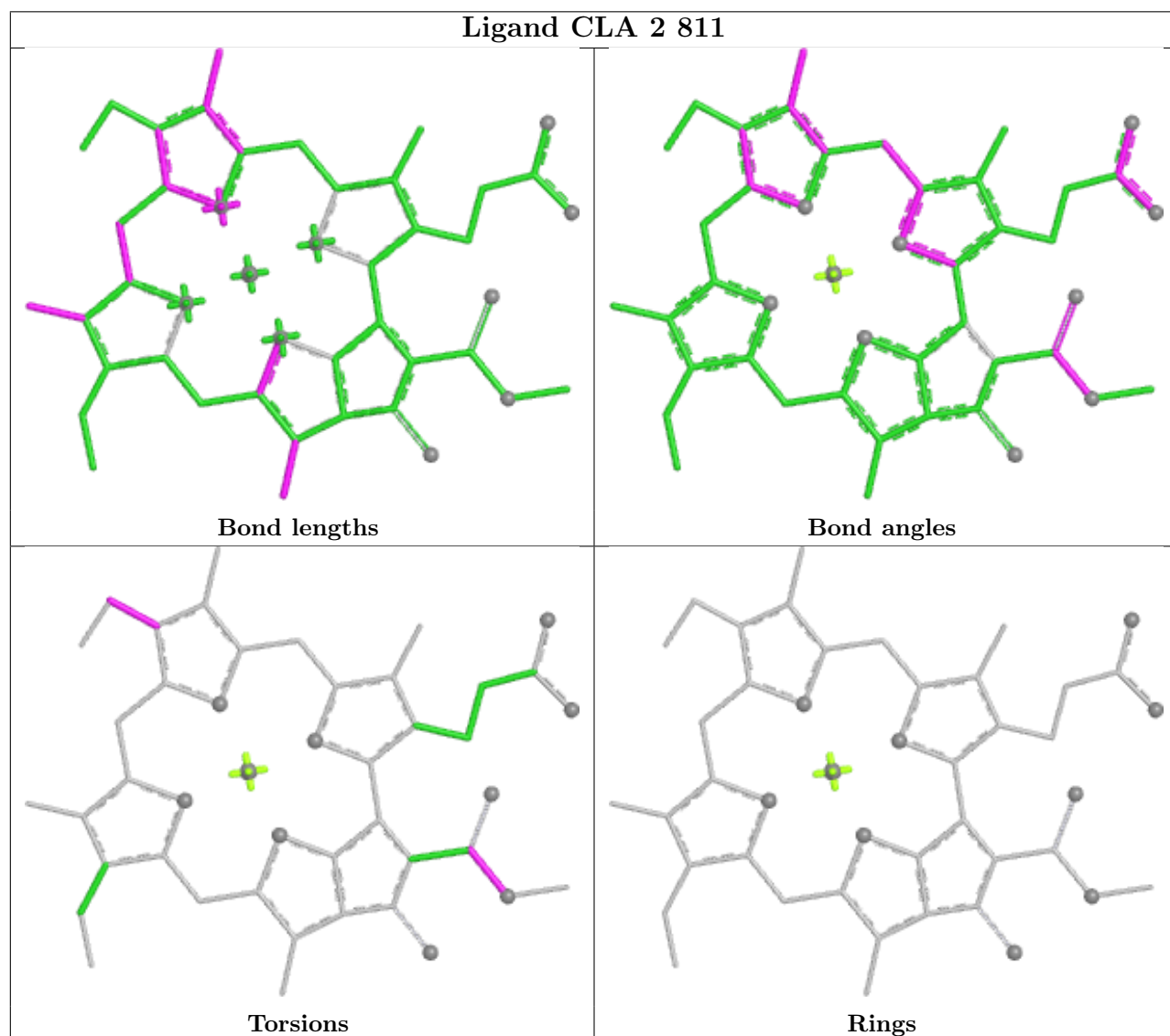
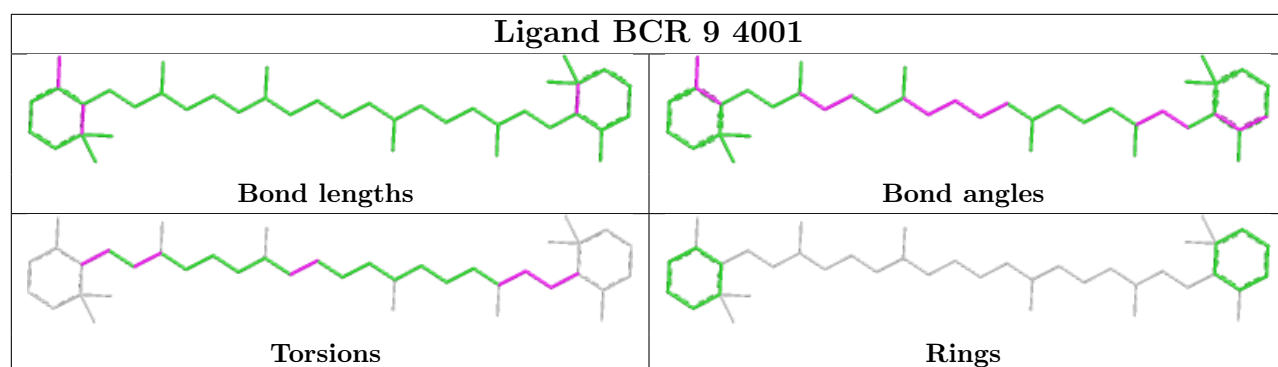
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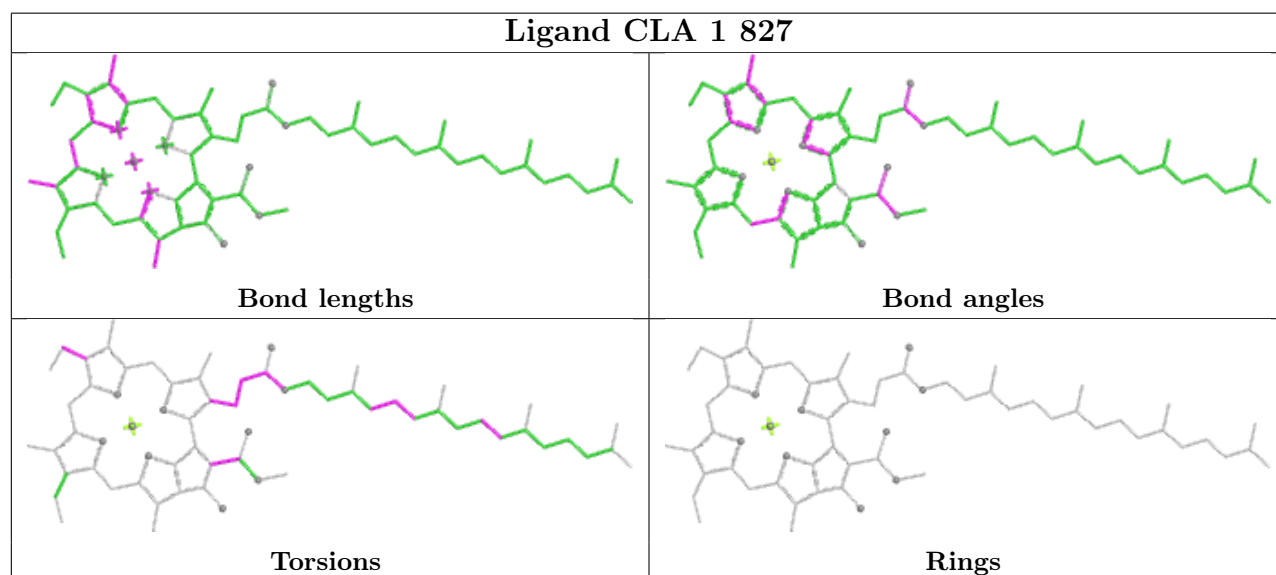
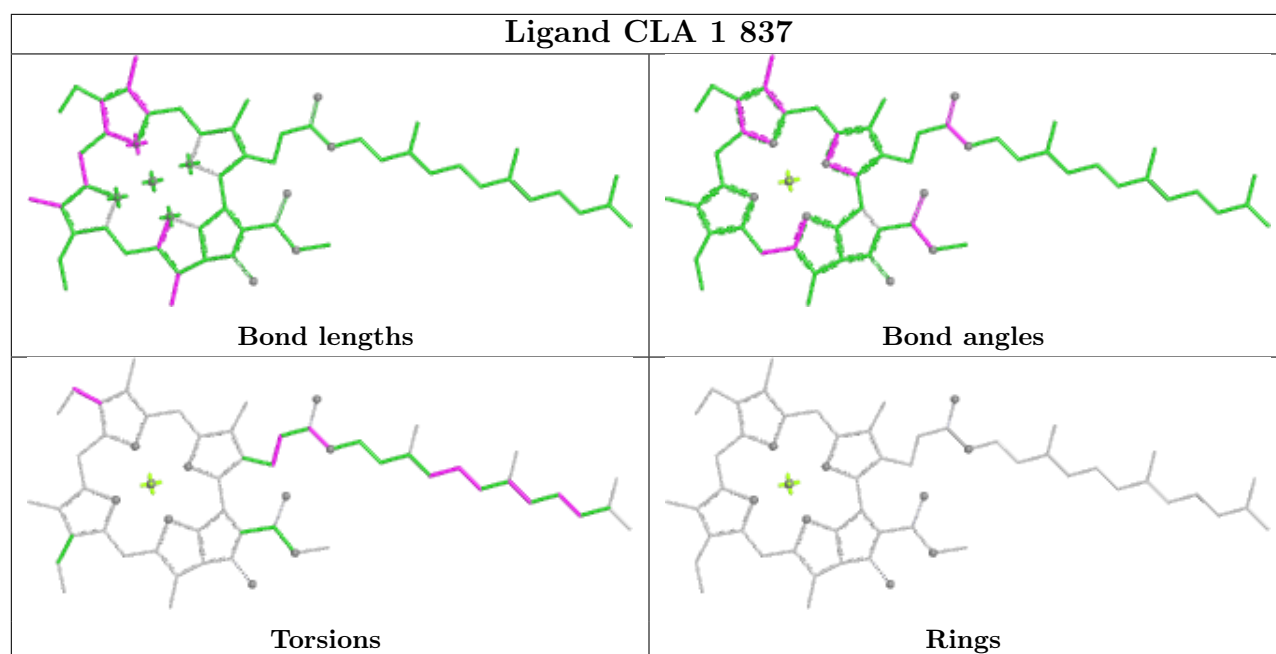
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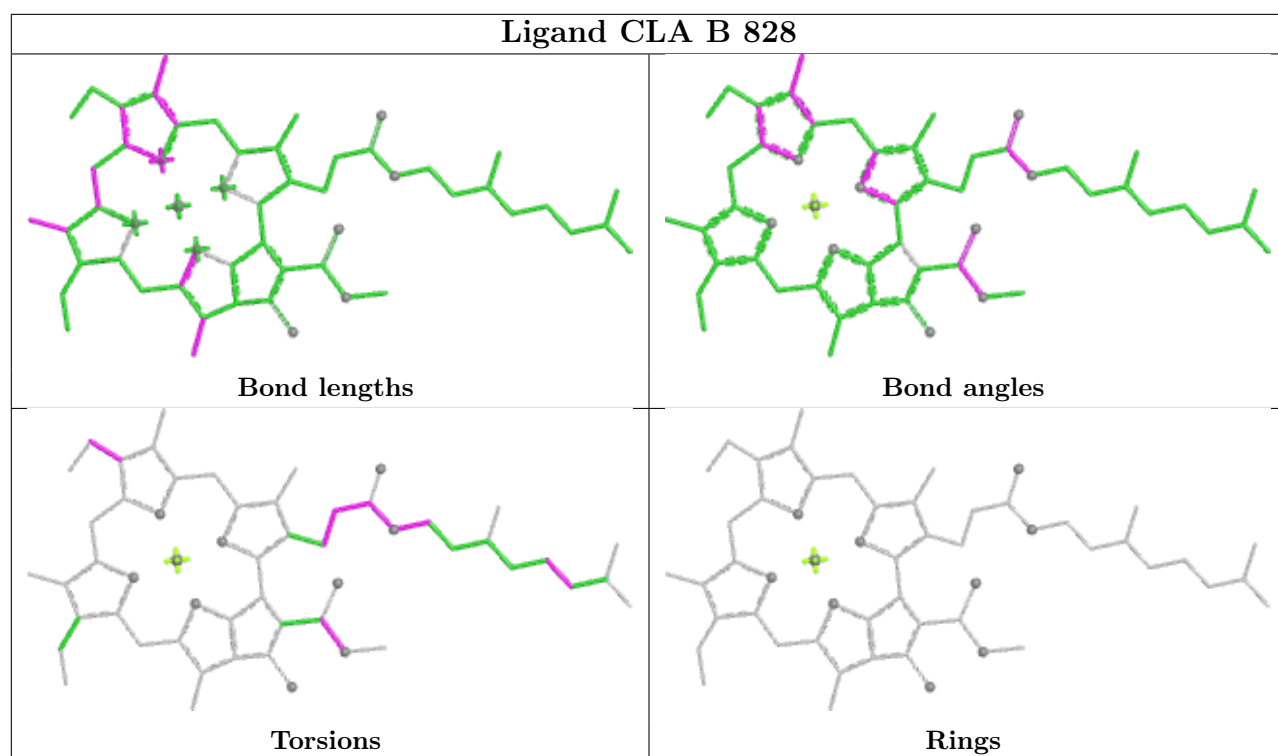
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	j	1105	BCR	2	0
17	a	850	LHG	1	0
13	B	813	CLA	1	0
13	2	815	CLA	1	0
16	b	848	BCR	4	0
18	B	846	LMG	3	0
13	A	821	CLA	6	0
13	b	831	CLA	2	0
13	a	806	CLA	5	0
13	2	820	CLA	7	0
13	A	805	CLA	2	0
13	A	817	CLA	3	0
13	2	801	CLA	1	0
13	0	208	CLA	5	0
13	A	837	CLA	4	0
13	1	804	CLA	3	0
13	B	809	CLA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

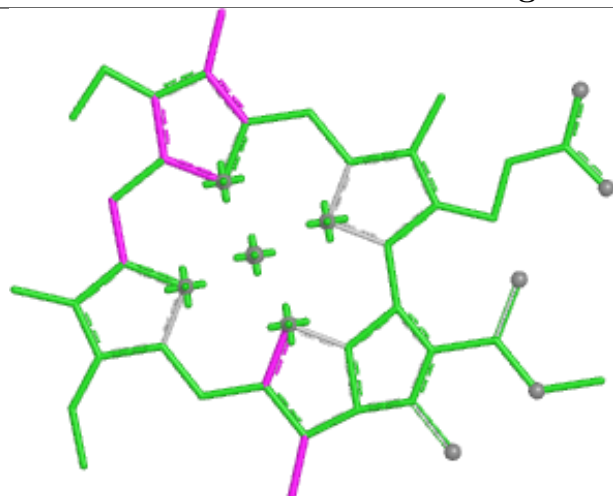




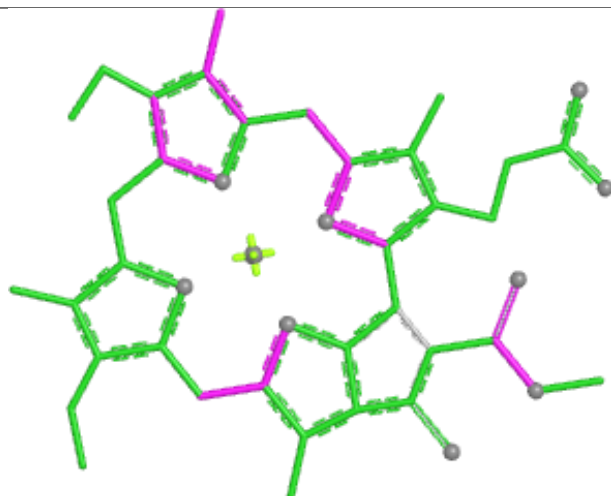




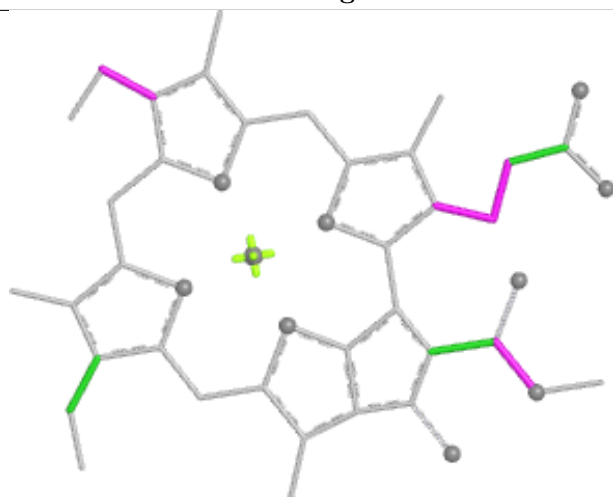
Ligand CLA 2 808



Bond lengths



Bond angles

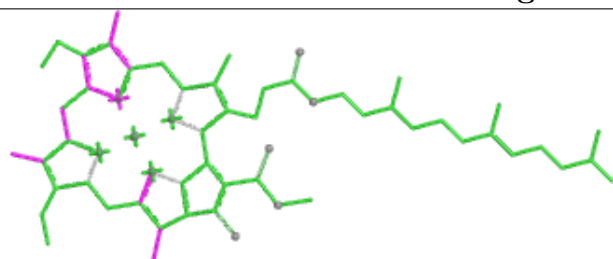


Torsions

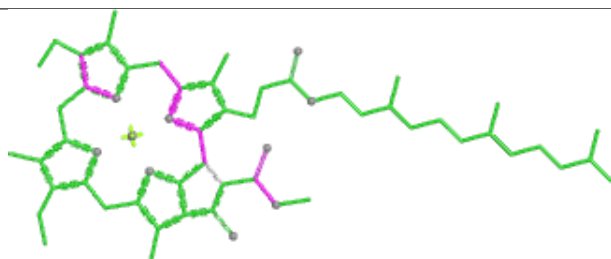


Rings

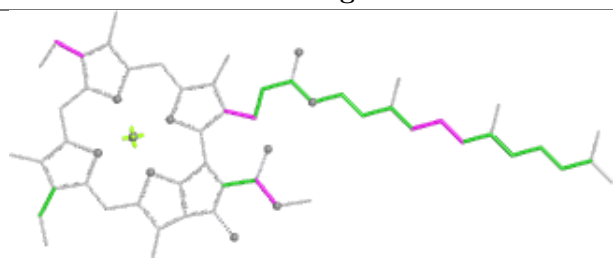
Ligand CLA b 816



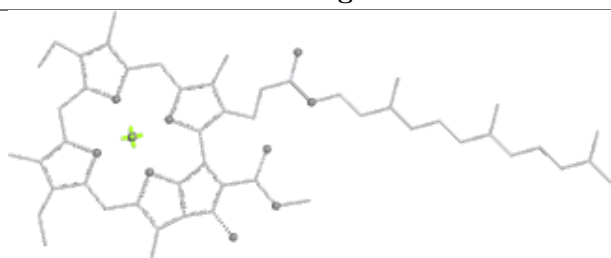
Bond lengths



Bond angles

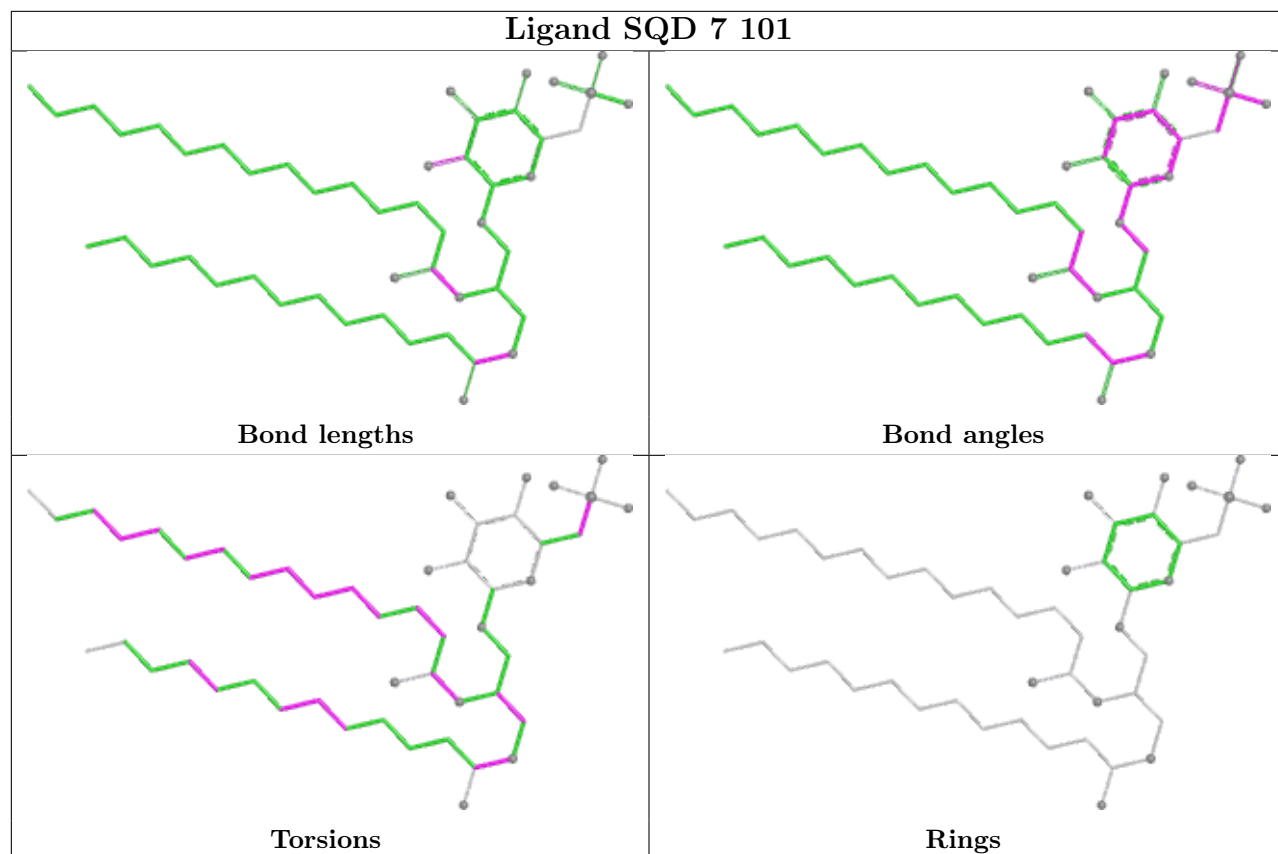


Torsions

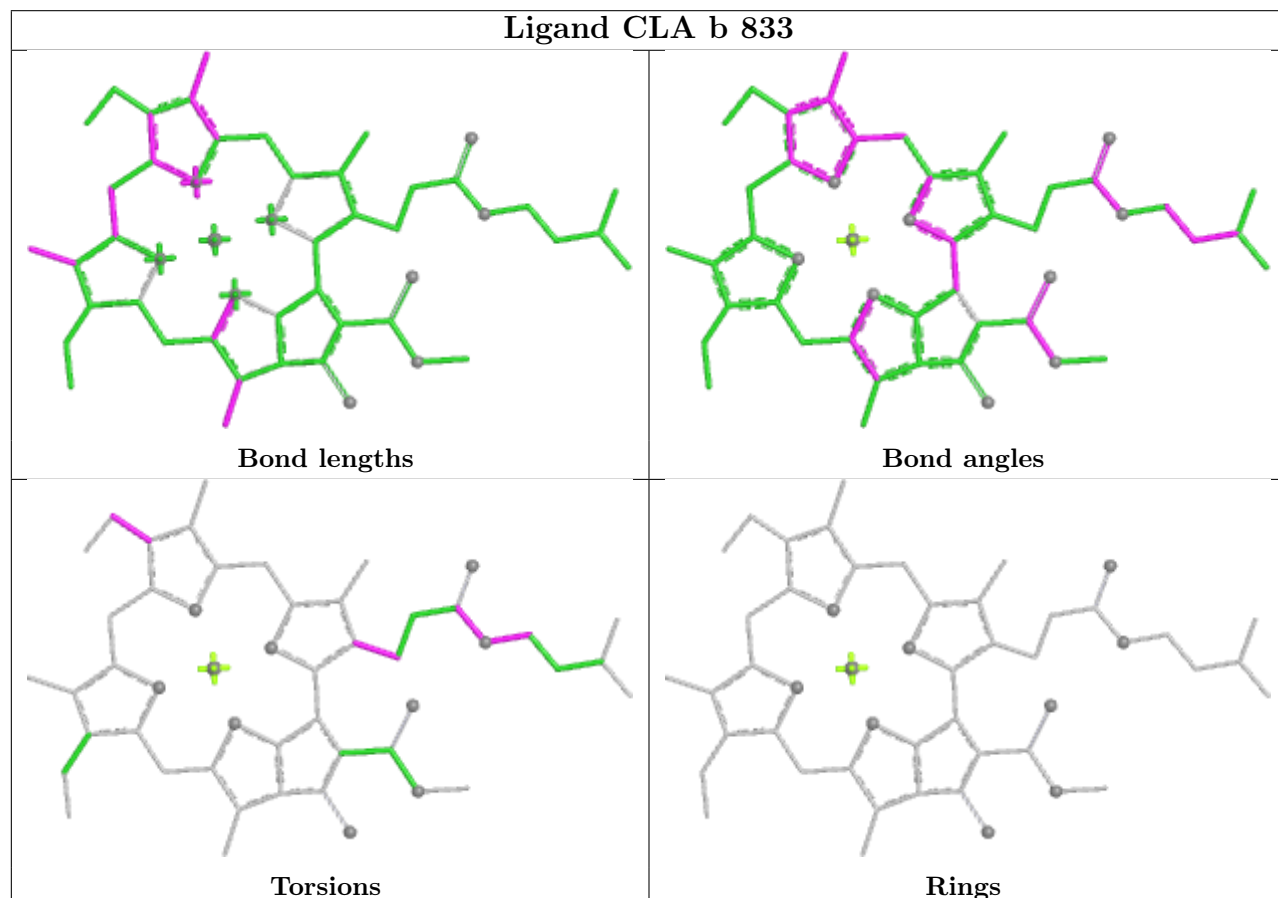


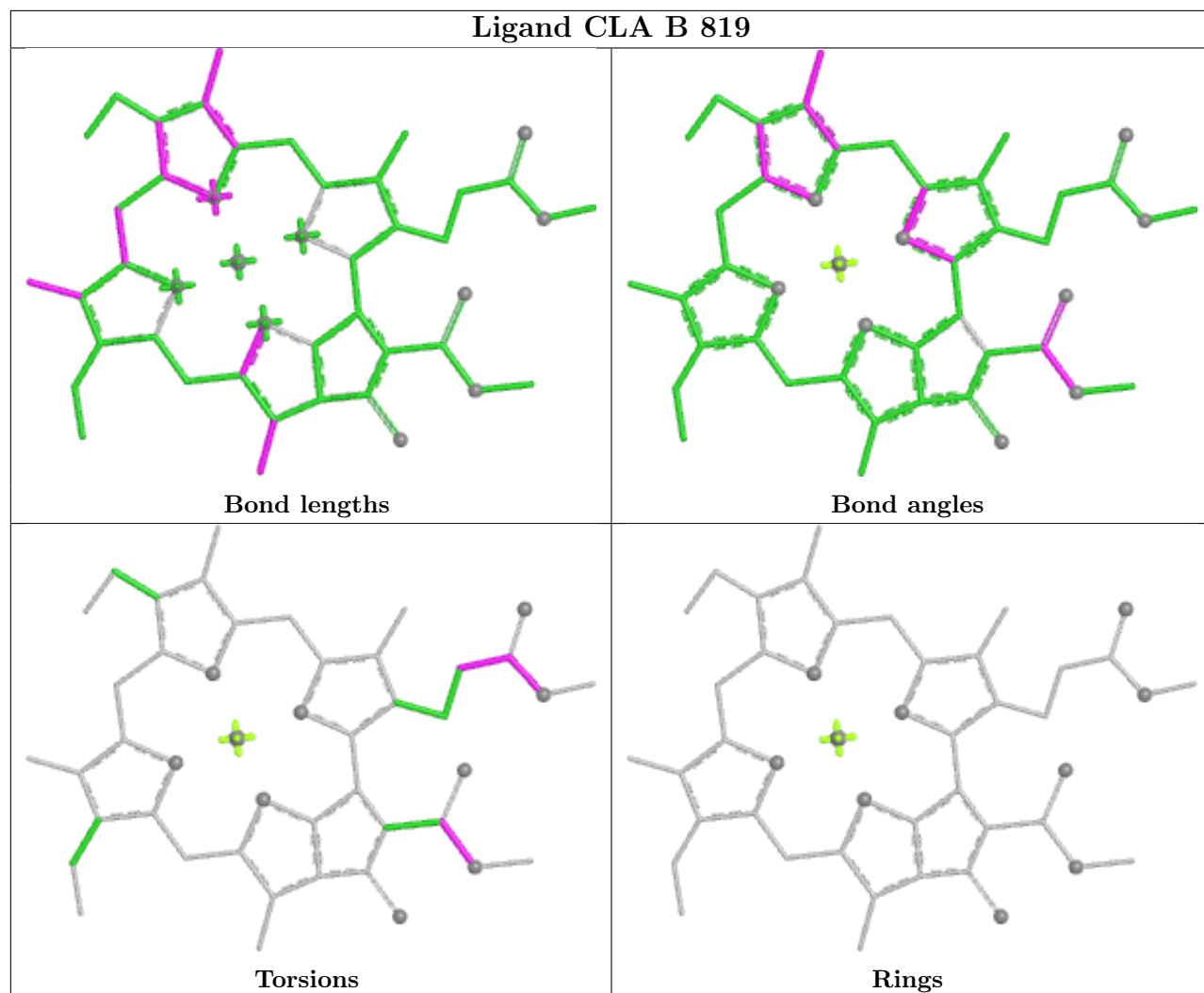
Rings

Ligand SQD 7 101

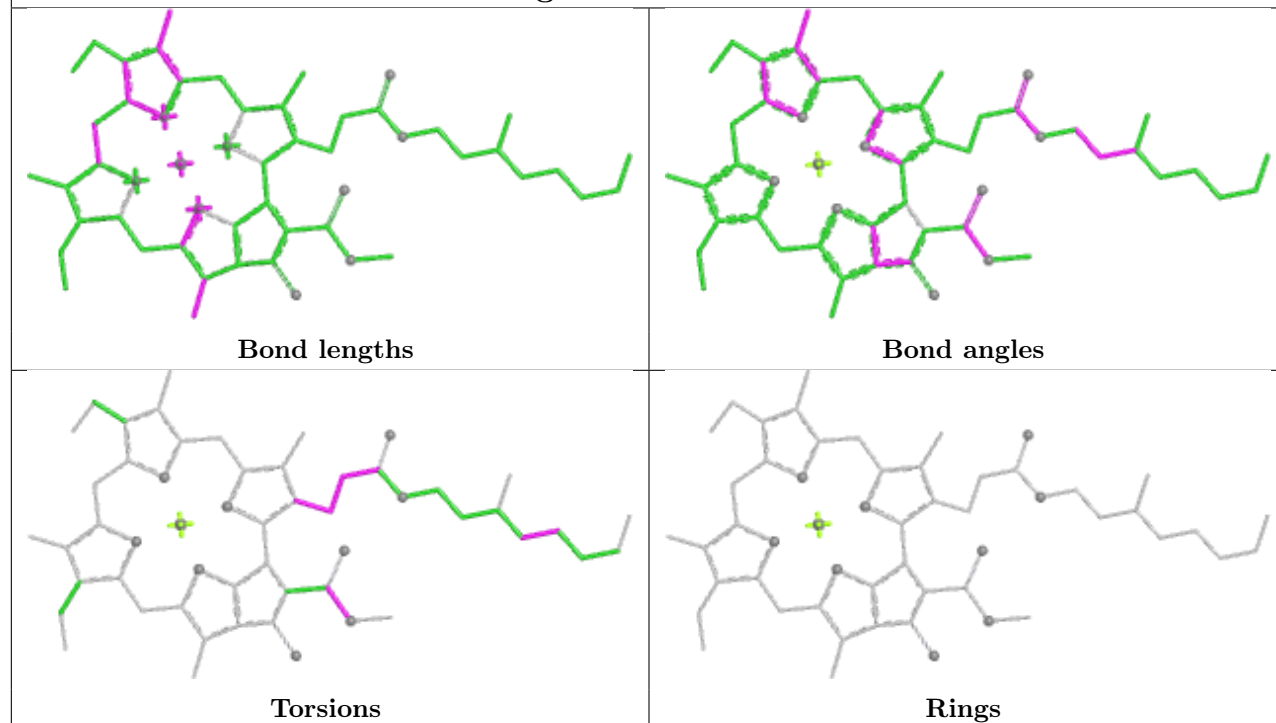


Ligand CLA b 833

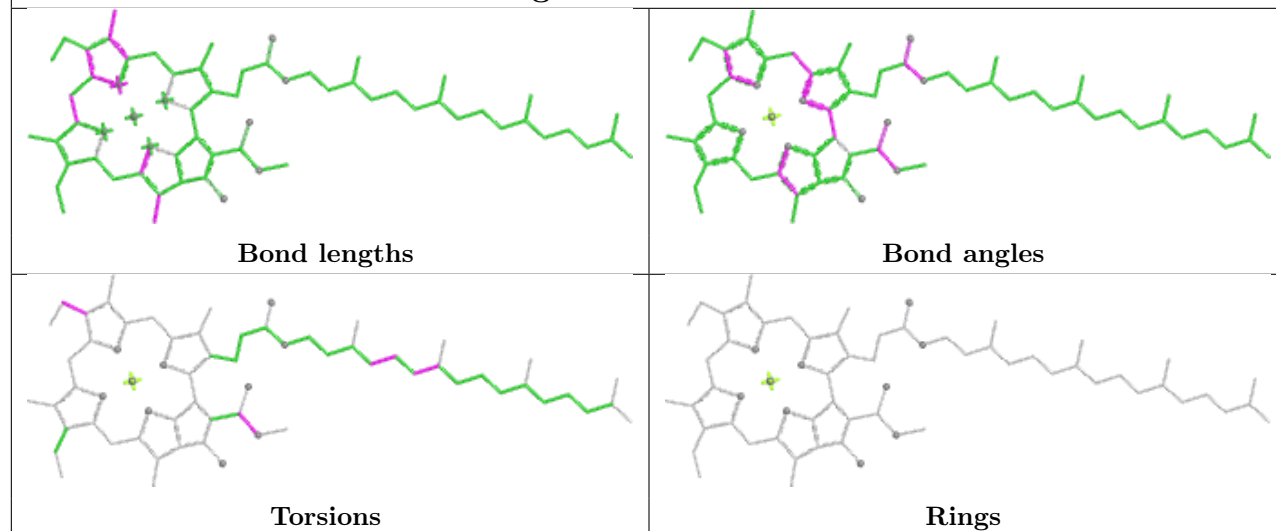




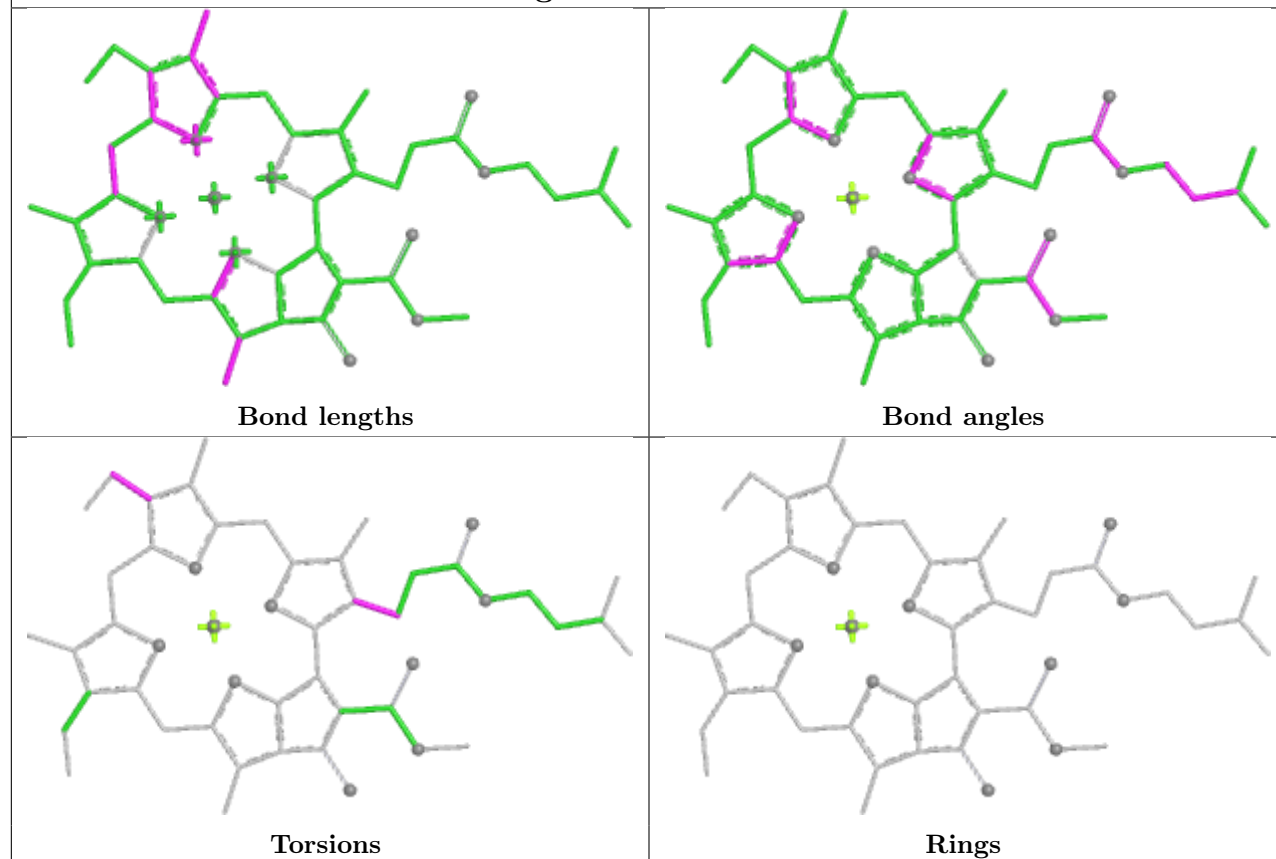
Ligand CLA 1 818



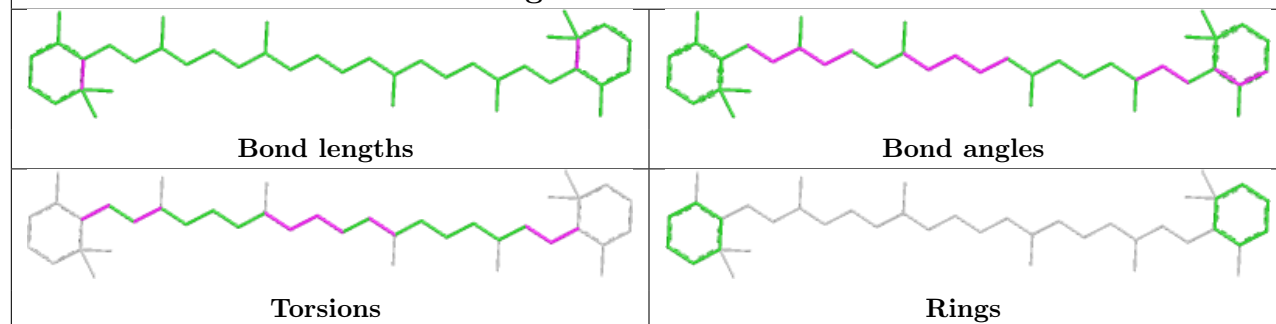
Ligand CLA B 831



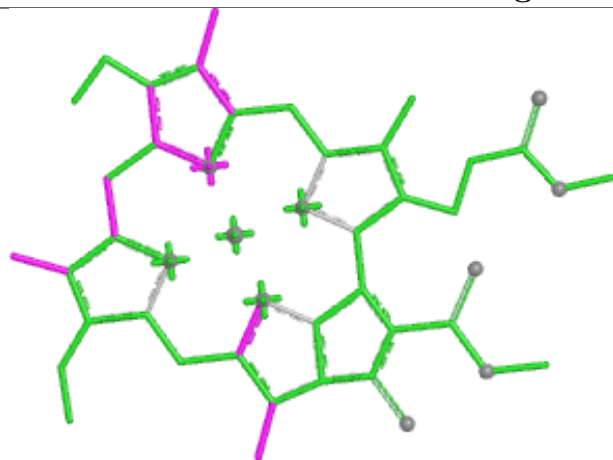
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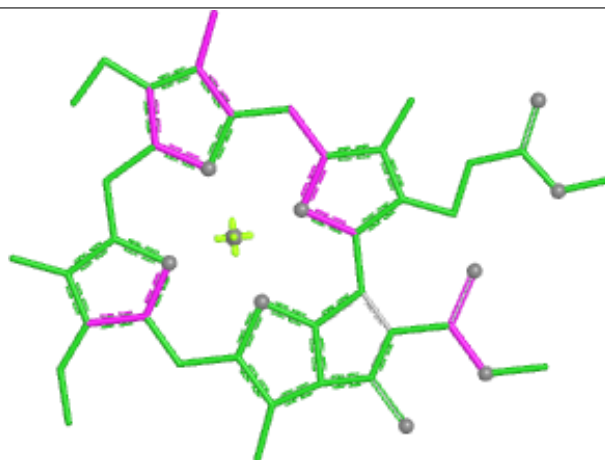
Ligand BCR 9 4004



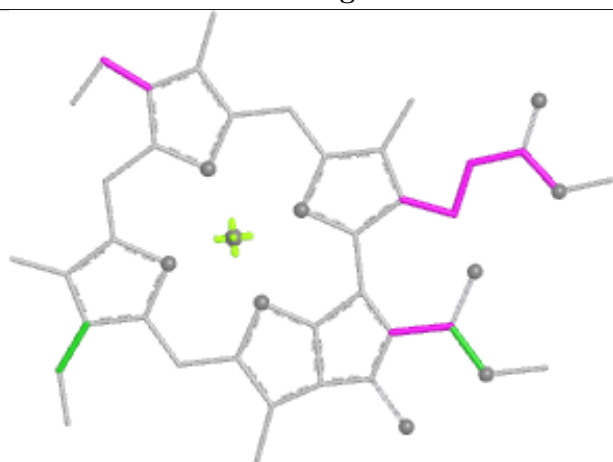
Ligand CLA B 818



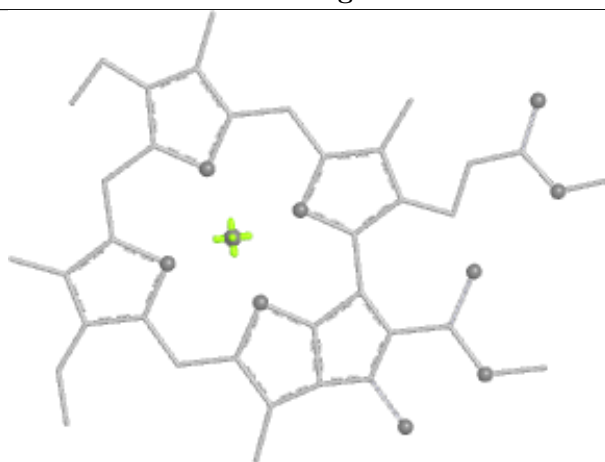
Bond lengths



Bond angles

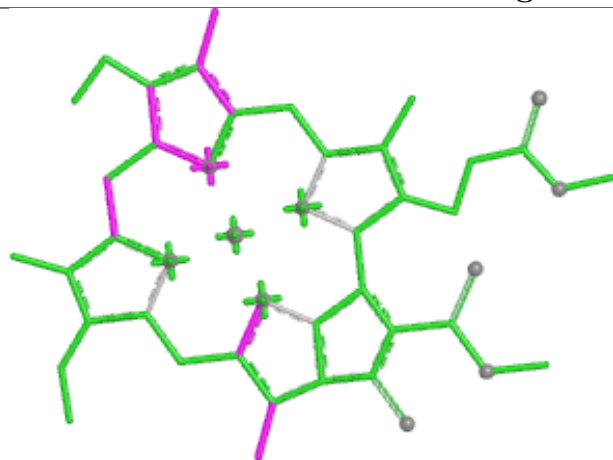


Torsions

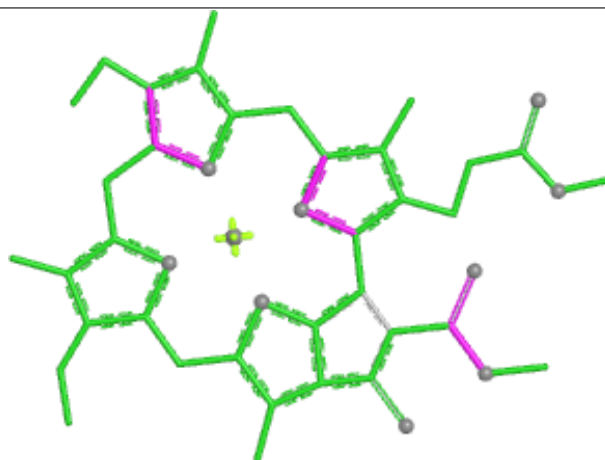


Rings

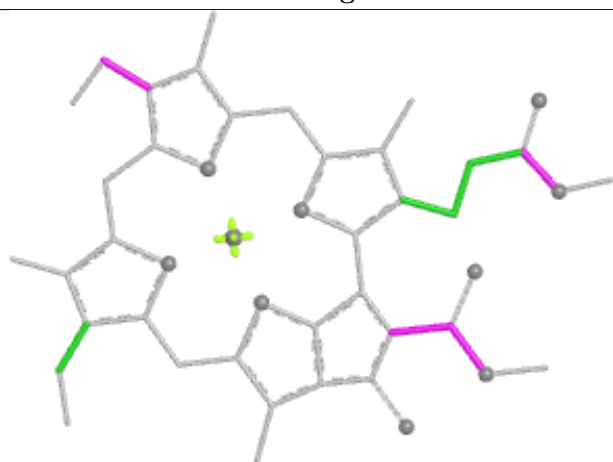
Ligand CLA F 204



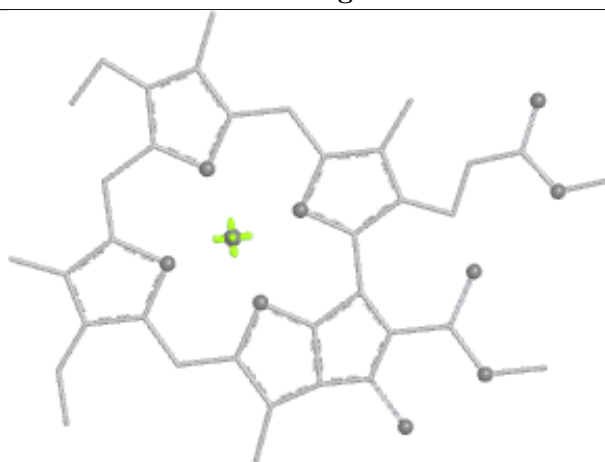
Bond lengths



Bond angles

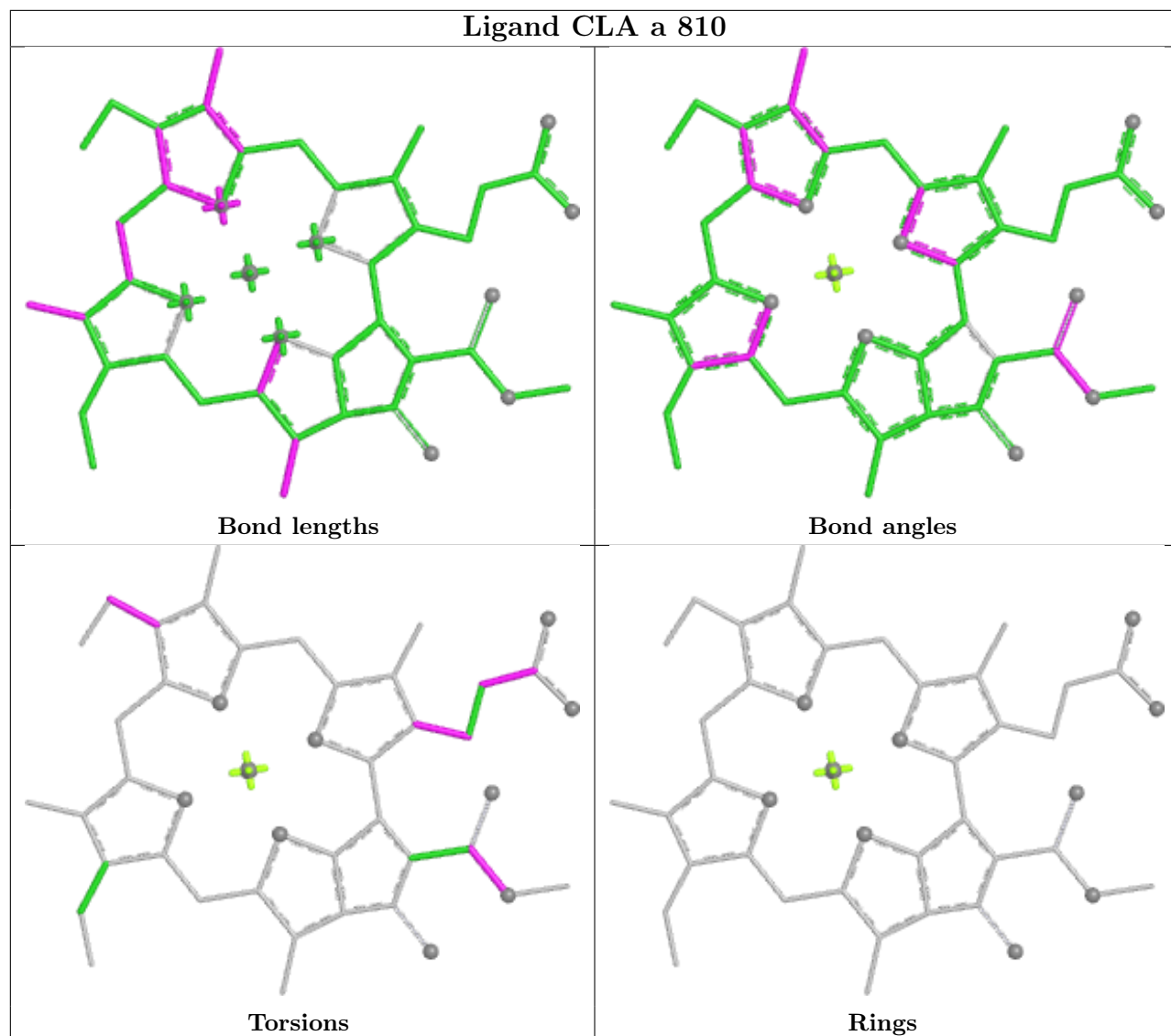


Torsions

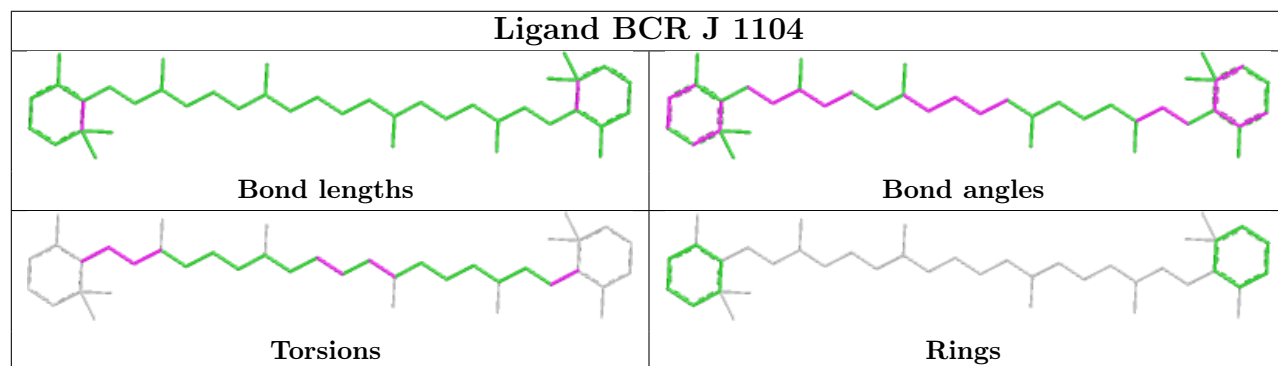


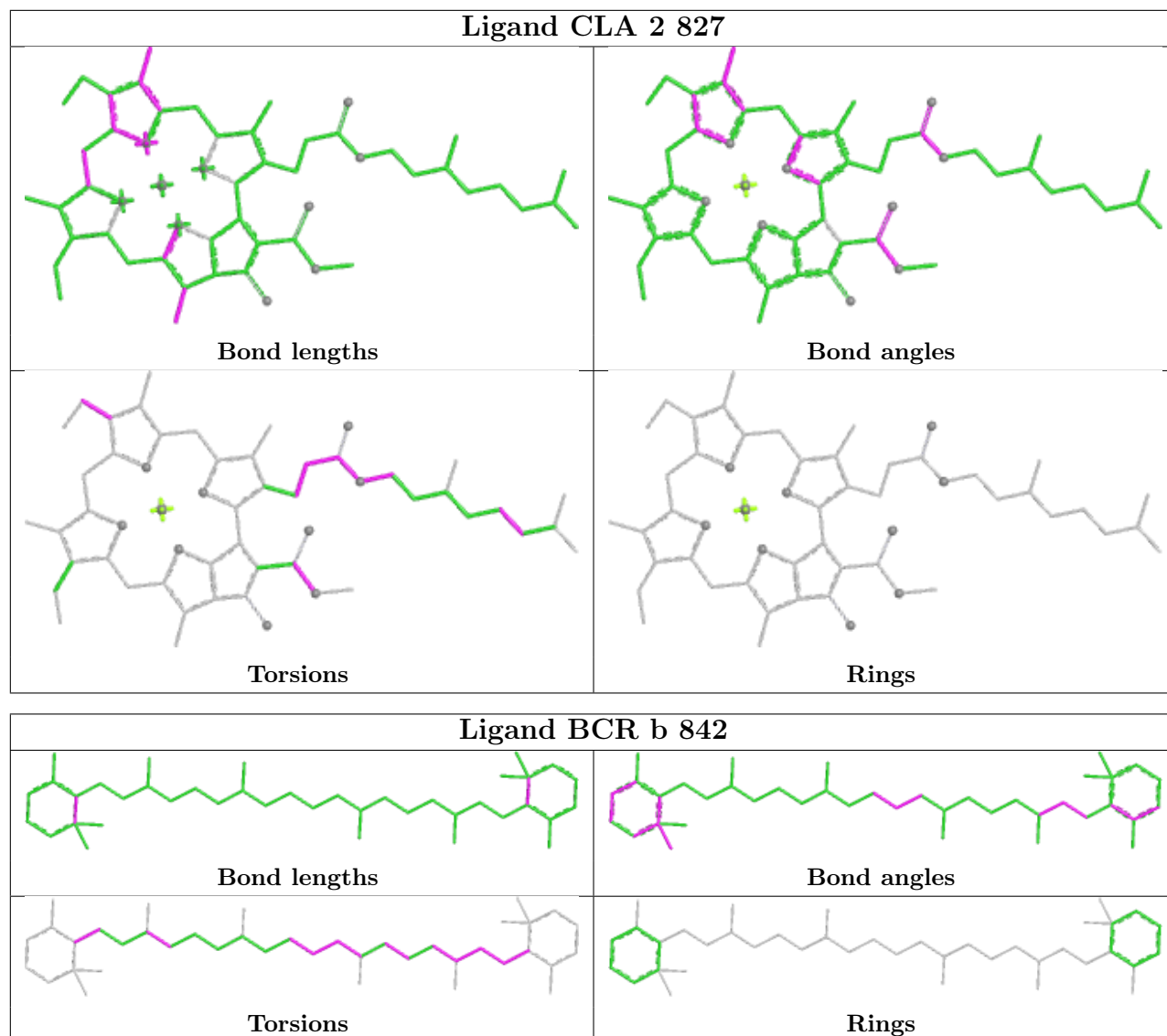
Rings

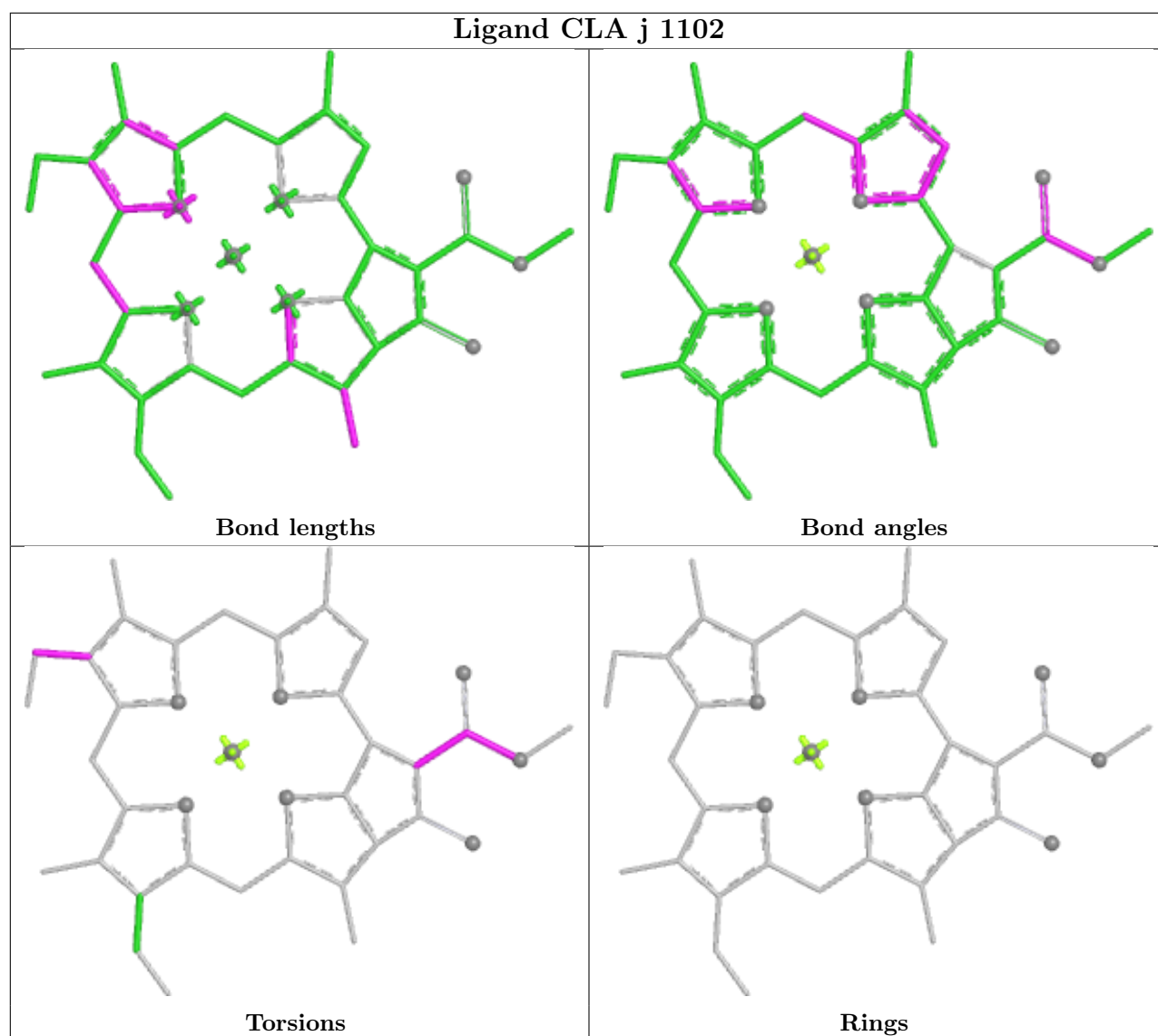
Ligand CLA a 810

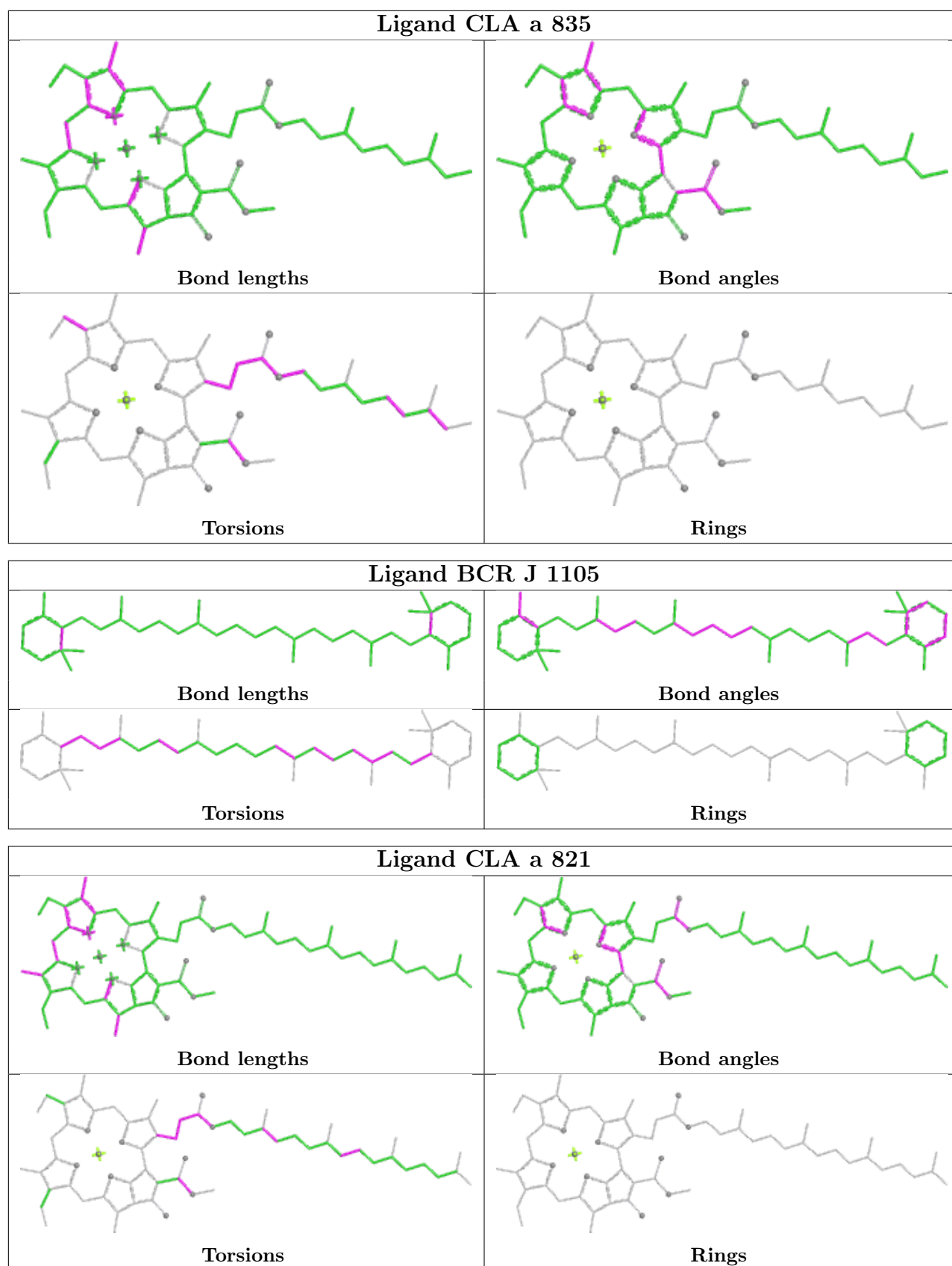


Ligand BCR J 1104

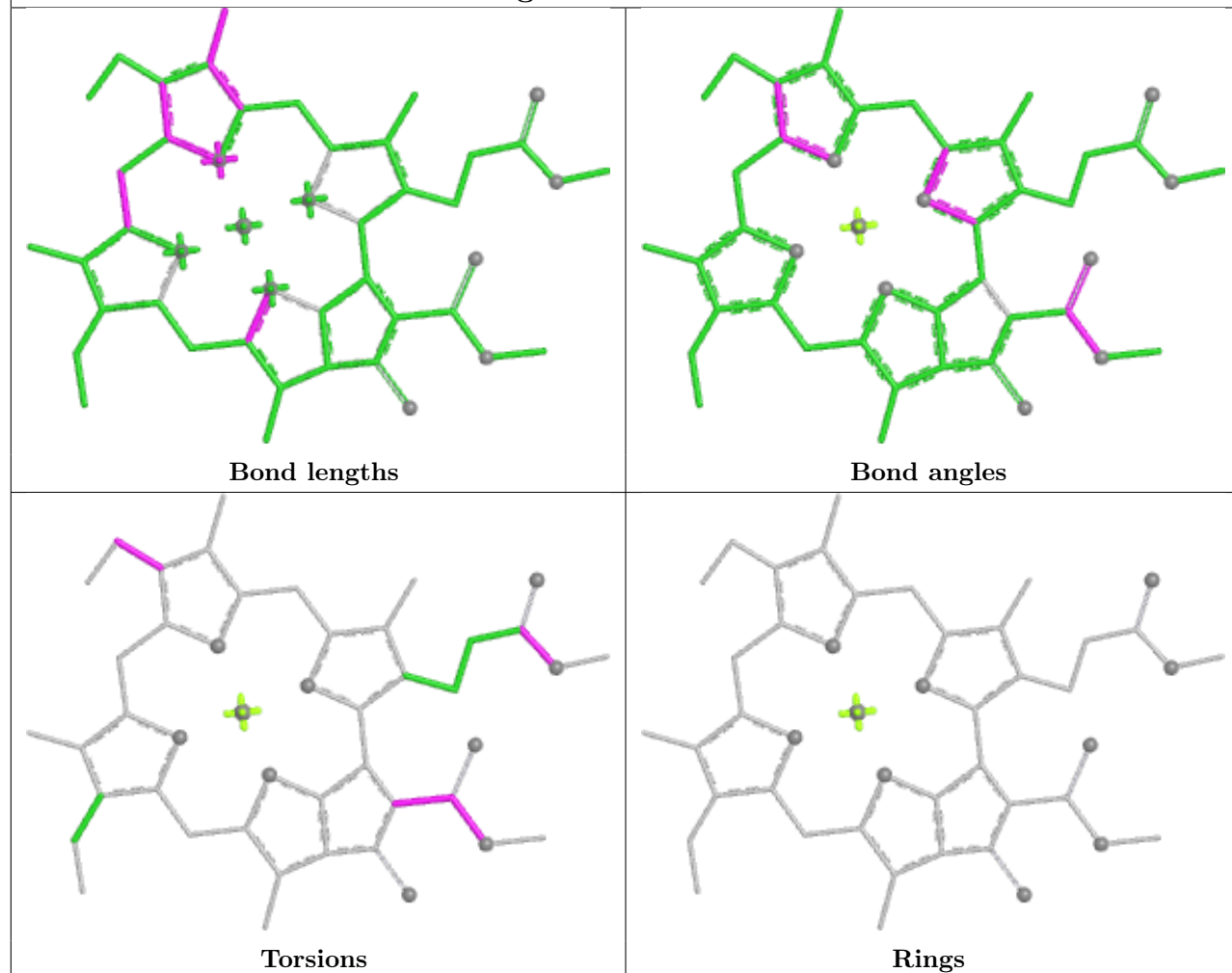




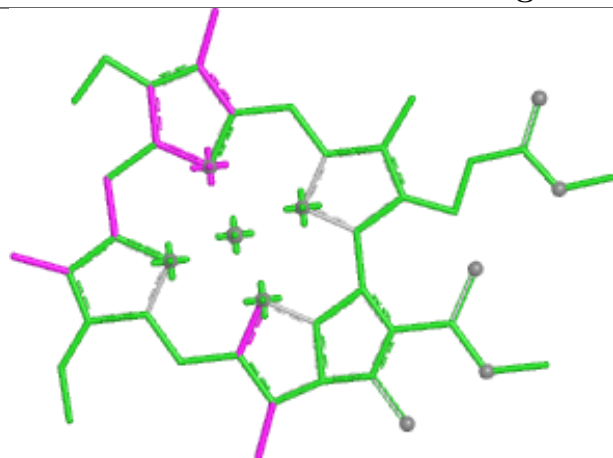




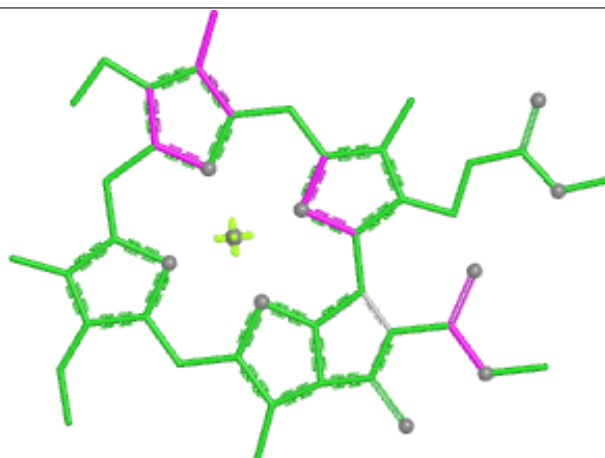
Ligand CLA 6 204



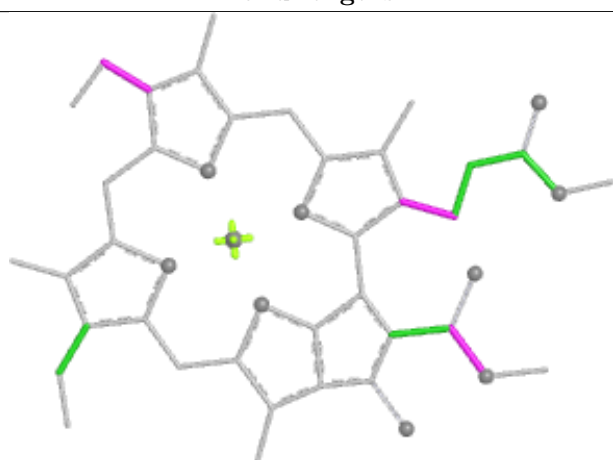
Ligand CLA L 204



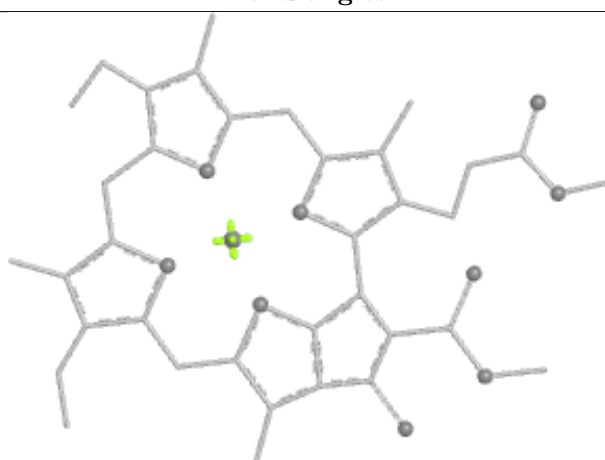
Bond lengths



Bond angles

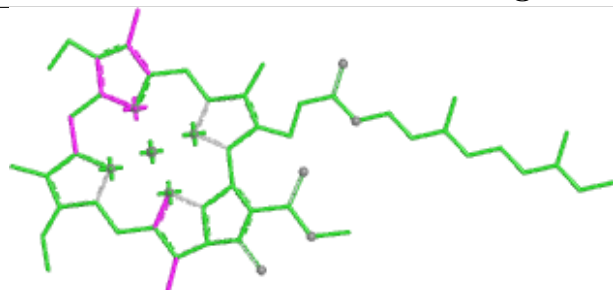


Torsions

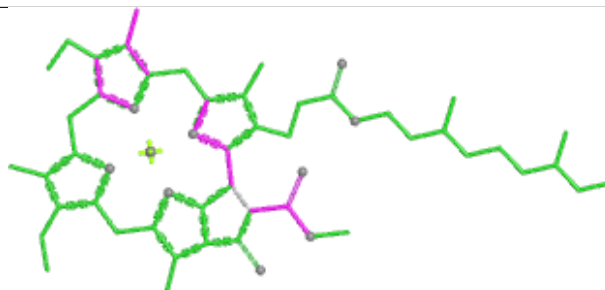


Rings

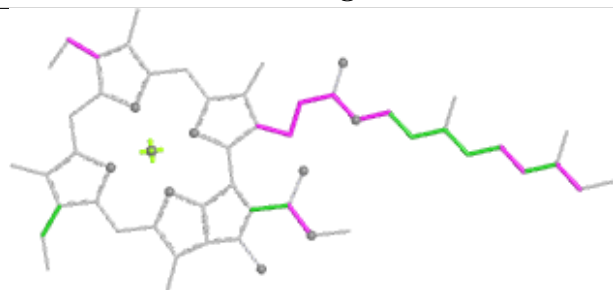
Ligand CLA A 835



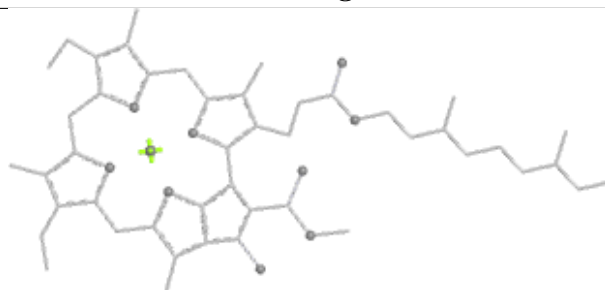
Bond lengths



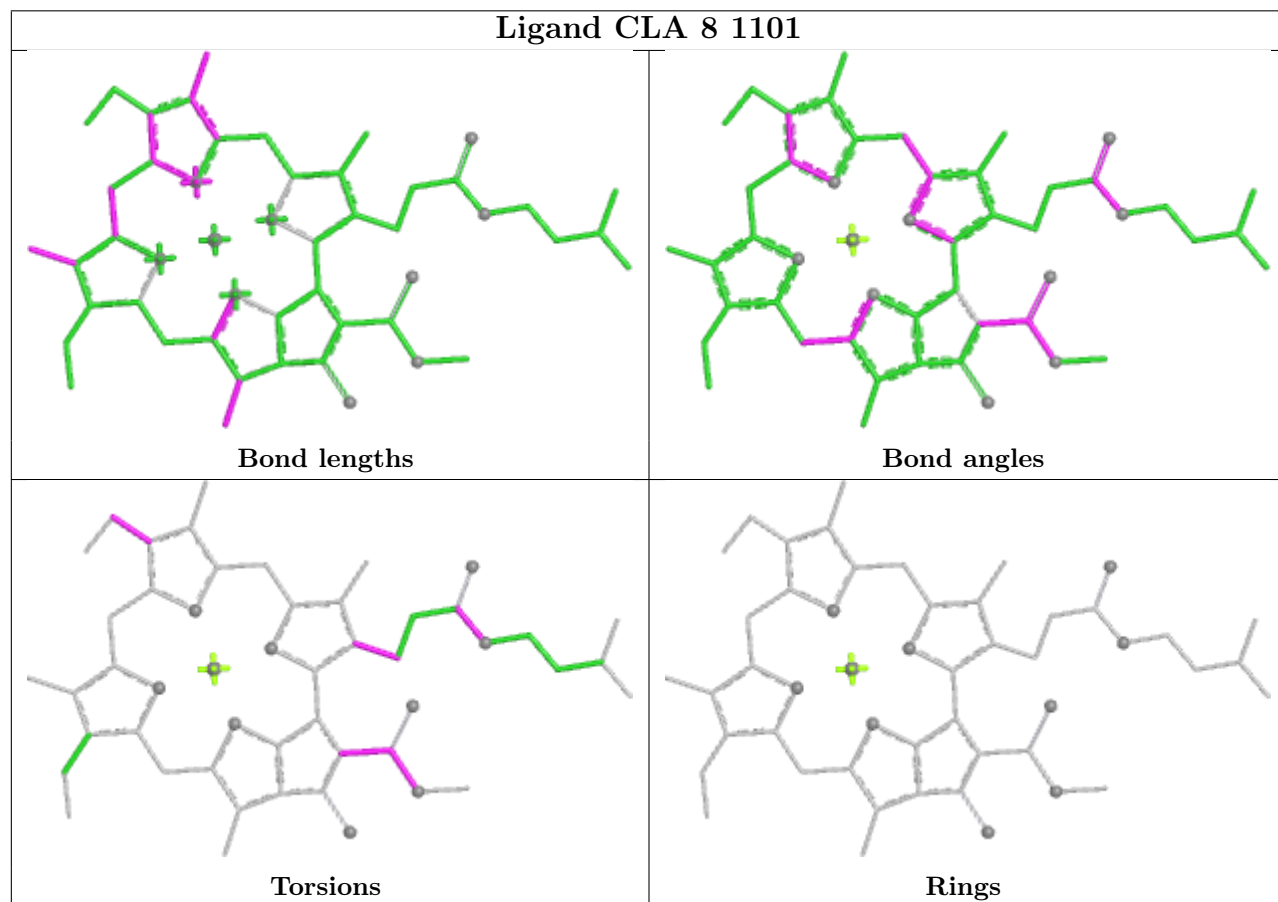
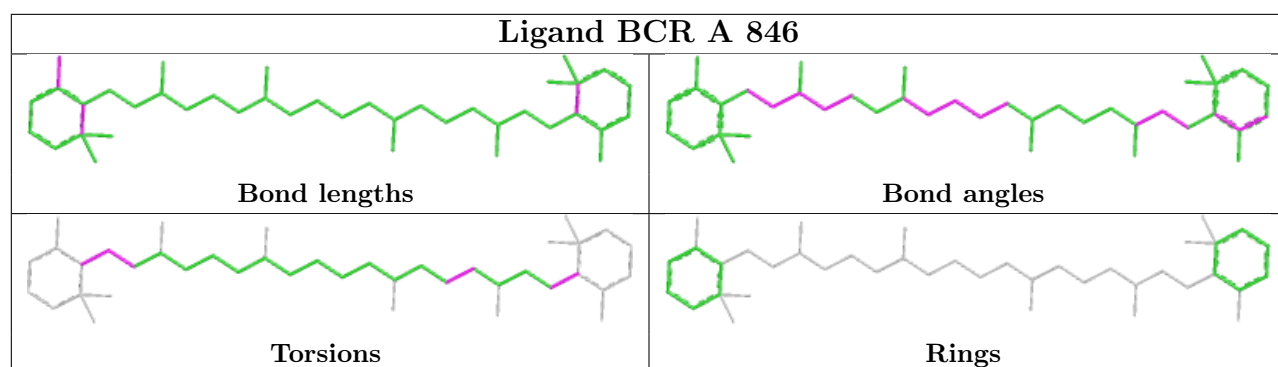
Bond angles

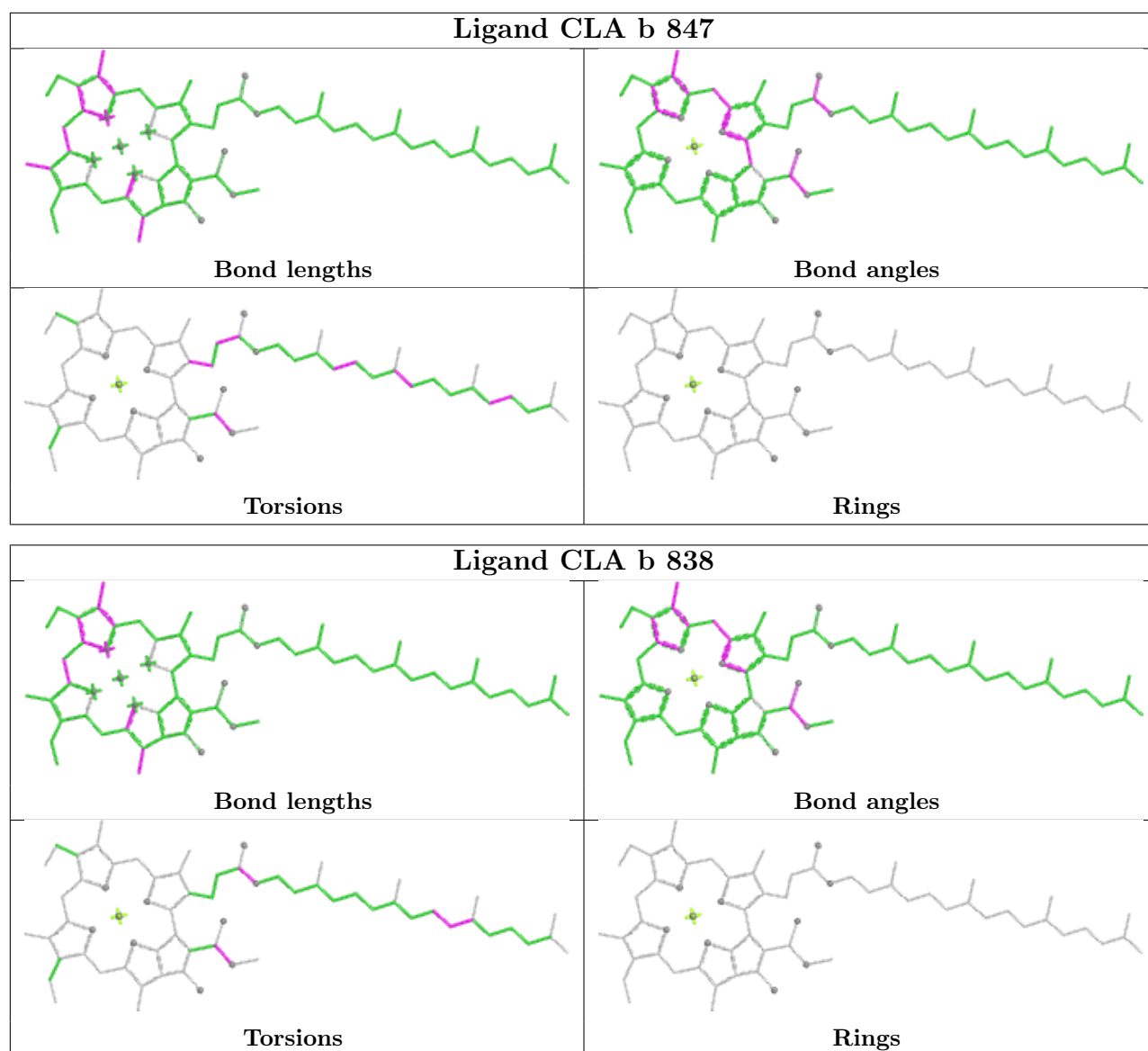


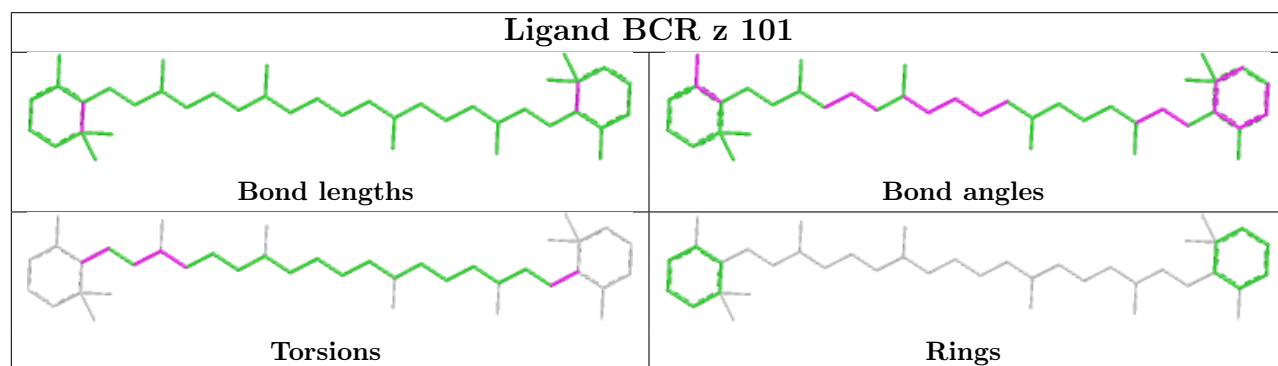
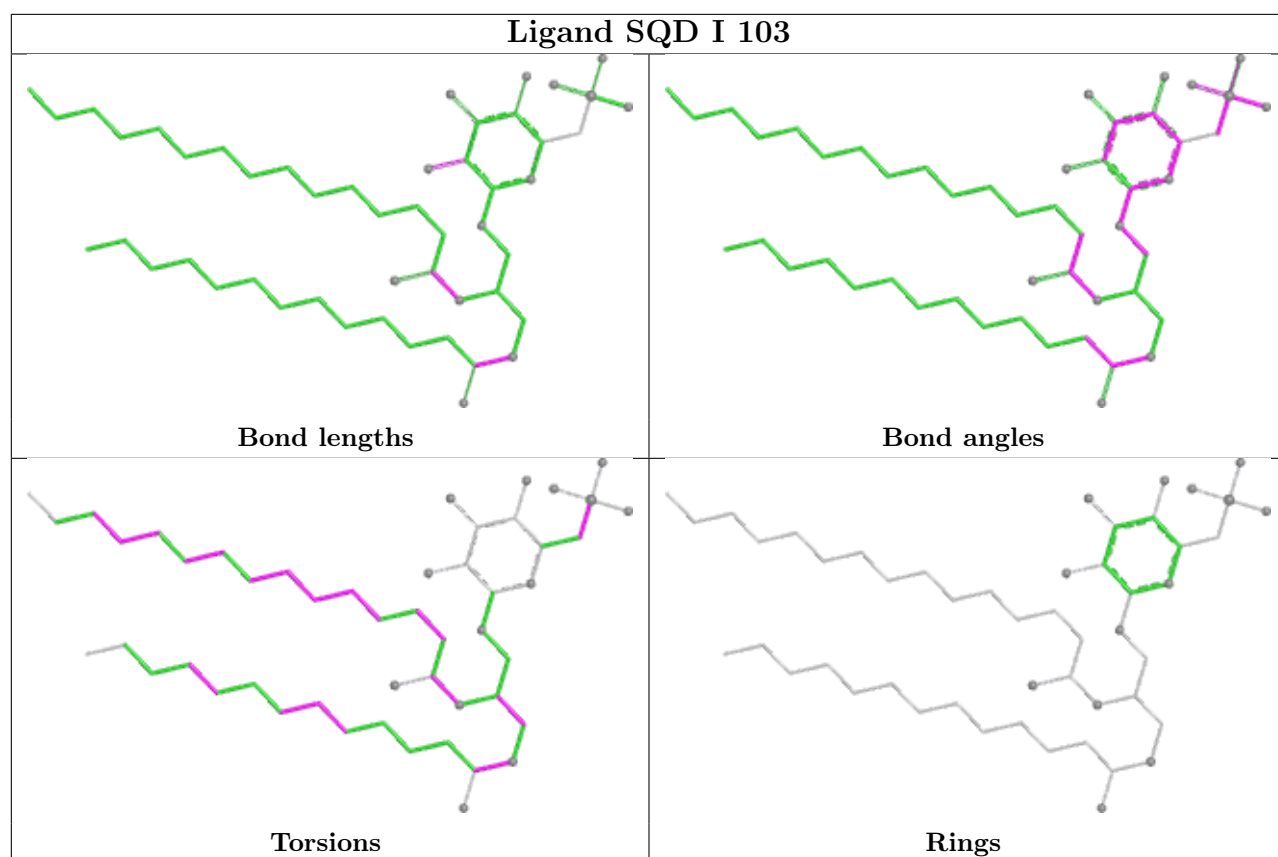
Torsions

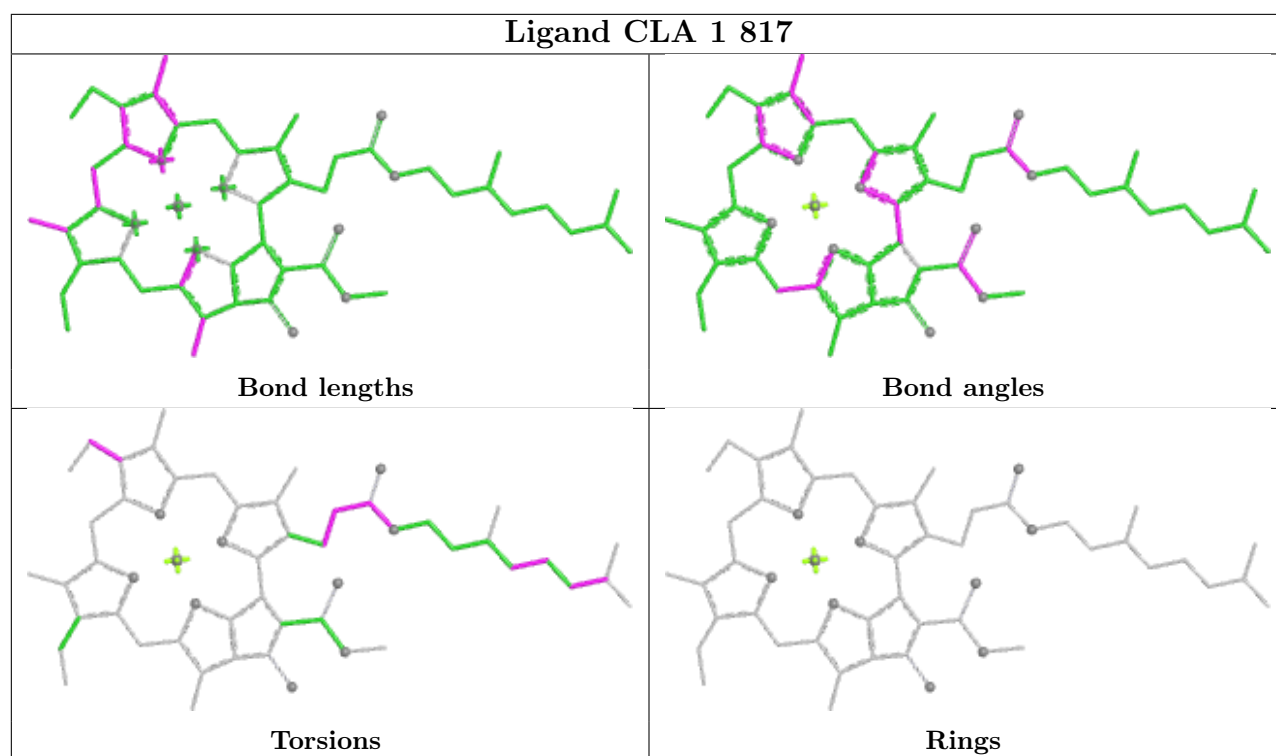


Rings

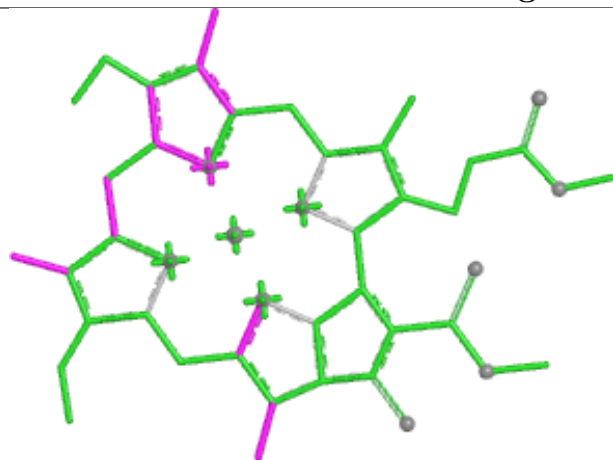




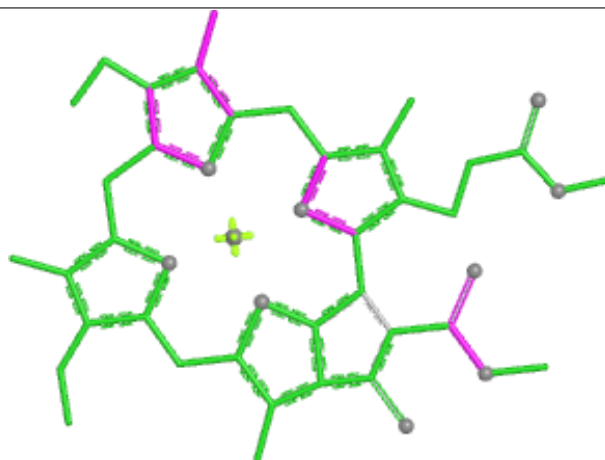




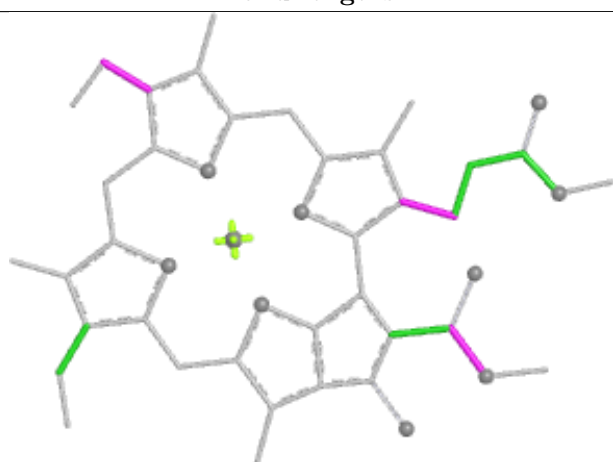
Ligand CLA 0 206



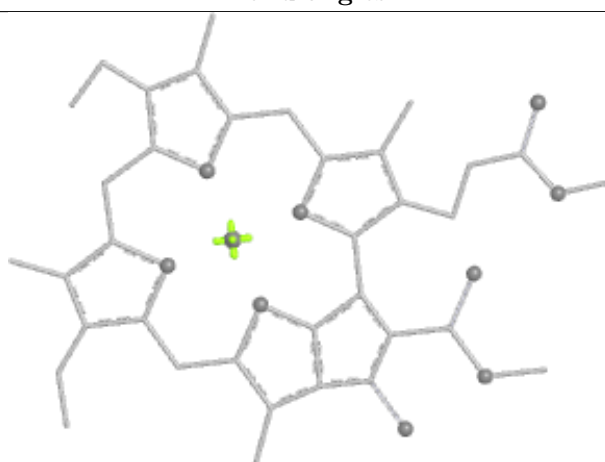
Bond lengths



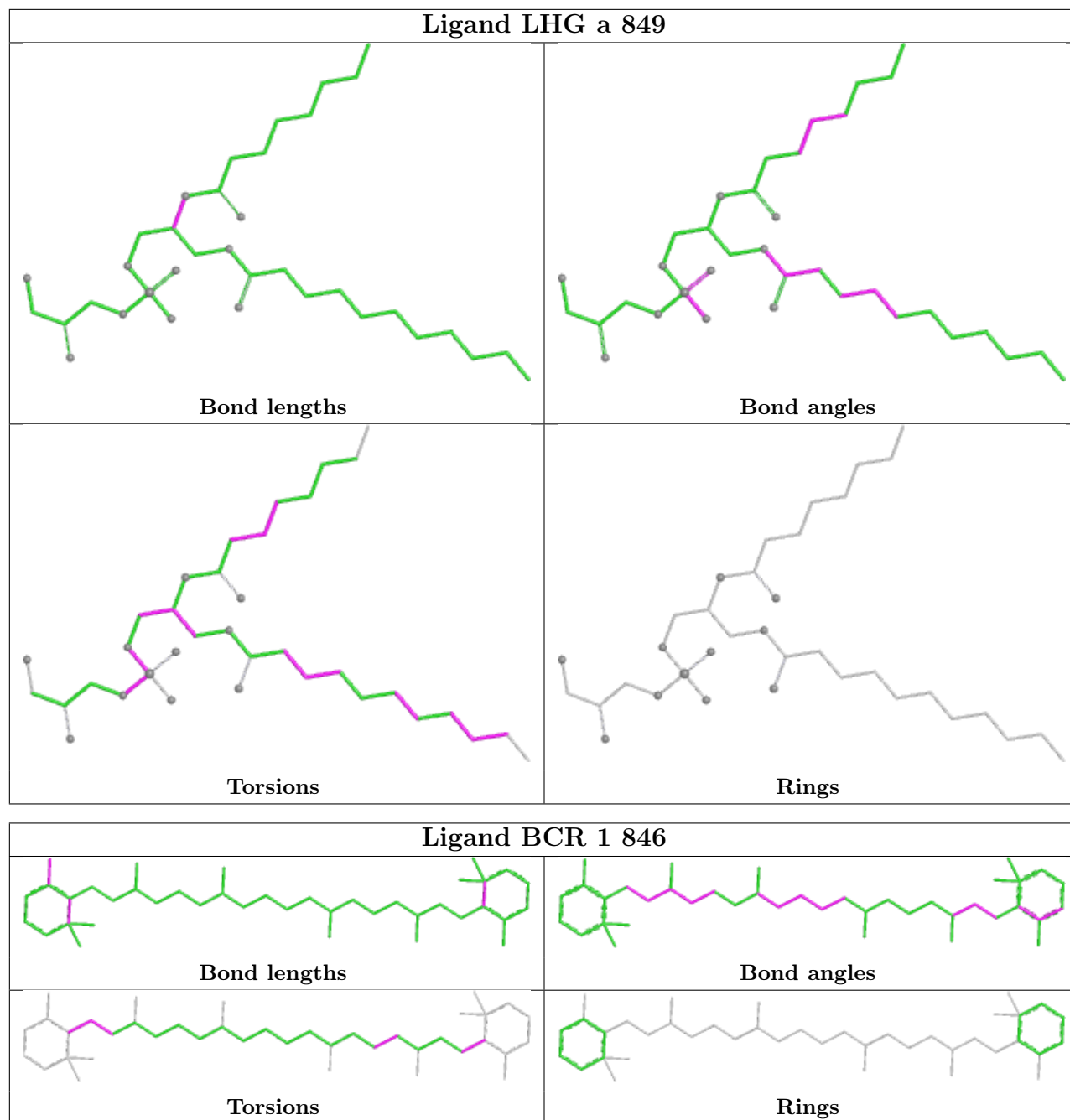
Bond angles

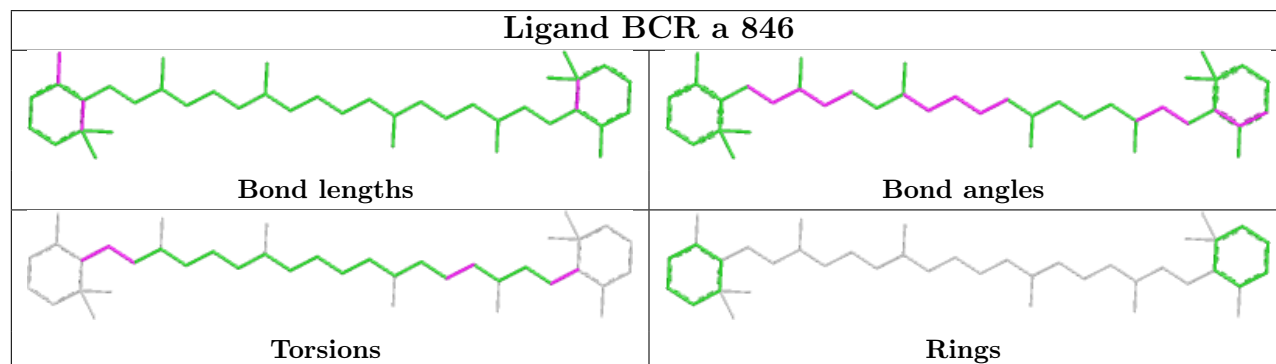
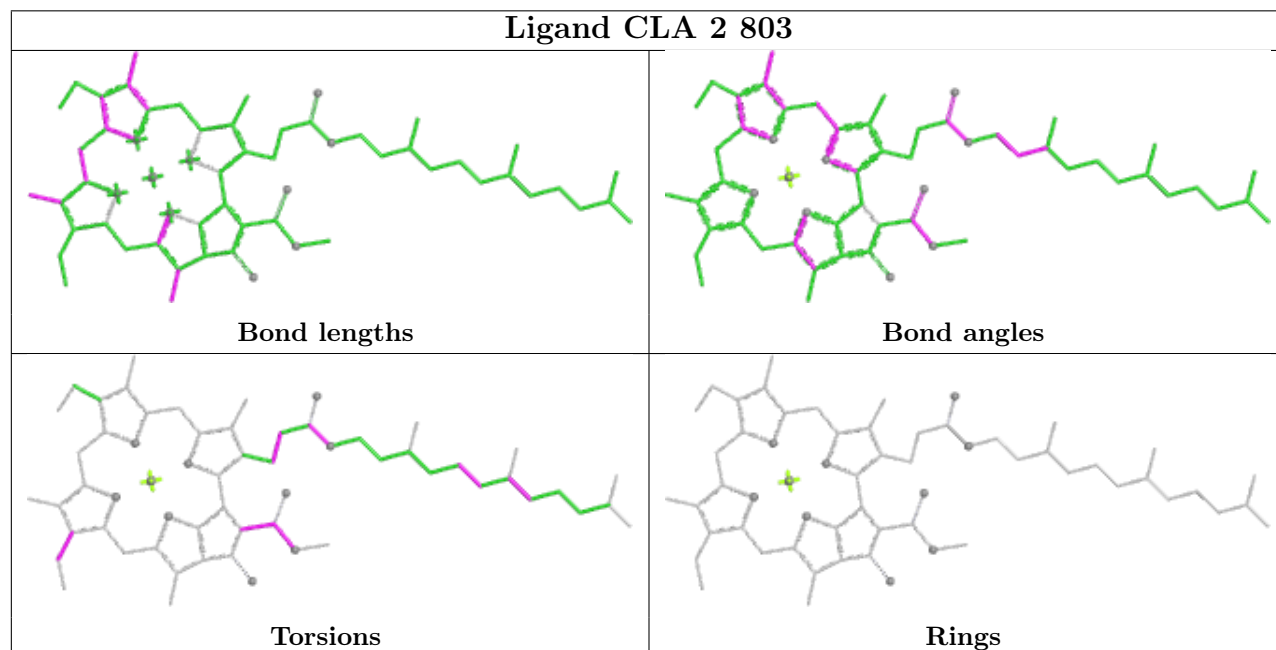
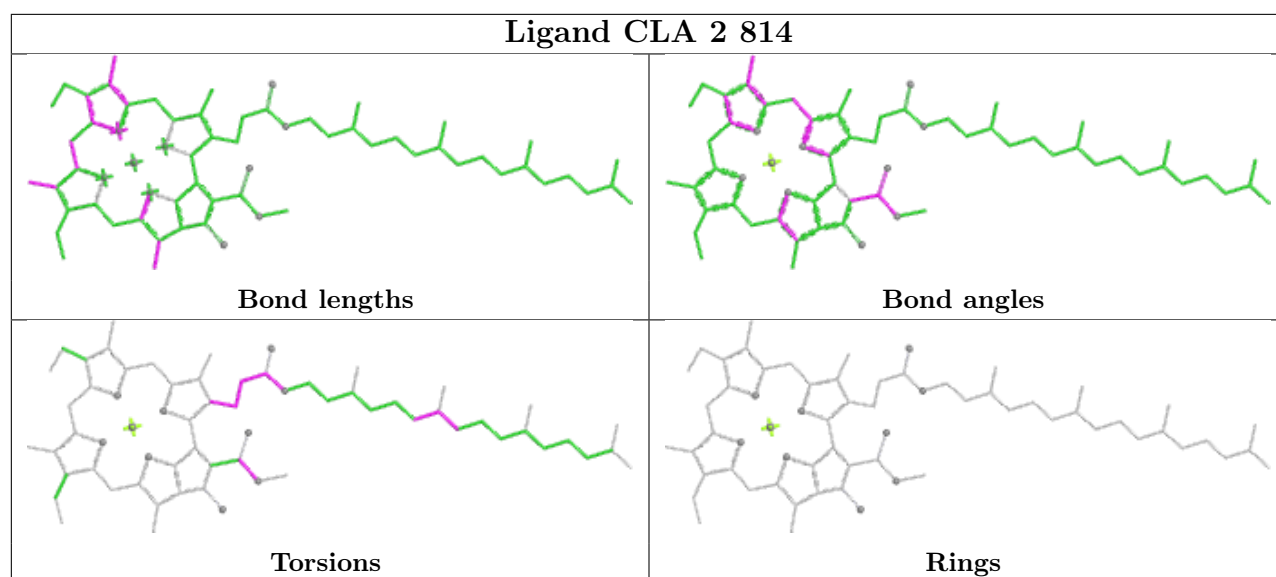


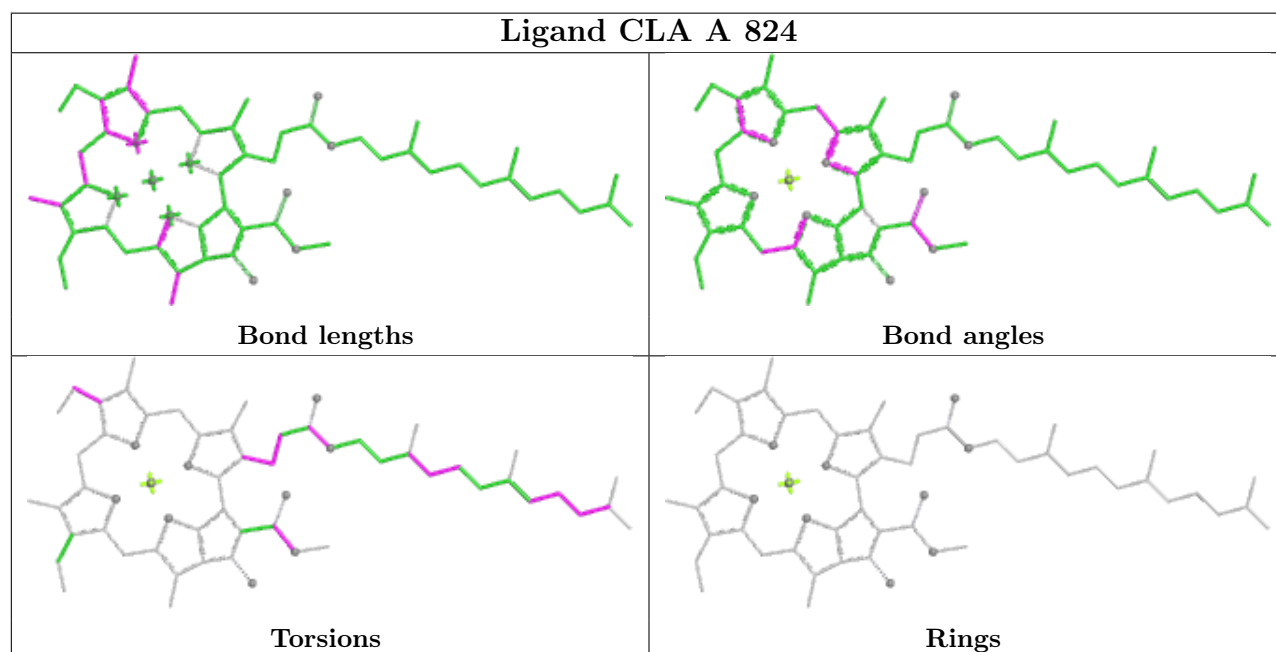
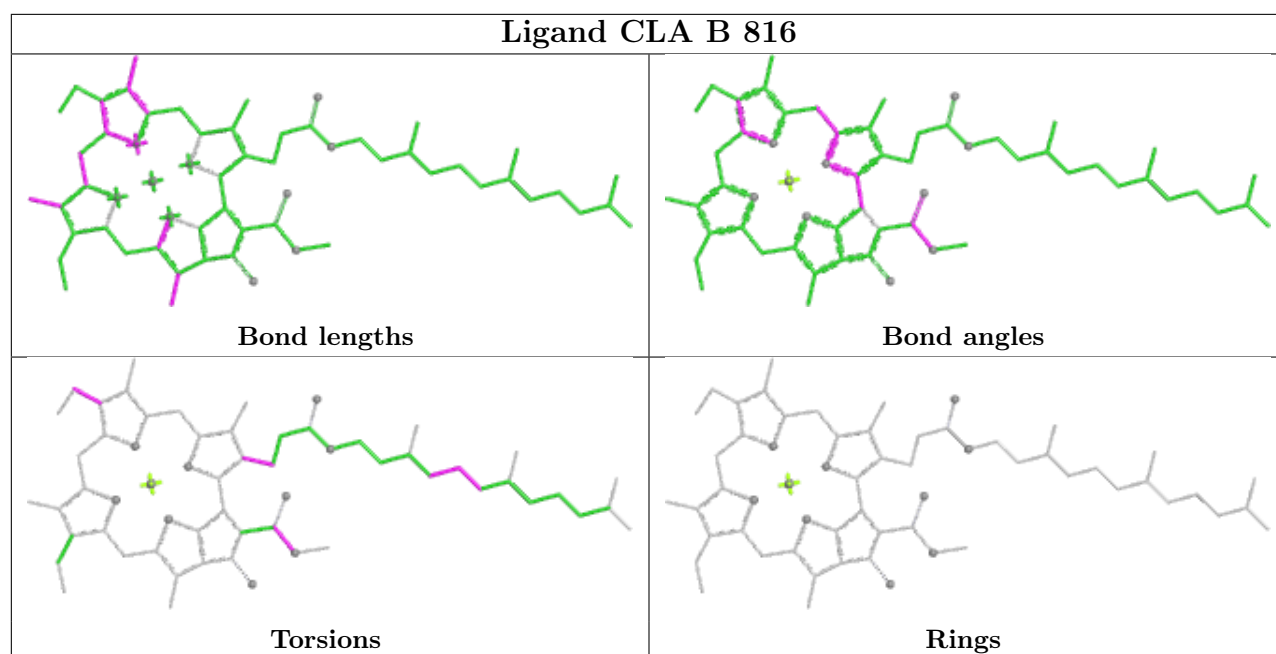
Torsions

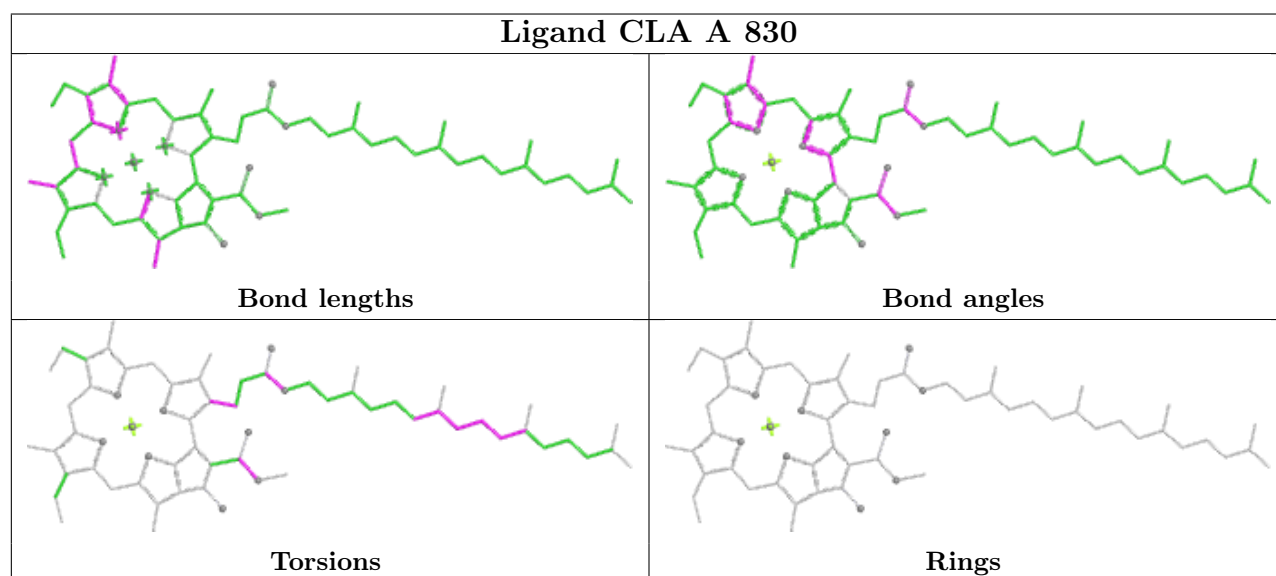
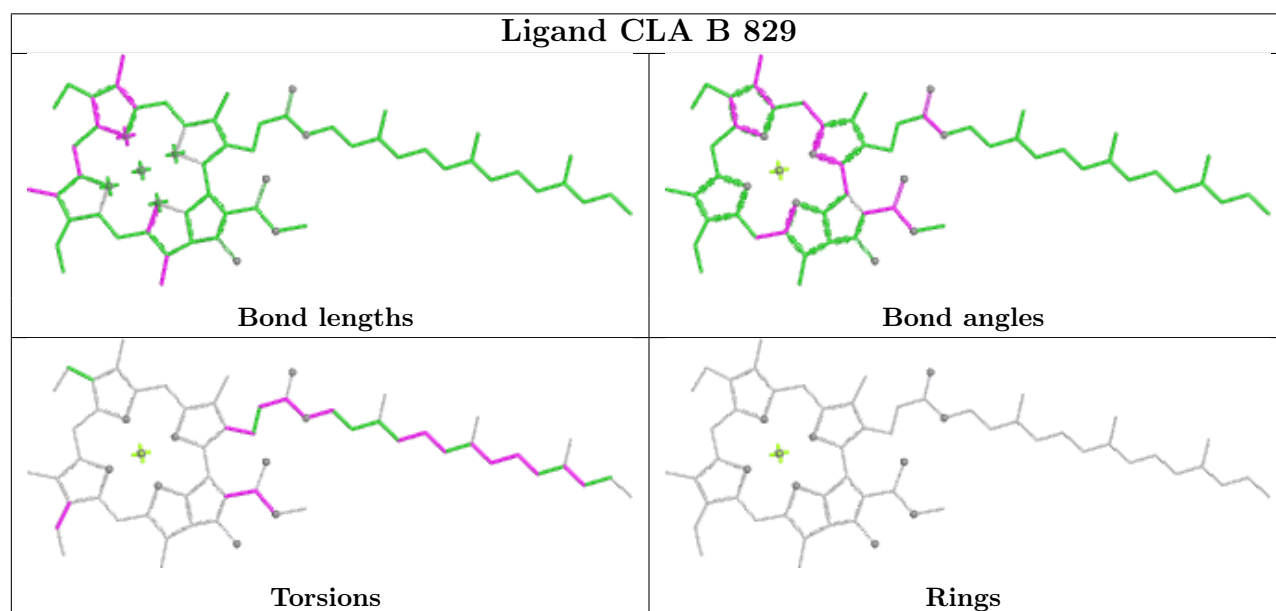
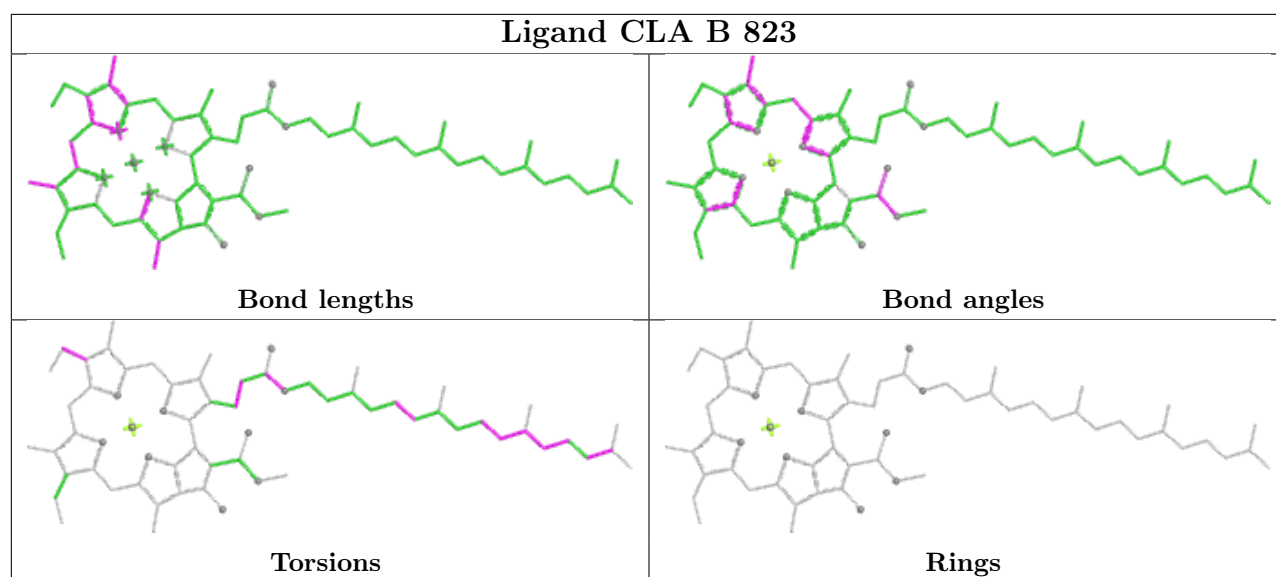


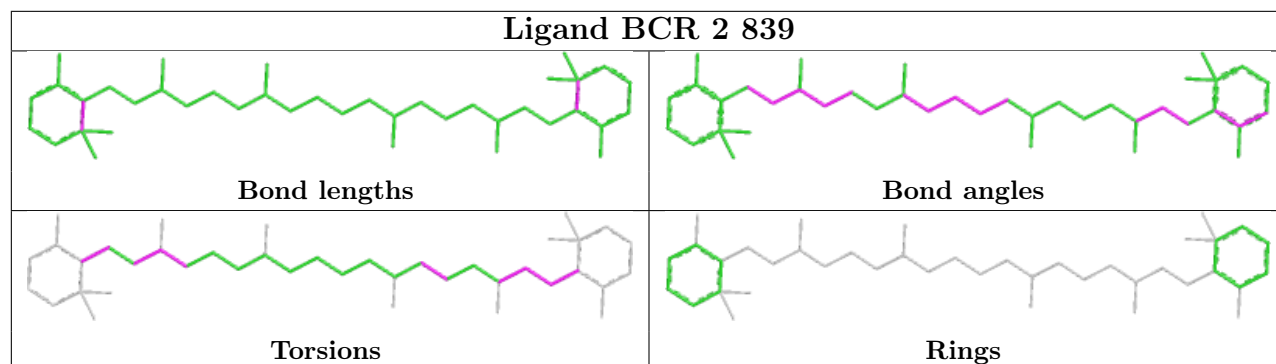
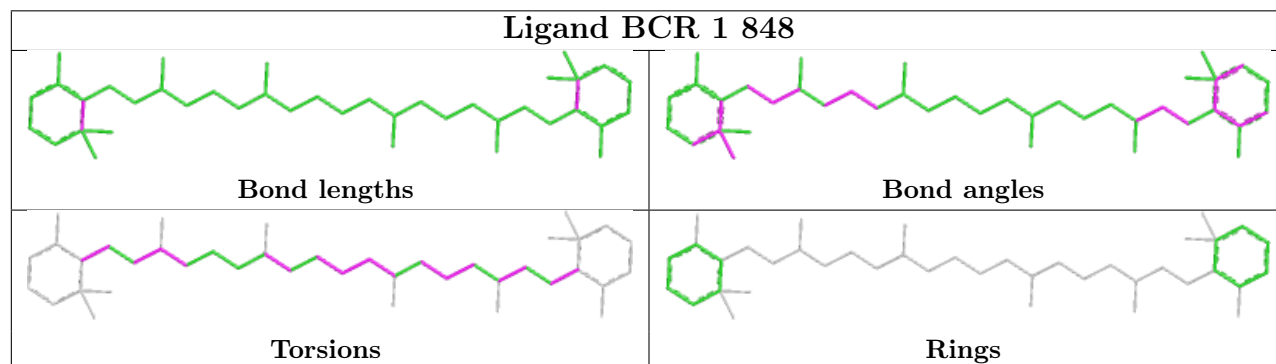
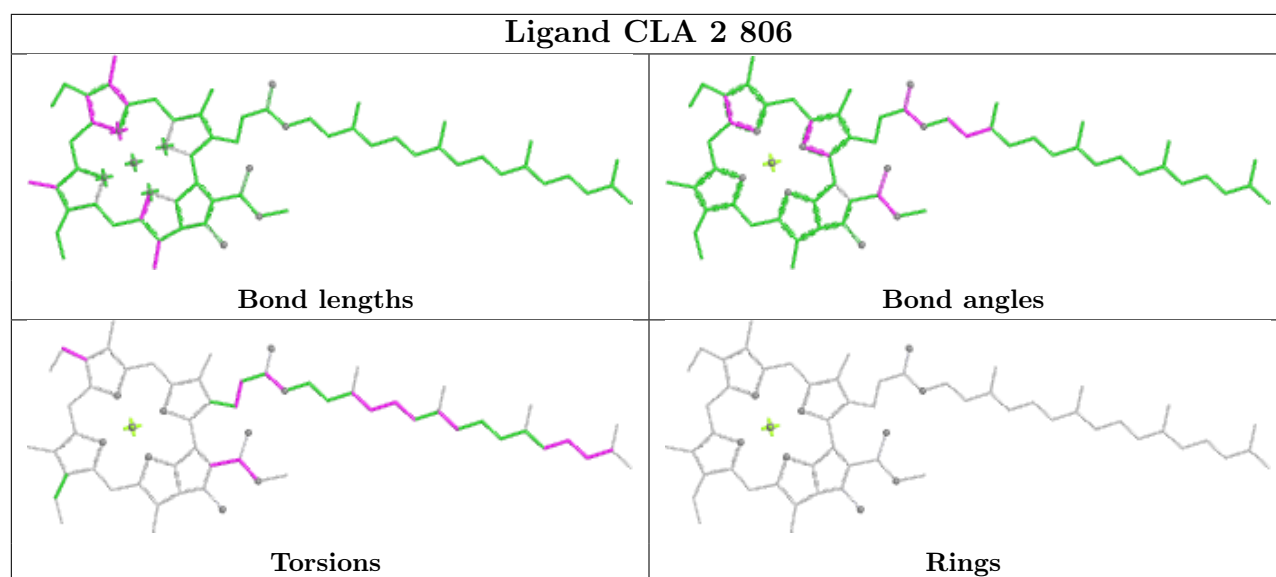
Rings

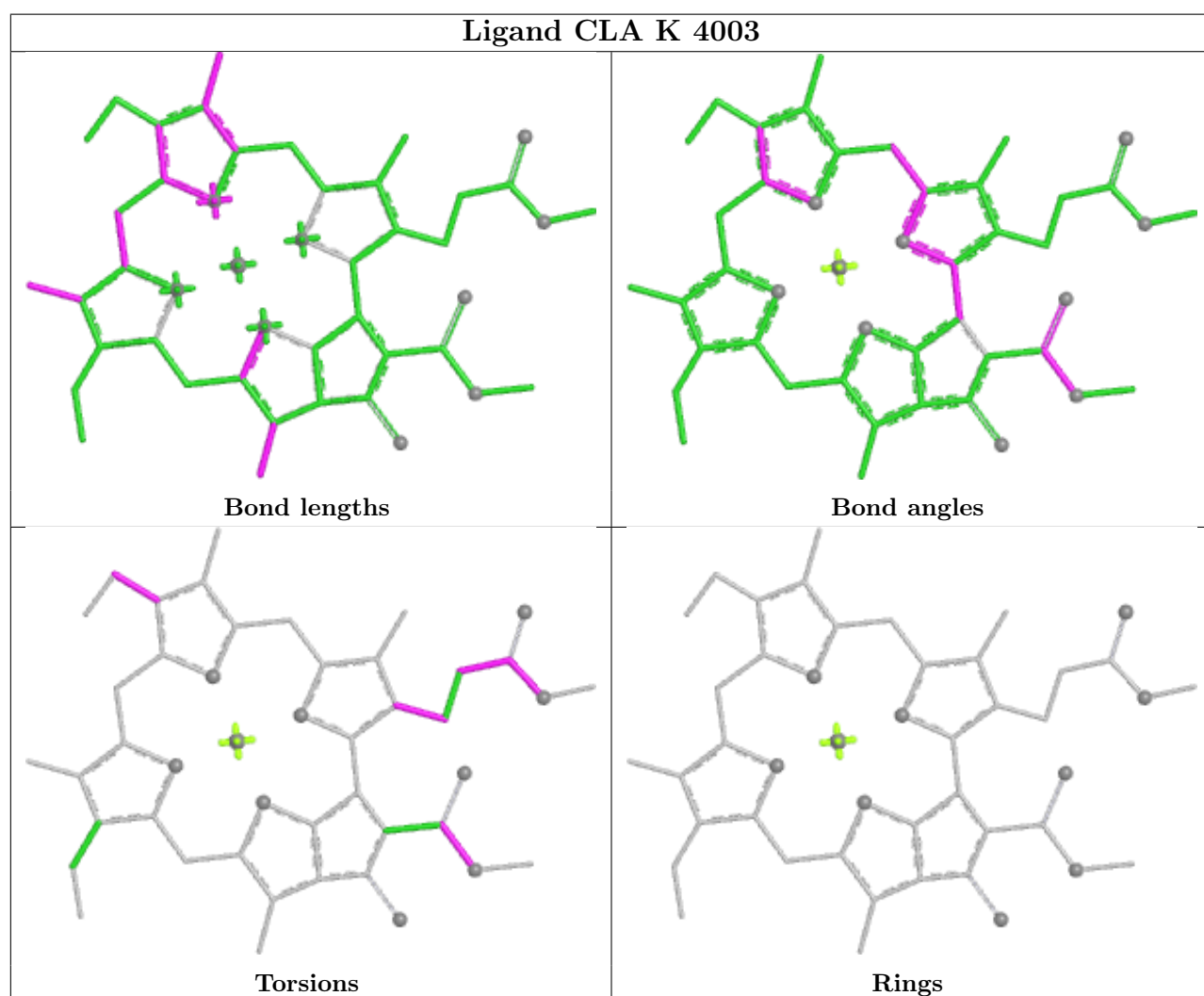
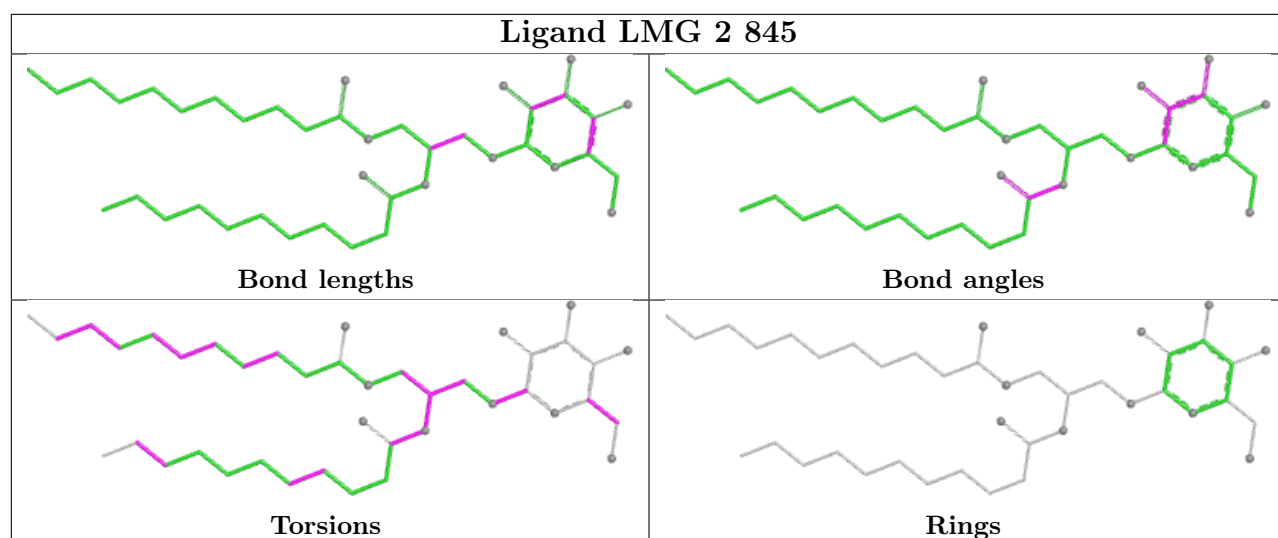




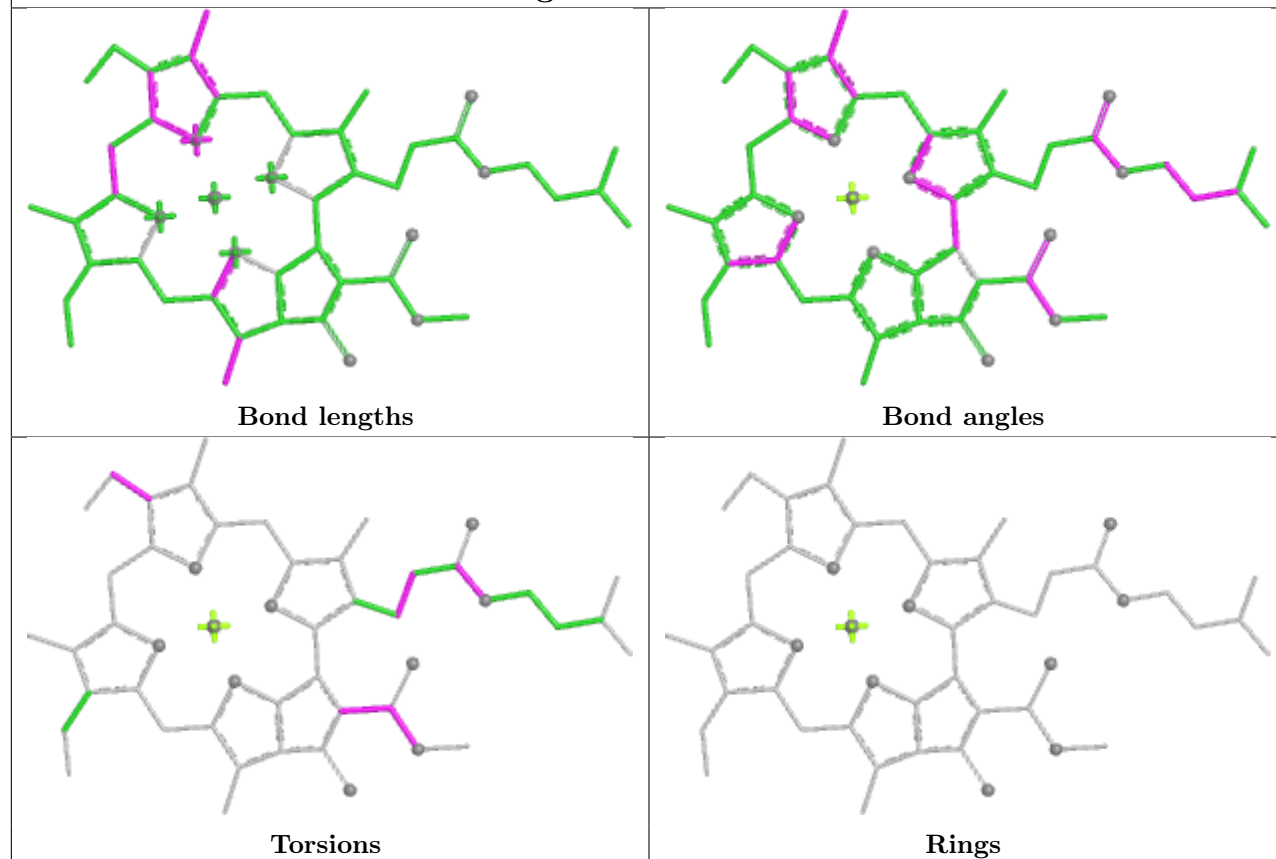




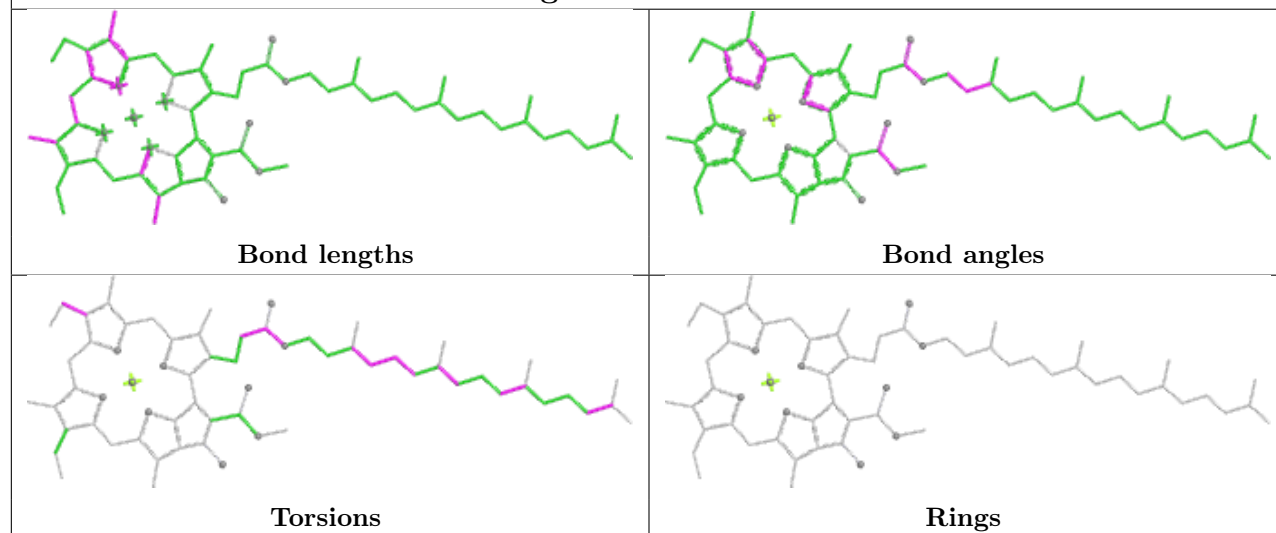


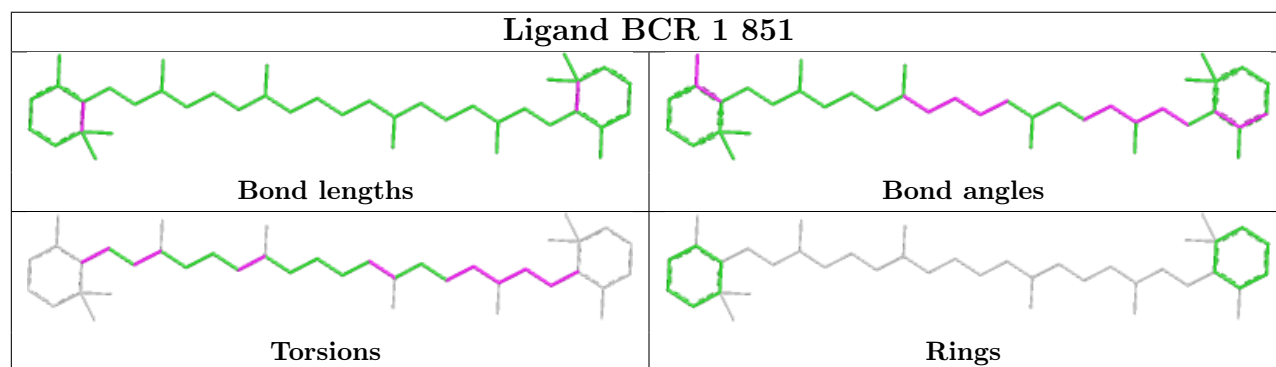
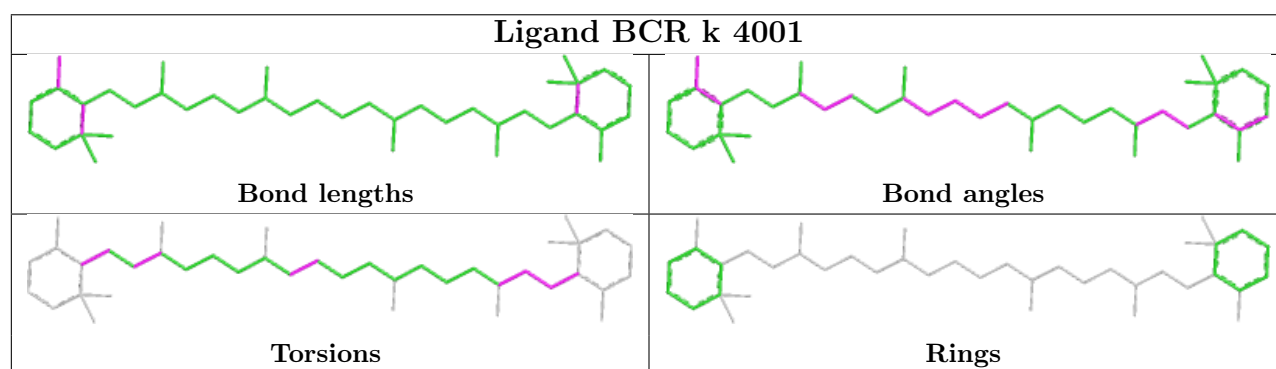
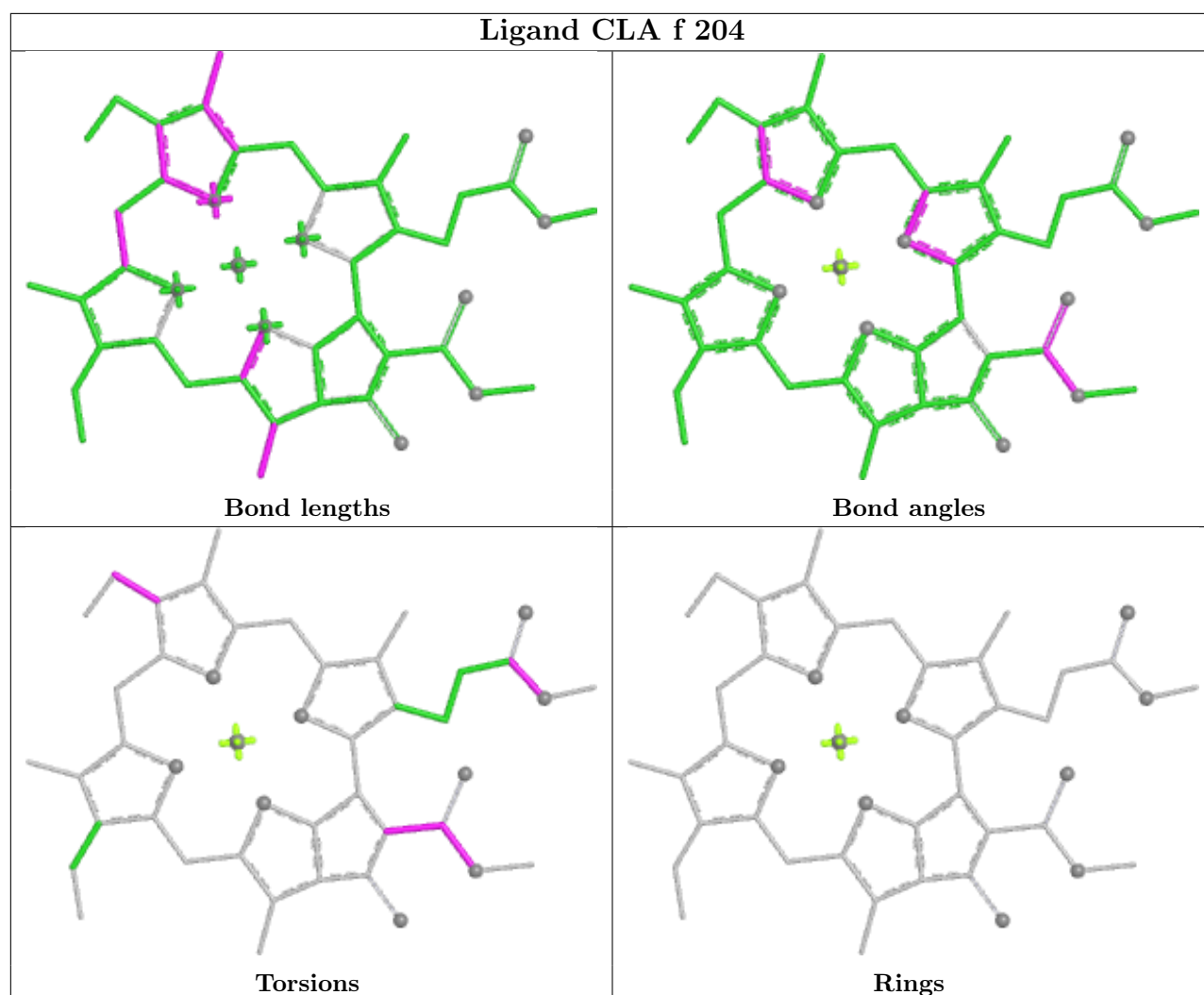


Ligand CLA 1 822

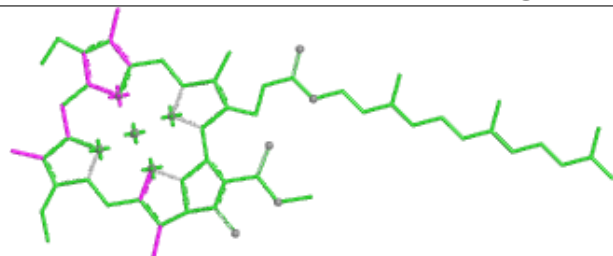


Ligand CL0 1 801

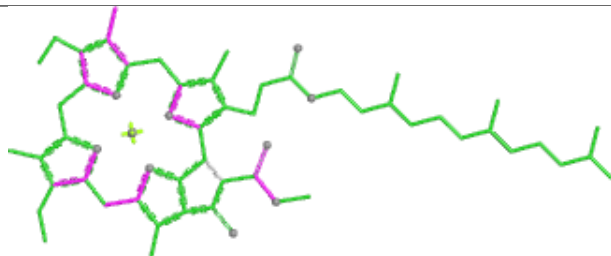




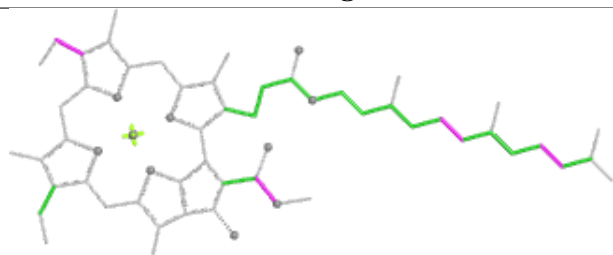
Ligand CLA b 834



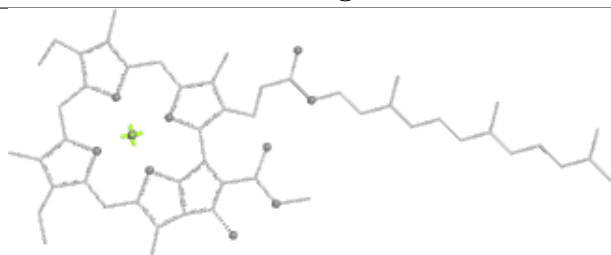
Bond lengths



Bond angles

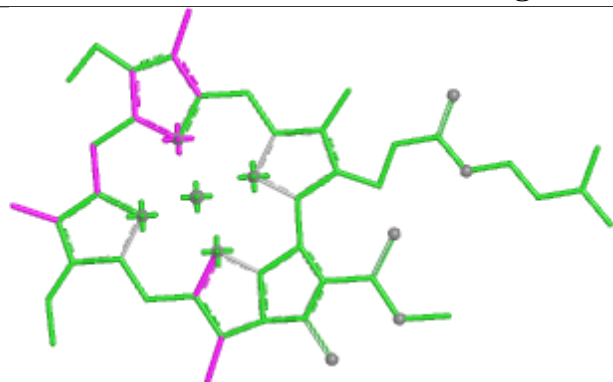


Torsions

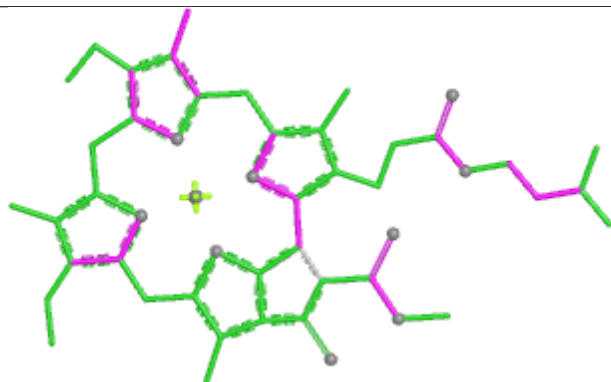


Rings

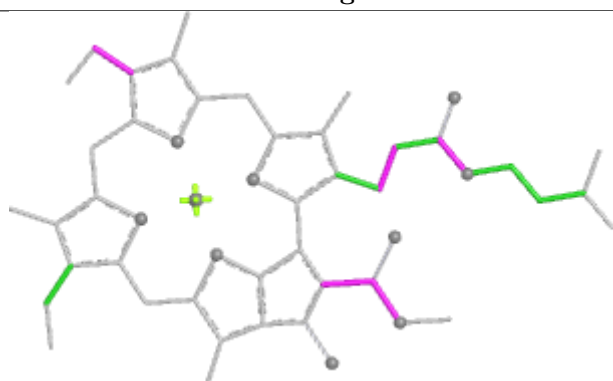
Ligand CLA A 822



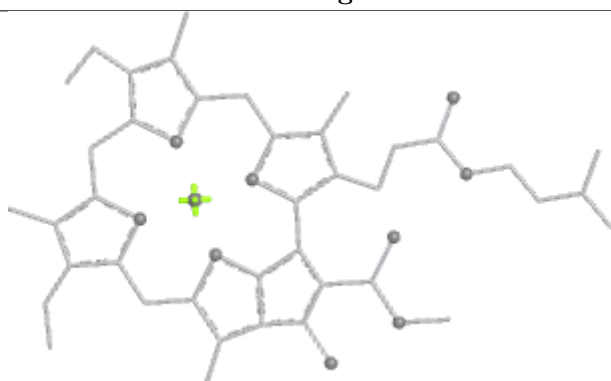
Bond lengths



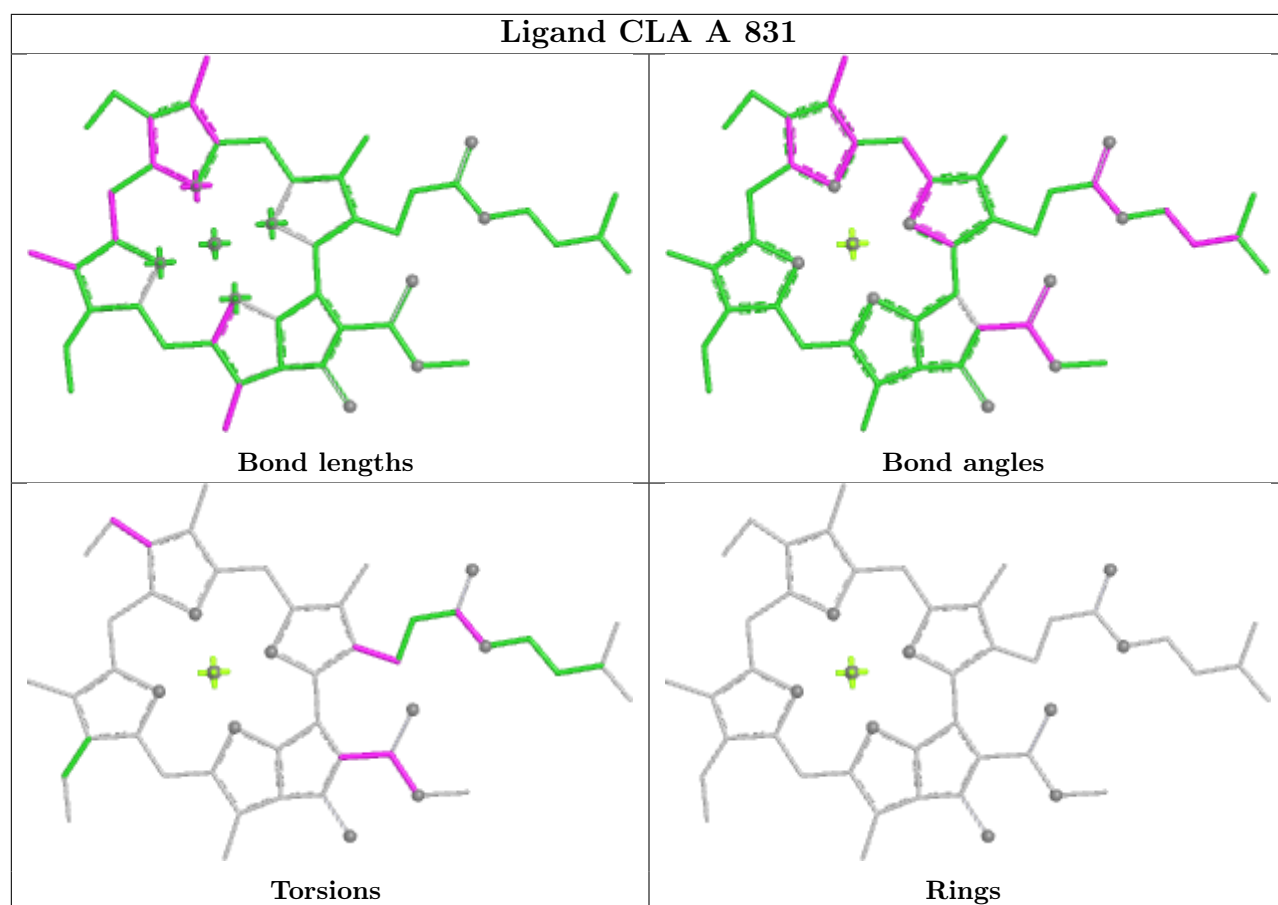
Bond angles



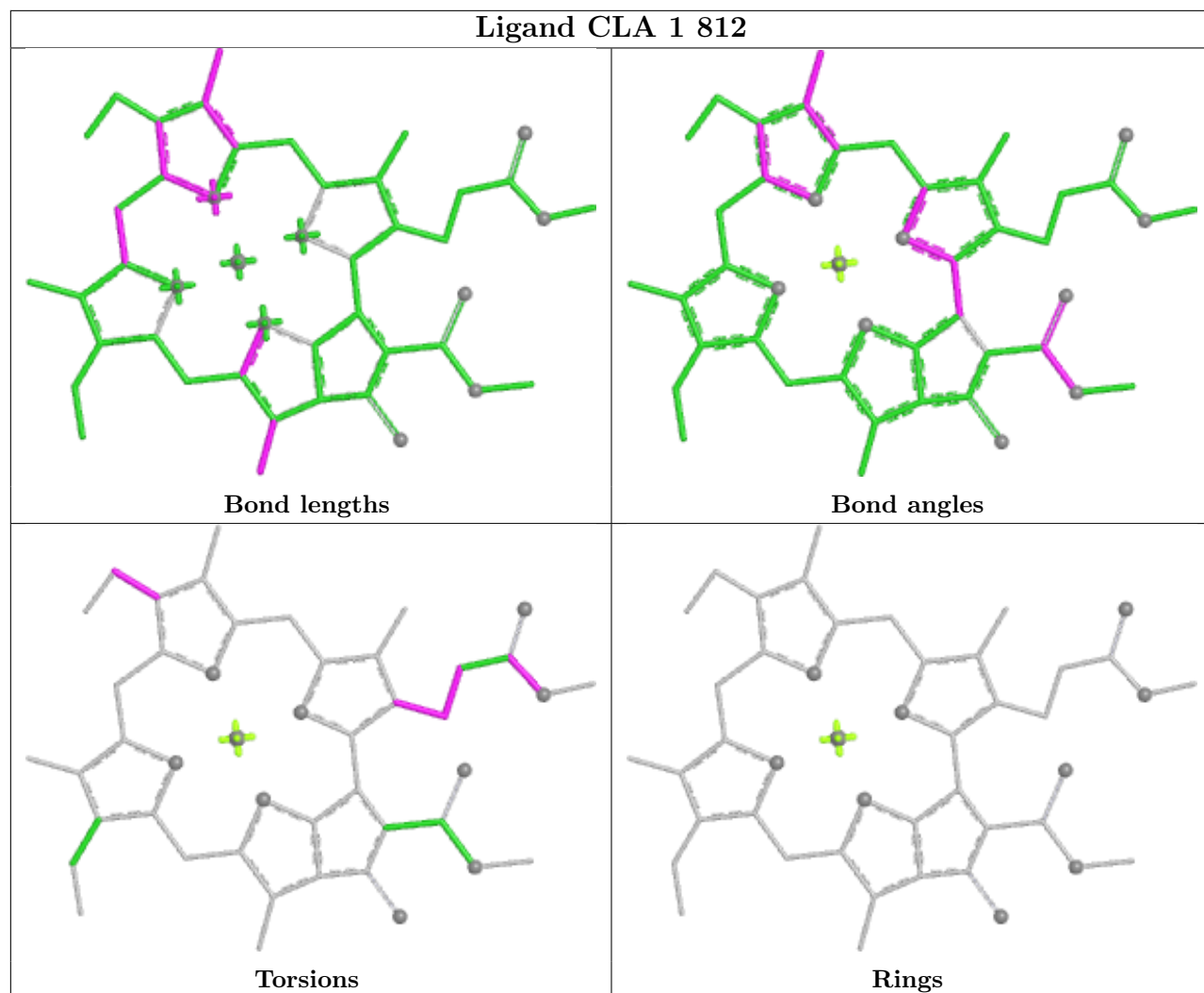
Torsions

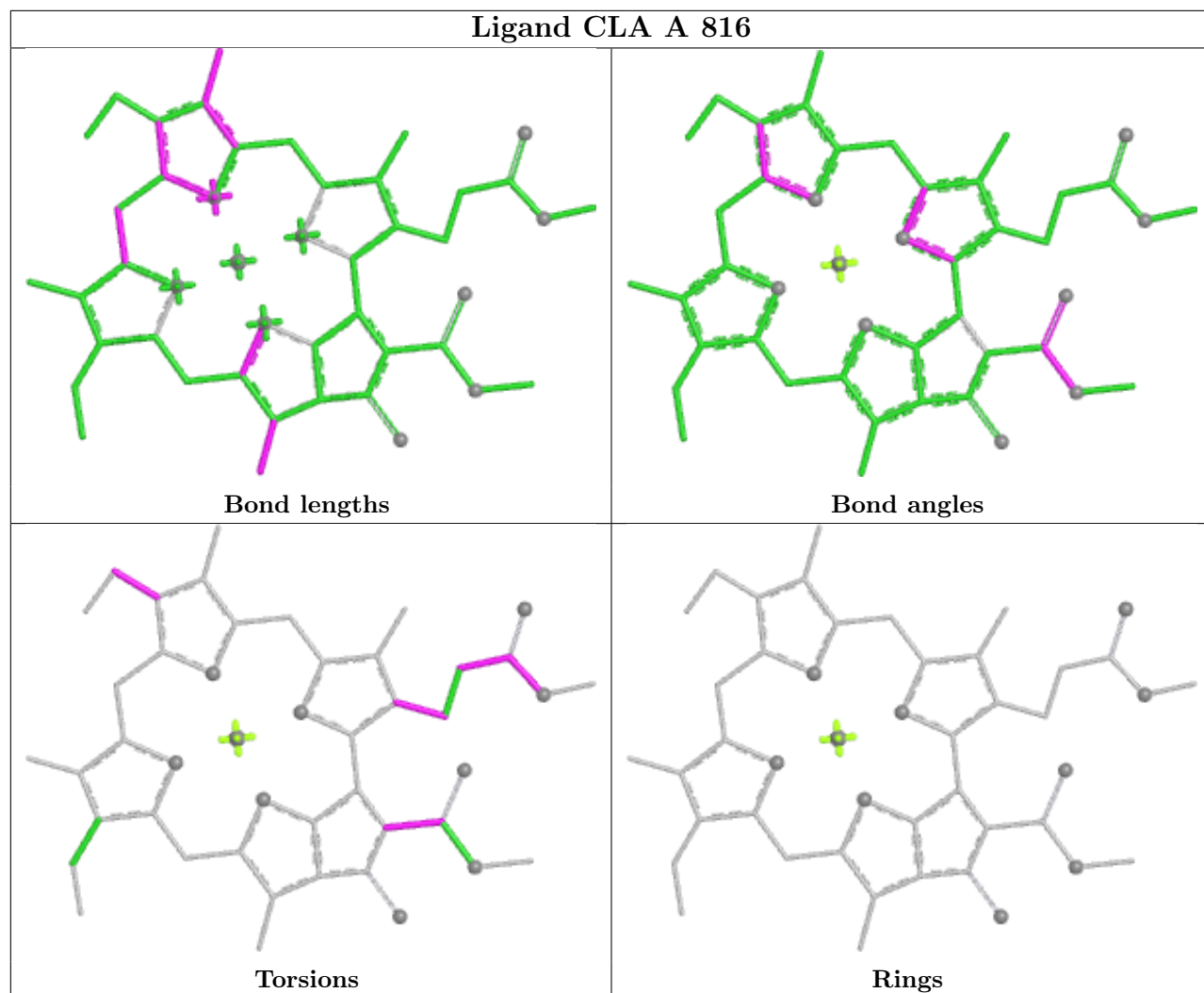


Rings

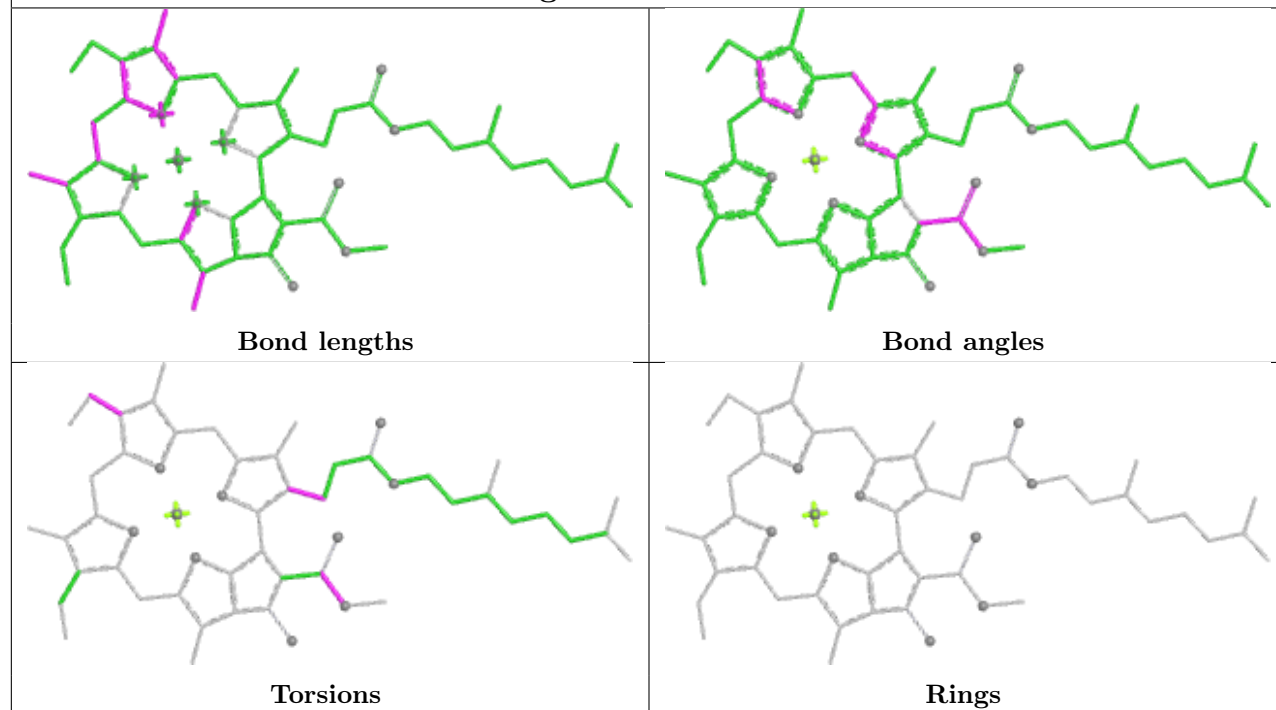


Ligand CLA 1 812

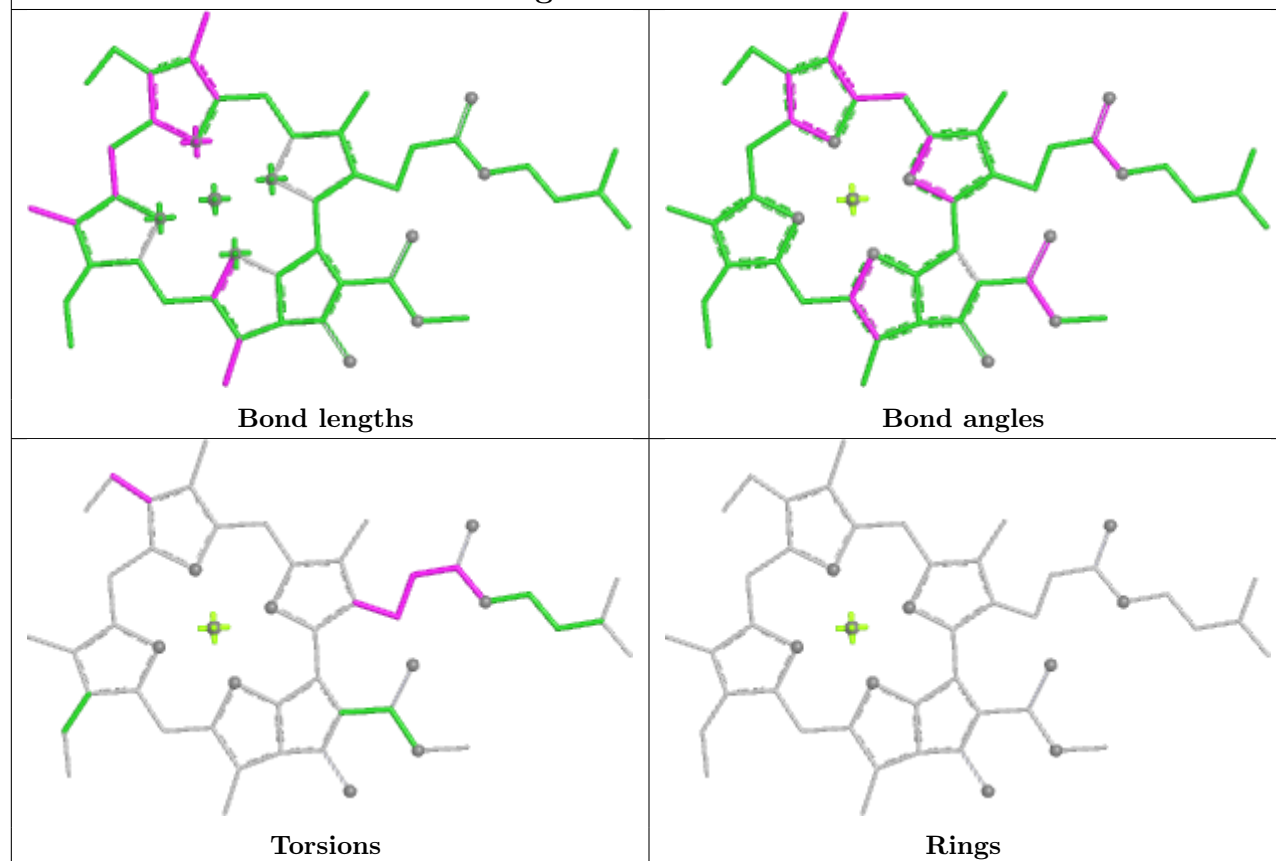




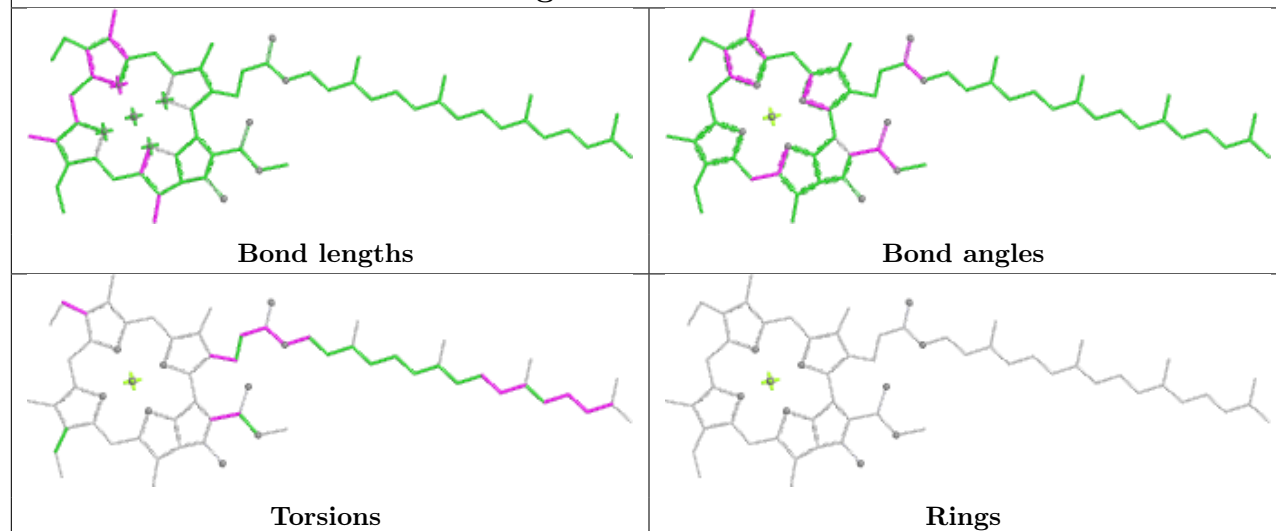
Ligand CLA f 201



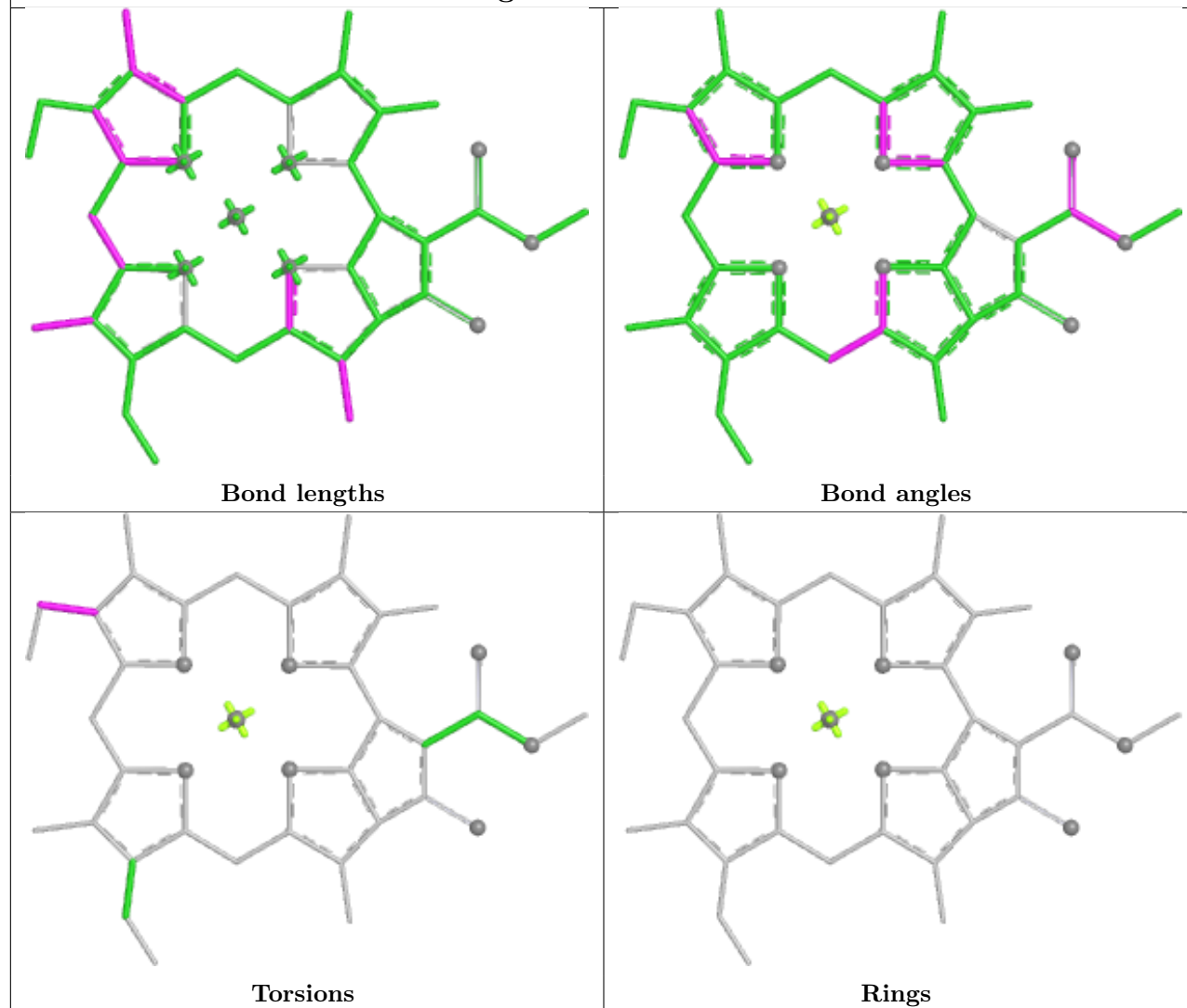
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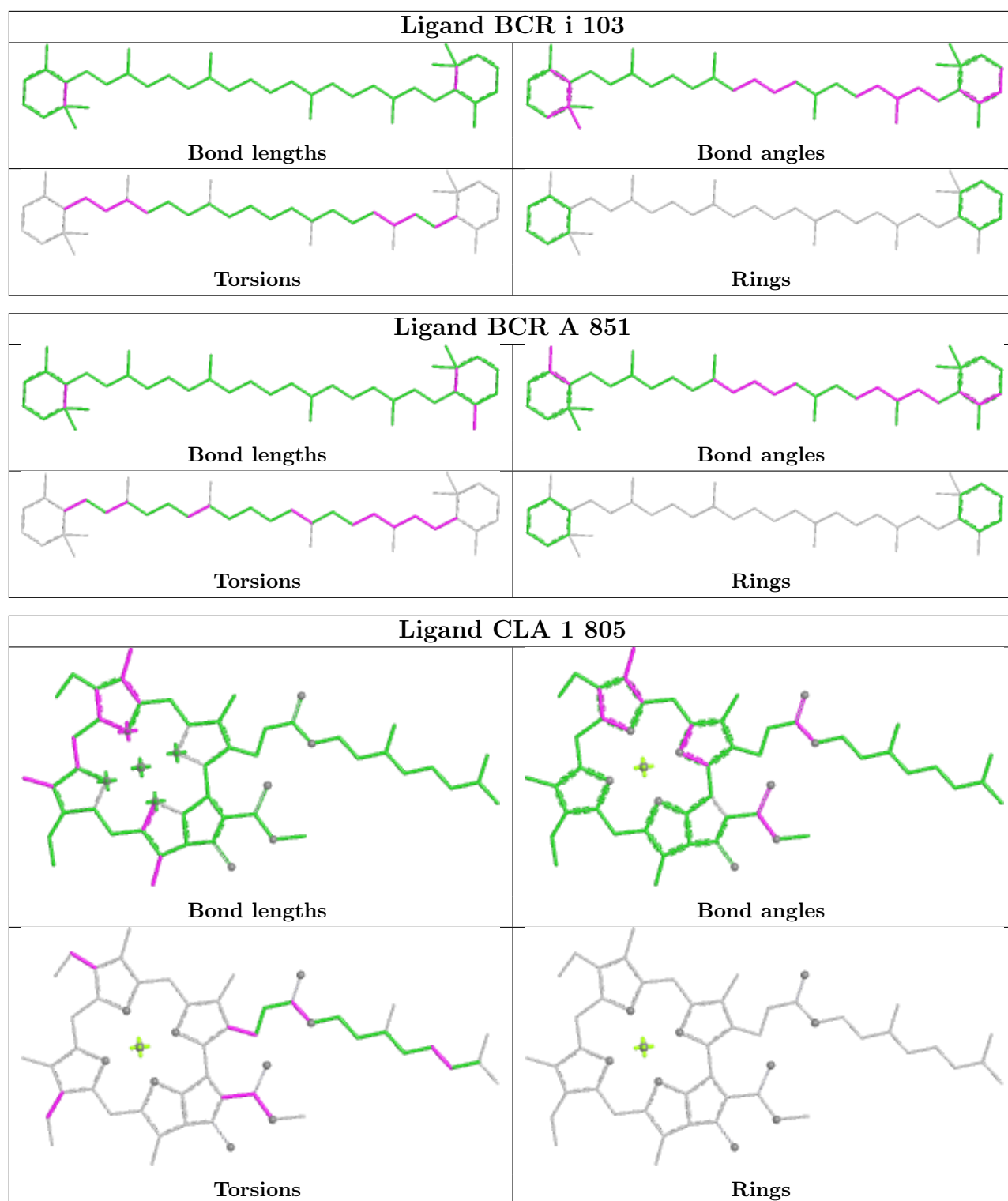


Ligand CLA 2 804

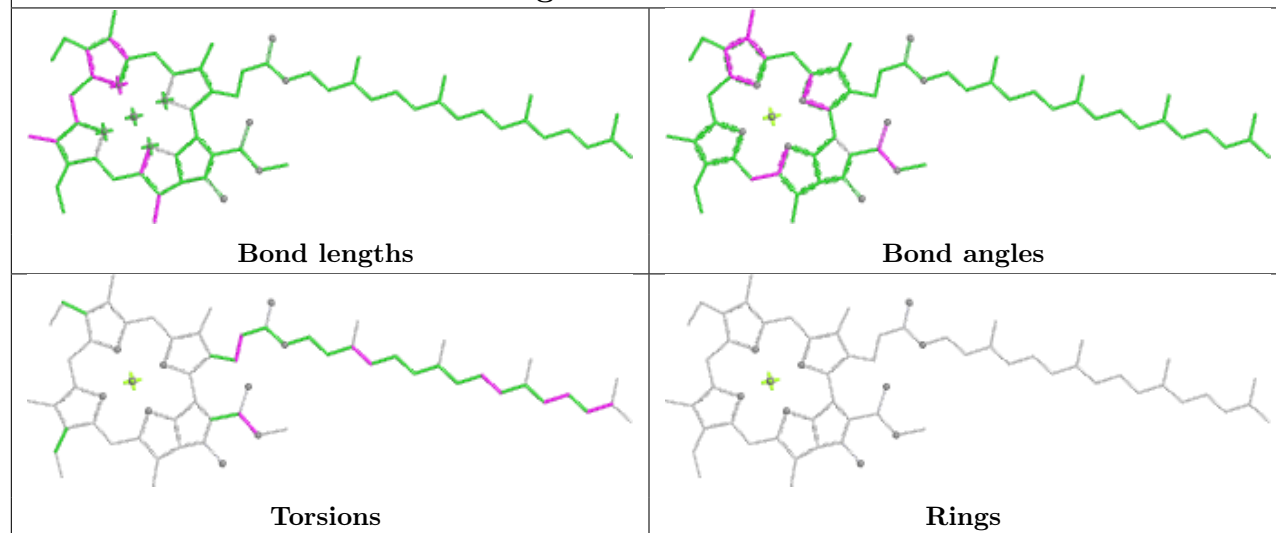


Ligand CLA b 817

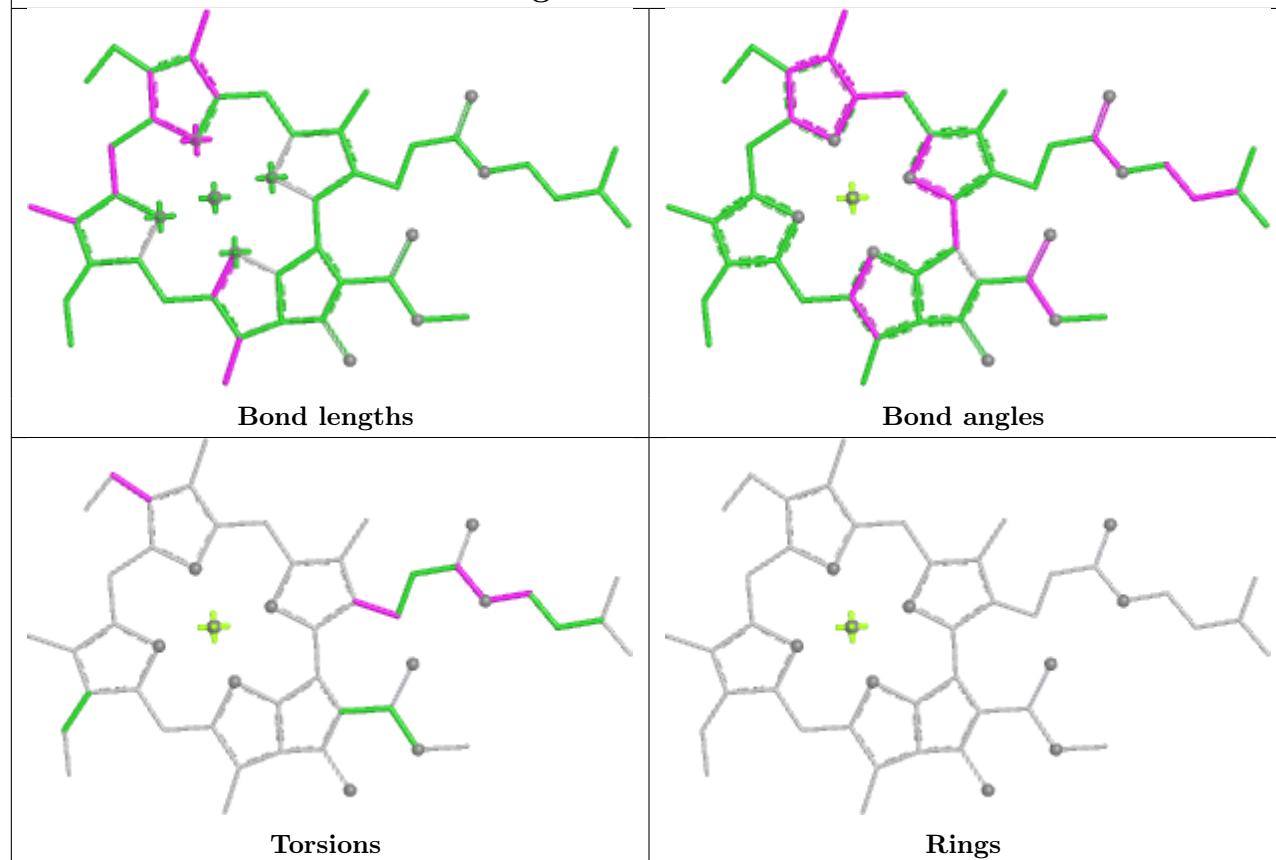




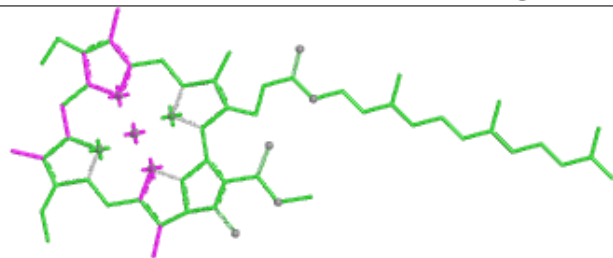
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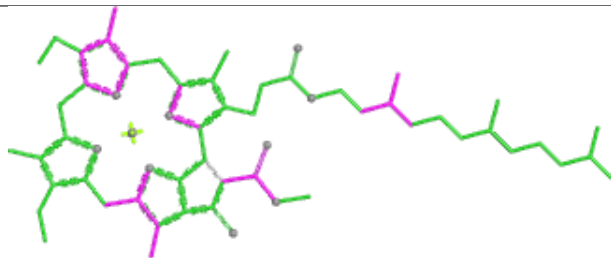
Ligand CLA B 833



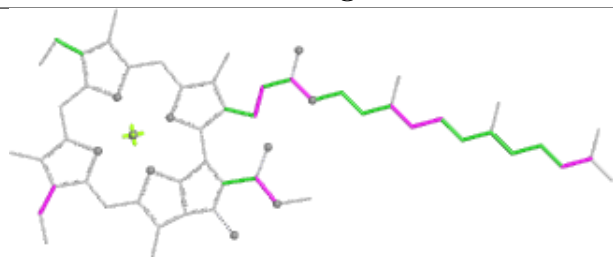
Ligand CLA A 802



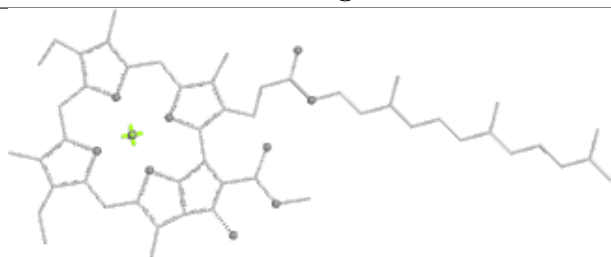
Bond lengths



Bond angles

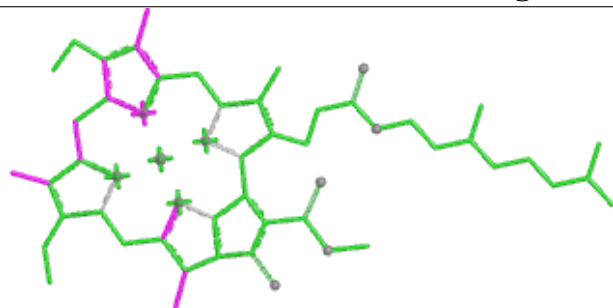


Torsions

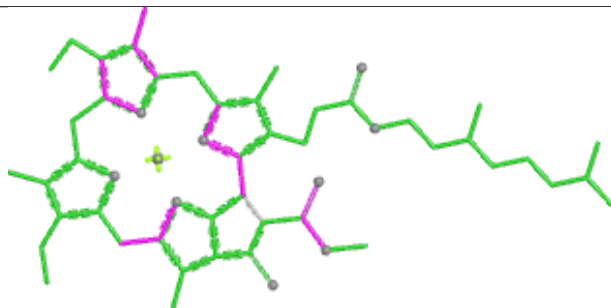


Rings

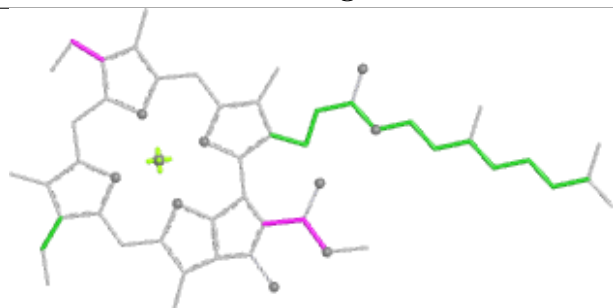
Ligand CLA A 807



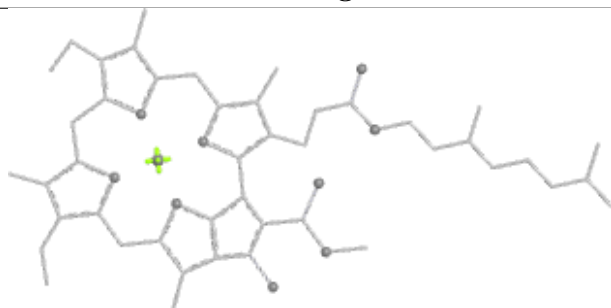
Bond lengths



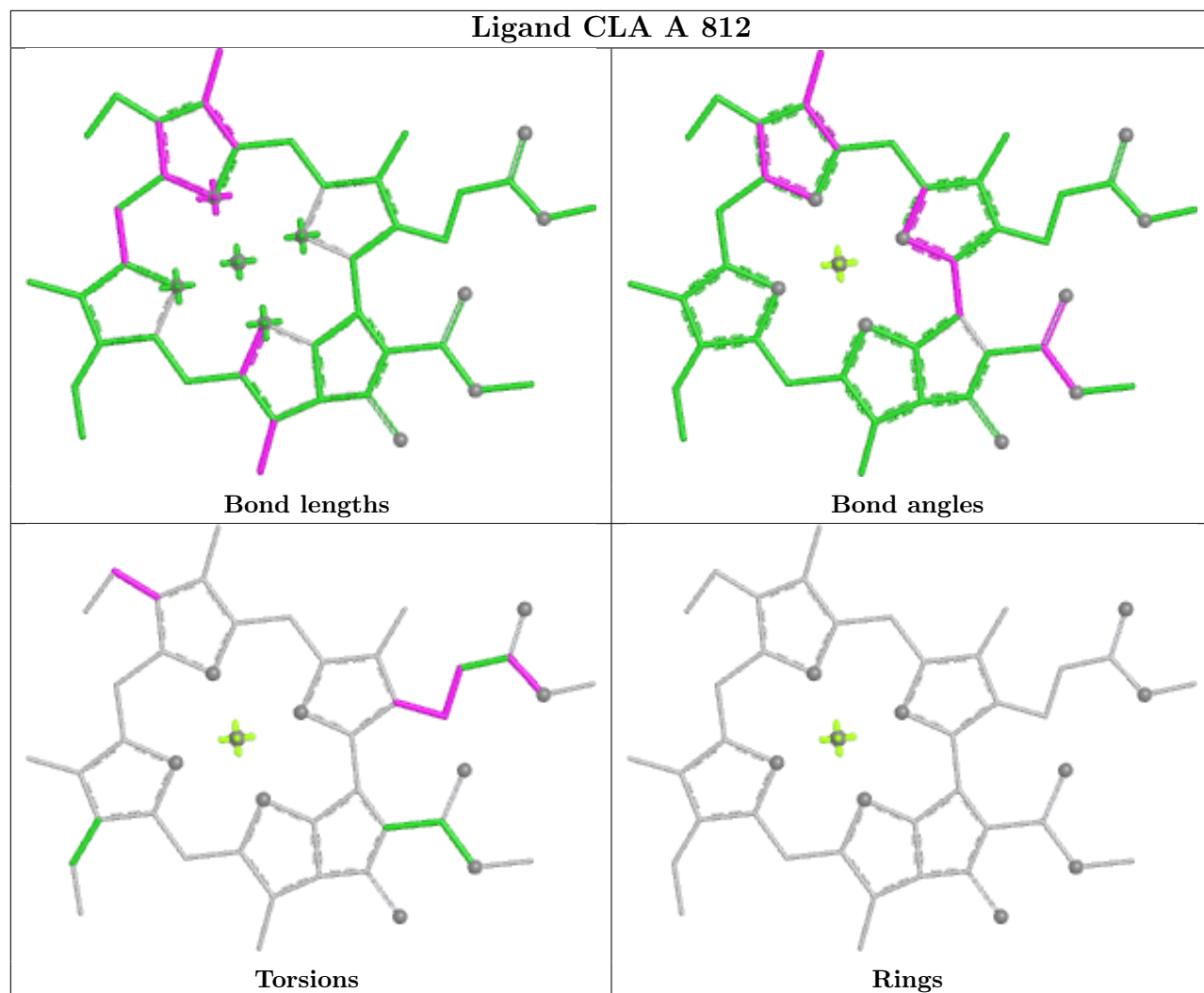
Bond angles



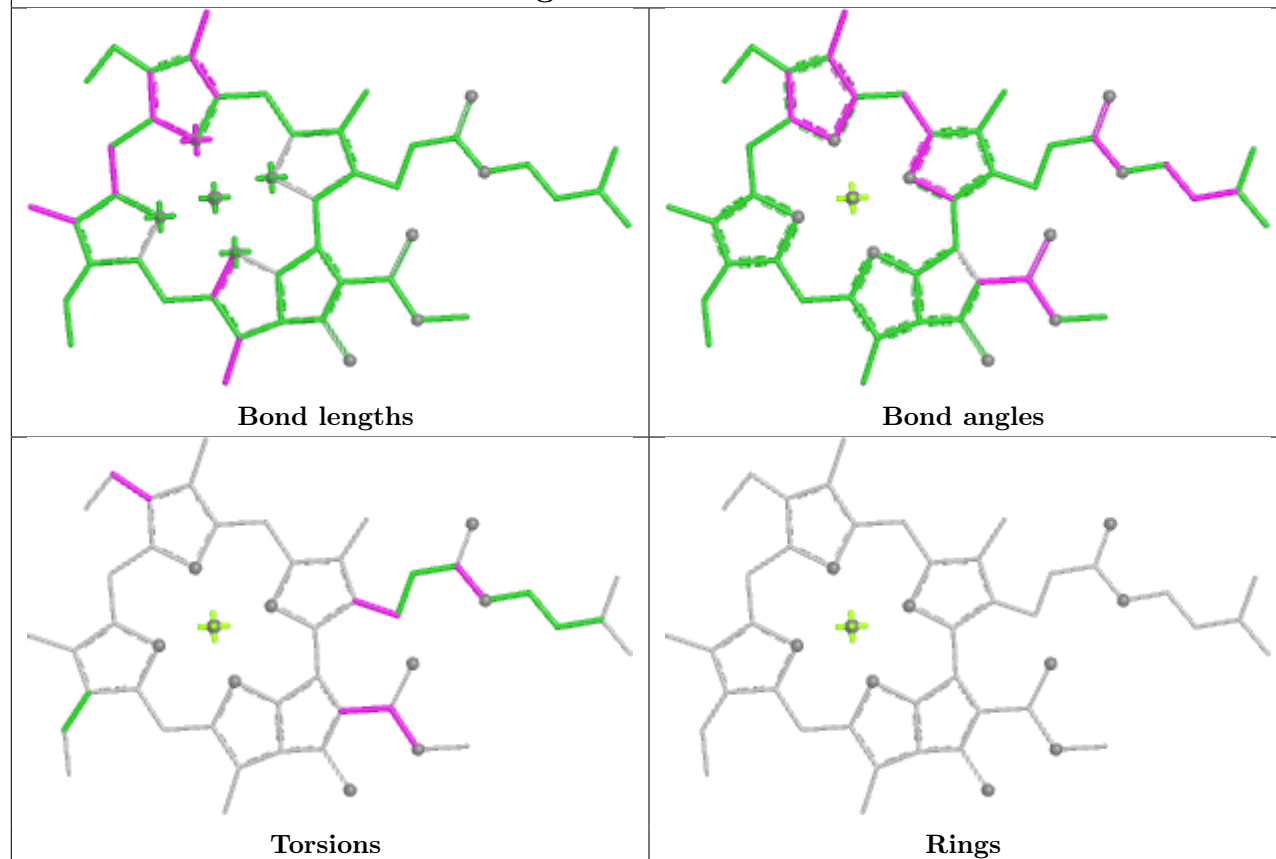
Torsions



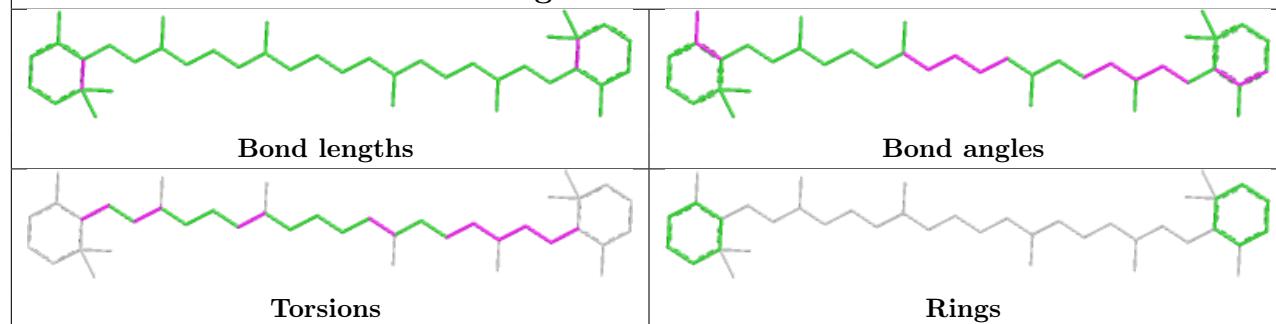
Rings

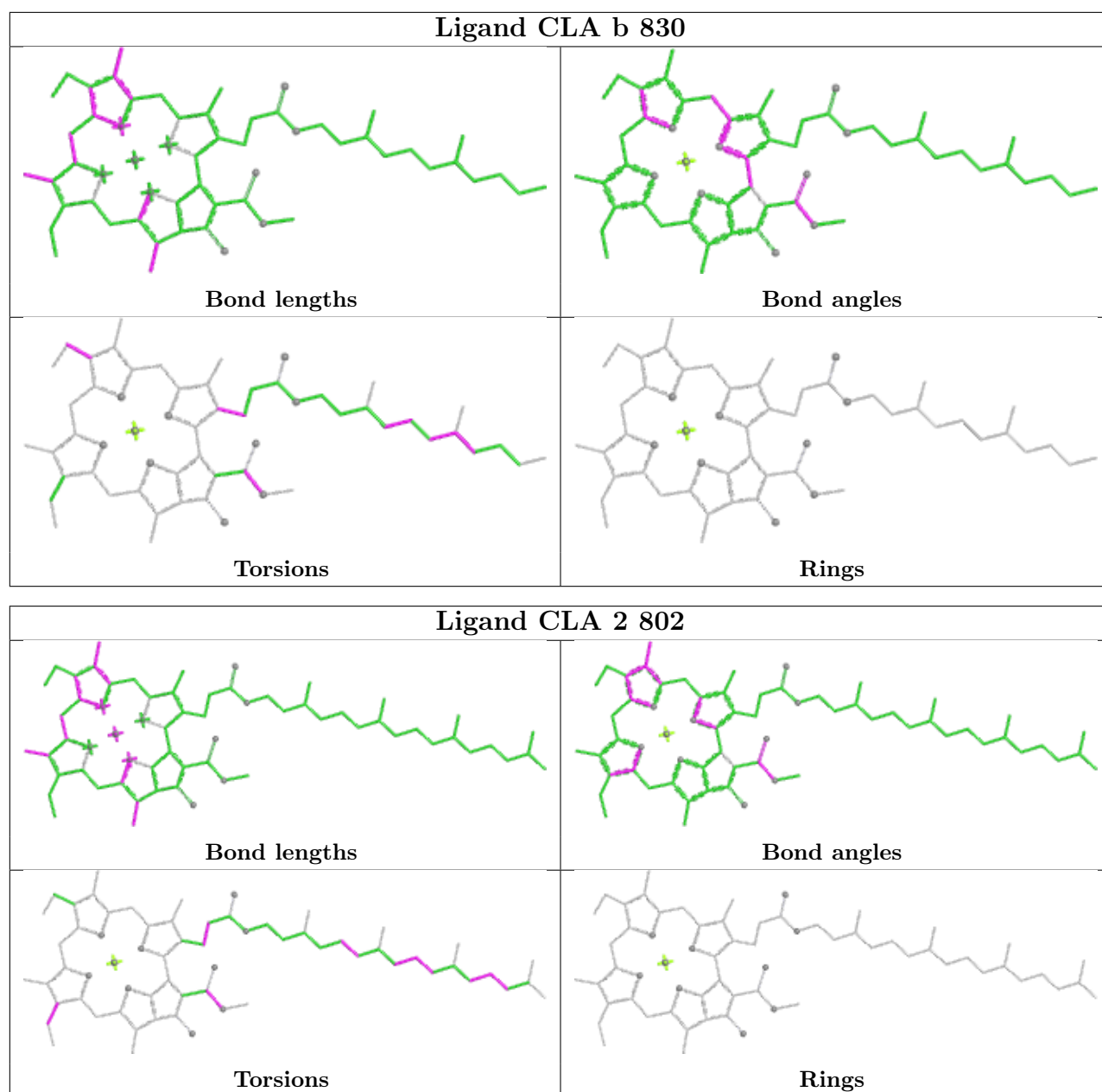


Ligand CLA a 831

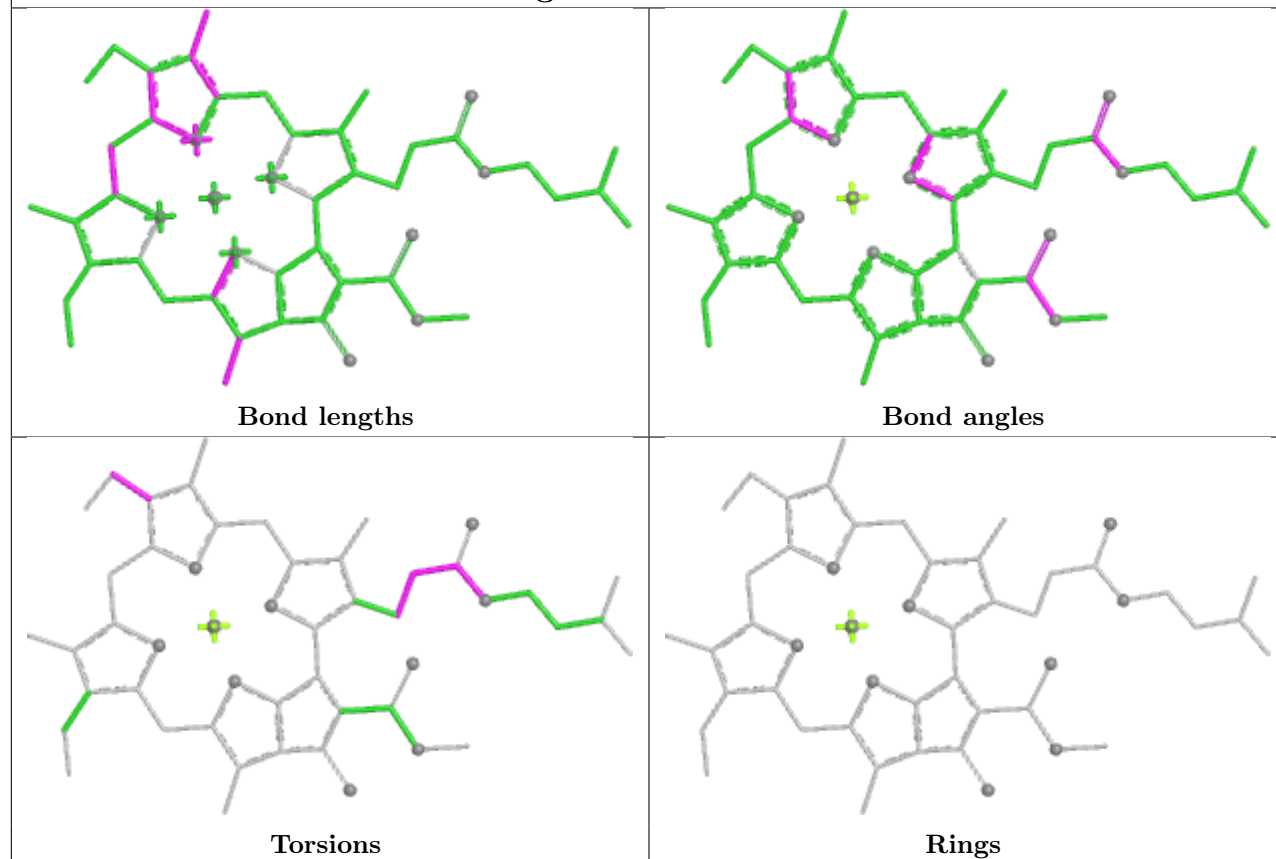


Ligand BCR a 851

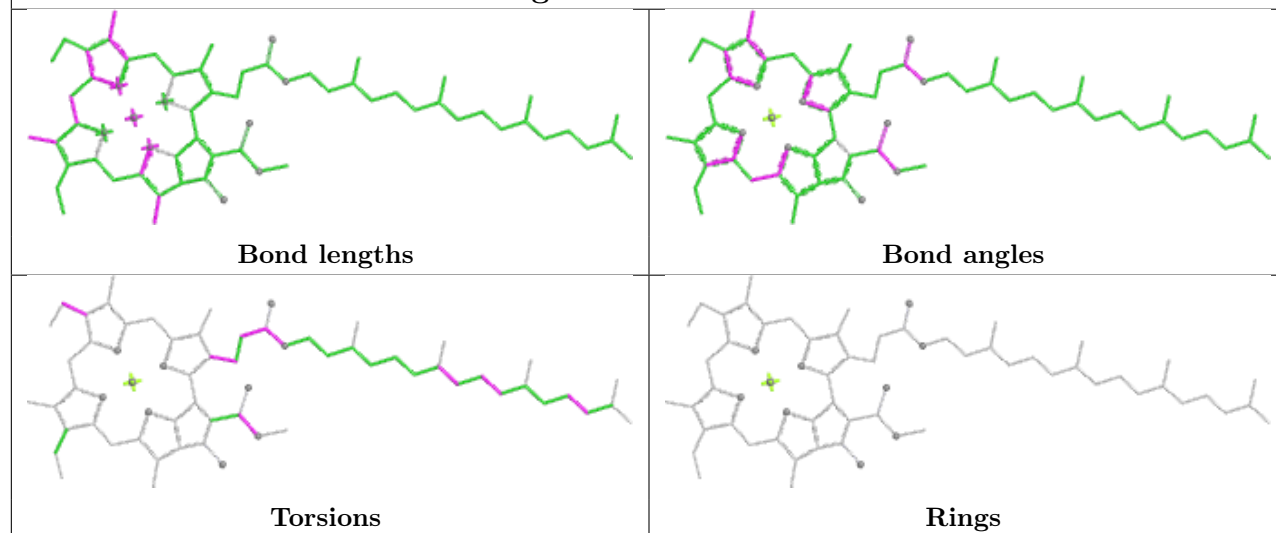


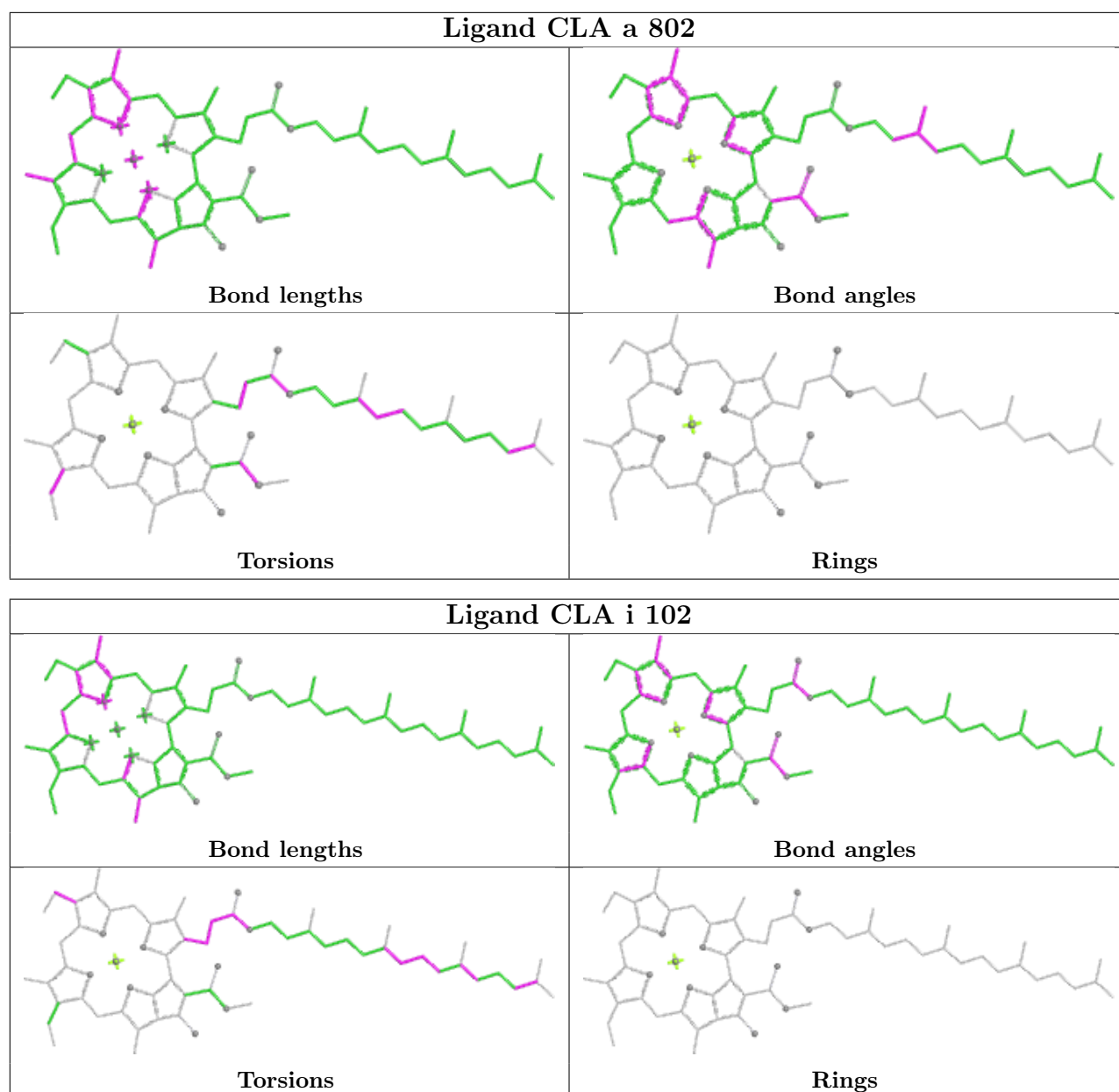


Ligand CLA a 823

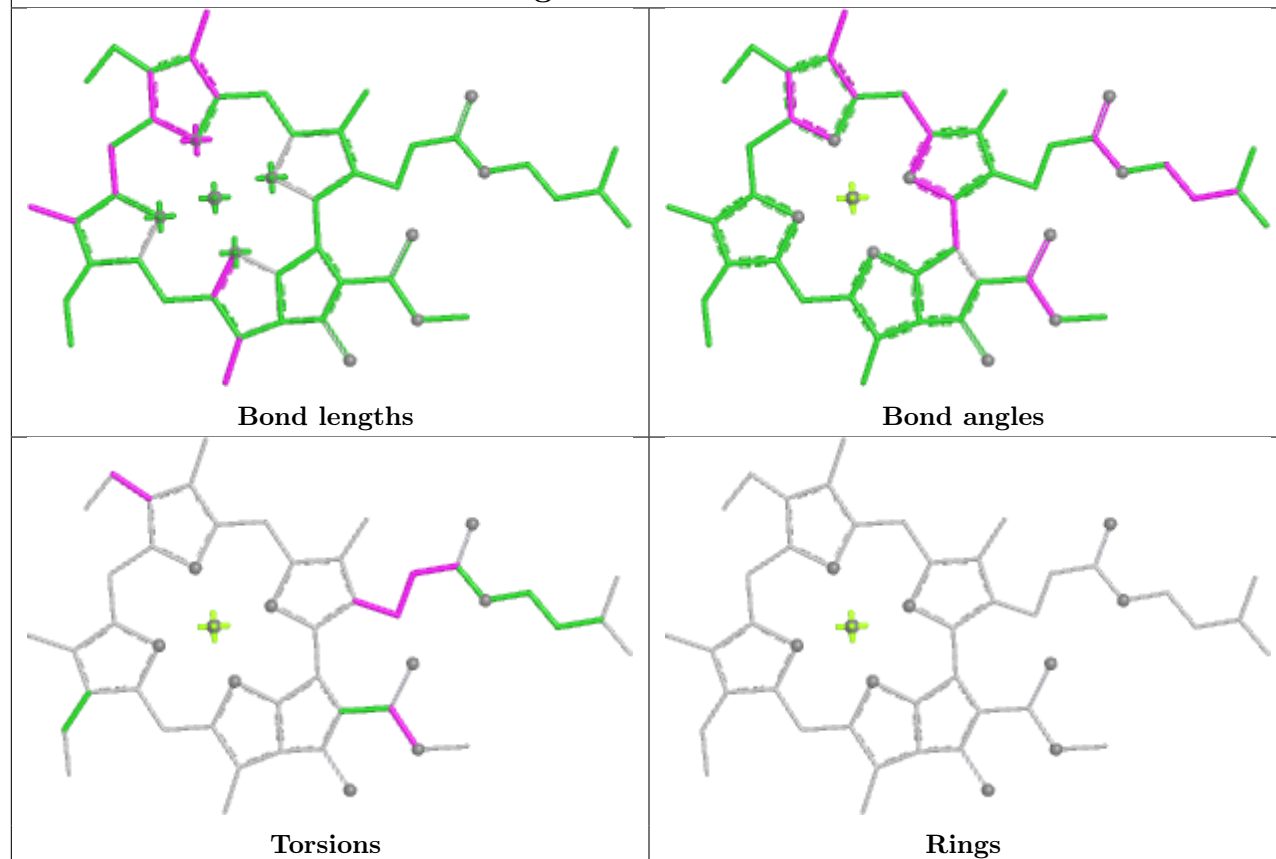


Ligand CLA A 806

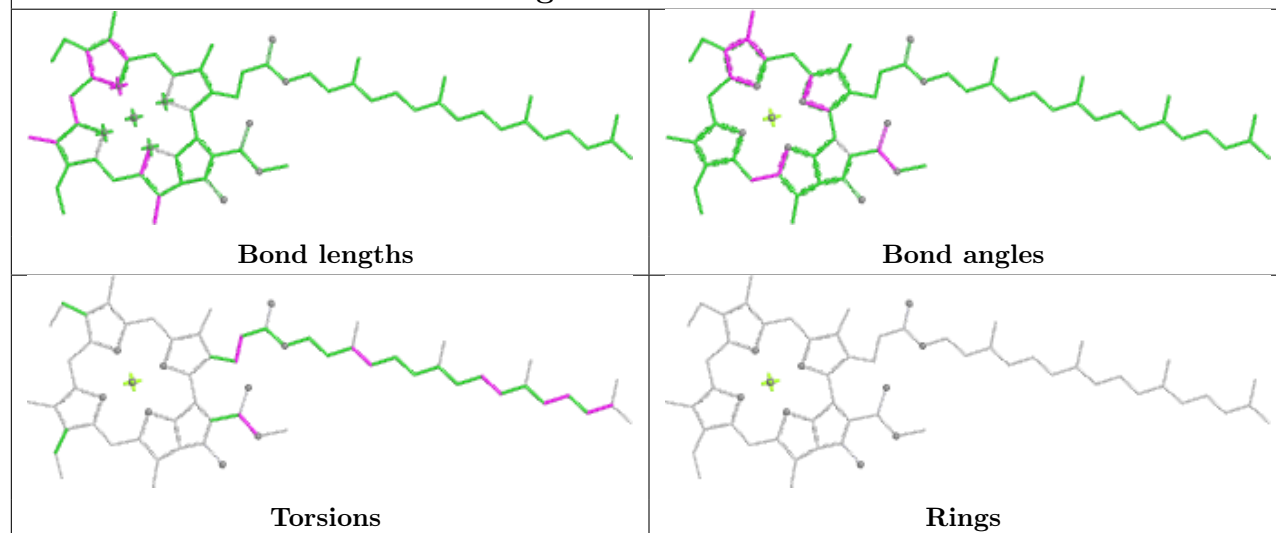


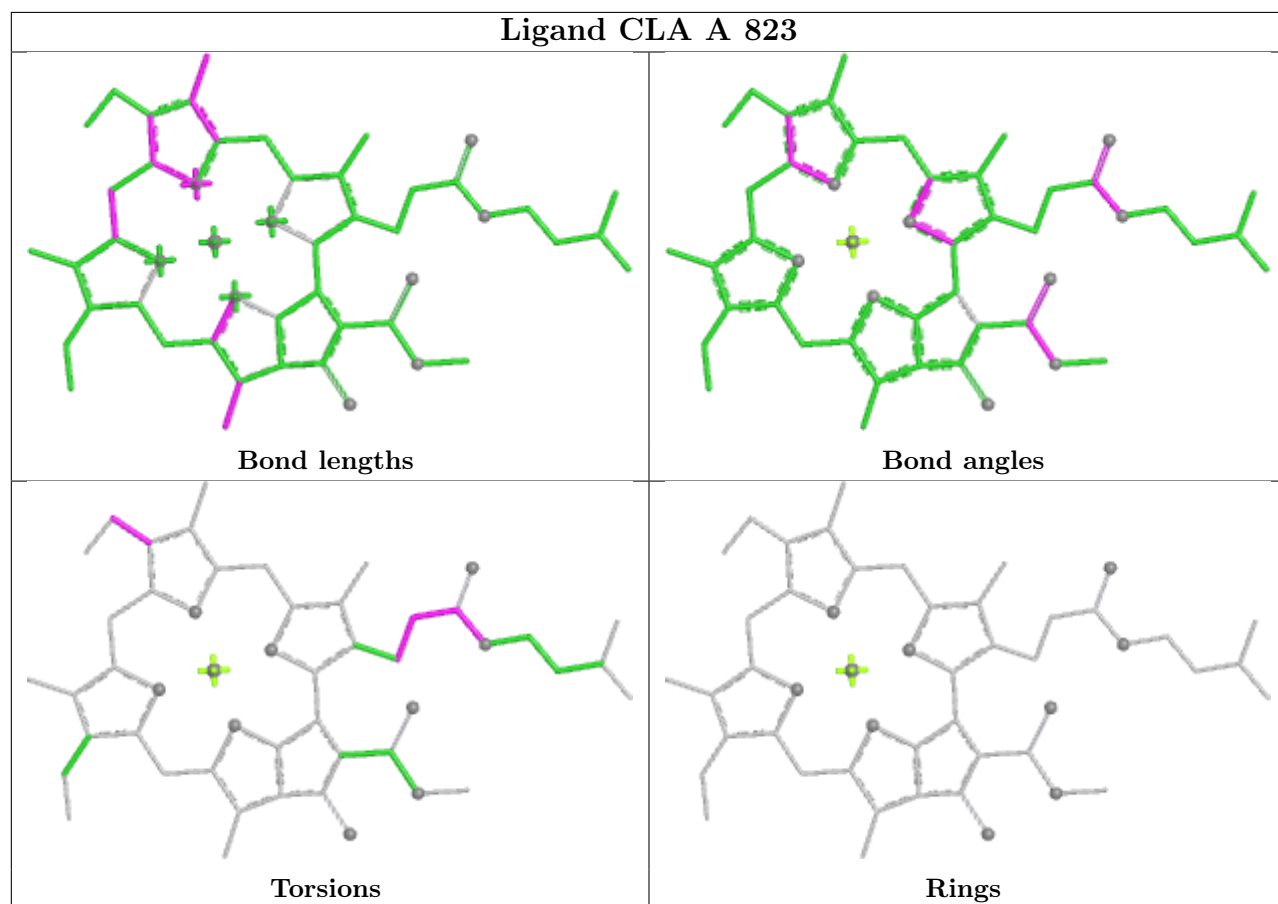
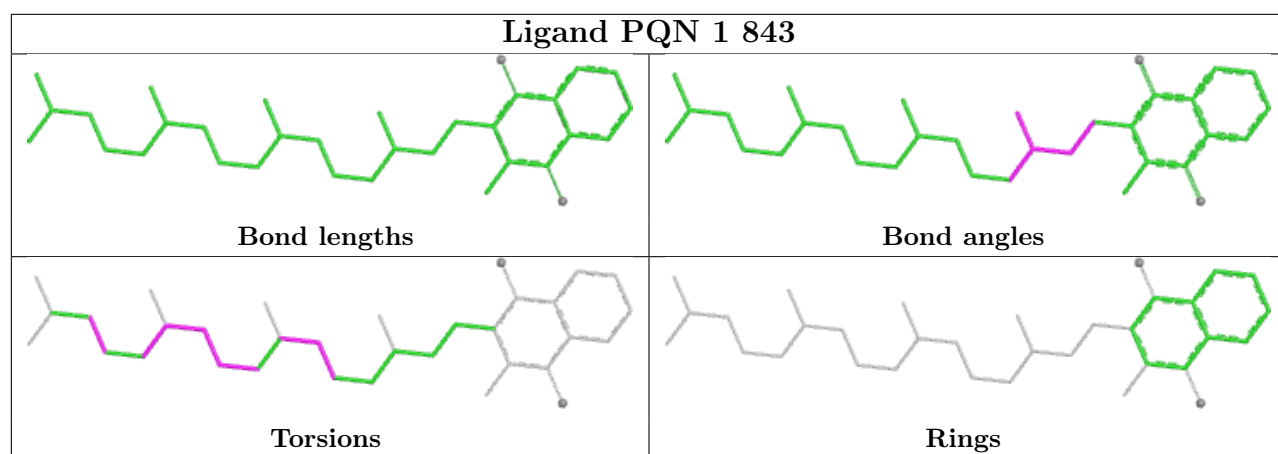


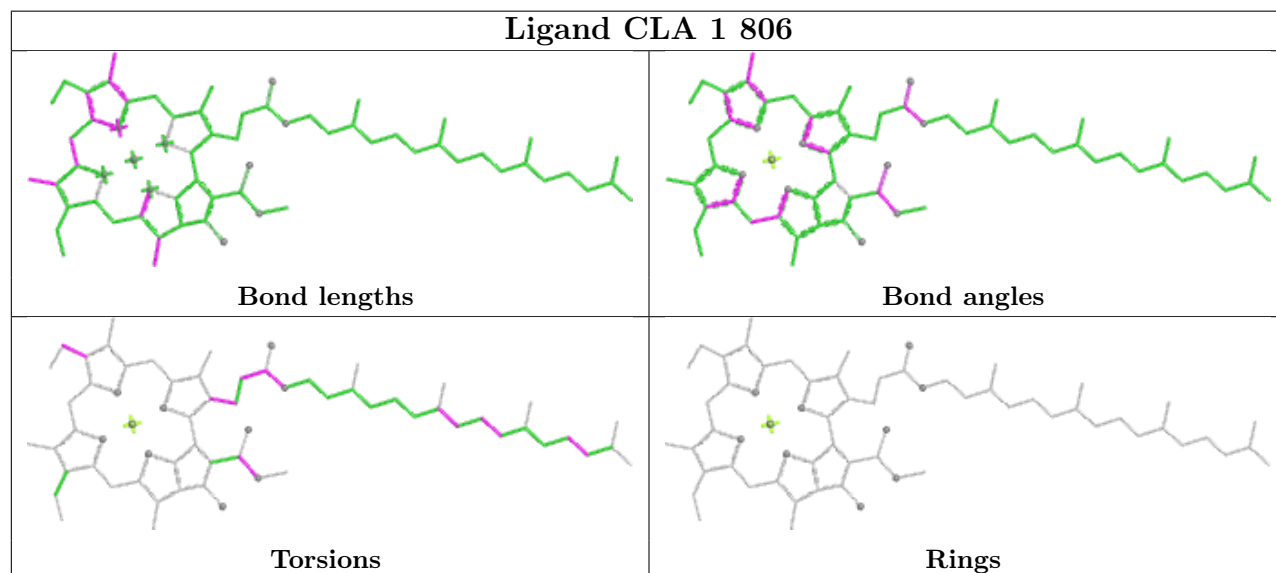
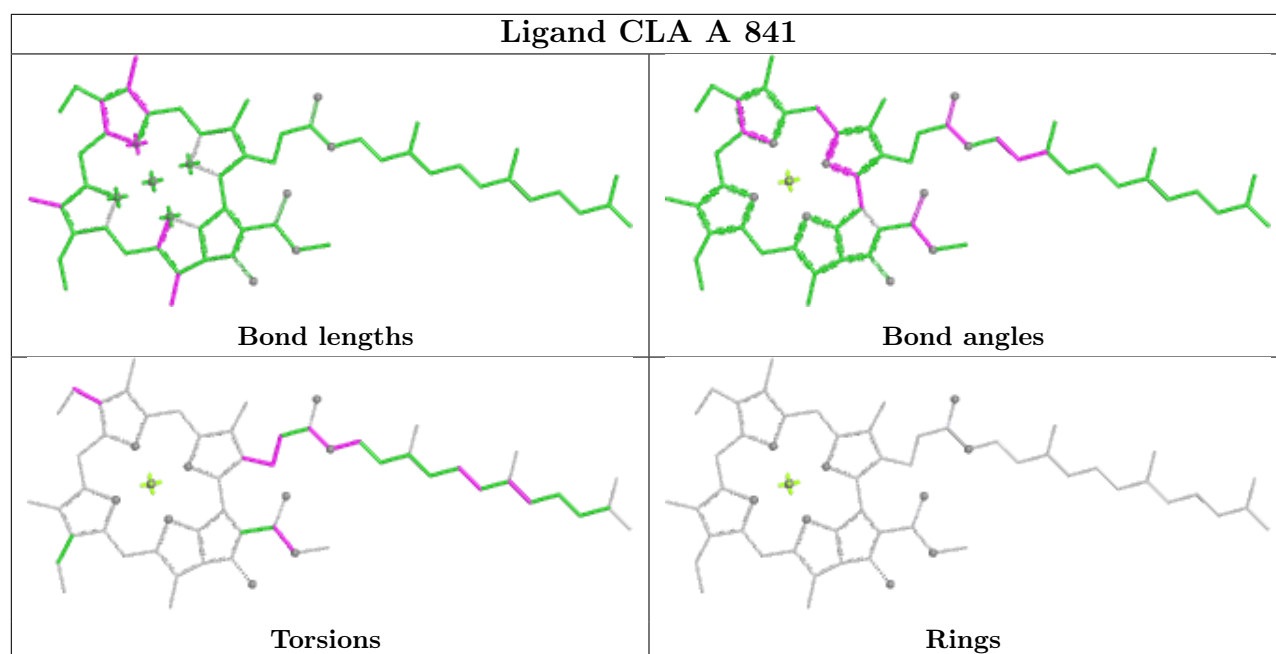
Ligand CLA L 203



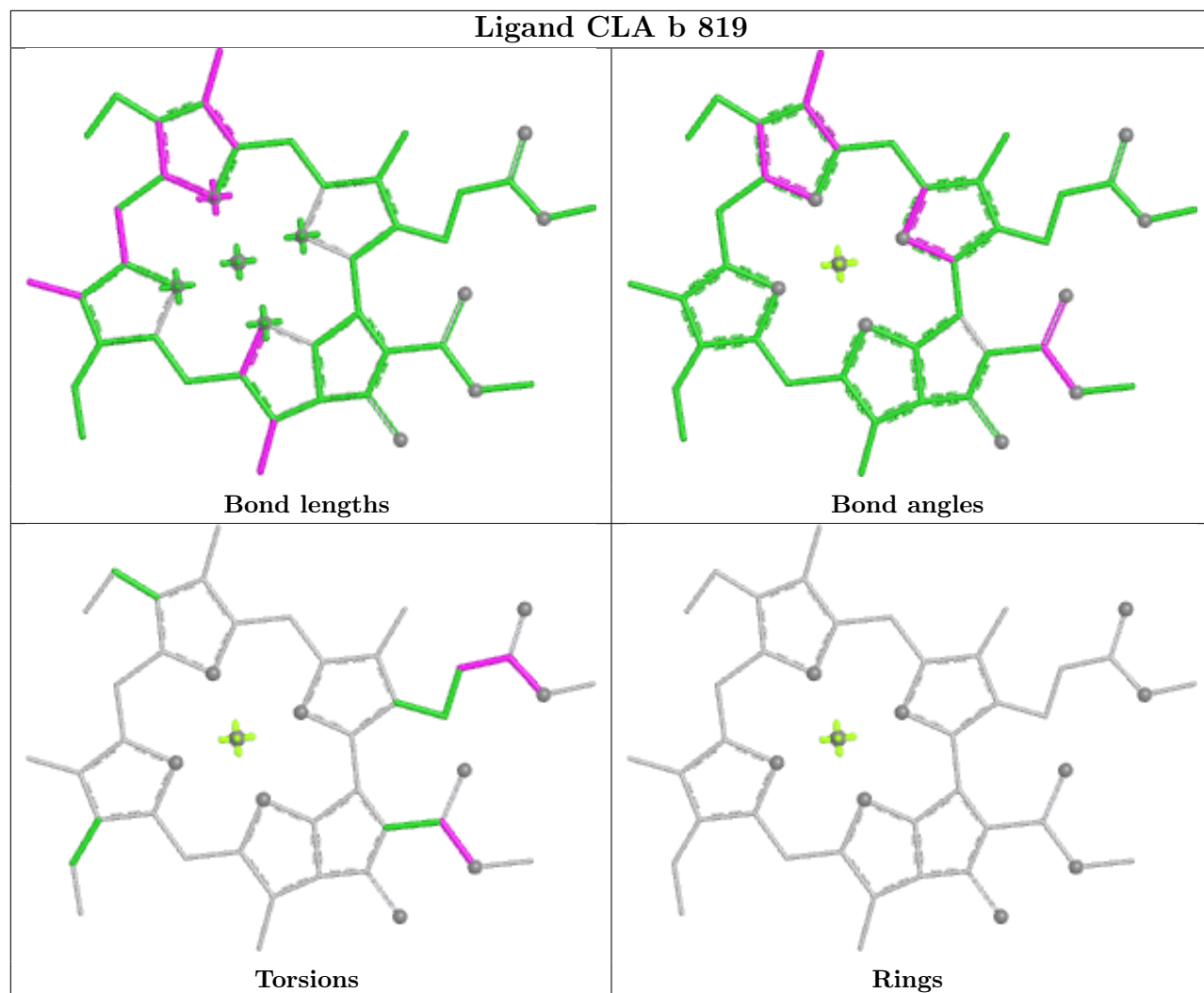
Ligand CLA a 828



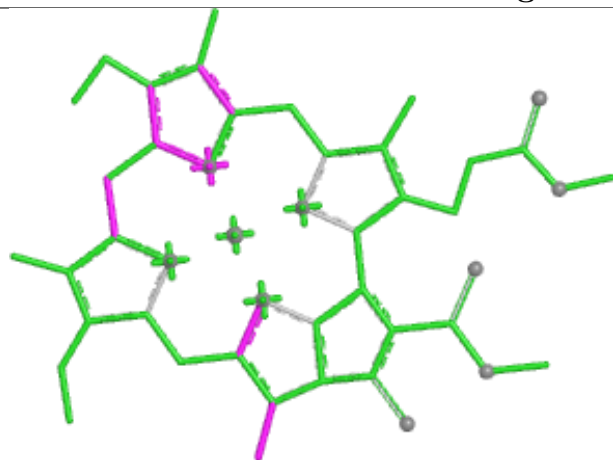




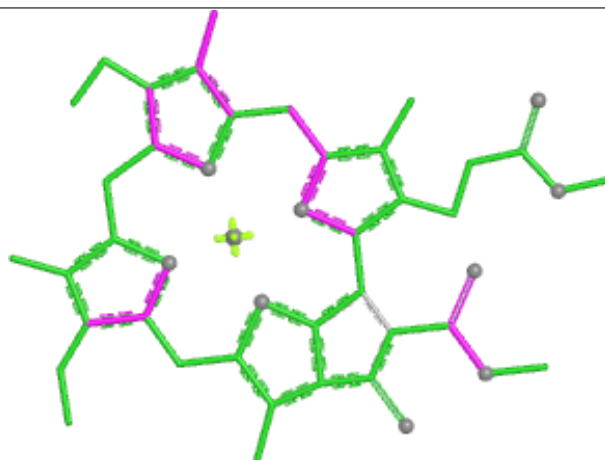
Ligand CLA b 819



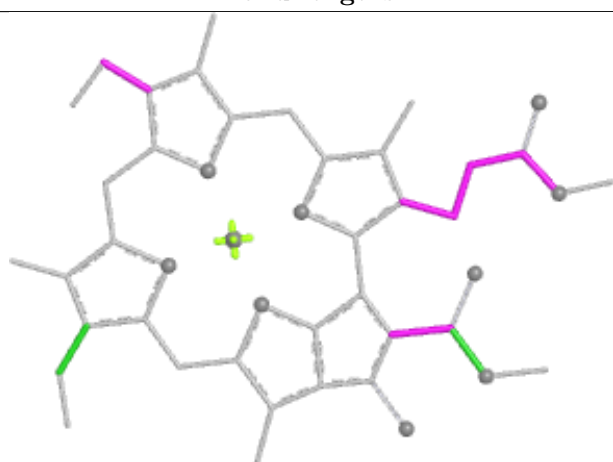
Ligand CLA b 818



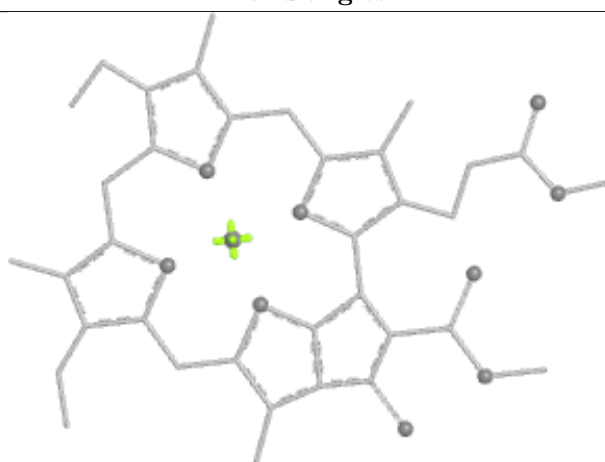
Bond lengths



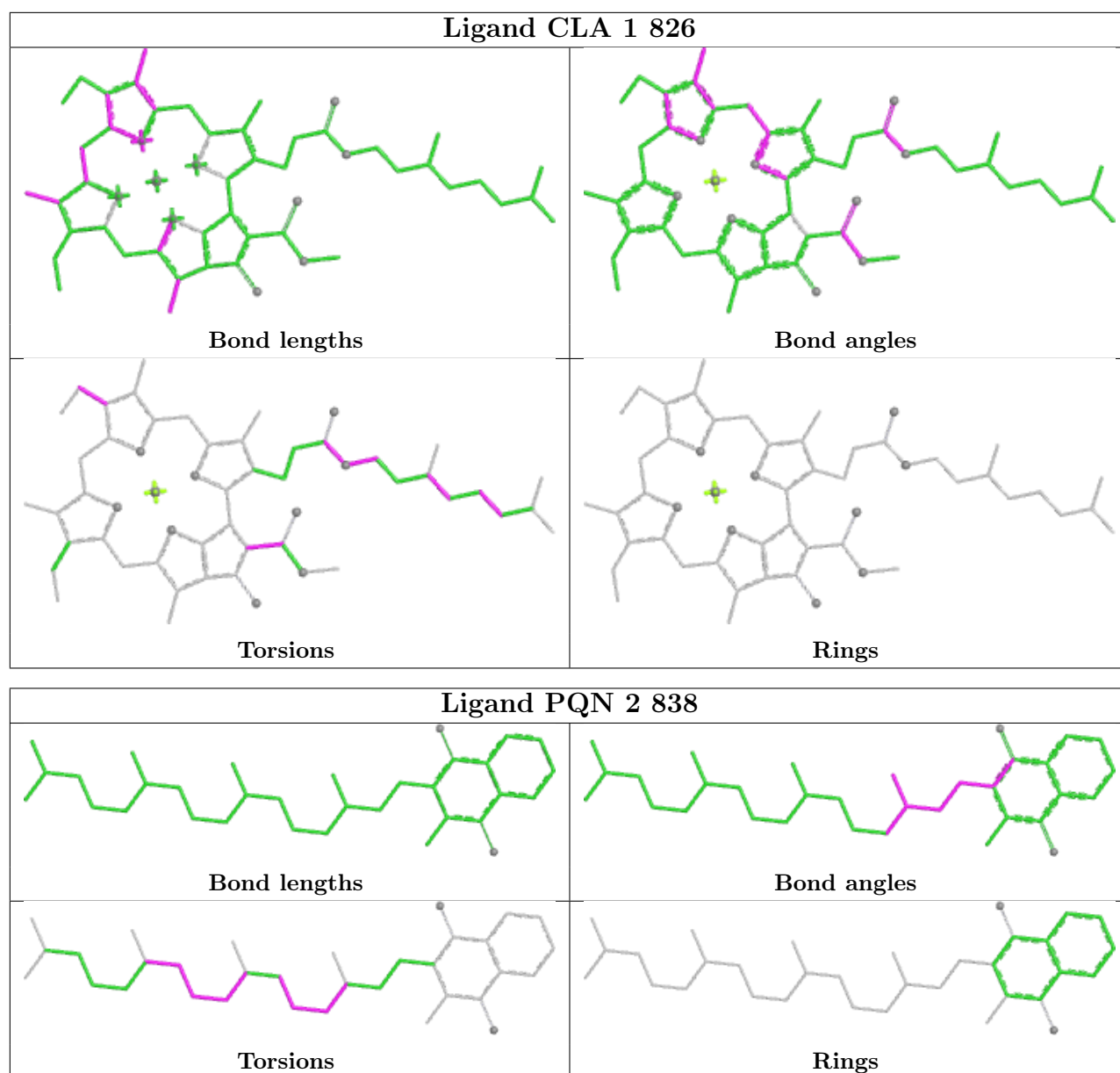
Bond angles

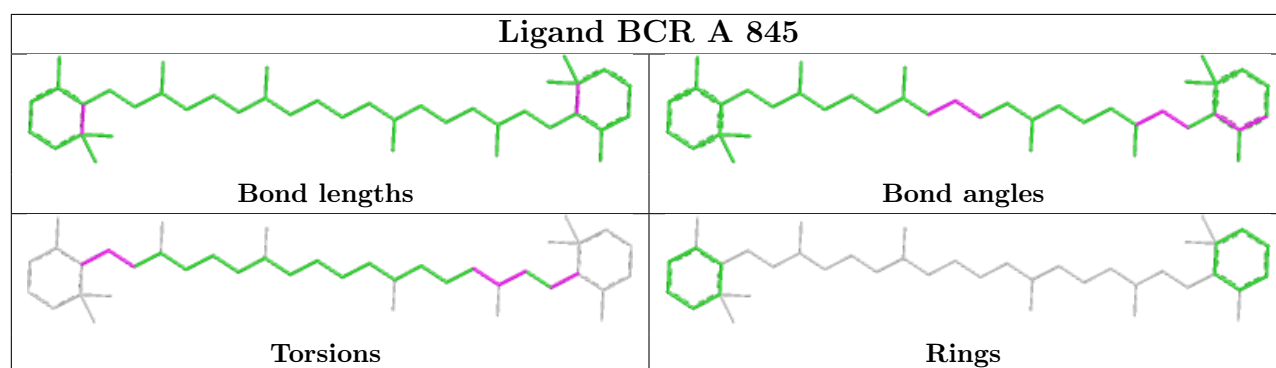
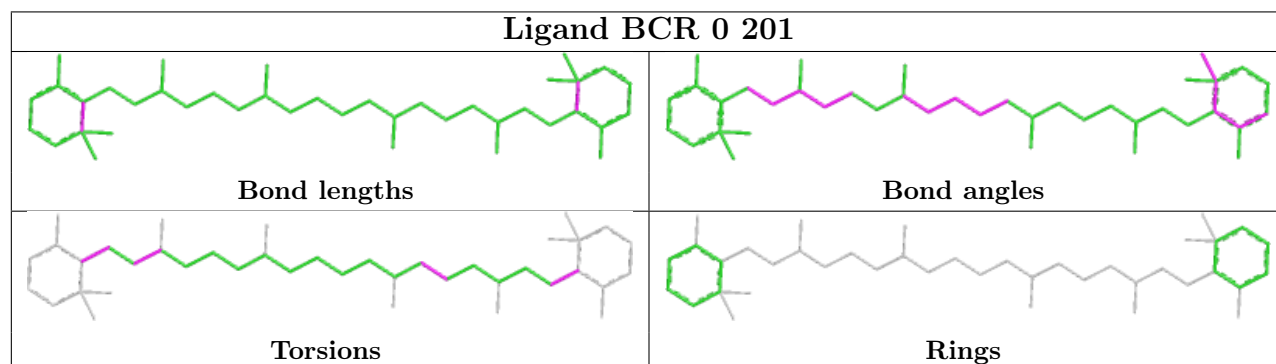
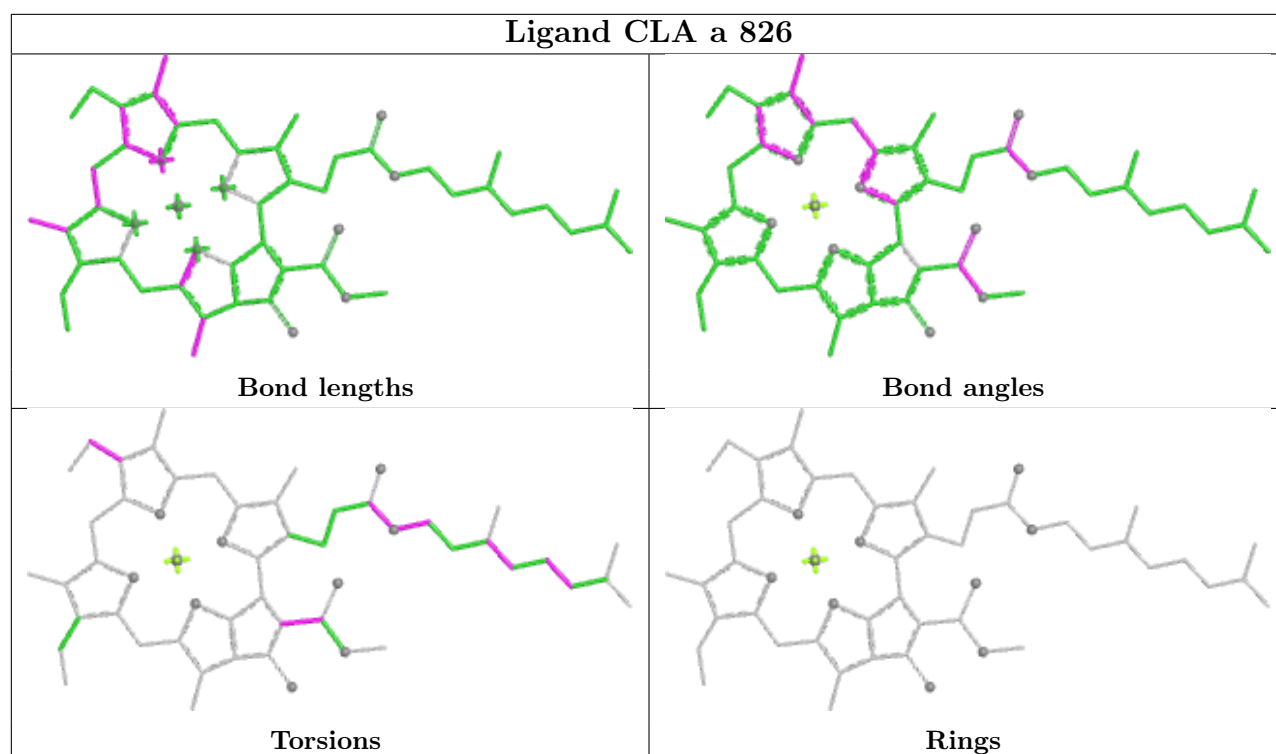


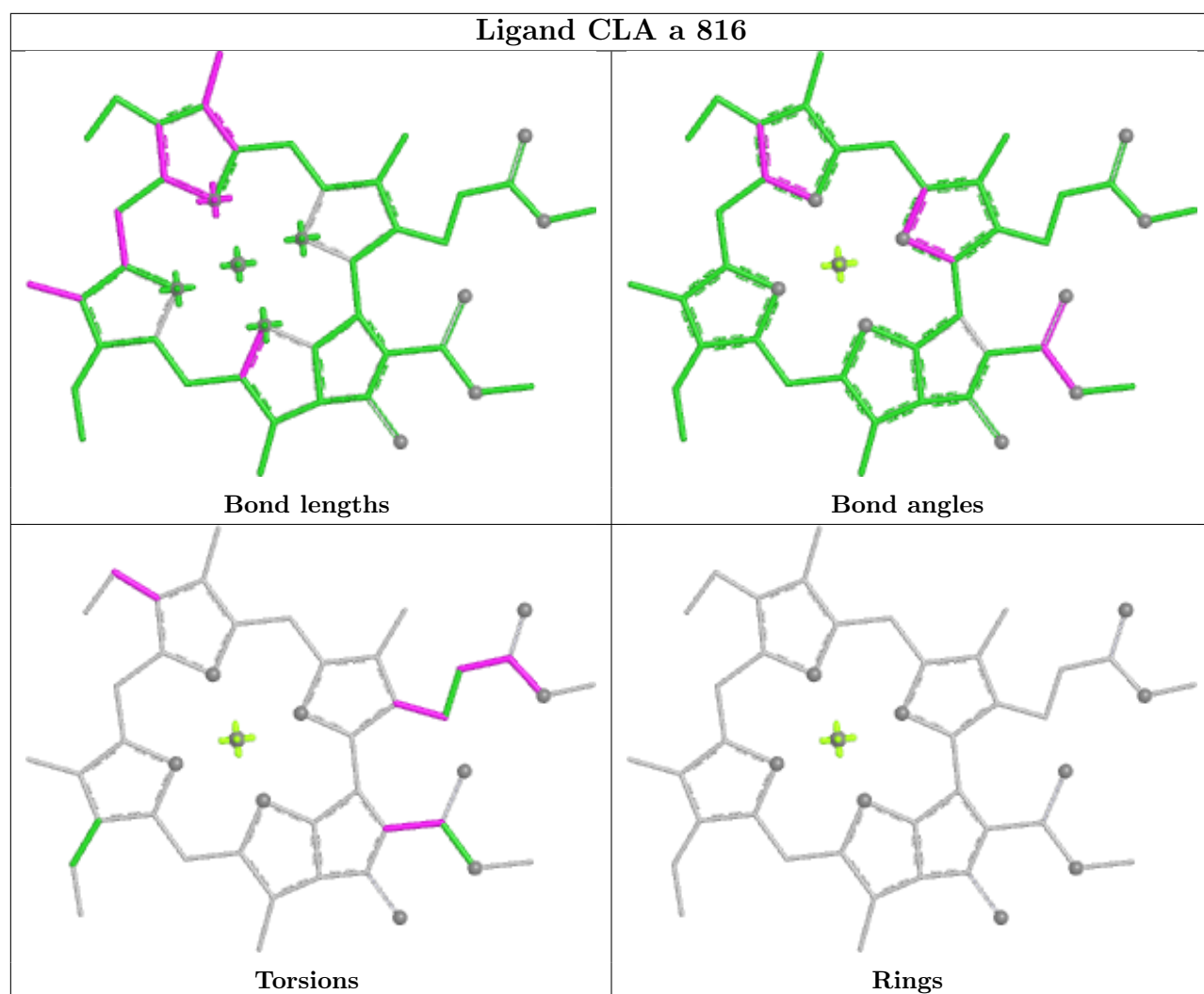
Torsions

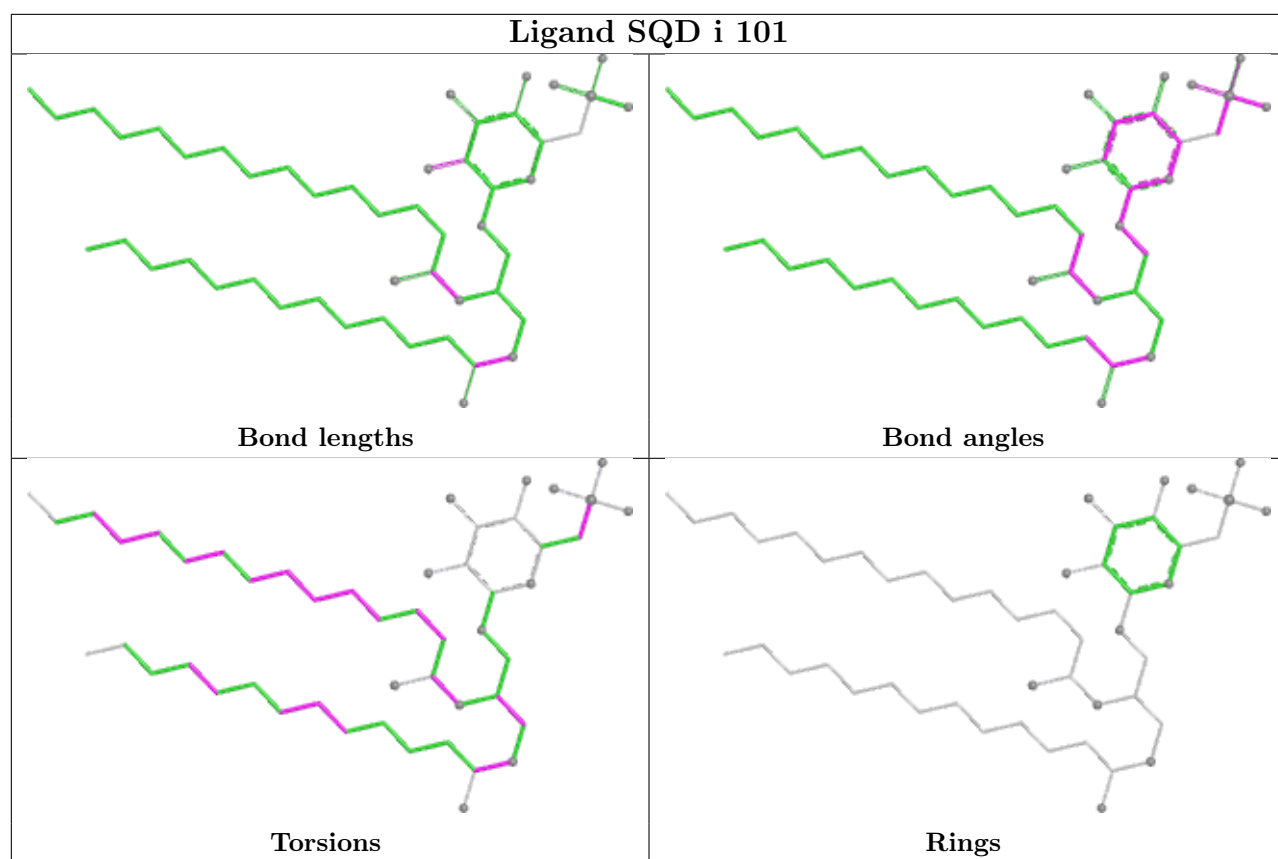


Rings

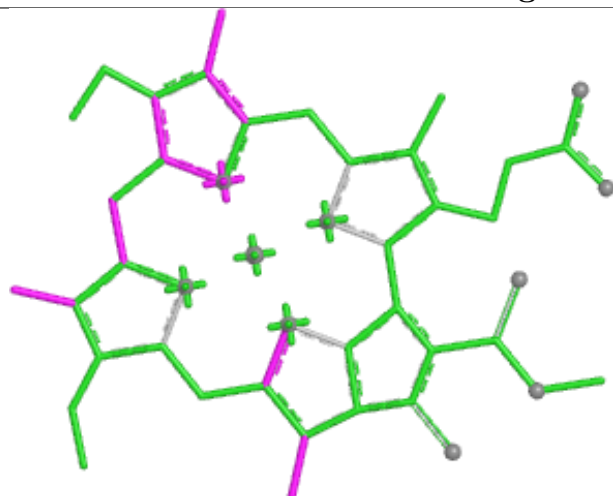




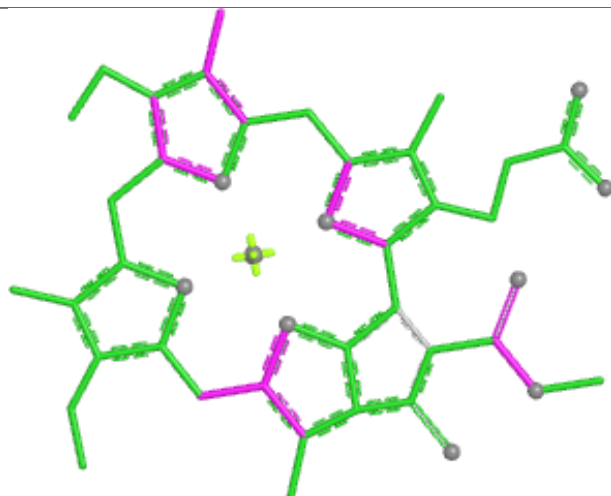




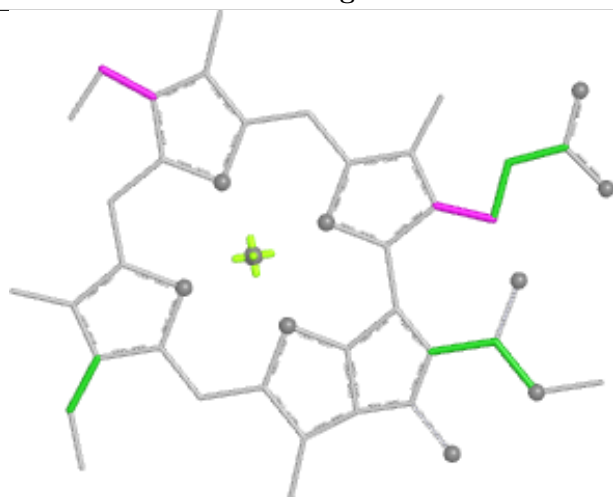
Ligand CLA a 815



Bond lengths



Bond angles

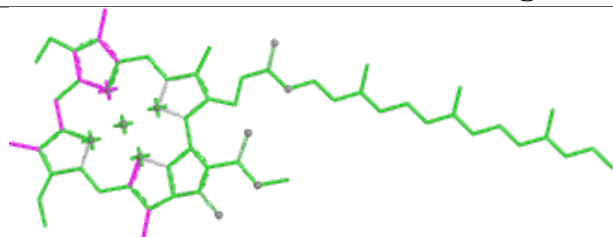


Torsions

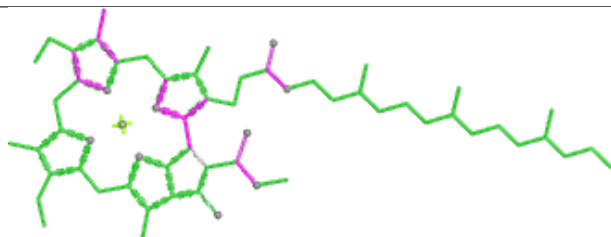


Rings

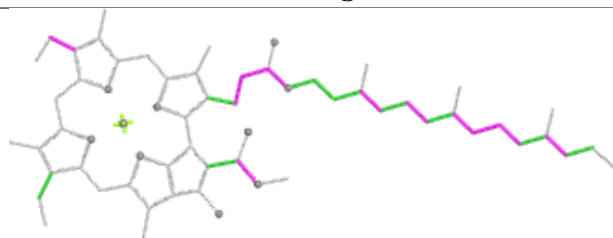
Ligand CLA a 825



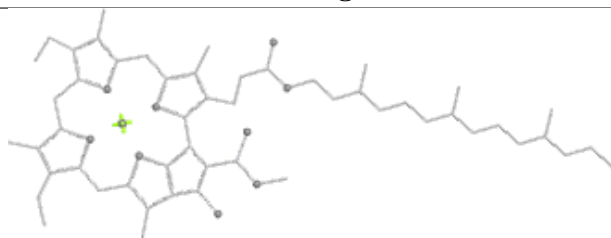
Bond lengths



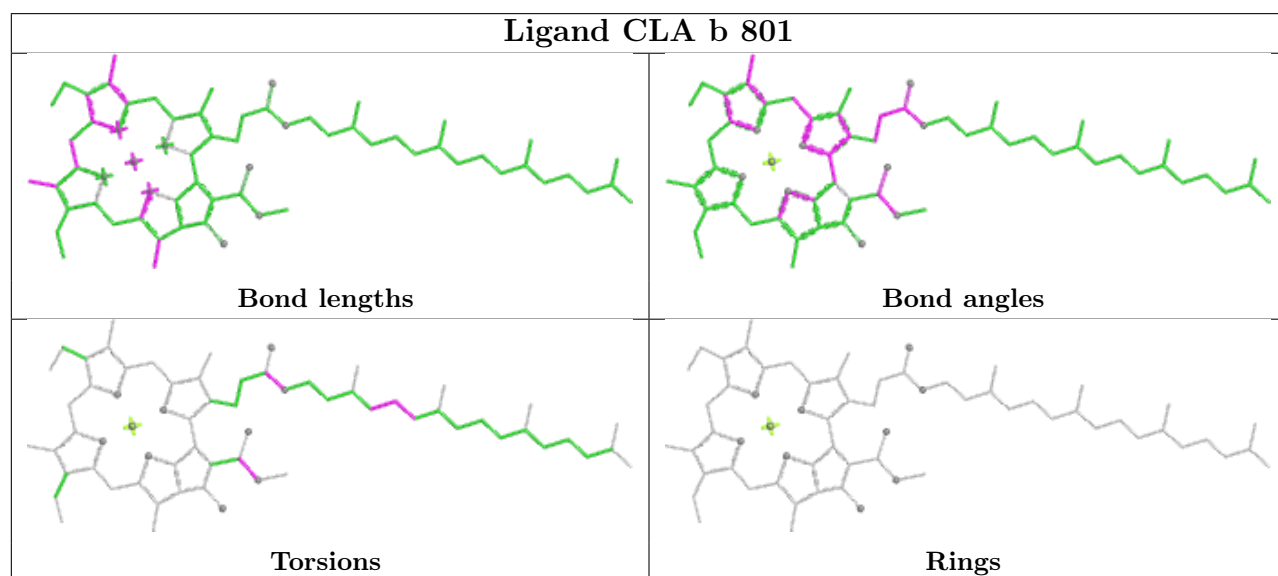
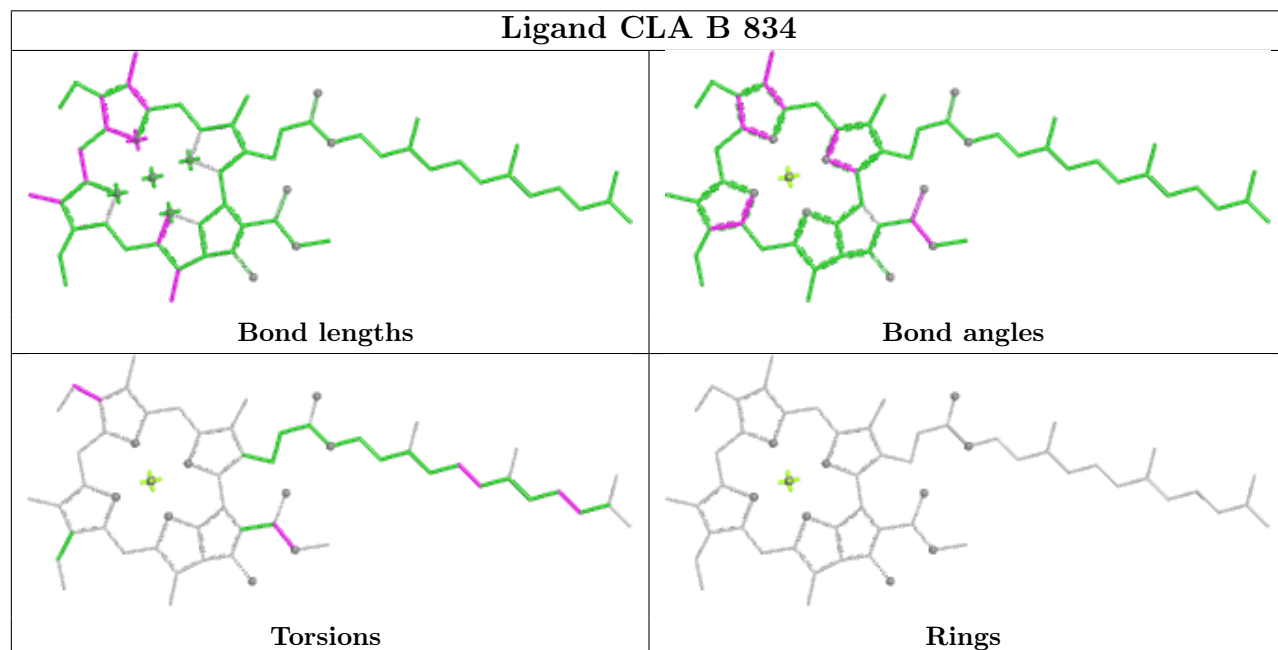
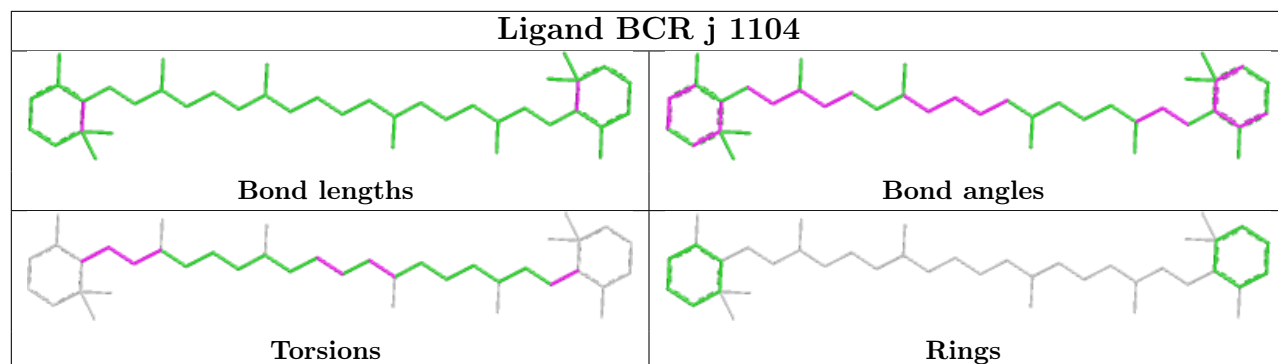
Bond angles

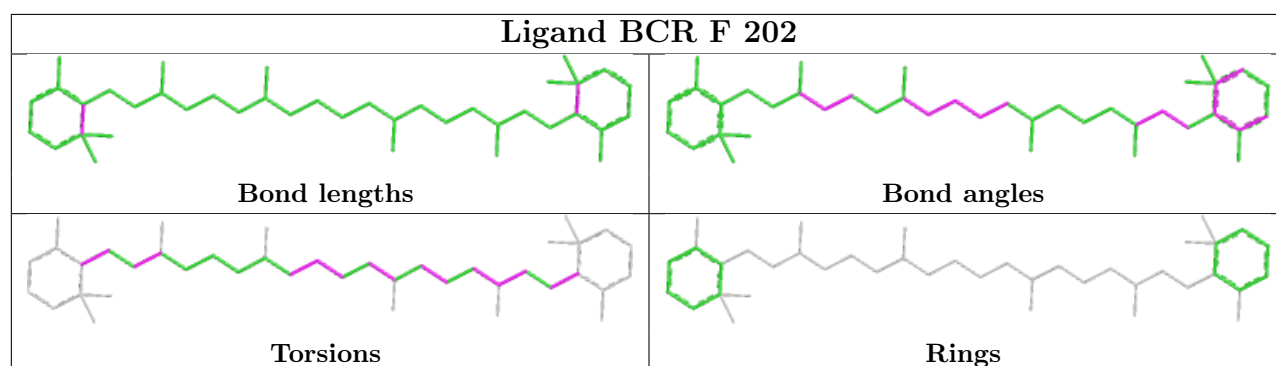
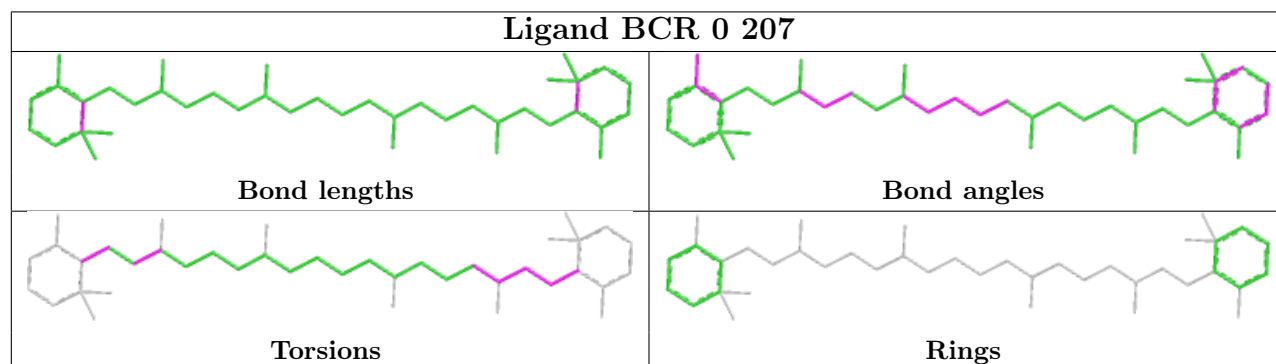
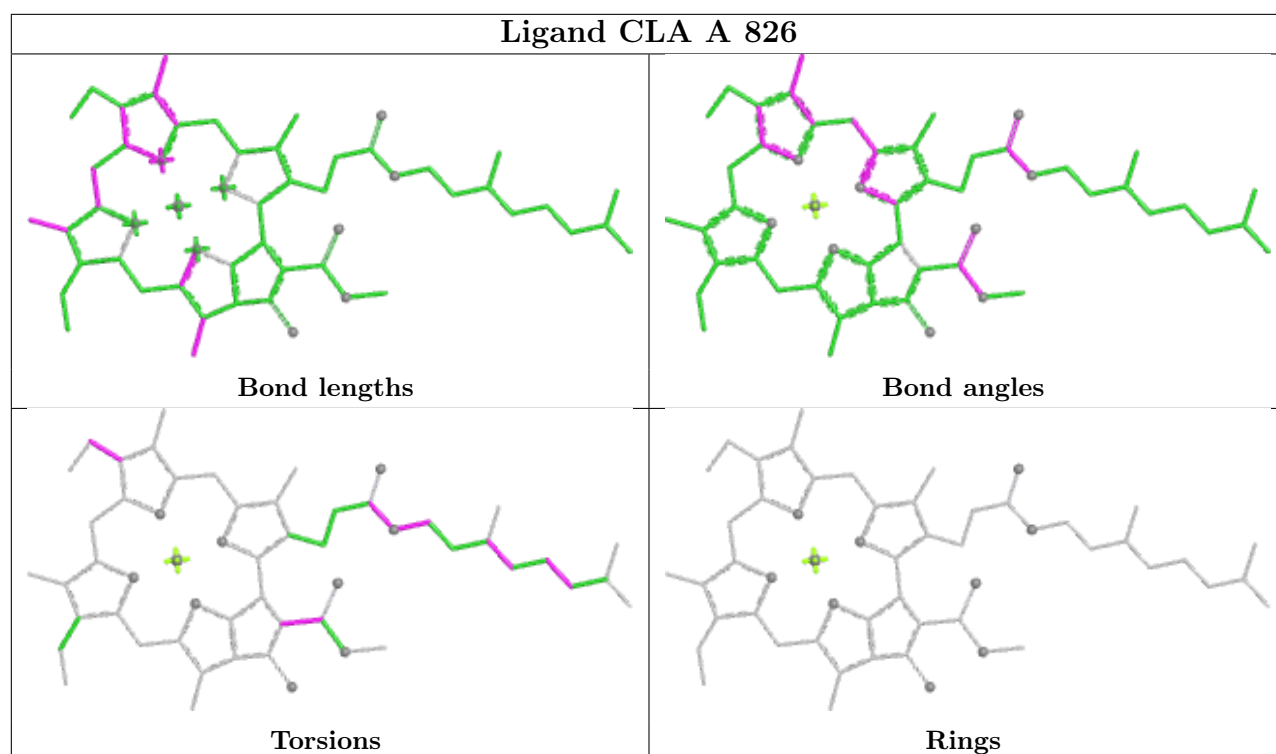


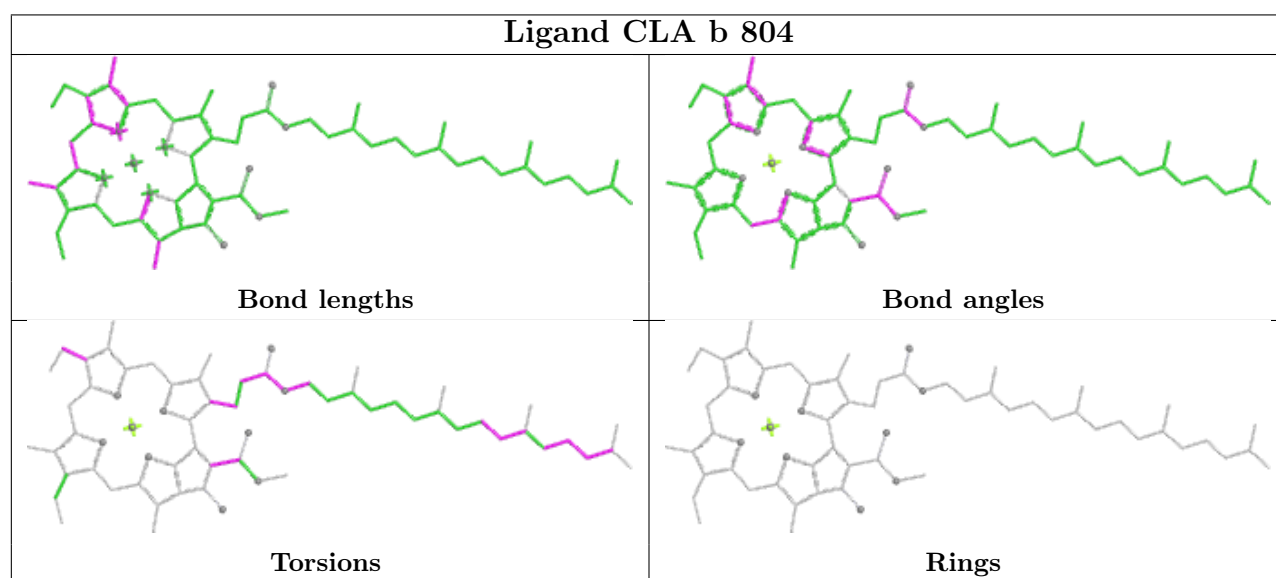
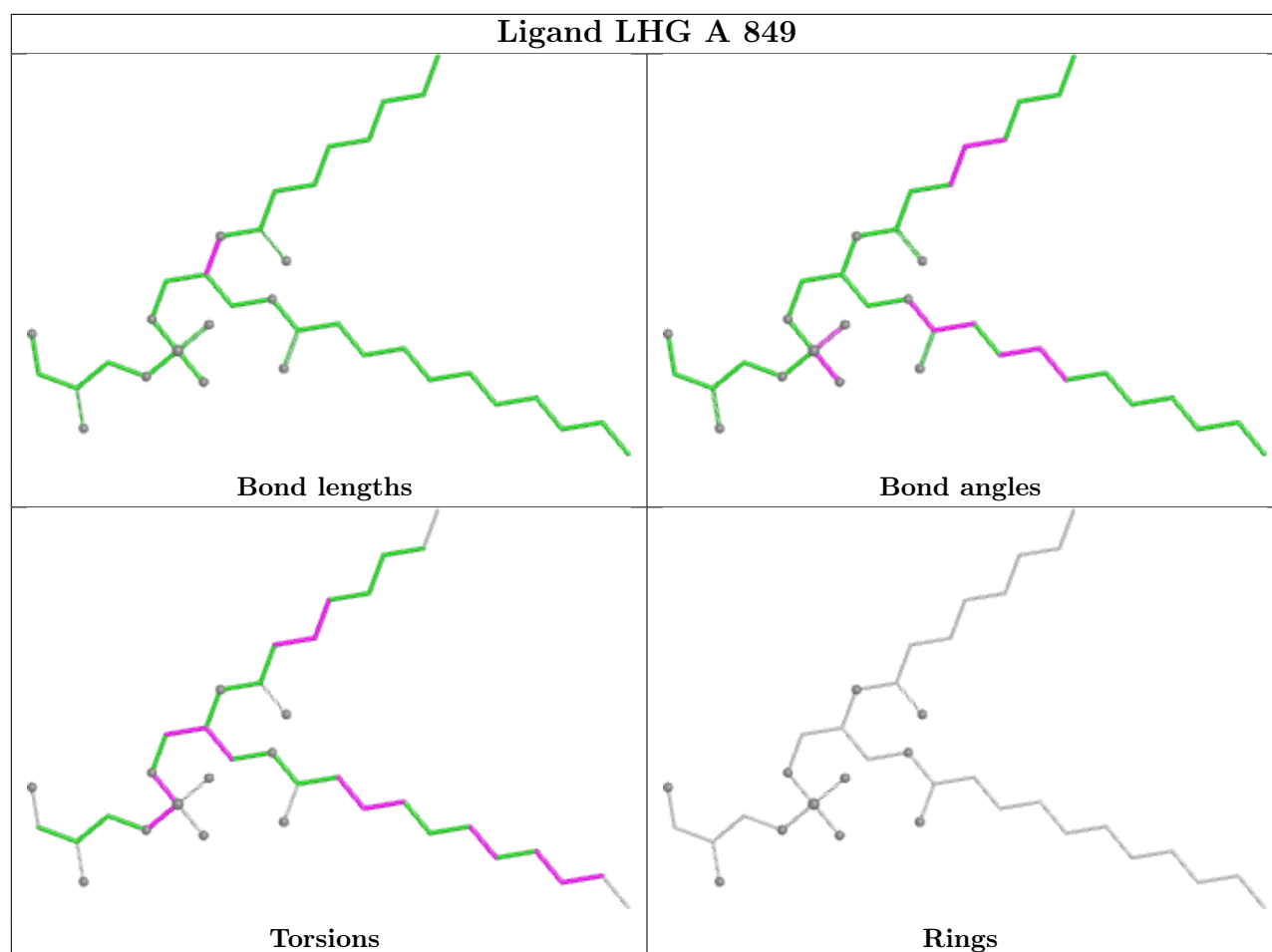
Torsions

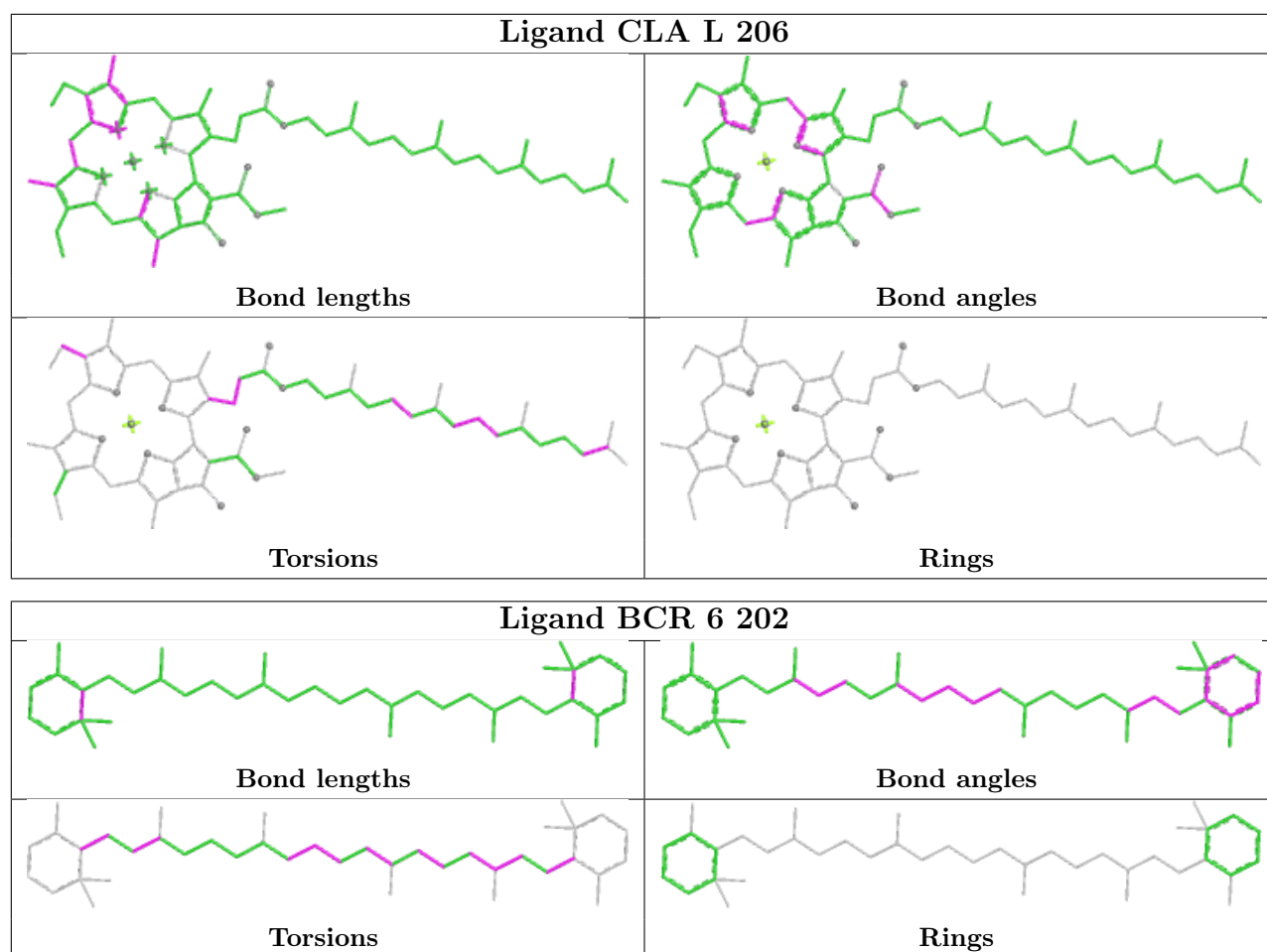


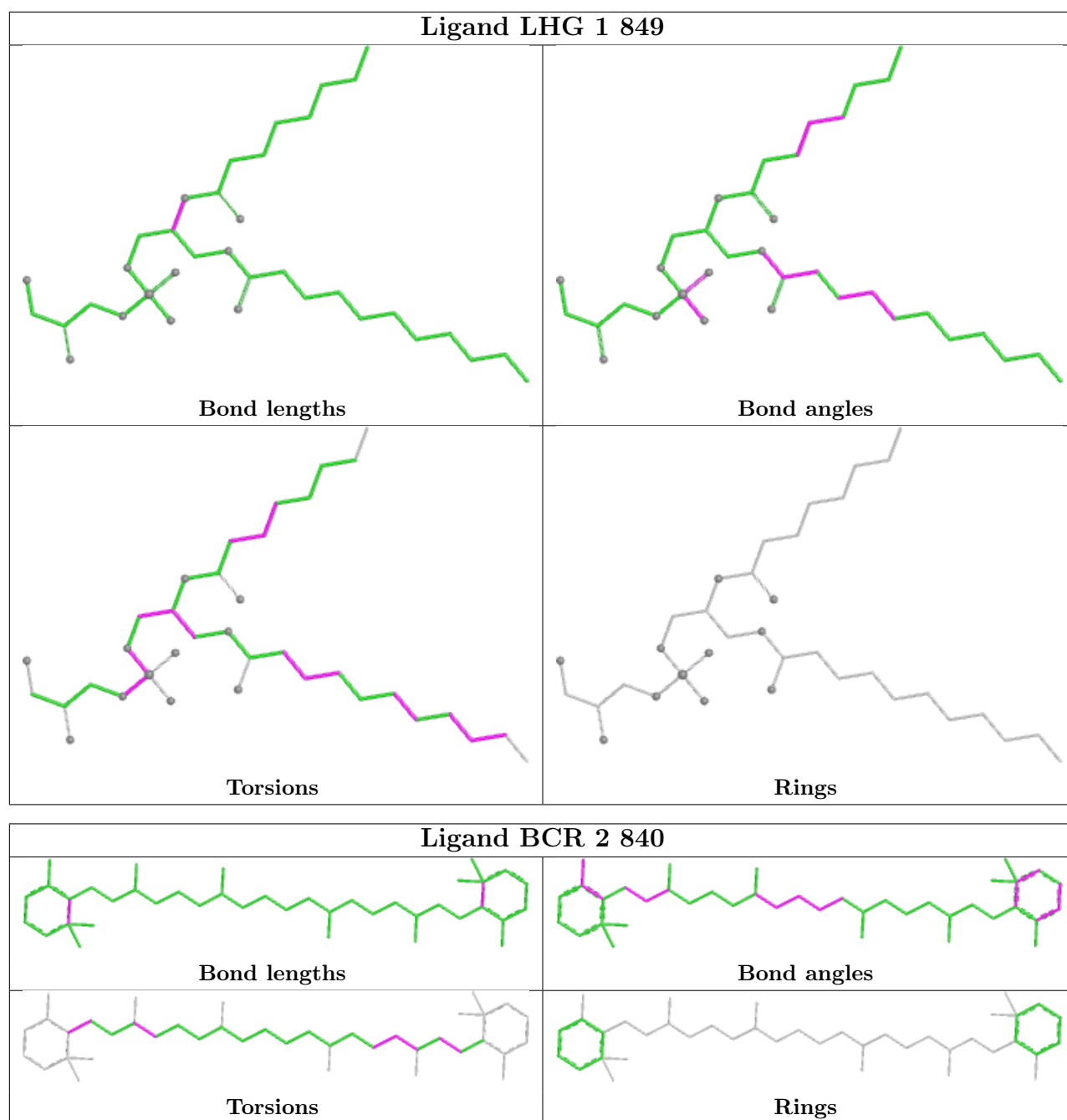
Rings



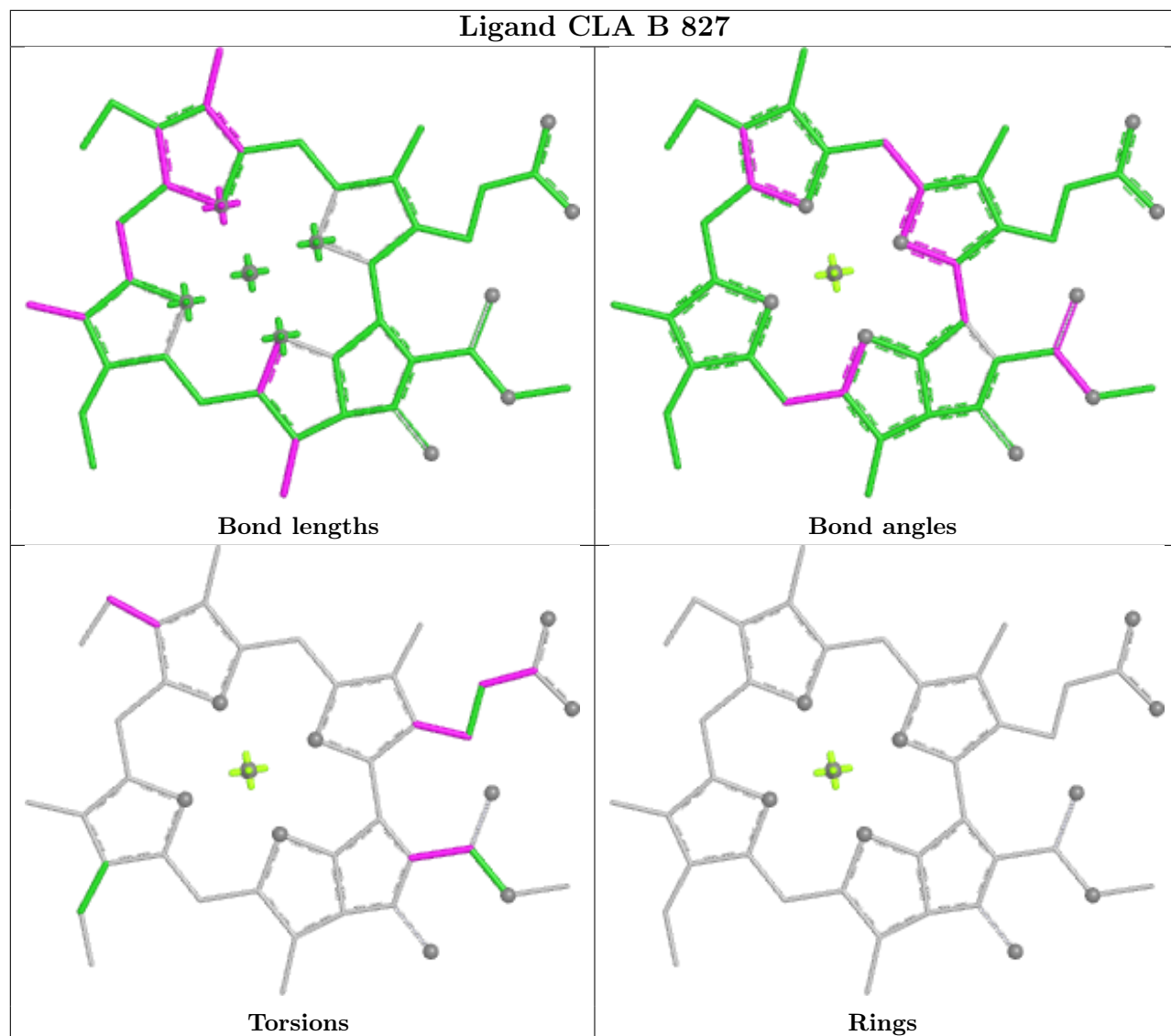




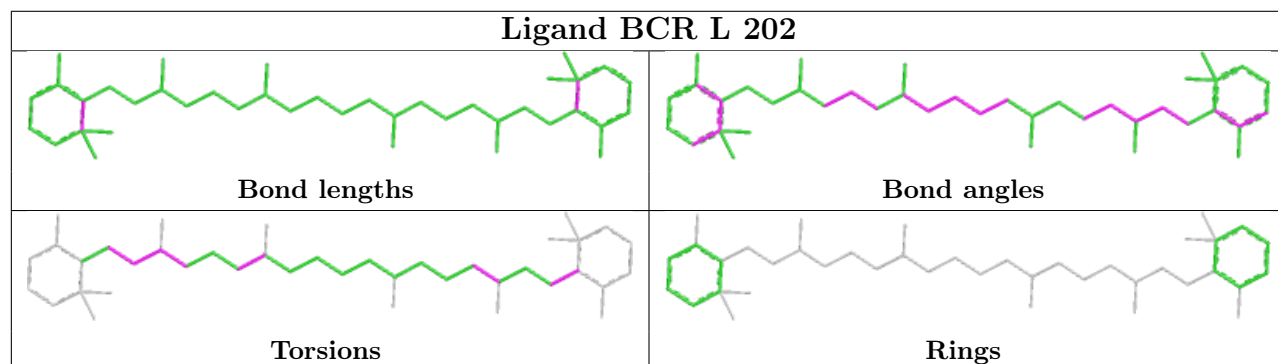


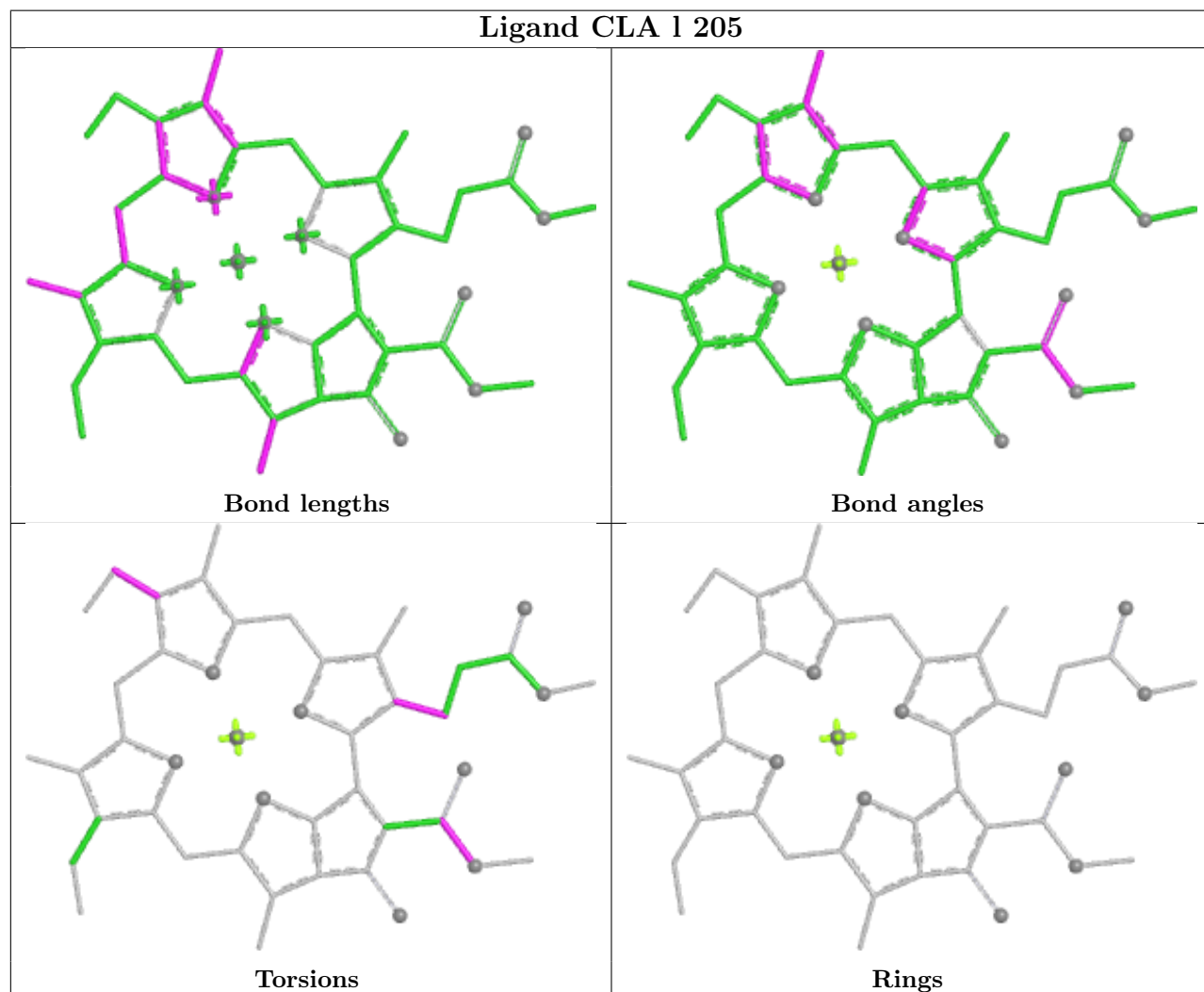
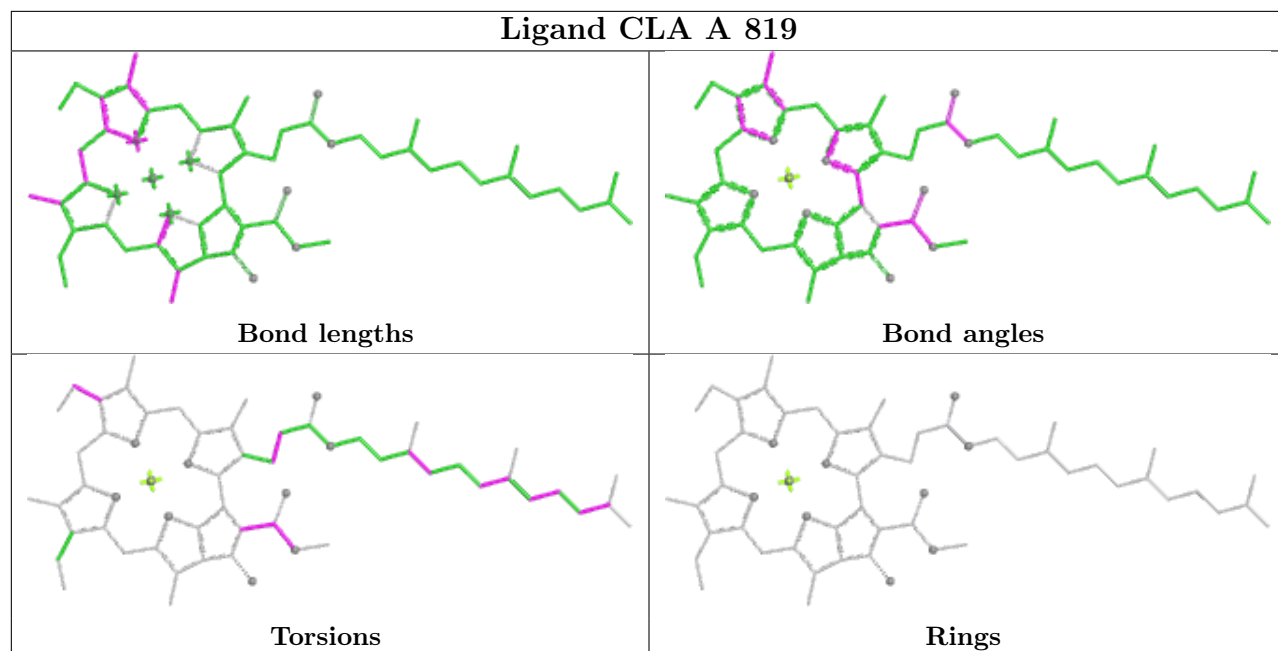


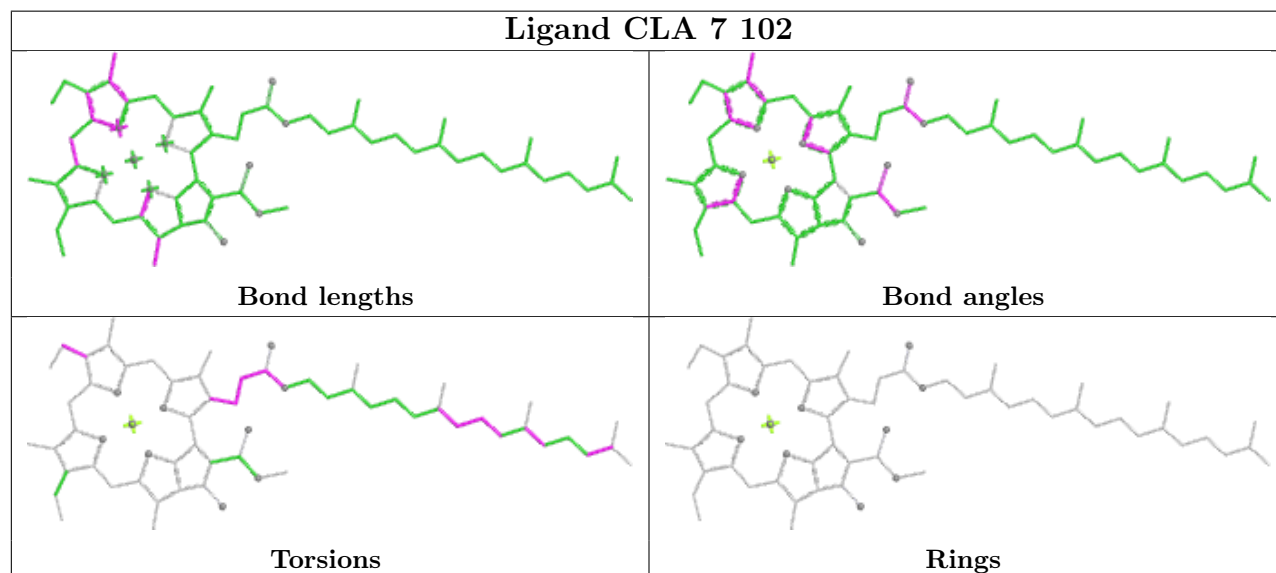
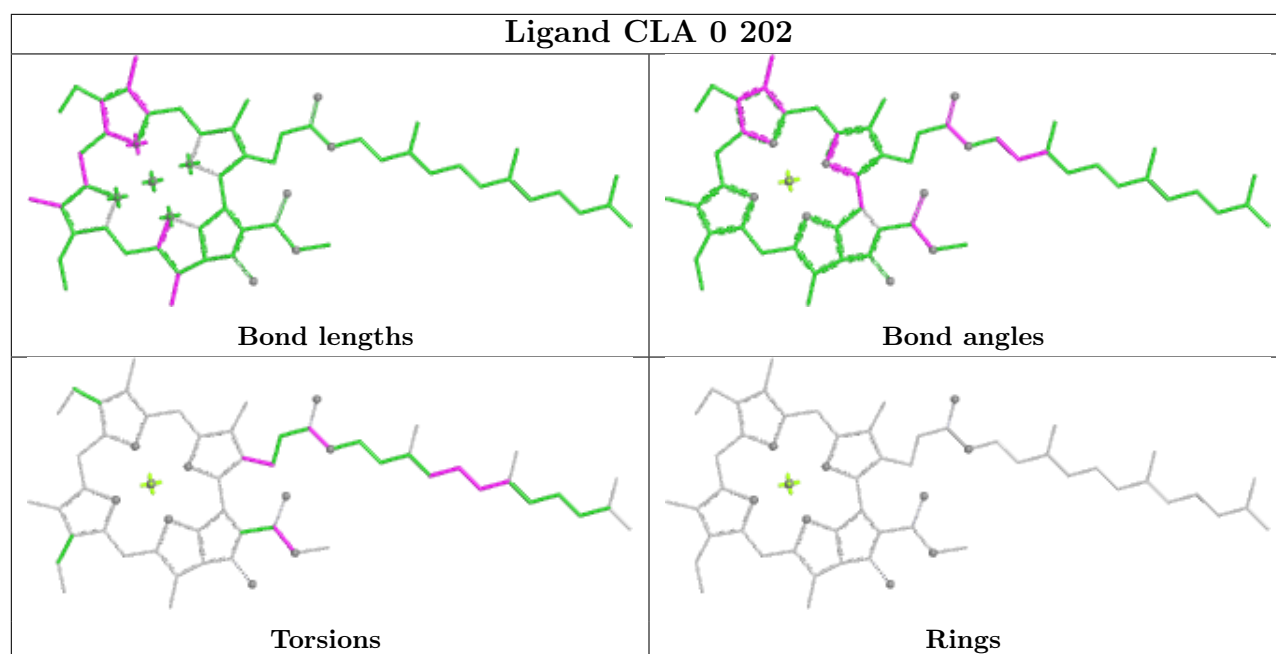
Ligand CLA B 827

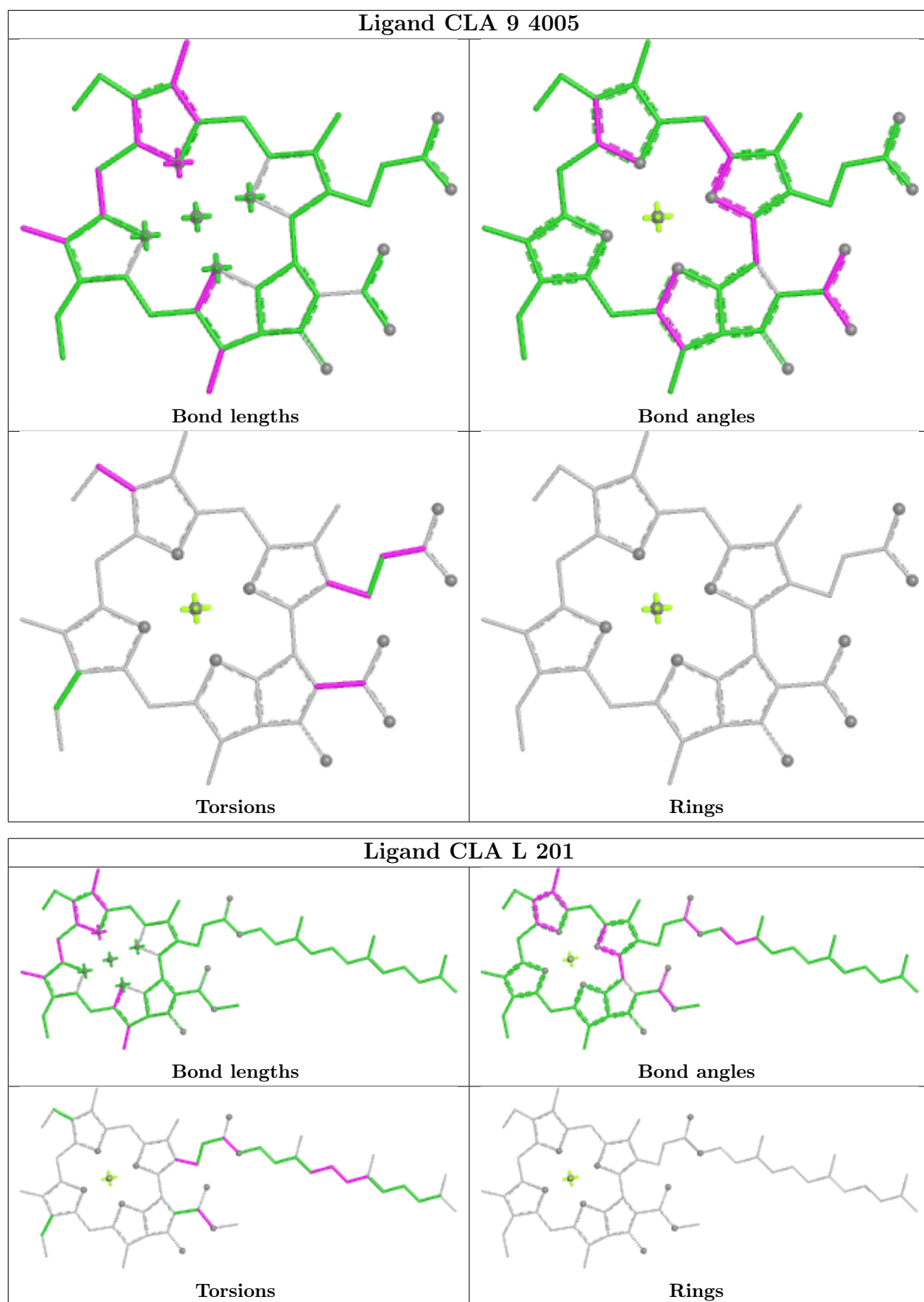


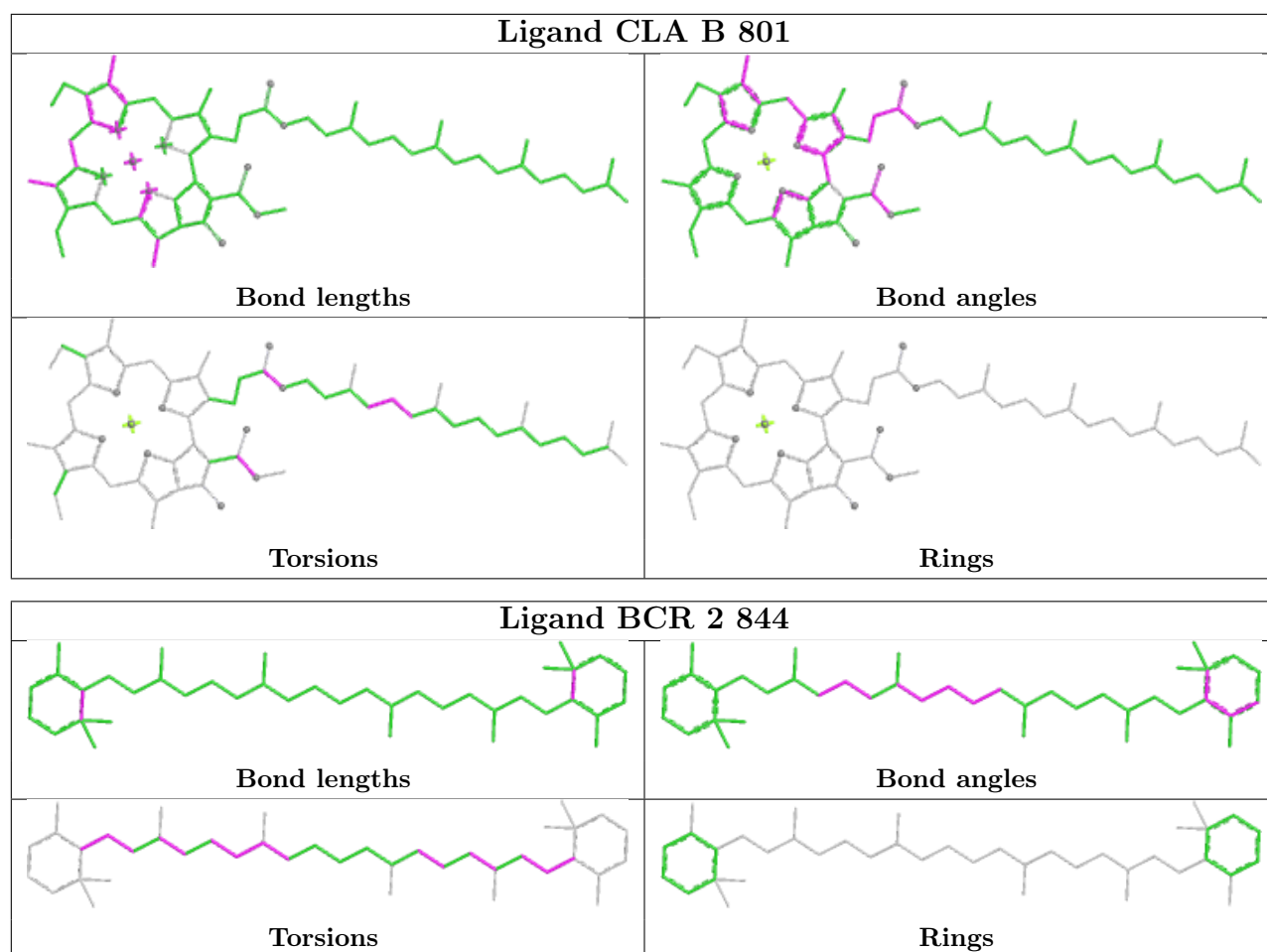
Ligand BCR L 202



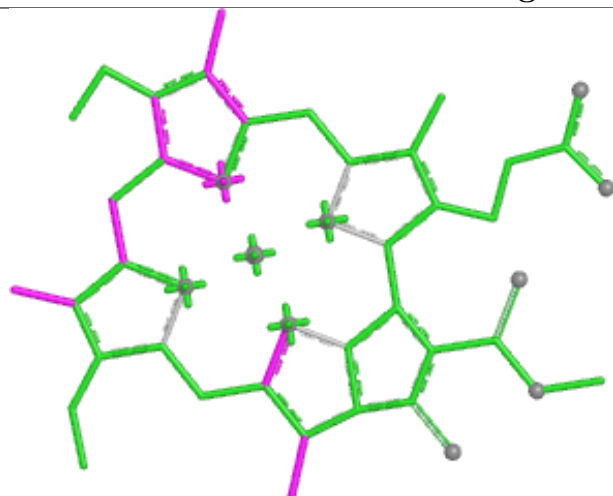




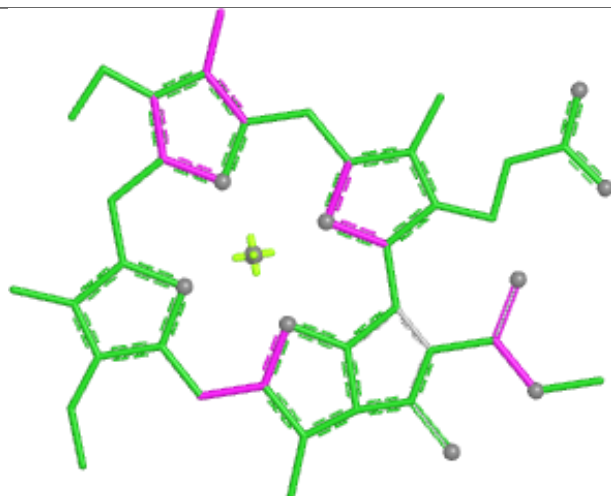




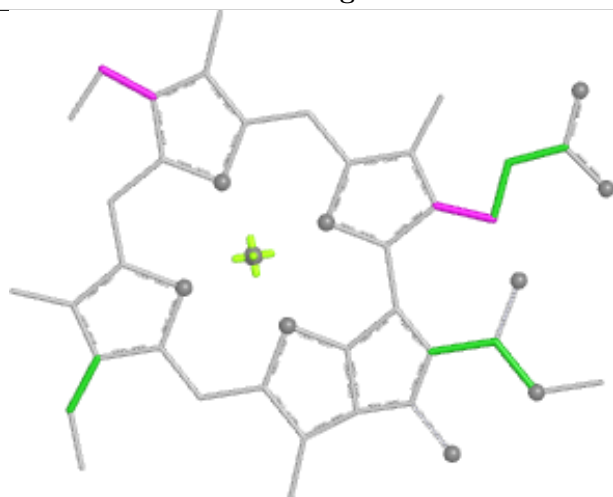
Ligand CLA 1 815



Bond lengths



Bond angles

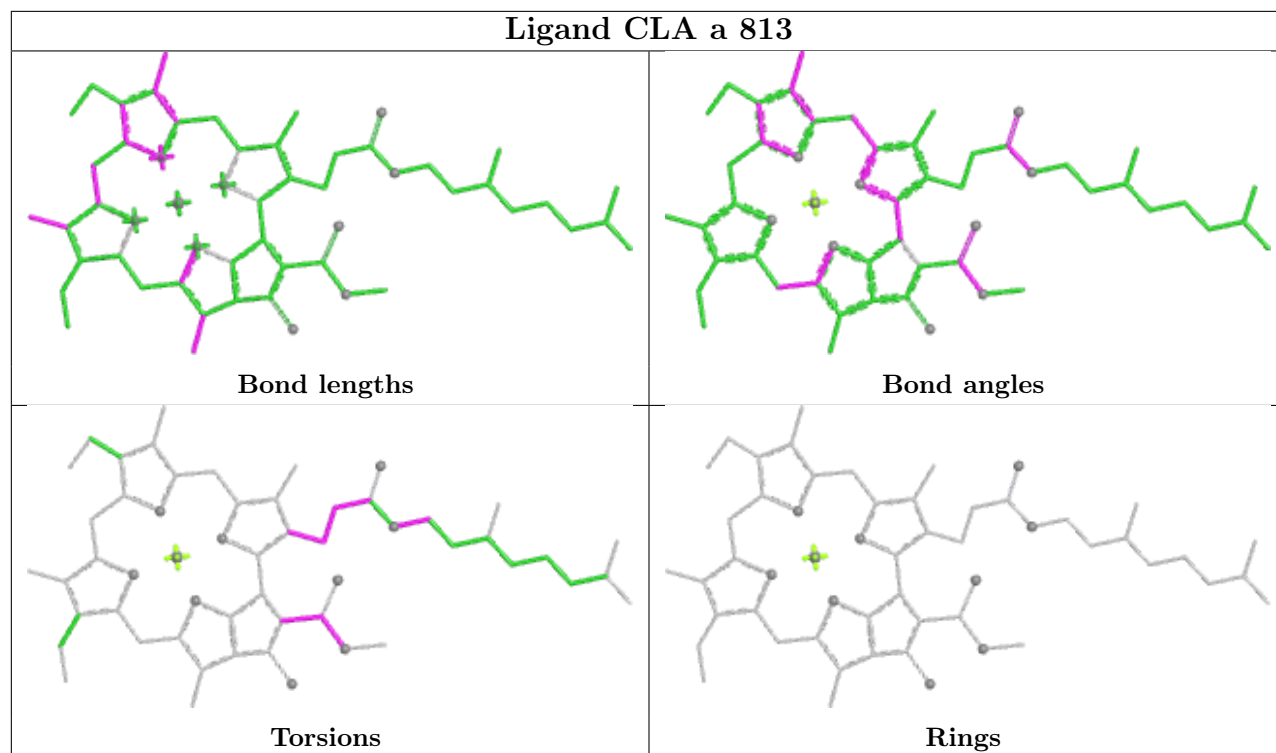


Torsions

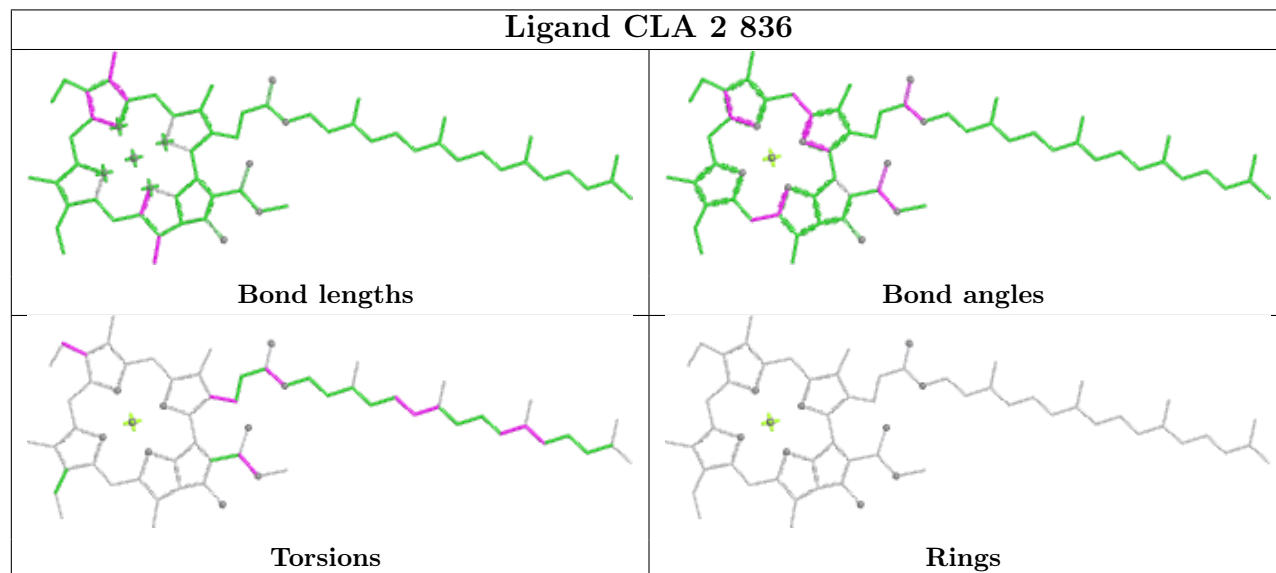


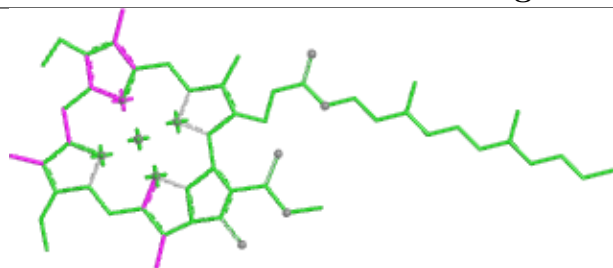
Rings

Ligand CLA a 813

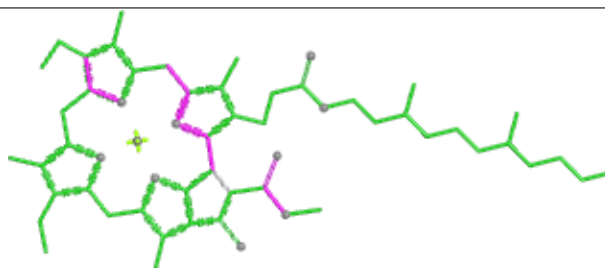


Ligand CLA 2 836

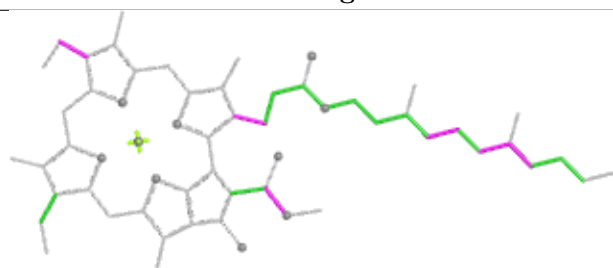


Ligand CLA B 830

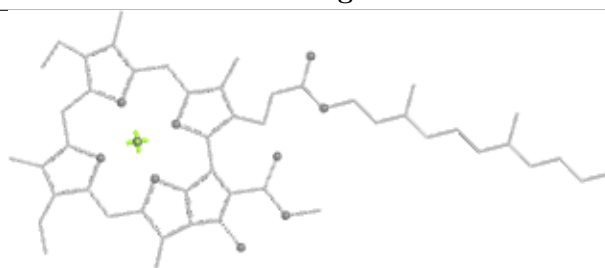
Bond lengths



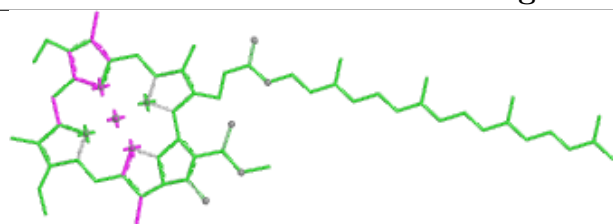
Bond angles



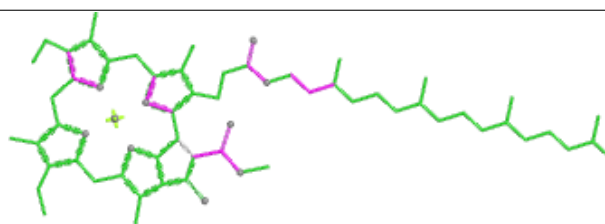
Torsions



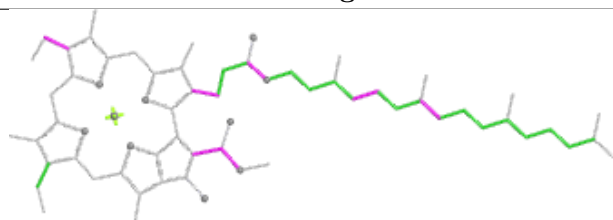
Rings

Ligand CLA 1 838

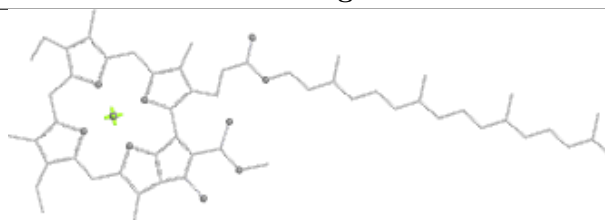
Bond lengths



Bond angles

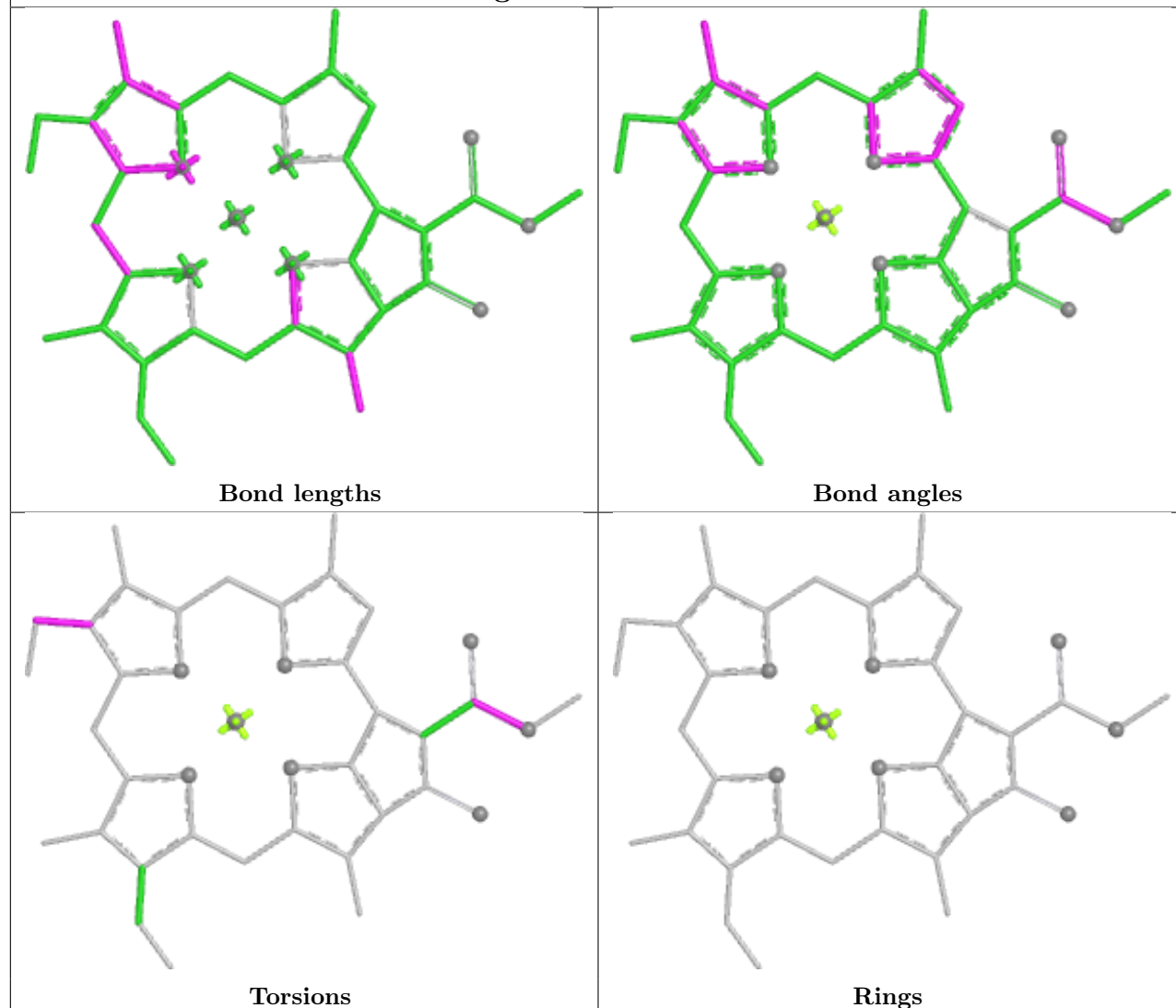


Torsions

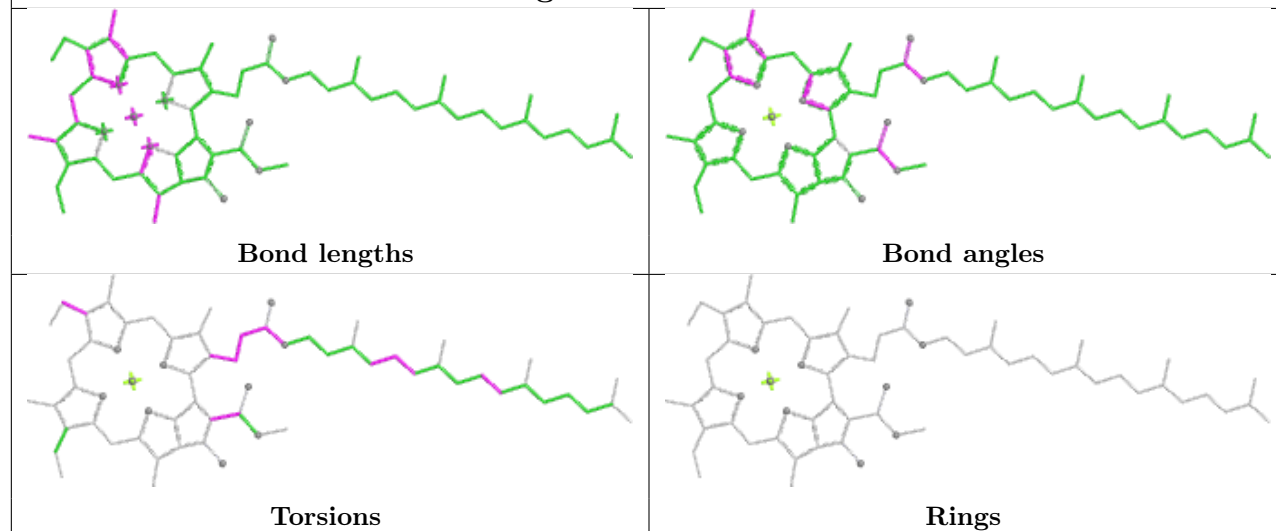


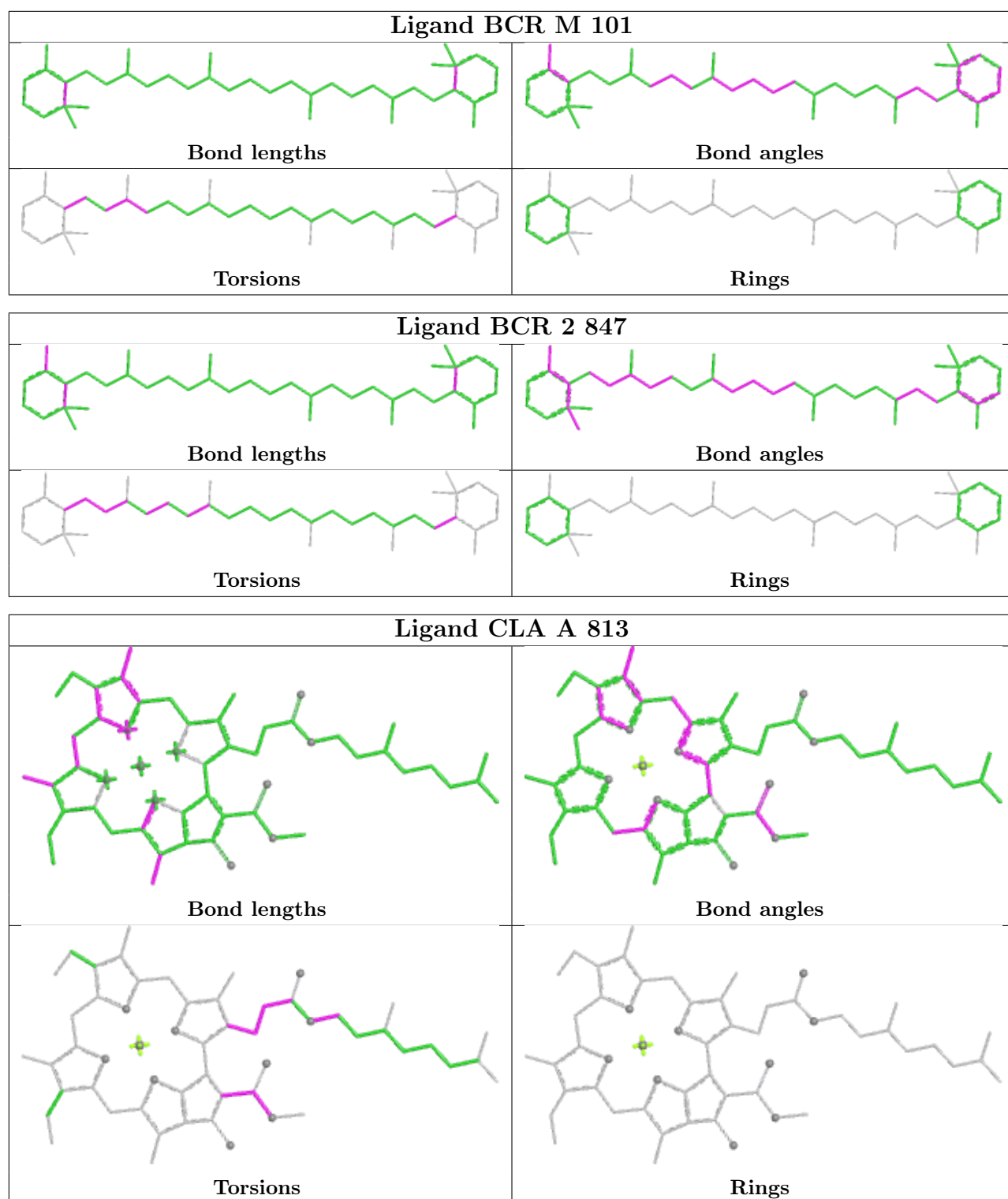
Rings

Ligand CLA 2 831

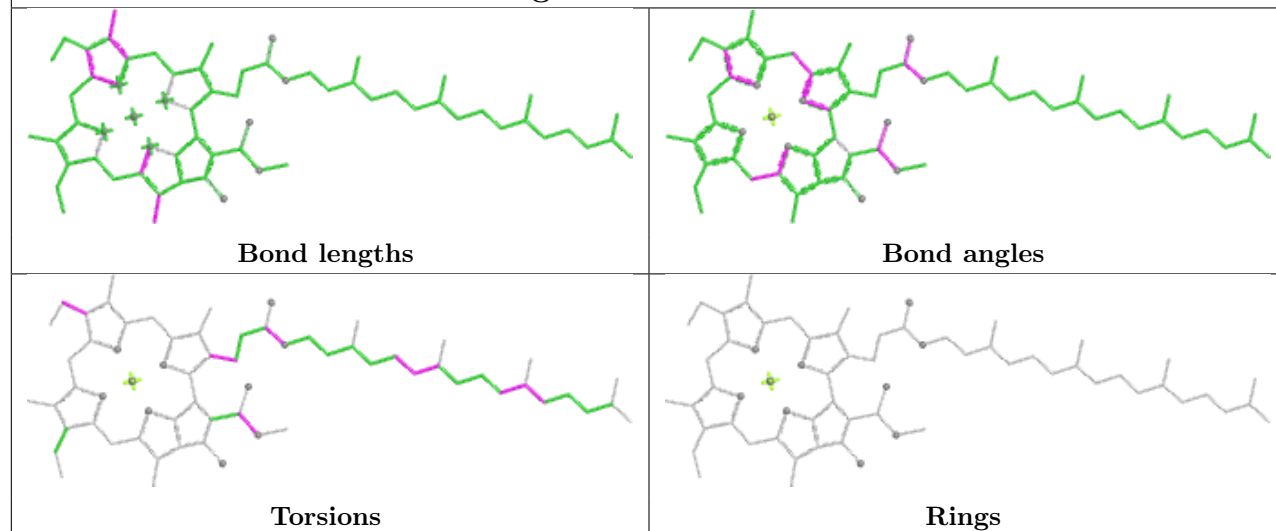


Ligand CLA a 827

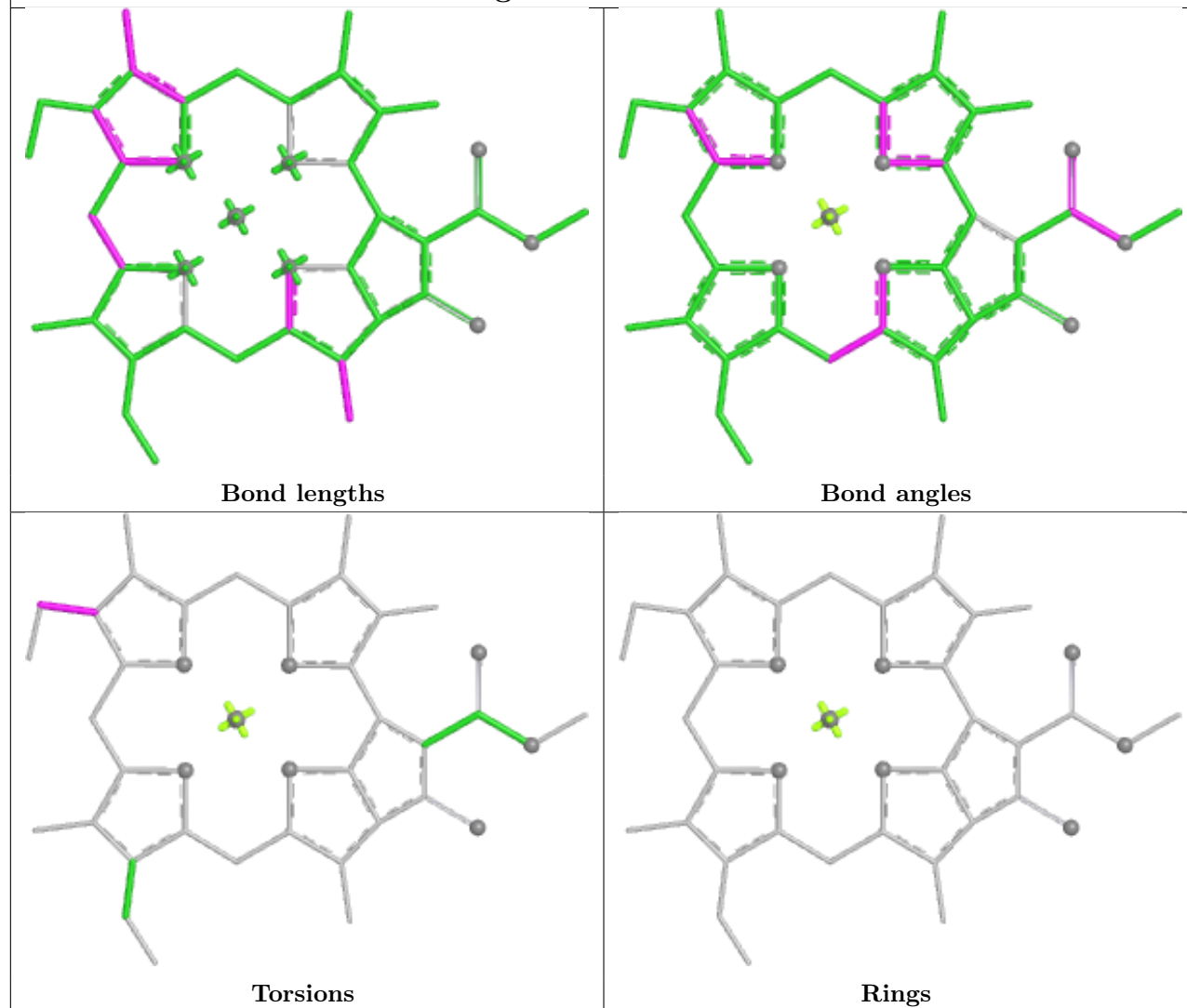




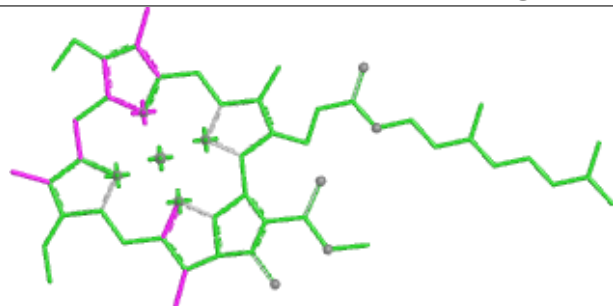
Ligand CLA B 837



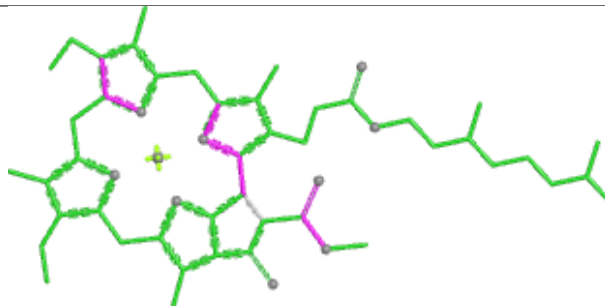
Ligand CLA B 817



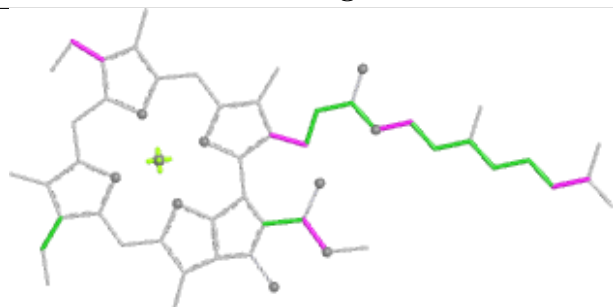
Ligand CLA B 820



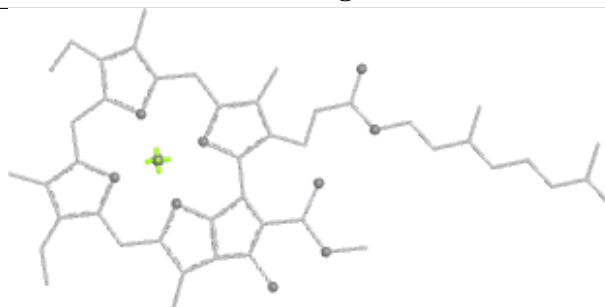
Bond lengths



Bond angles

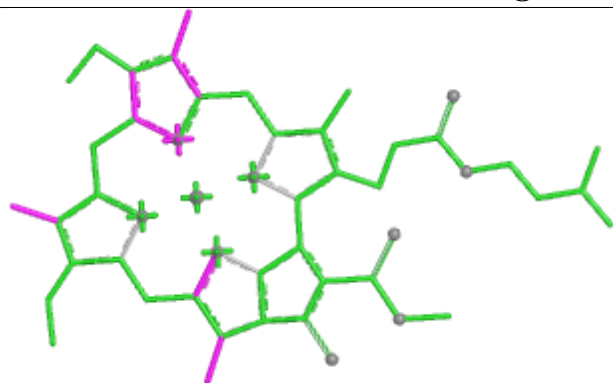


Torsions

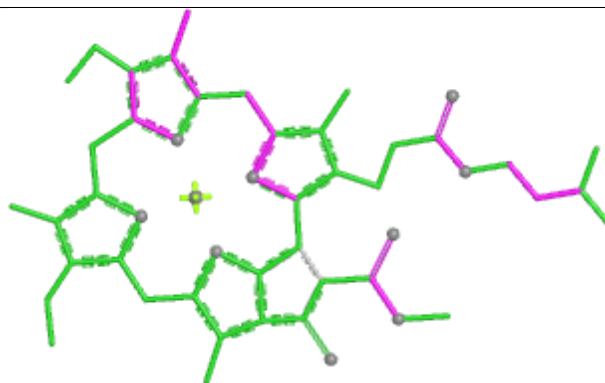


Rings

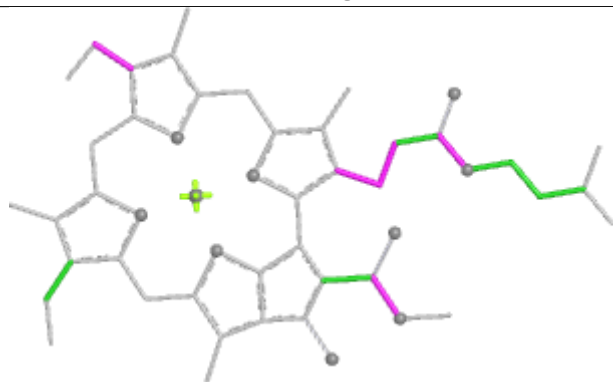
Ligand CLA A 809



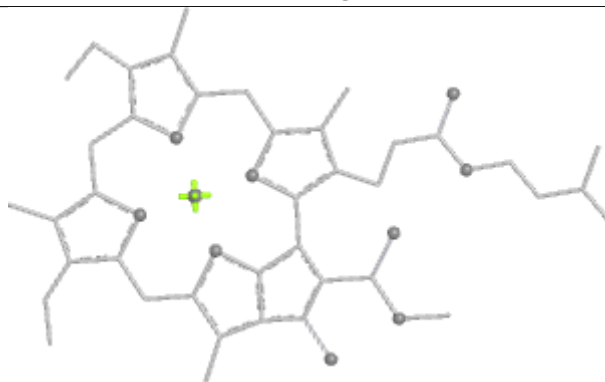
Bond lengths



Bond angles

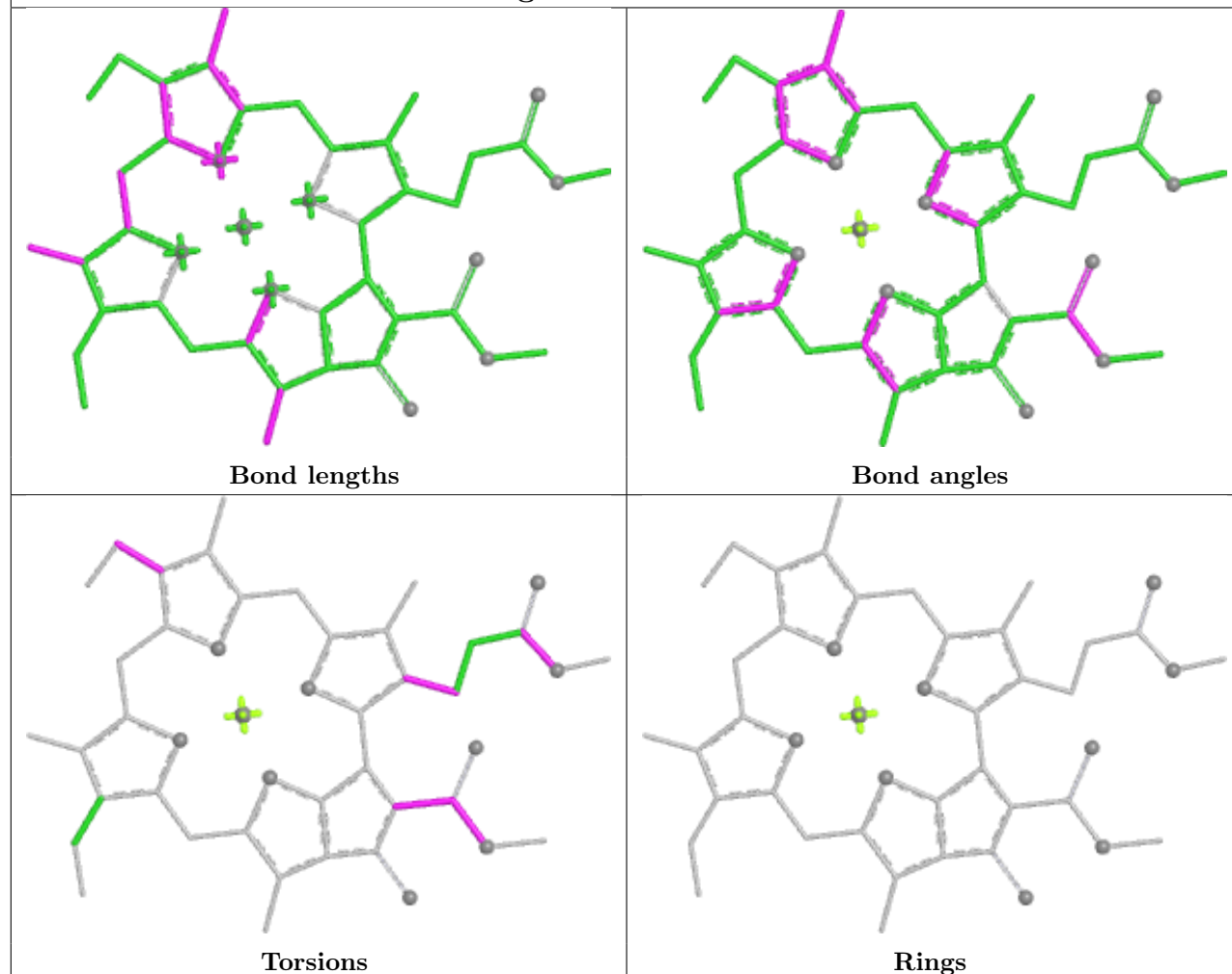


Torsions

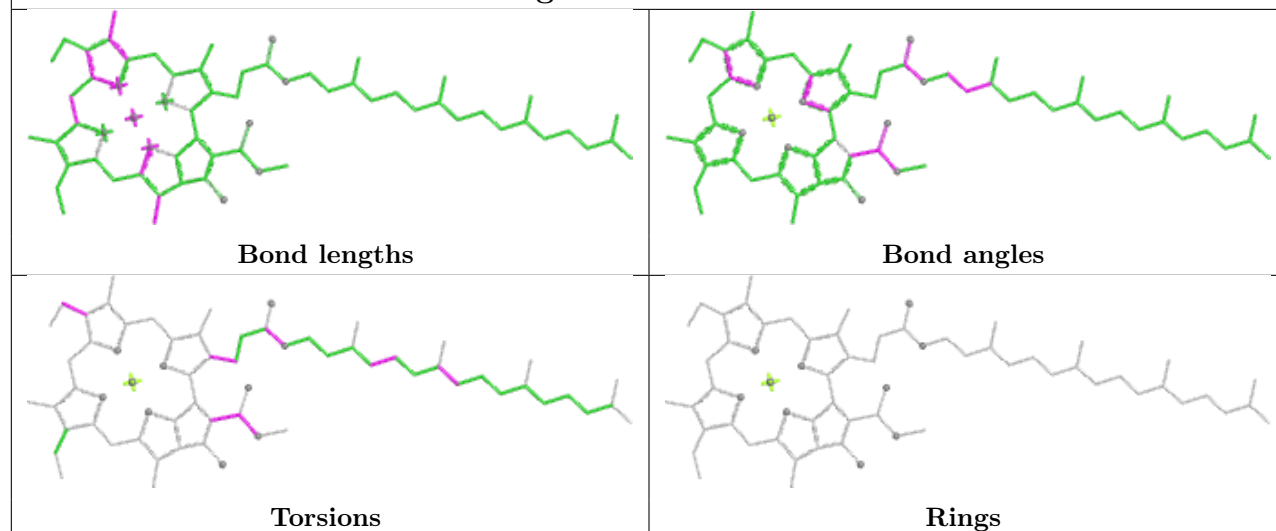


Rings

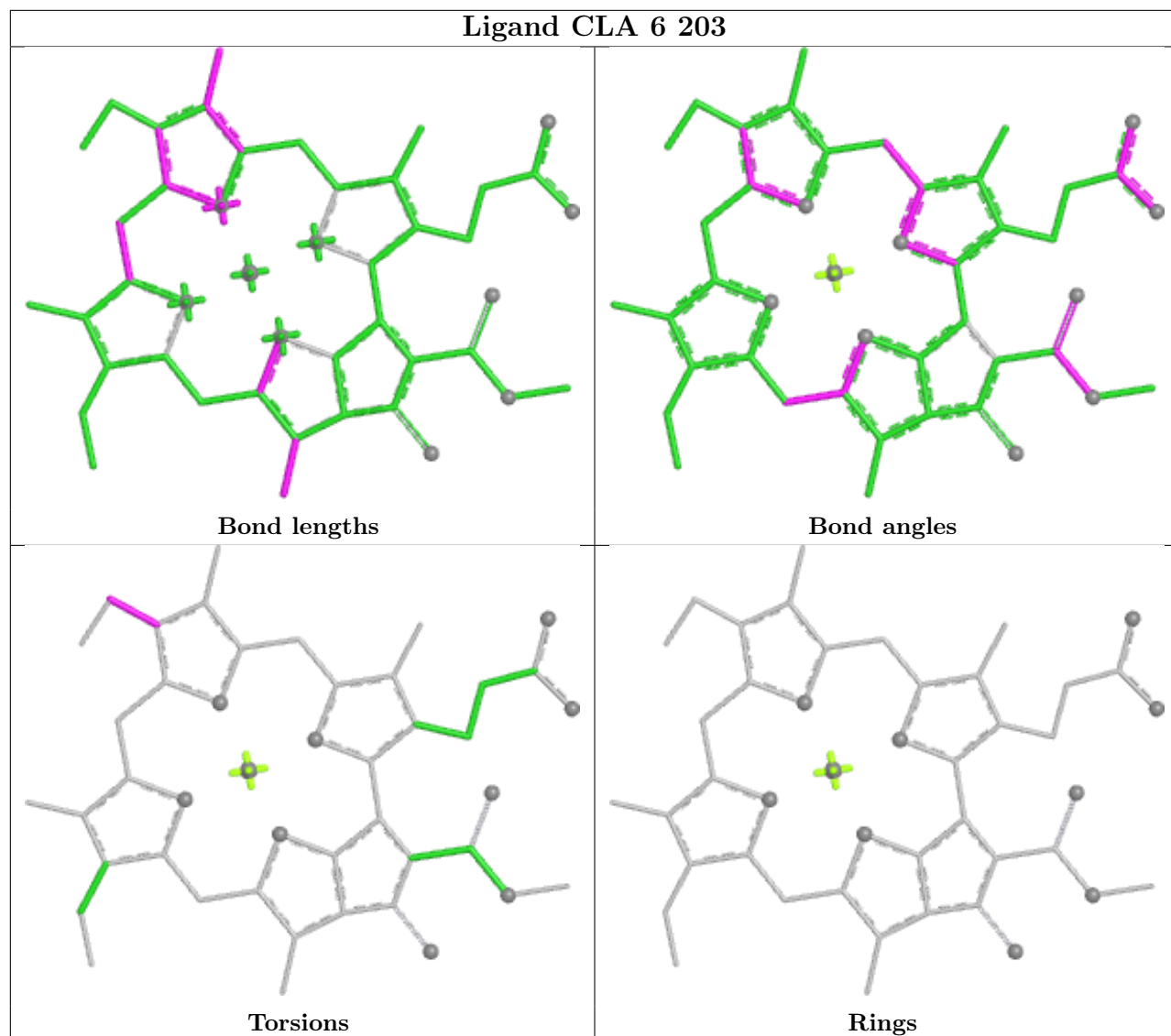
Ligand CLA 2 810



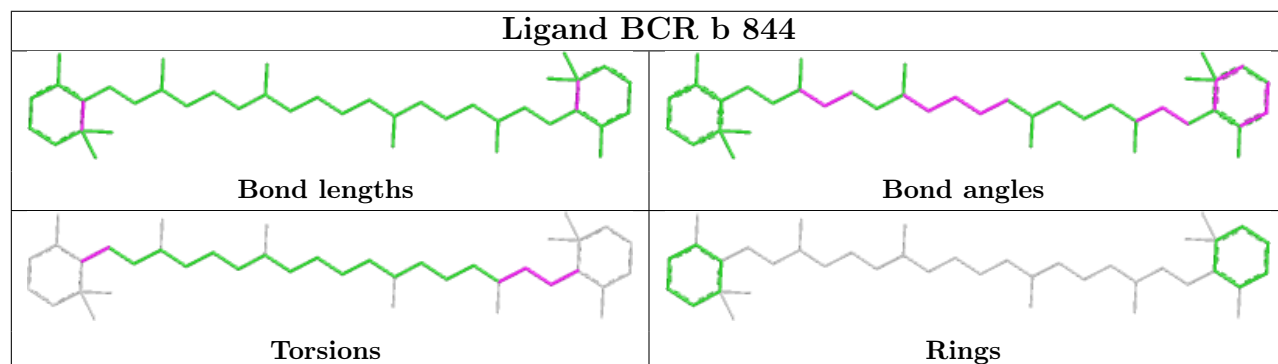
Ligand CLA a 838

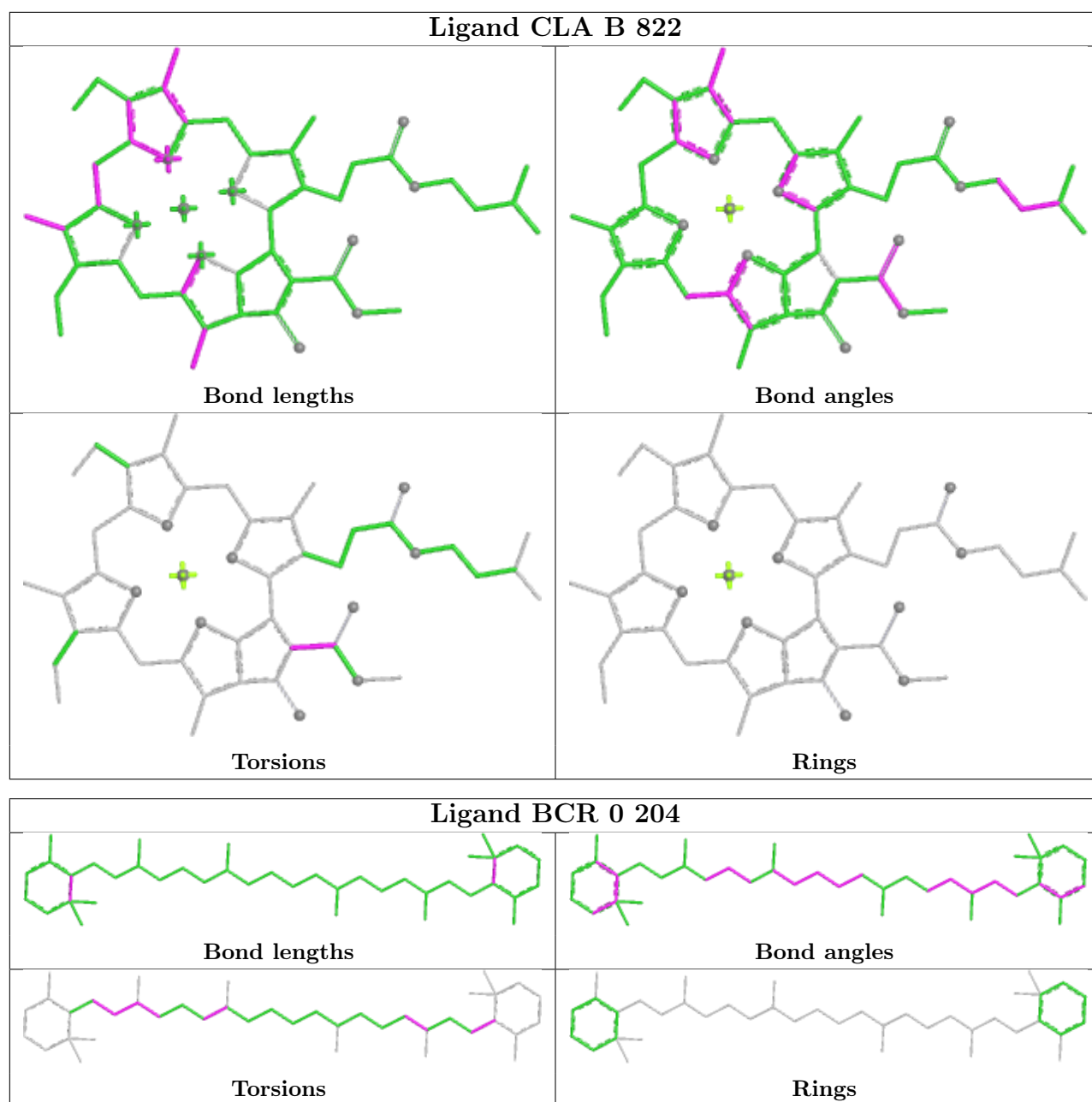


Ligand CLA 6 203

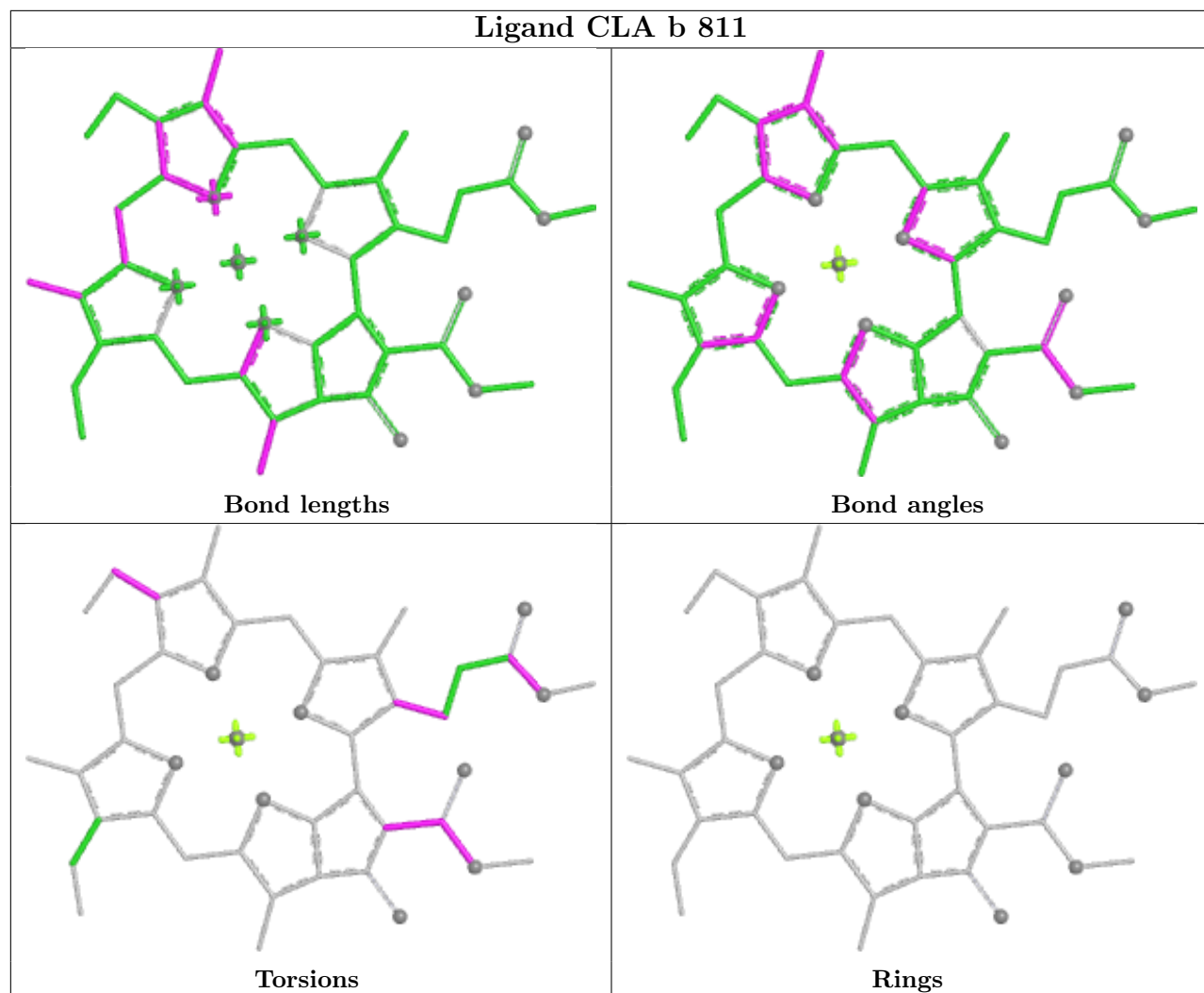


Ligand BCR b 844

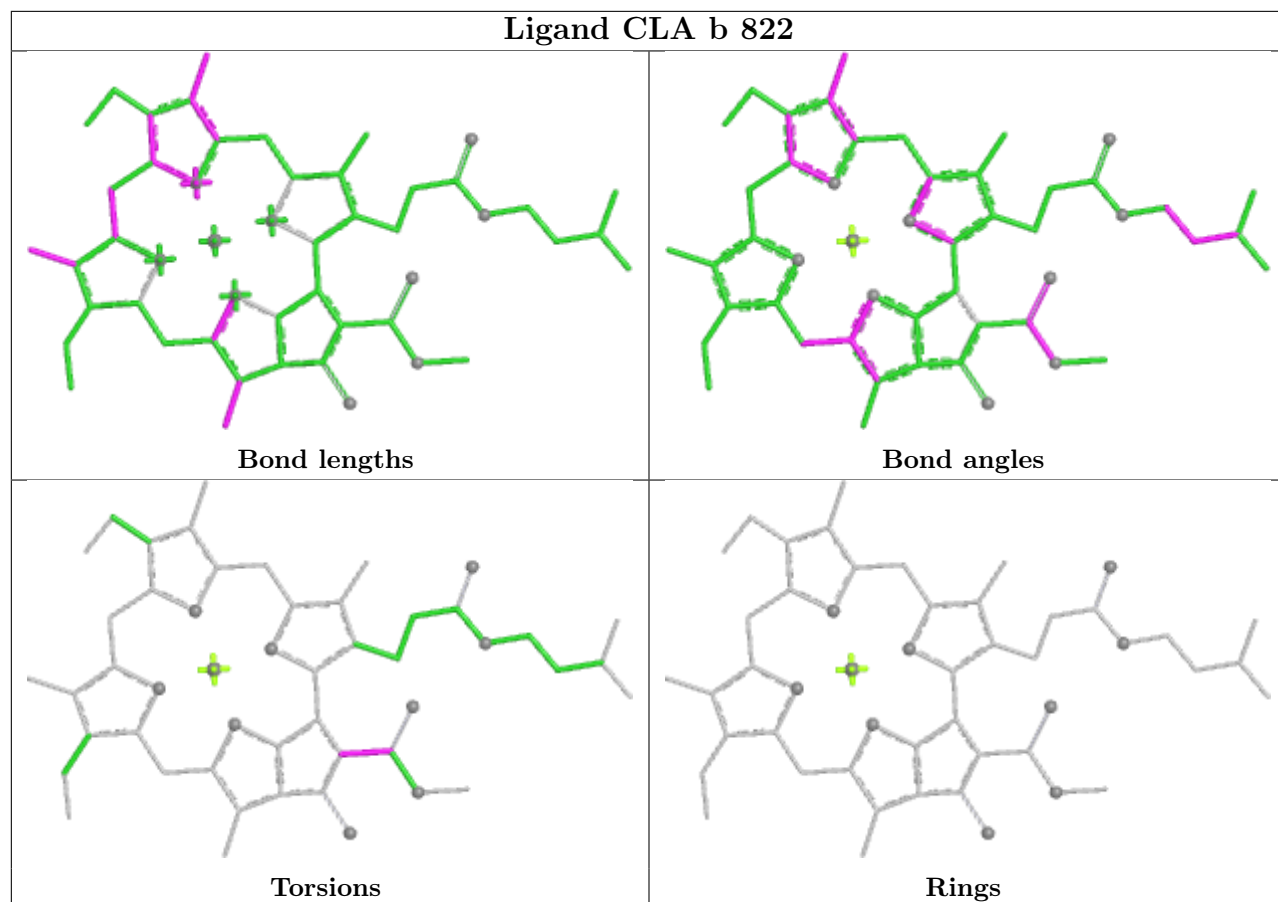




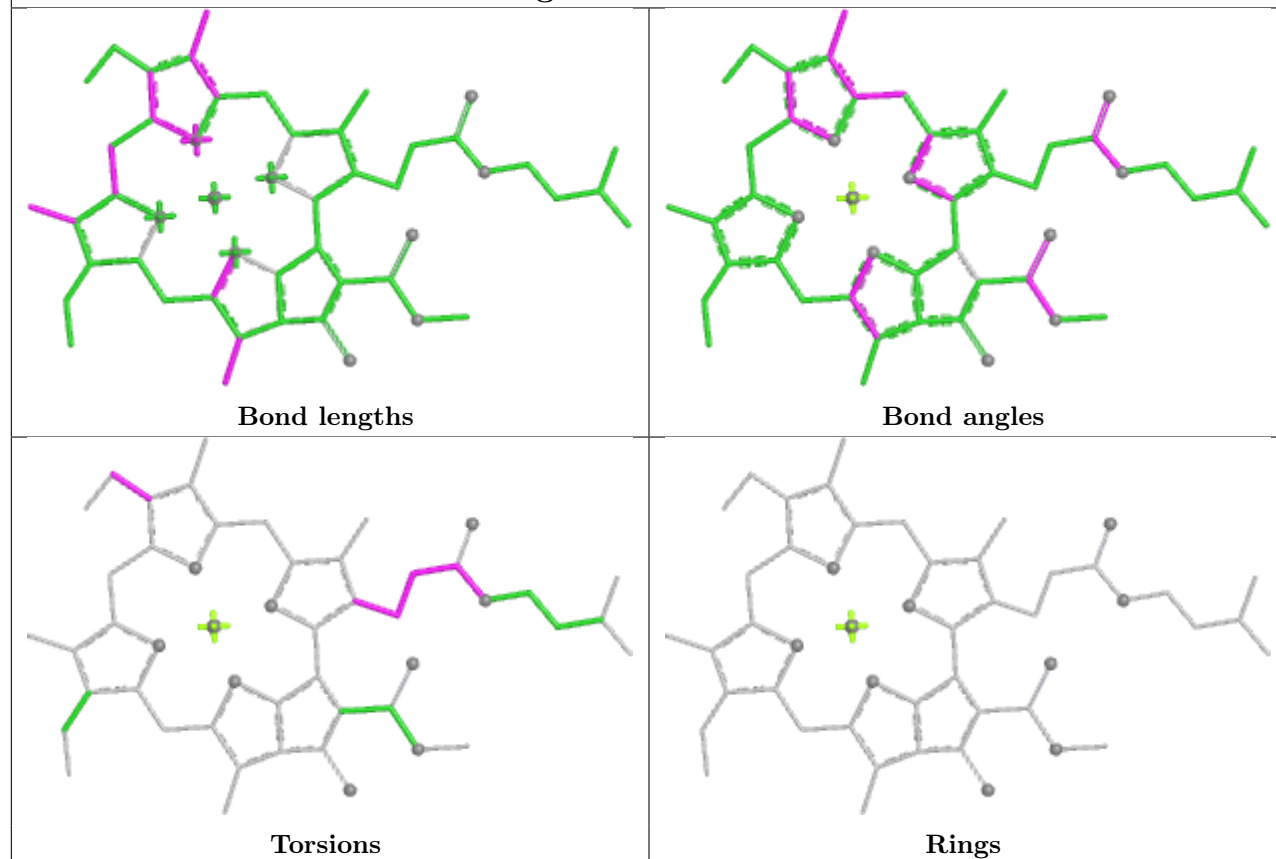
Ligand CLA b 811



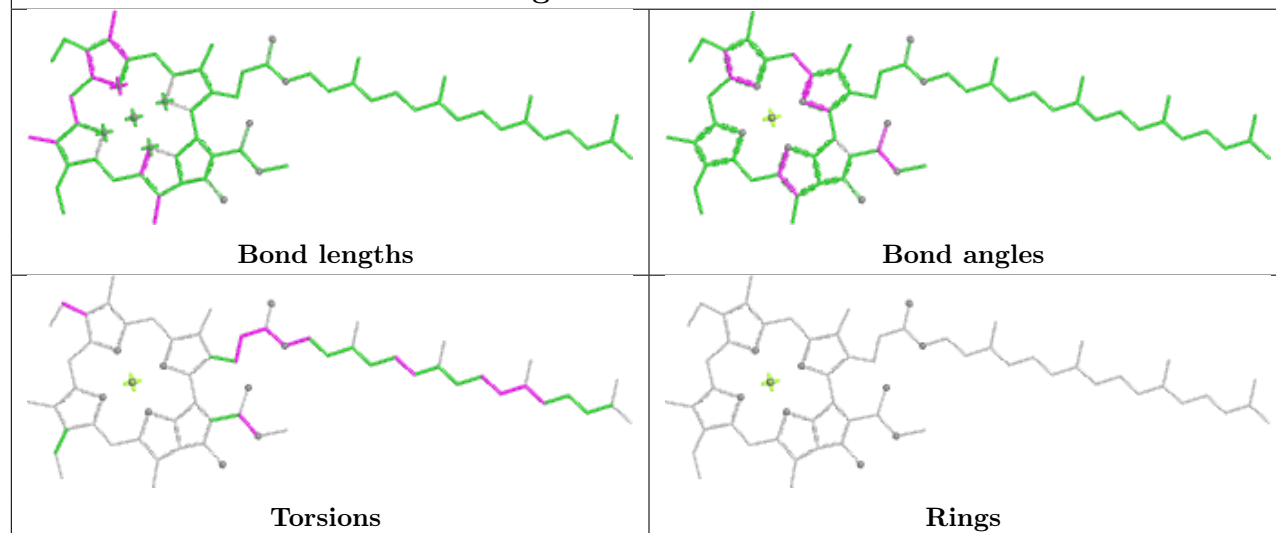
Ligand CLA b 822

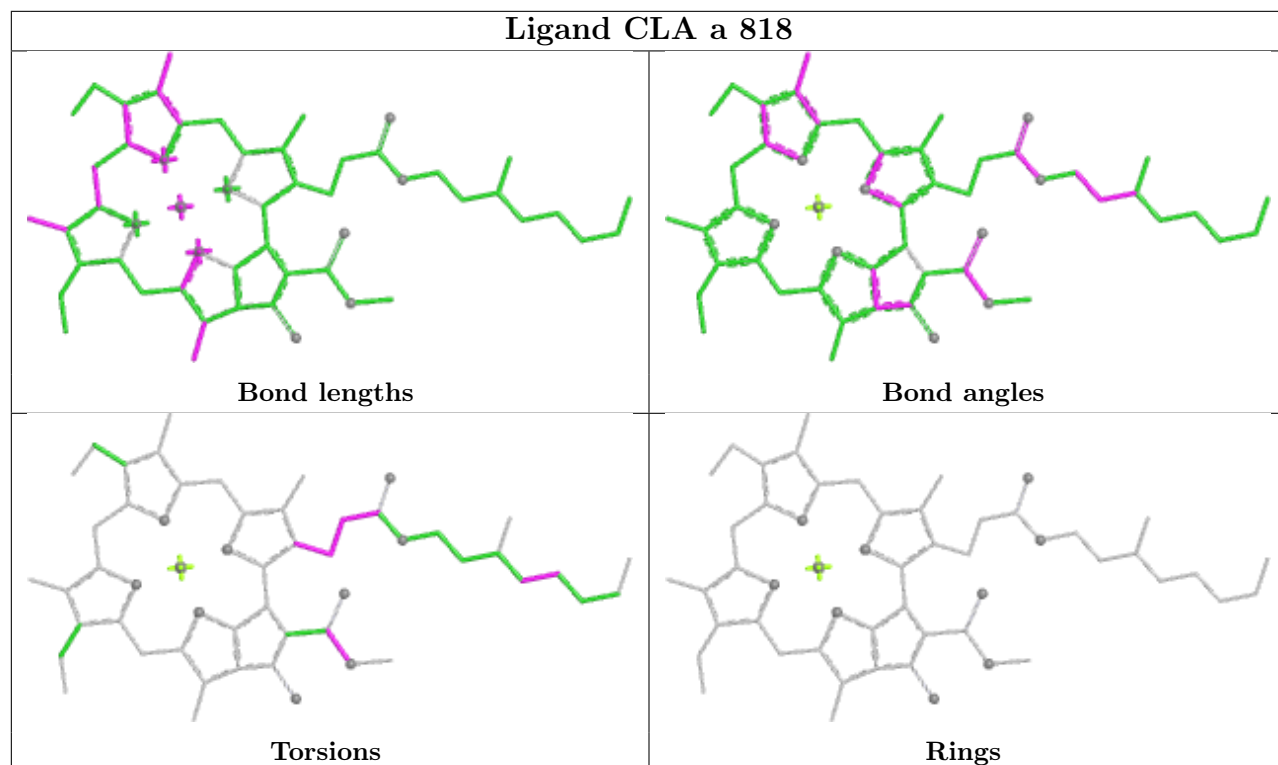
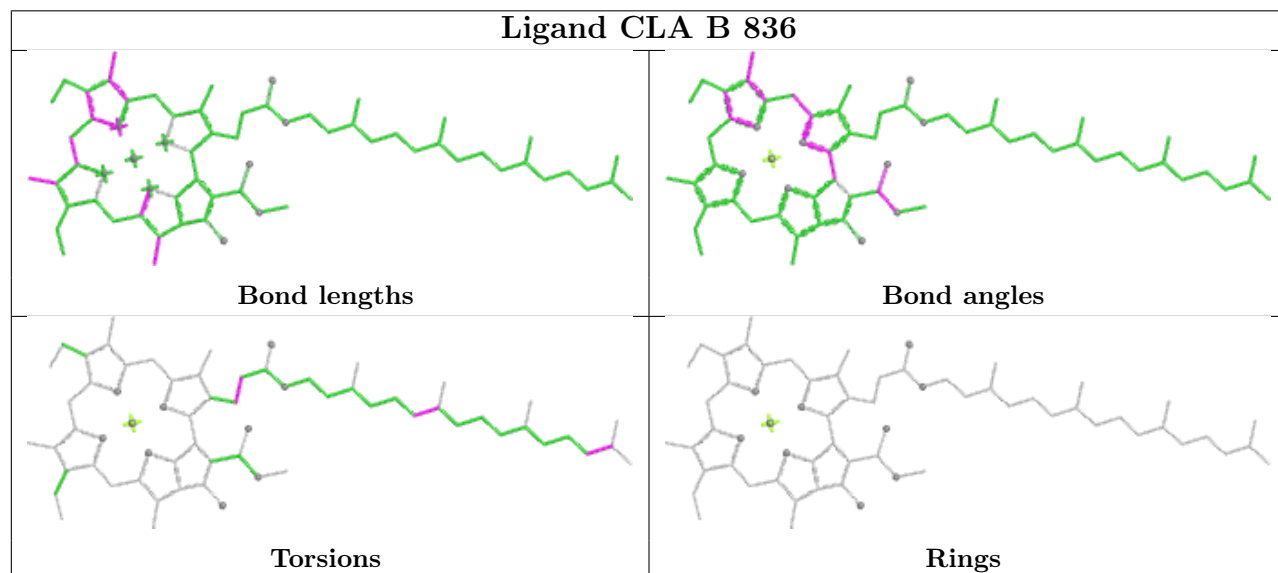
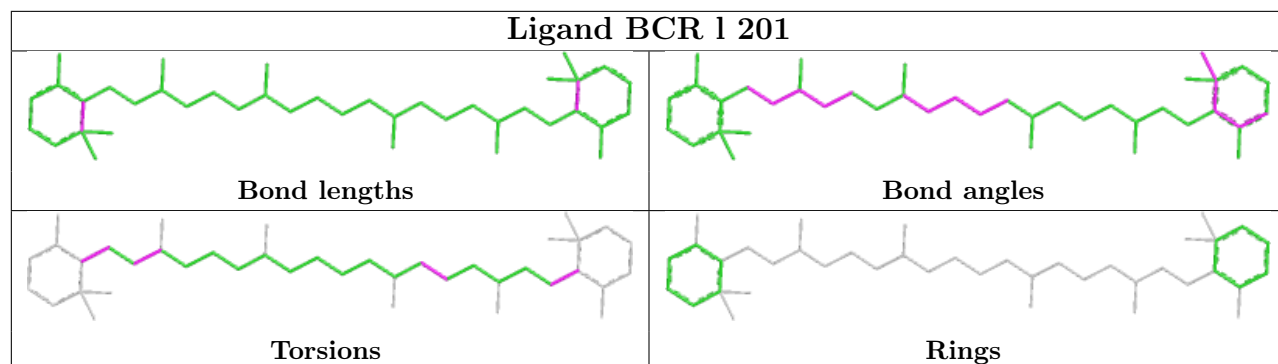


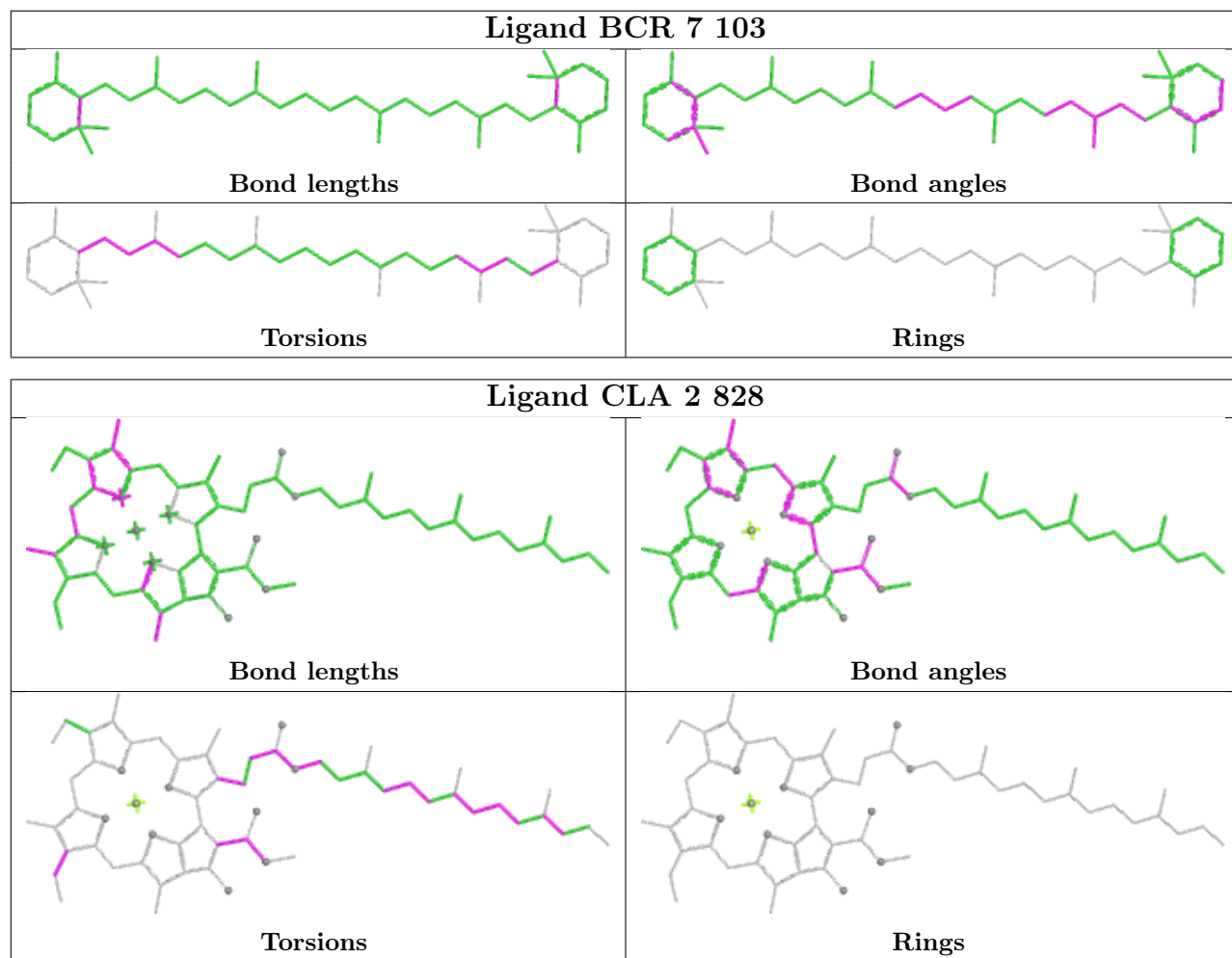
Ligand CLA 2 813



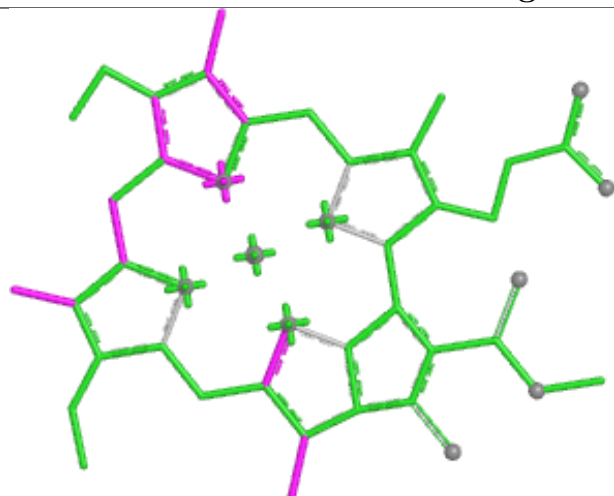
Ligand CLA B 807



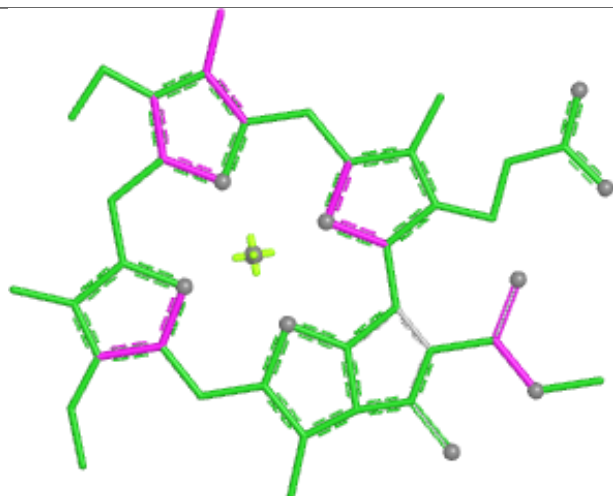




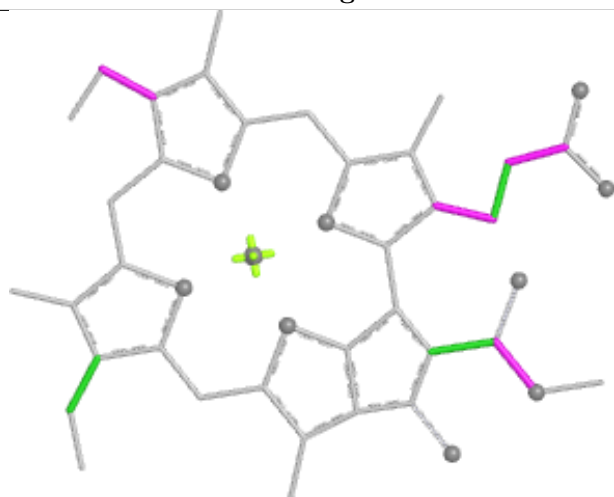
Ligand CLA 1 810



Bond lengths



Bond angles

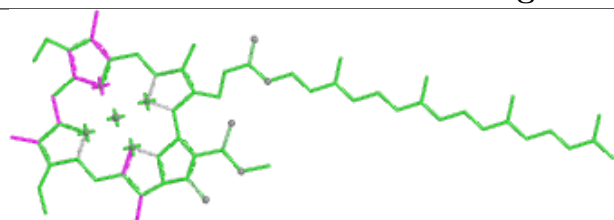


Torsions

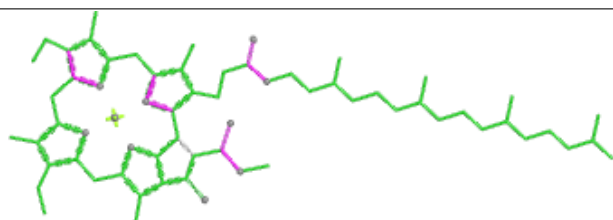


Rings

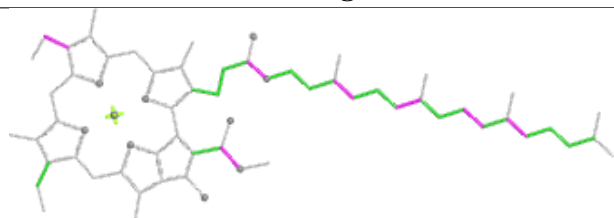
Ligand CLA b 805



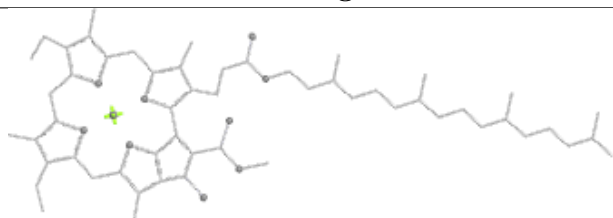
Bond lengths



Bond angles

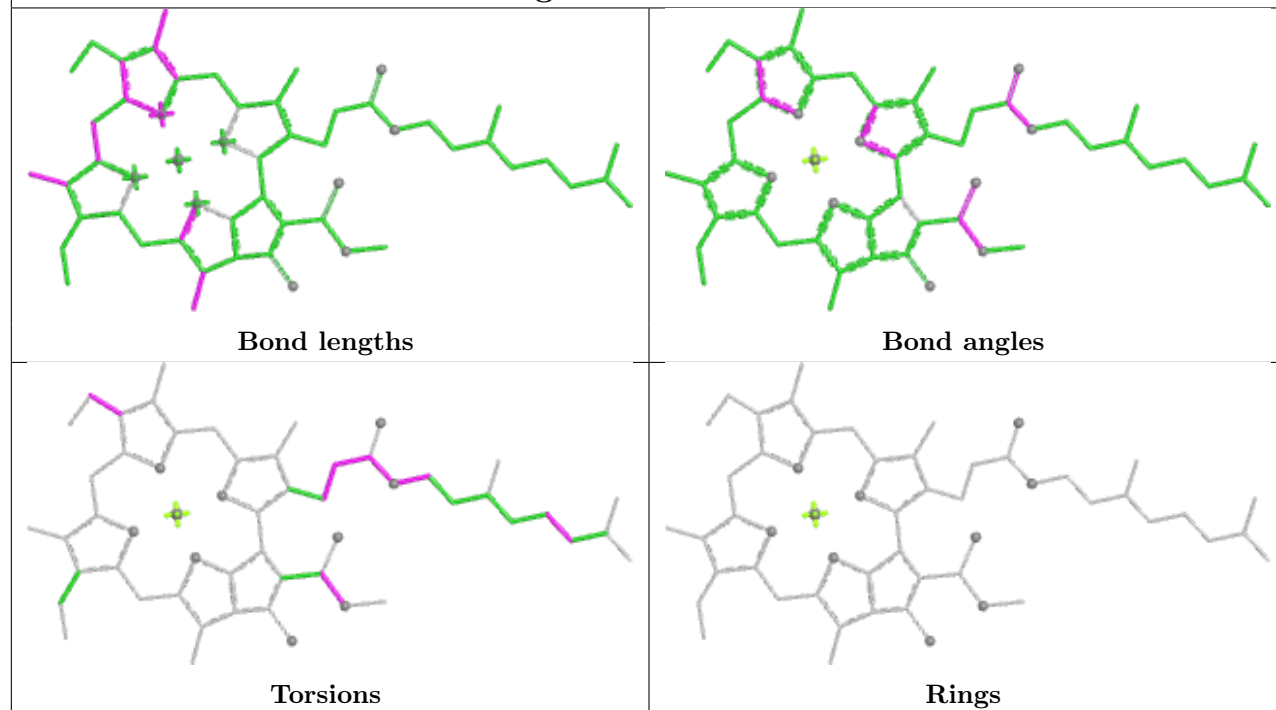


Torsions

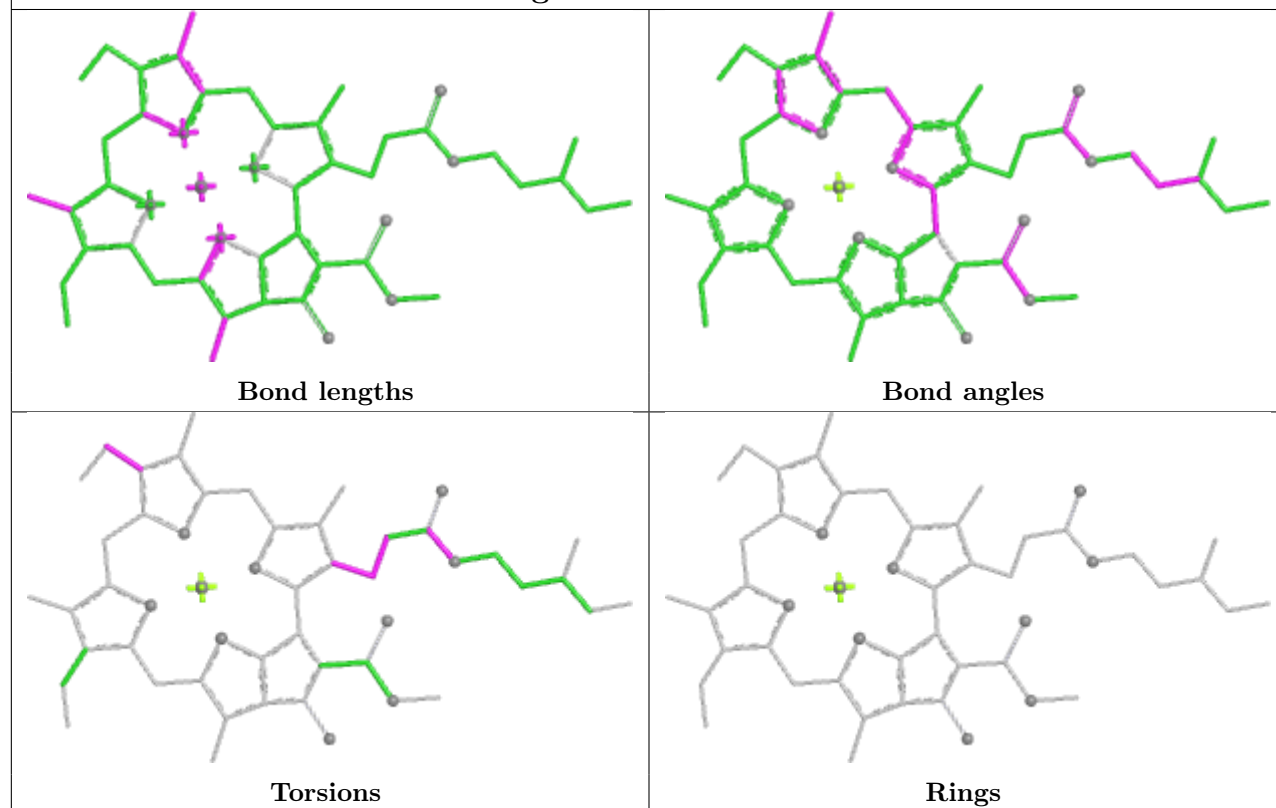


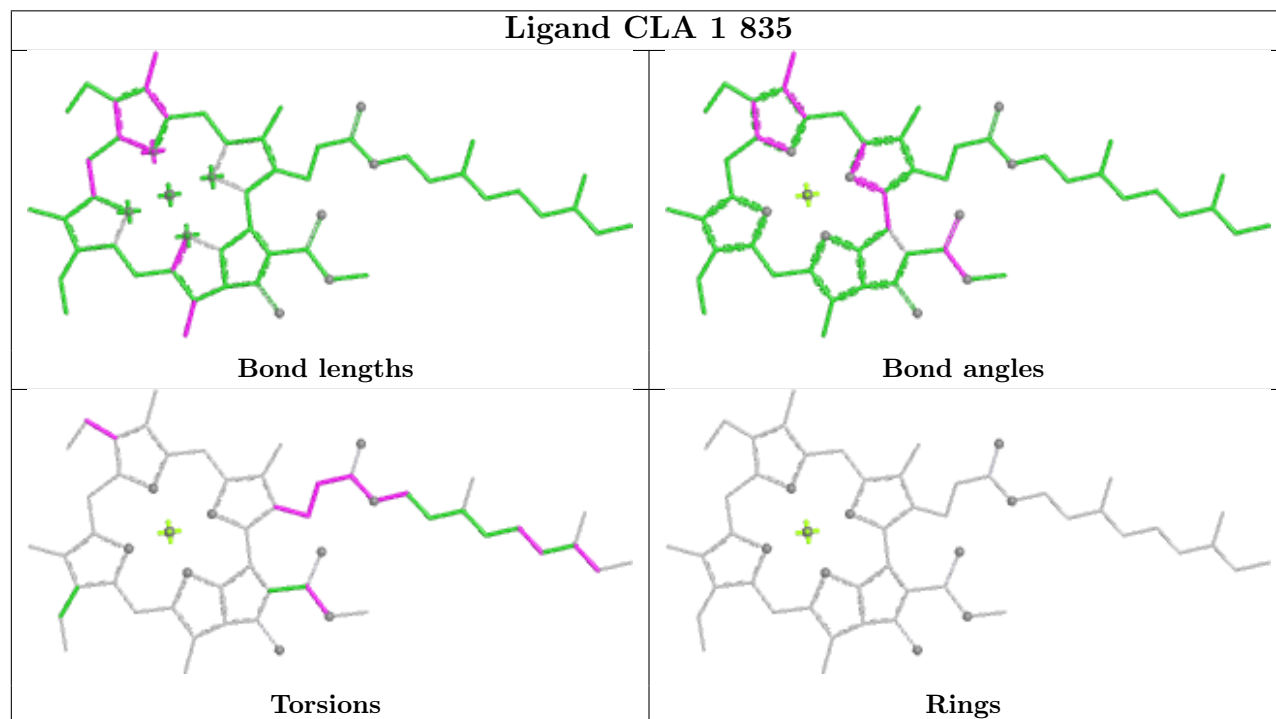
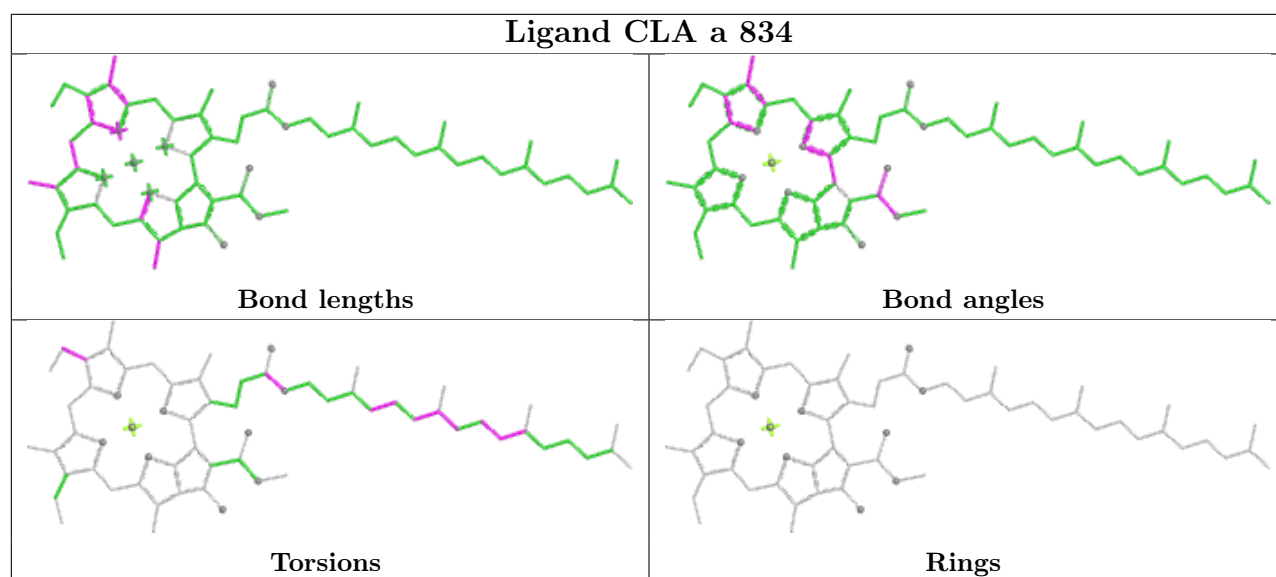
Rings

Ligand CLA b 828

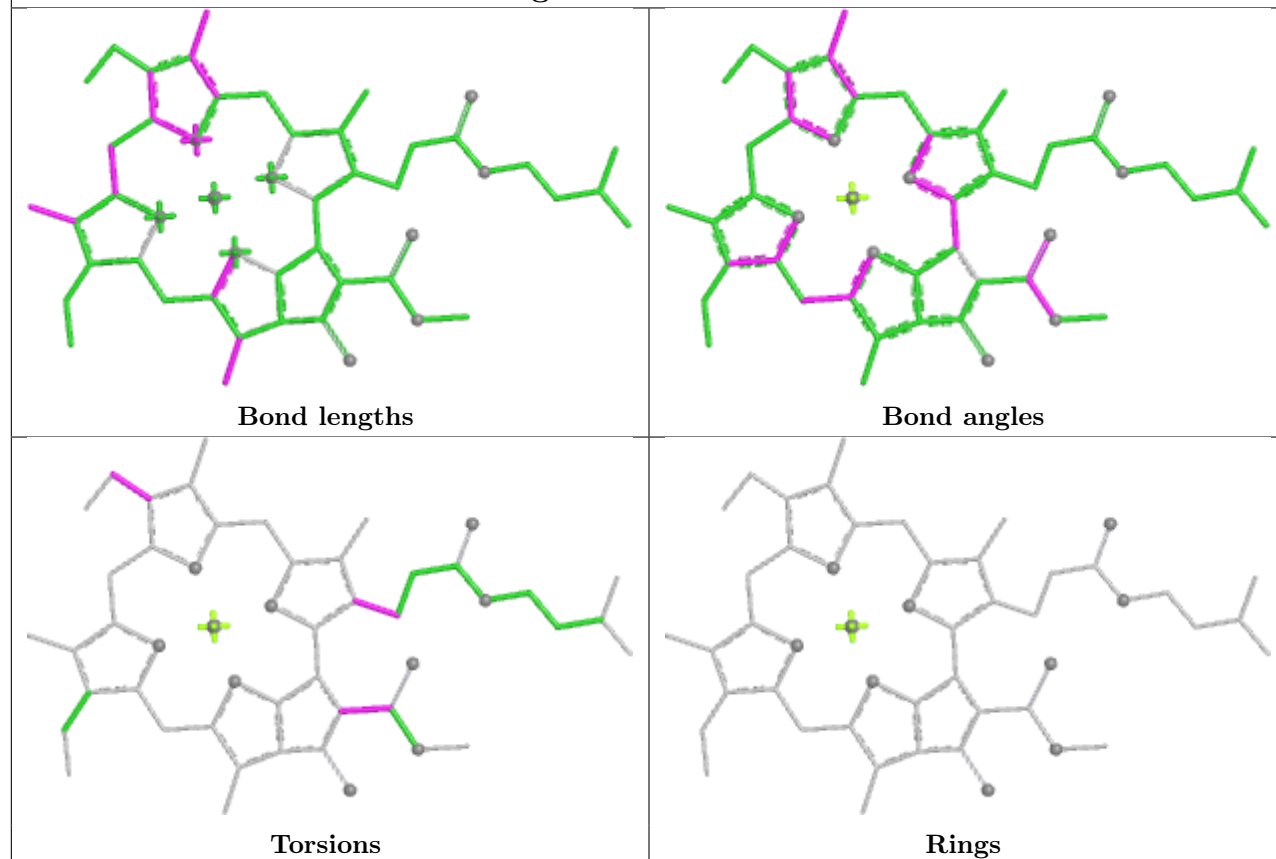


Ligand CLA A 836

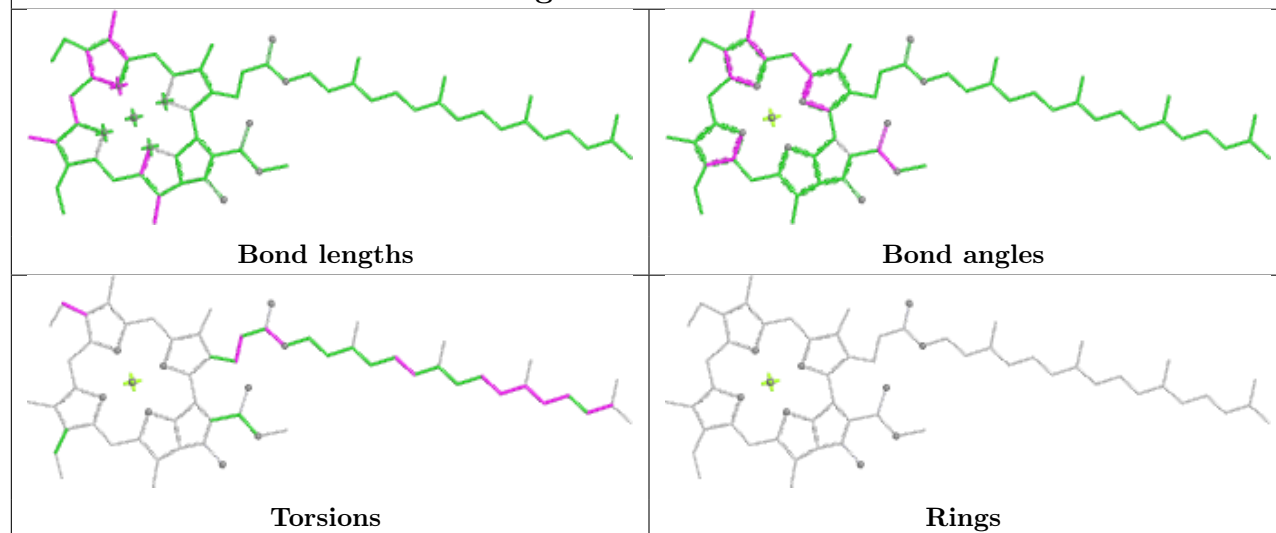


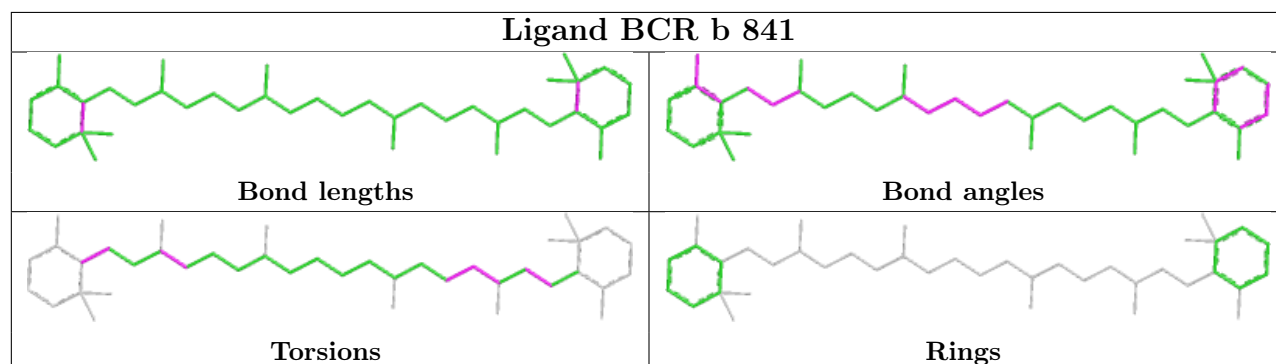
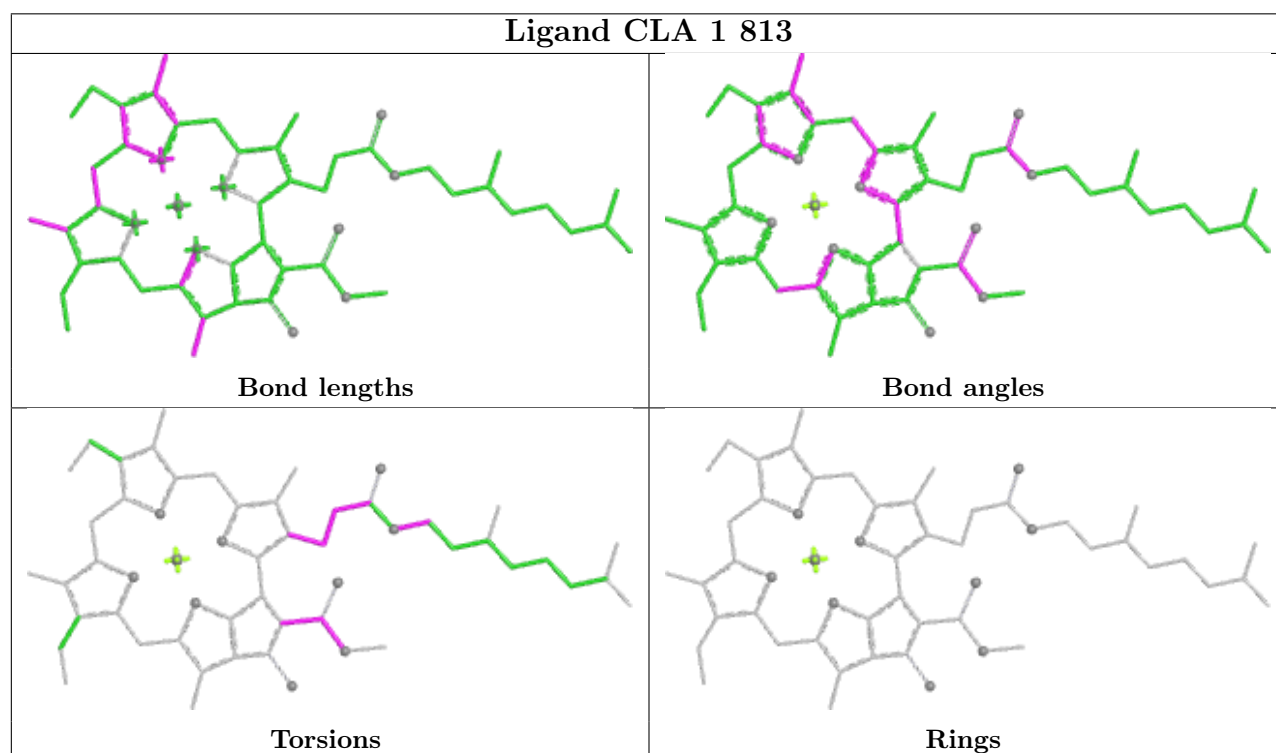
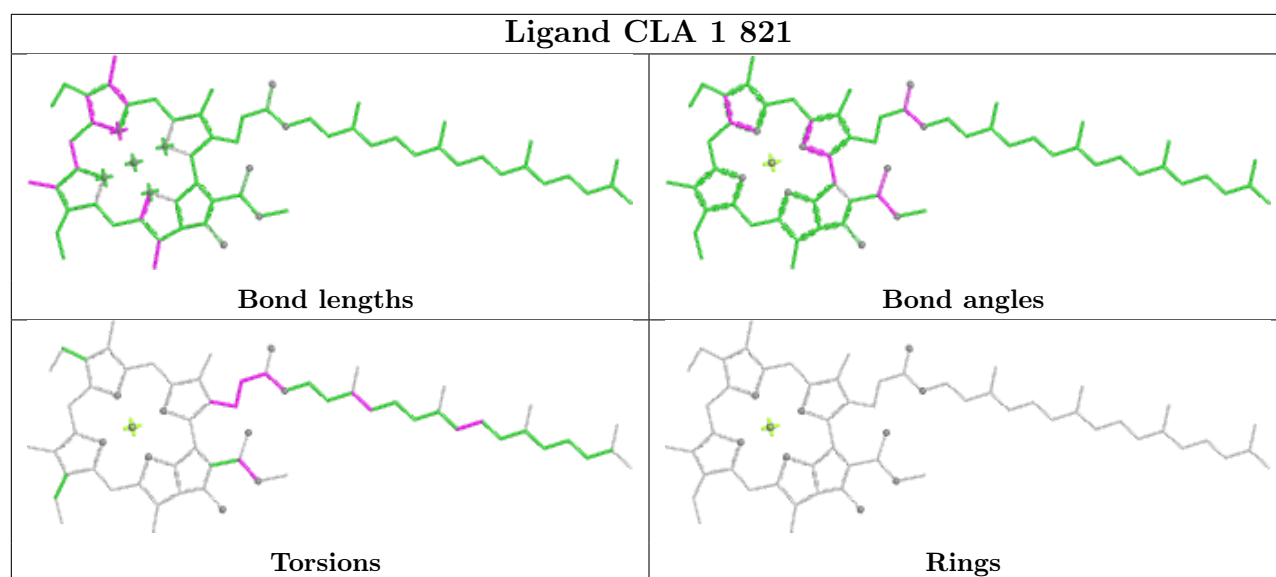


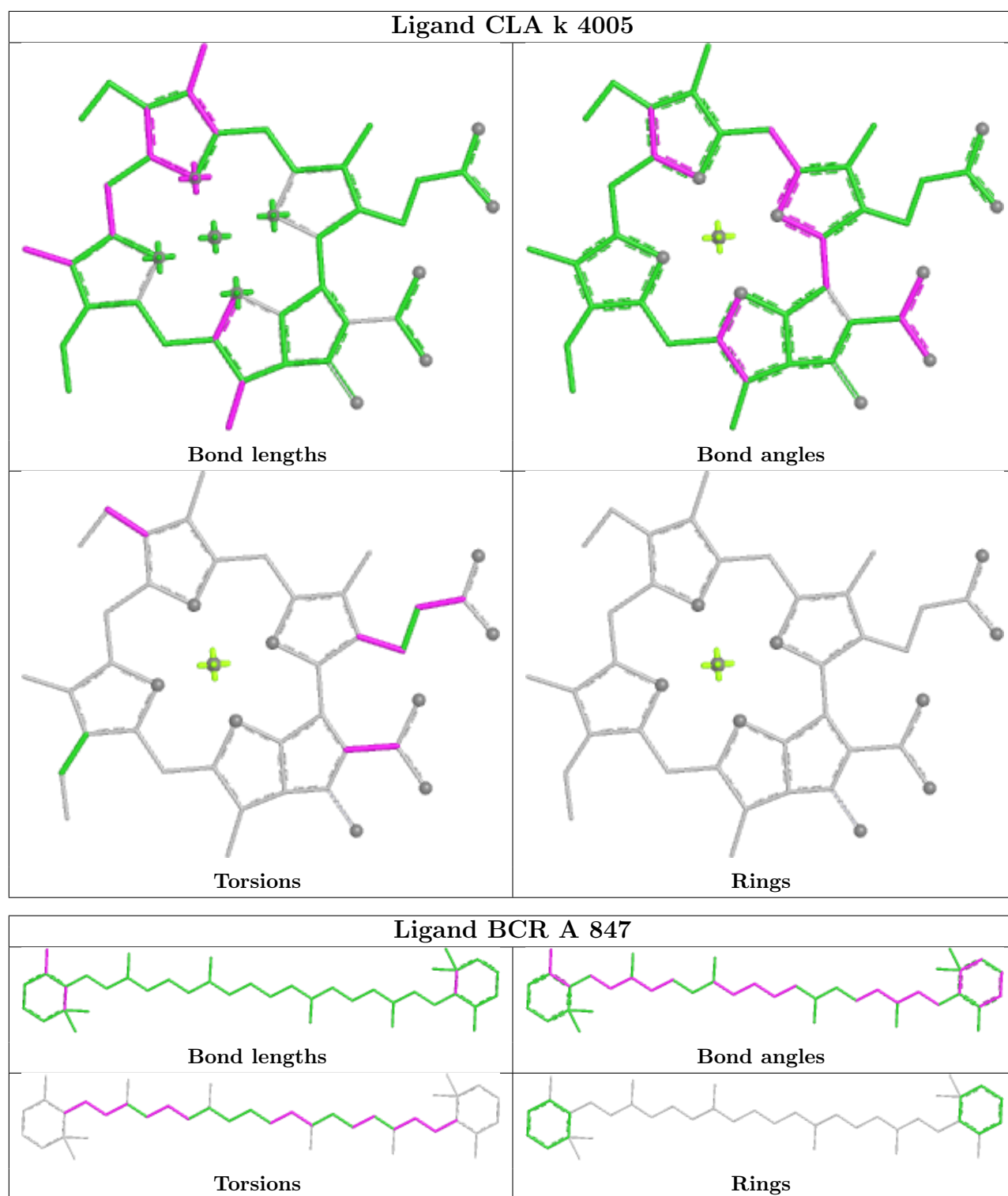
Ligand CLA A 808

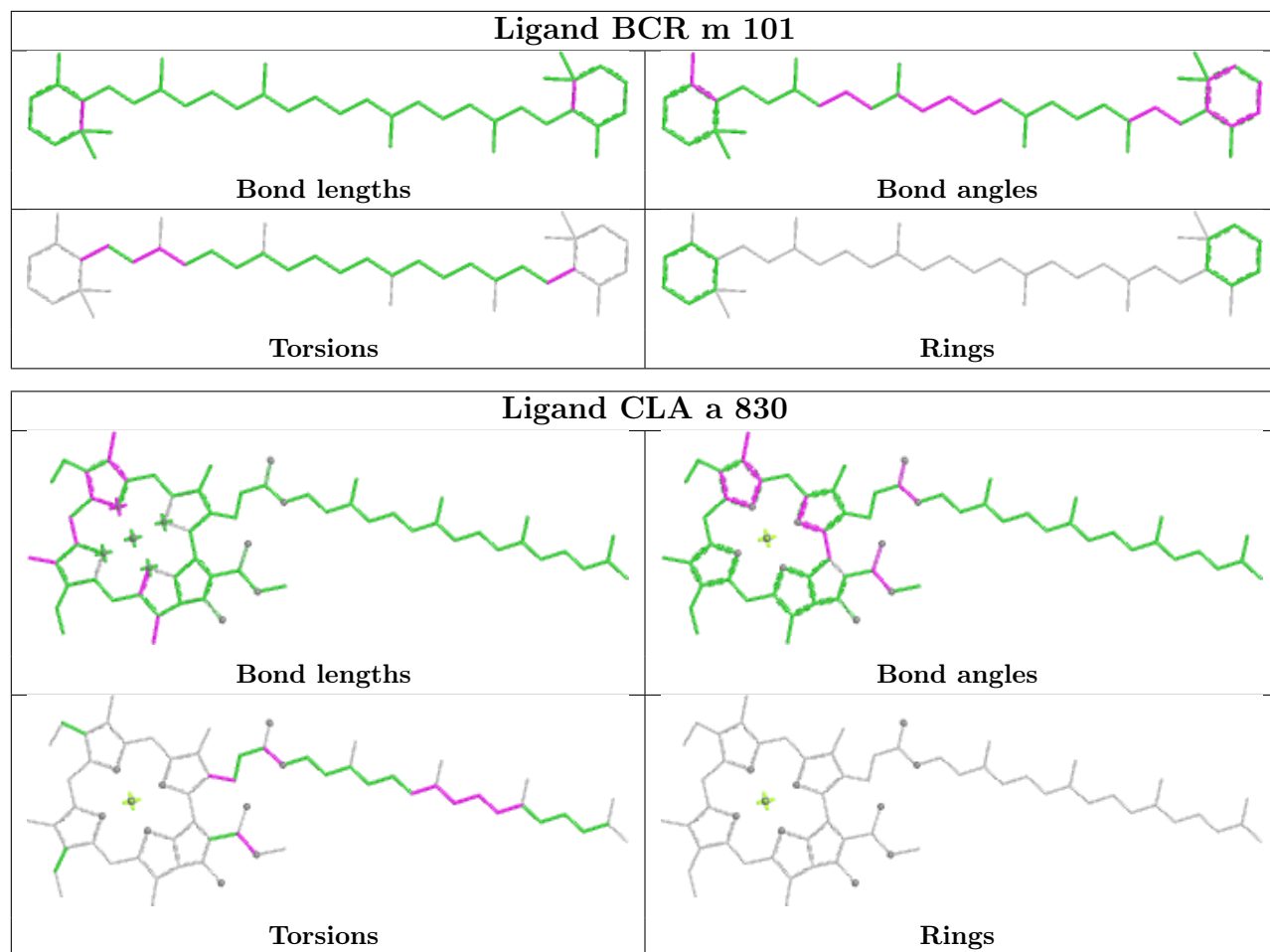


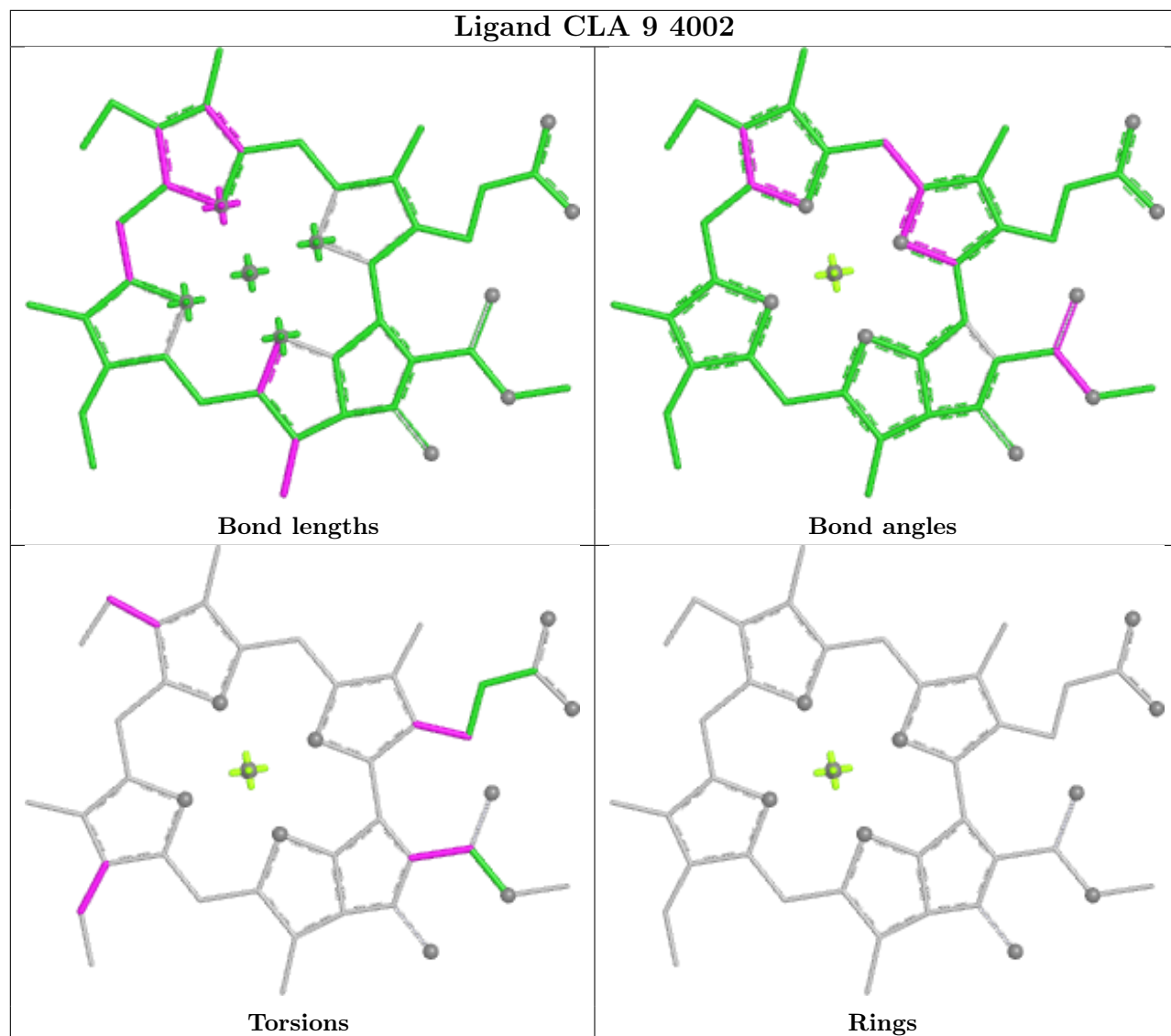
Ligand CLA b 823



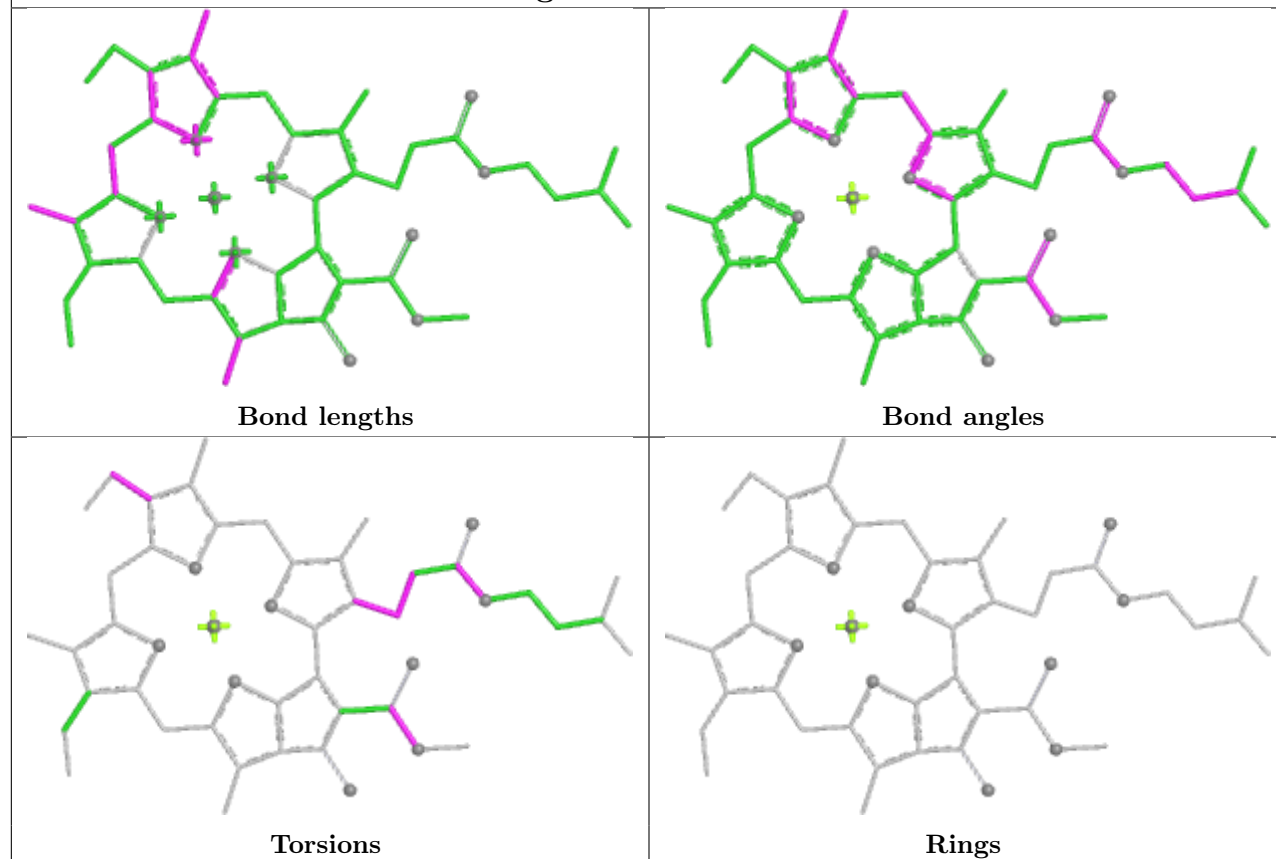




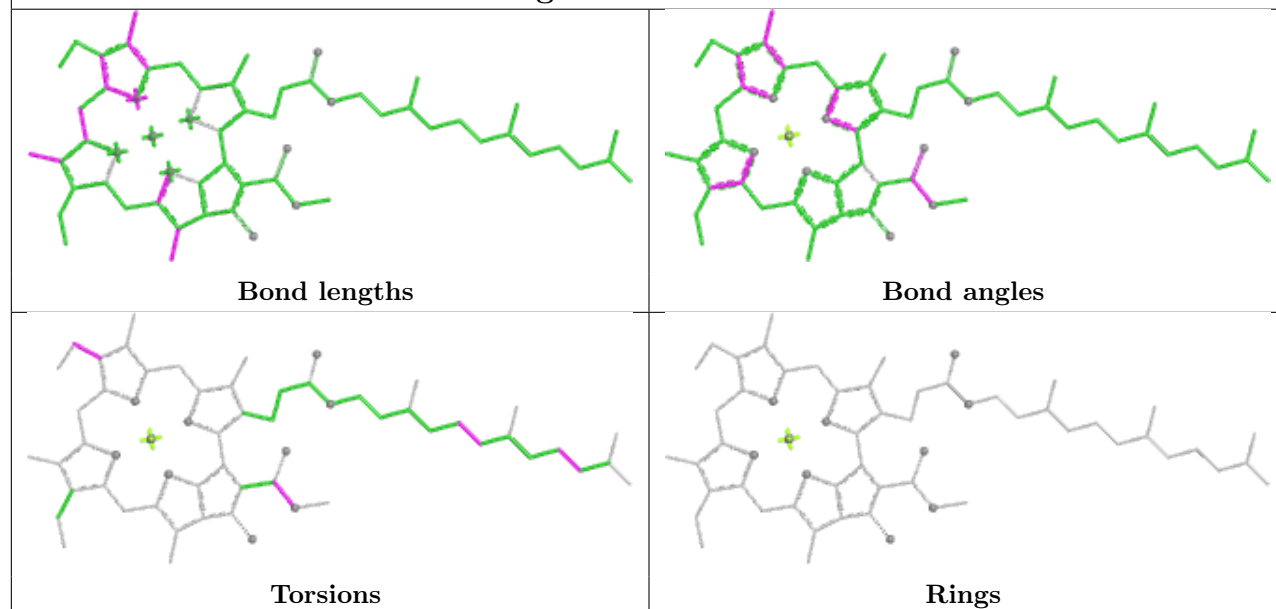


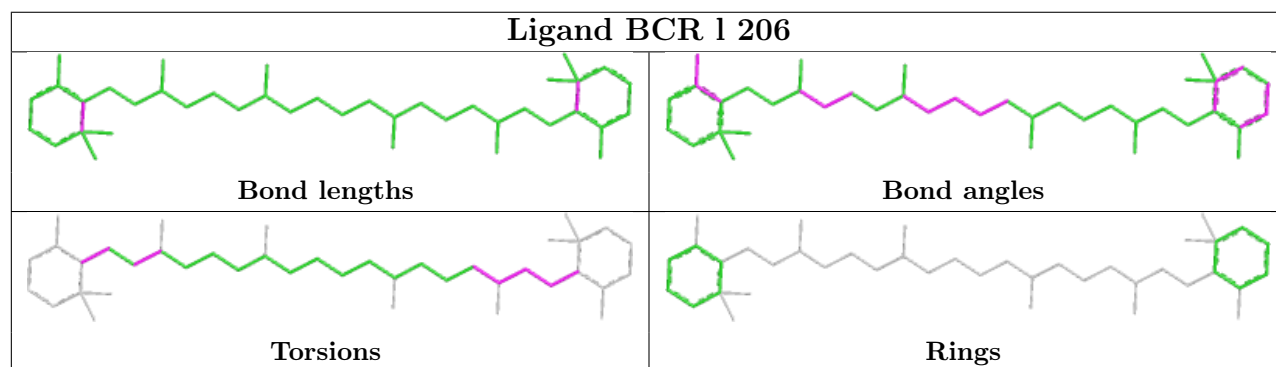
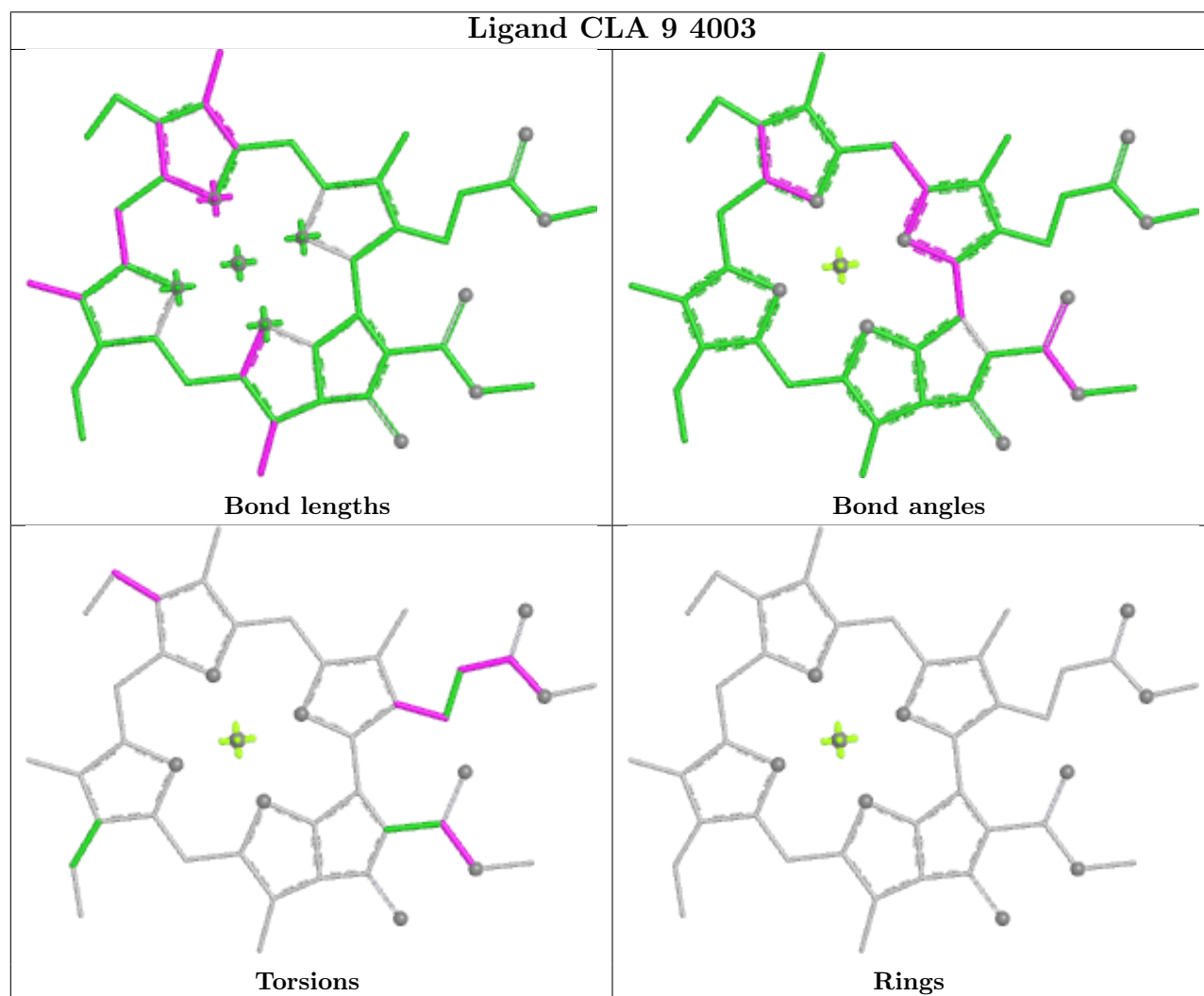
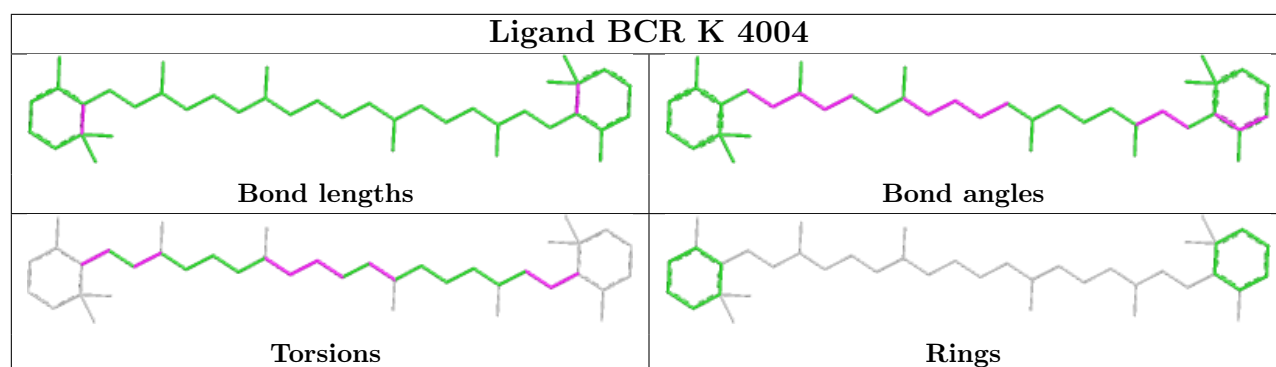


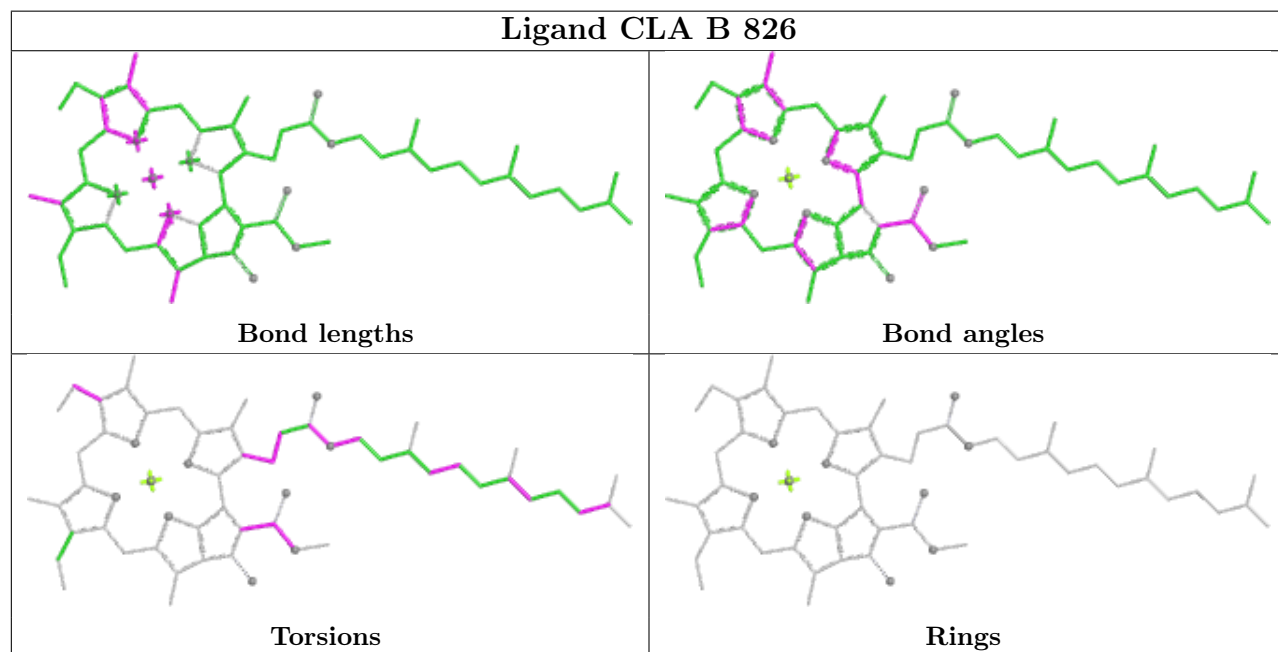
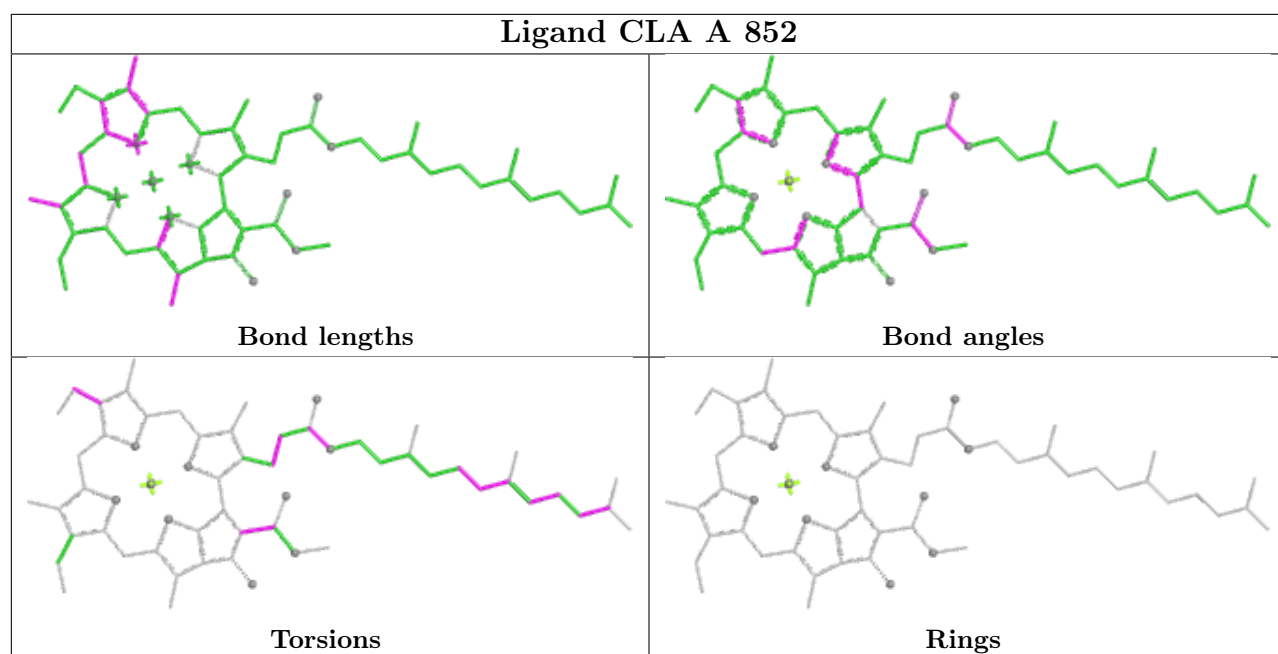
Ligand CLA a 809

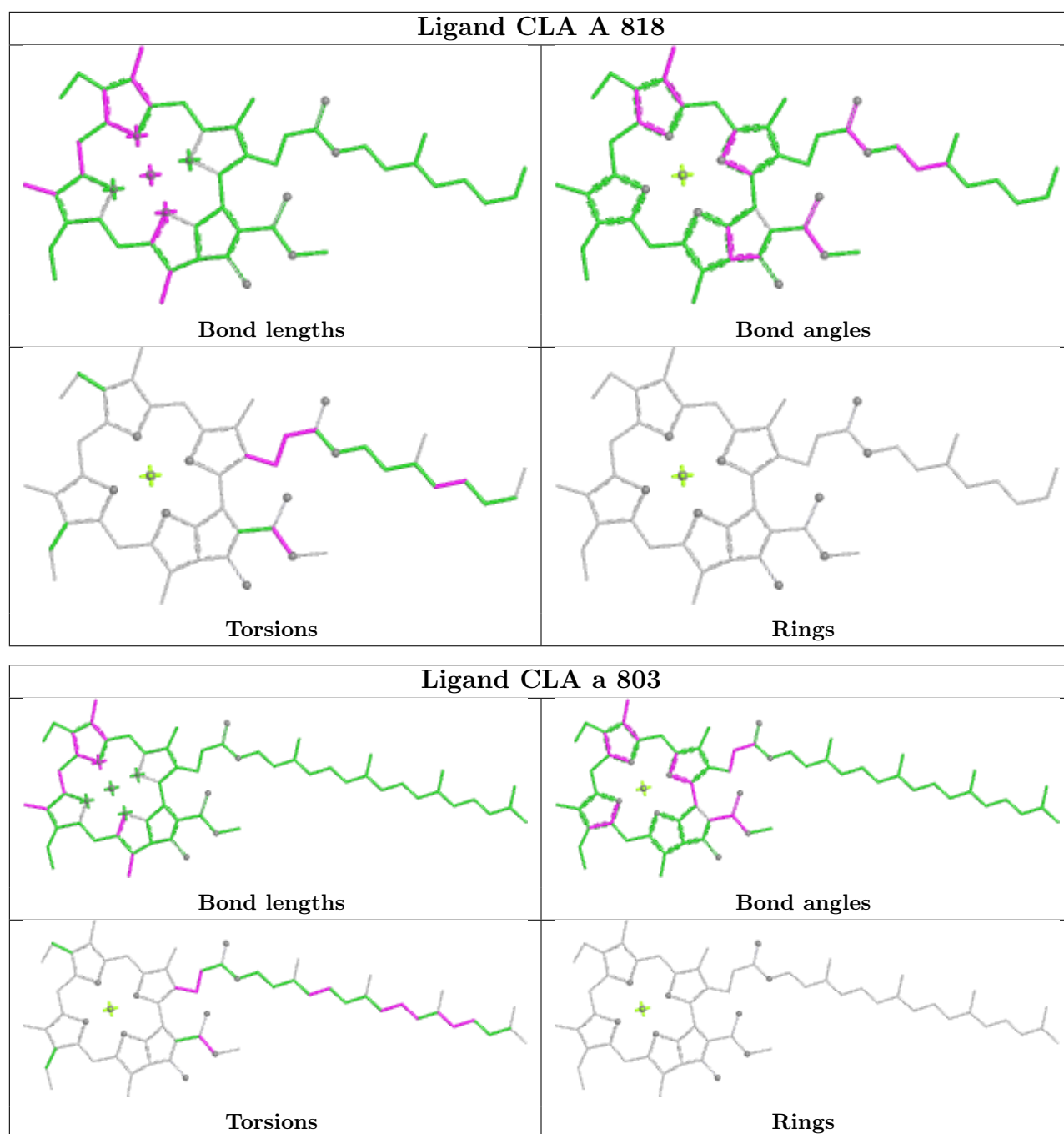


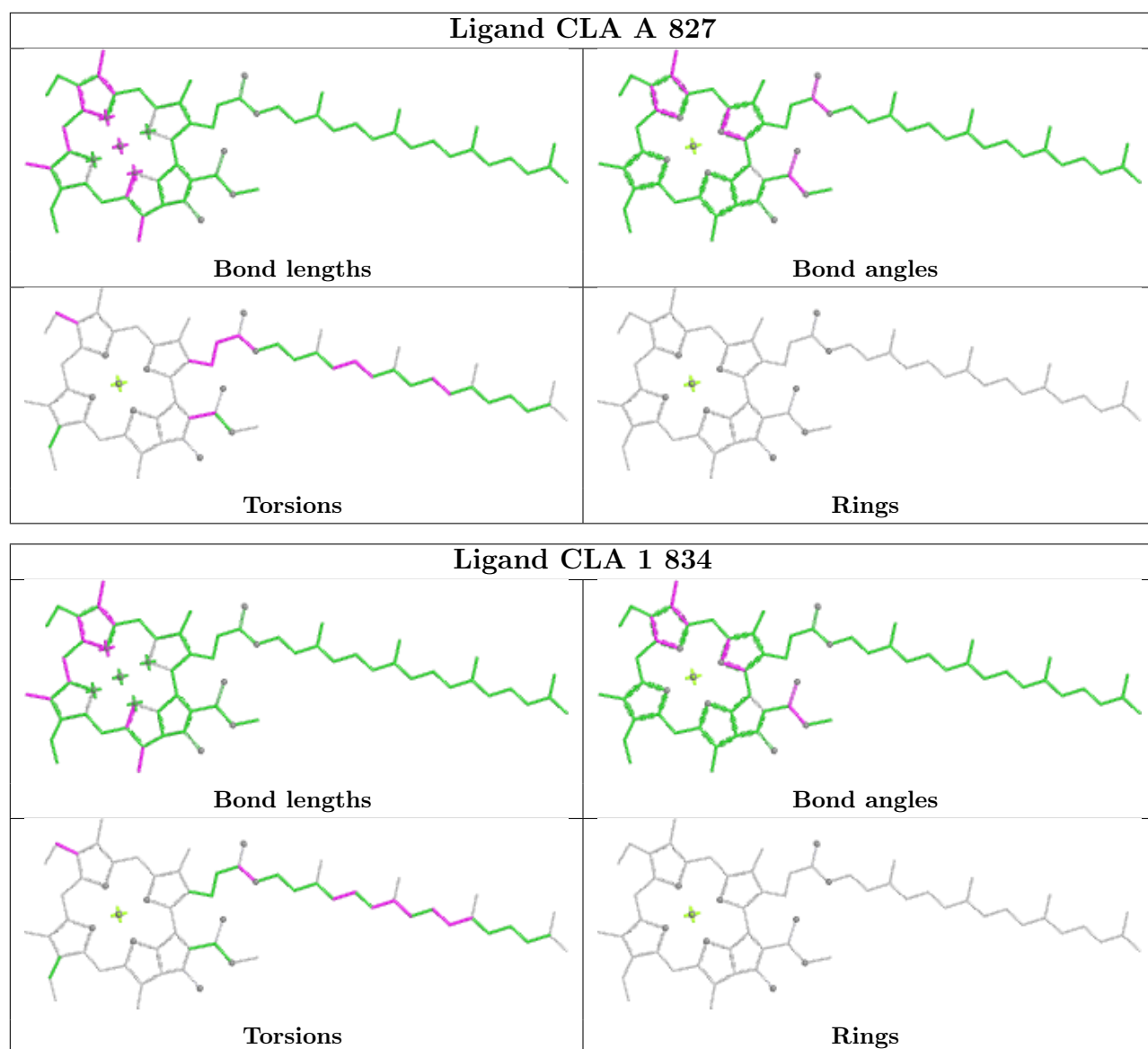
Ligand CLA 2 833

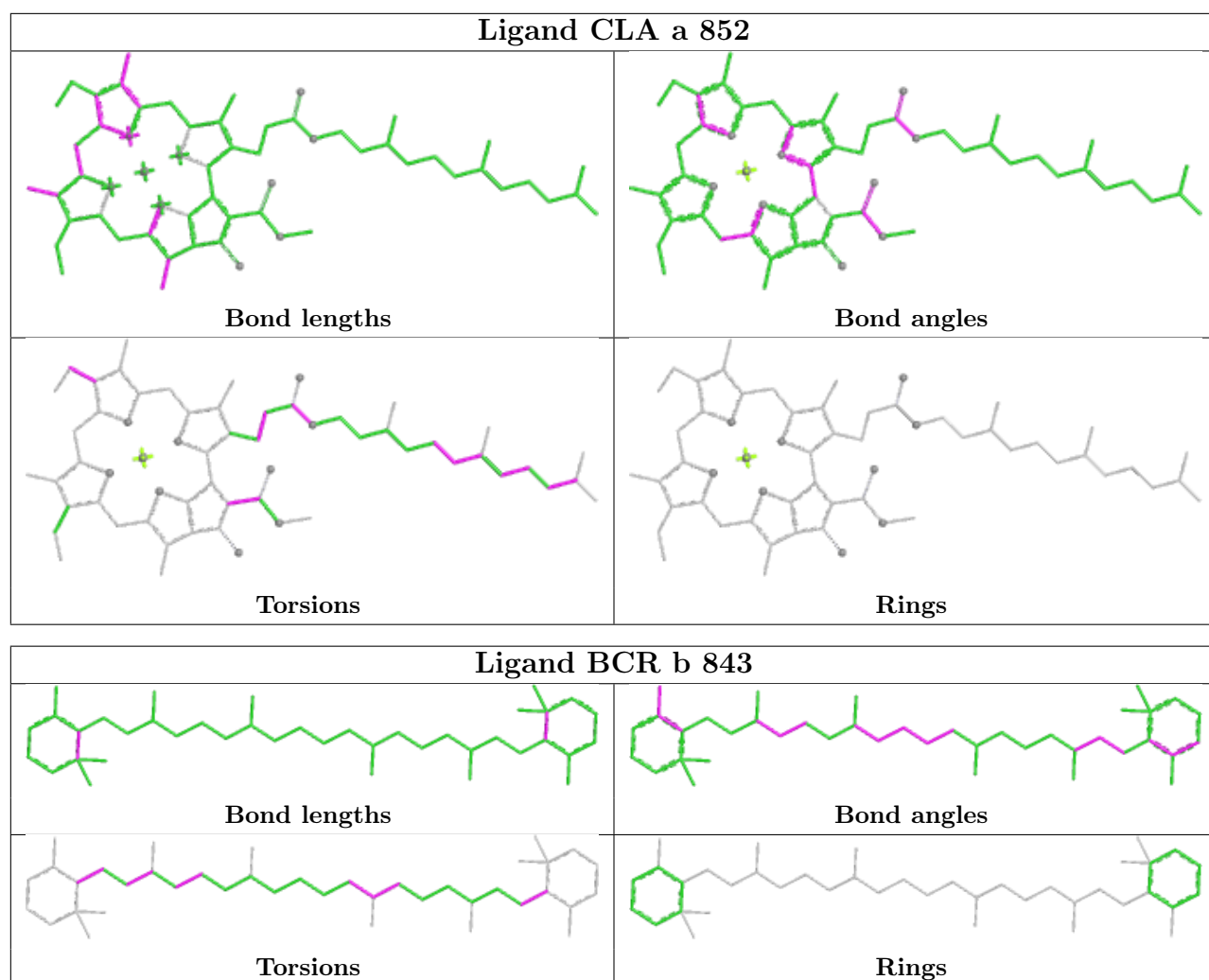




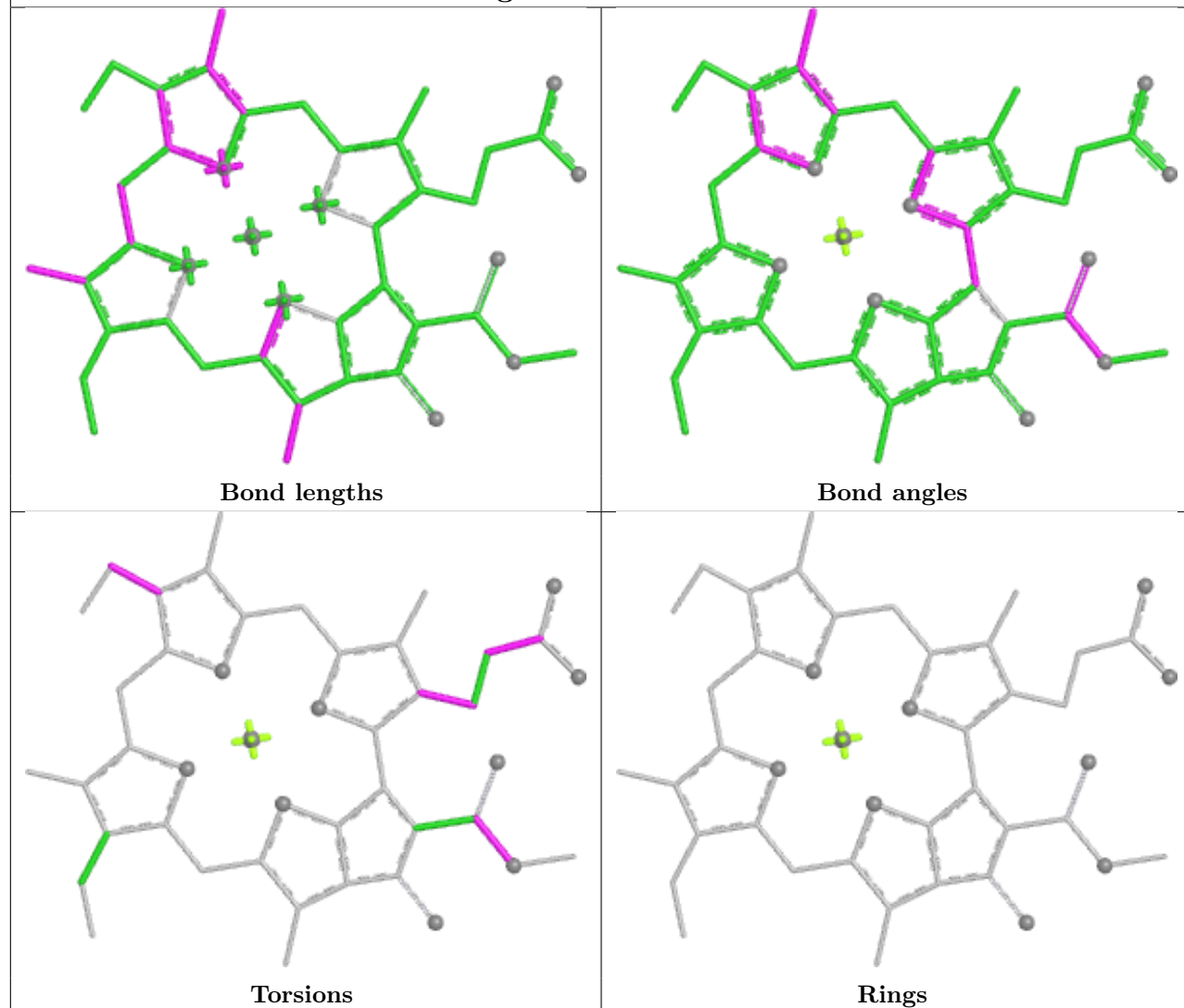




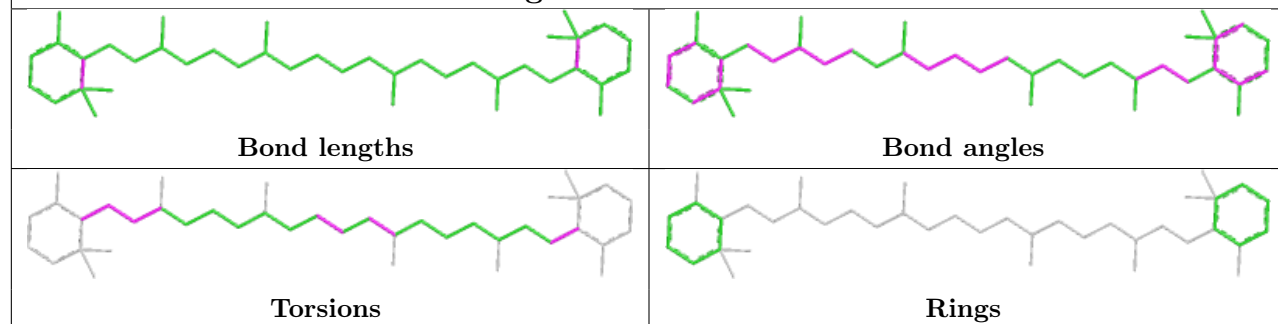


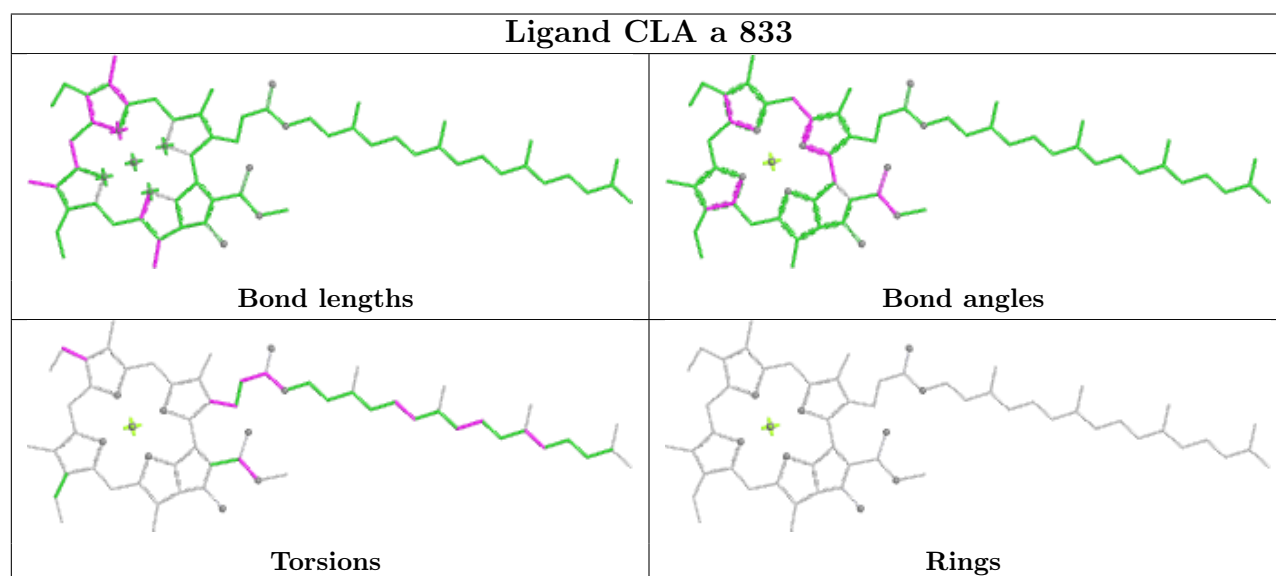
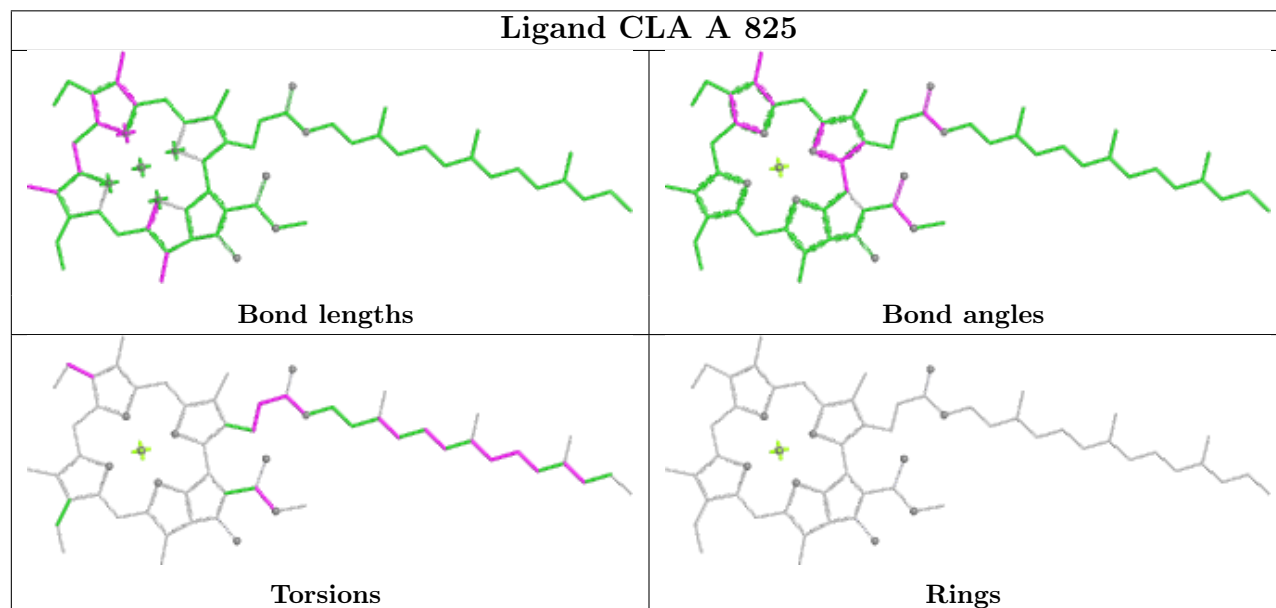
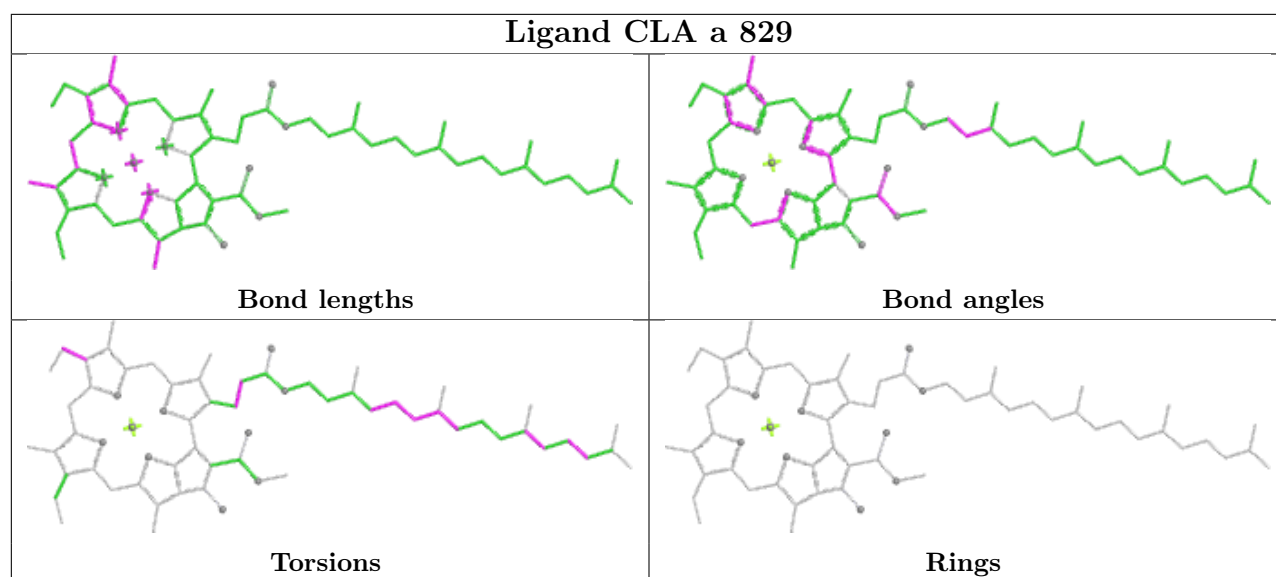


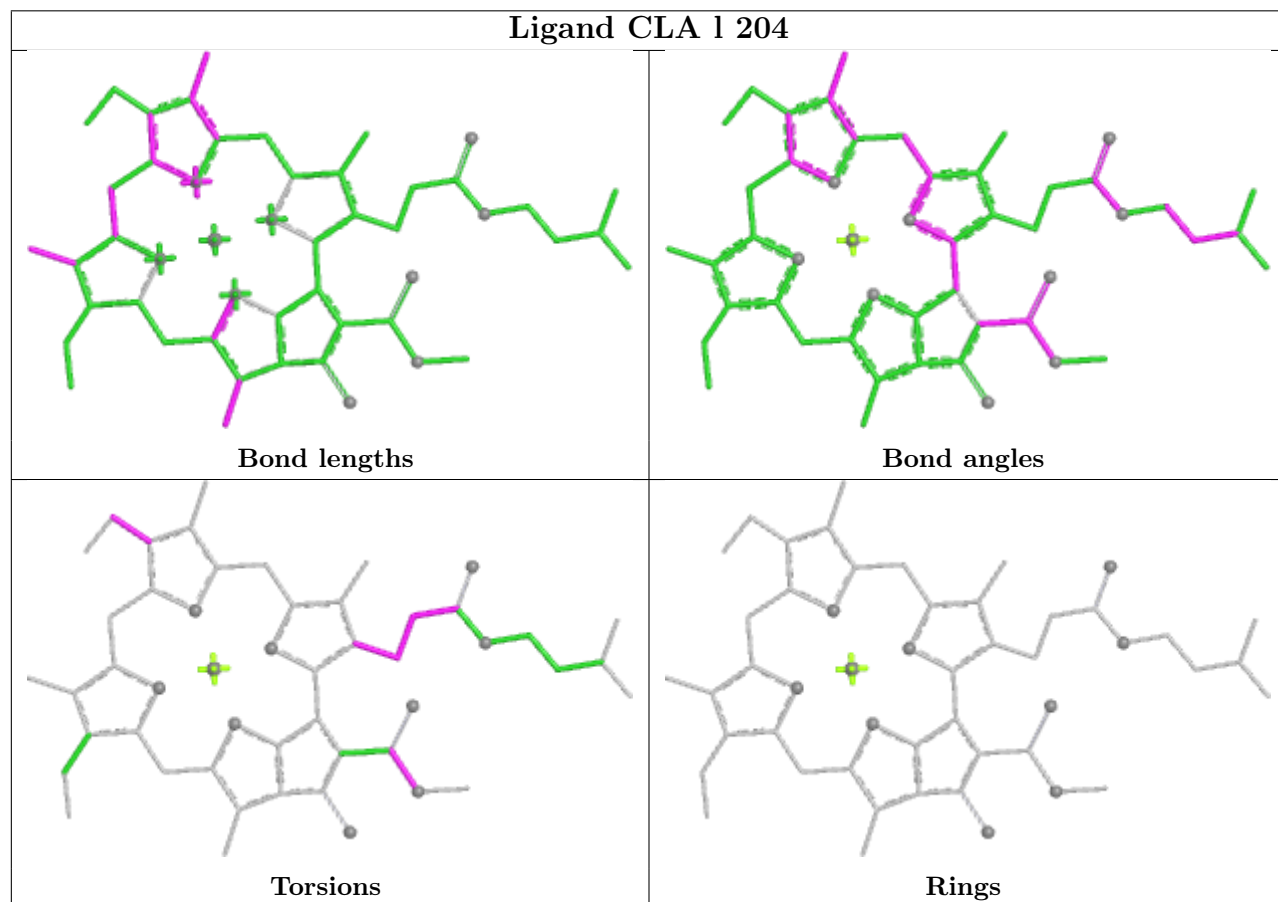
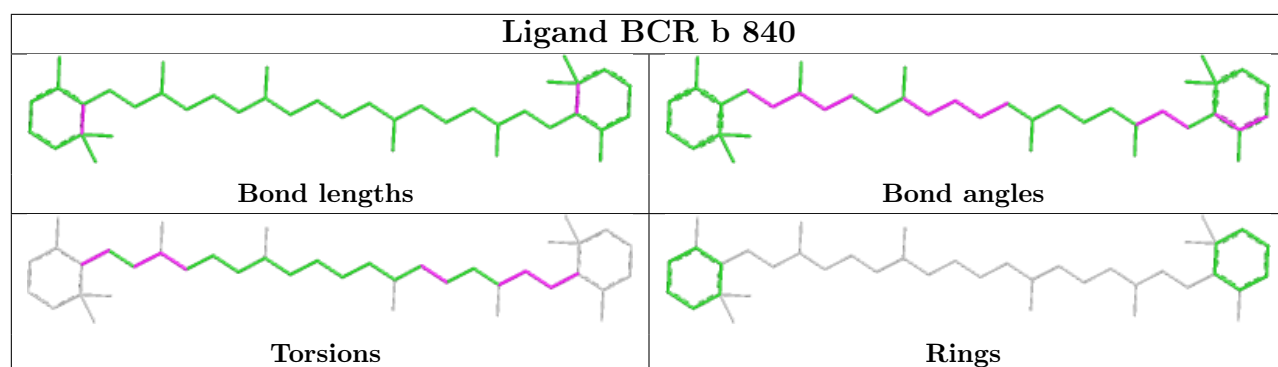
Ligand CLA 1 842



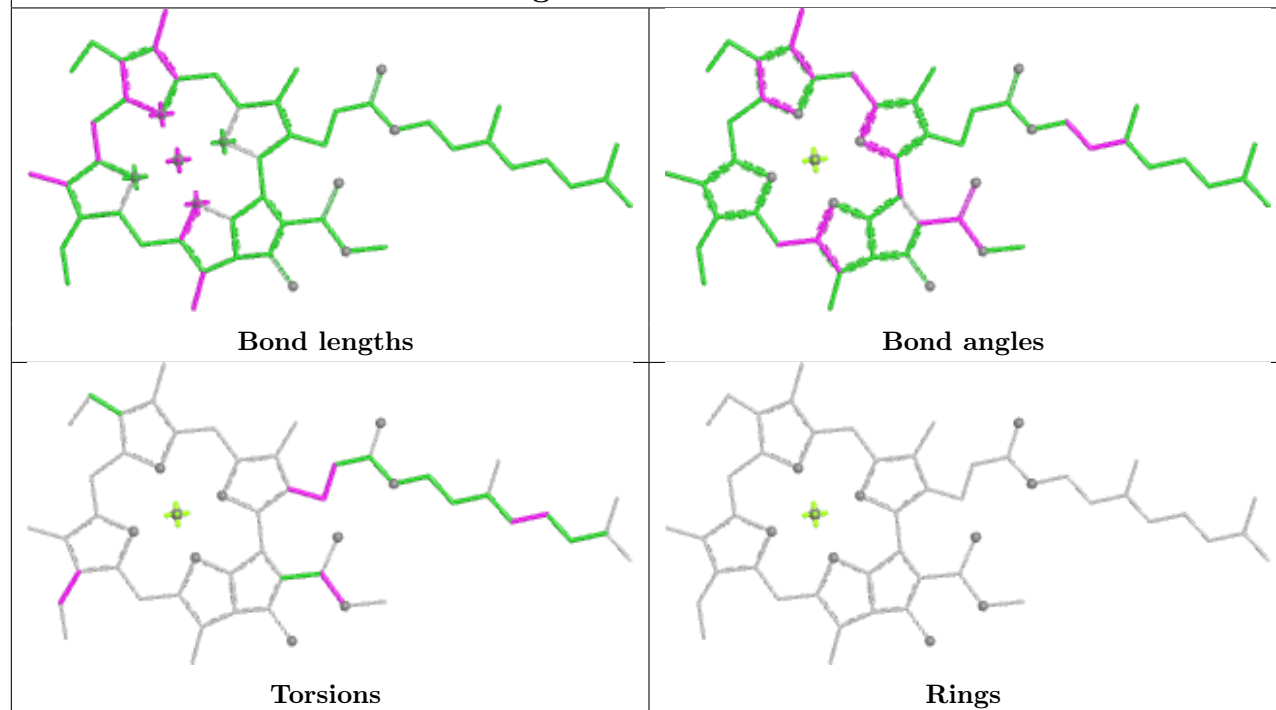
Ligand BCR 8 1104



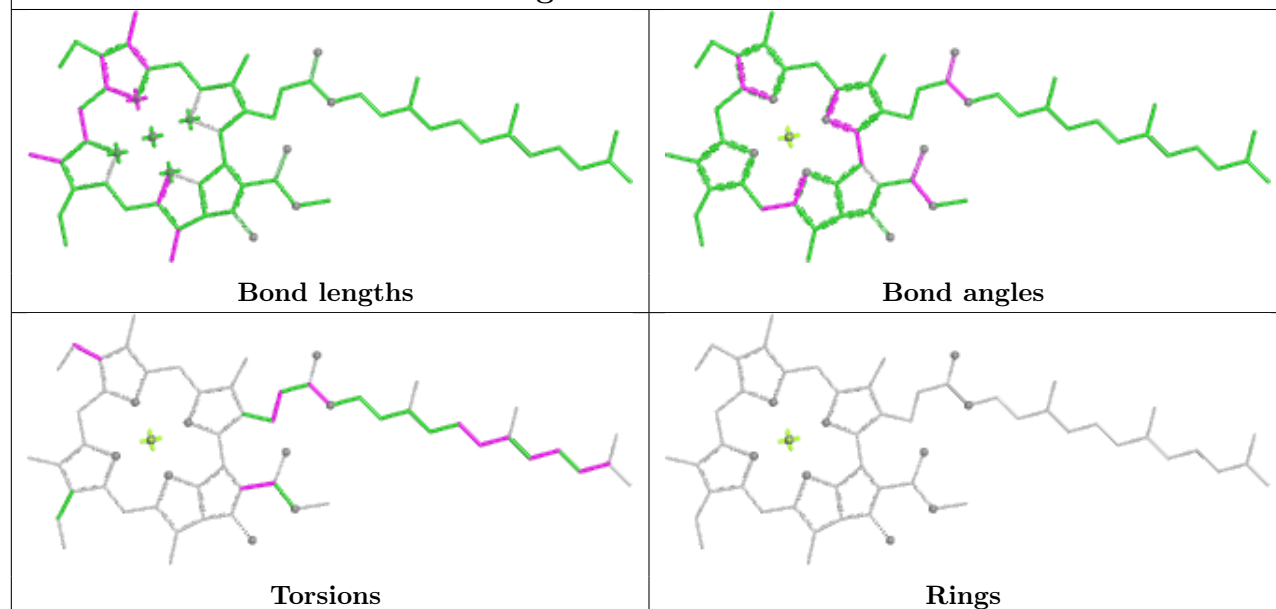




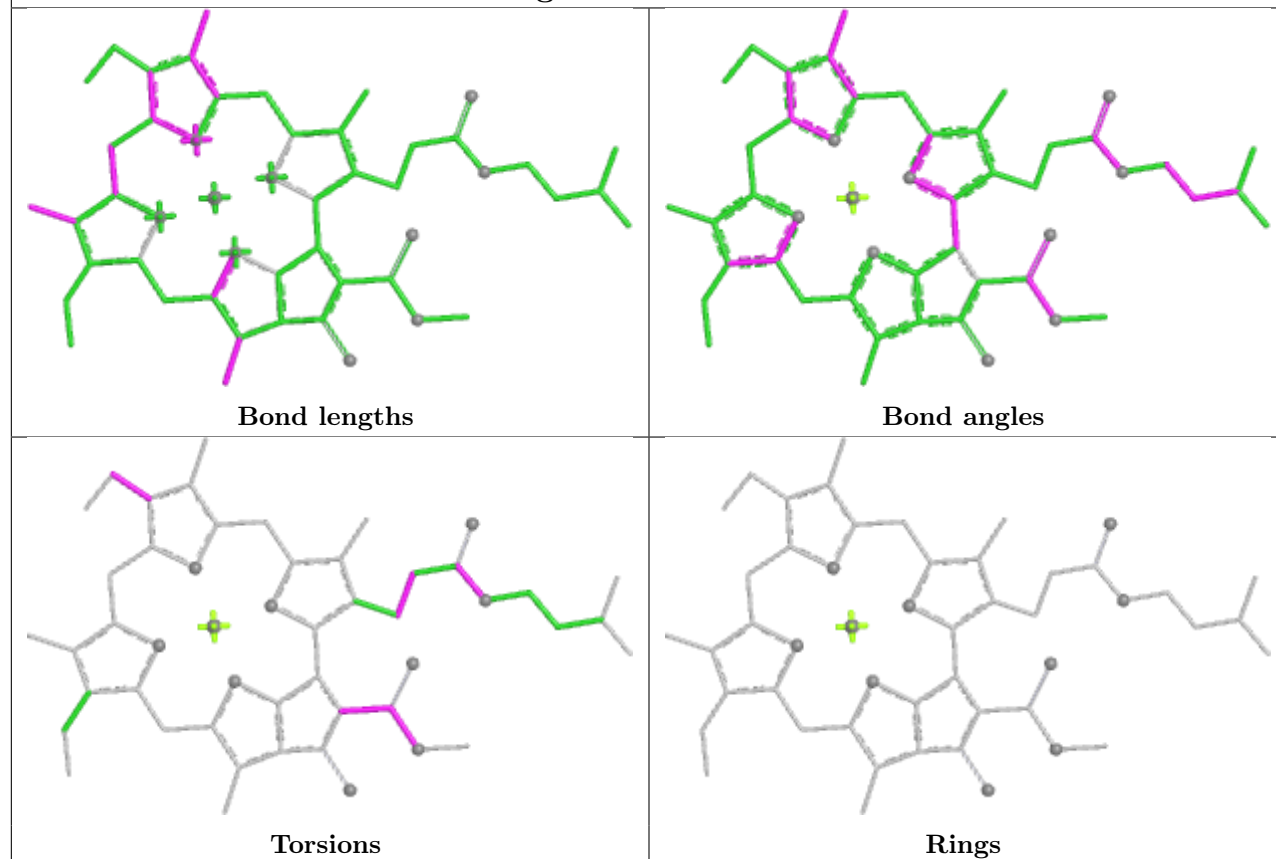
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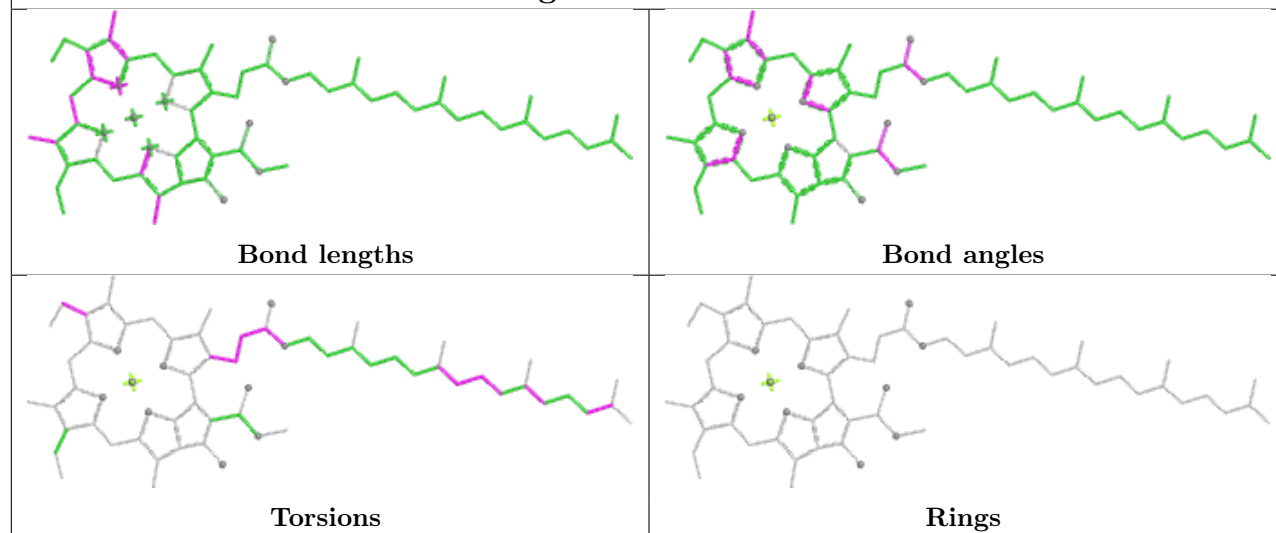
Ligand CLA 1 852

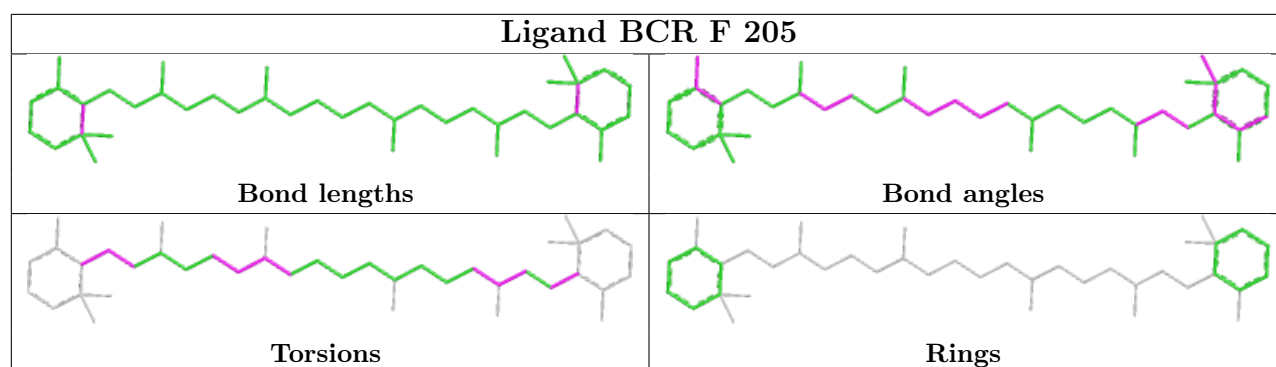
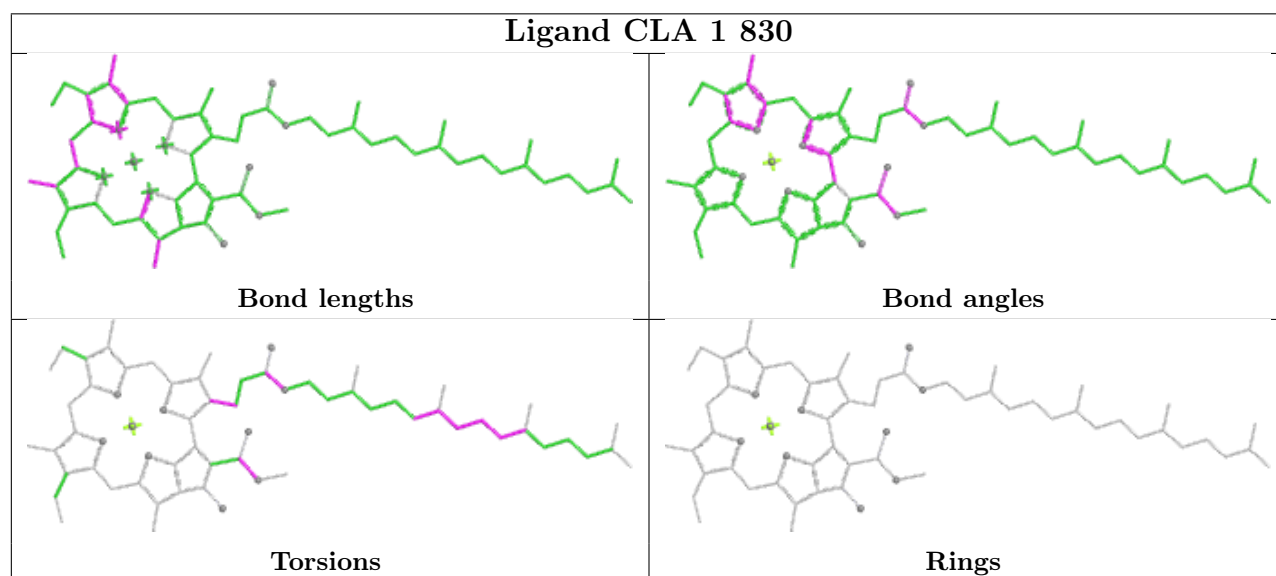
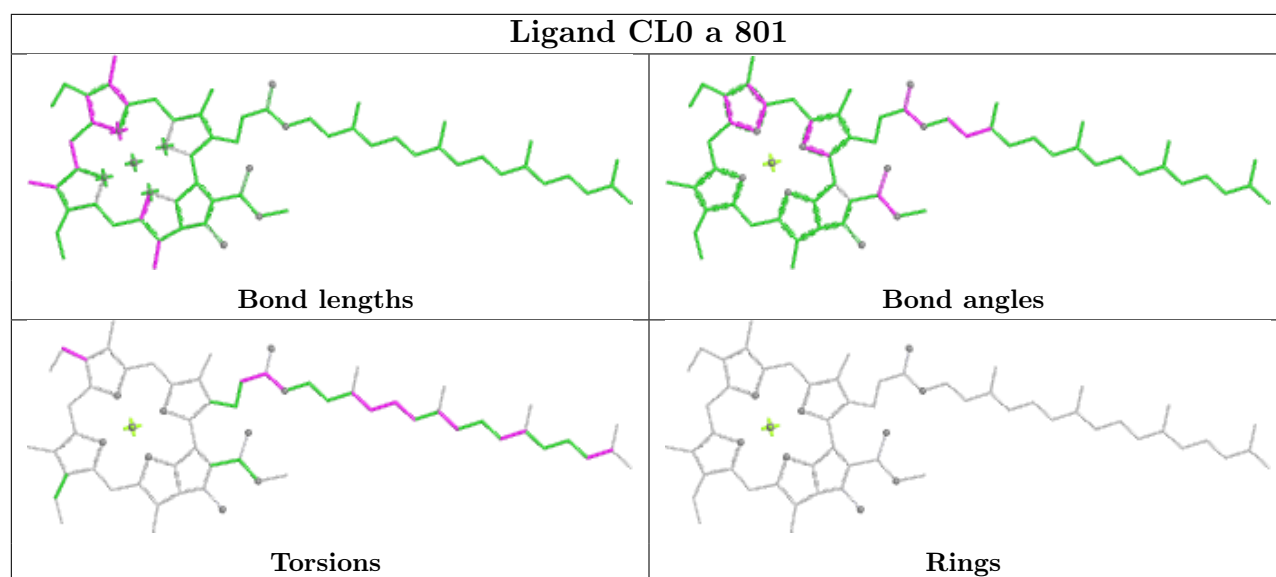


Ligand CLA a 822

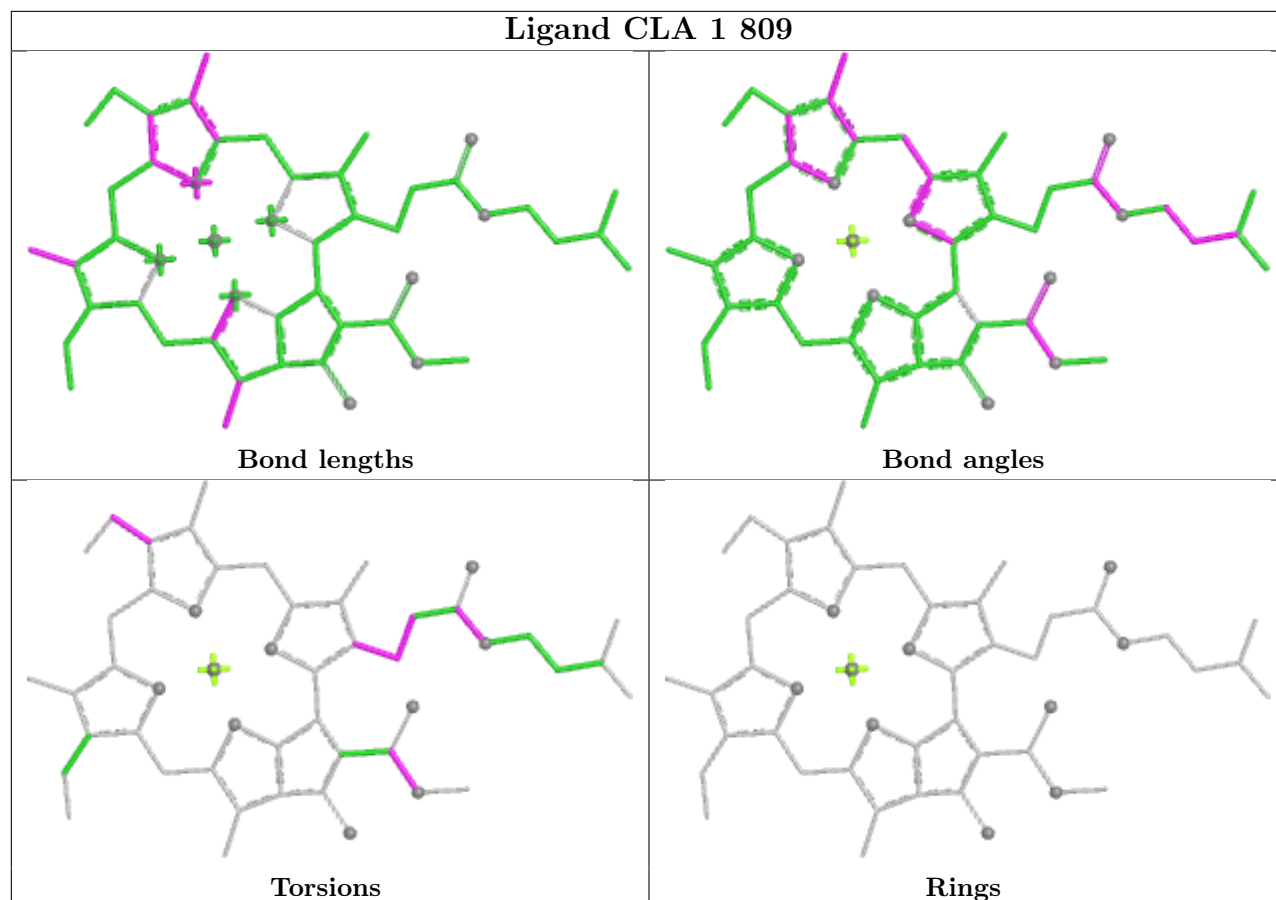


Ligand CLA I 101

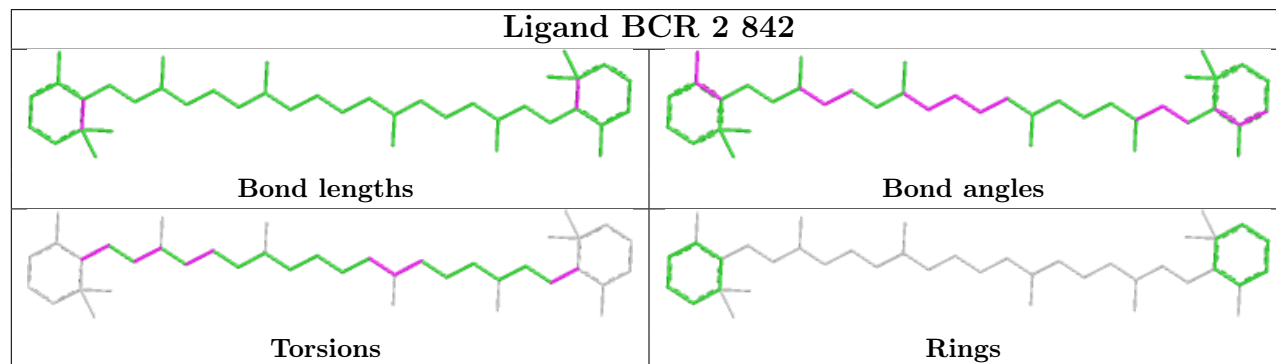


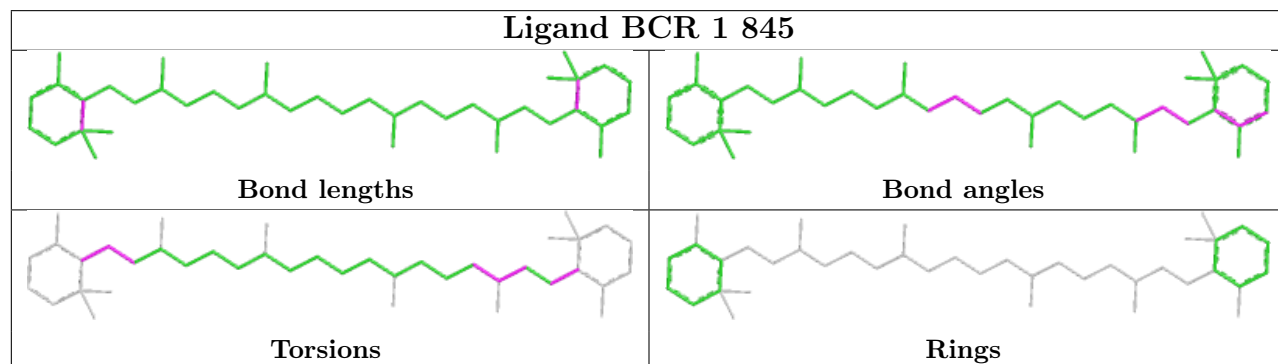
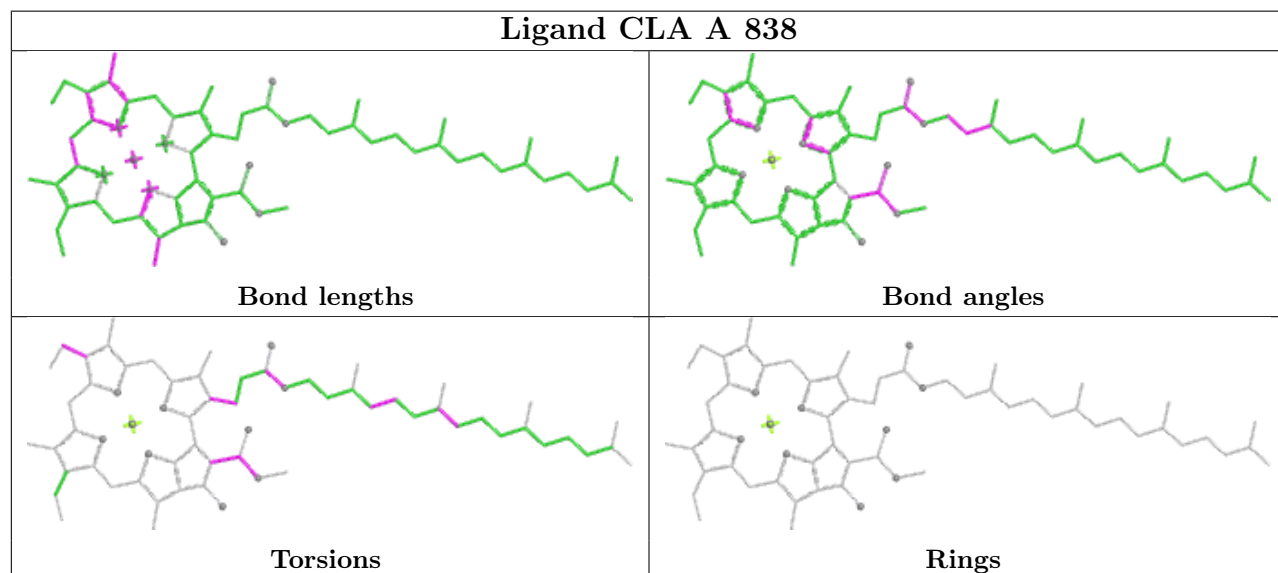
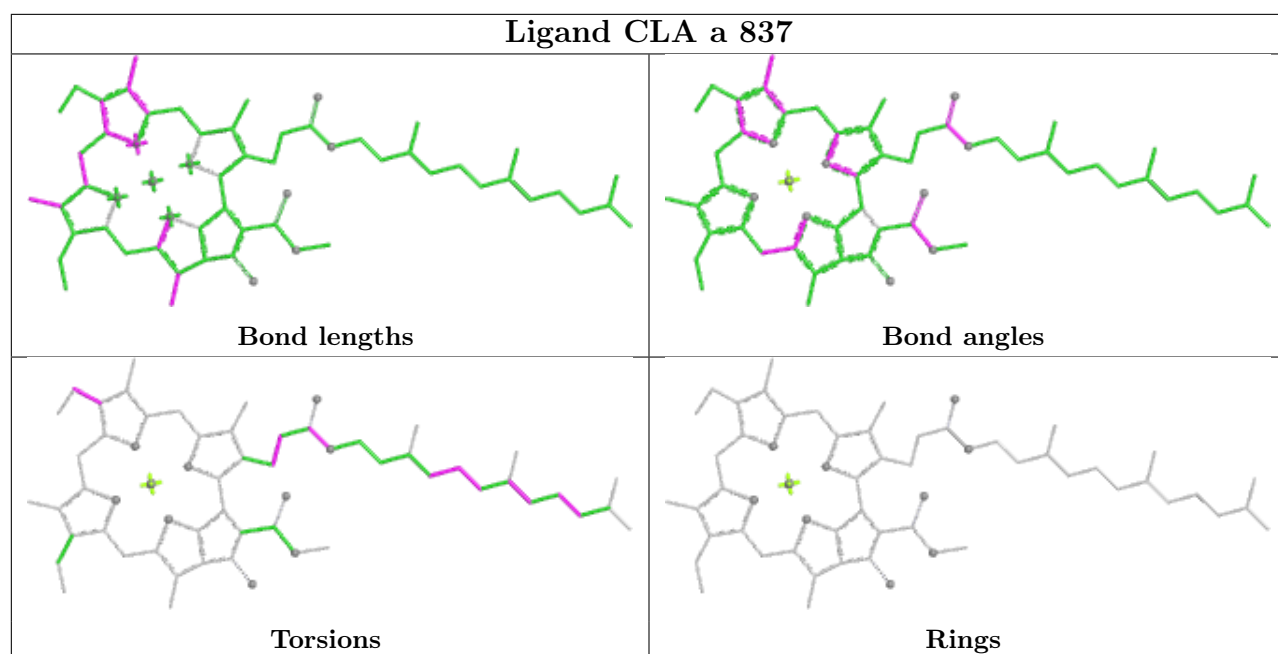


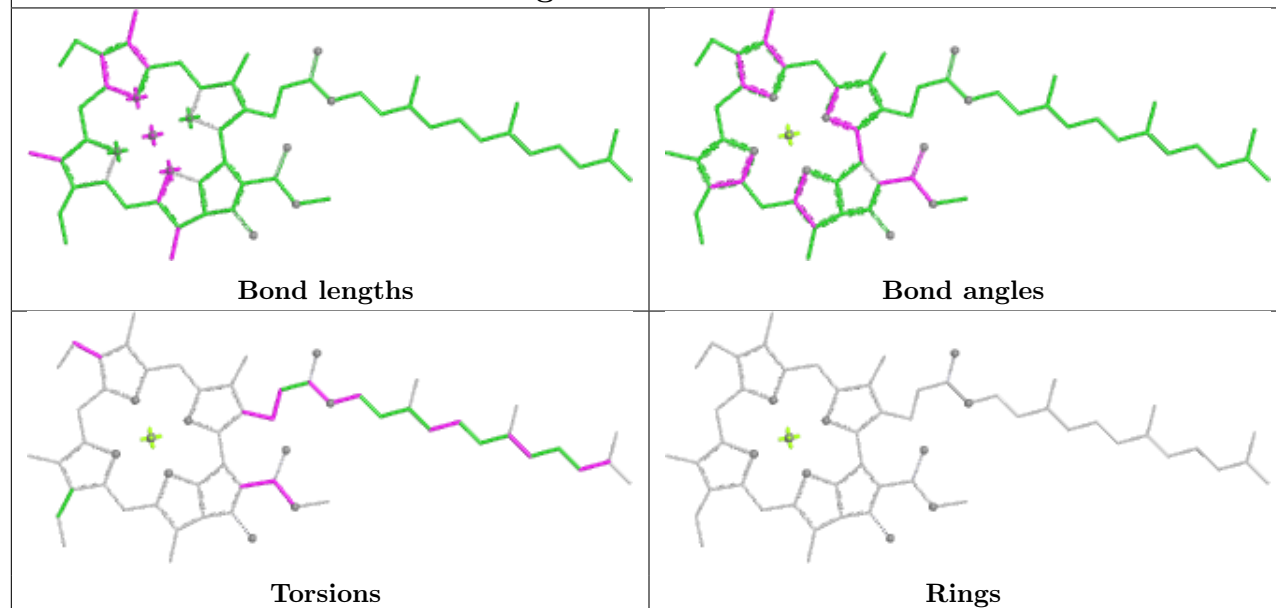
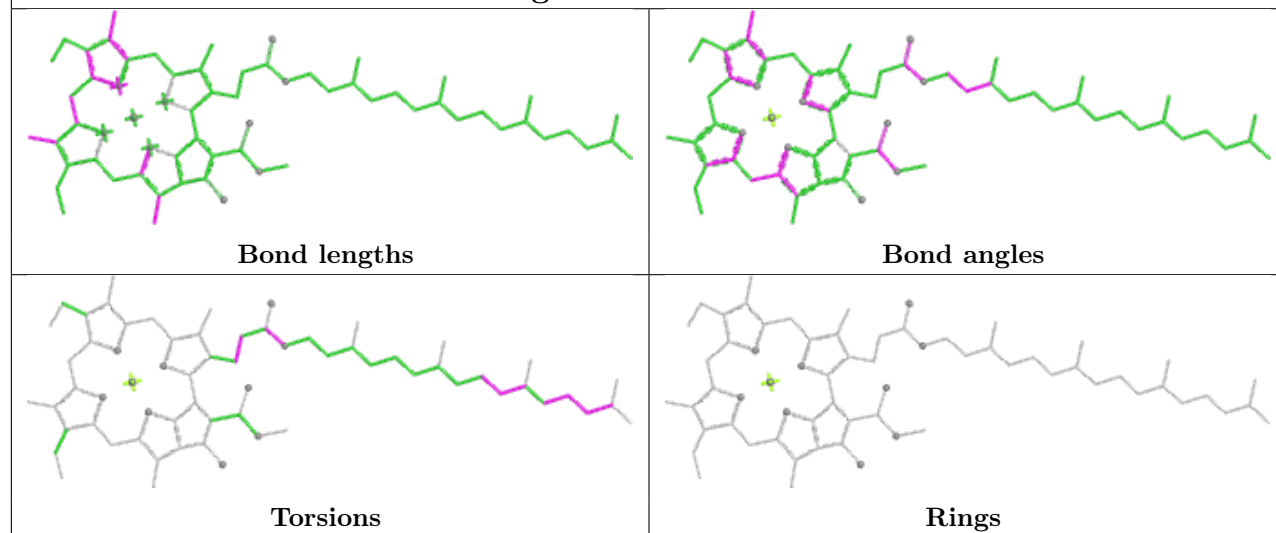
Ligand CLA 1 809

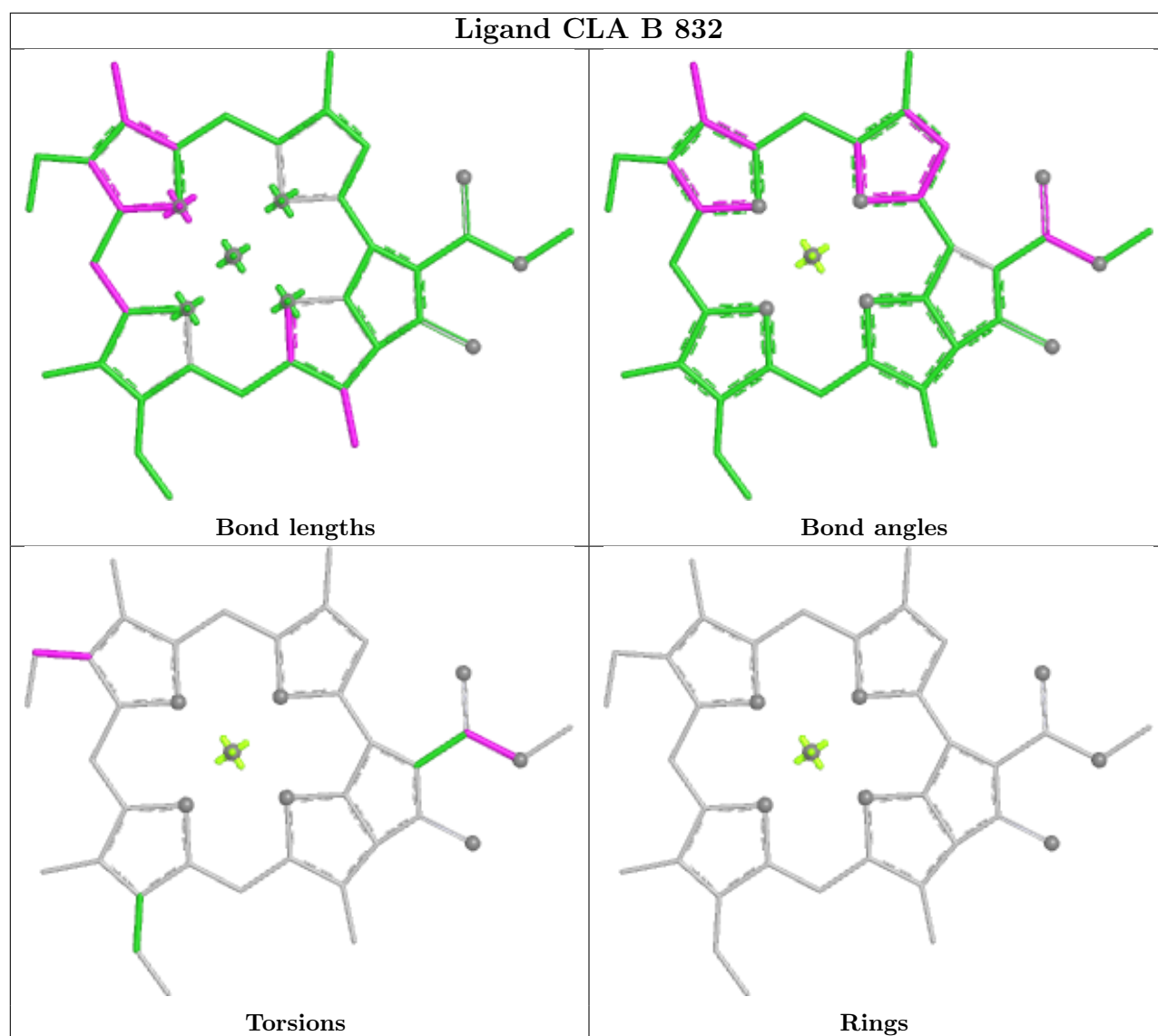


Ligand BCR 2 842

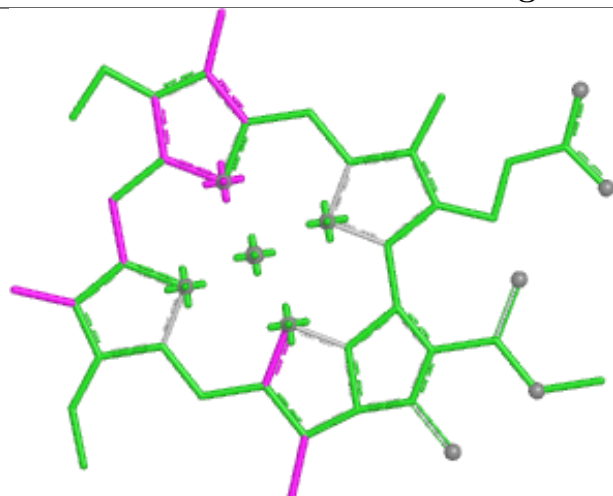




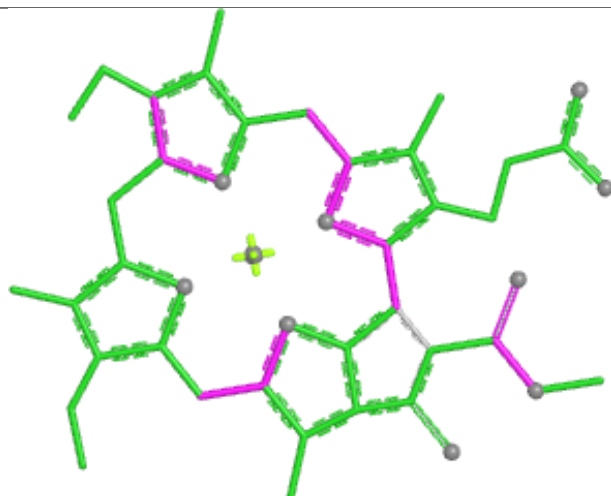
Ligand CLA 2 825**Ligand CLA A 839**



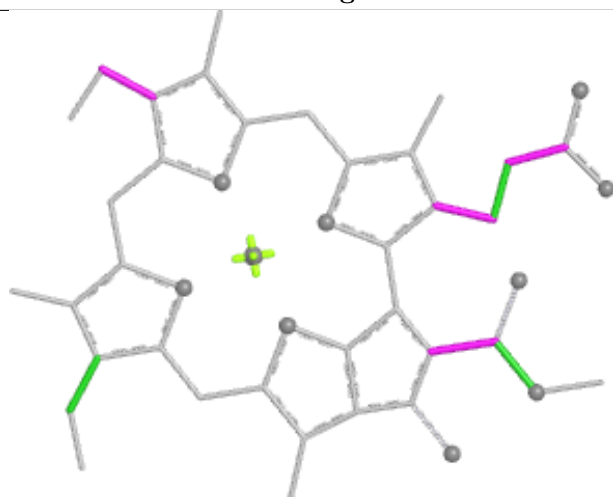
Ligand CLA 2 826



Bond lengths



Bond angles

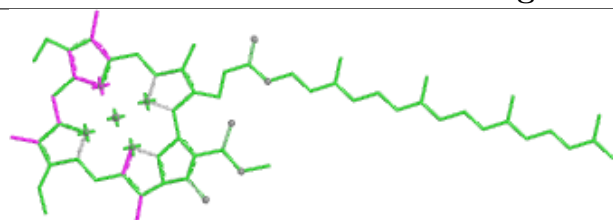


Torsions

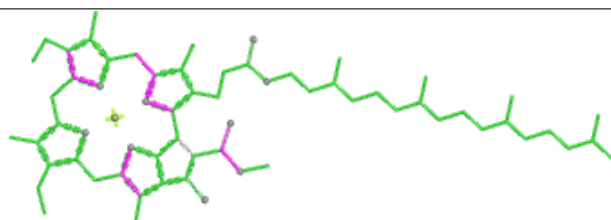


Rings

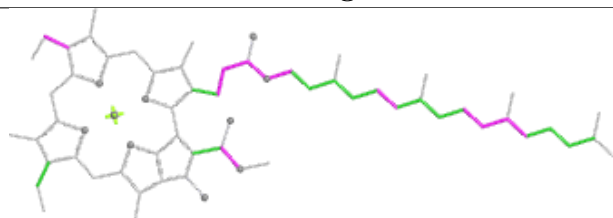
Ligand CLA b 807



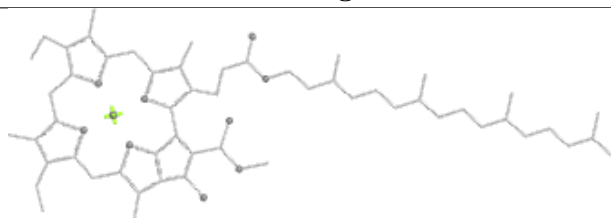
Bond lengths



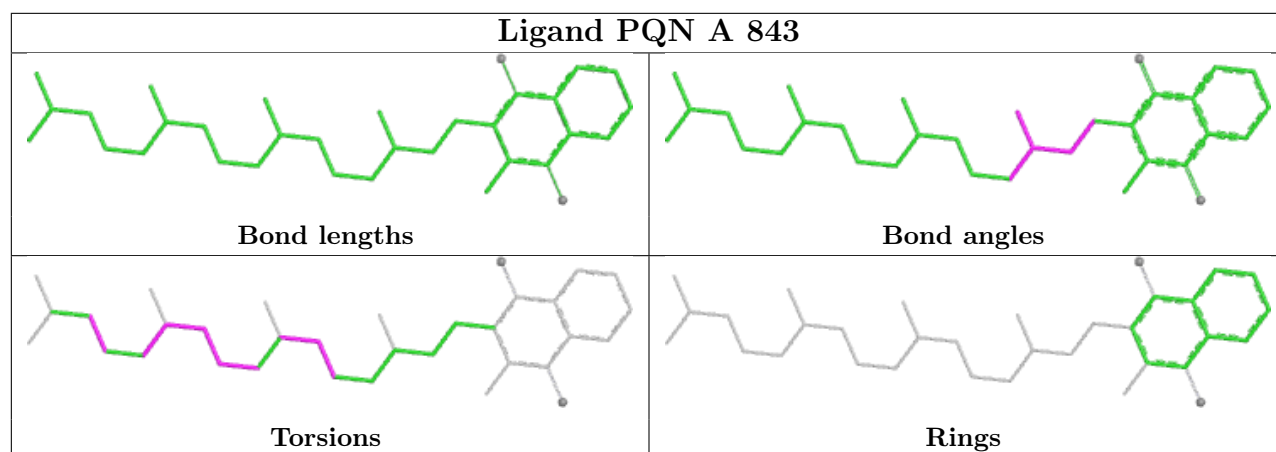
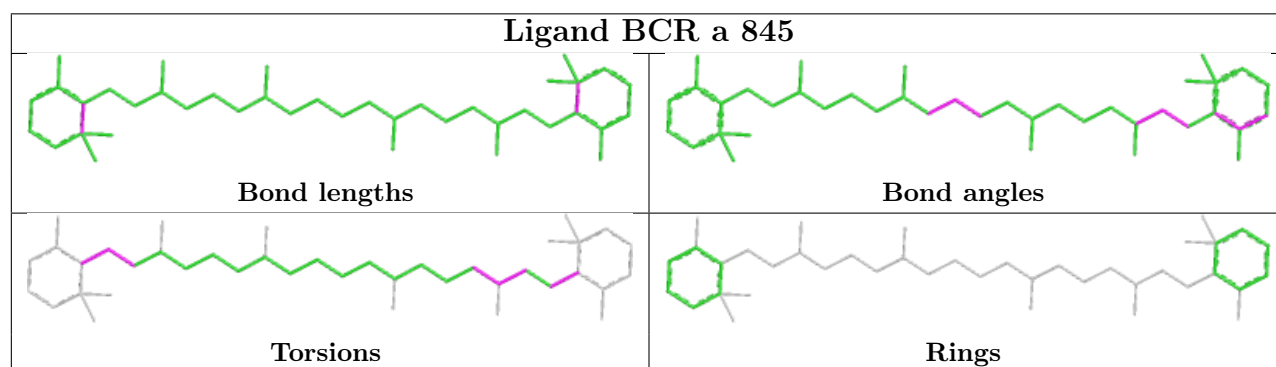
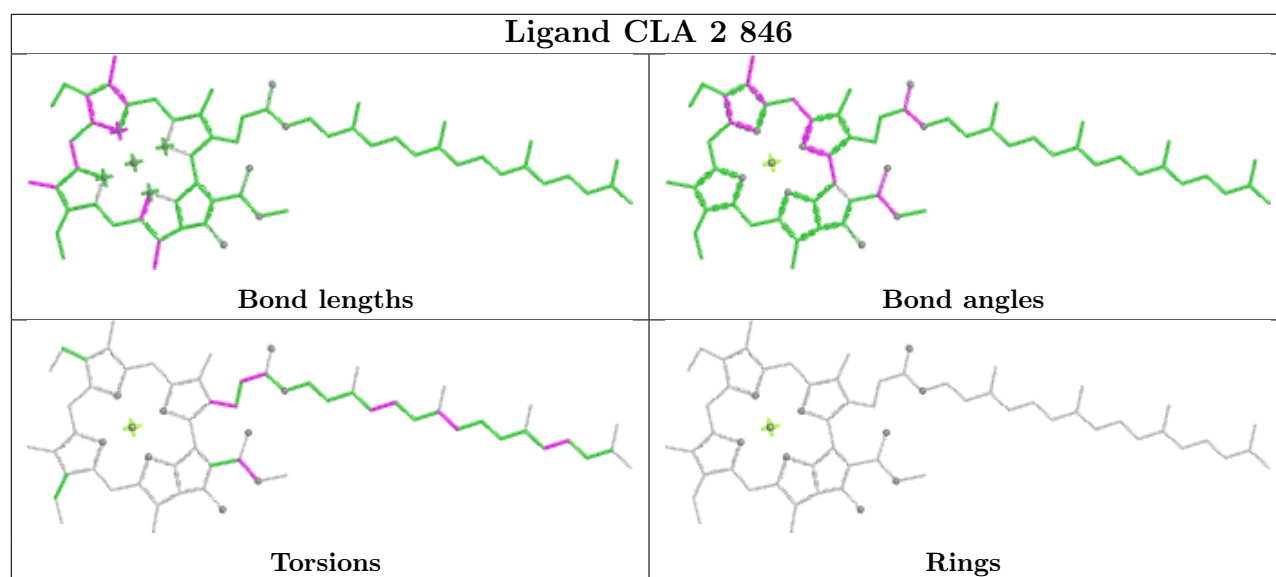
Bond angles

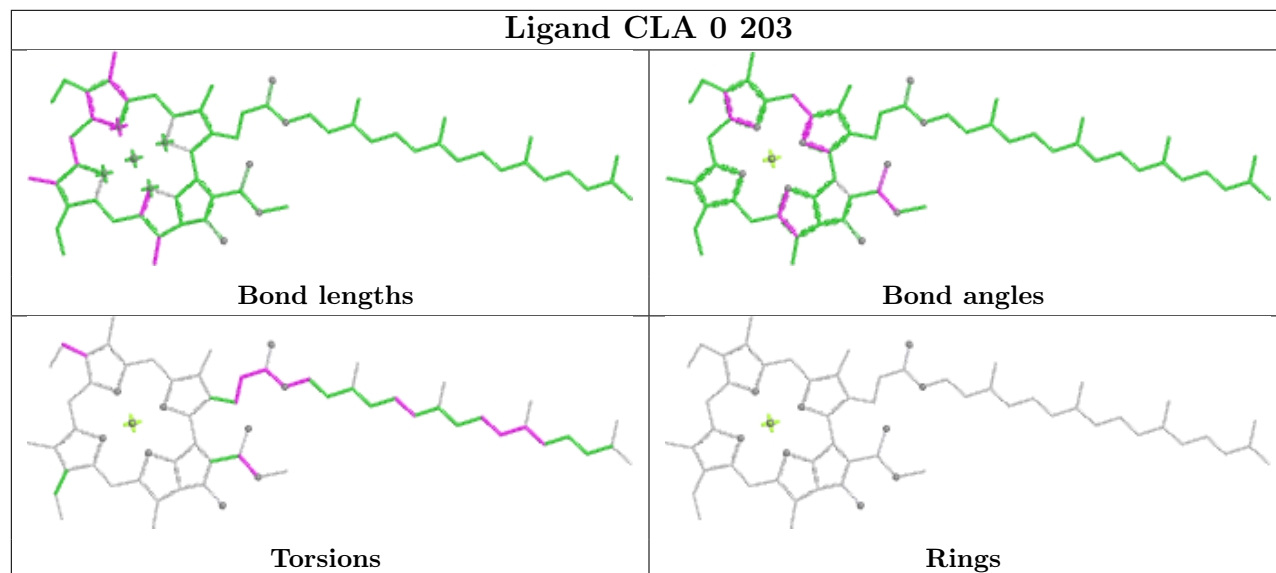
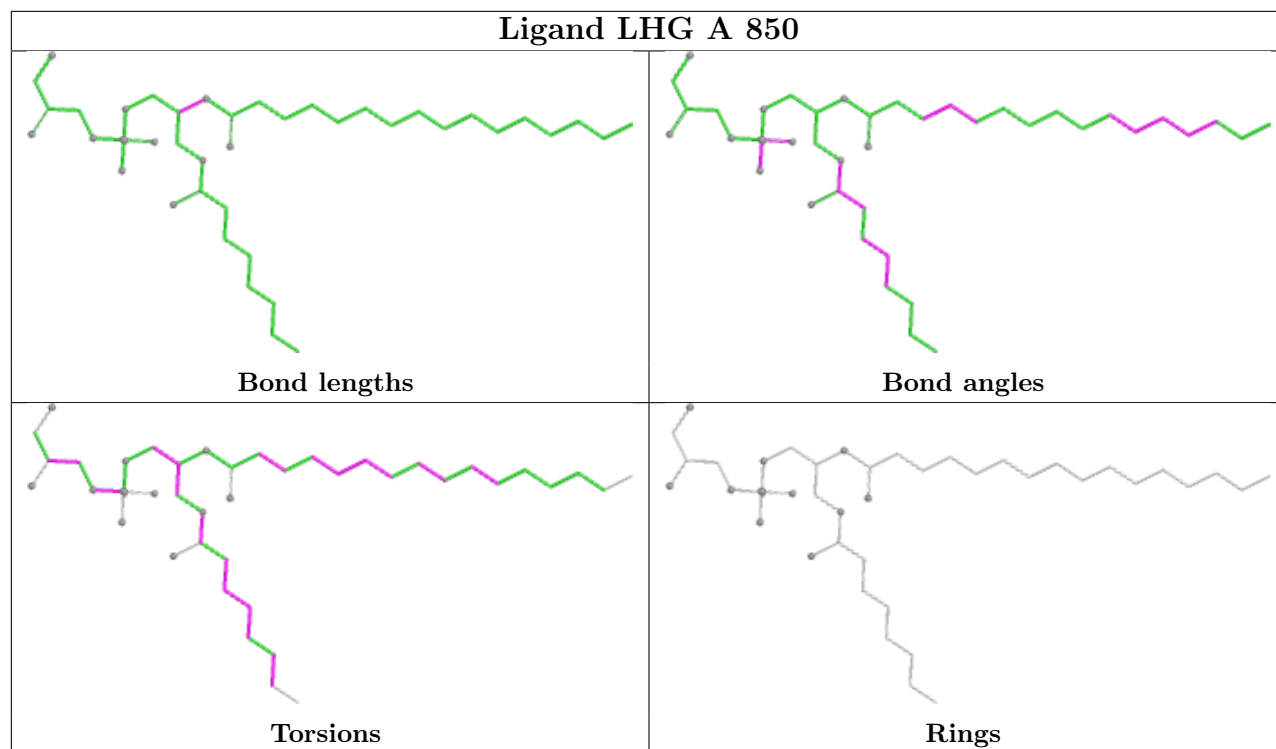


Torsions

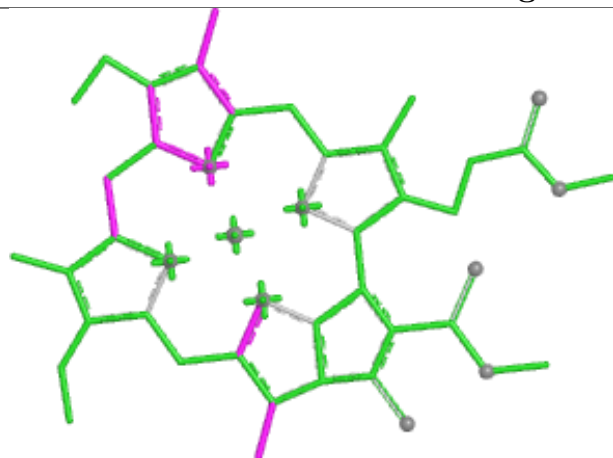


Rings

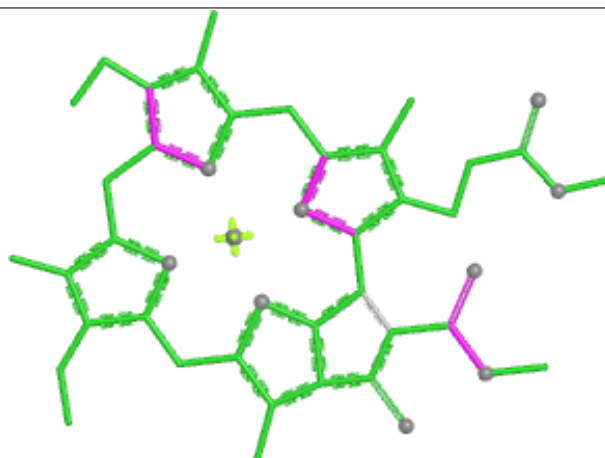




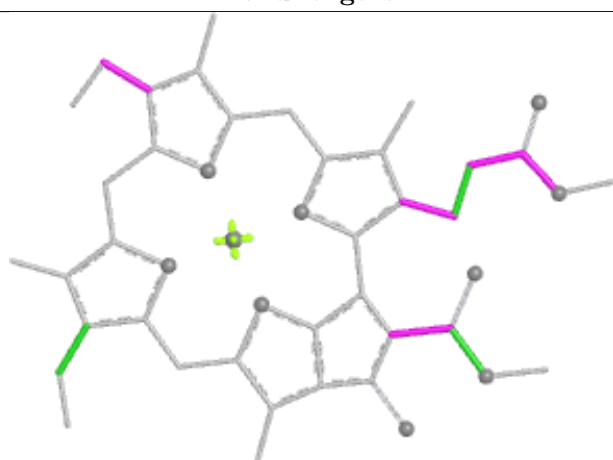
Ligand CLA 1 816



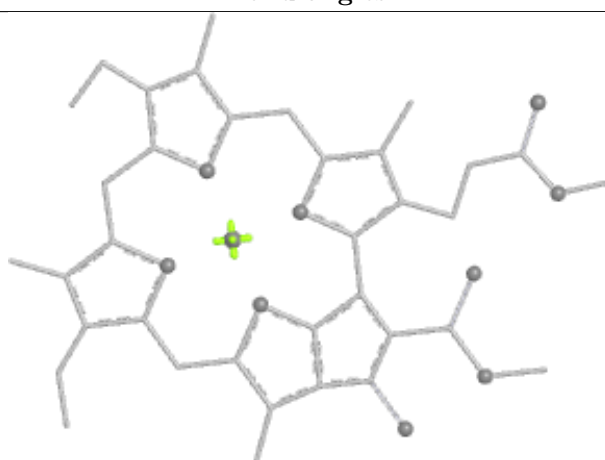
Bond lengths



Bond angles

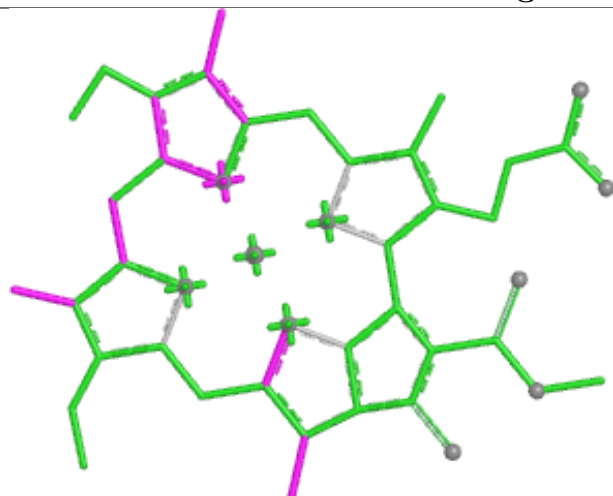


Torsions

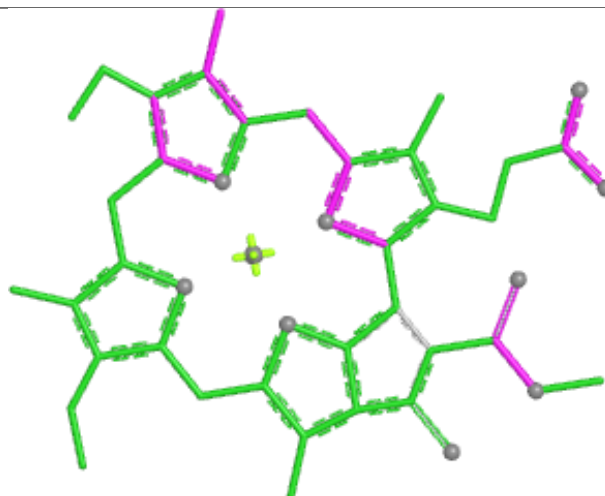


Rings

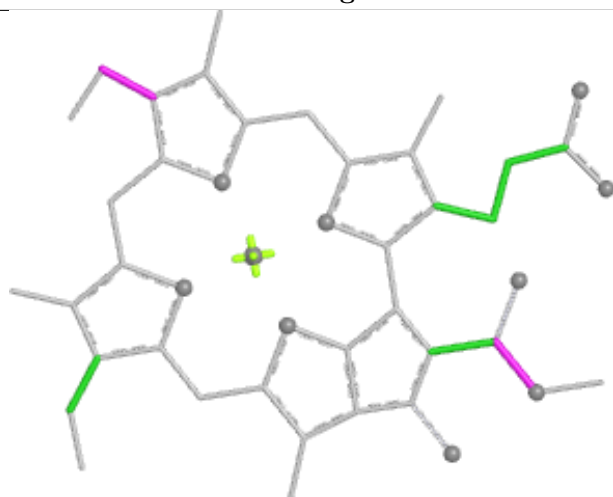
Ligand CLA b 812



Bond lengths



Bond angles

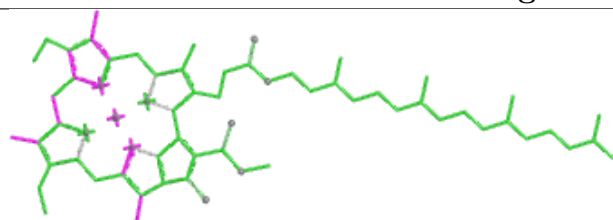


Torsions

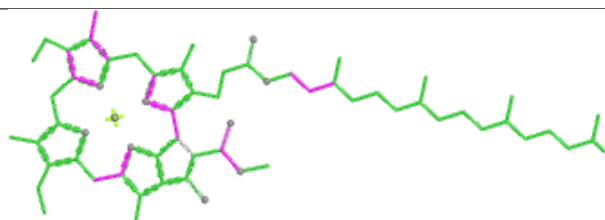


Rings

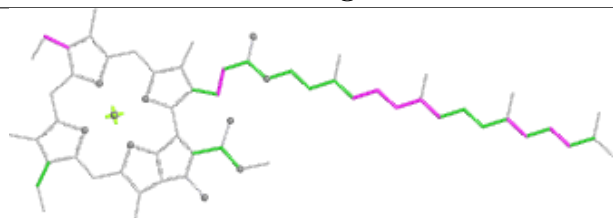
Ligand CLA 1 829



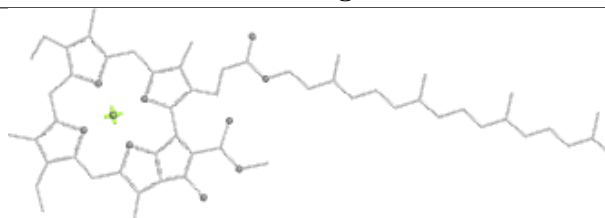
Bond lengths



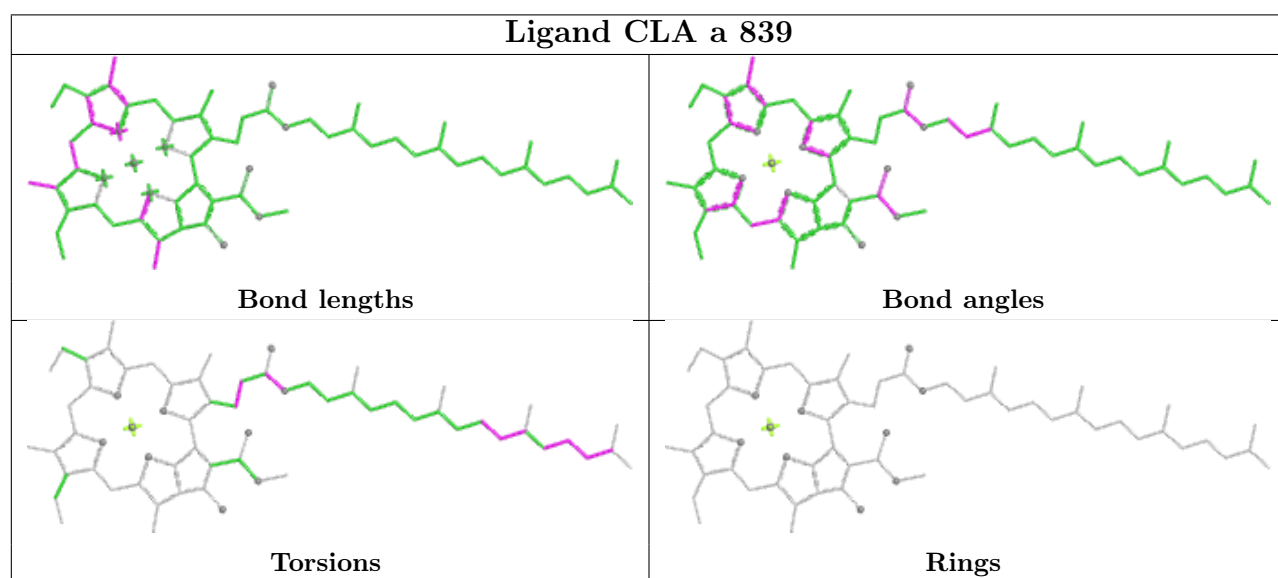
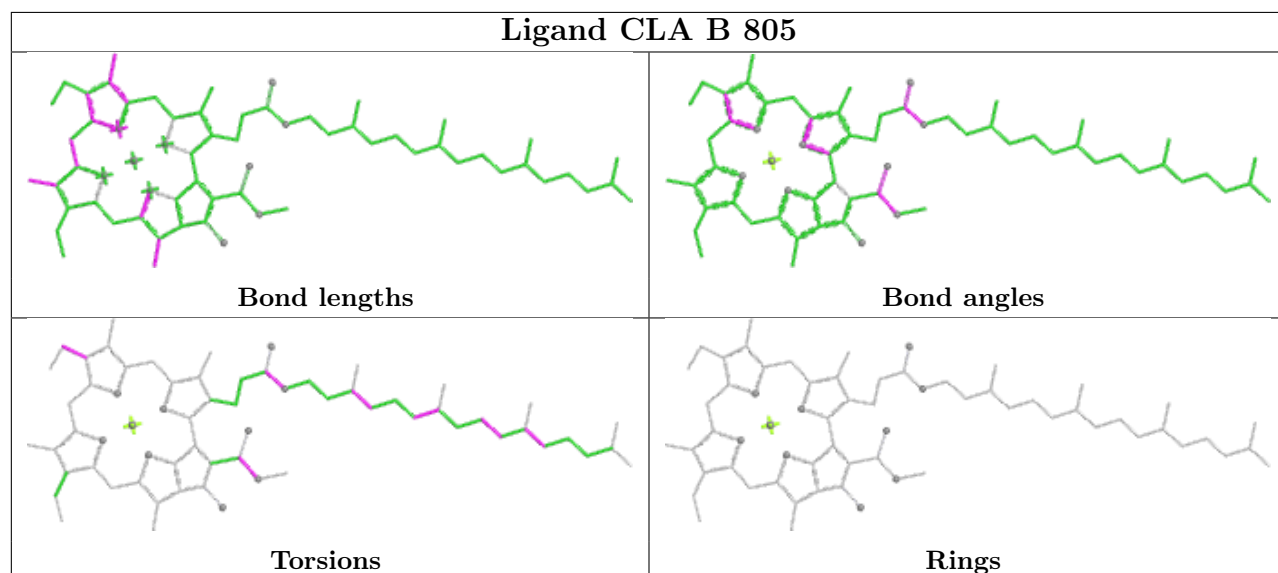
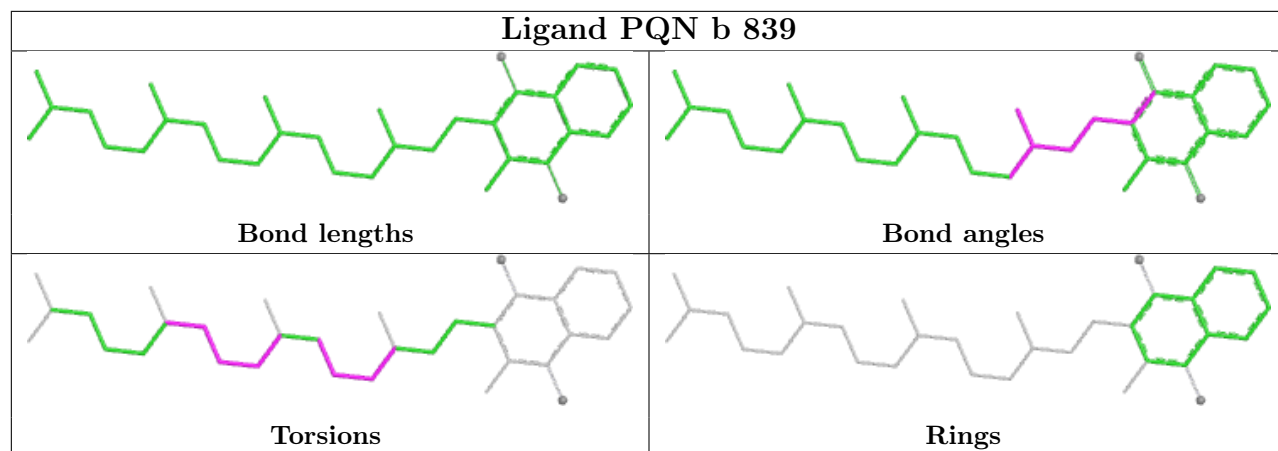
Bond angles

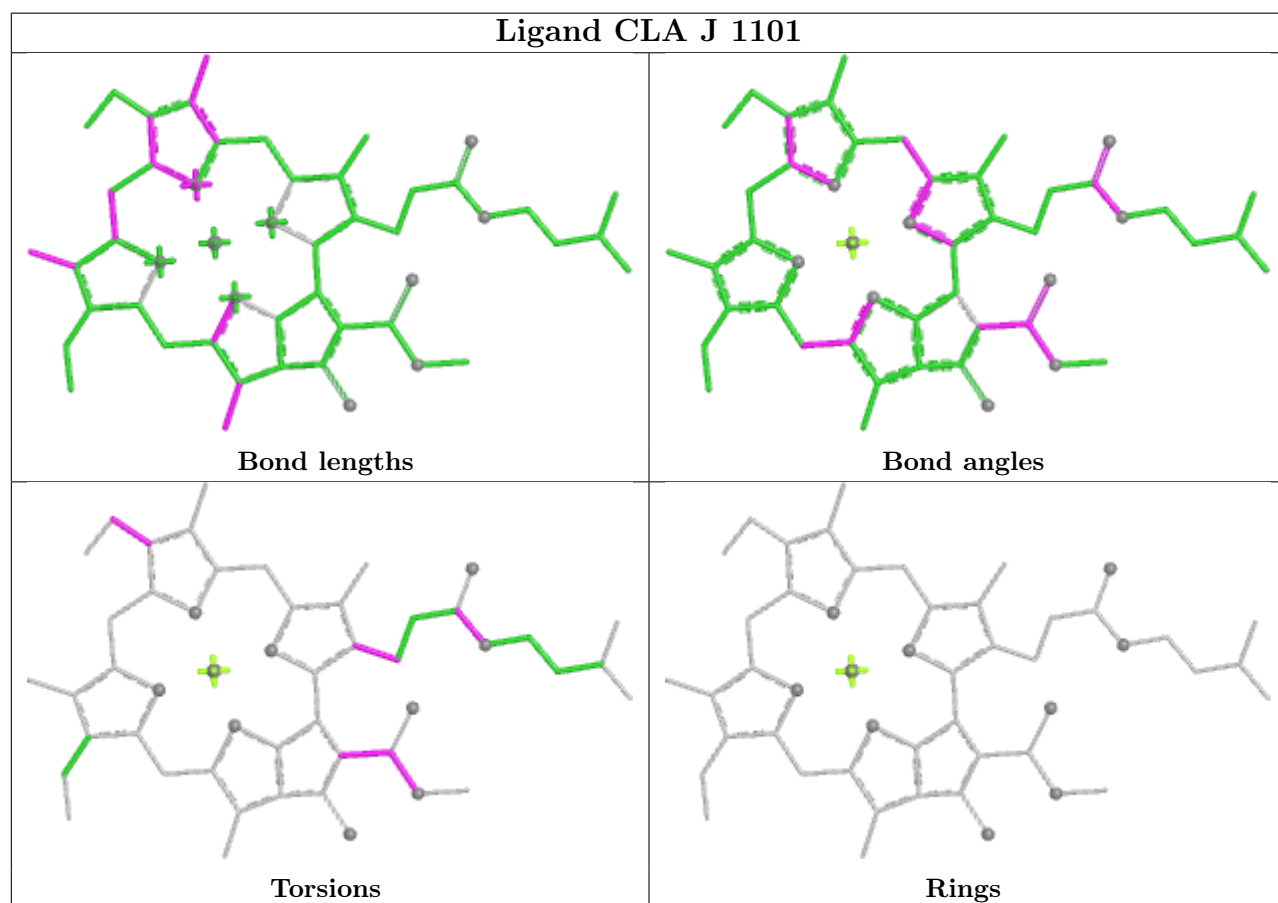
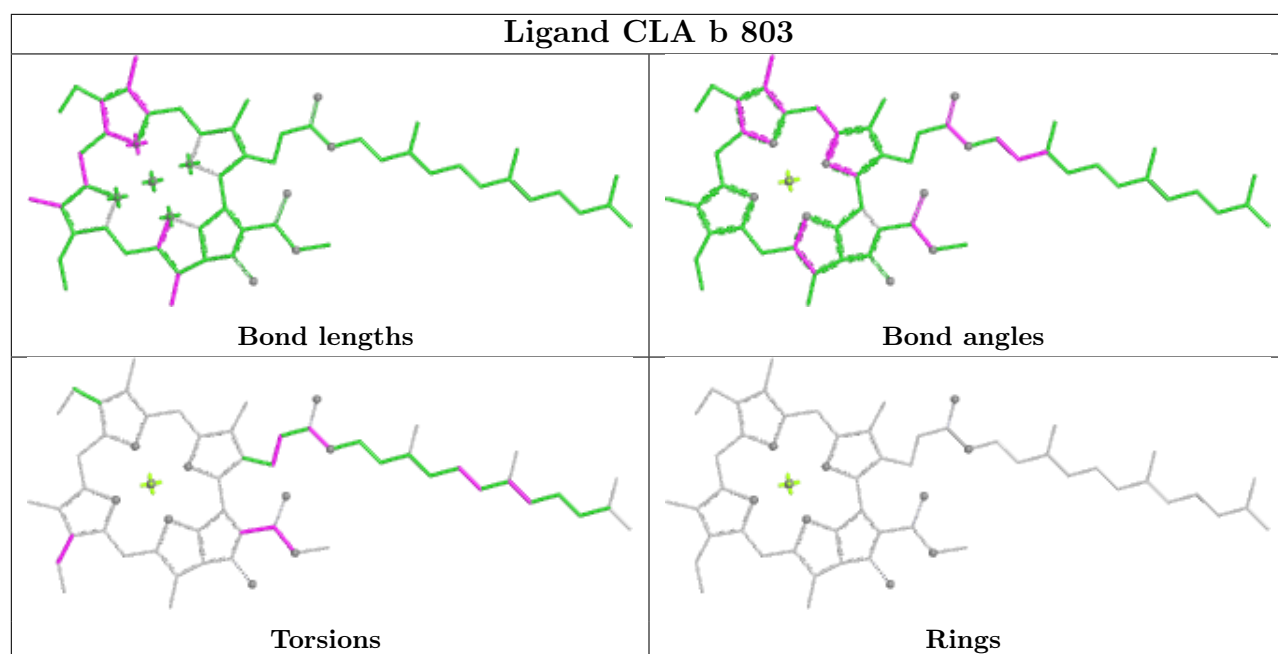


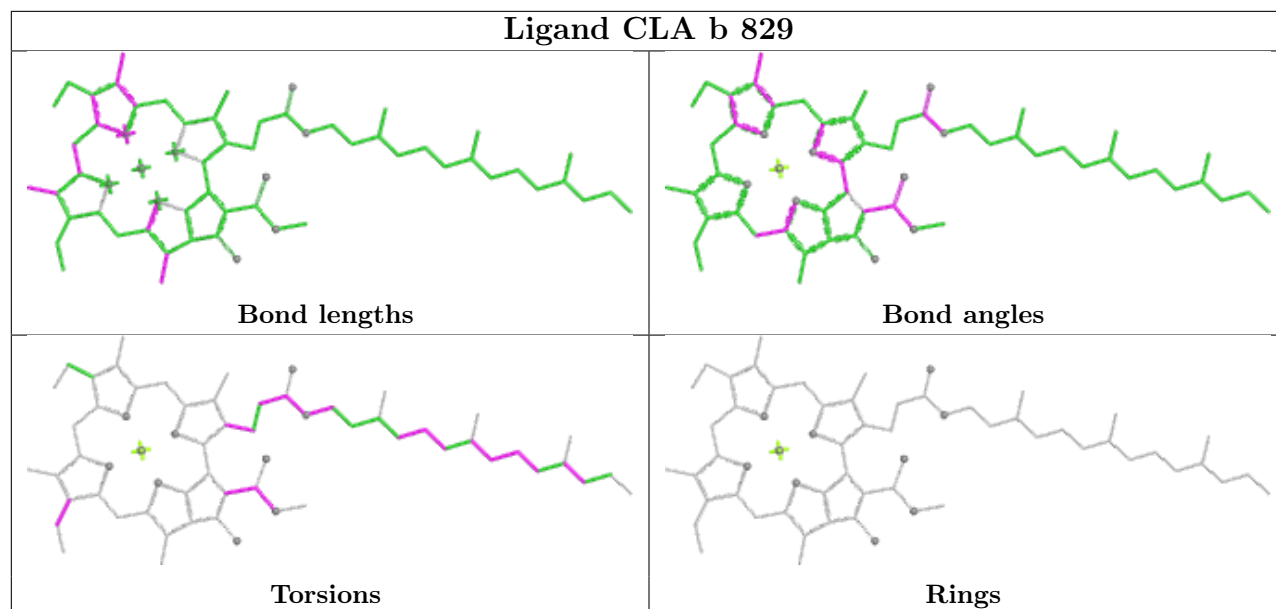
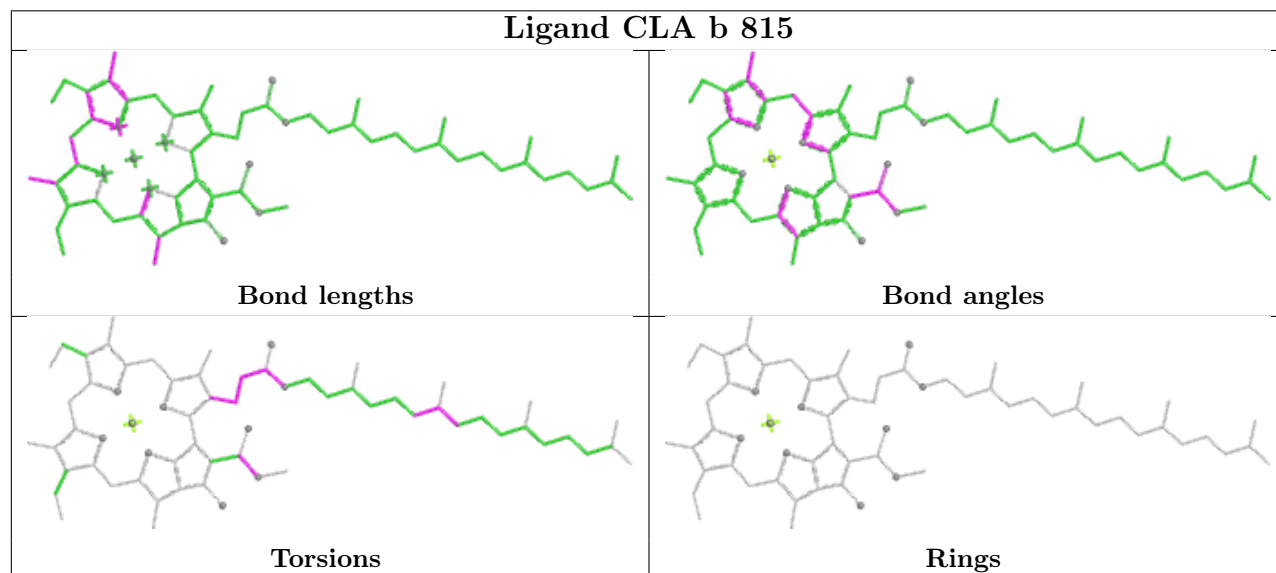
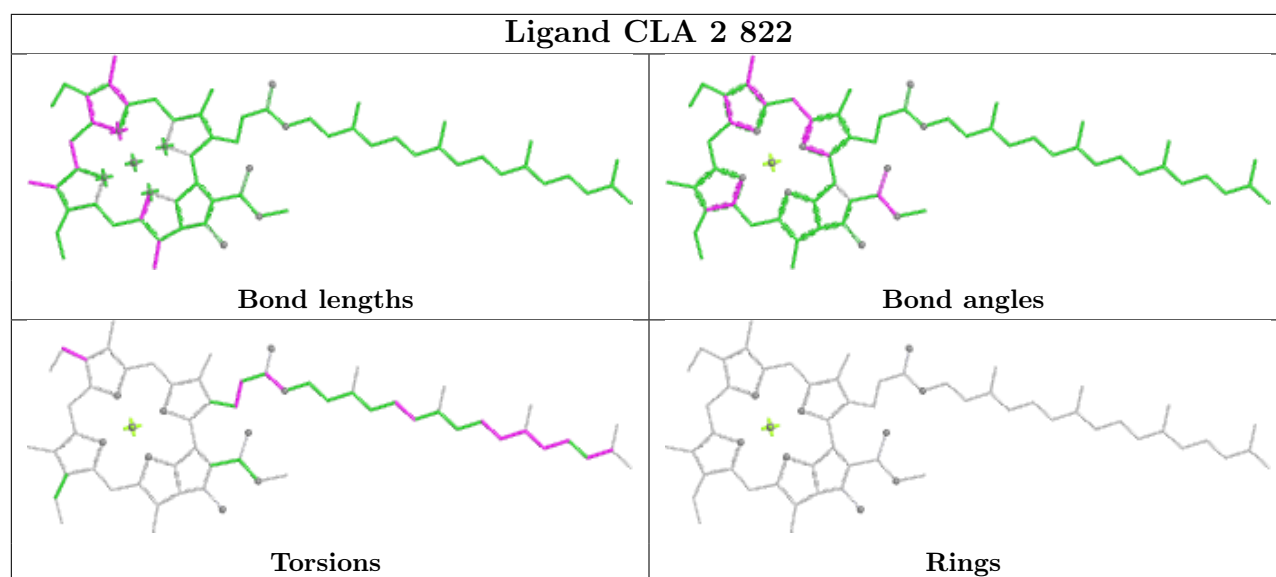
Torsions



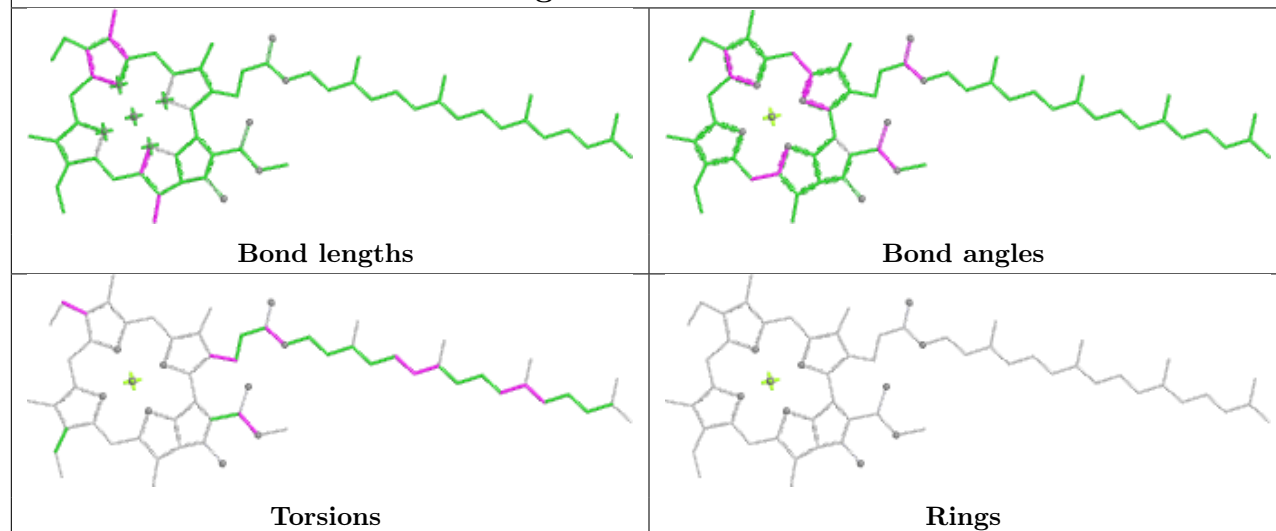
Rings



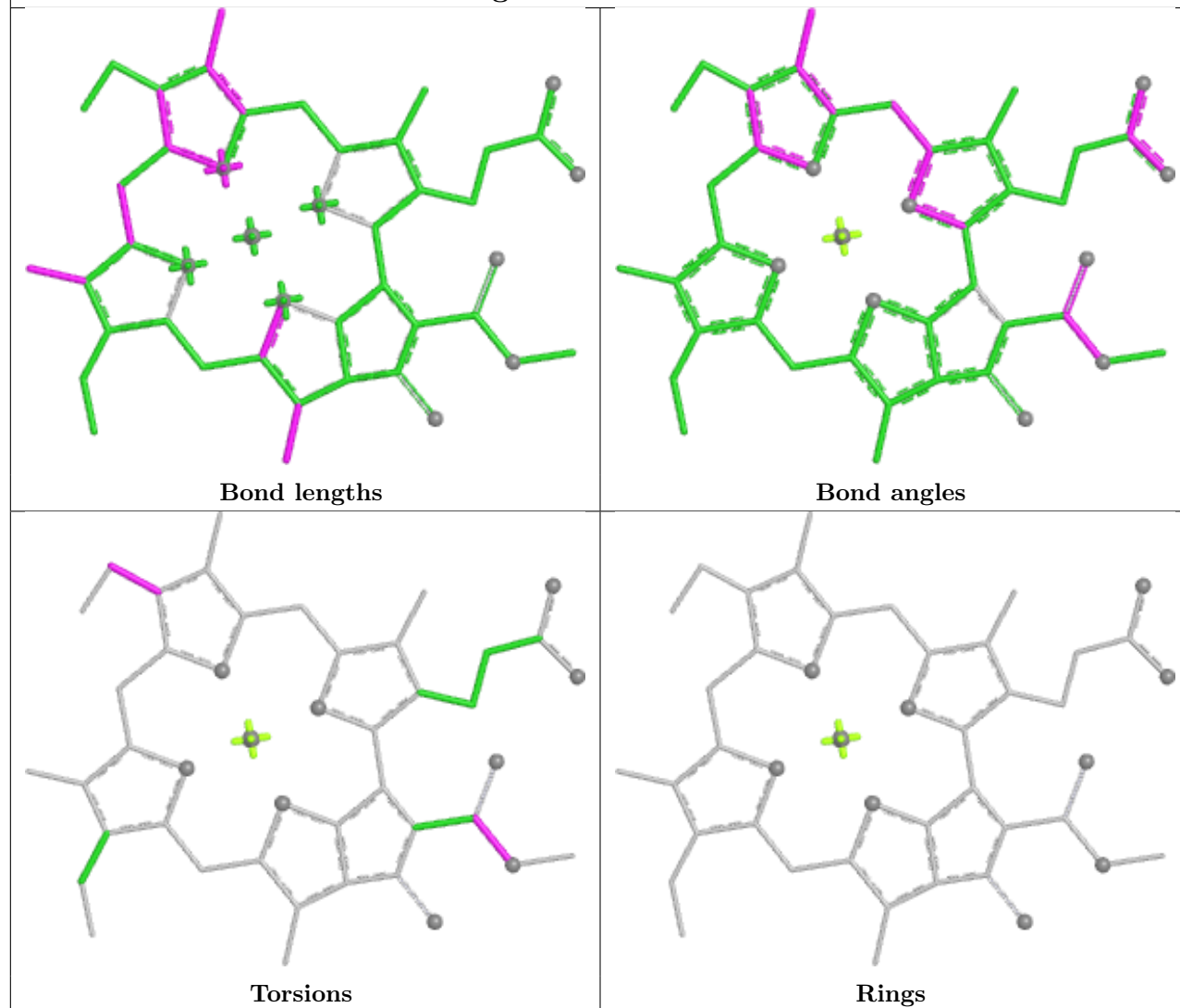


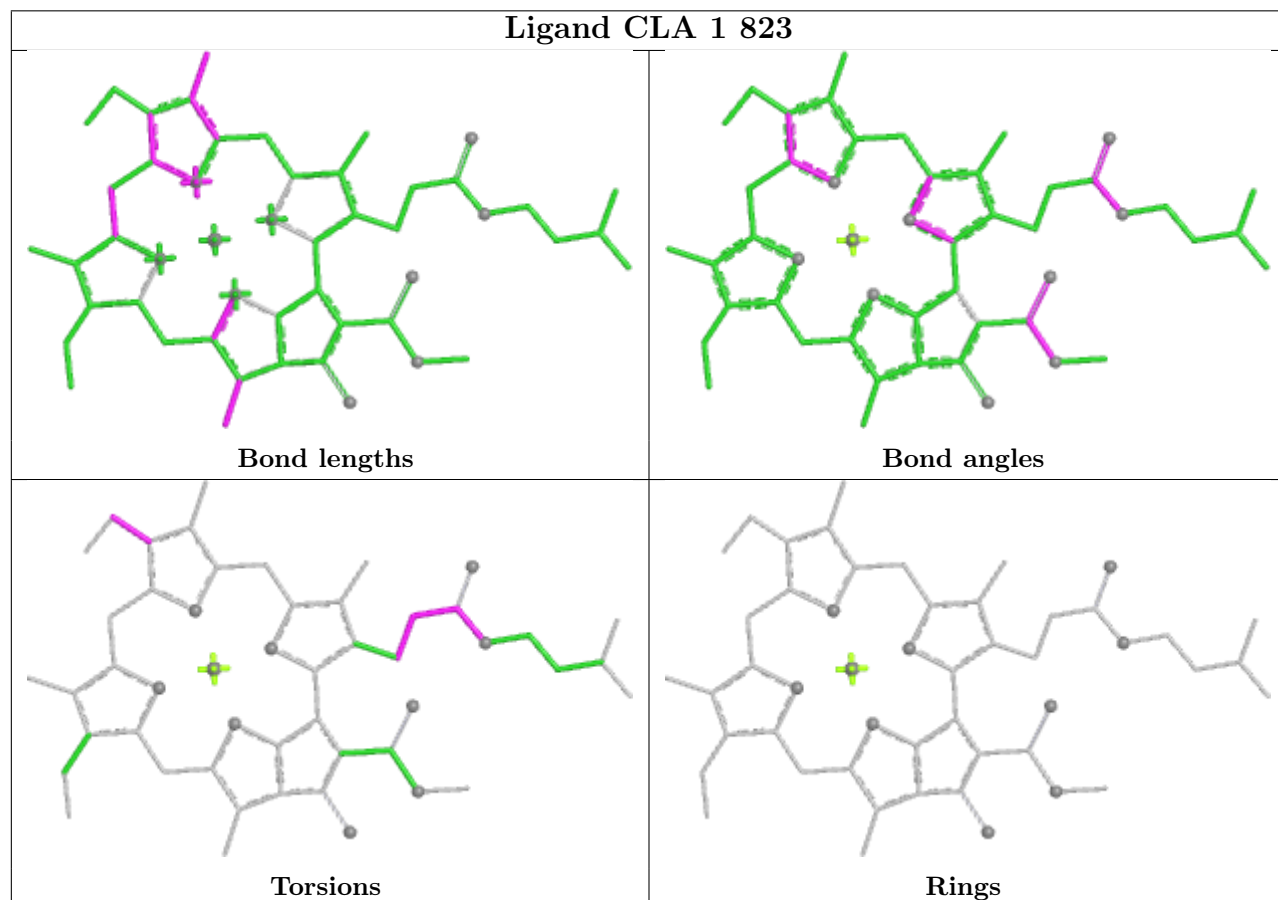
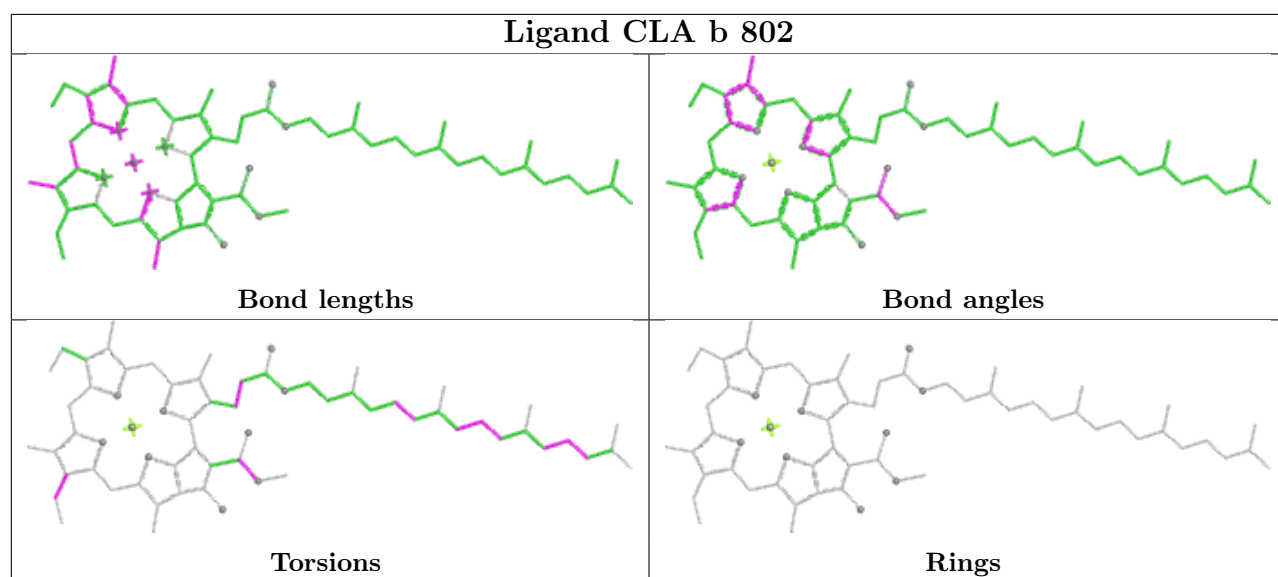


Ligand CLA b 837

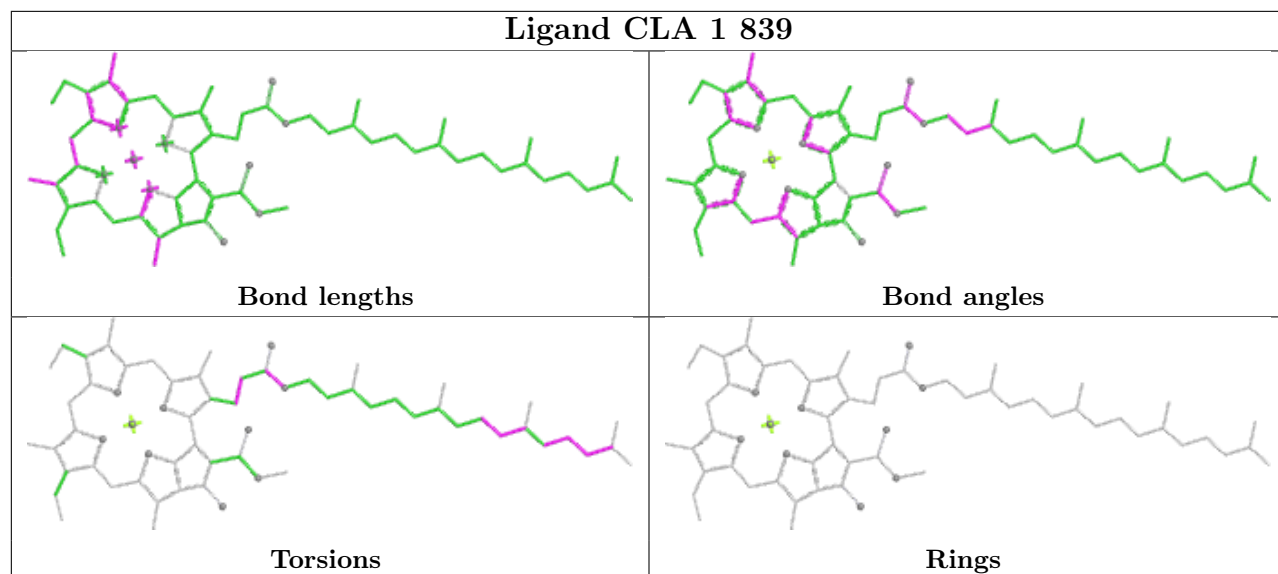


Ligand CLA B 812

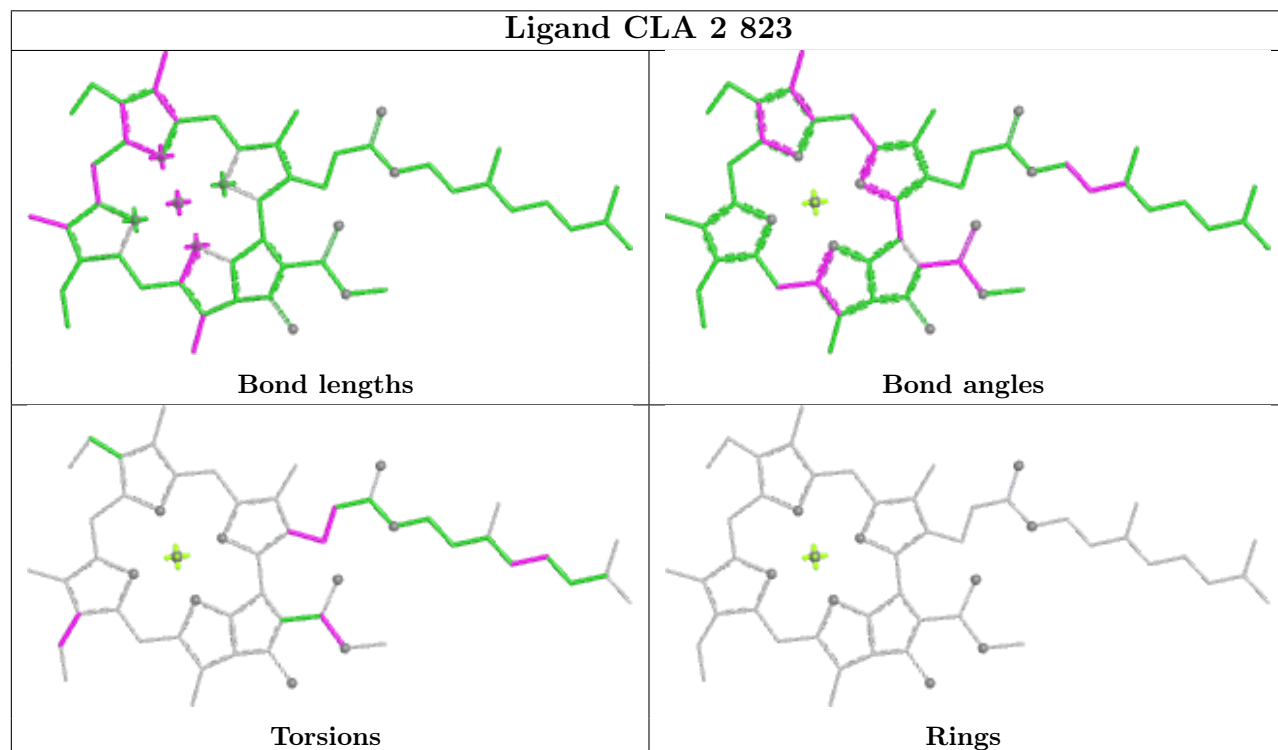


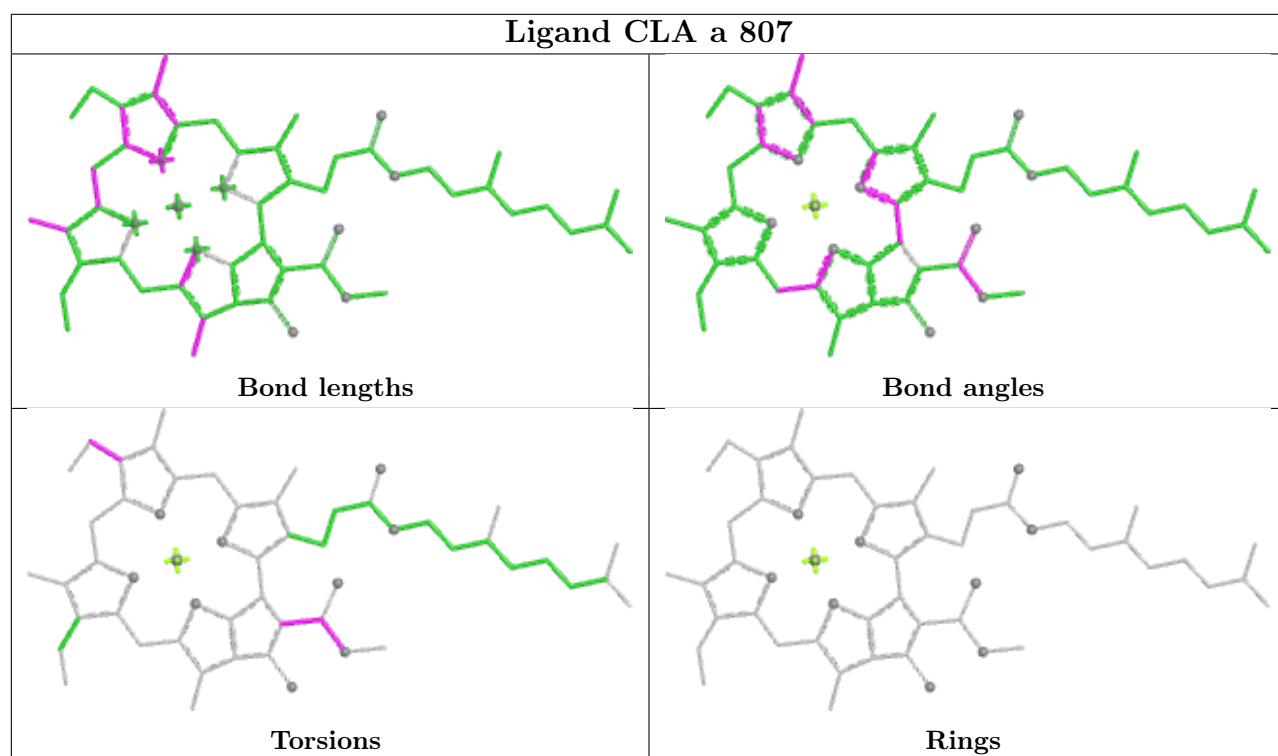


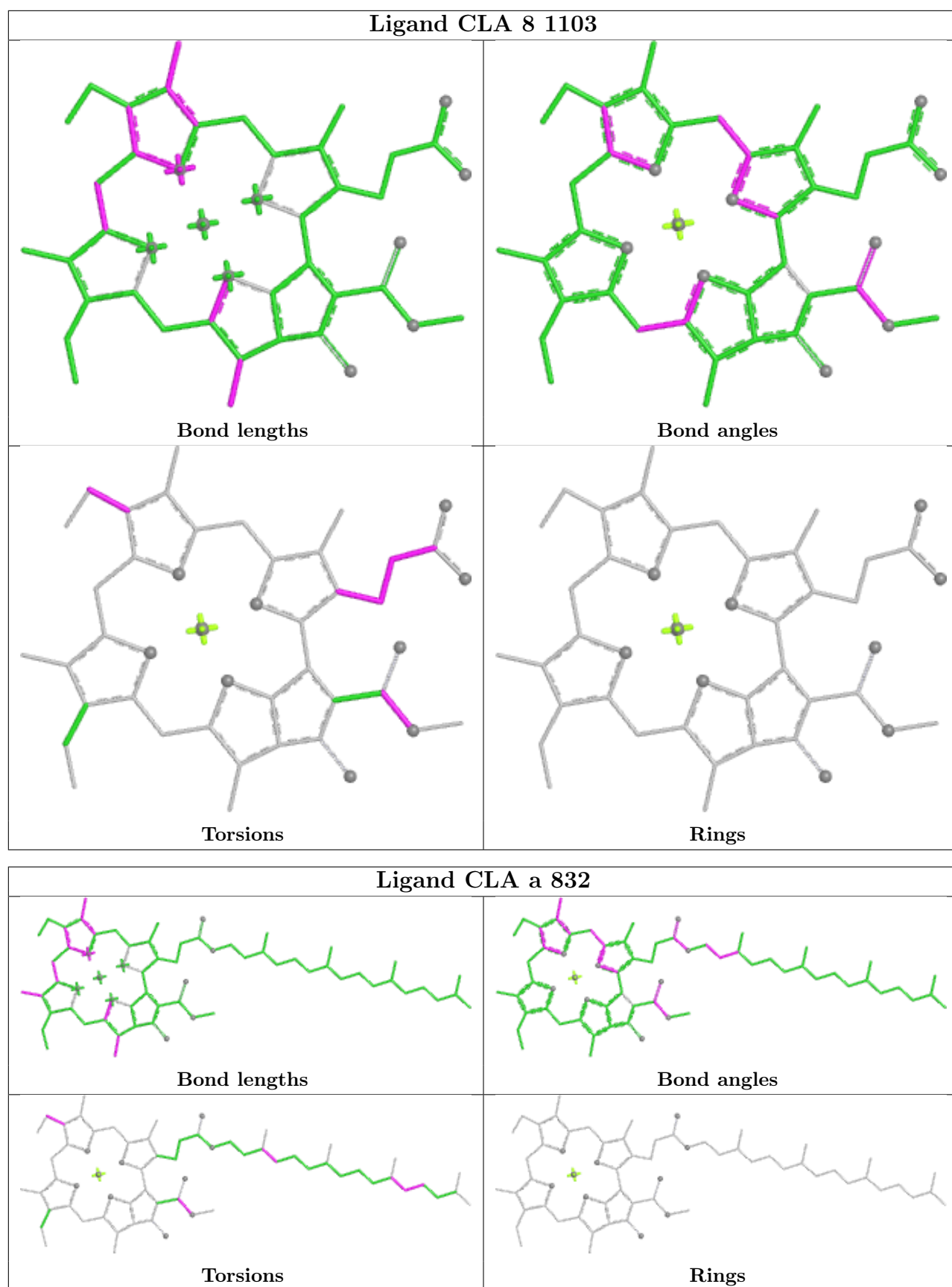
Ligand CLA 1 839

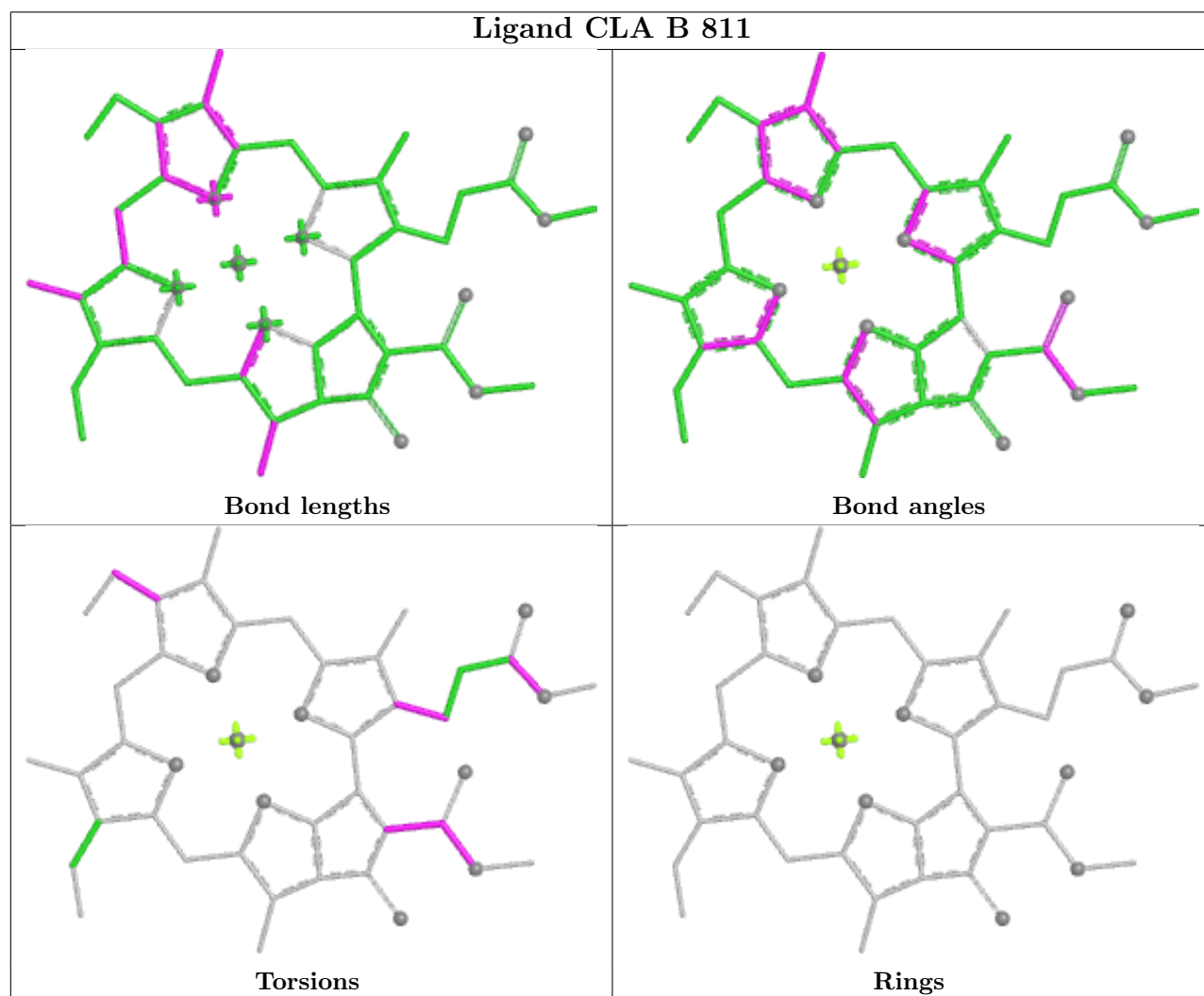
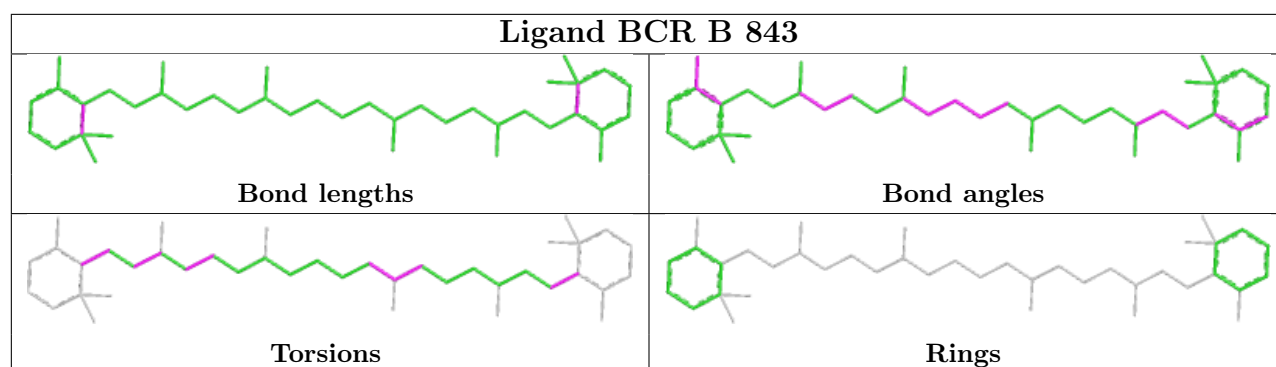


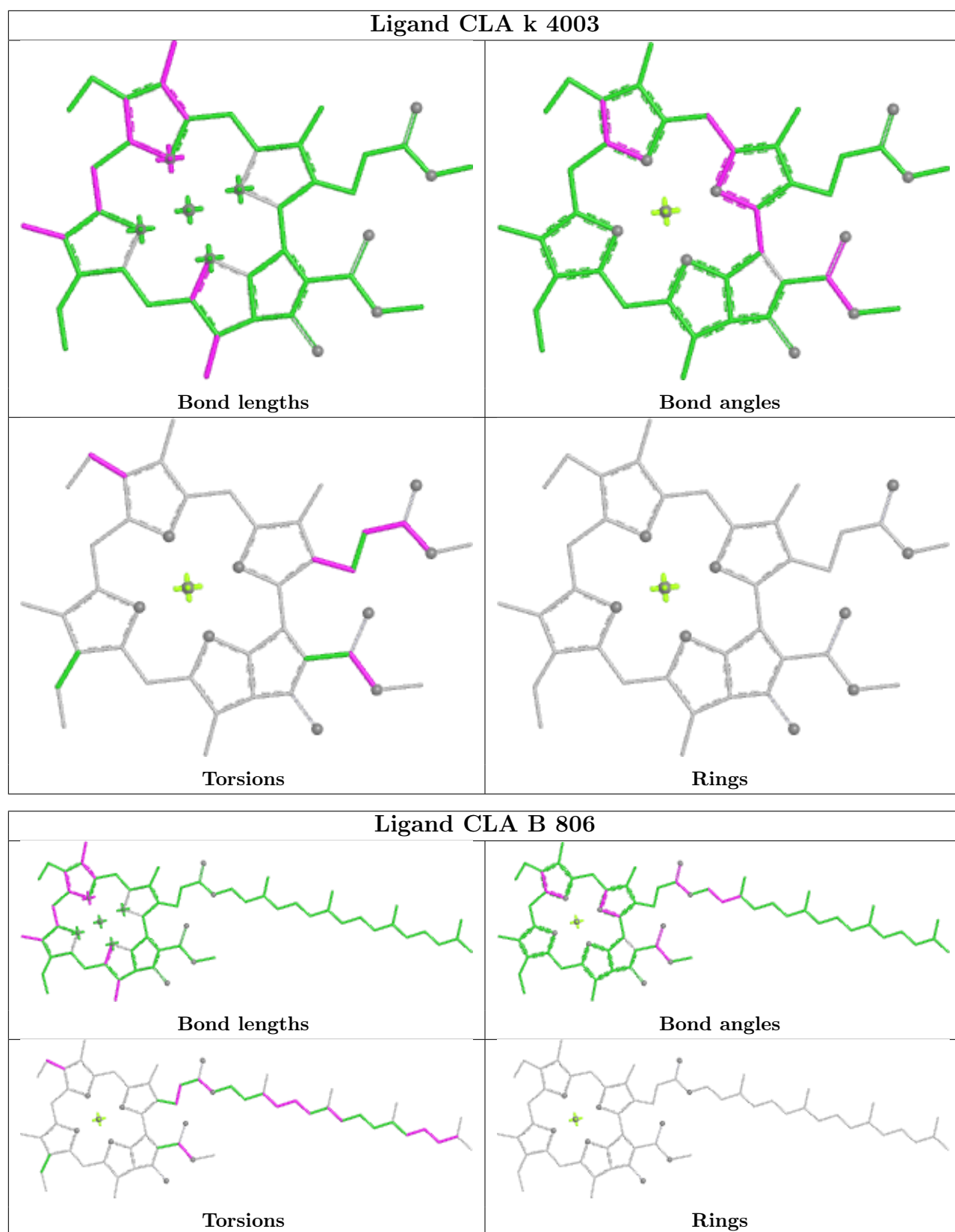
Ligand CLA 2 823

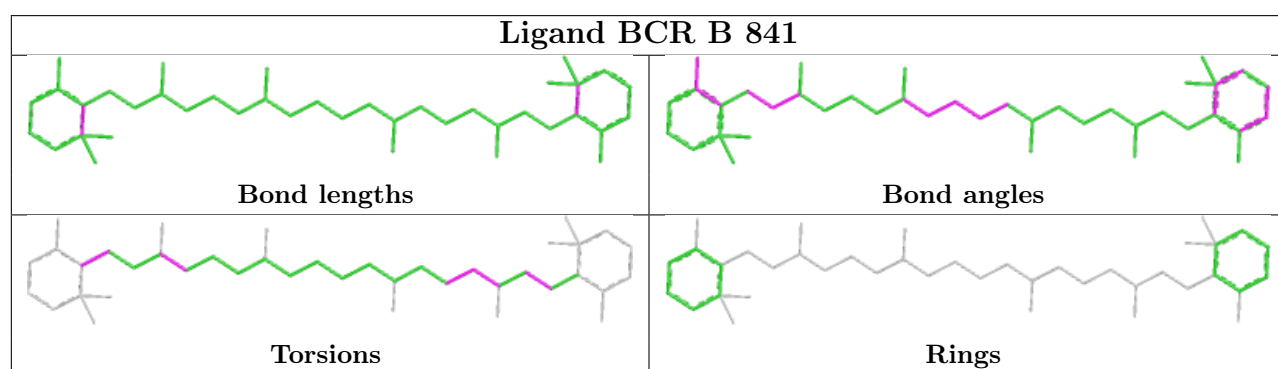
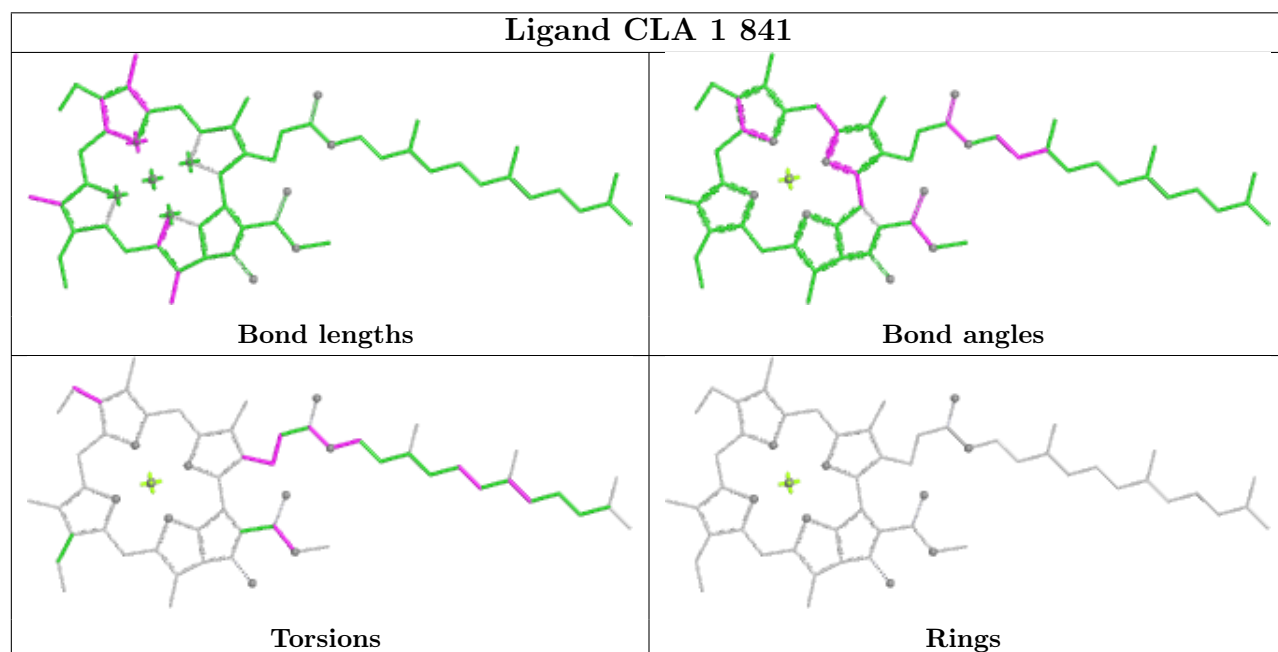
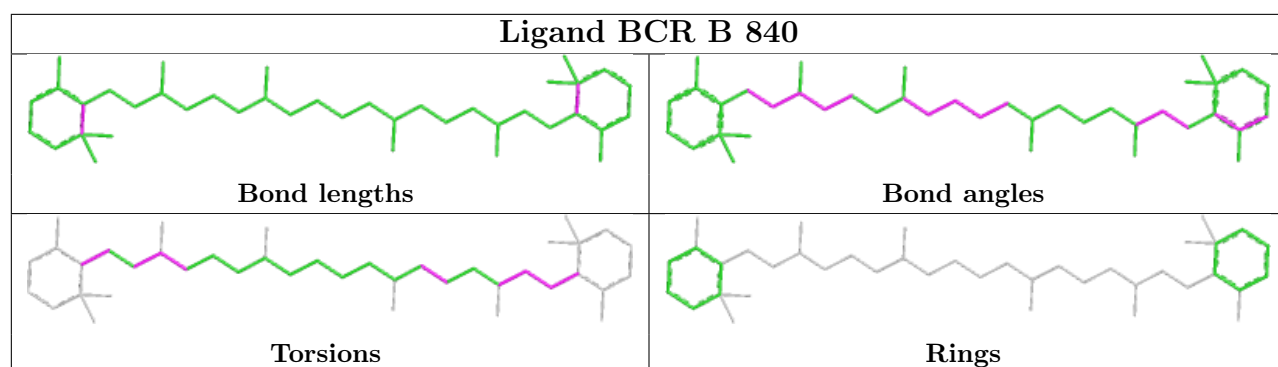




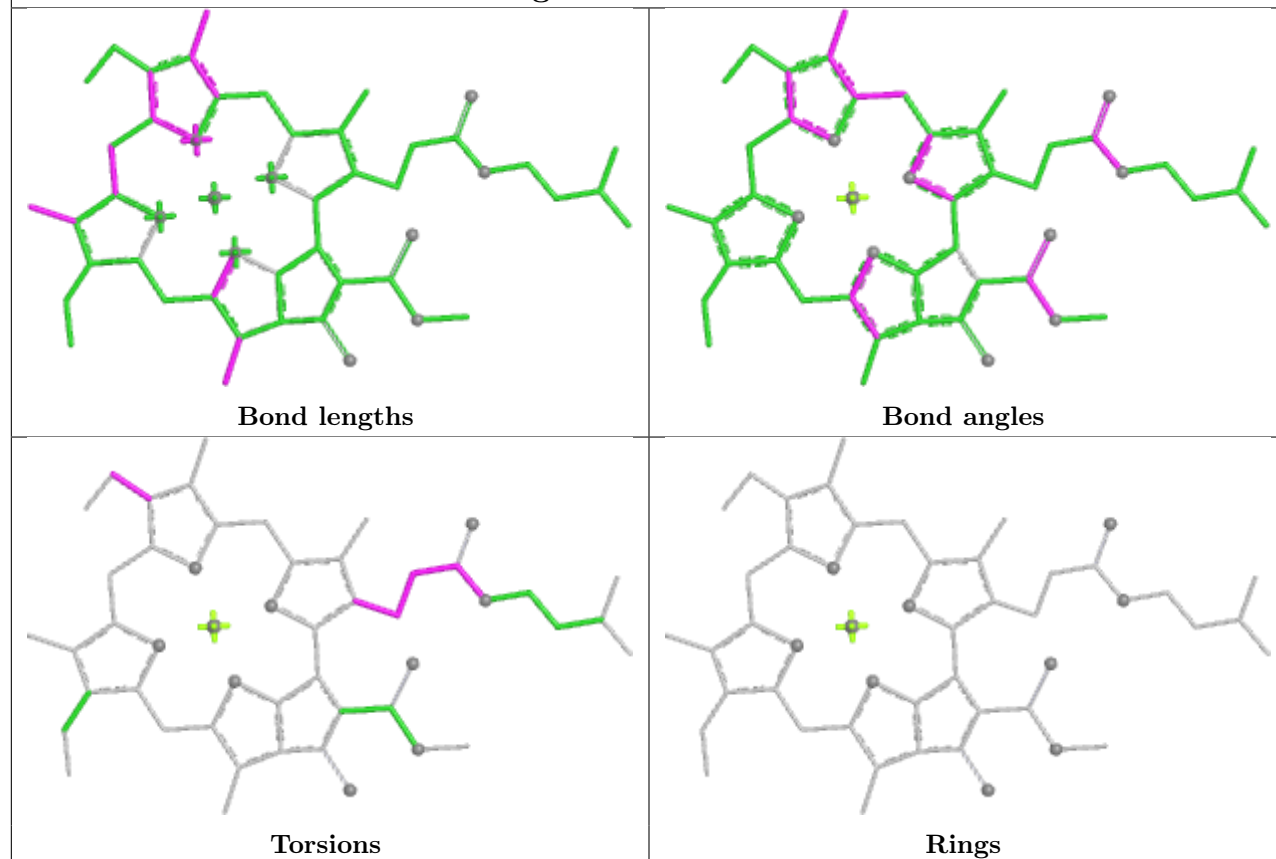




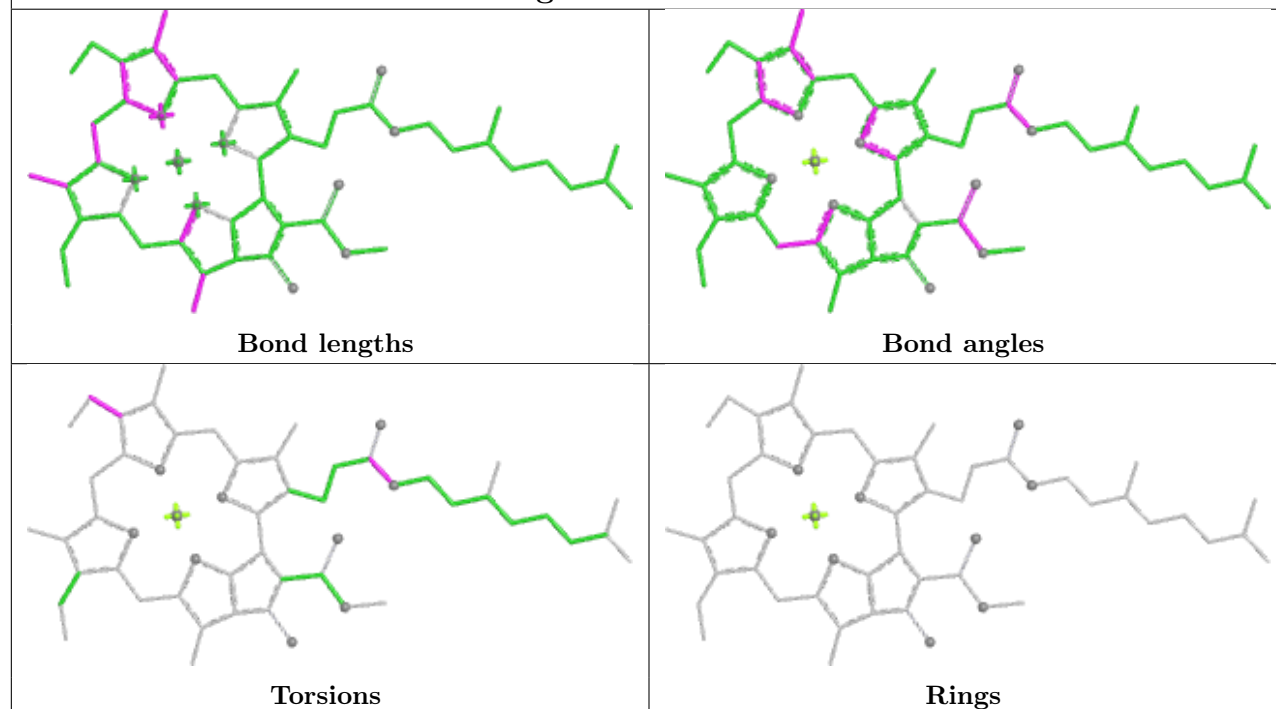


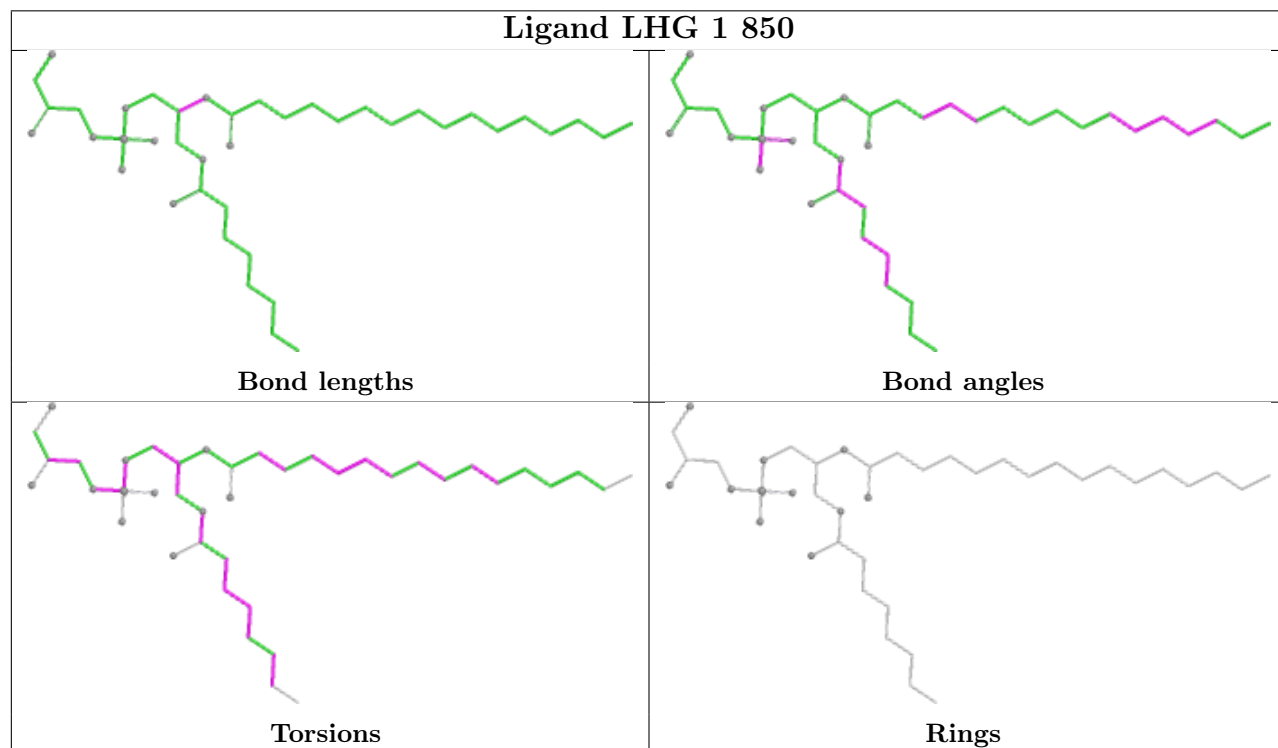
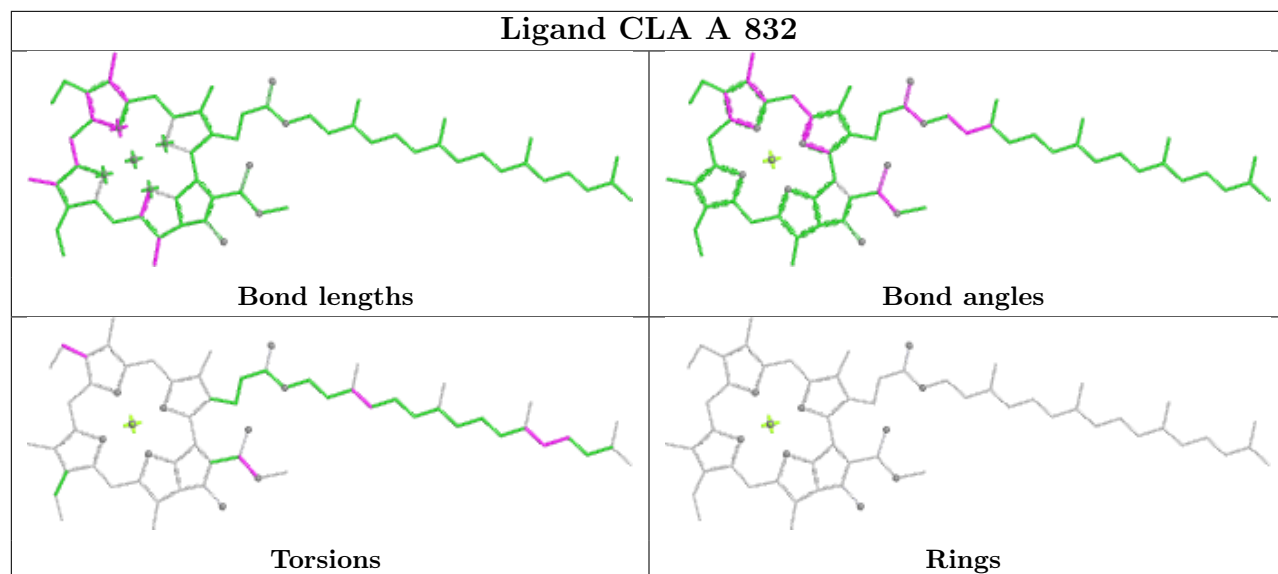


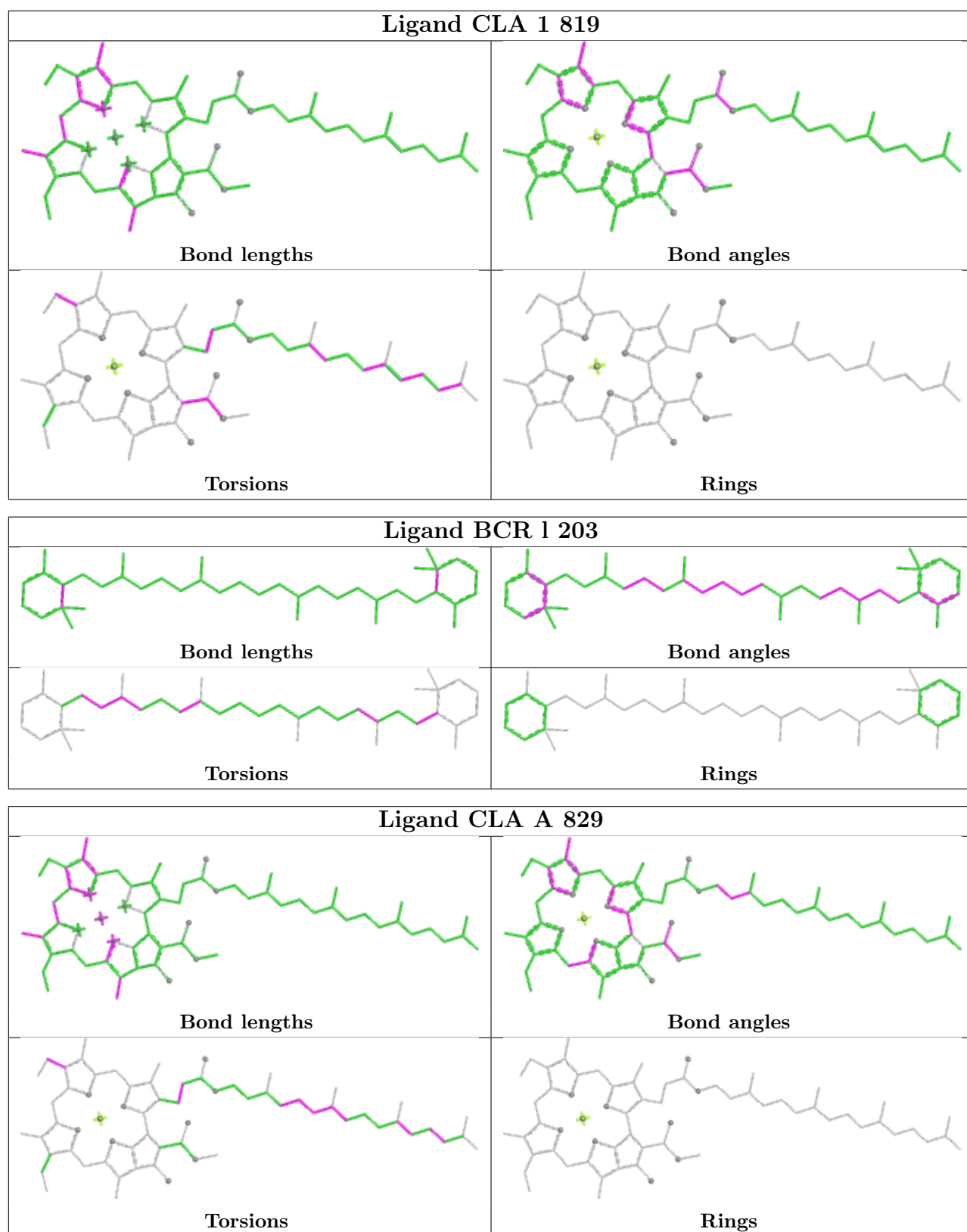
Ligand CLA B 814

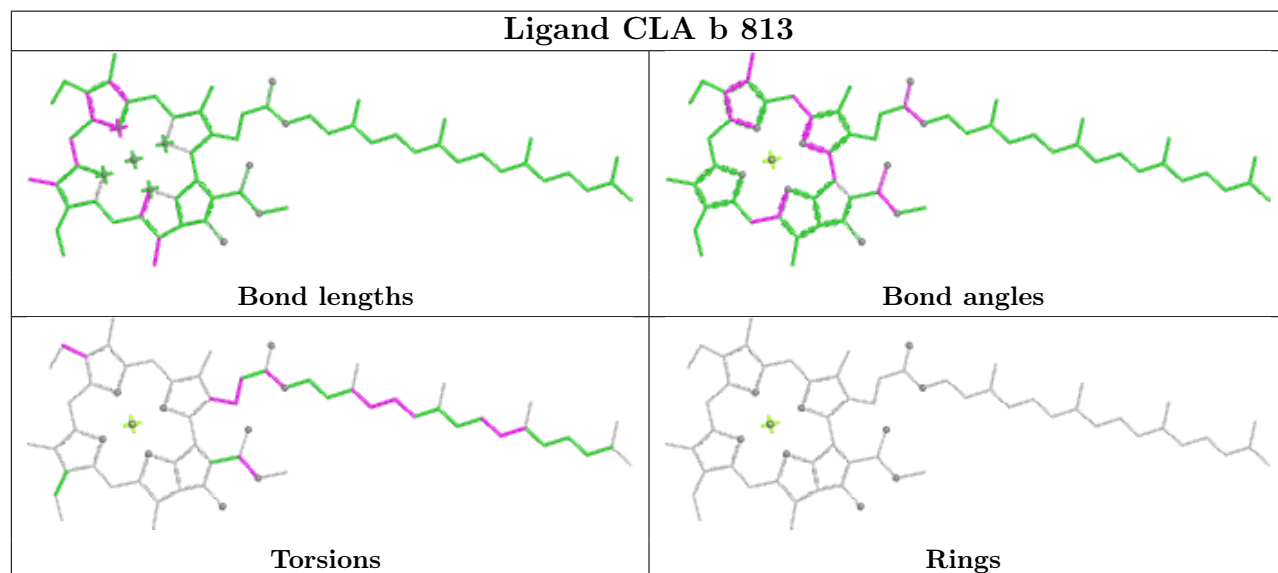
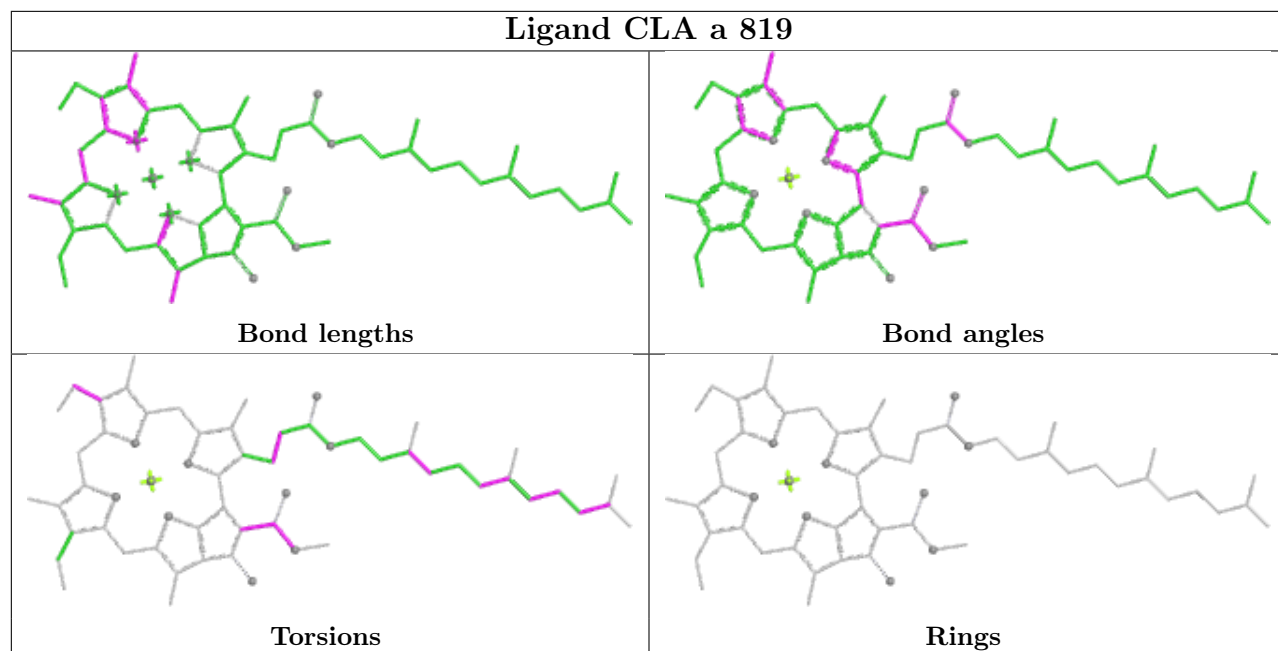


Ligand CLA a 804

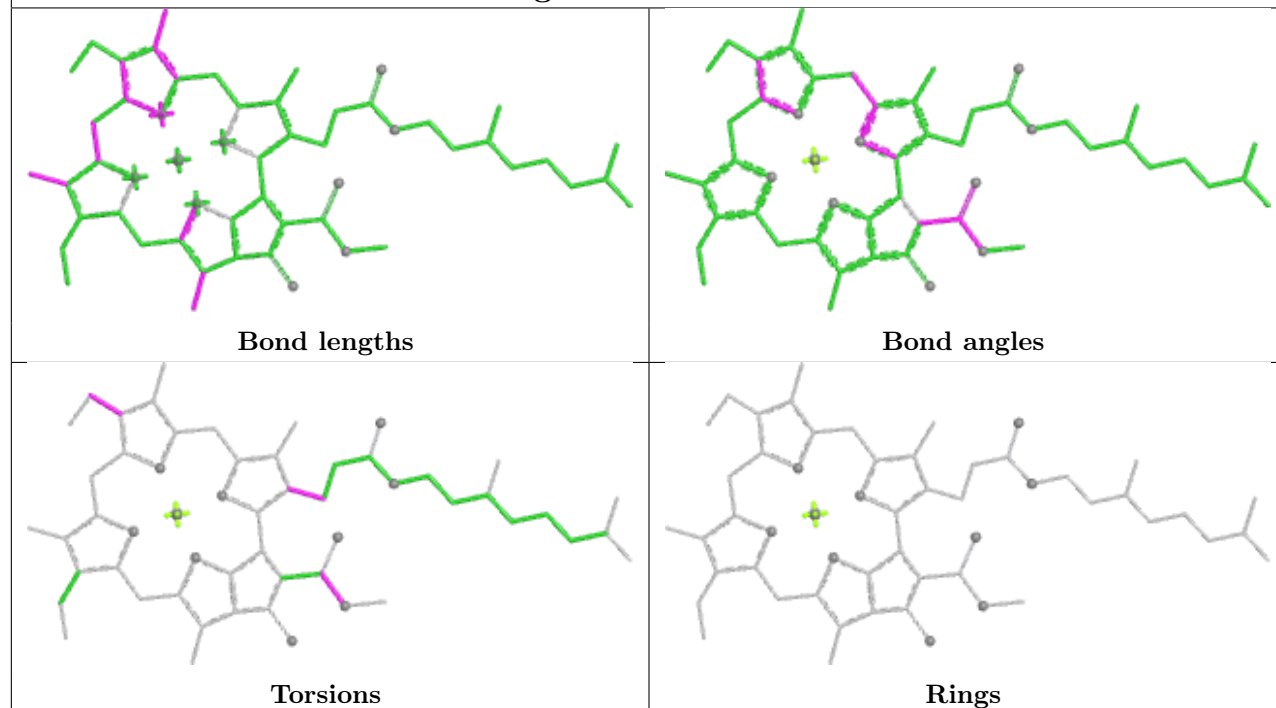




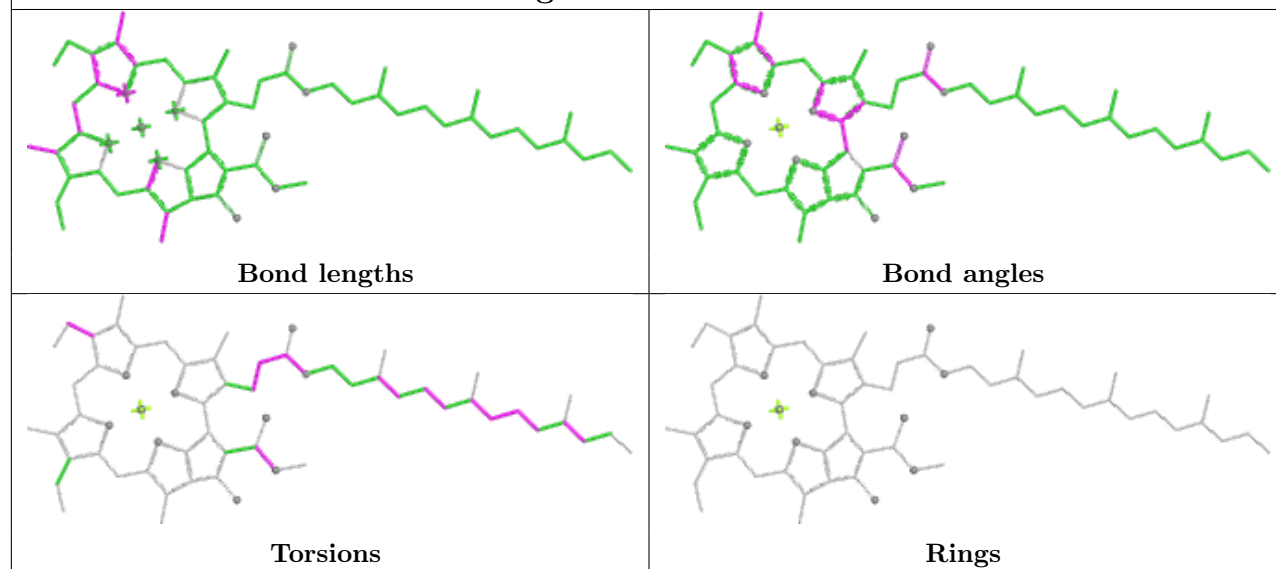




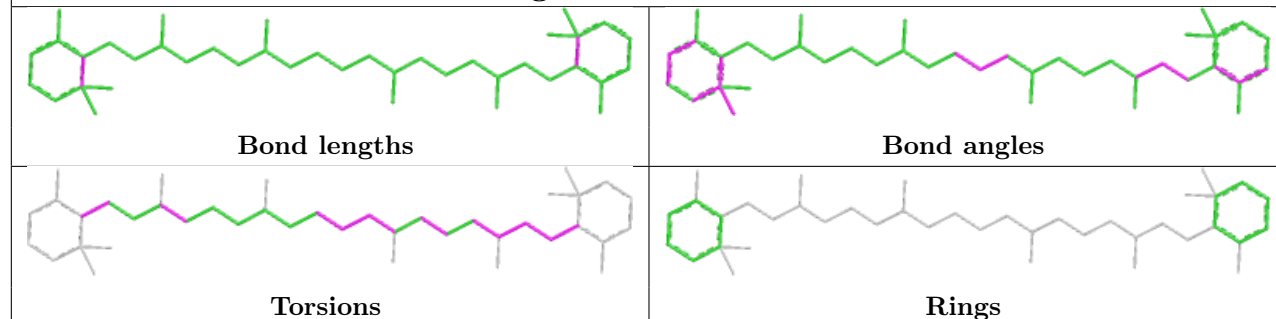
Ligand CLA F 201

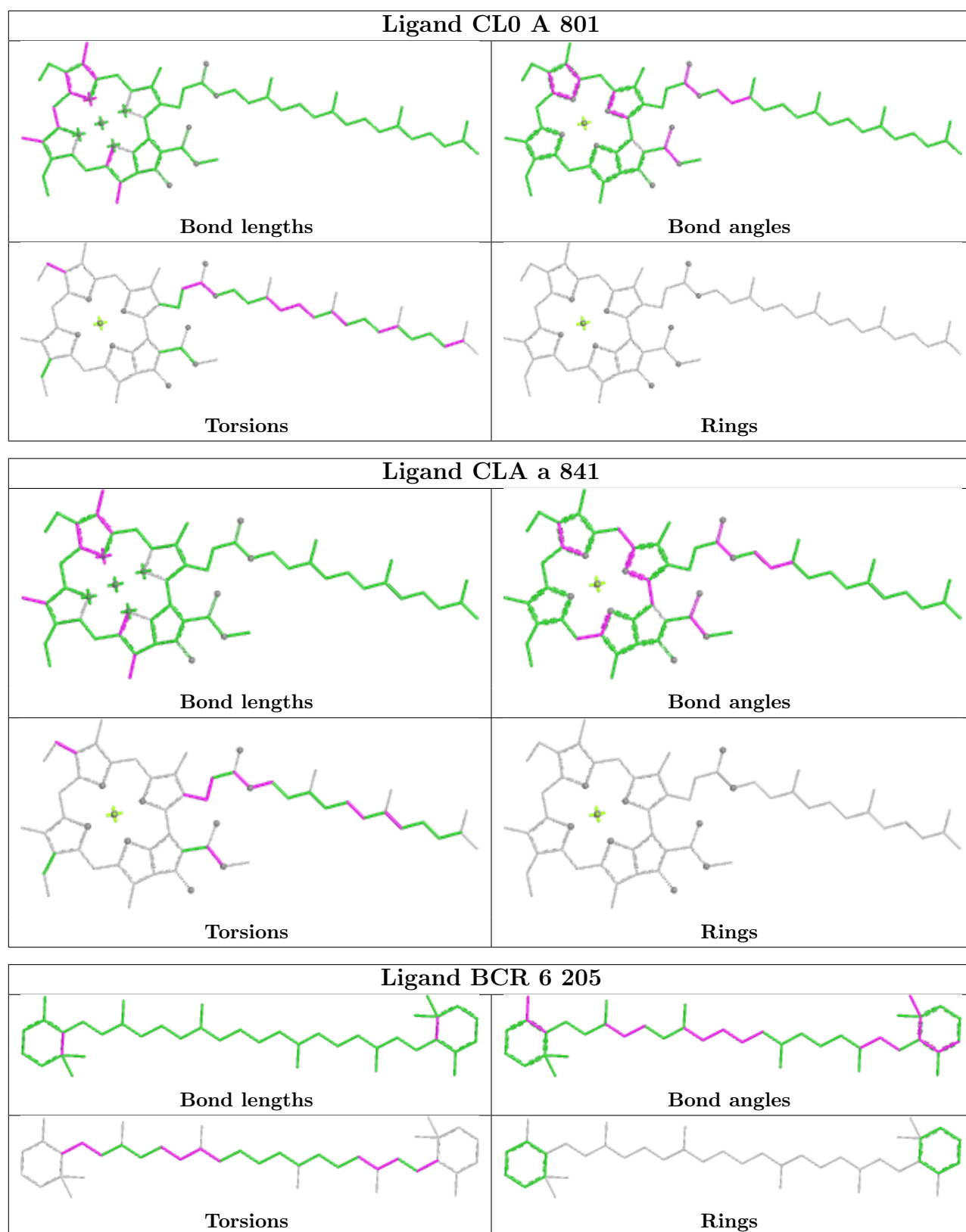


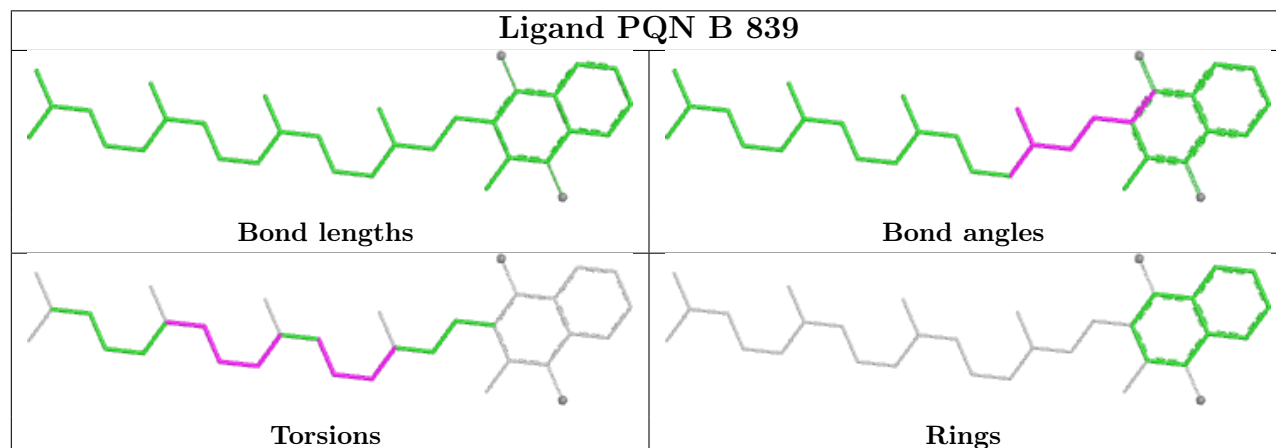
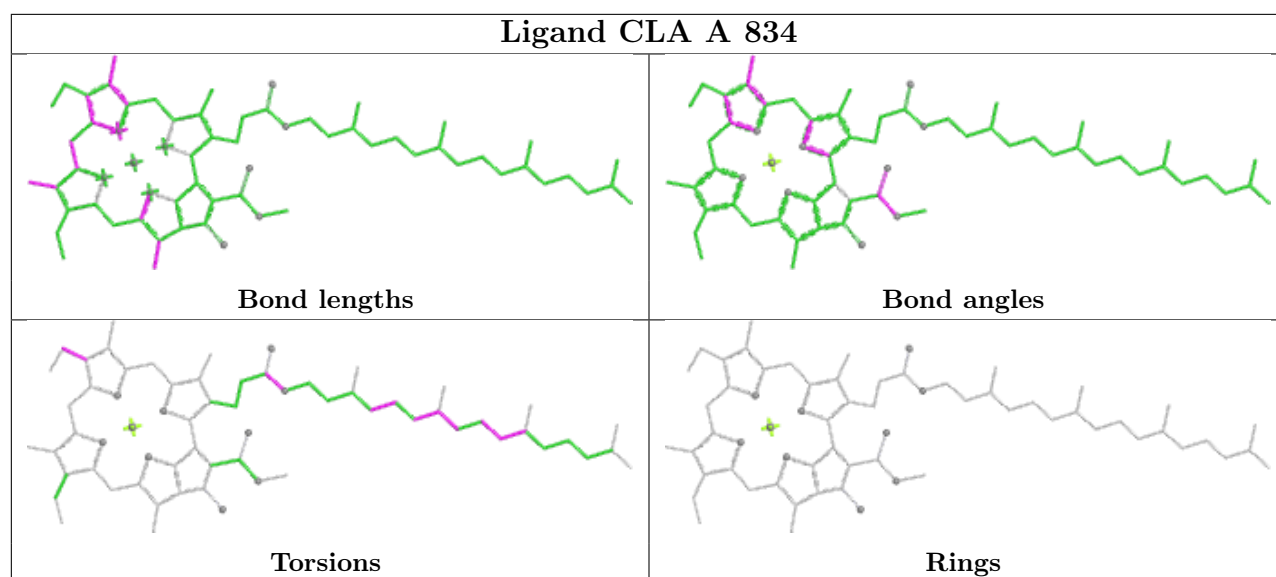
Ligand CLA 1 825



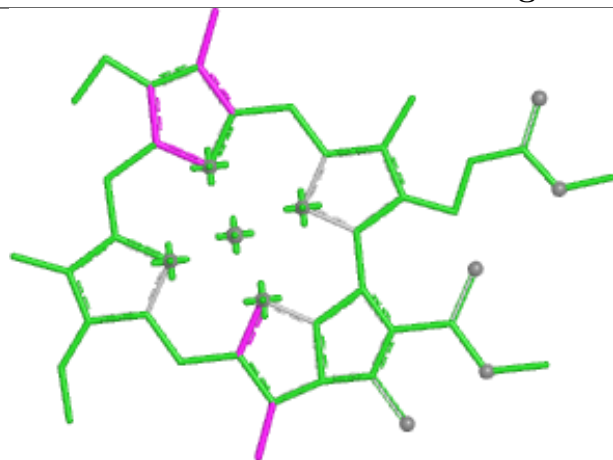
Ligand BCR B 842



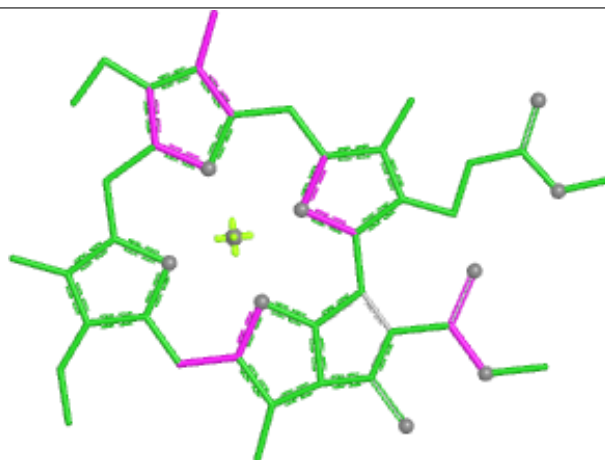




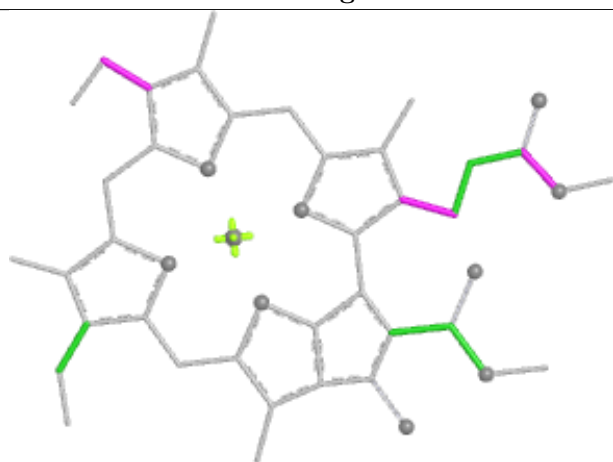
Ligand CLA a 820



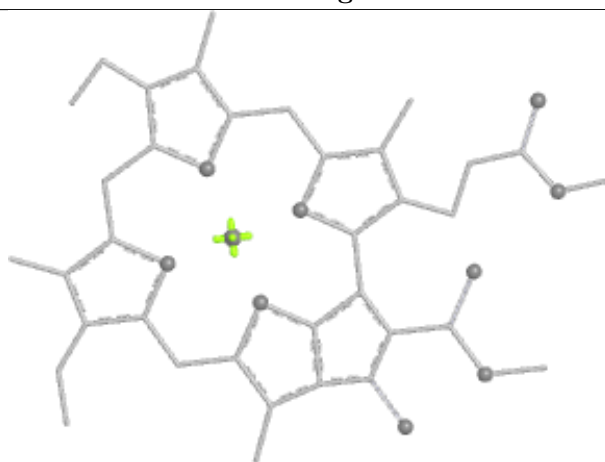
Bond lengths



Bond angles

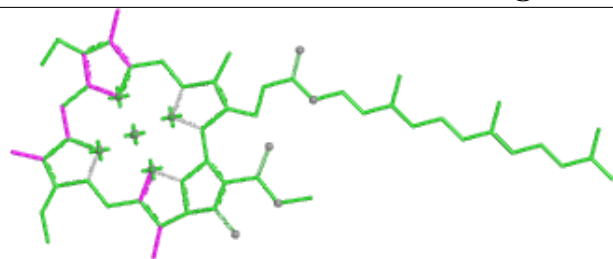


Torsions

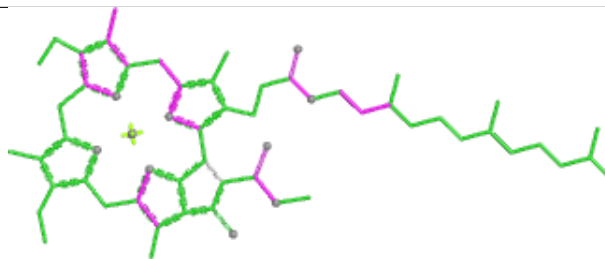


Rings

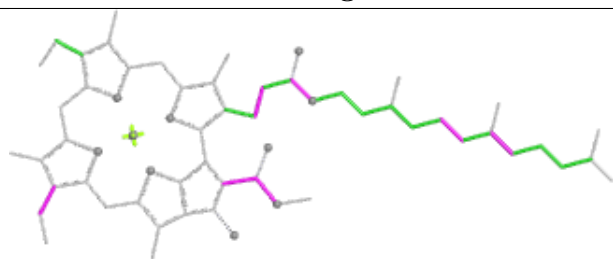
Ligand CLA B 803



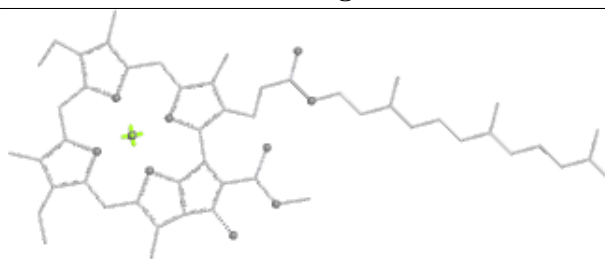
Bond lengths



Bond angles

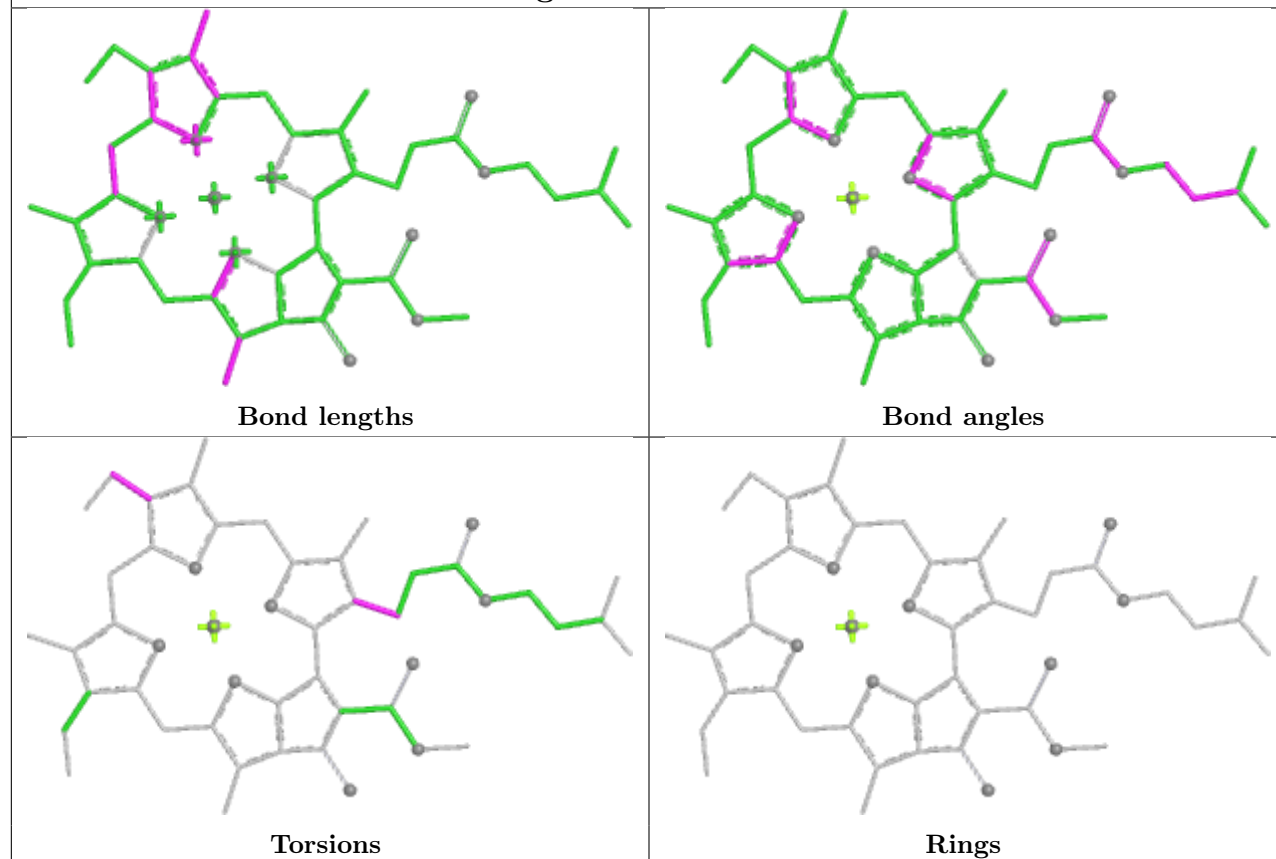


Torsions

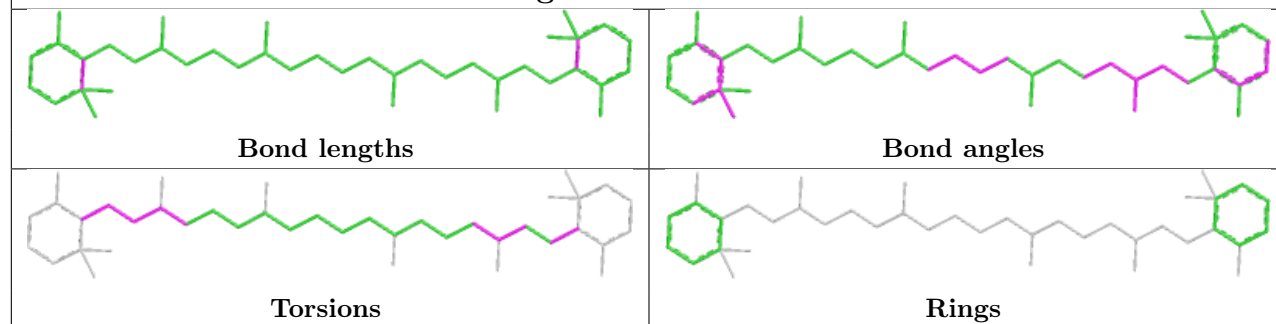


Rings

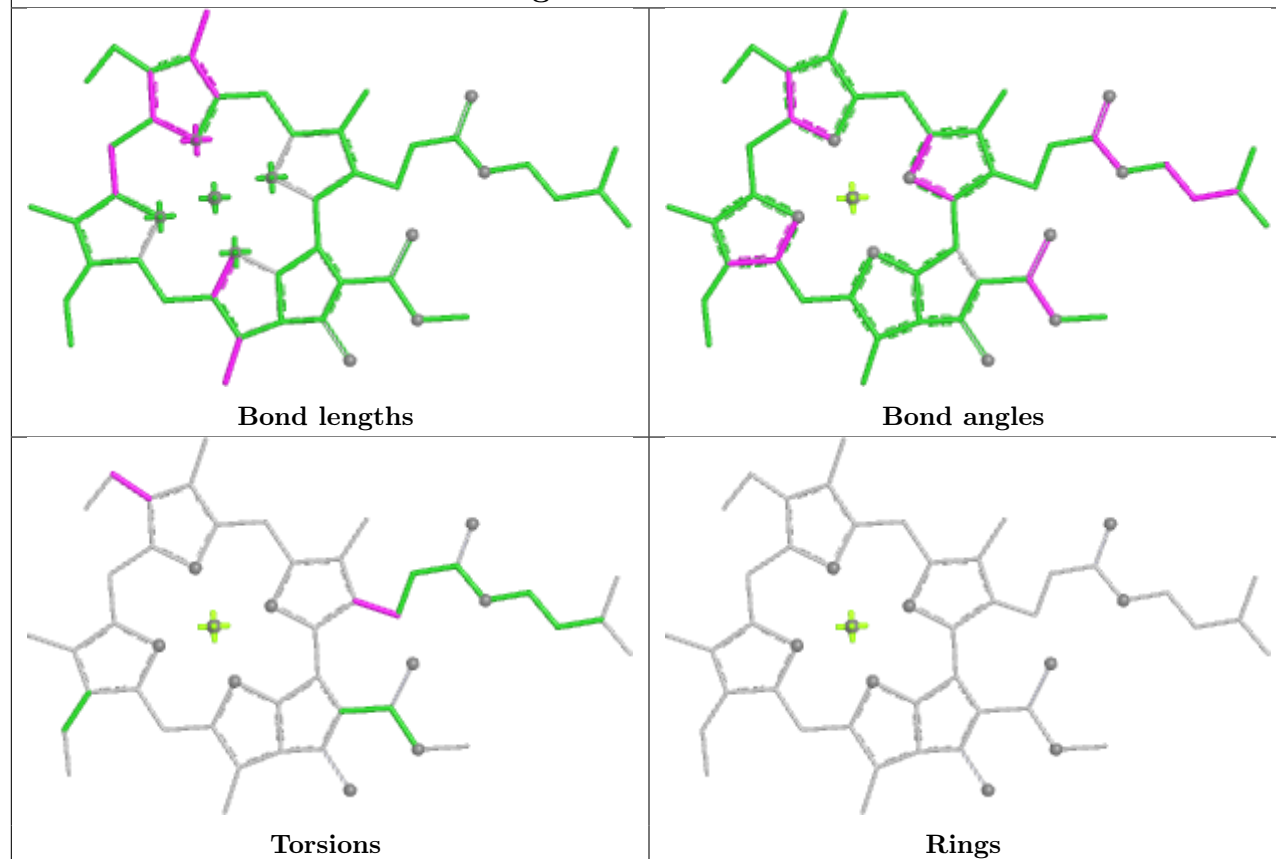
Ligand CLA 2 834



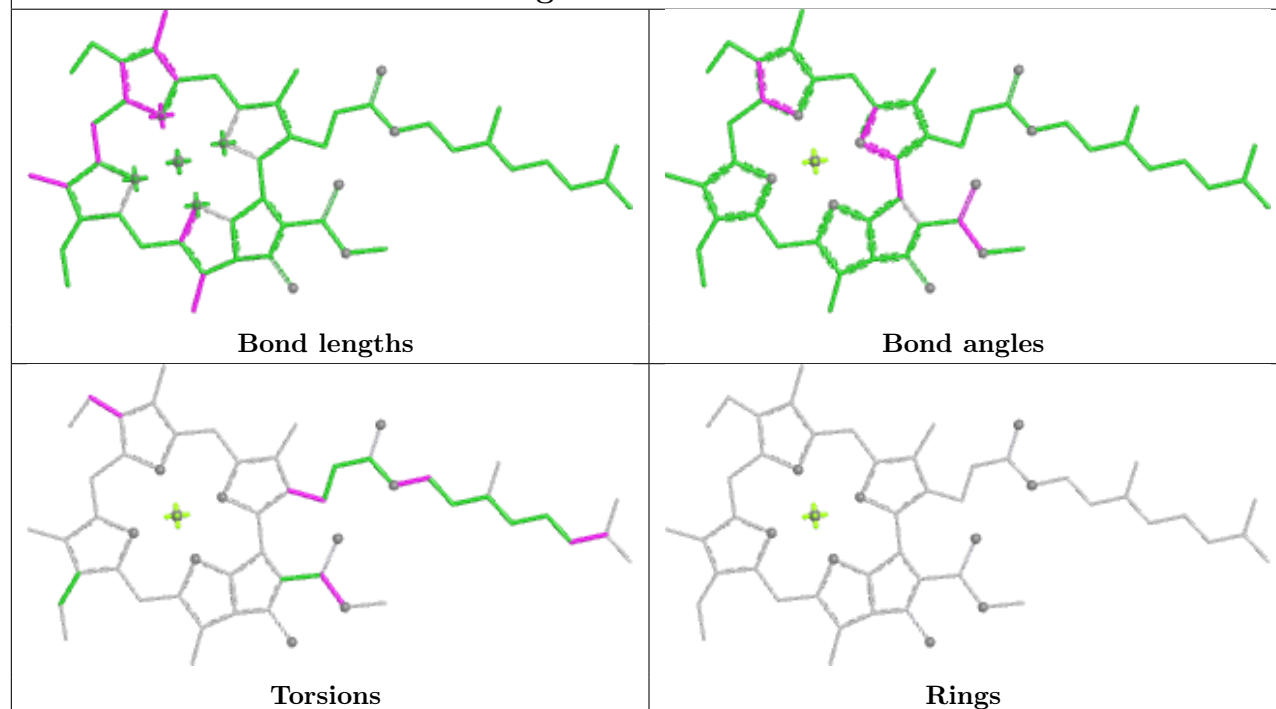
Ligand BCR I 102

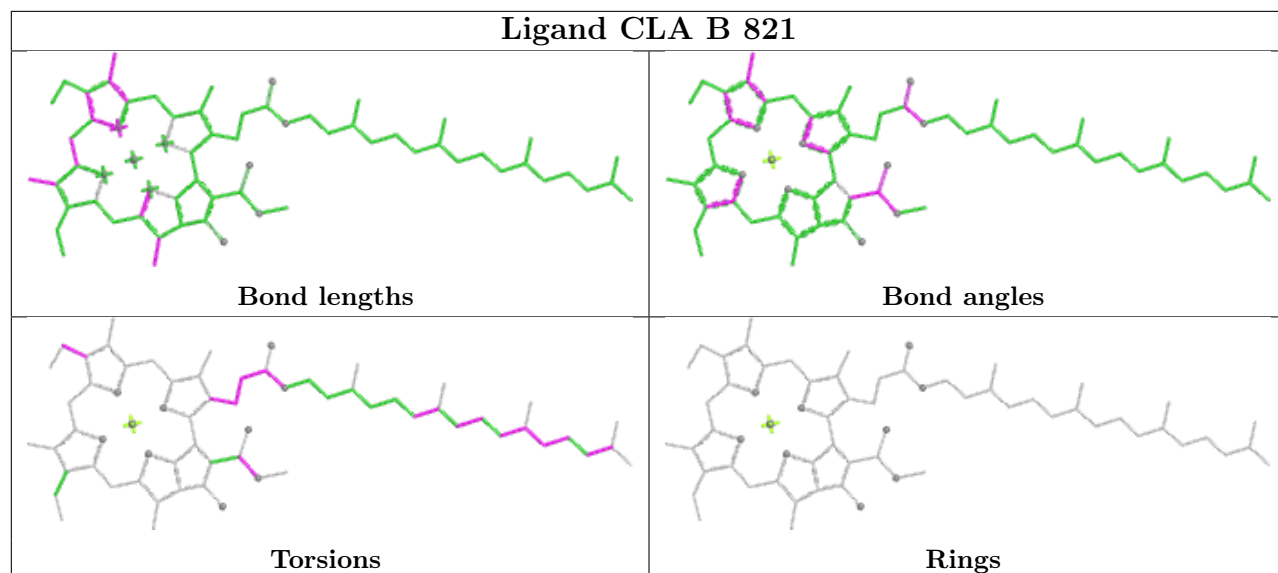
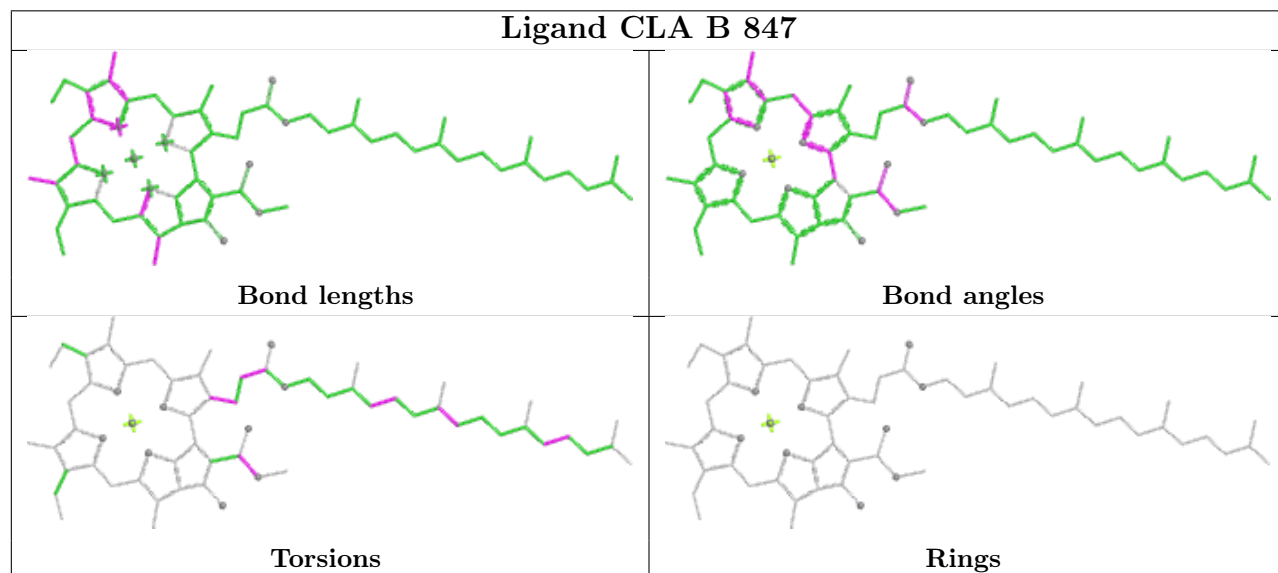
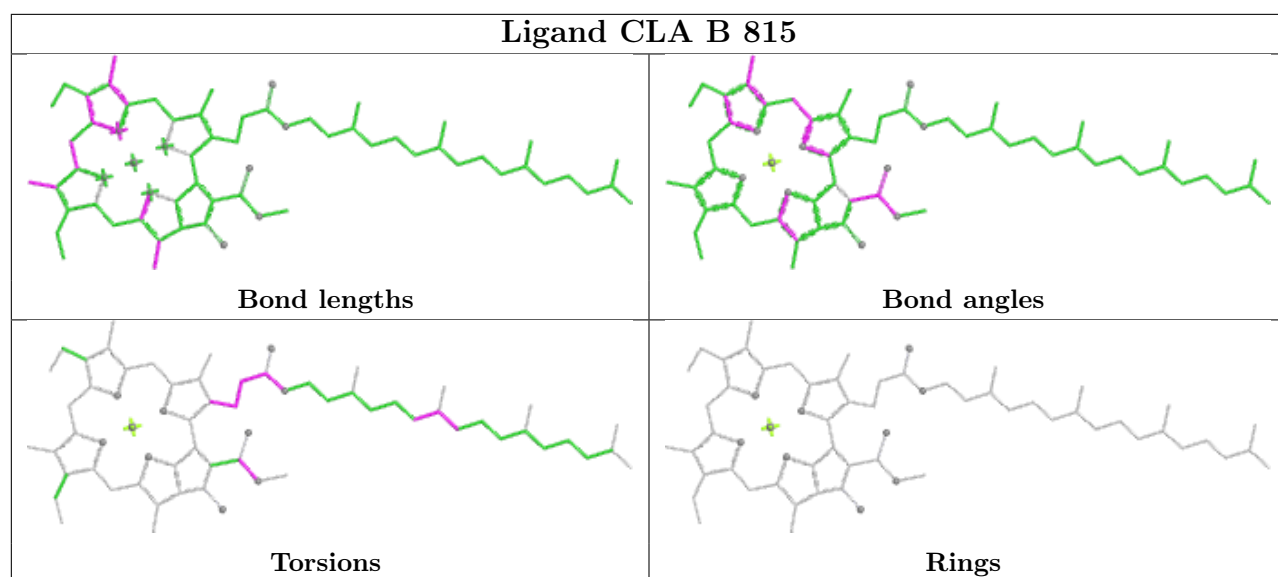


Ligand CLA B 835

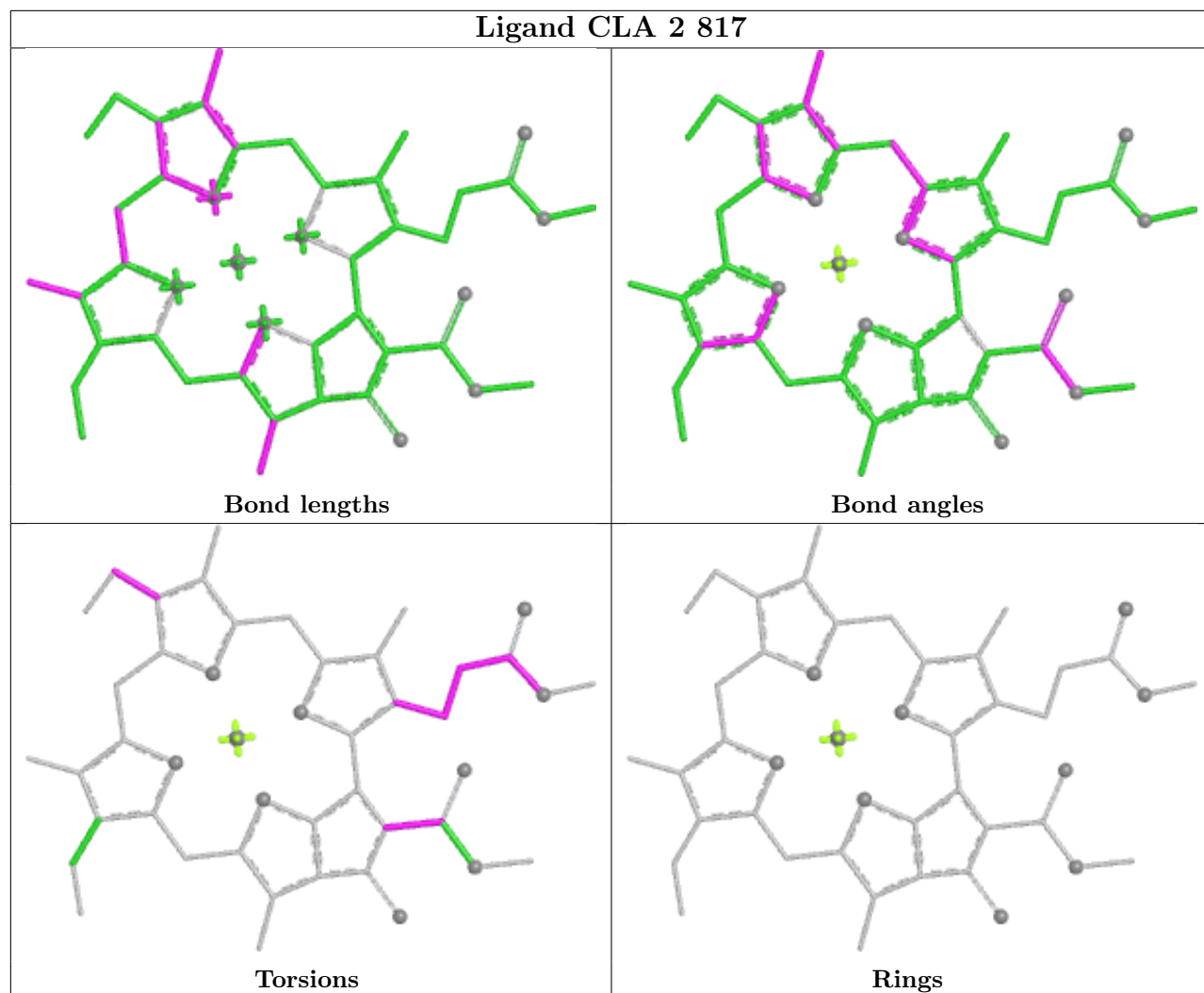


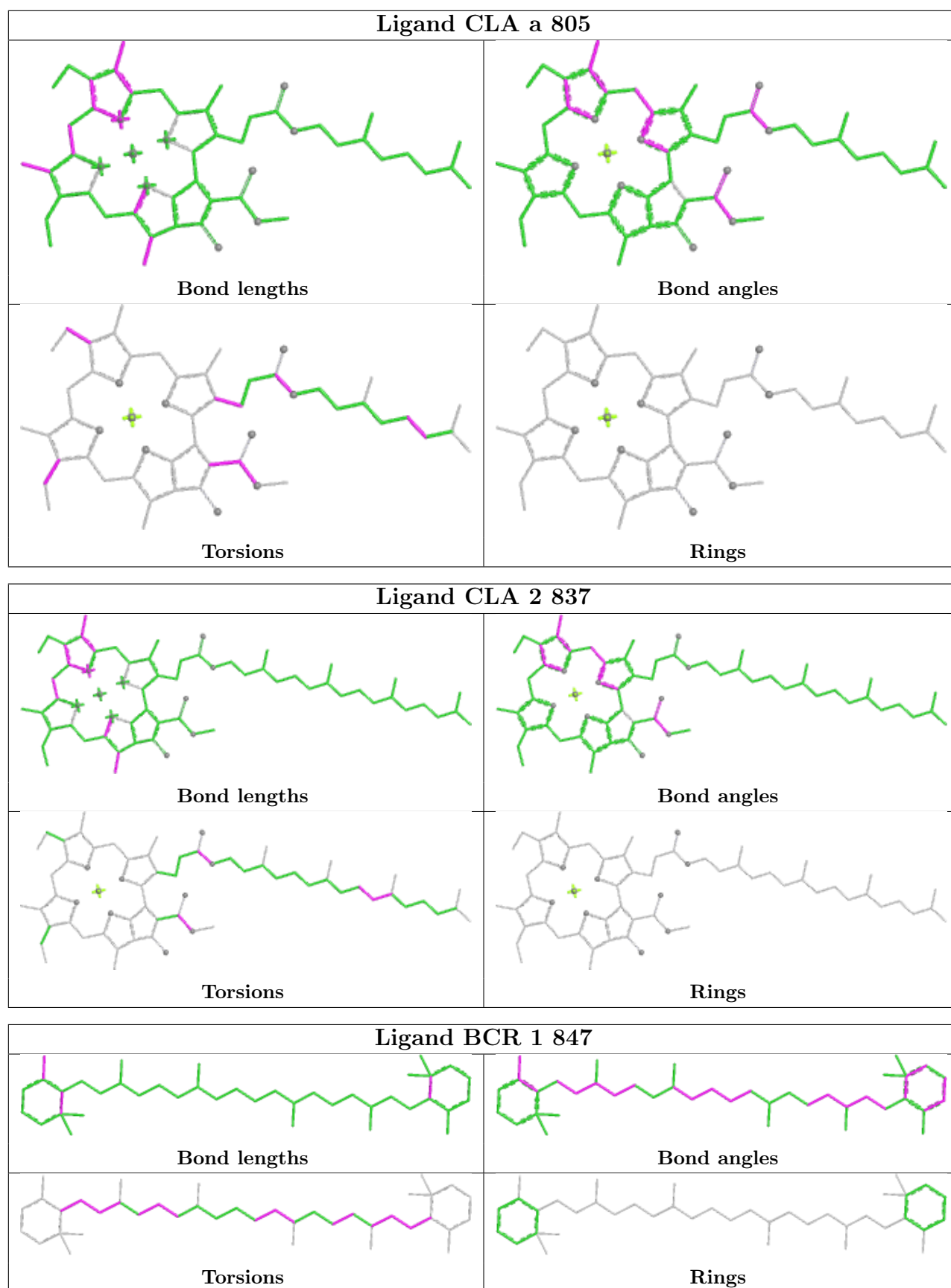
Ligand CLA 2 819

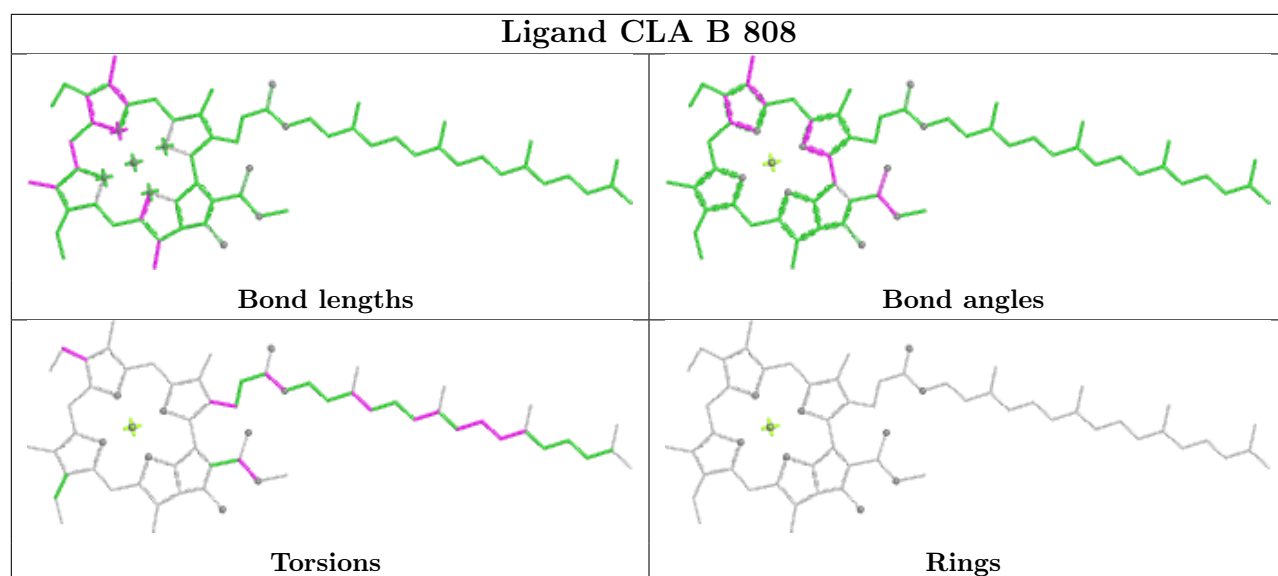
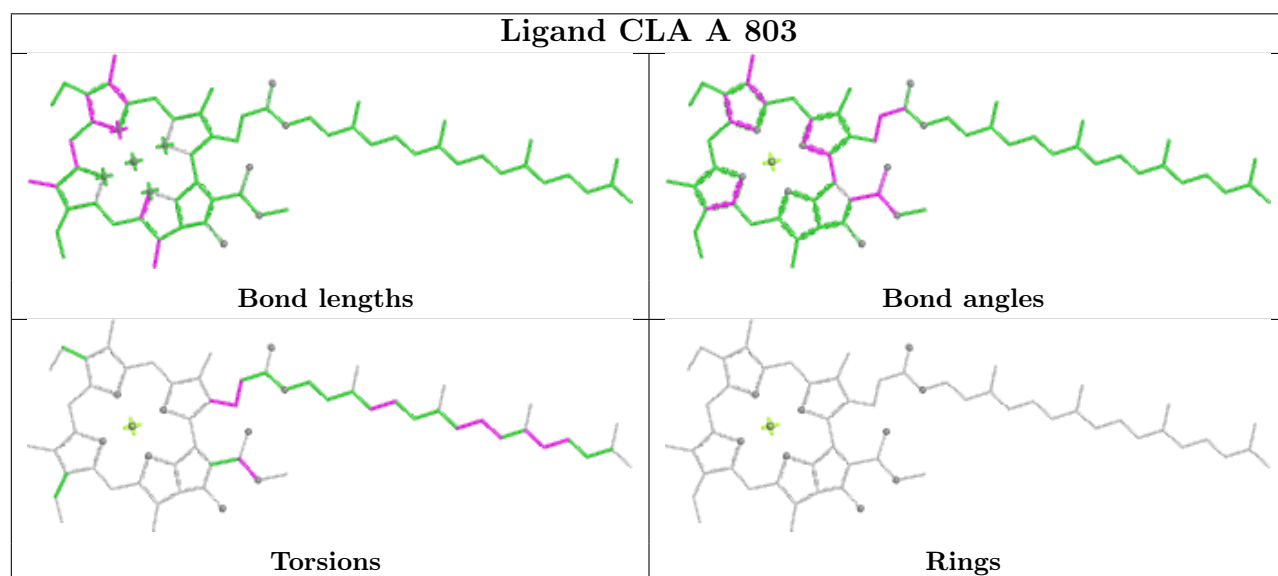
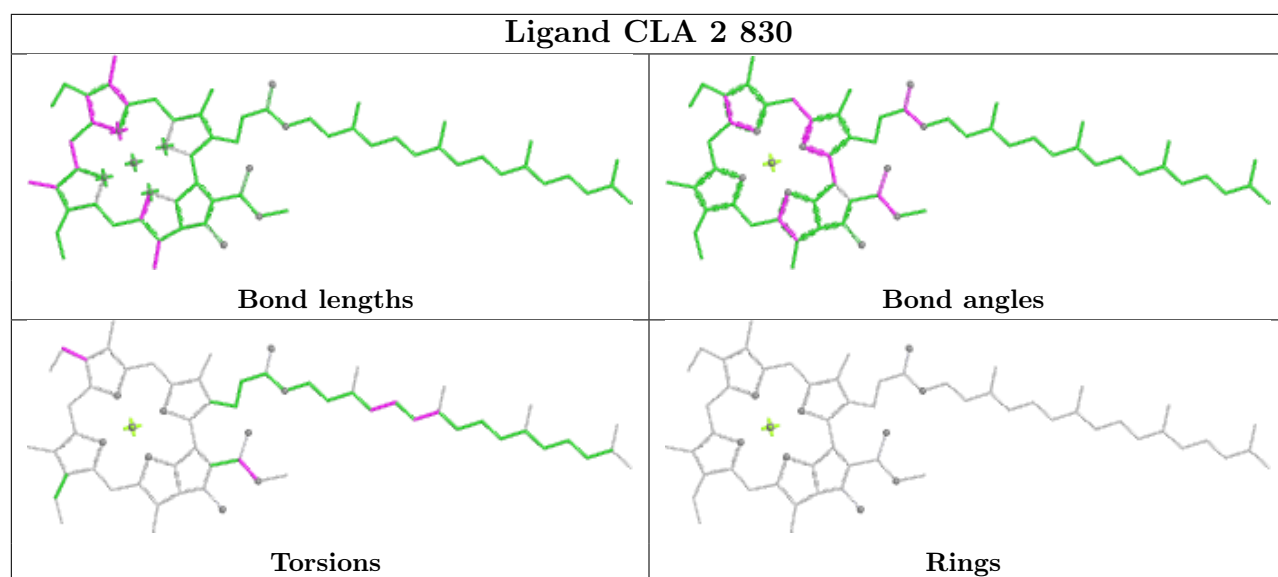


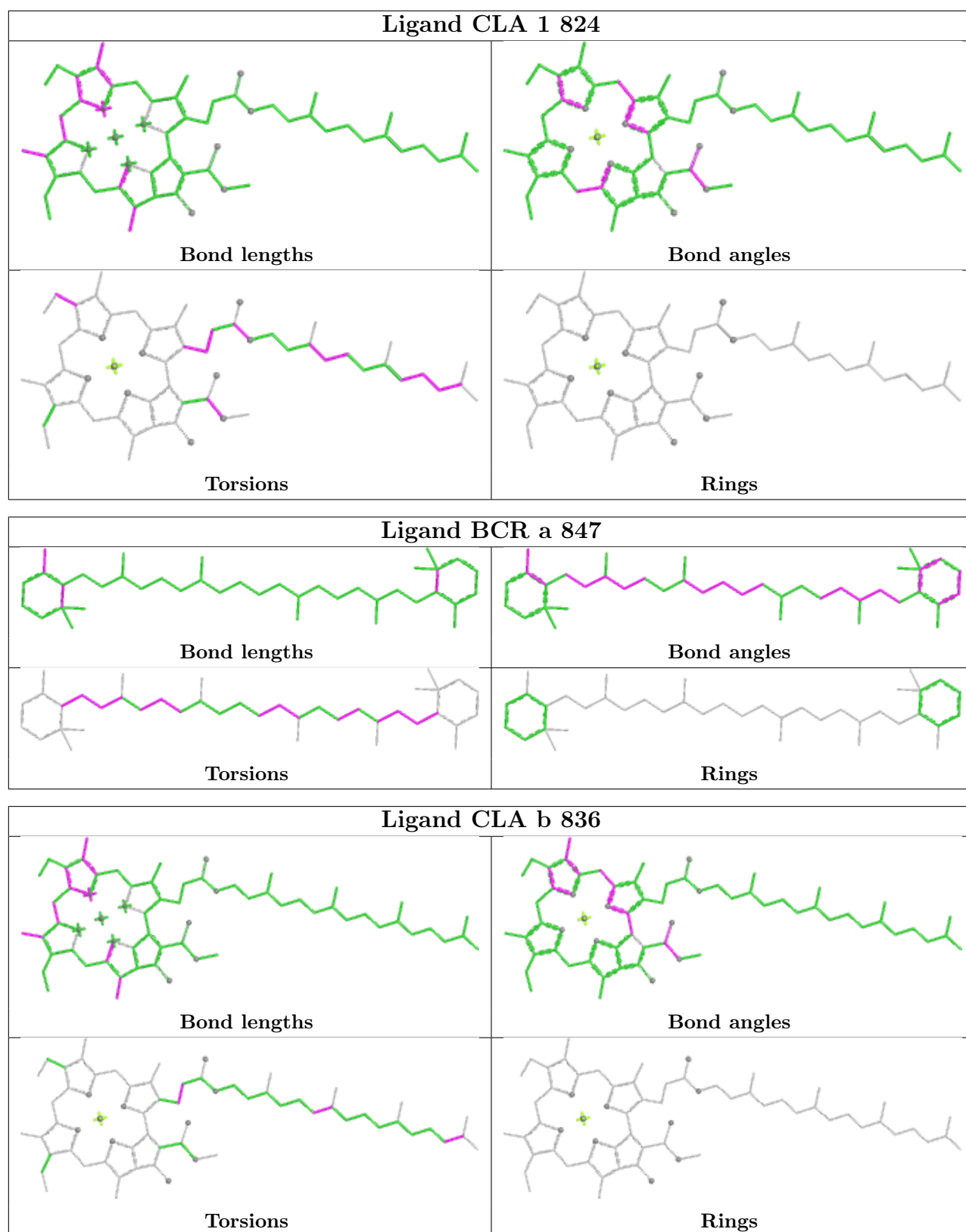


Ligand CLA 2 817

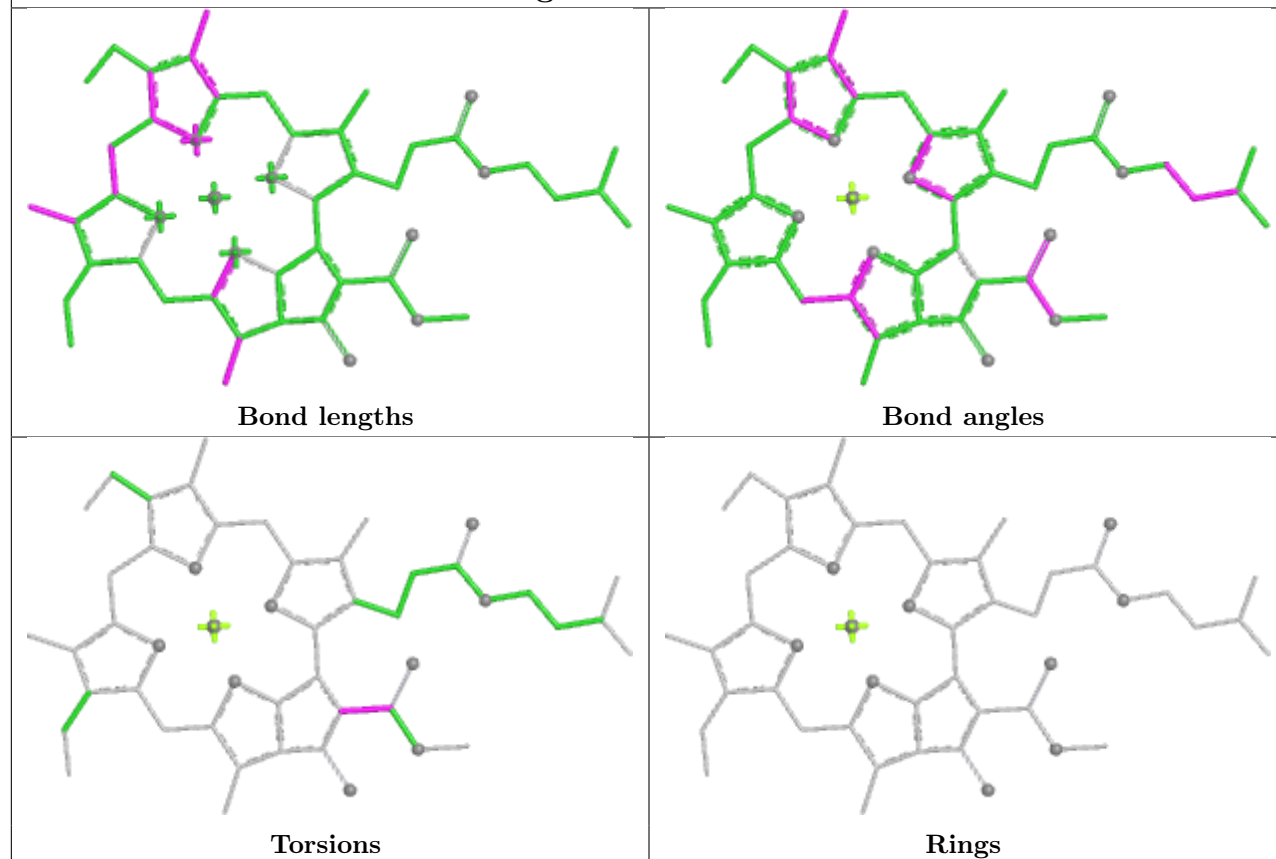




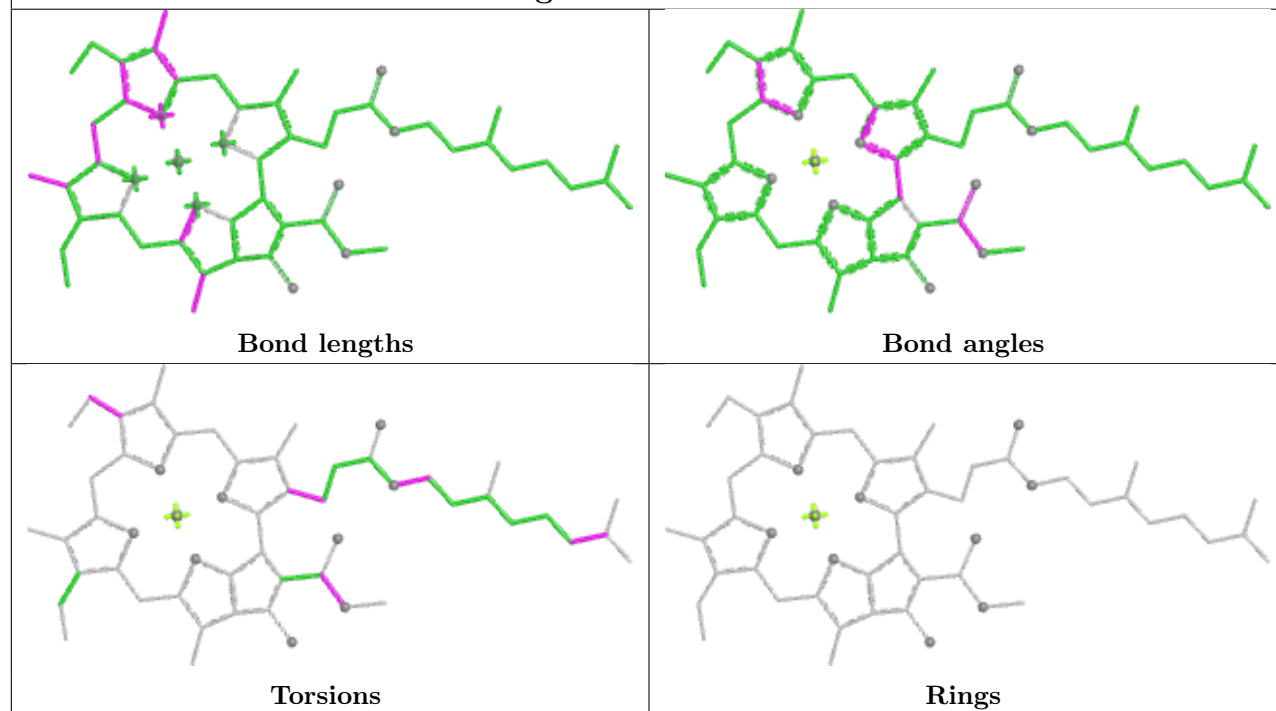


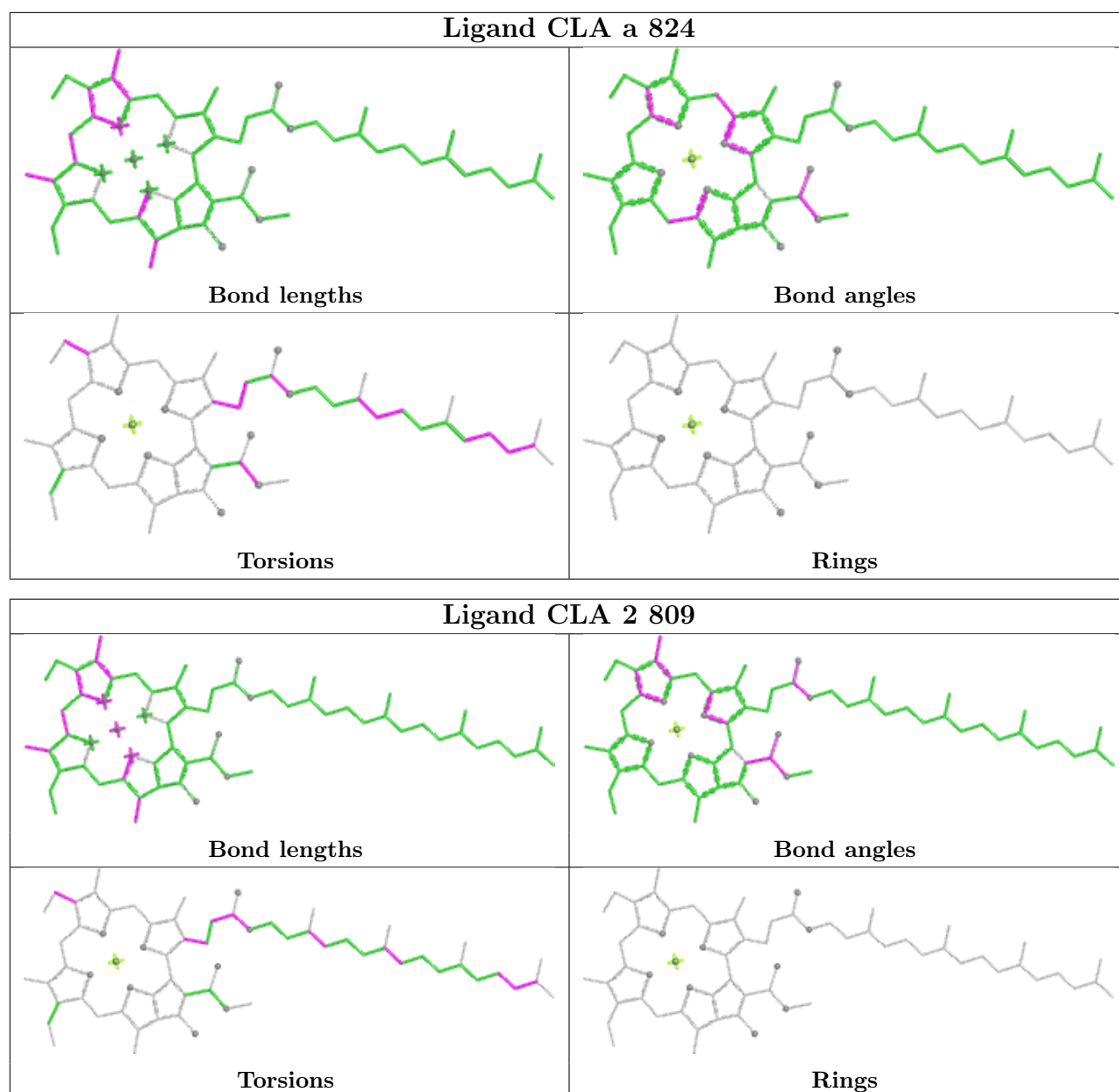


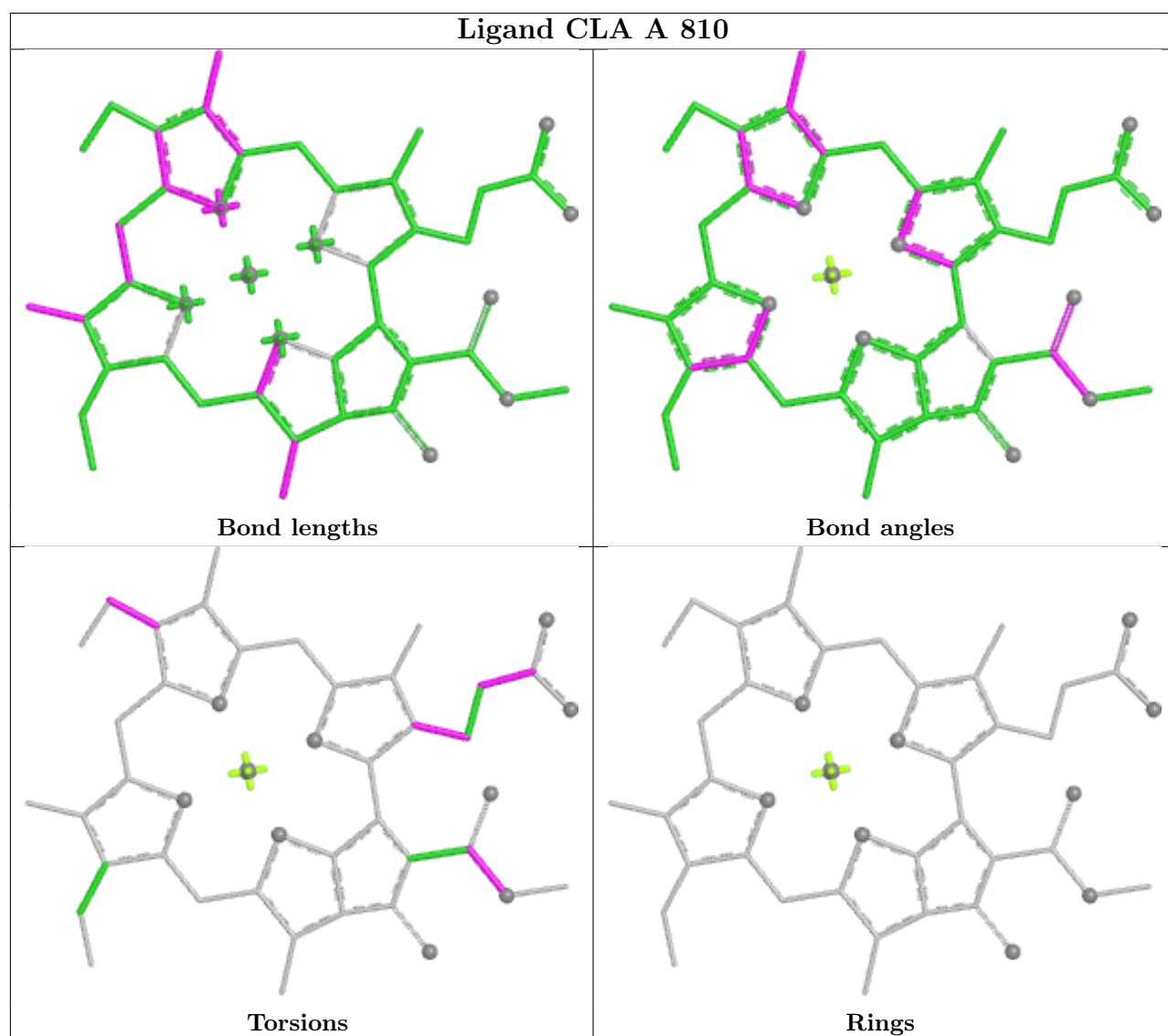
Ligand CLA 2 821



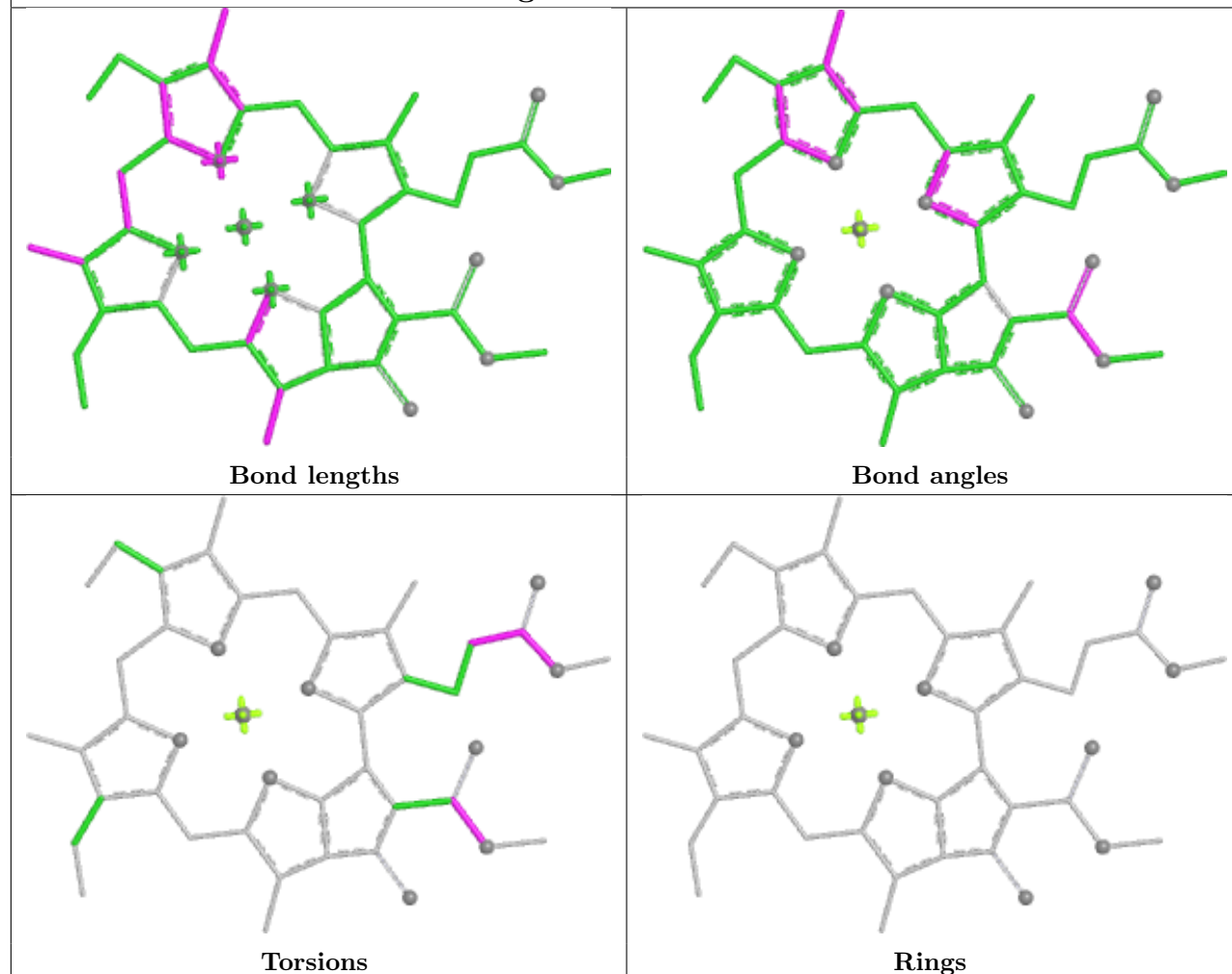
Ligand CLA b 820



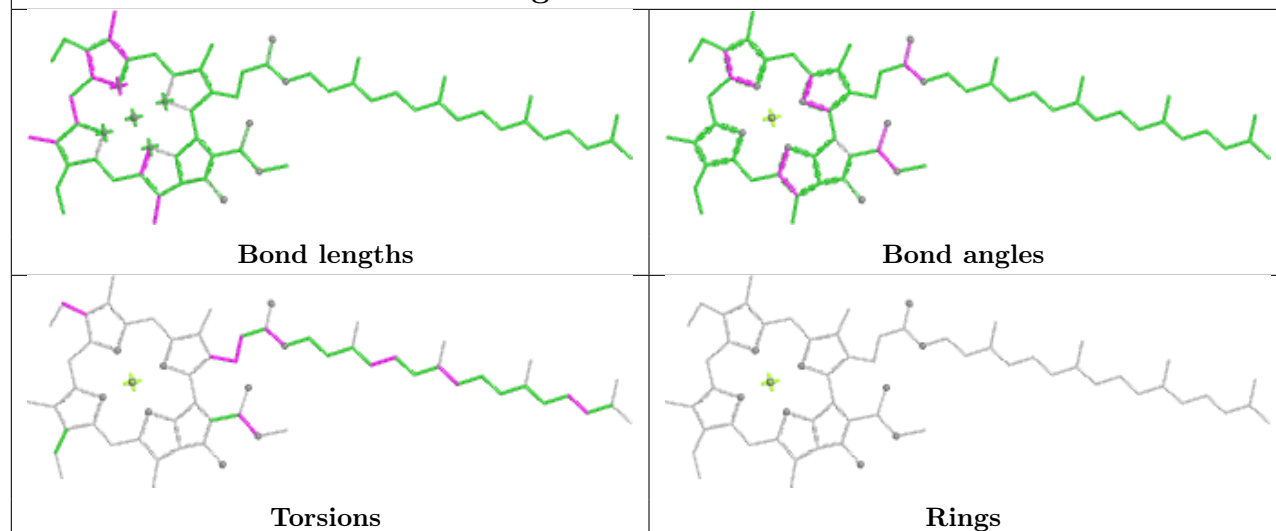




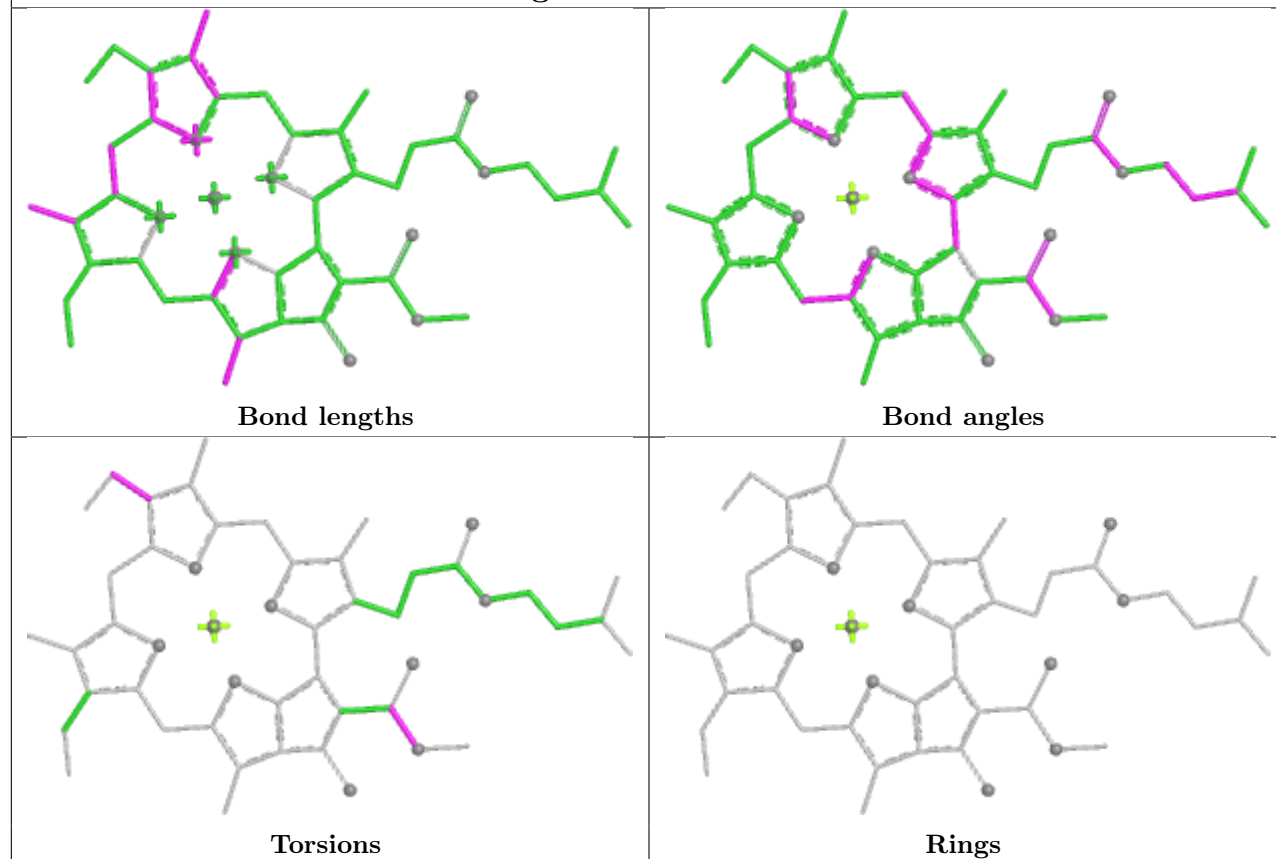
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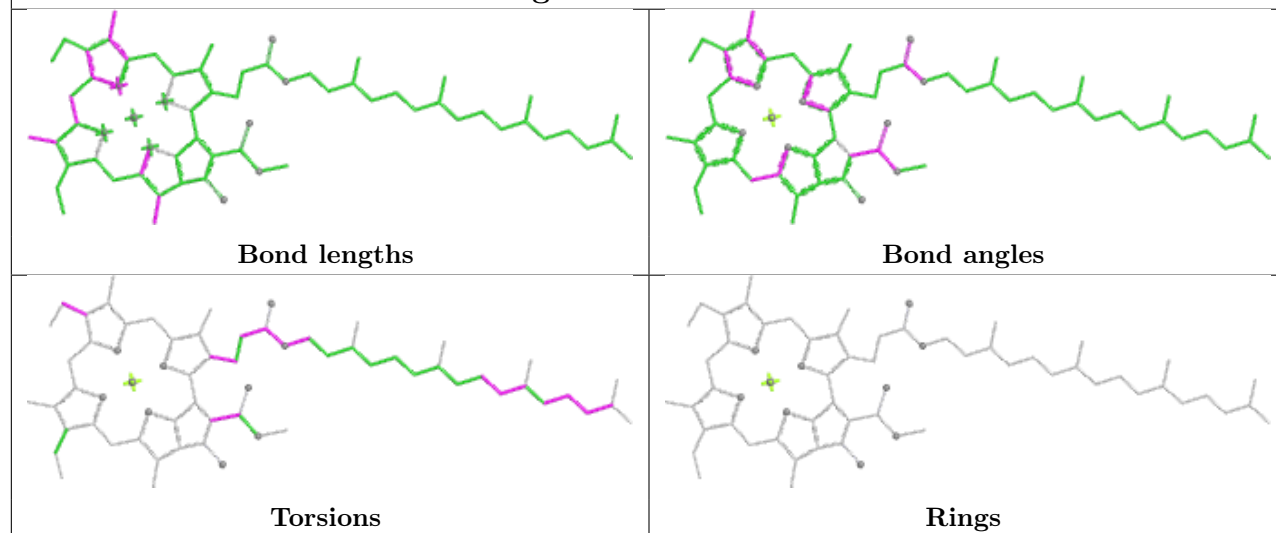
Ligand CLA A 840



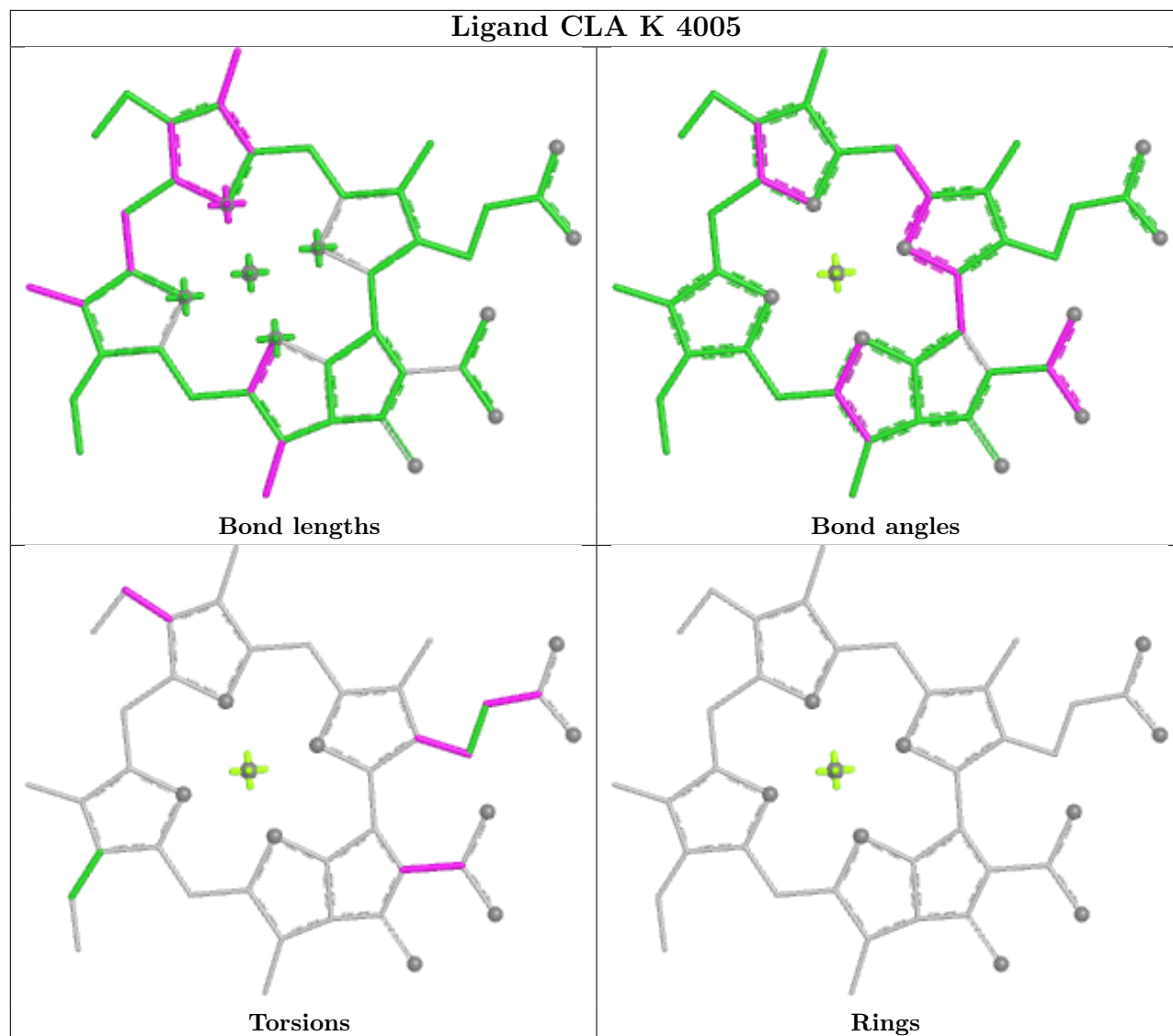
Ligand CLA A 814



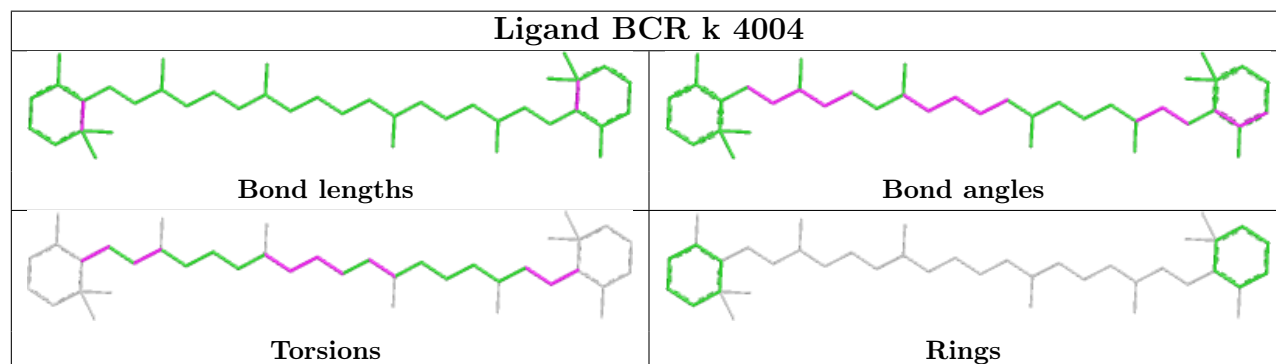
Ligand CLA B 804



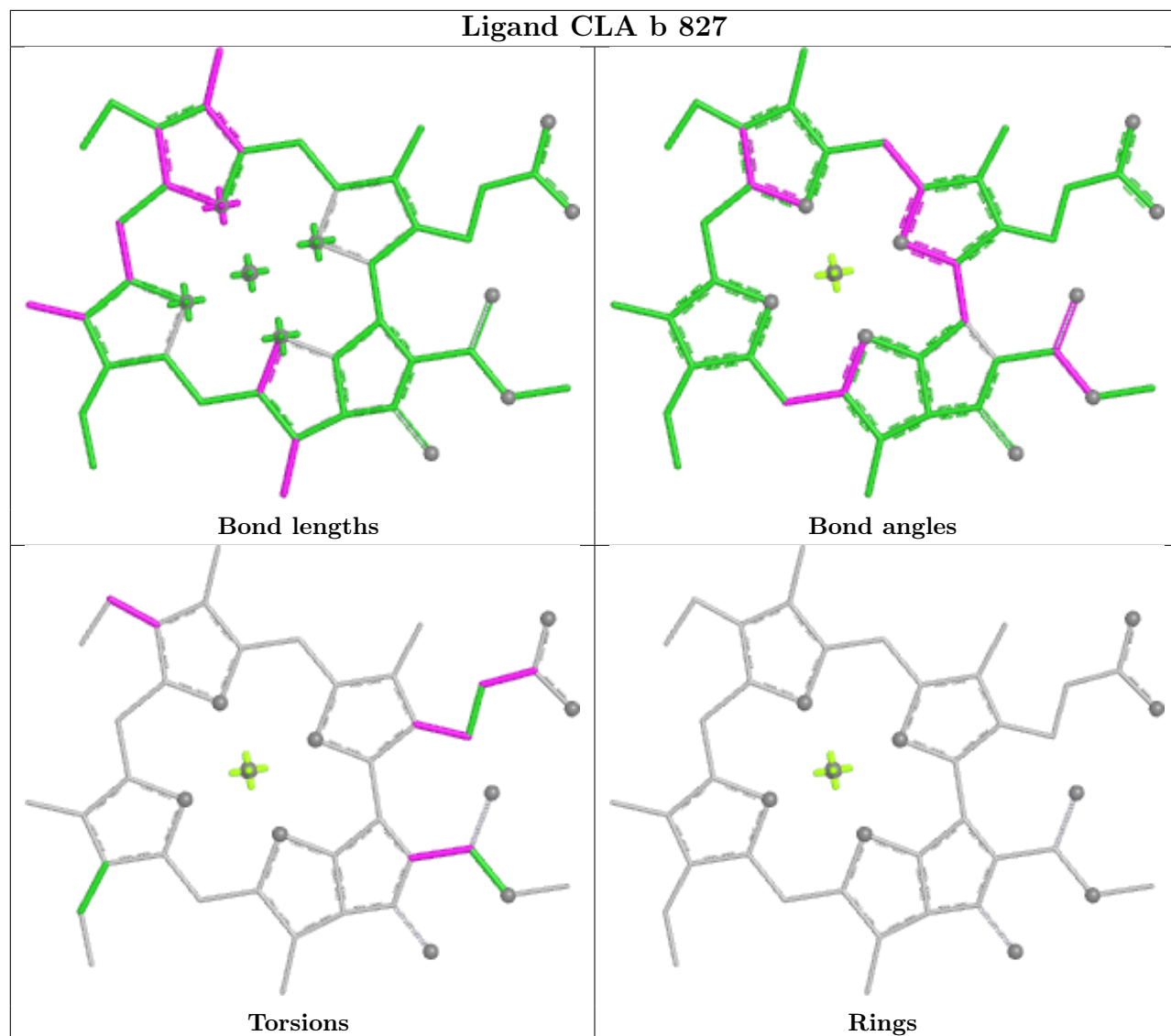
Ligand CLA K 4005

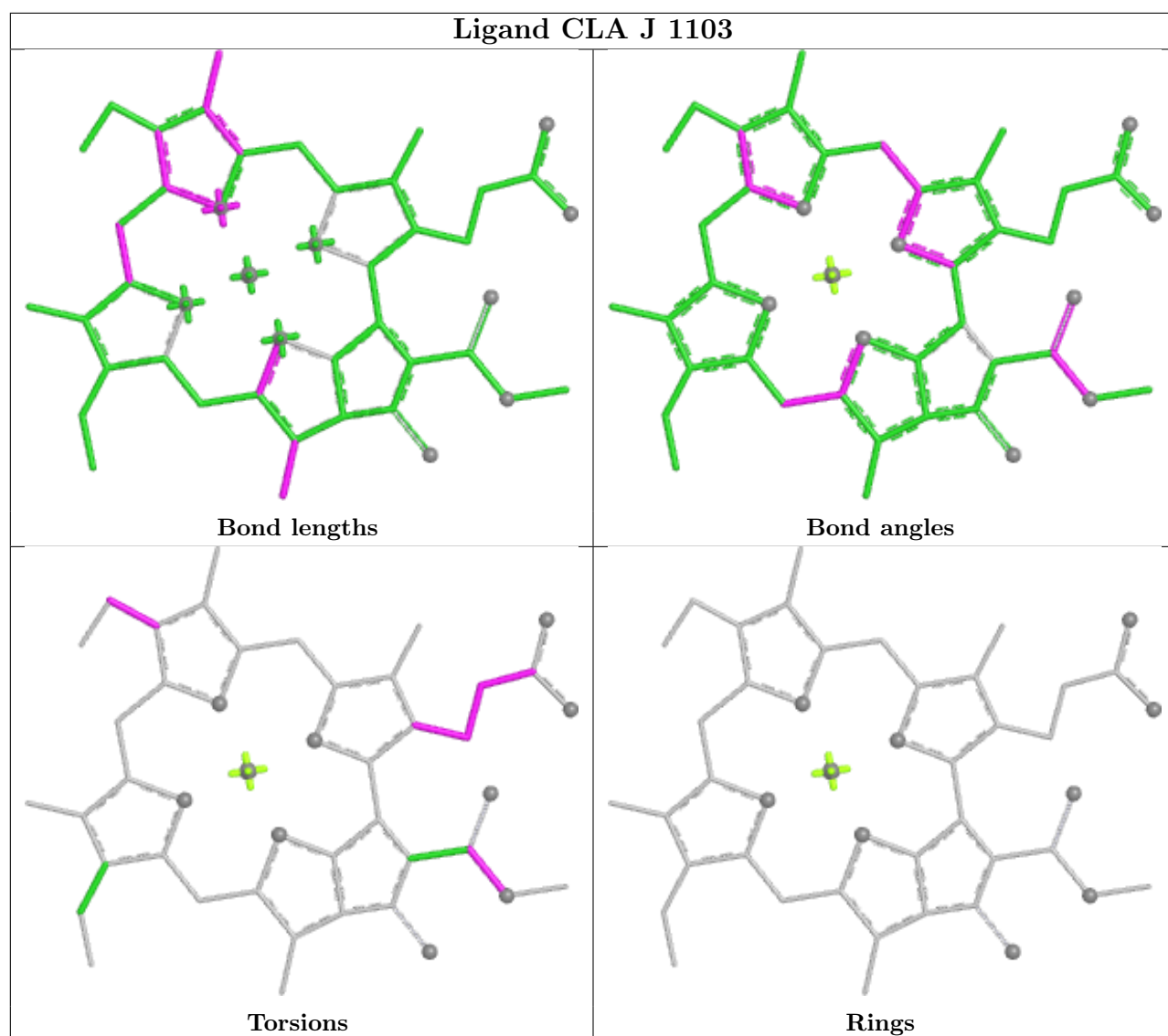


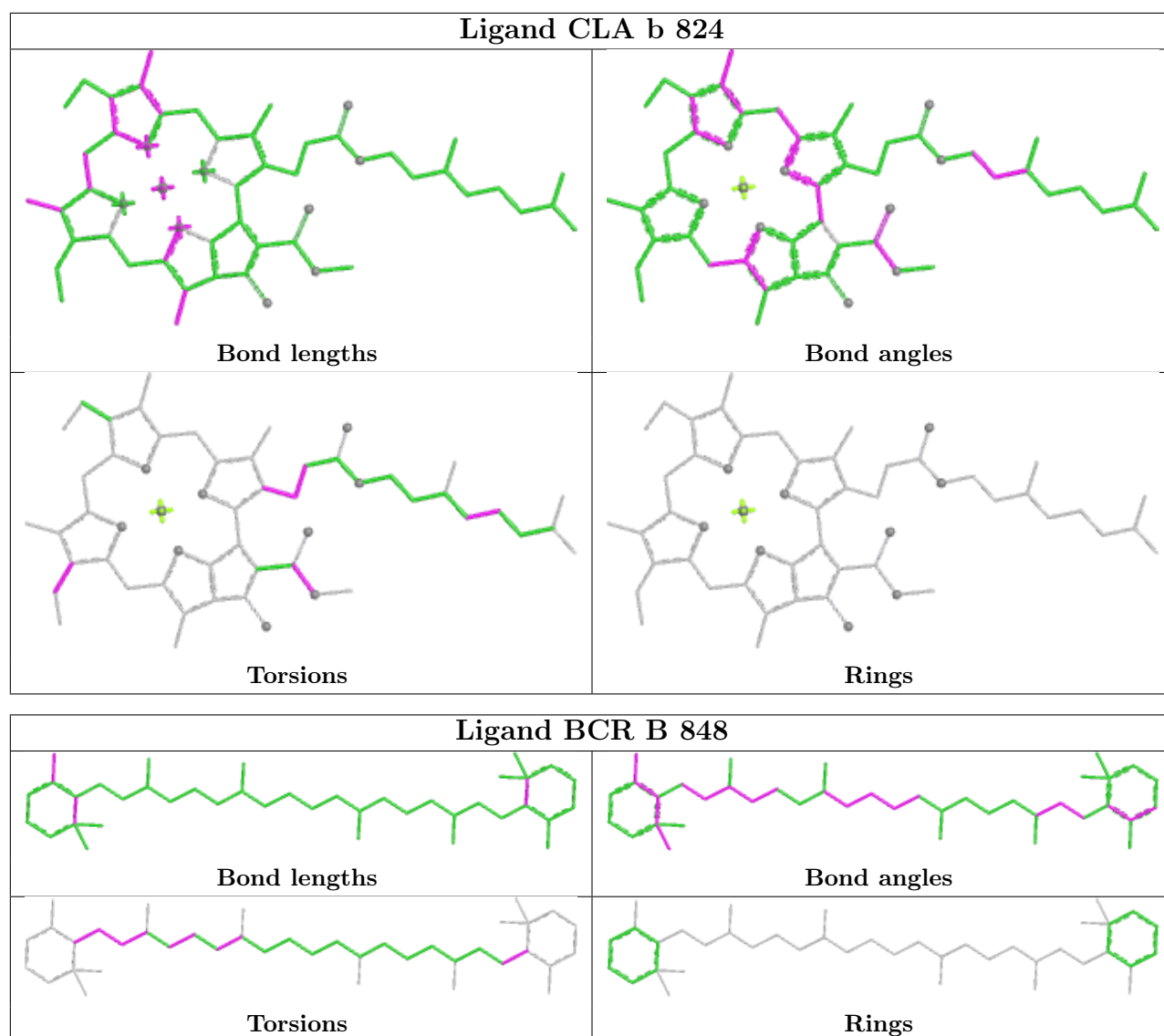
Ligand BCR k 4004



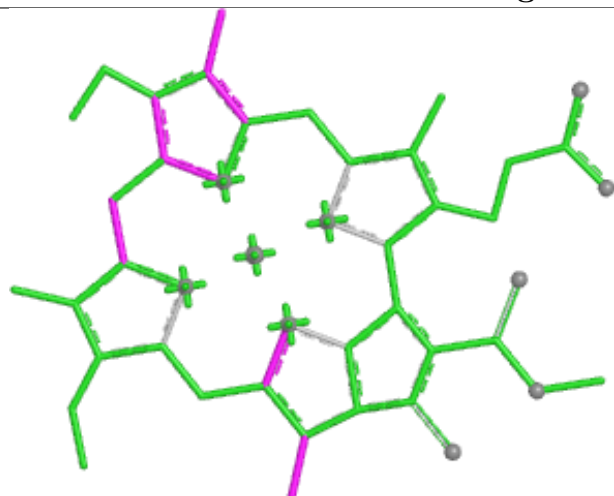
Ligand CLA b 827



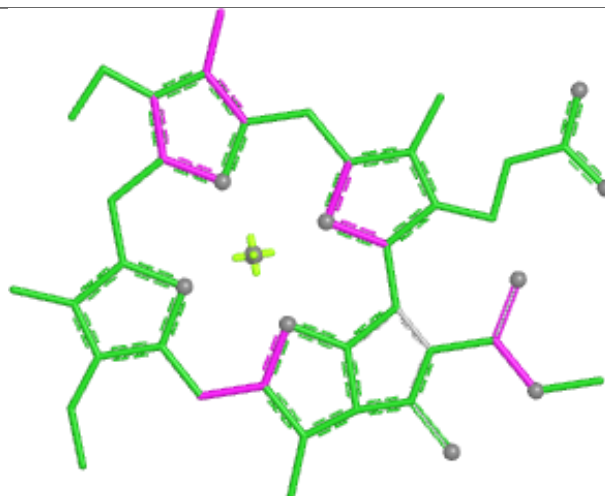




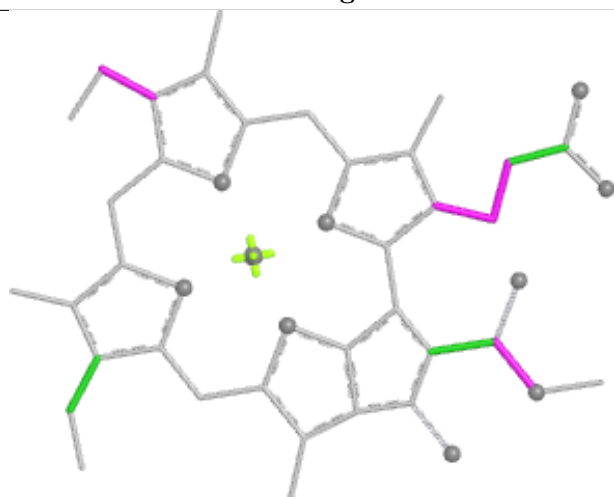
Ligand CLA b 809



Bond lengths



Bond angles

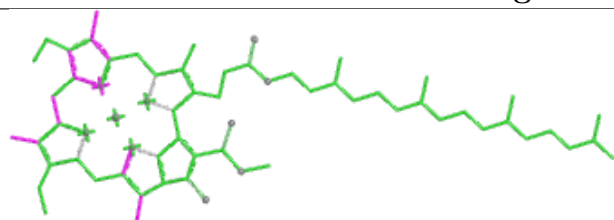


Torsions

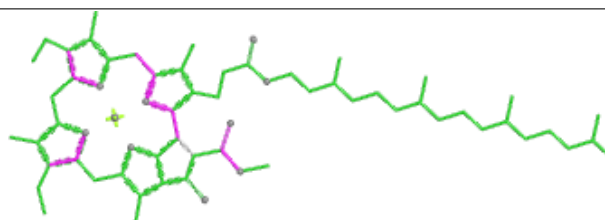


Rings

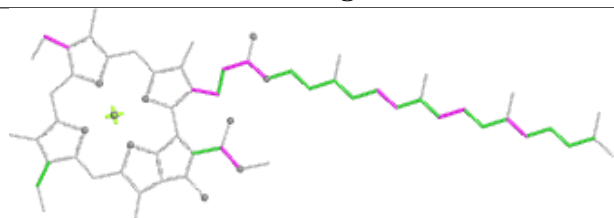
Ligand CLA A 833



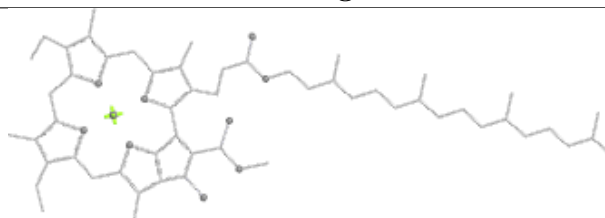
Bond lengths



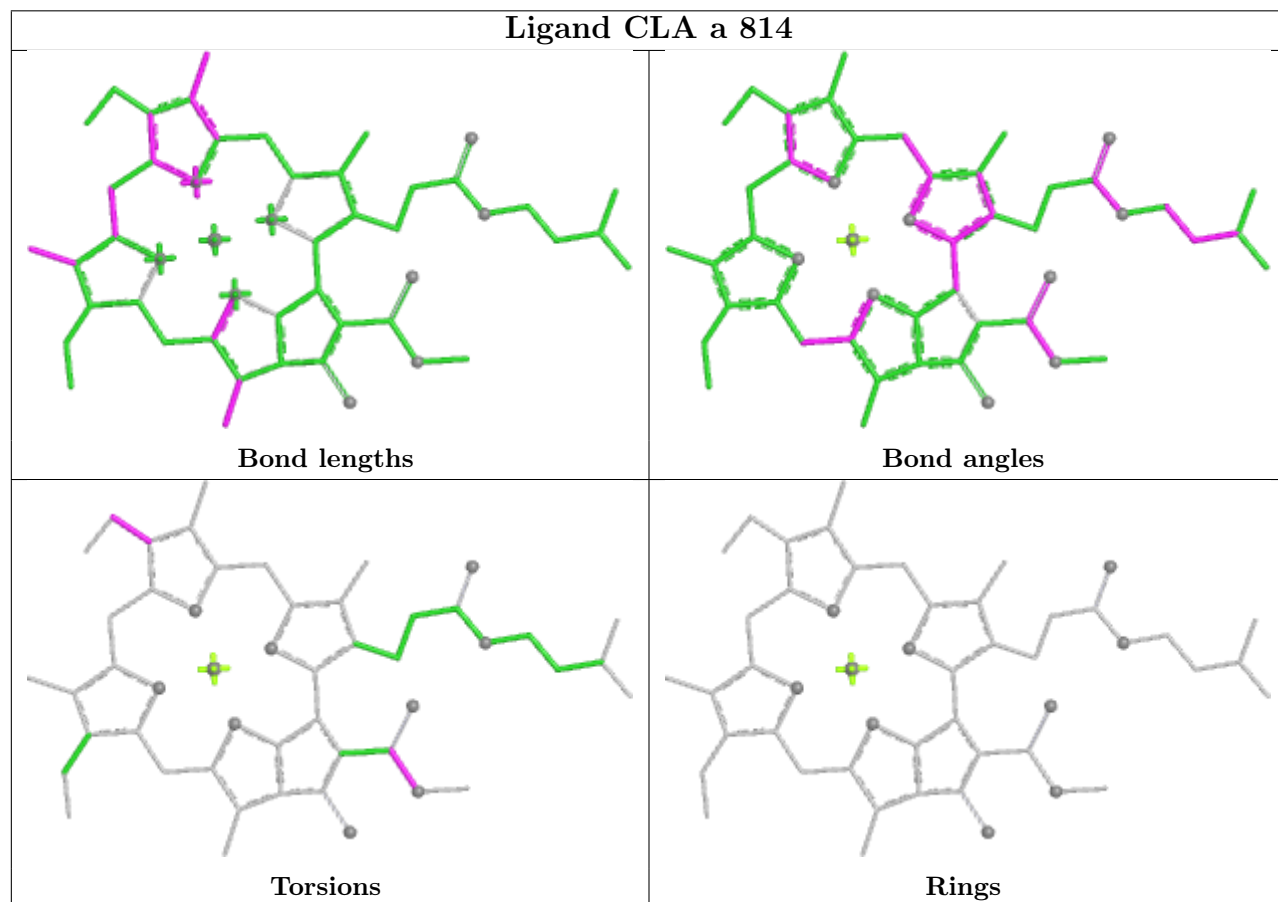
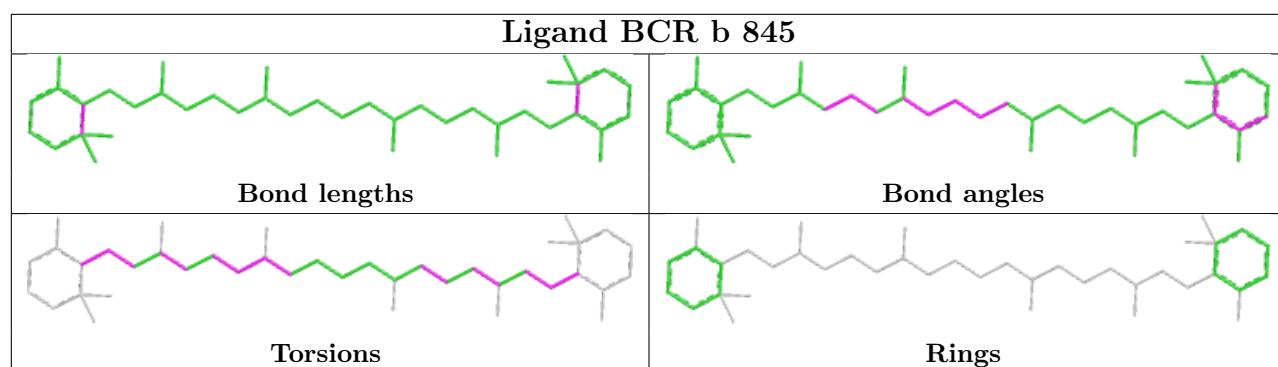
Bond angles

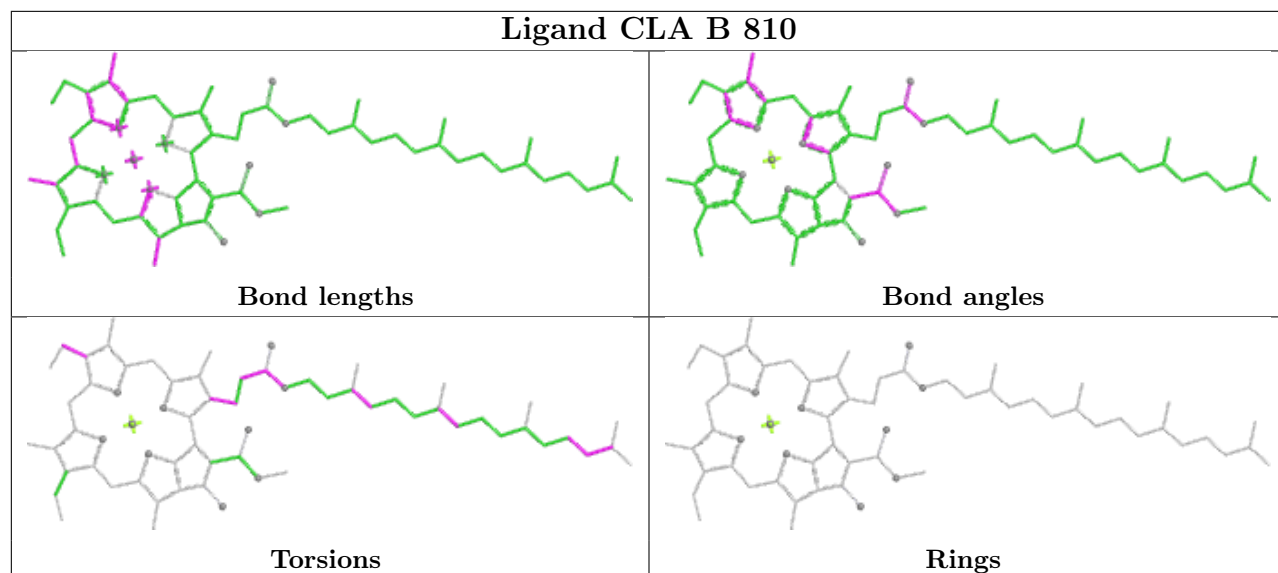
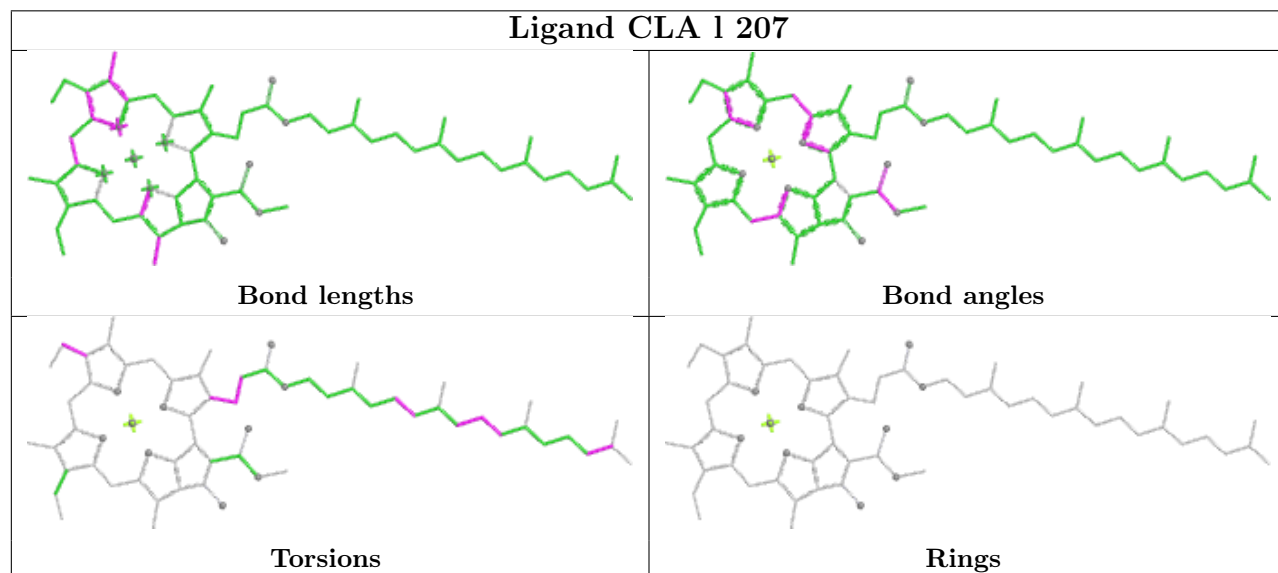
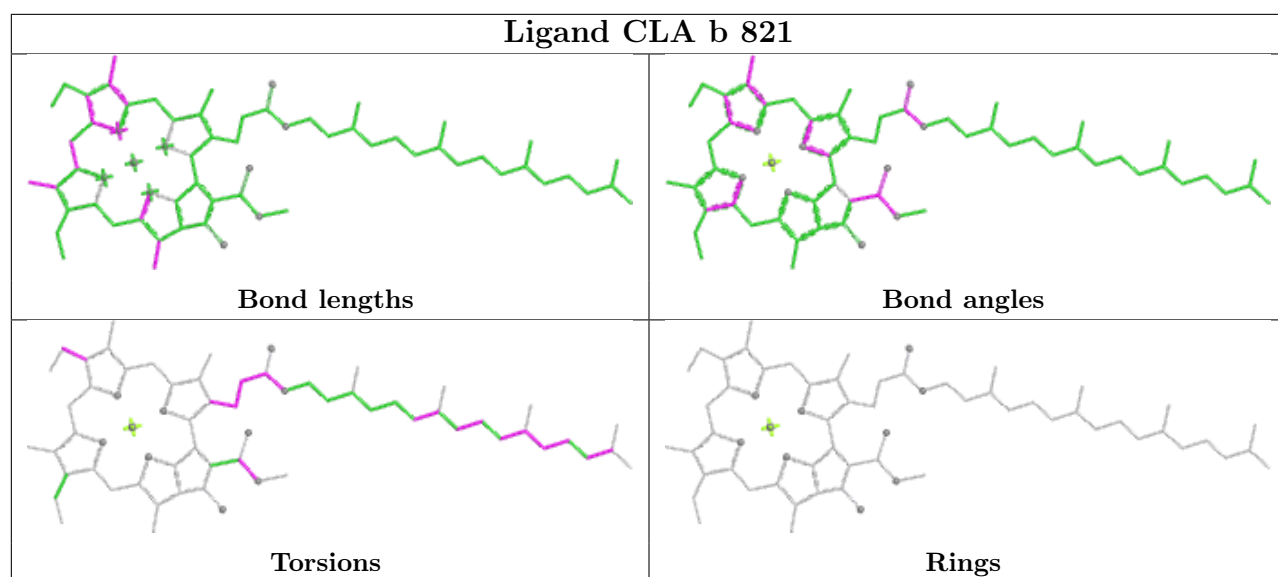


Torsions

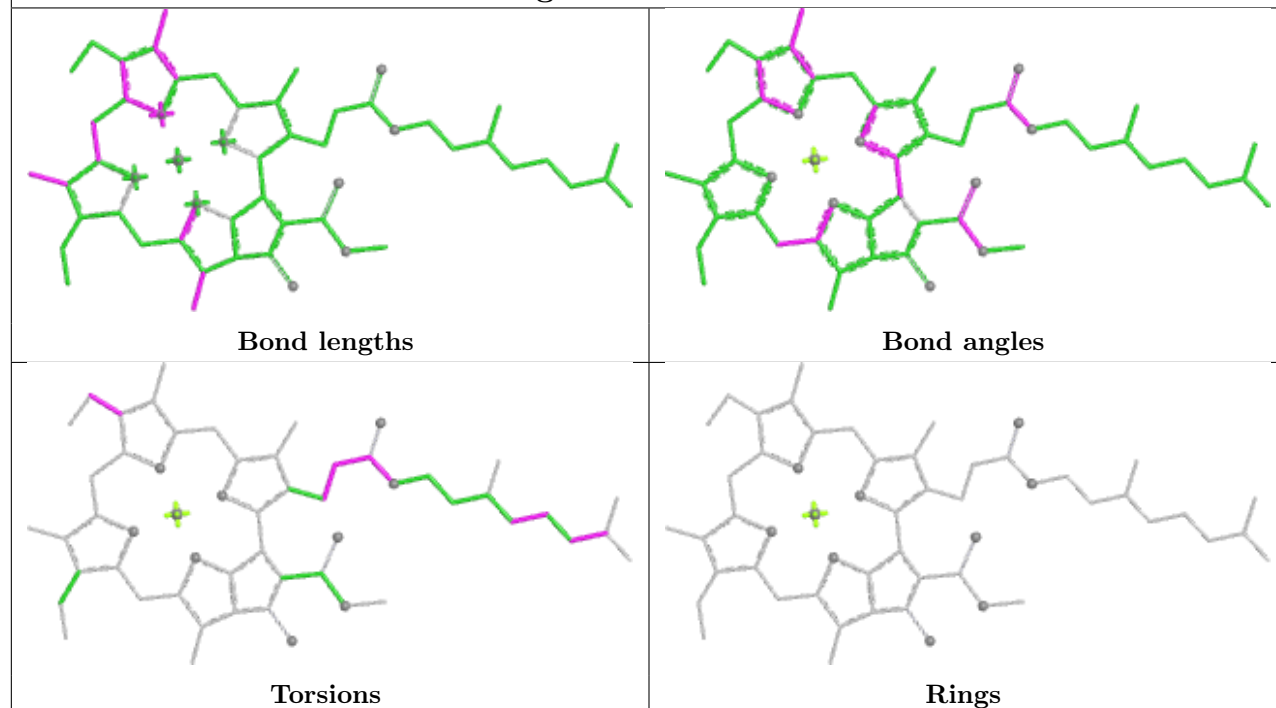


Rings

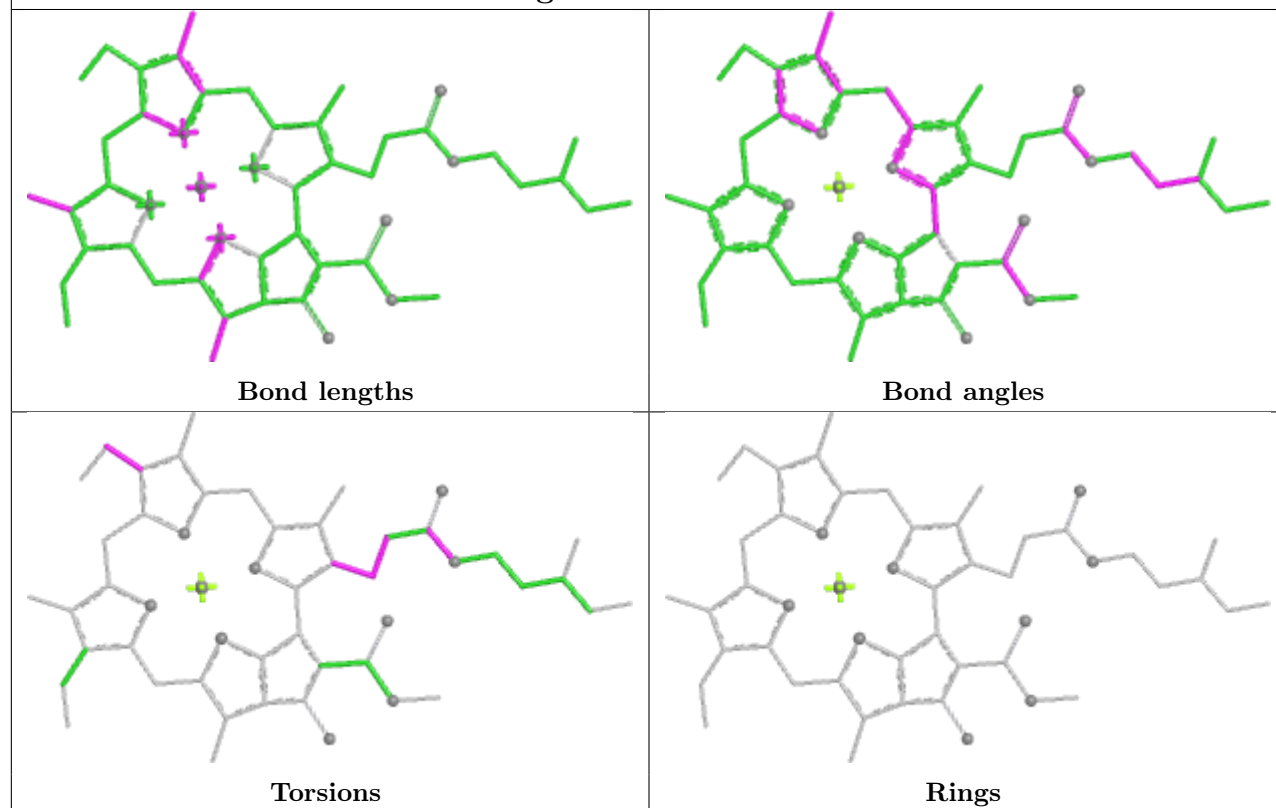


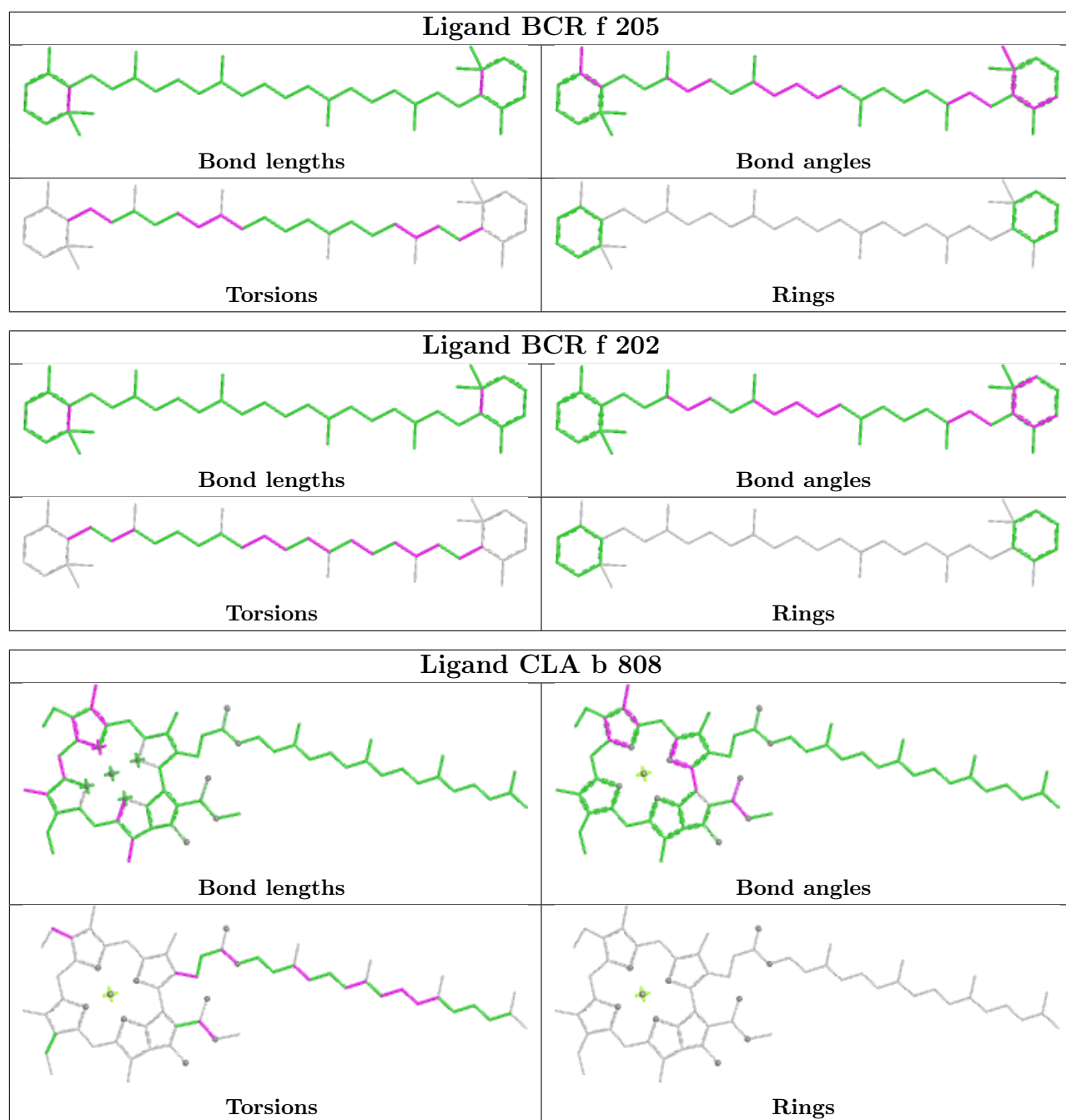


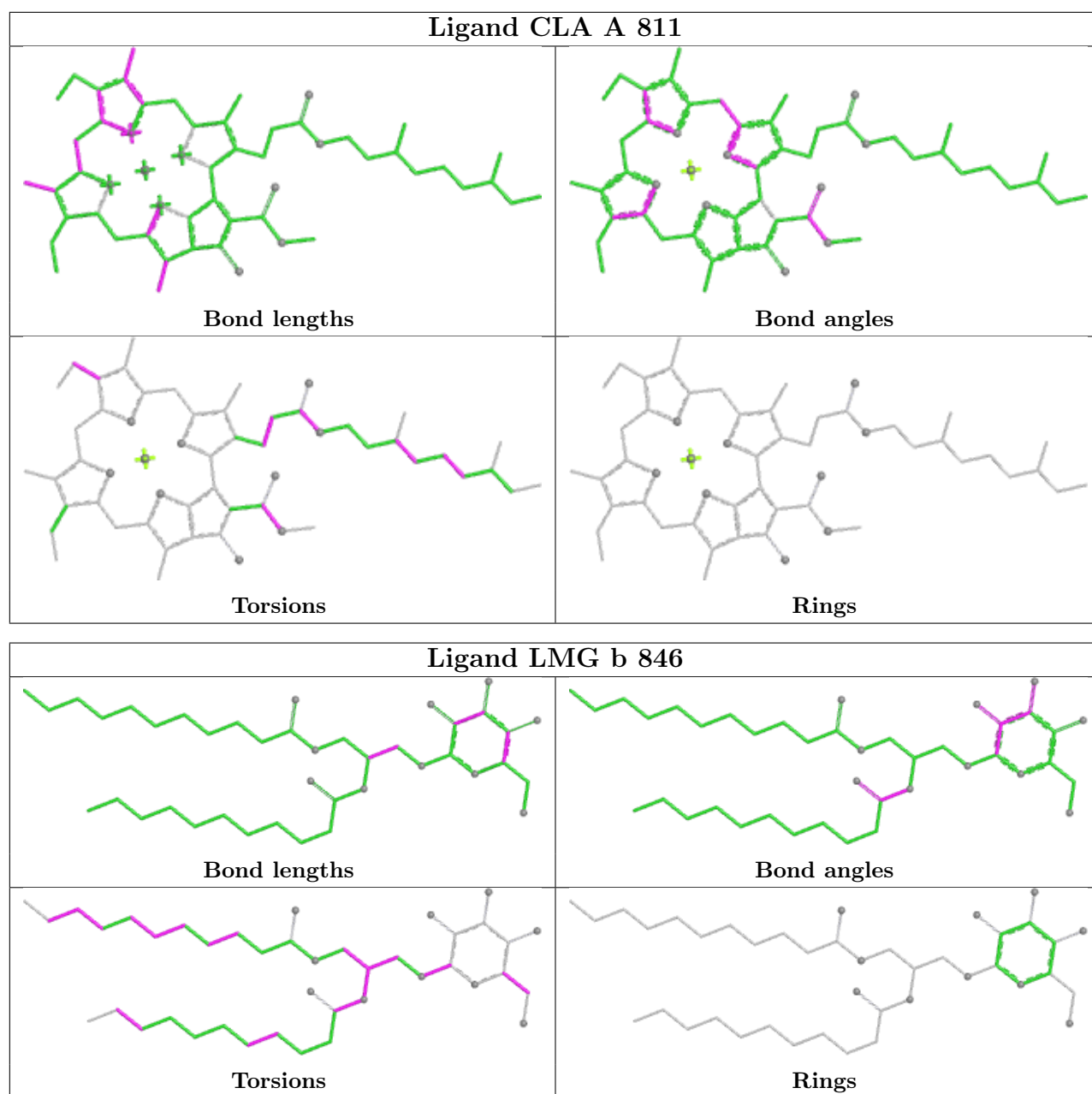
Ligand CLA a 817



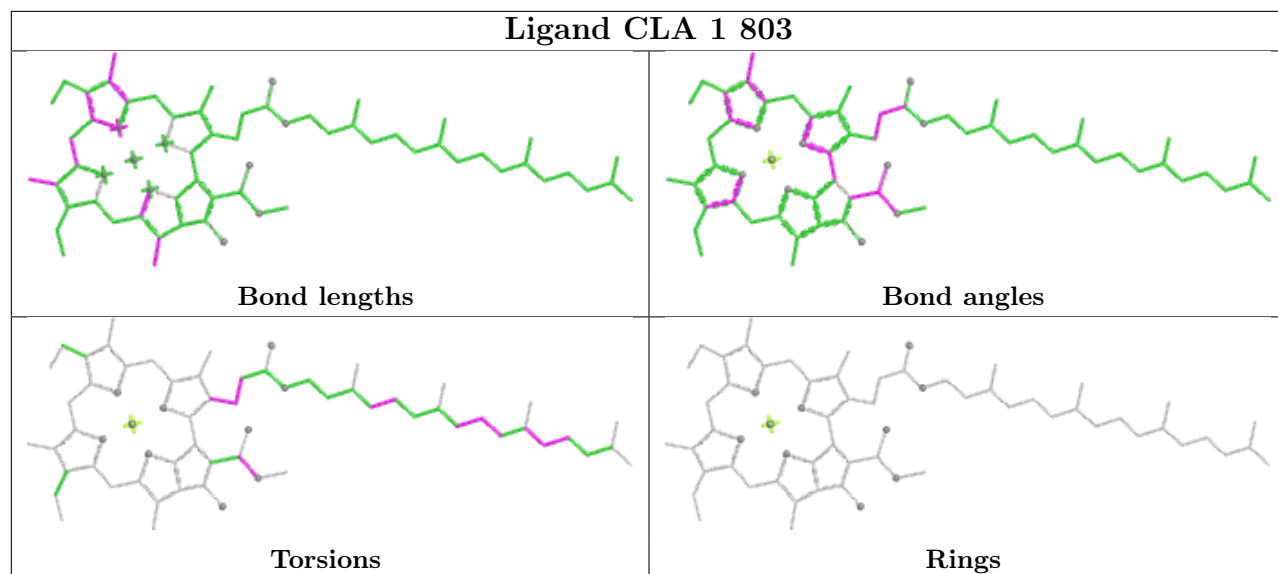
Ligand CLA a 836



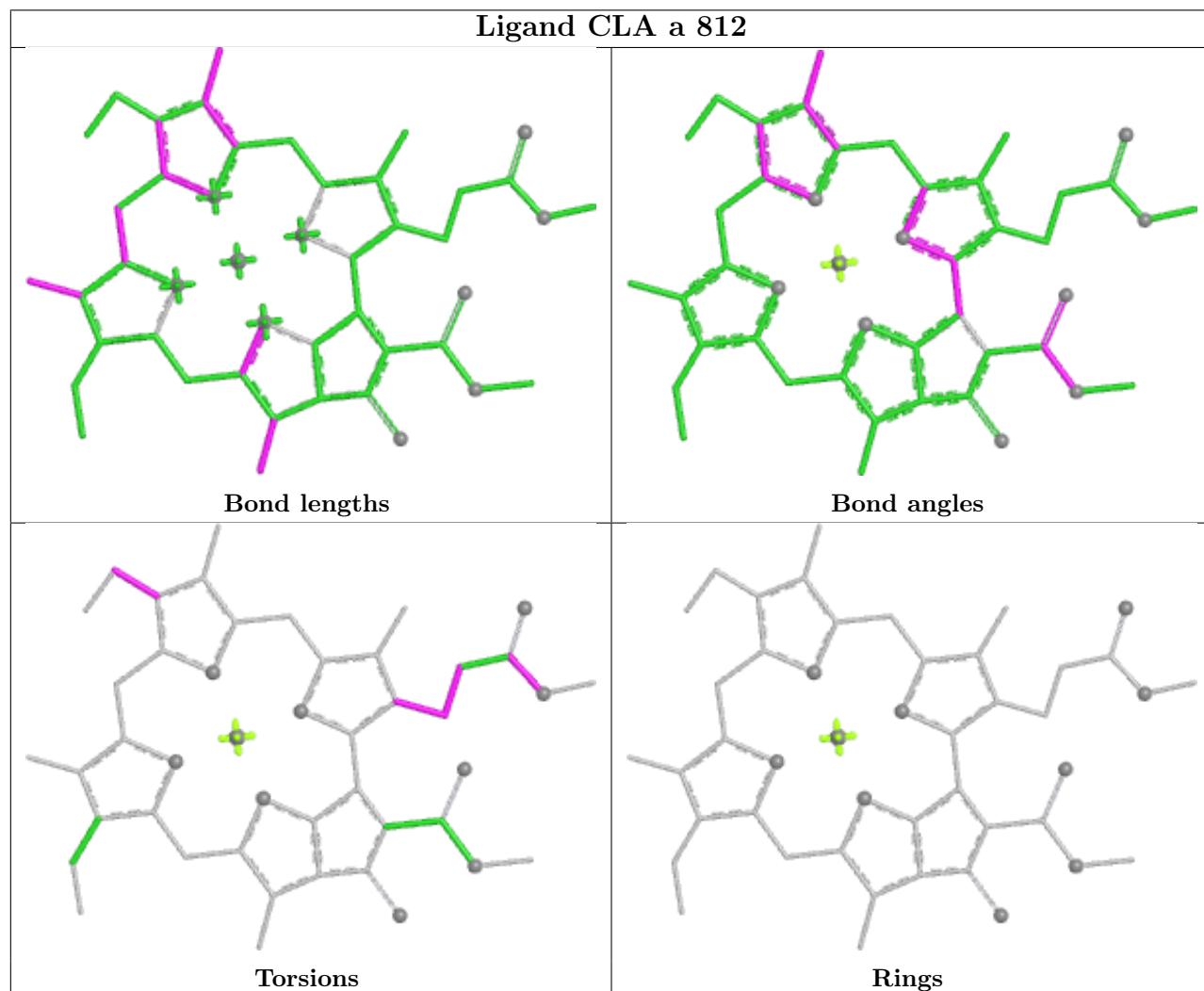


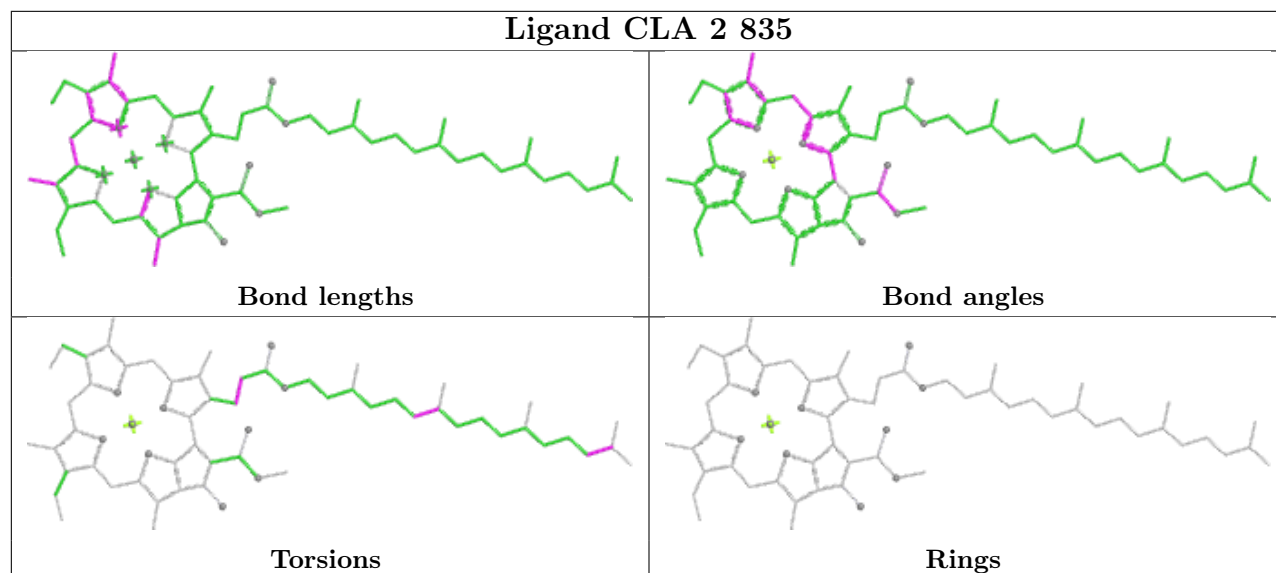
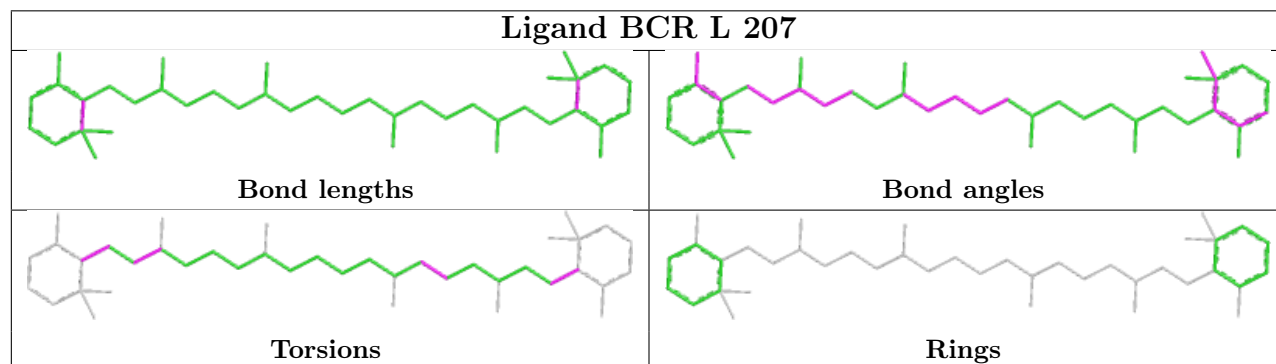
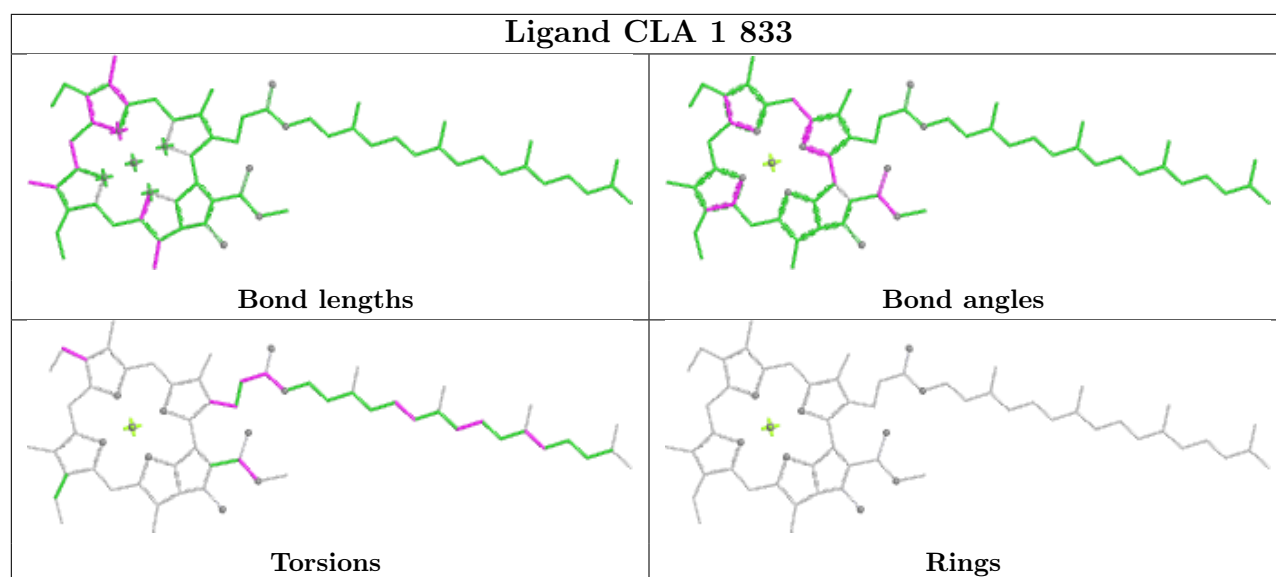


Ligand CLA 1 803

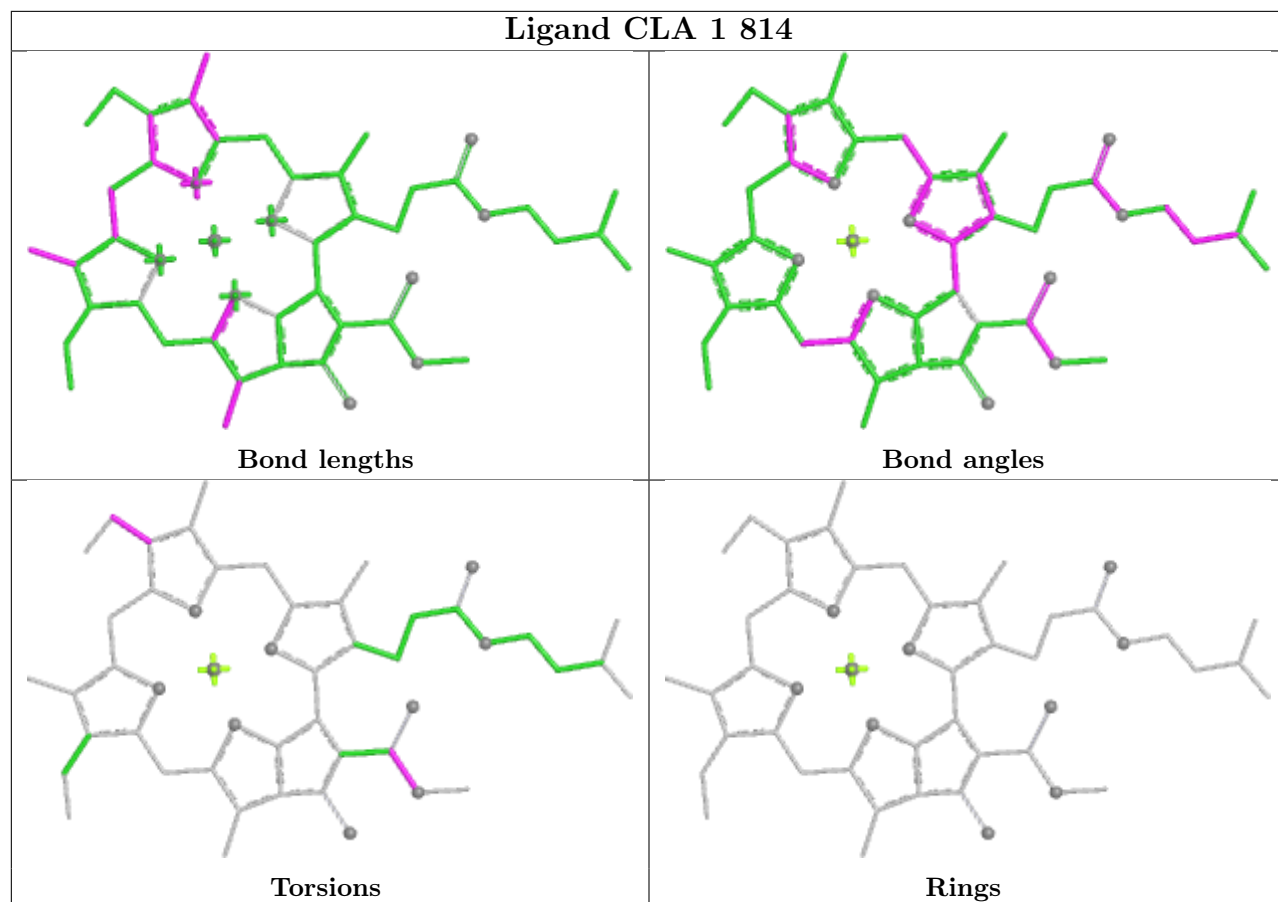


Ligand CLA a 812

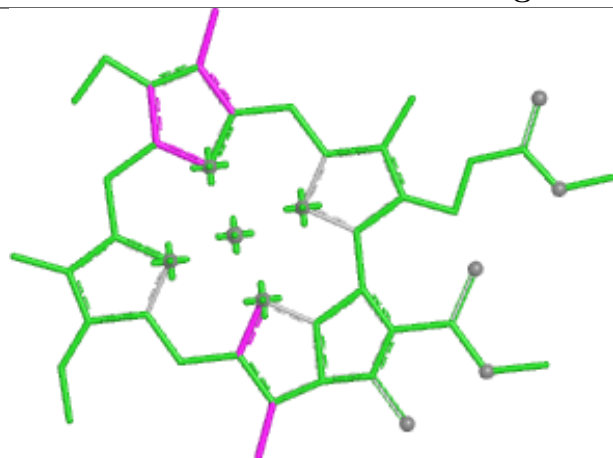




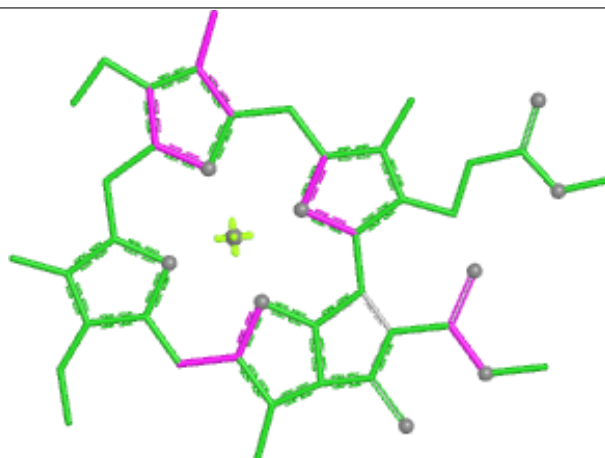
Ligand CLA 1 814



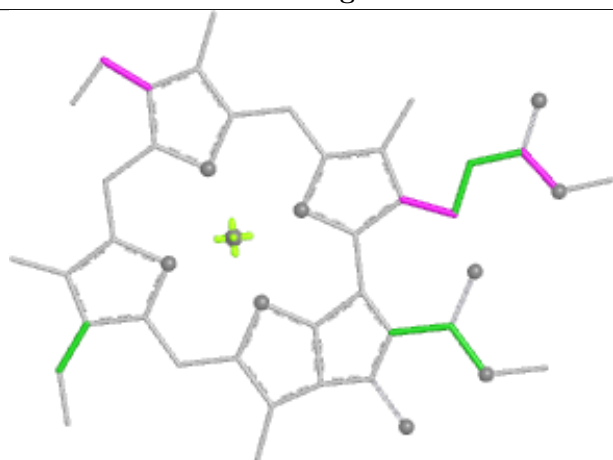
Ligand CLA A 820



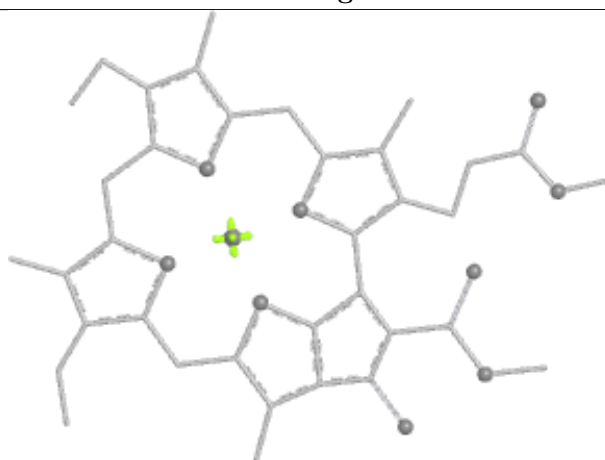
Bond lengths



Bond angles

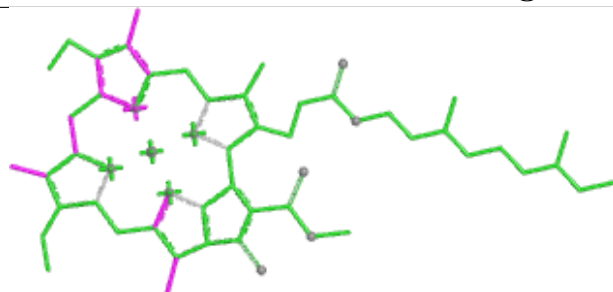


Torsions

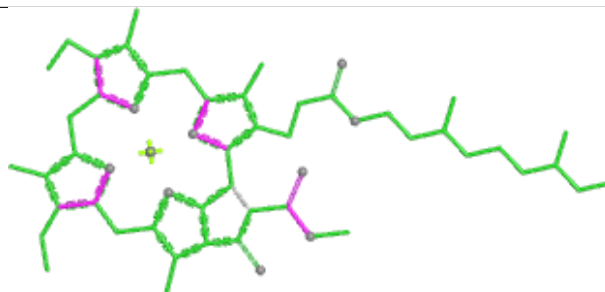


Rings

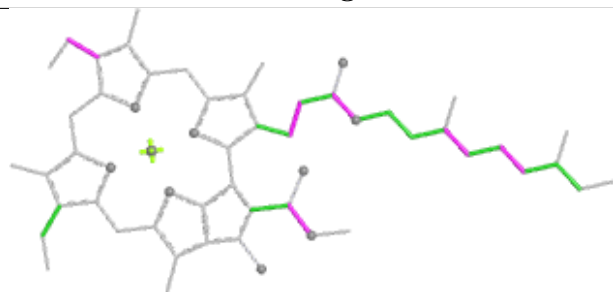
Ligand CLA 1 811



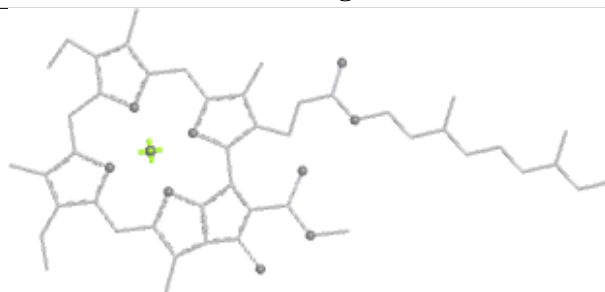
Bond lengths



Bond angles

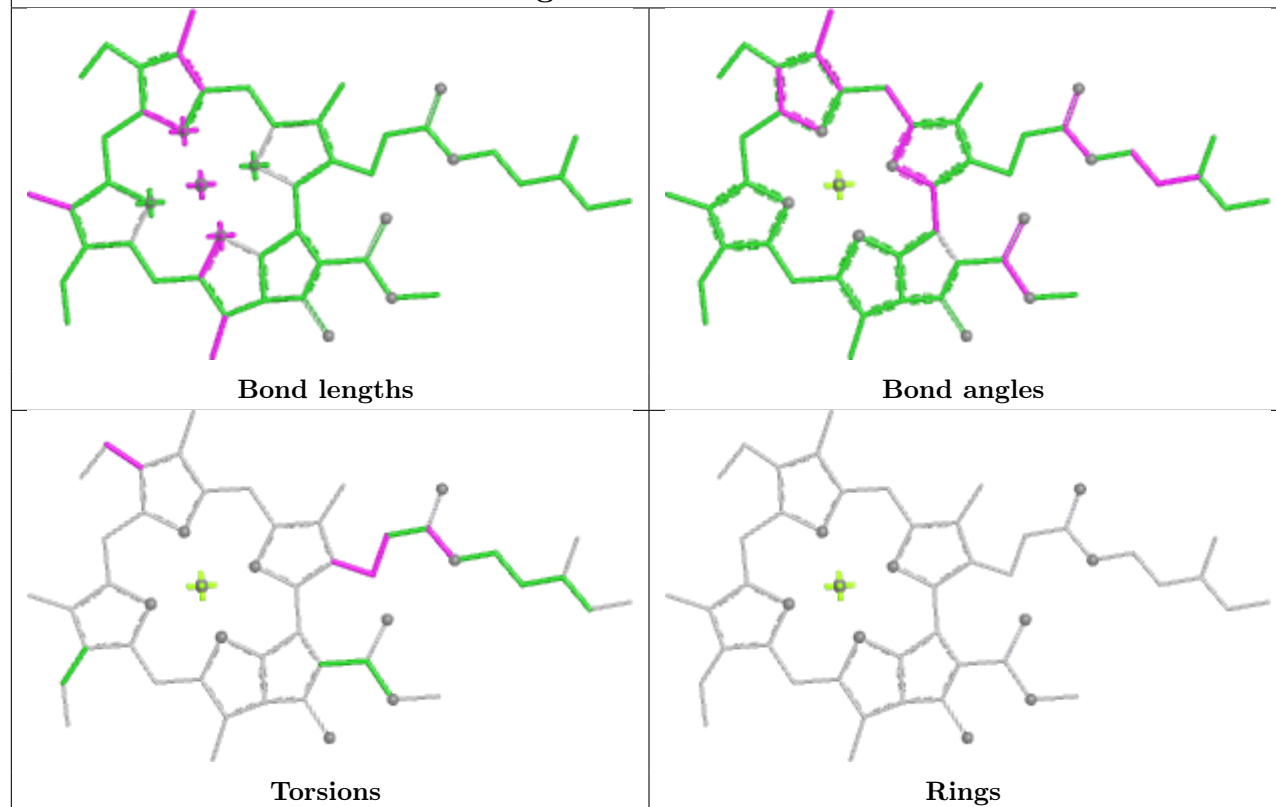


Torsions

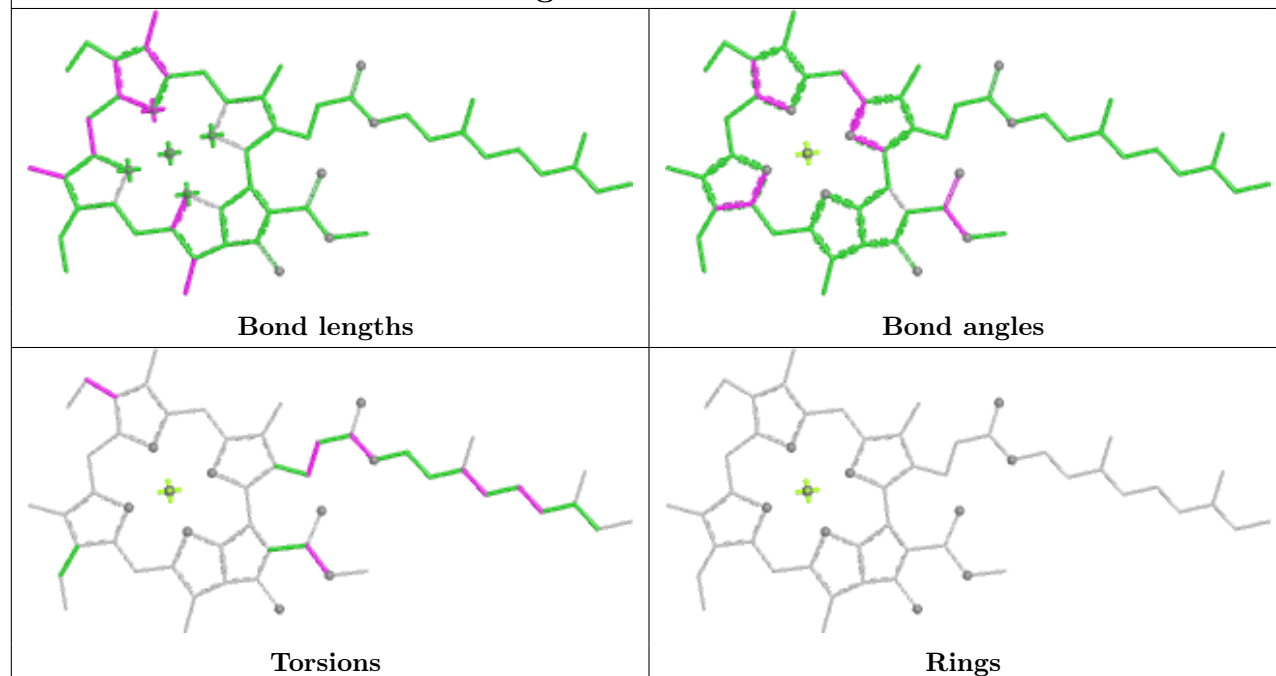


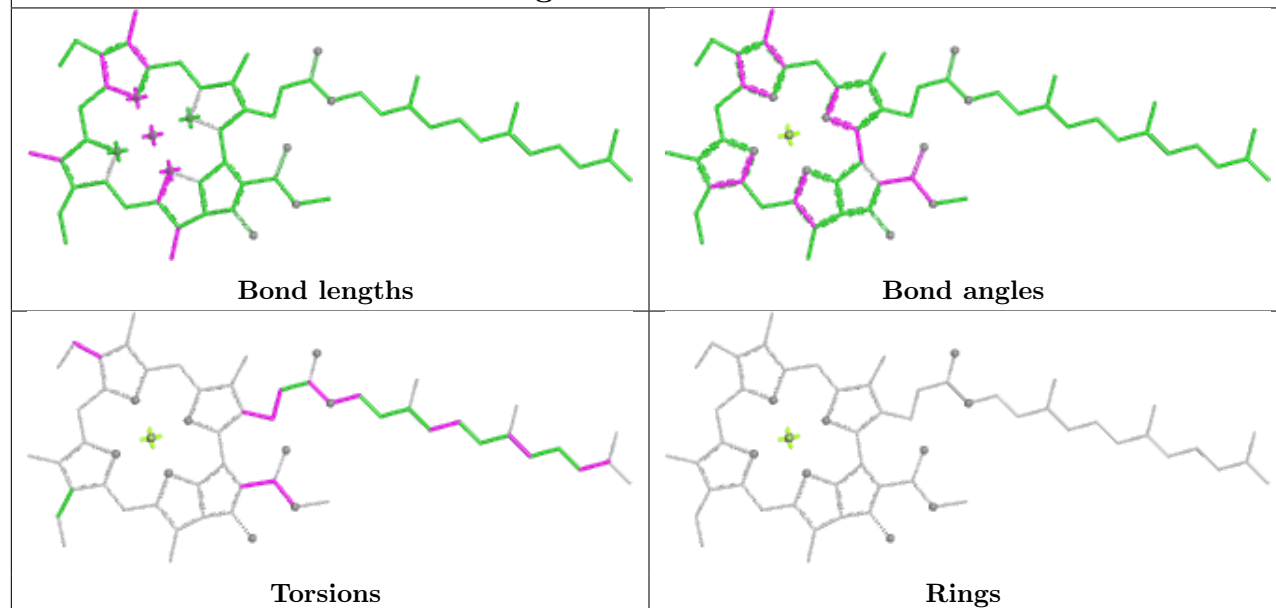
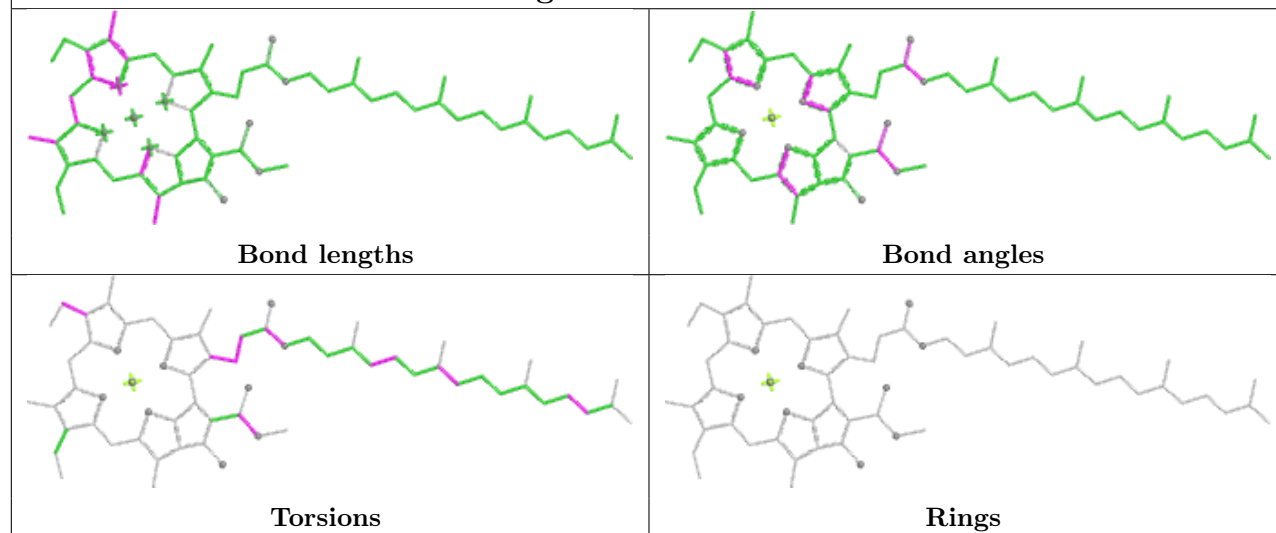
Rings

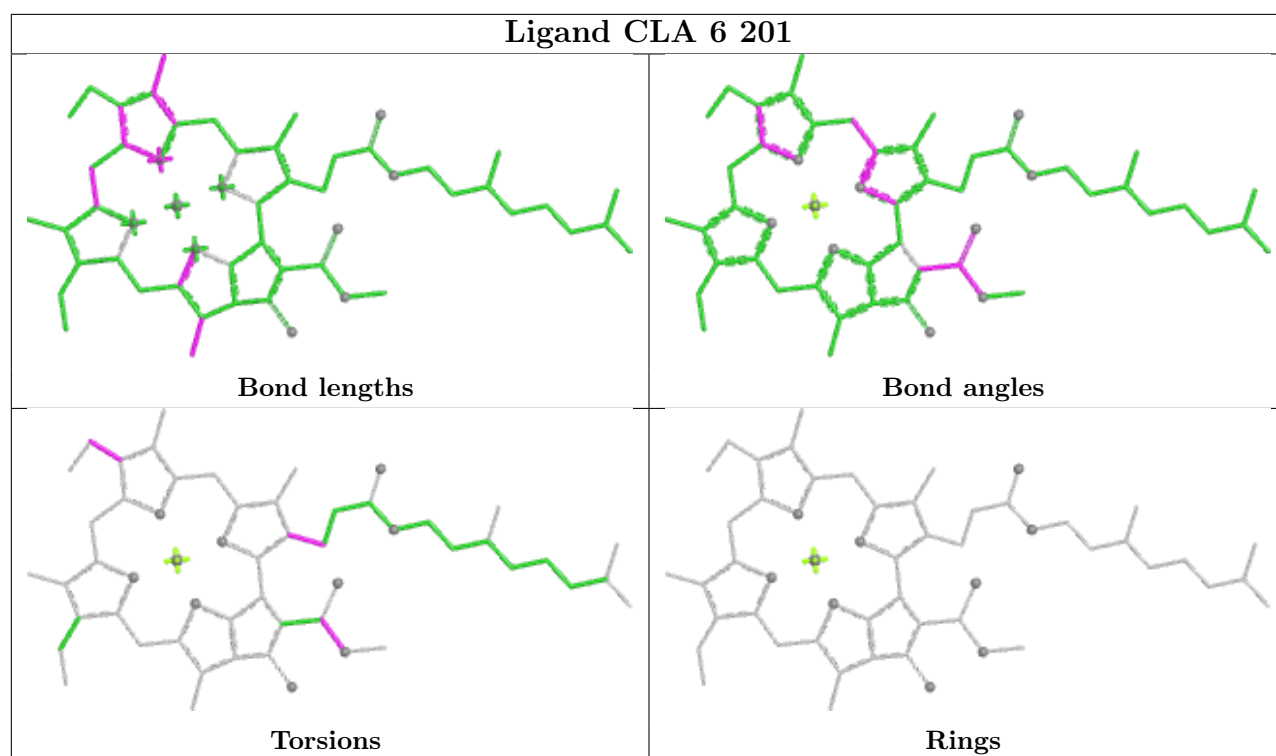
Ligand CLA 1 836



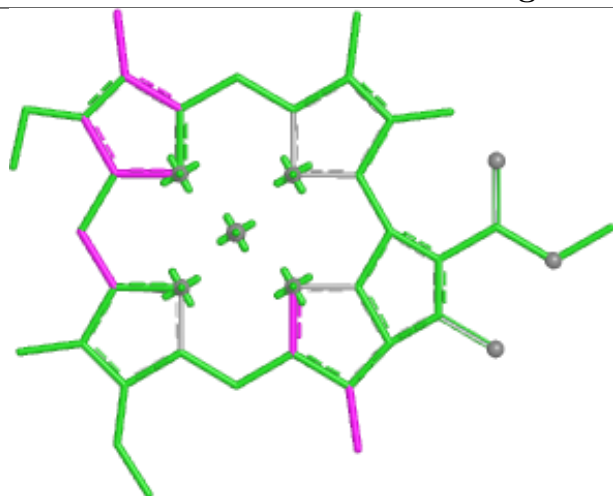
Ligand CLA a 811



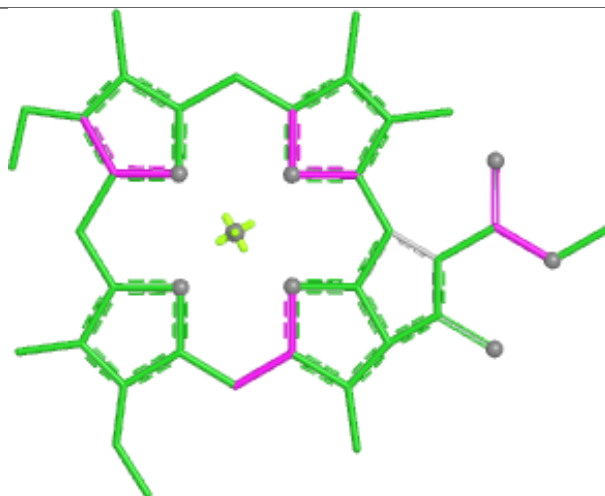
Ligand CLA b 826**Ligand CLA a 840**



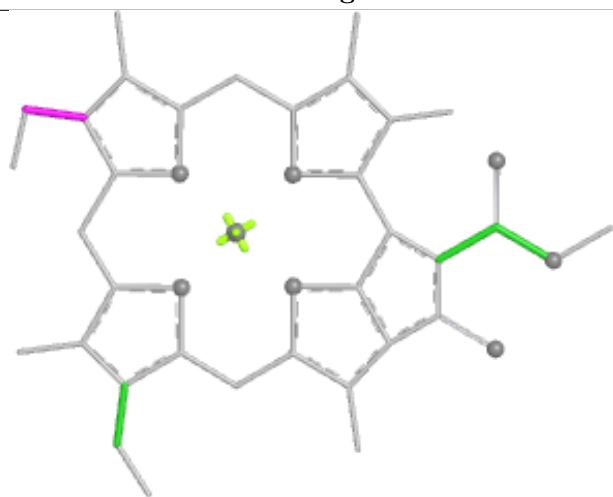
Ligand CLA 2 816



Bond lengths



Bond angles

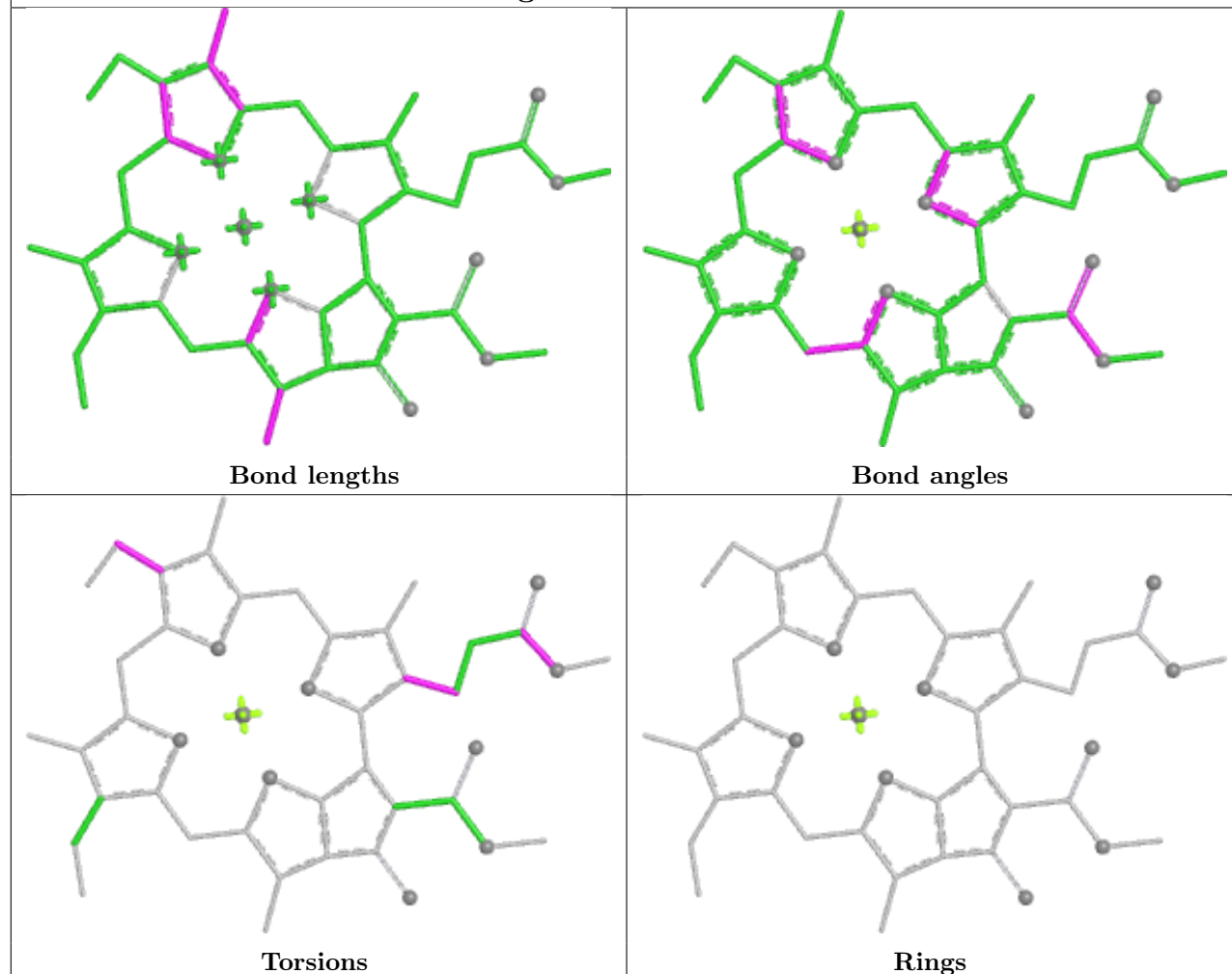


Torsions

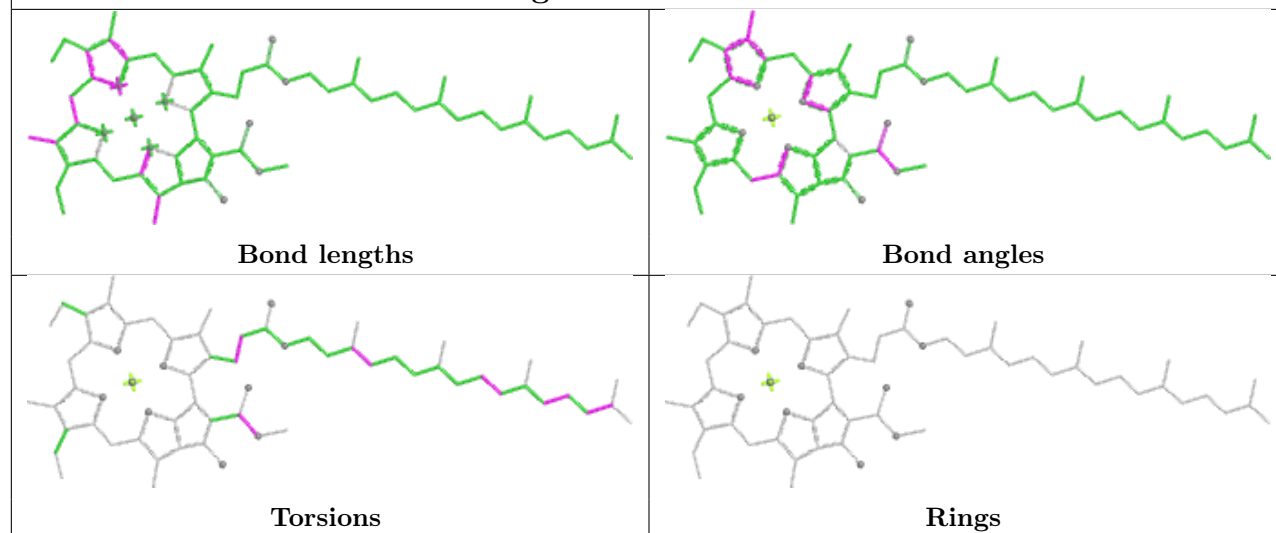


Rings

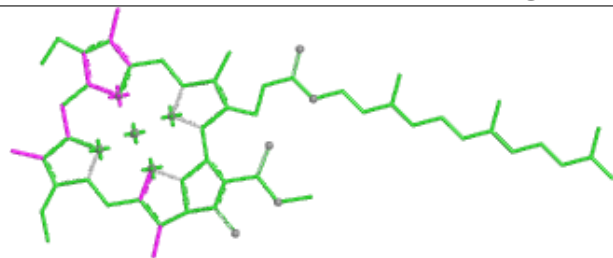
Ligand CLA 1 820



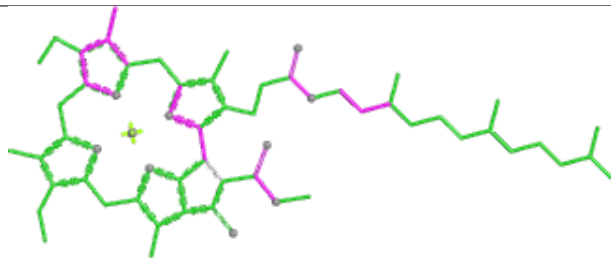
Ligand CLA A 828



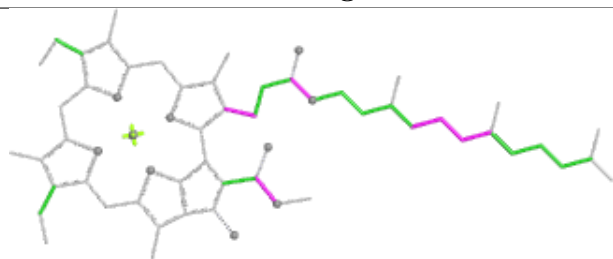
Ligand CLA I 202



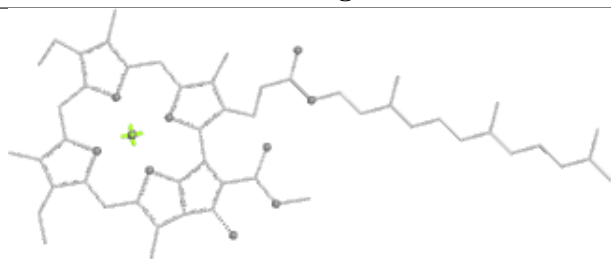
Bond lengths



Bond angles

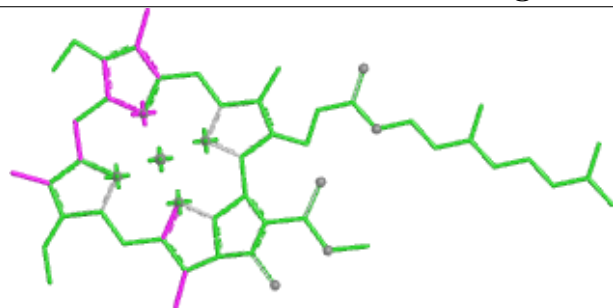


Torsions

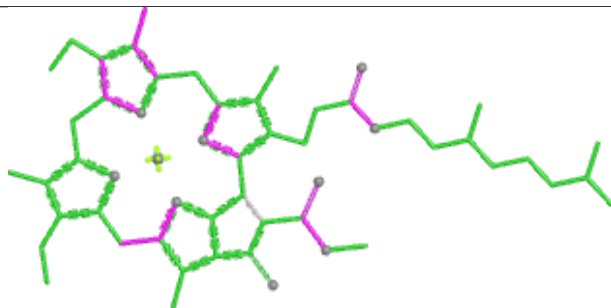


Rings

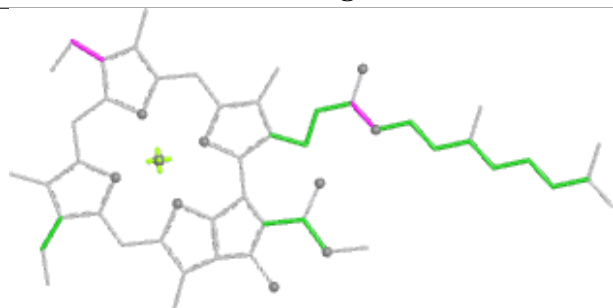
Ligand CLA A 804



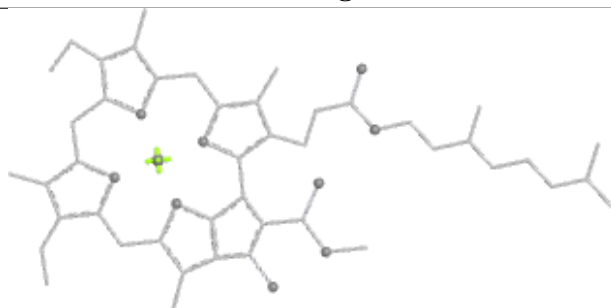
Bond lengths



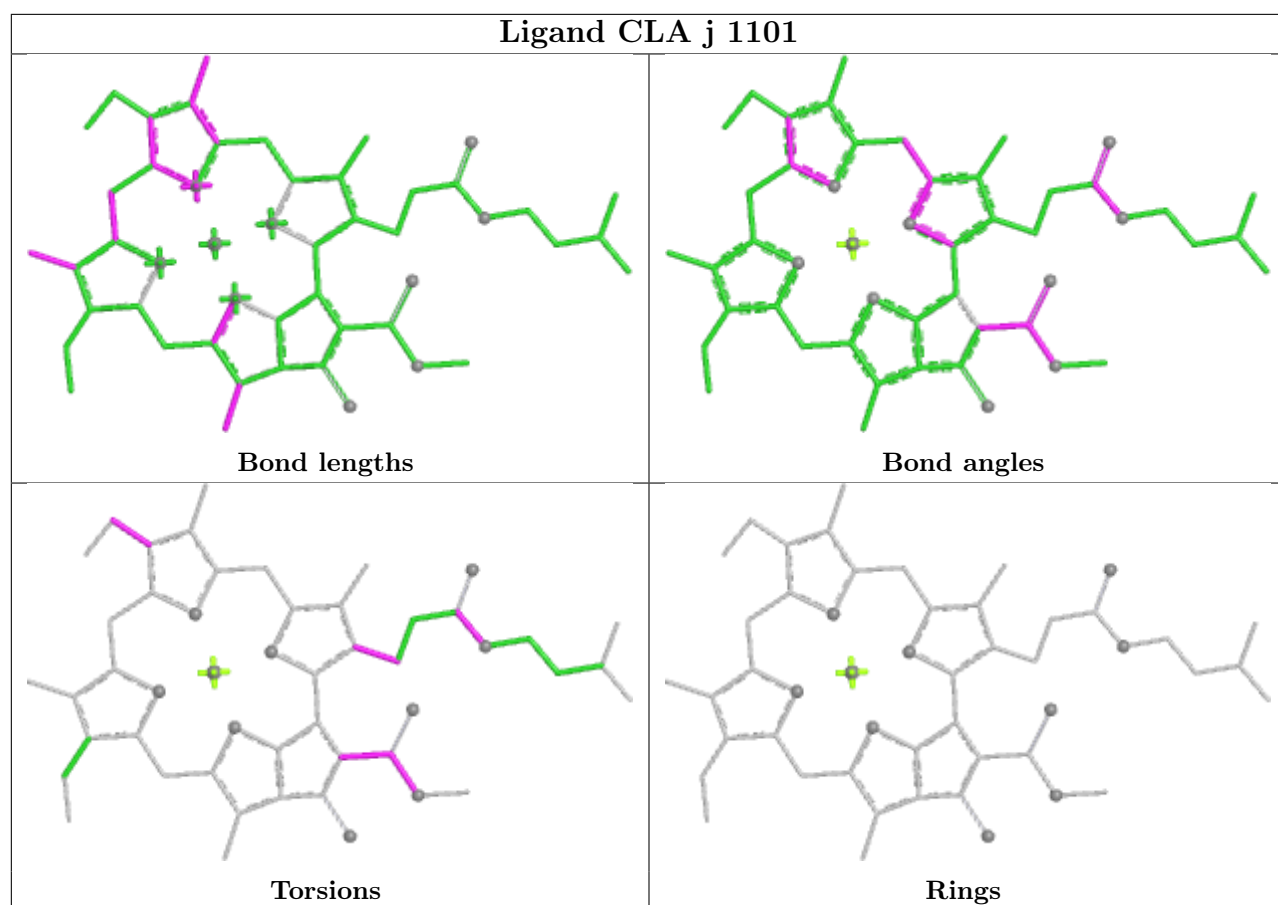
Bond angles



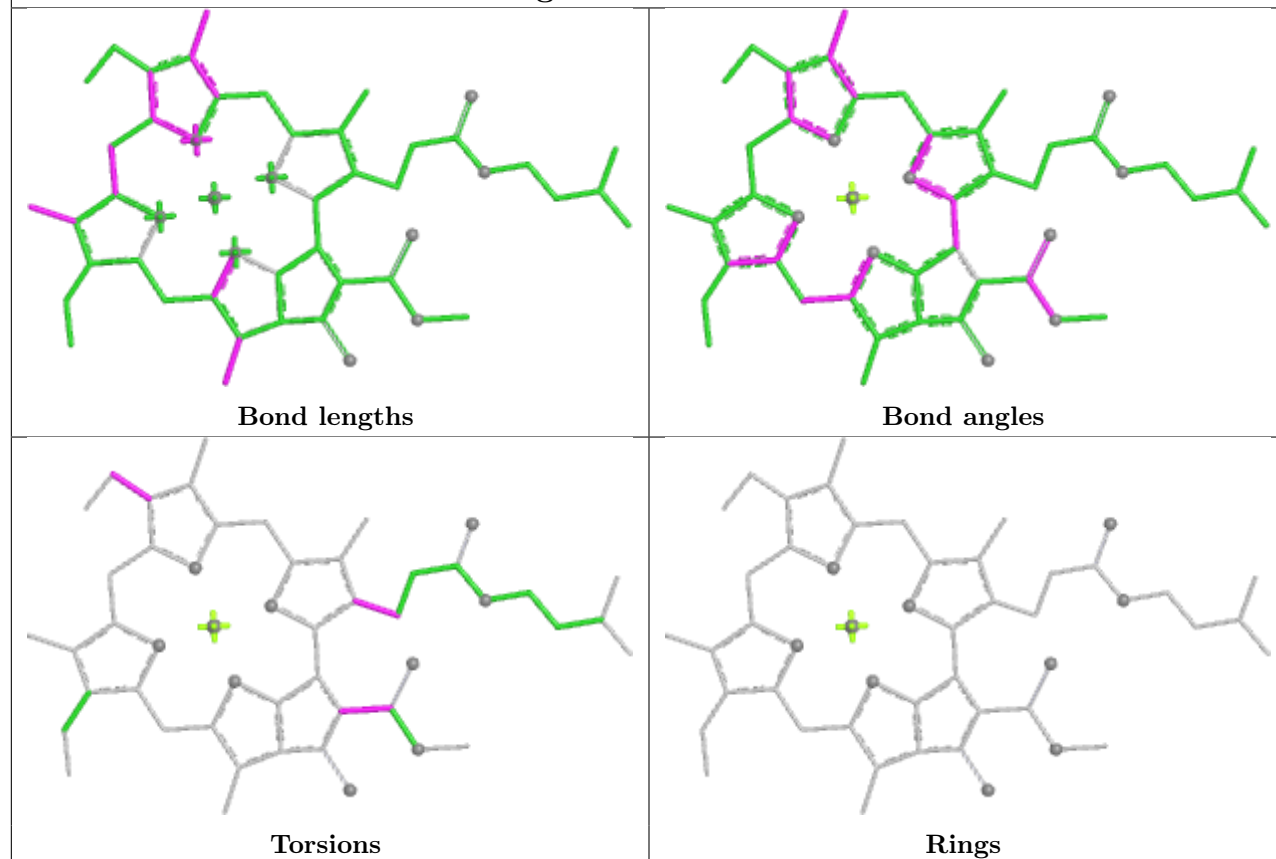
Torsions



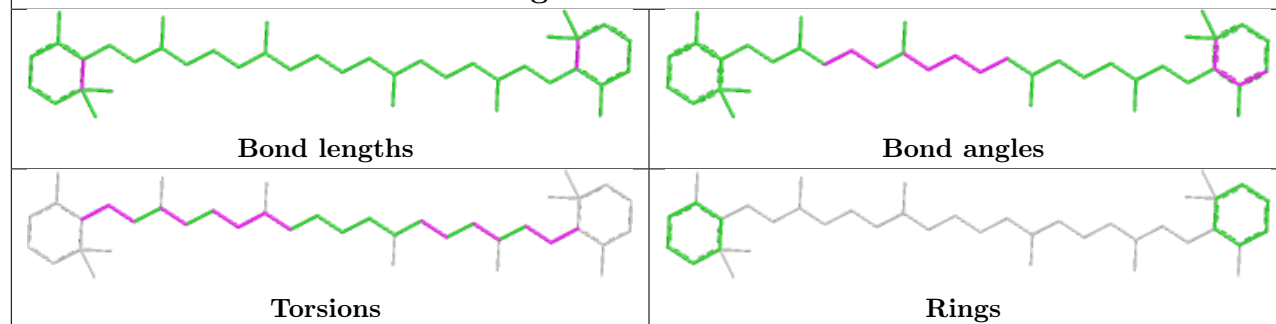
Rings

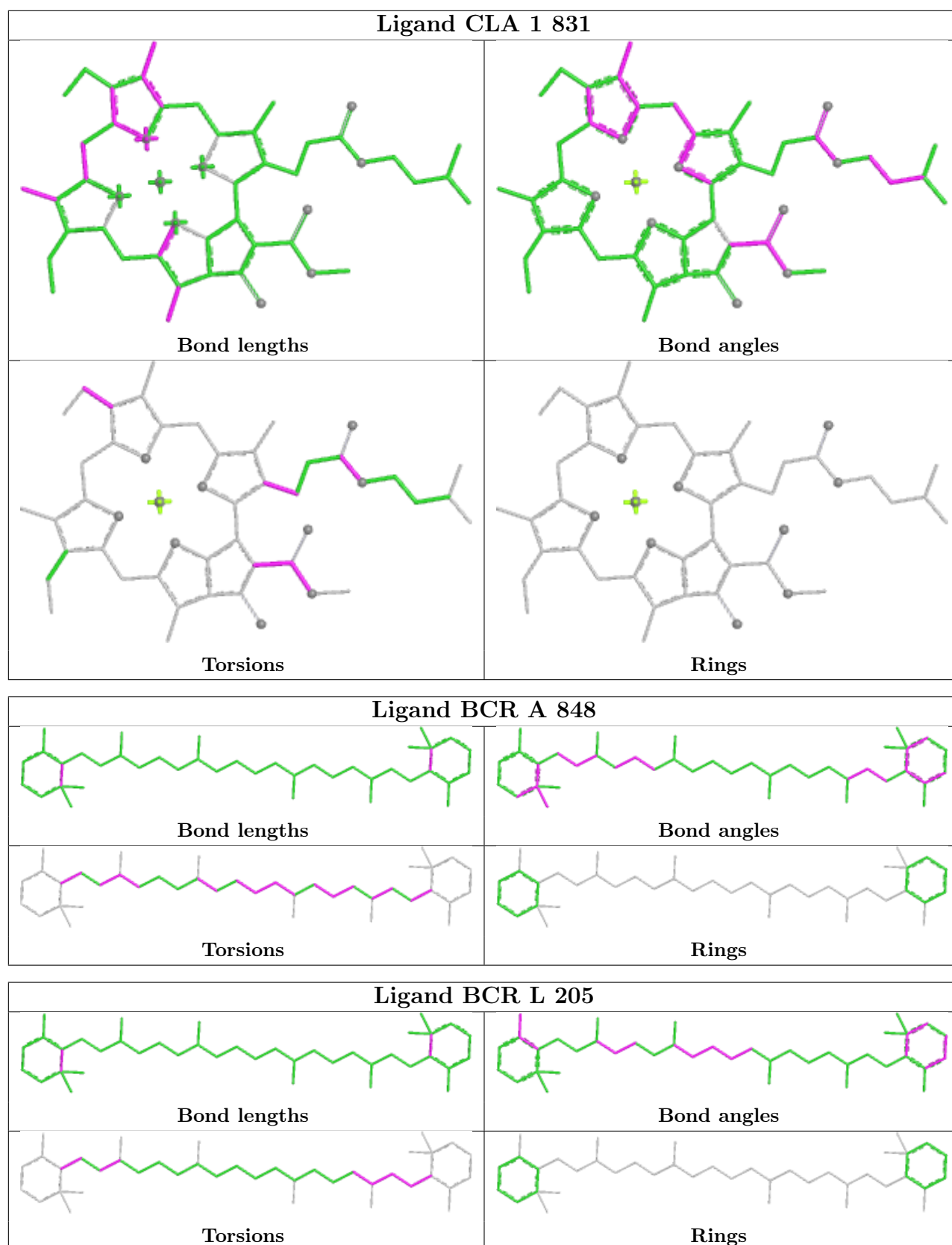


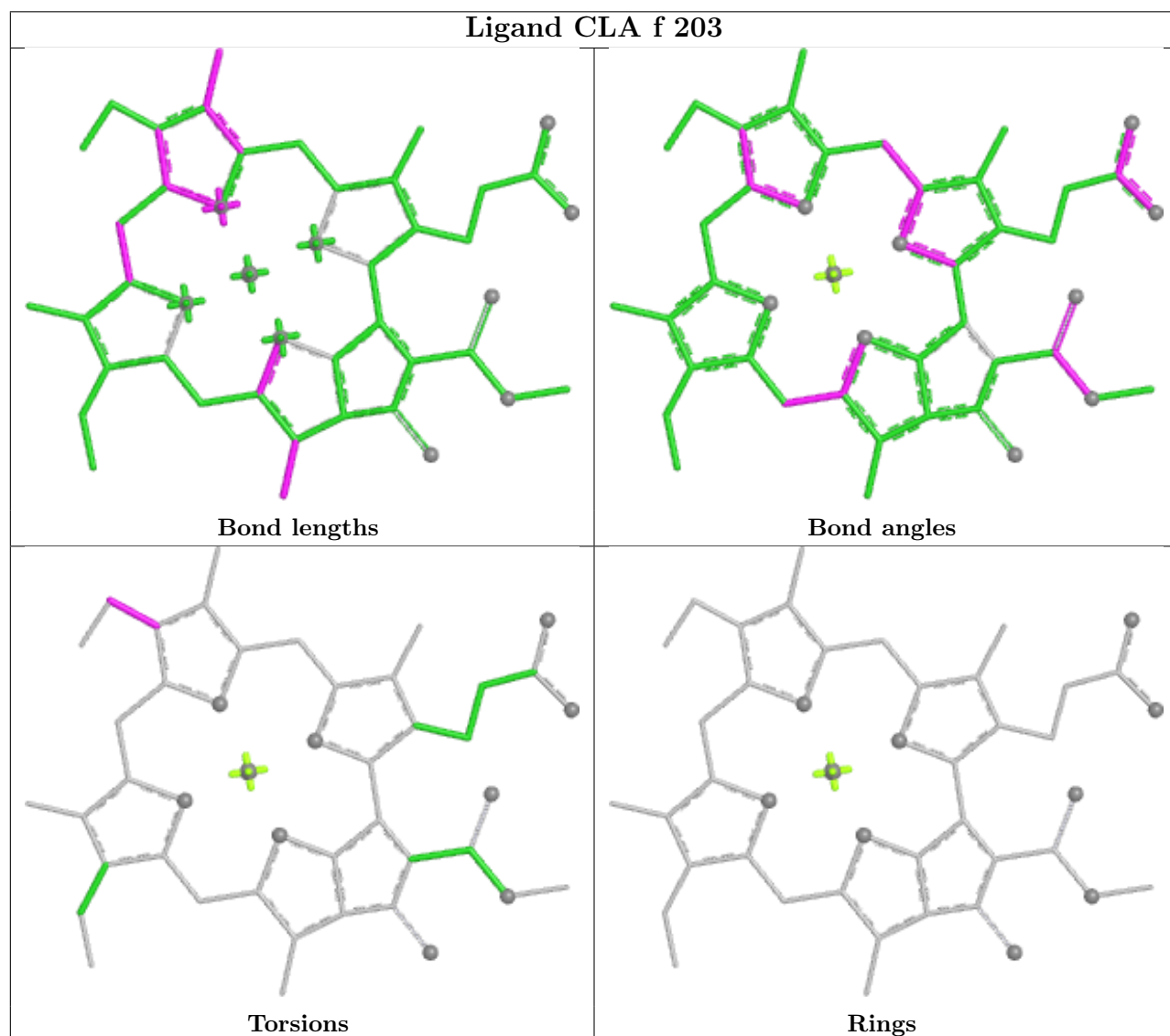
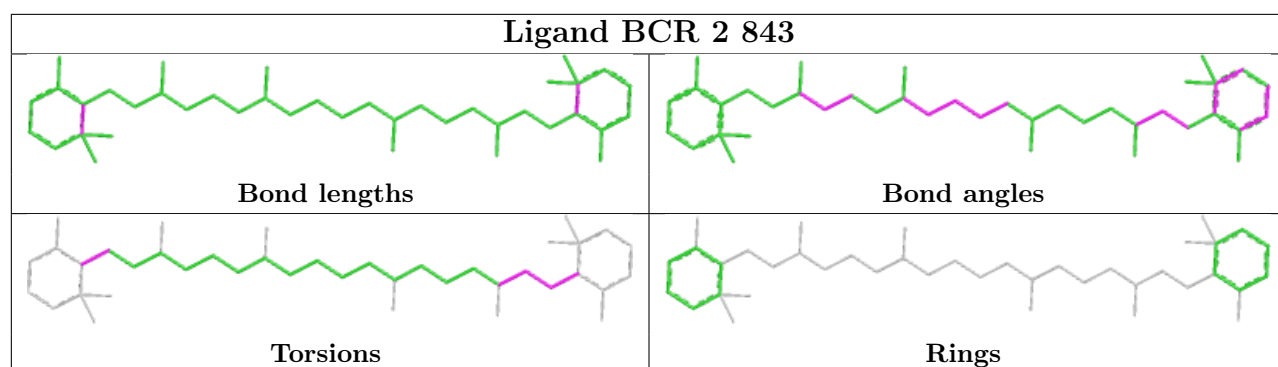
Ligand CLA a 808

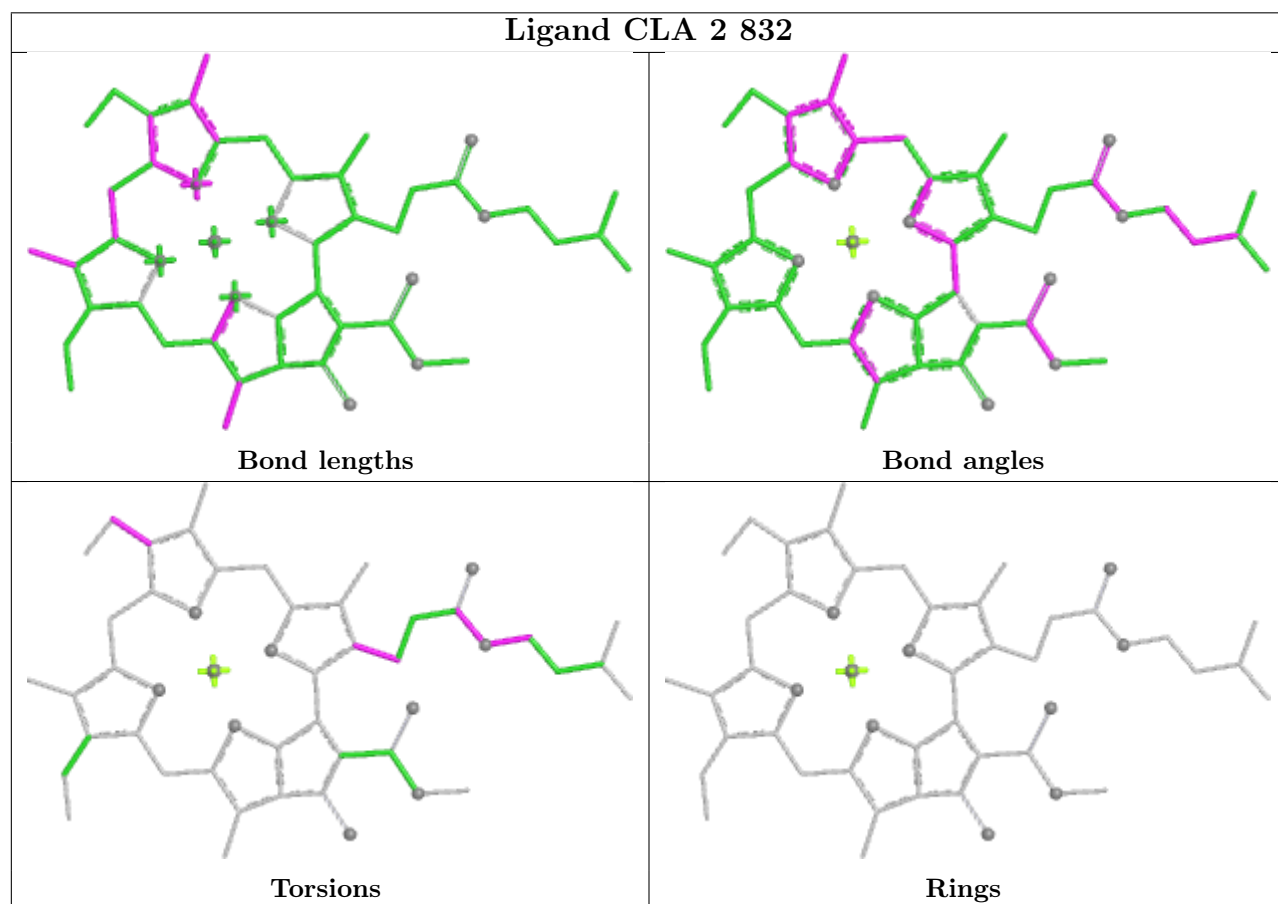
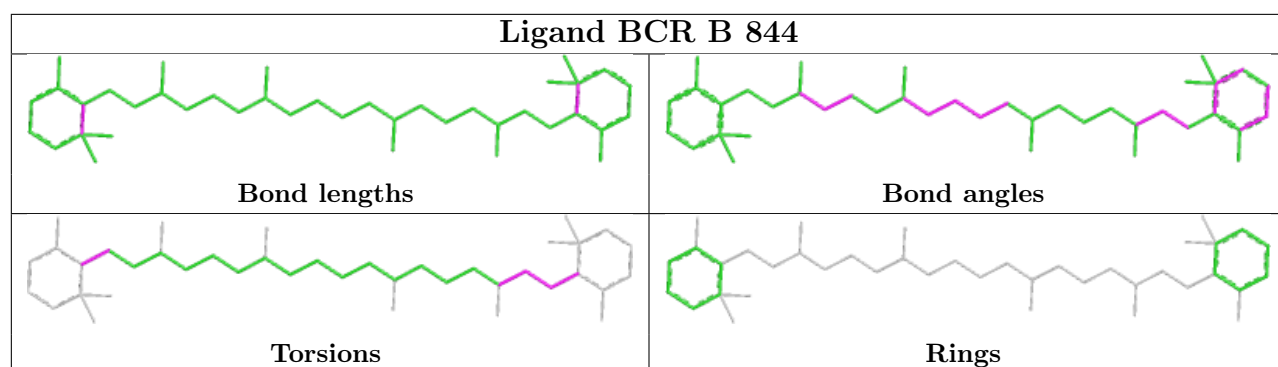


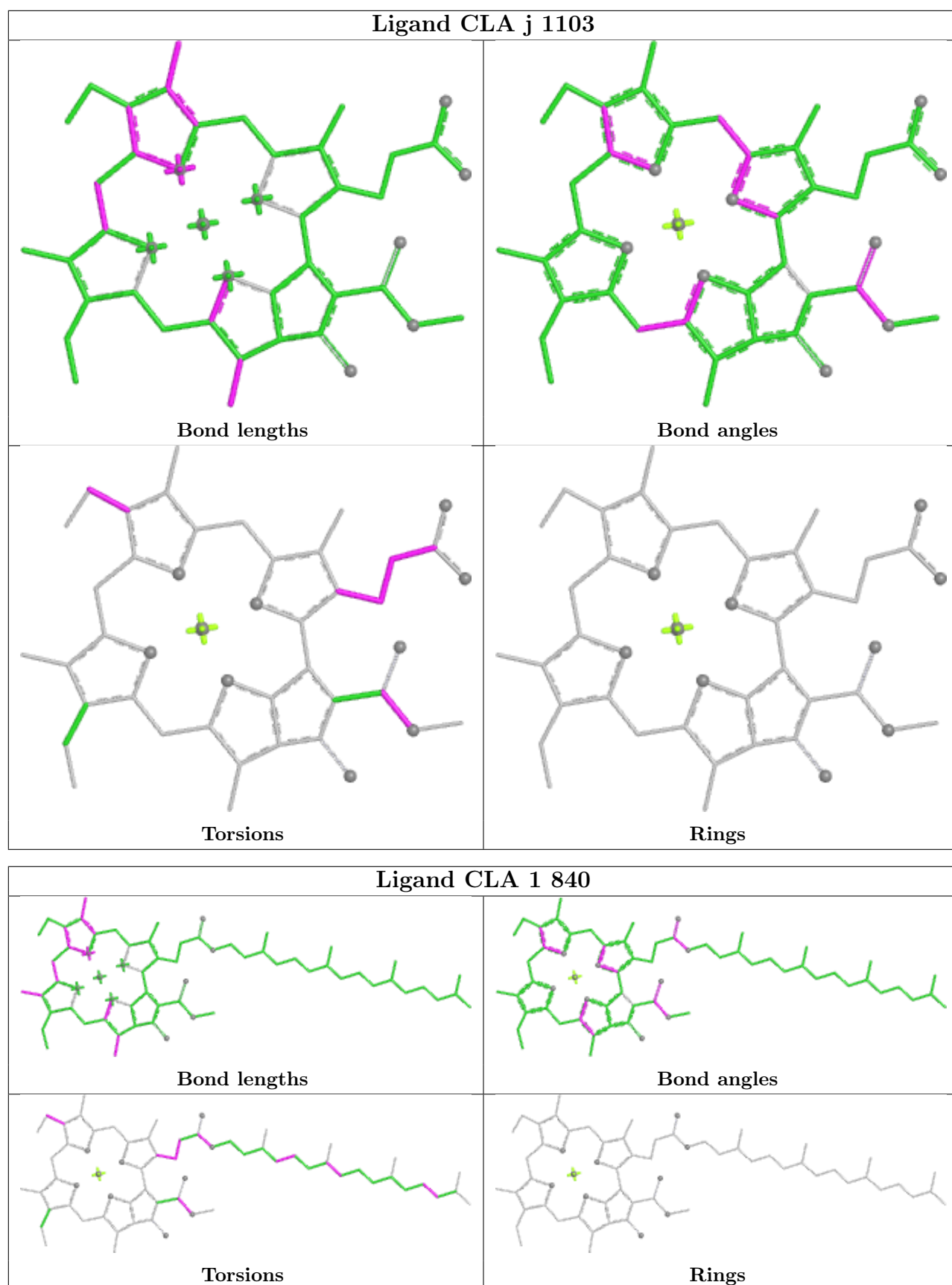
Ligand BCR B 845

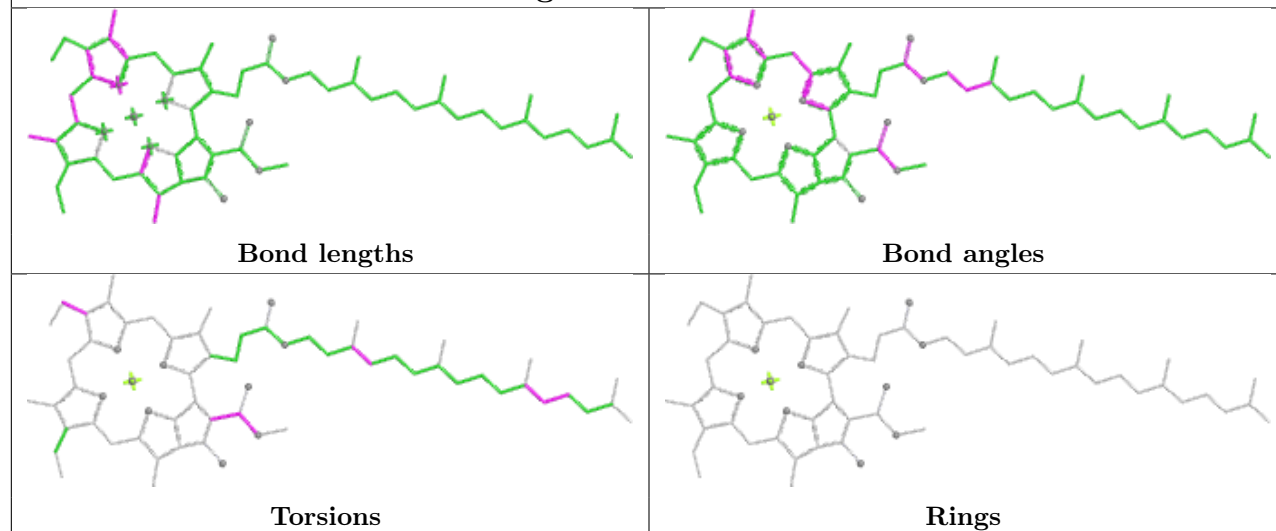
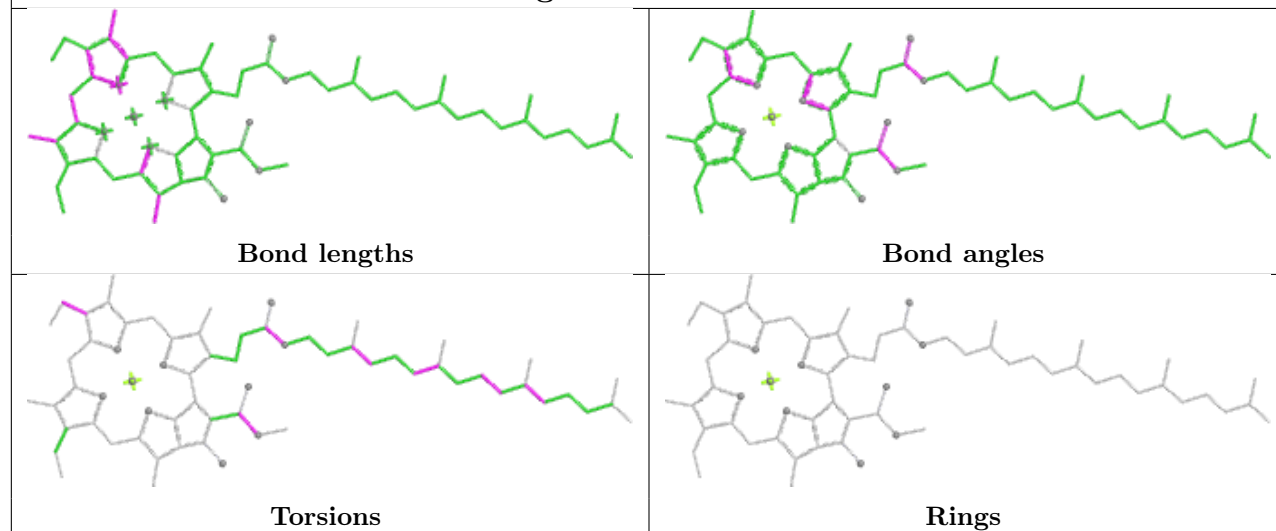


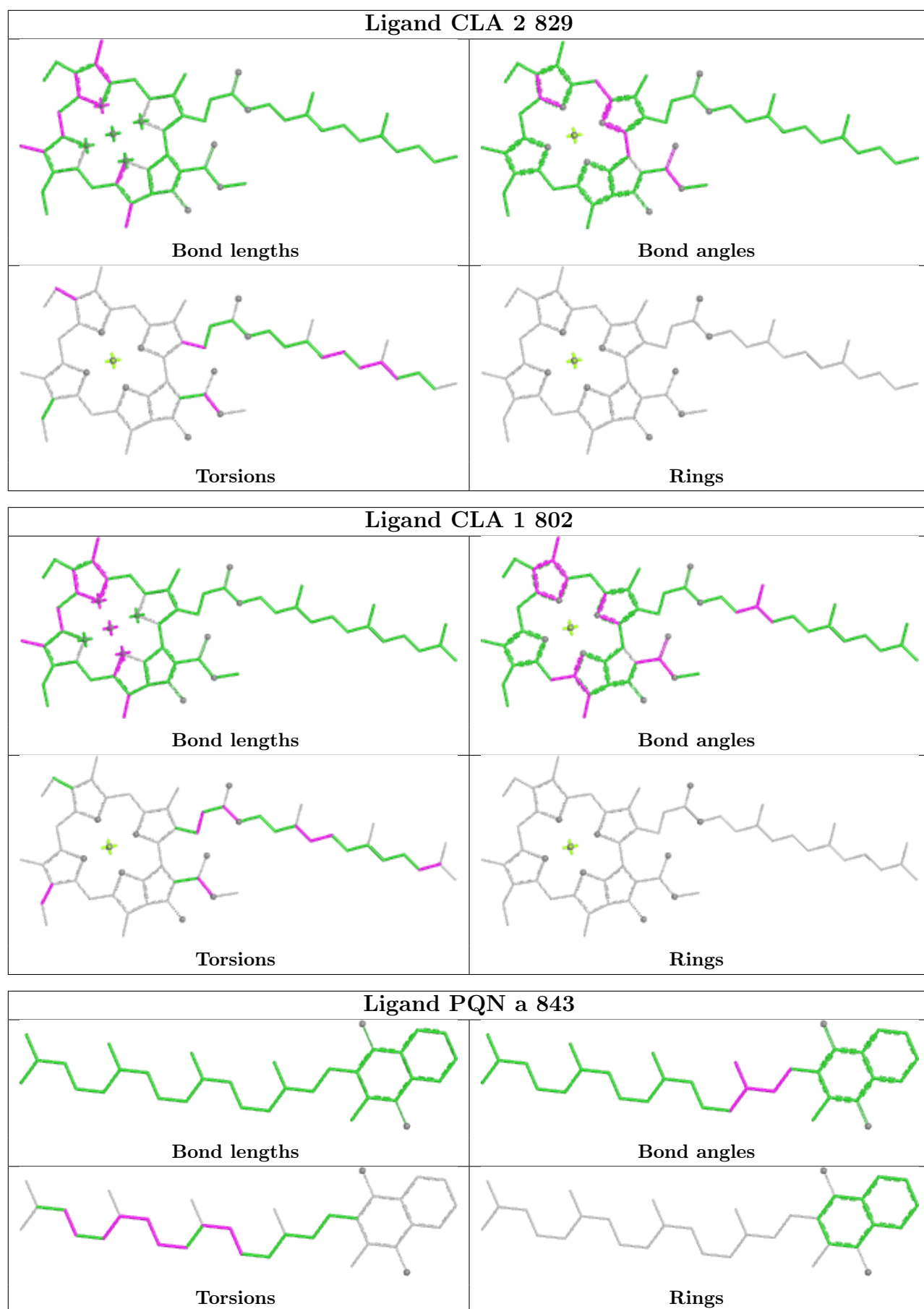


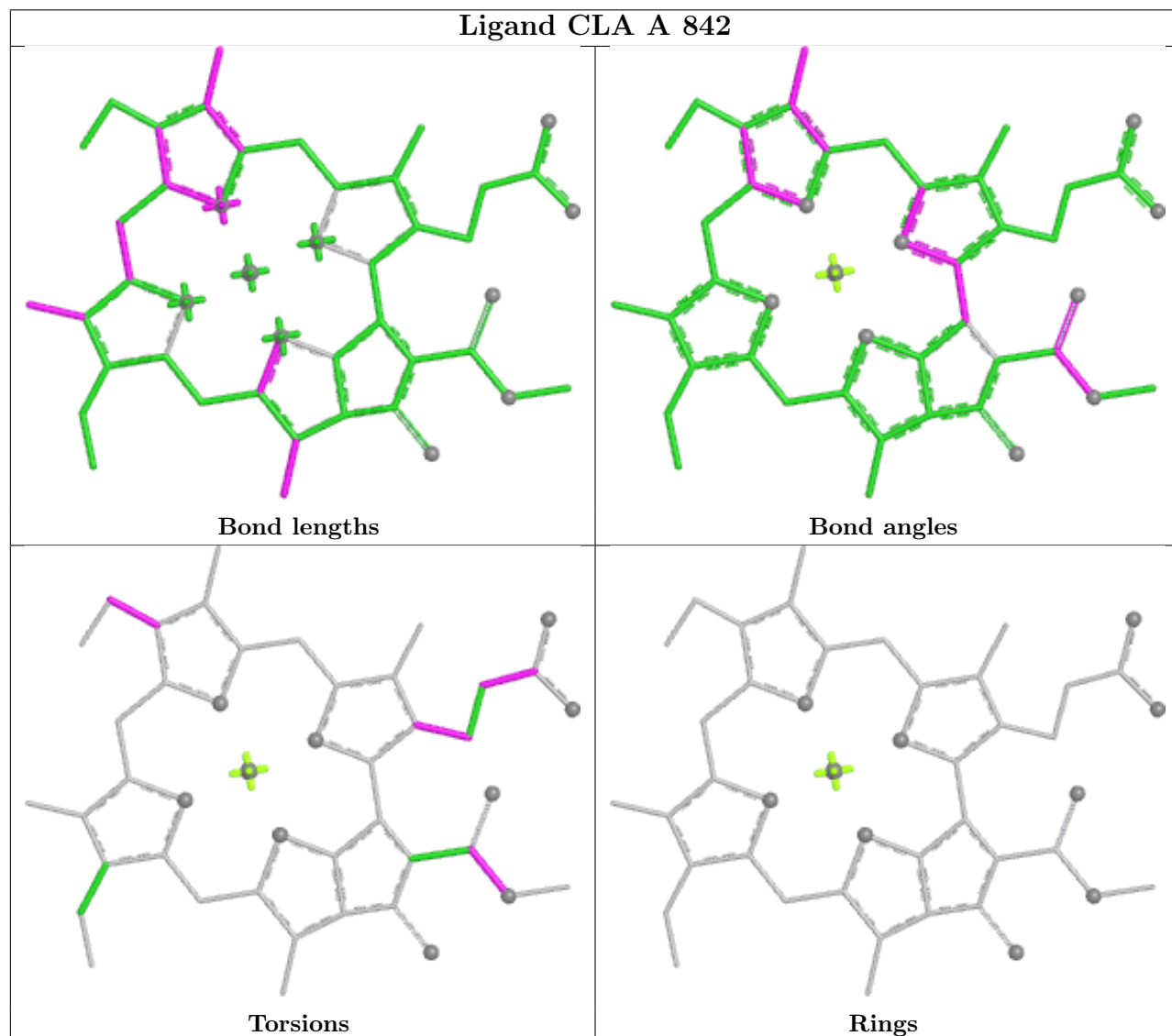
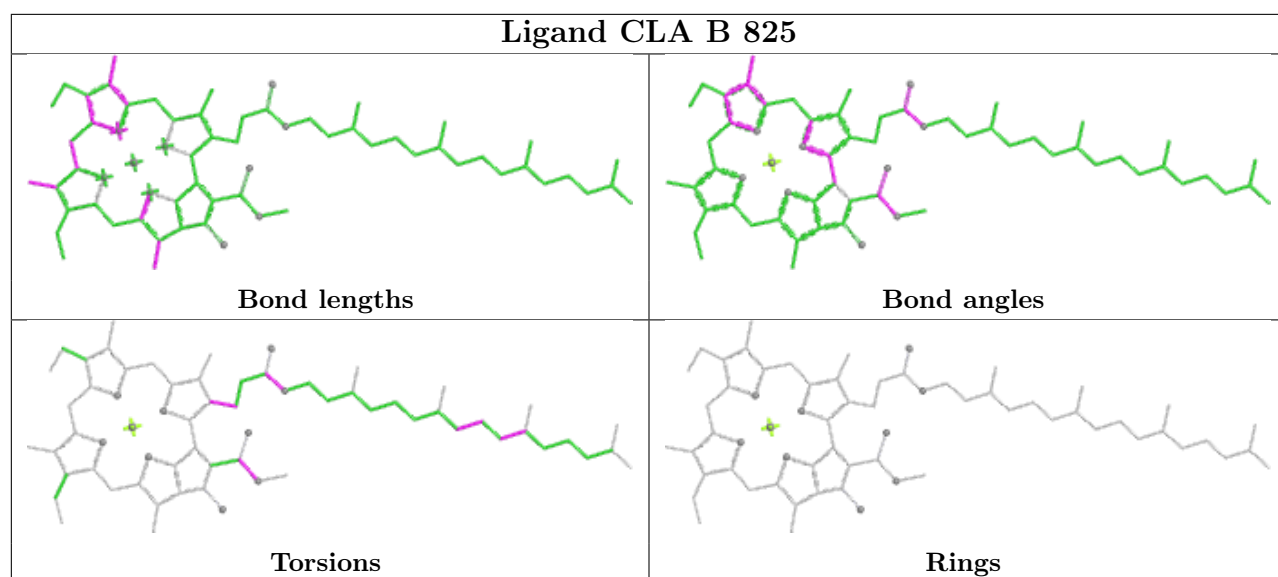




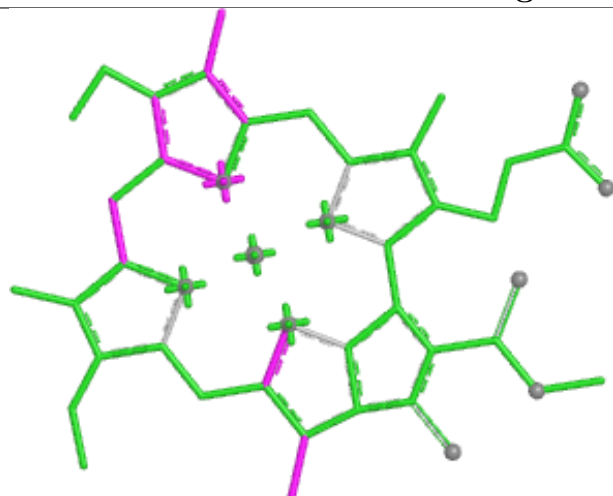


Ligand CLA 1 832**Ligand CLA 2 805**

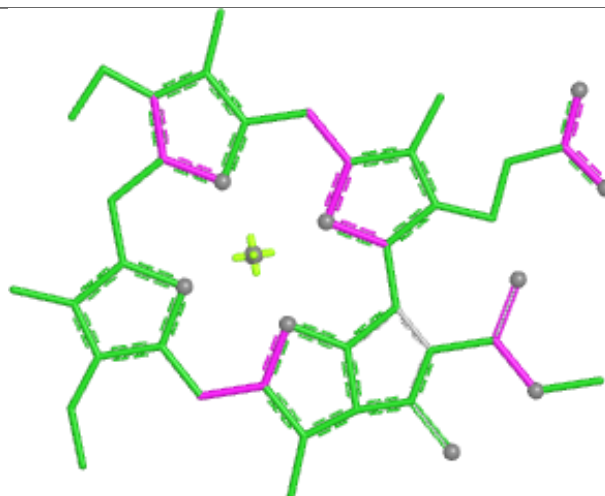




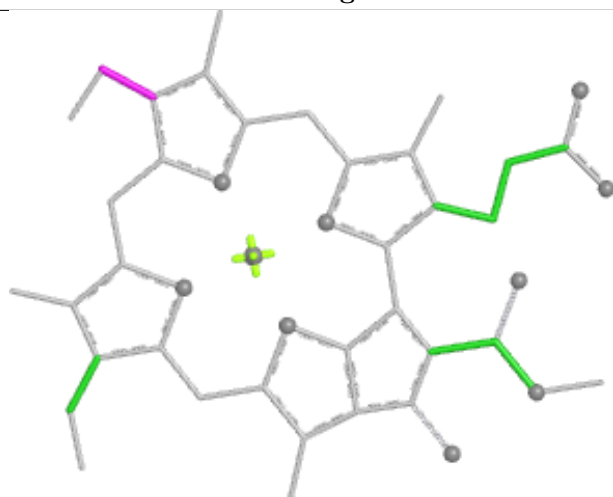
Ligand CLA F 203



Bond lengths



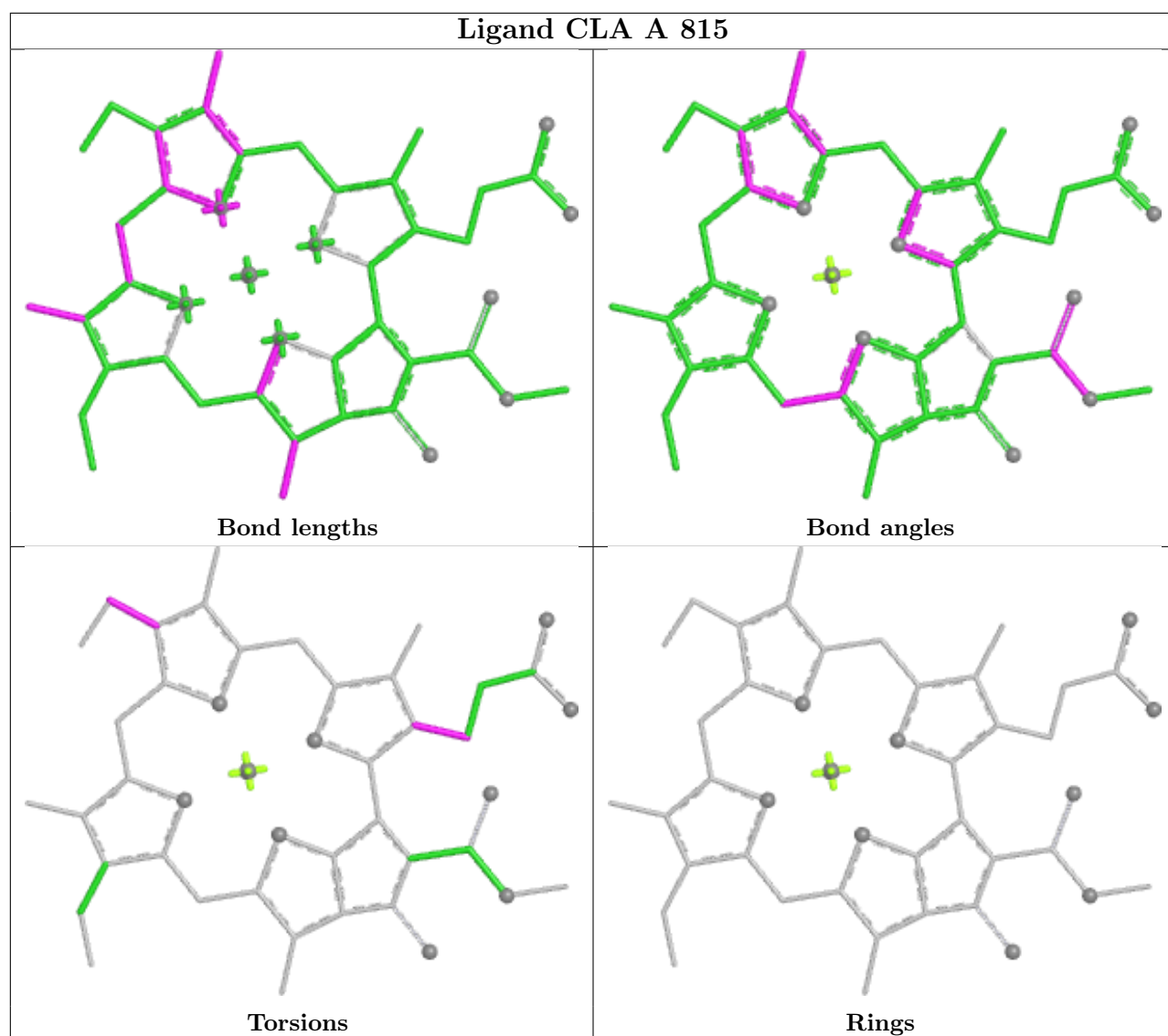
Bond angles



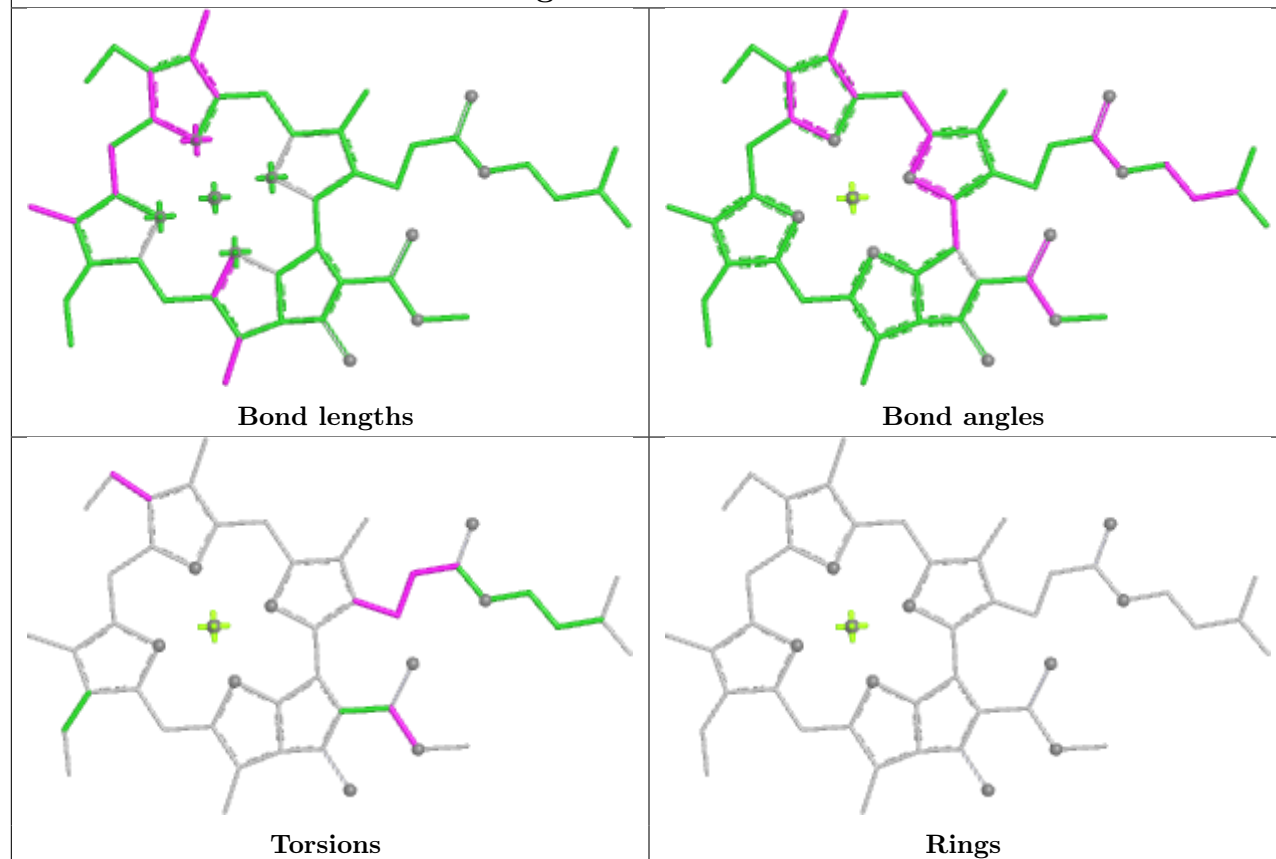
Torsions



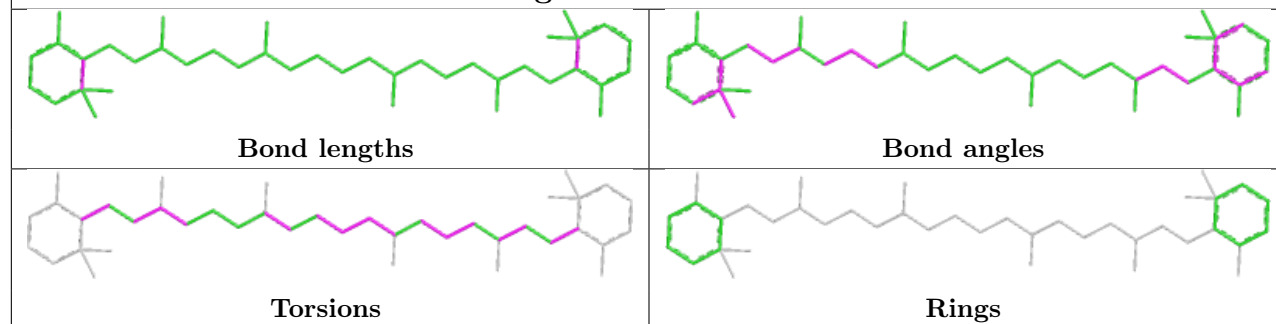
Rings

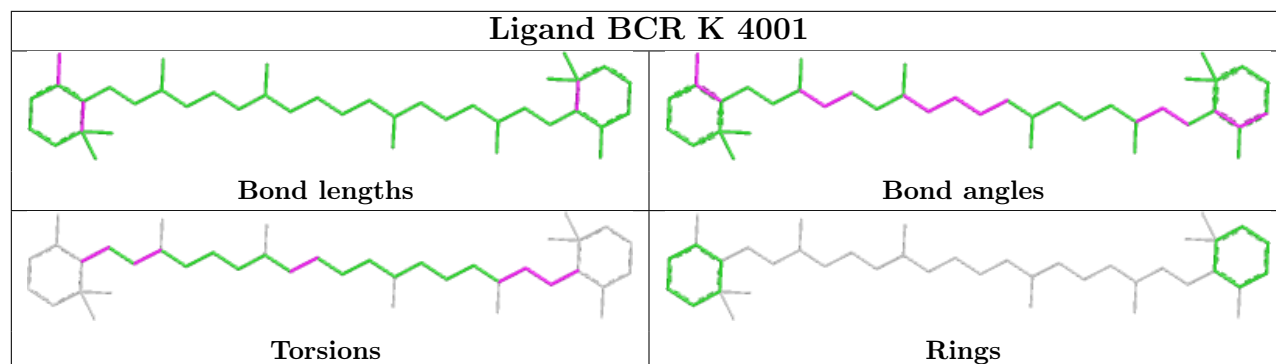
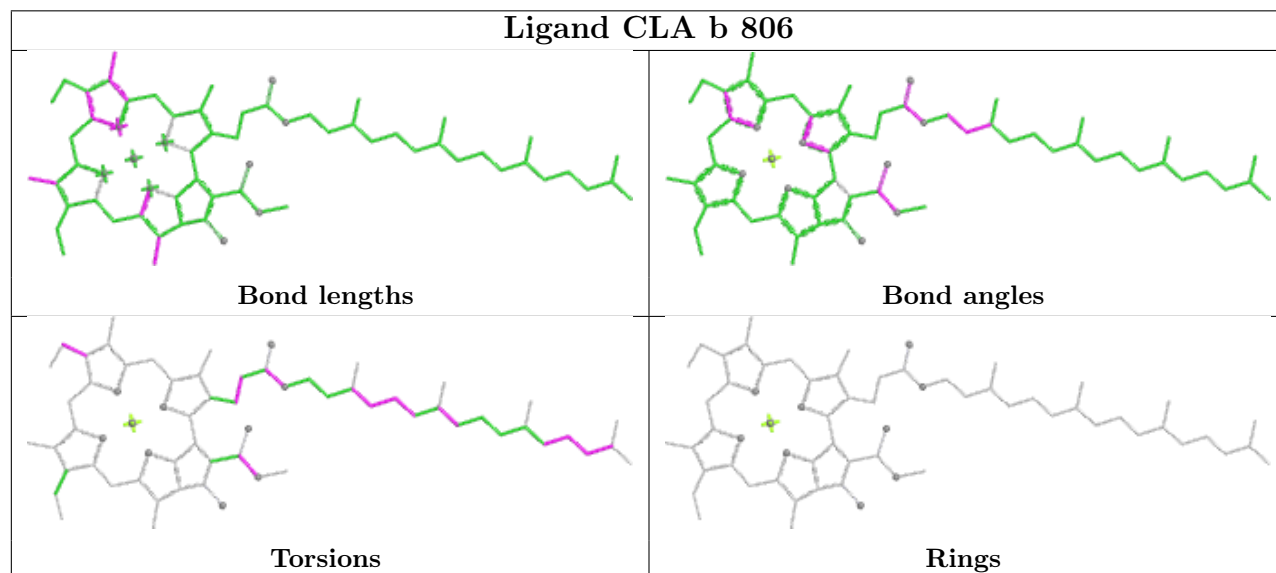
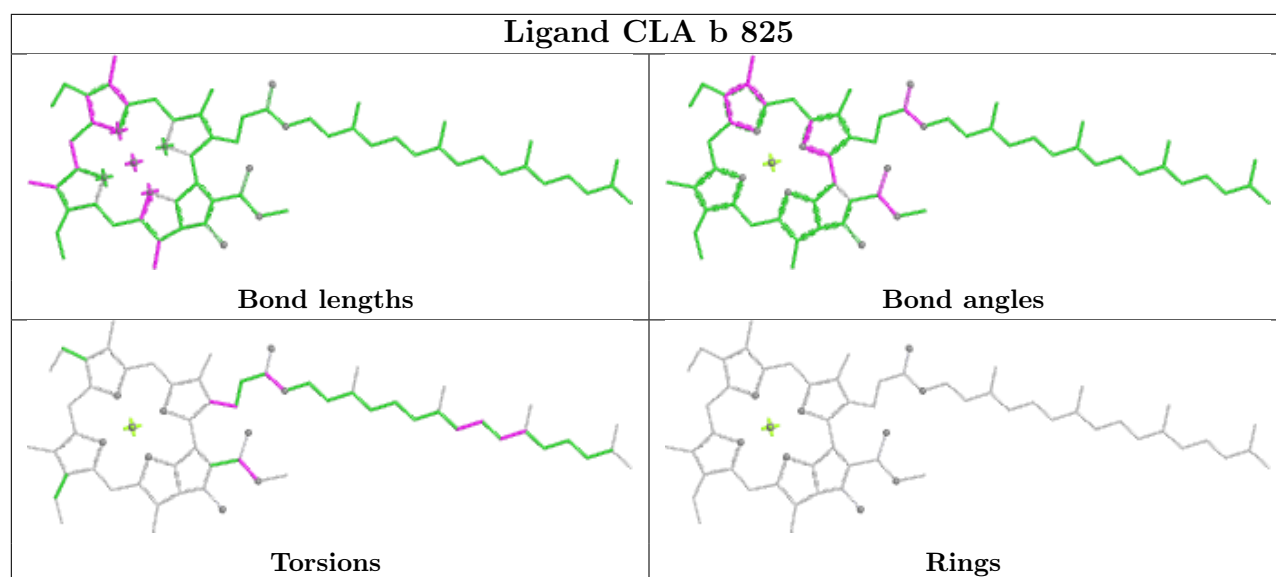


Ligand CLA 0 205

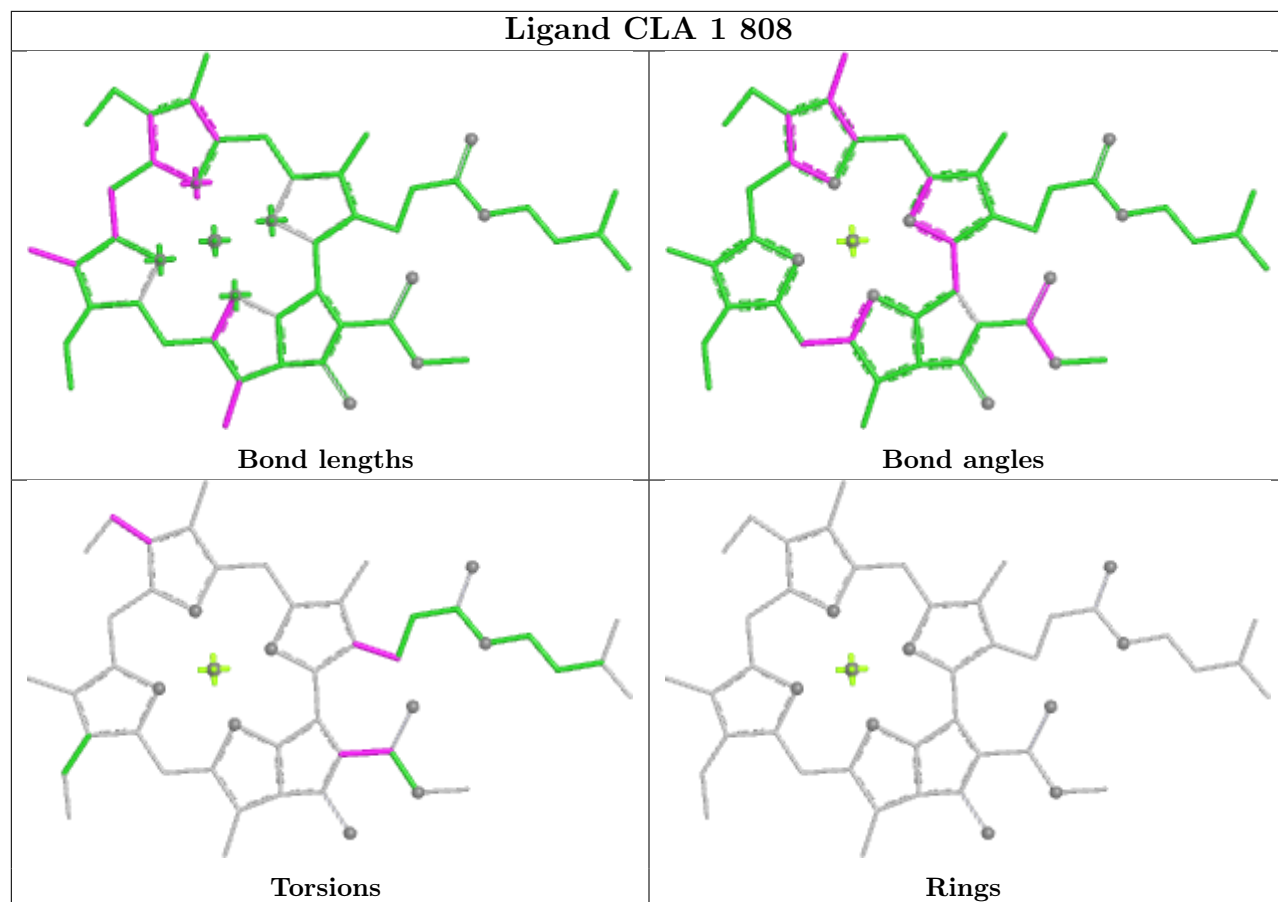


Ligand BCR a 848

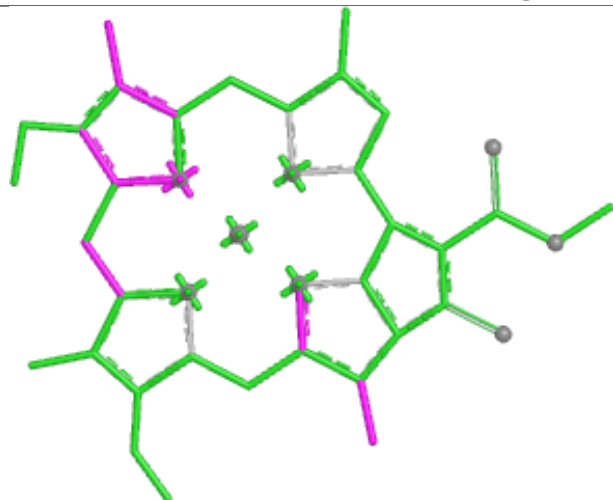




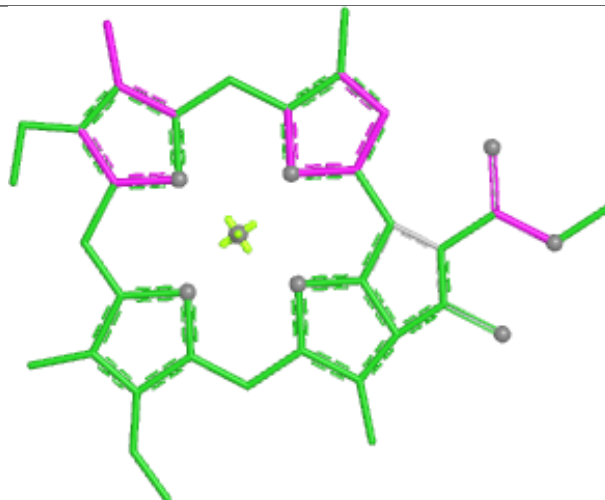
Ligand CLA 1 808



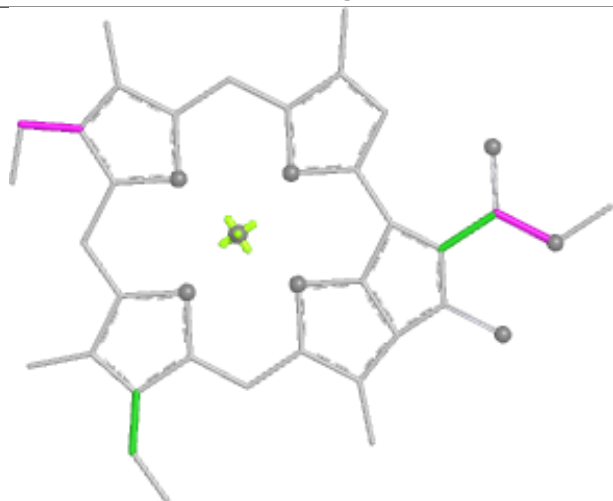
Ligand CLA b 832



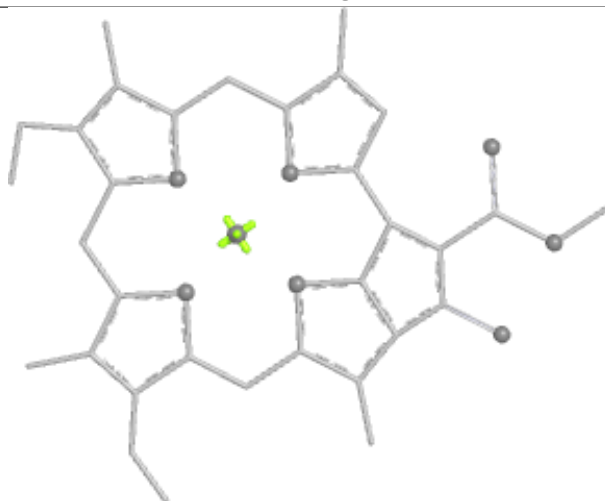
Bond lengths



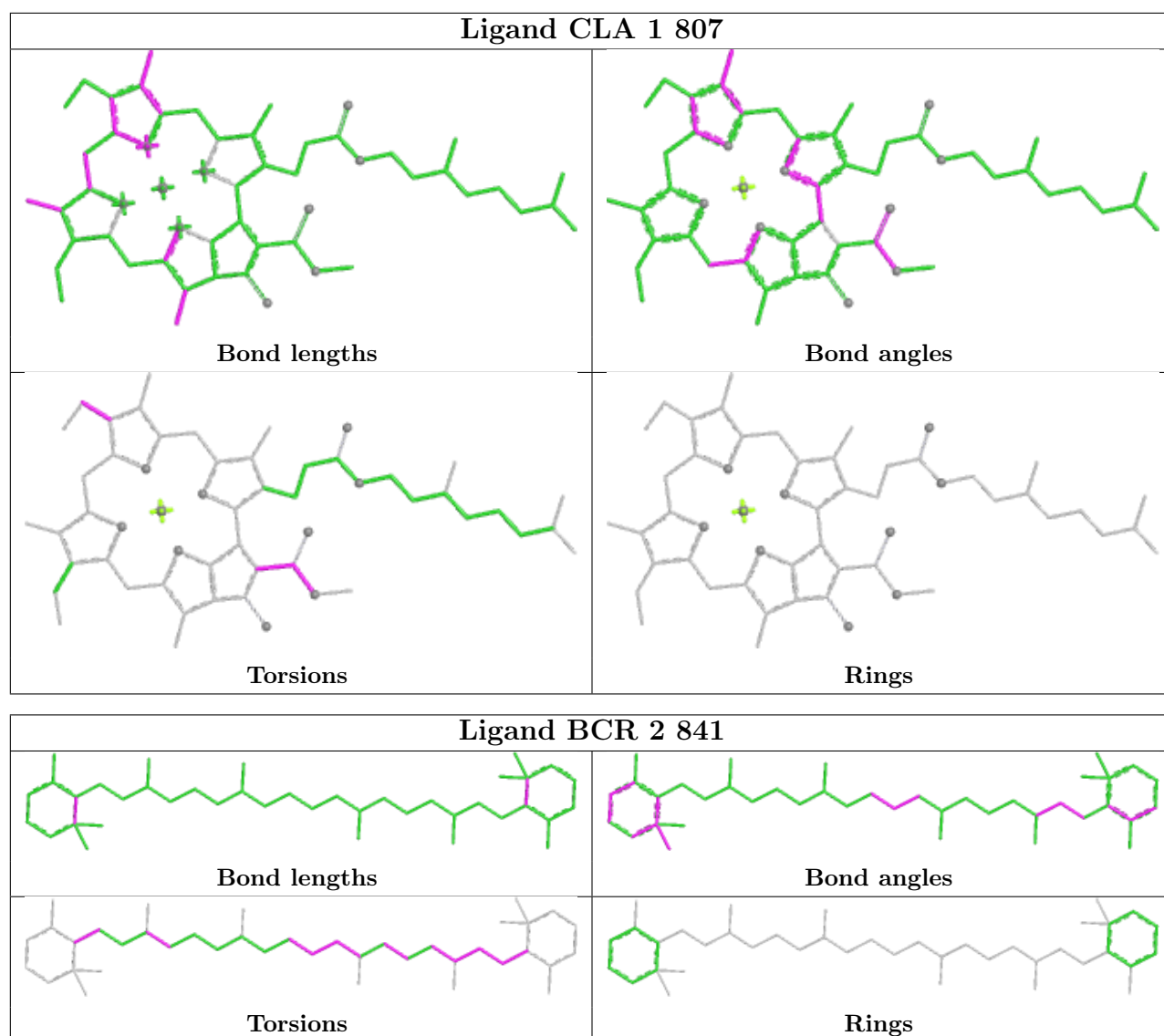
Bond angles



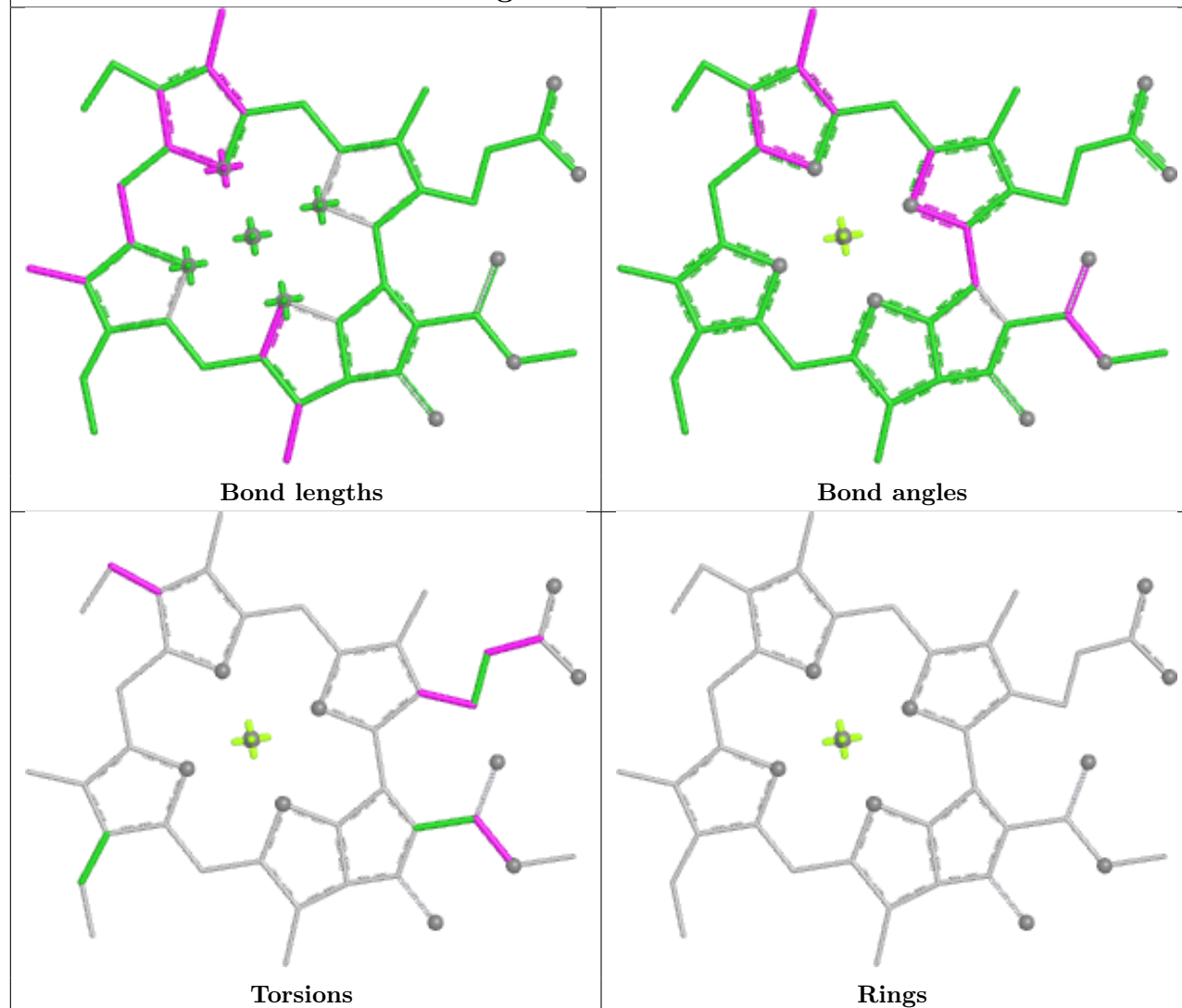
Torsions



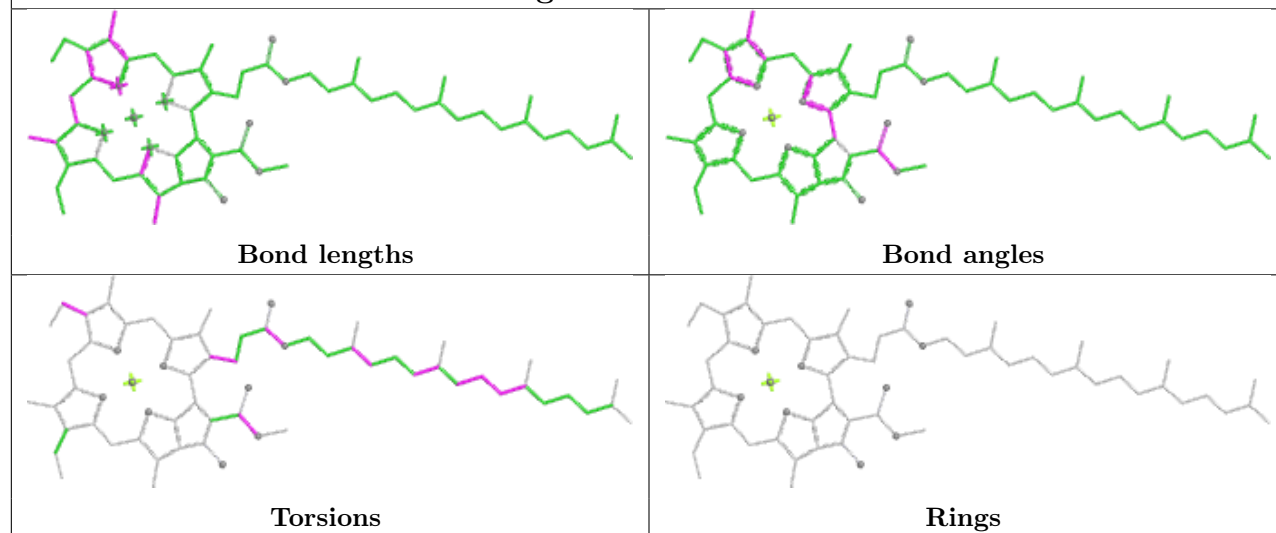
Rings

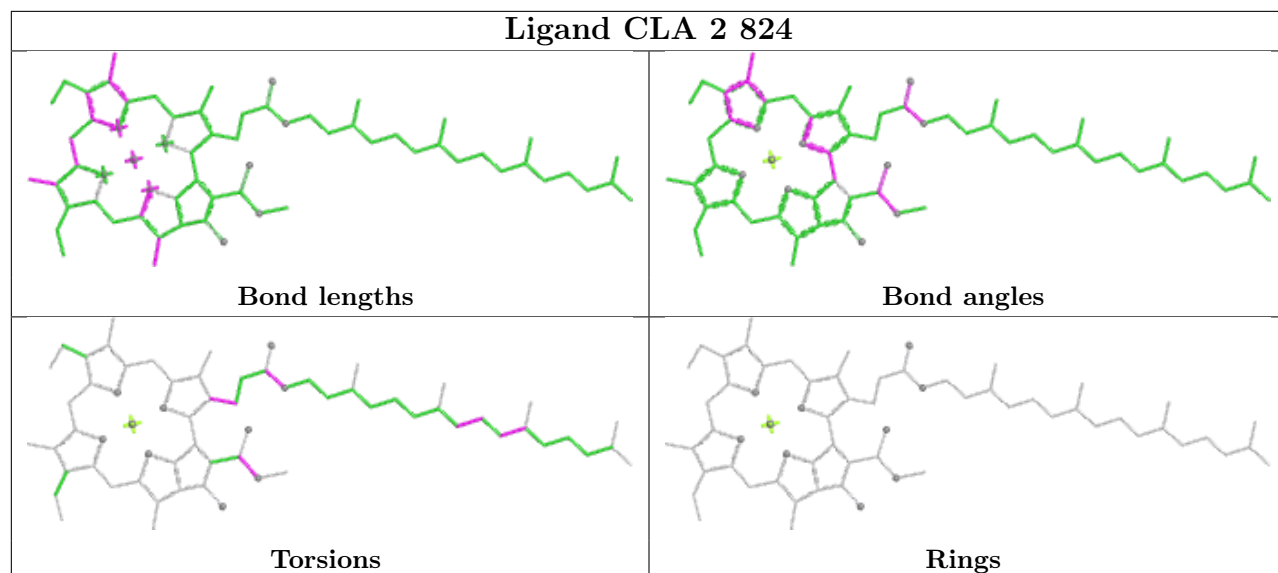
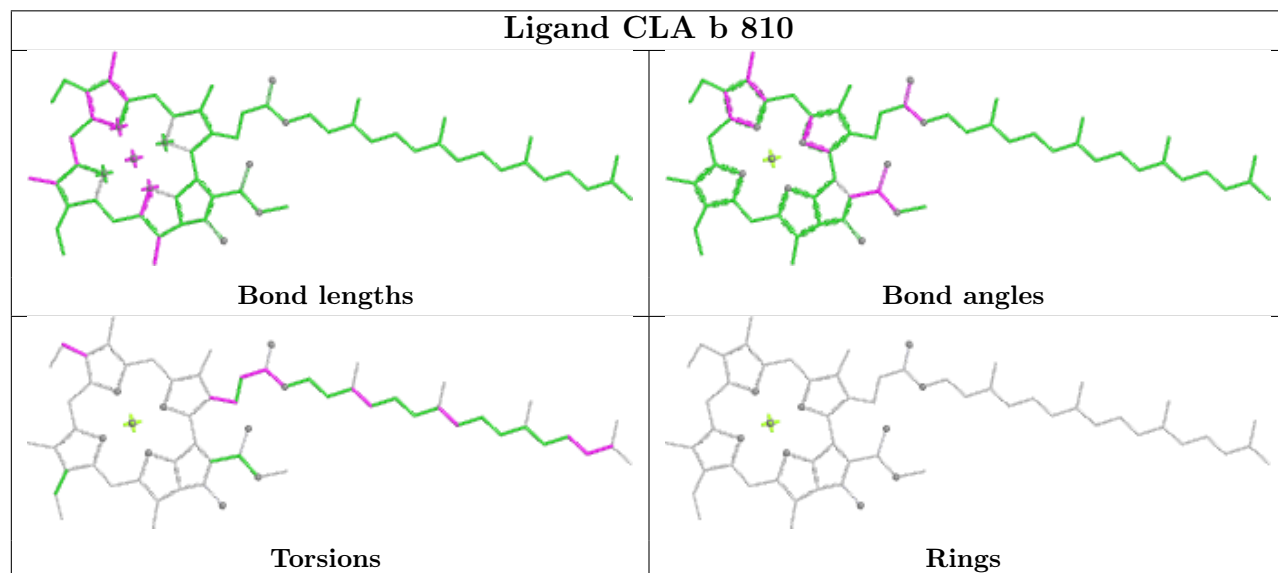
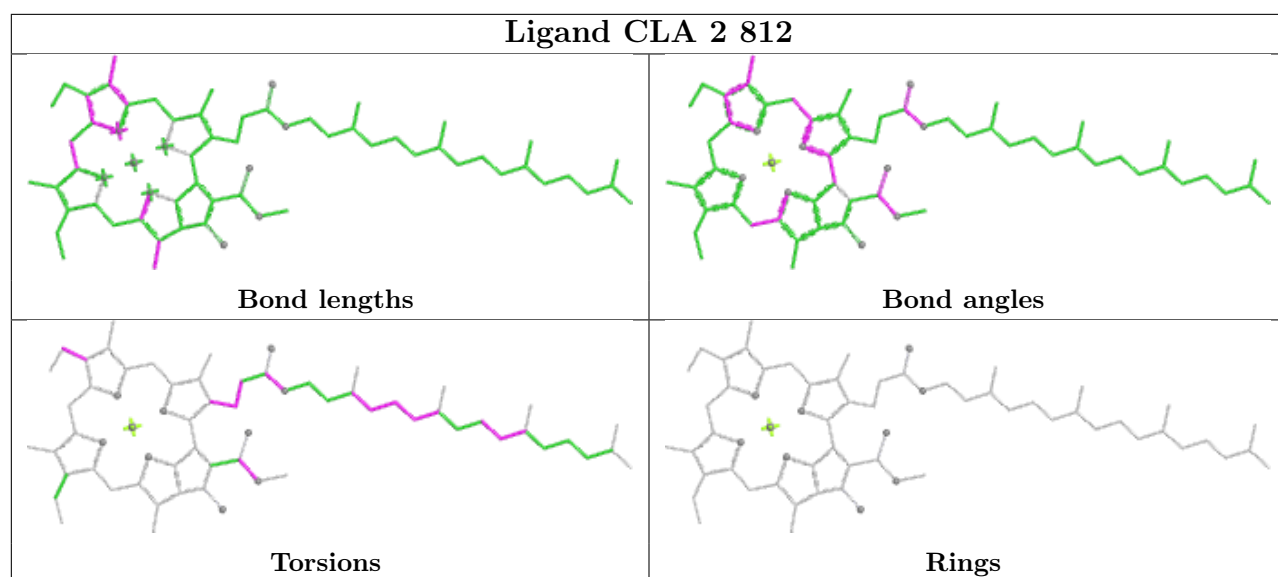


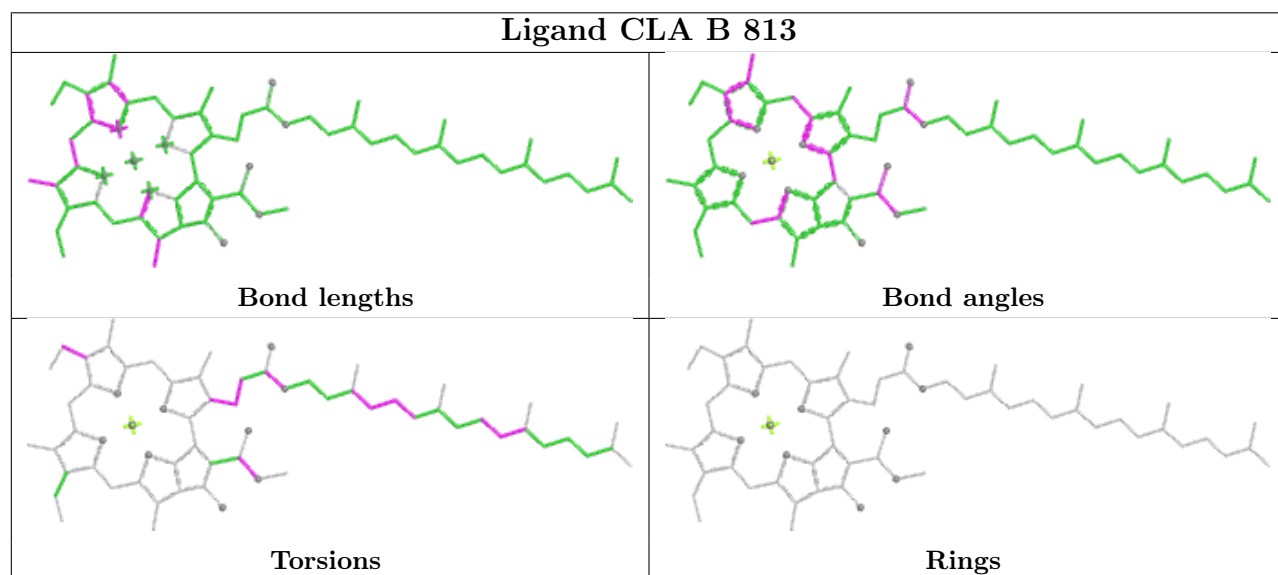
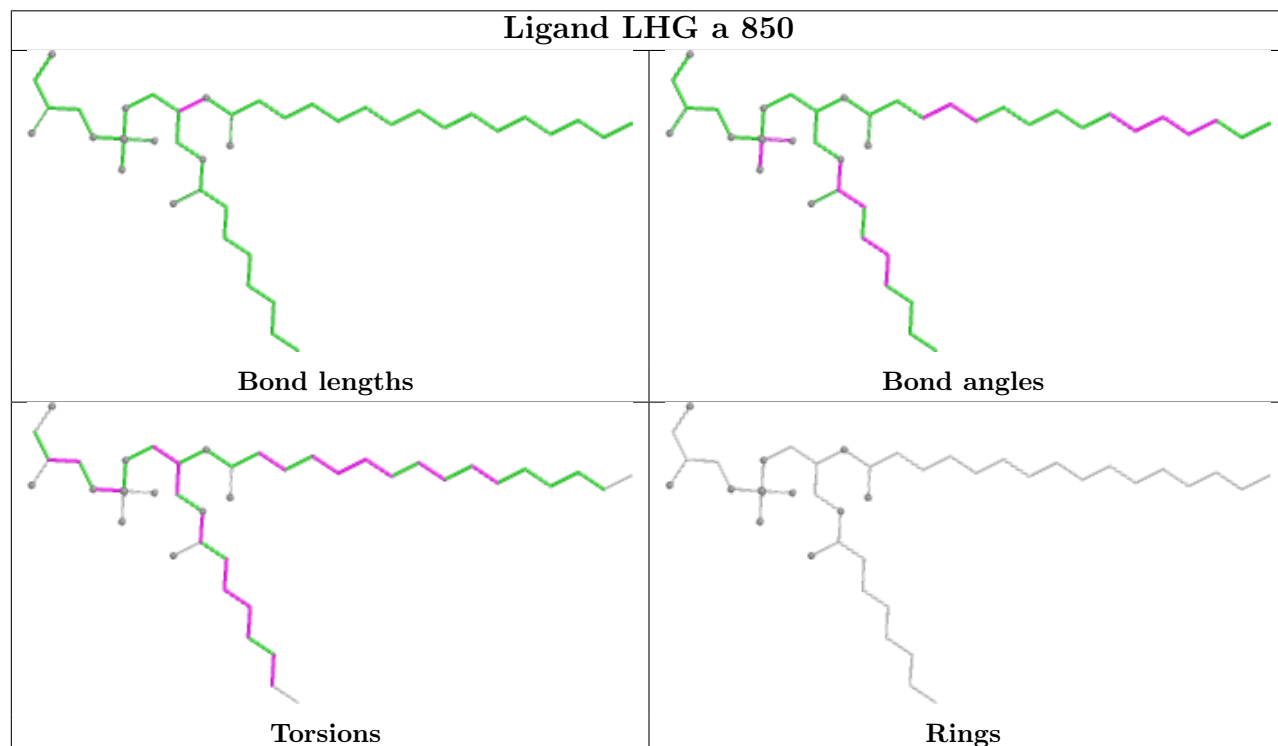
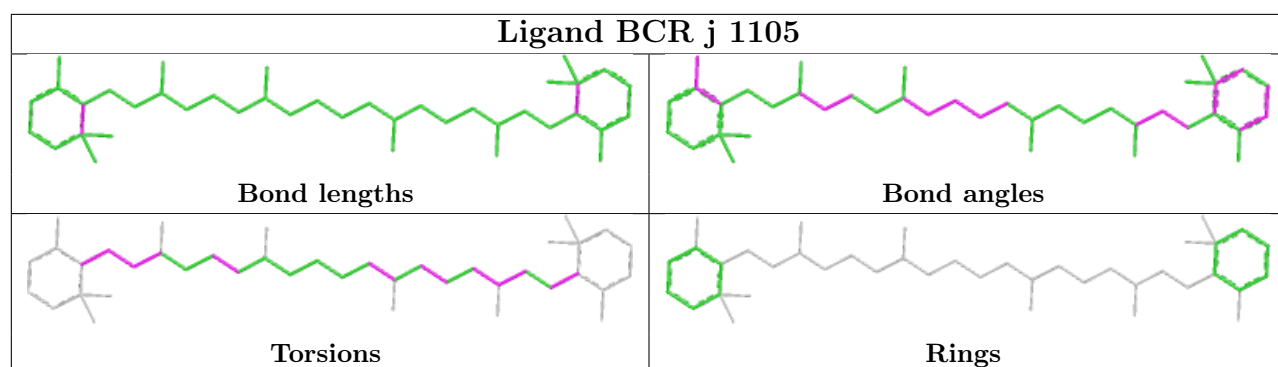
Ligand CLA a 842

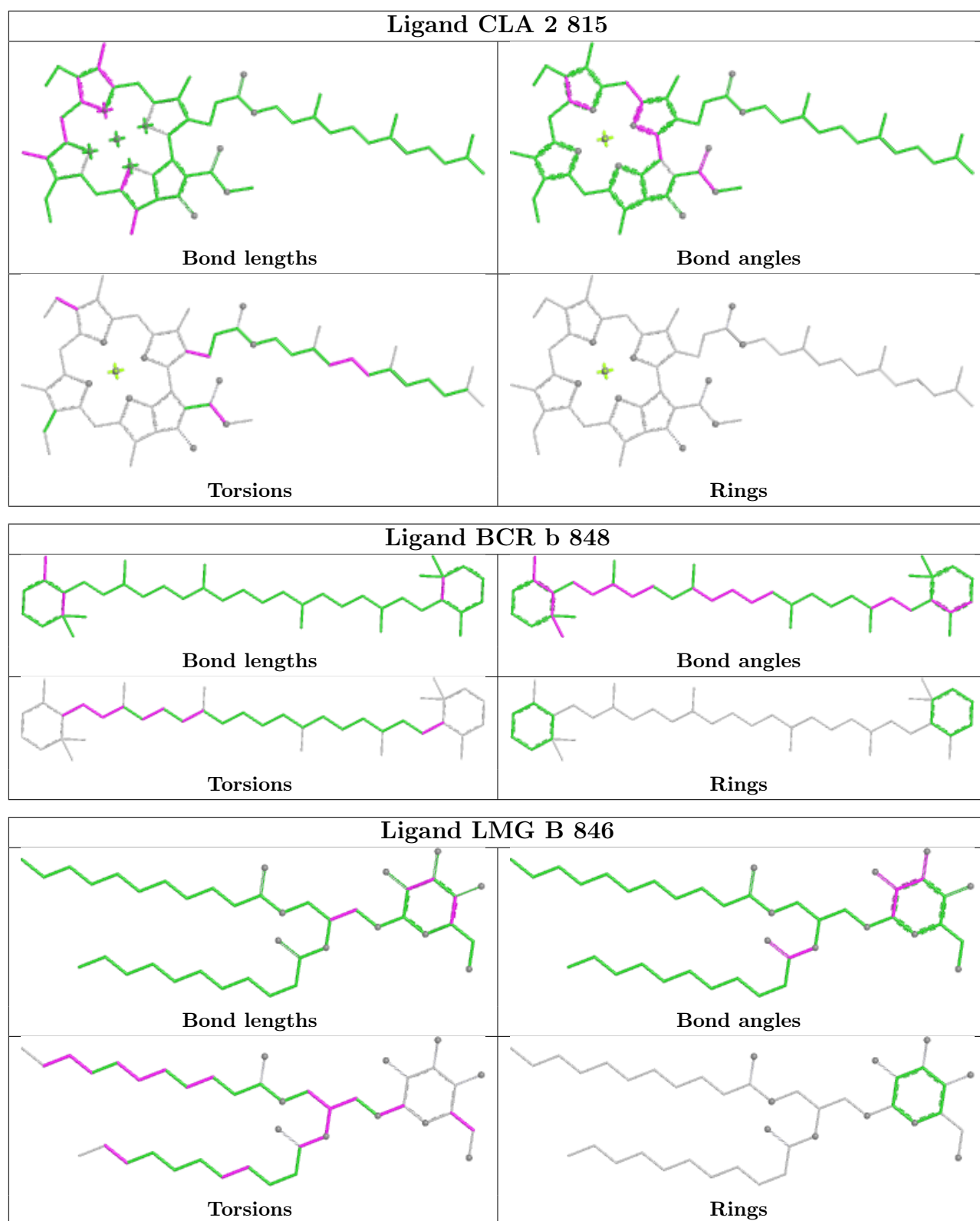


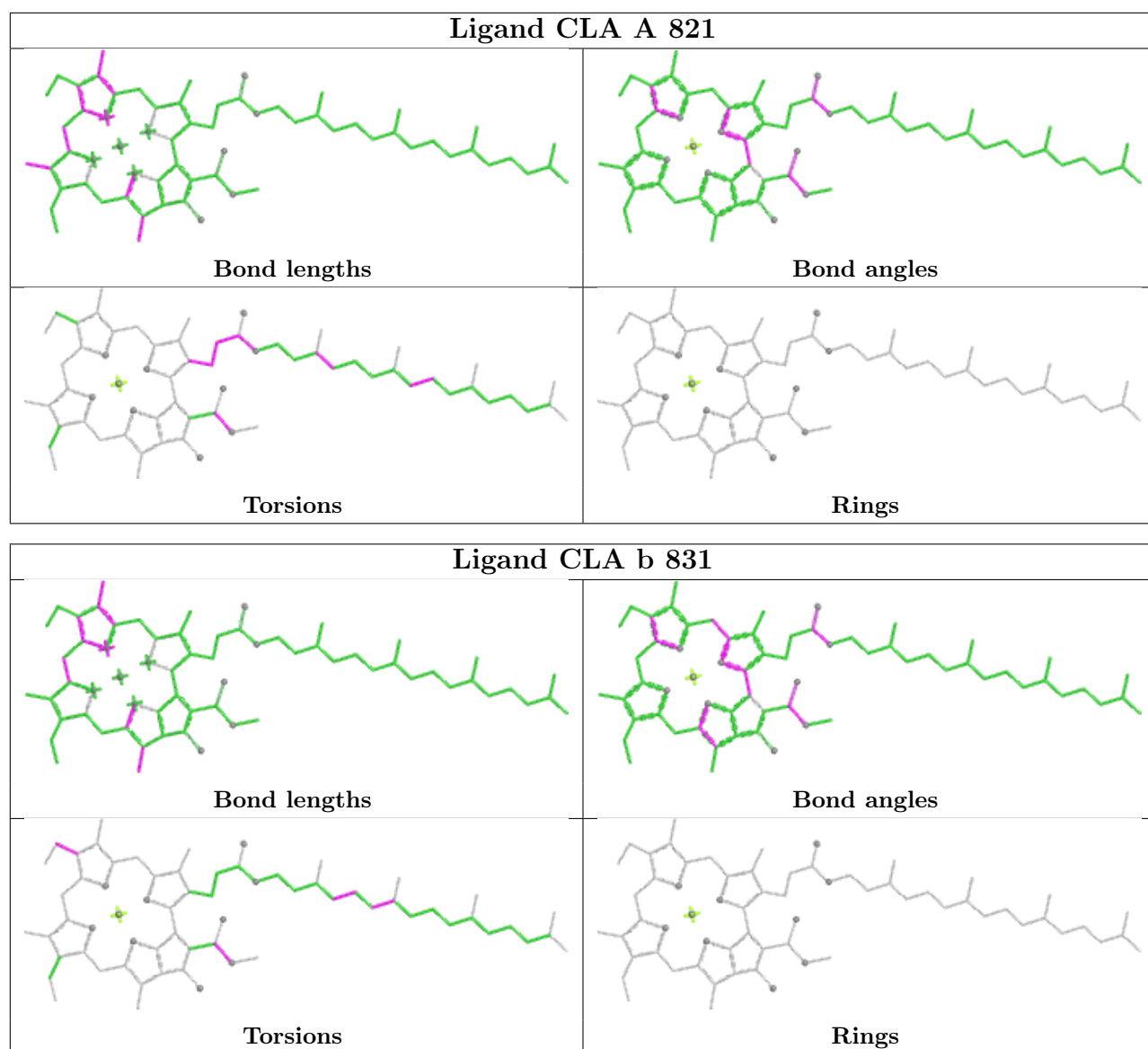
Ligand CLA 2 807



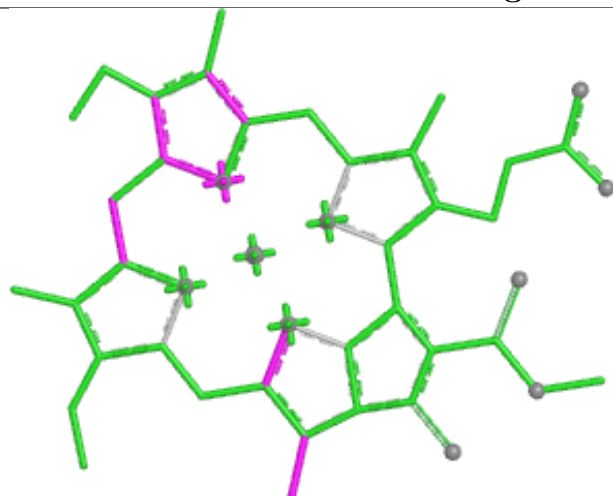




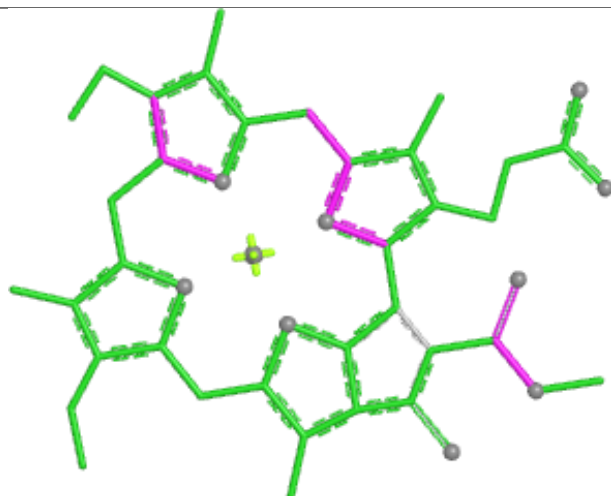




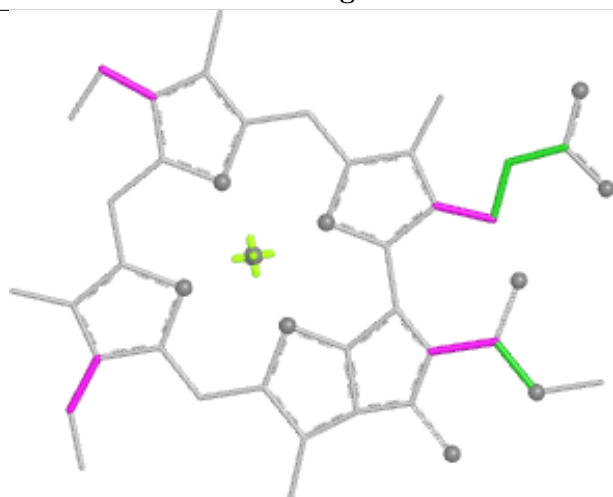
Ligand CLA K 4002



Bond lengths



Bond angles

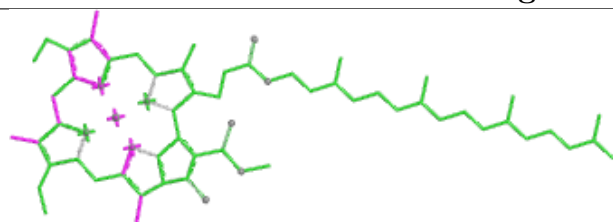


Torsions

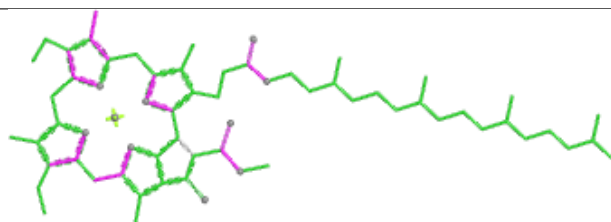


Rings

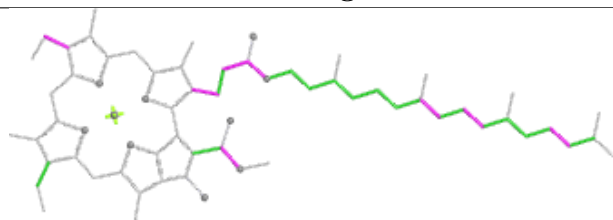
Ligand CLA a 806



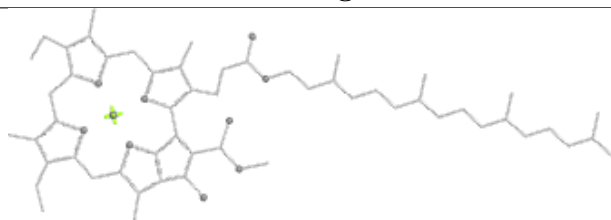
Bond lengths



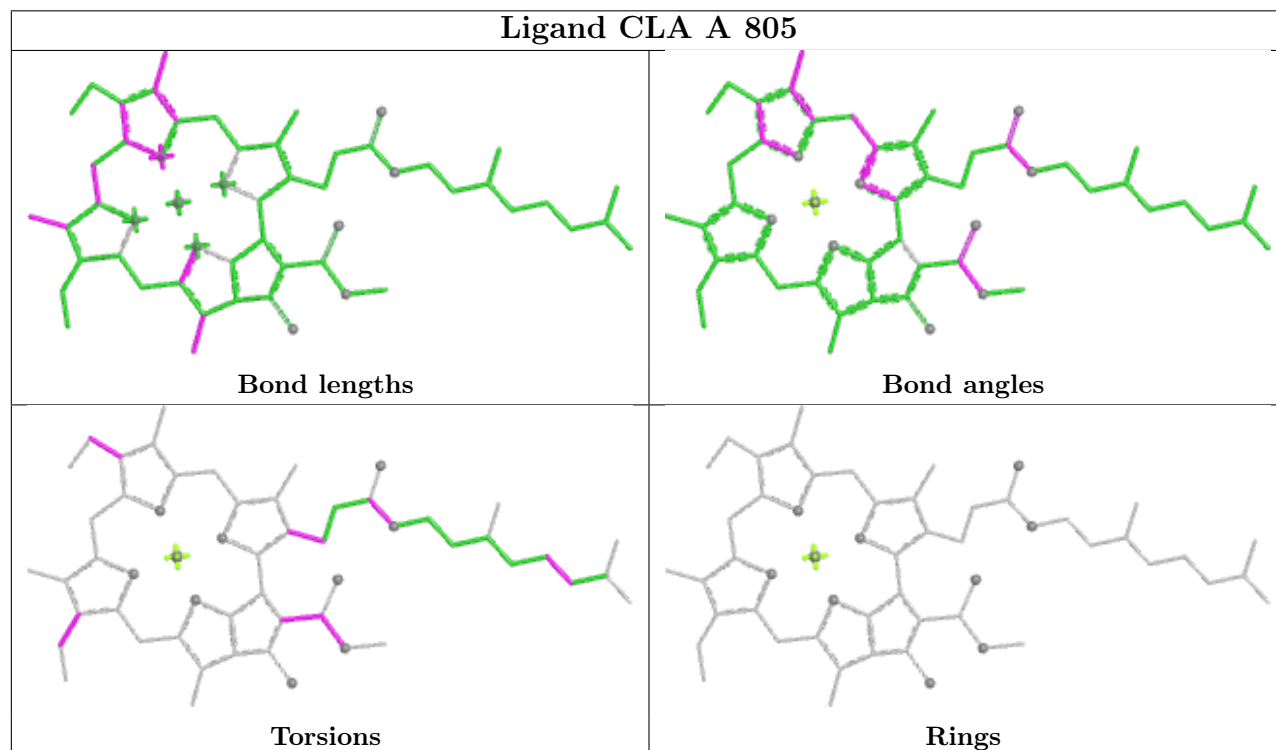
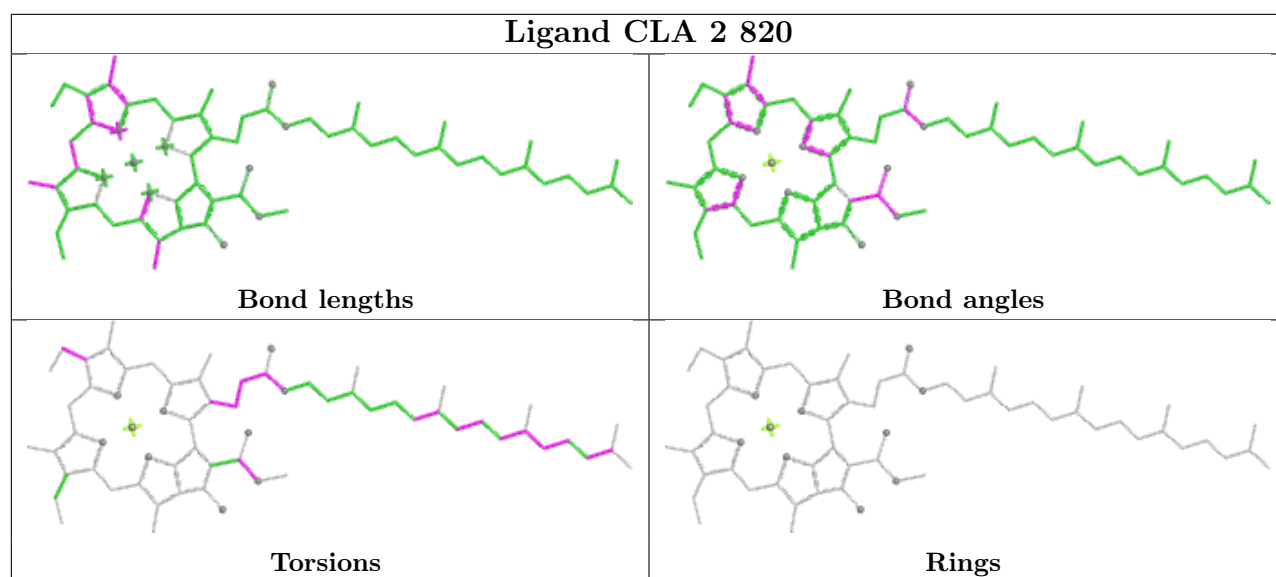
Bond angles

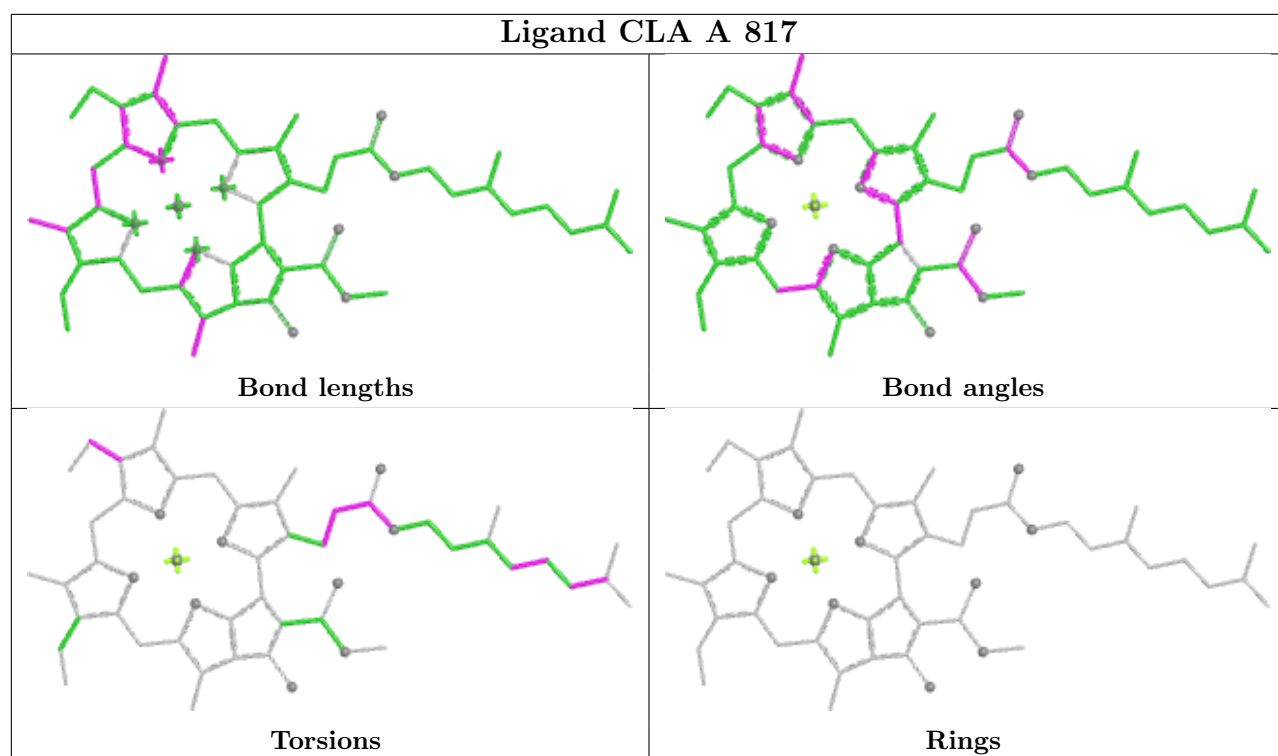


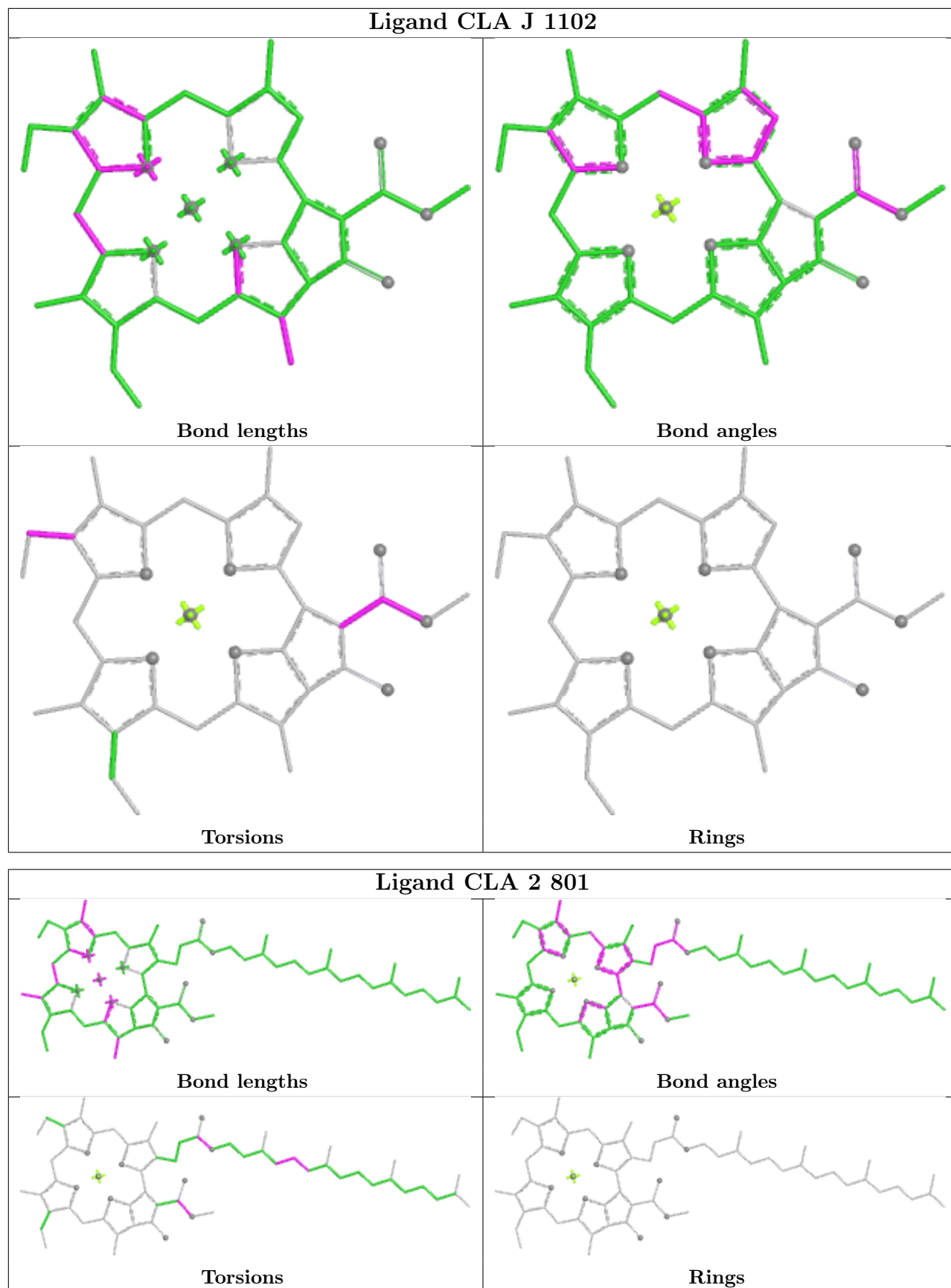
Torsions



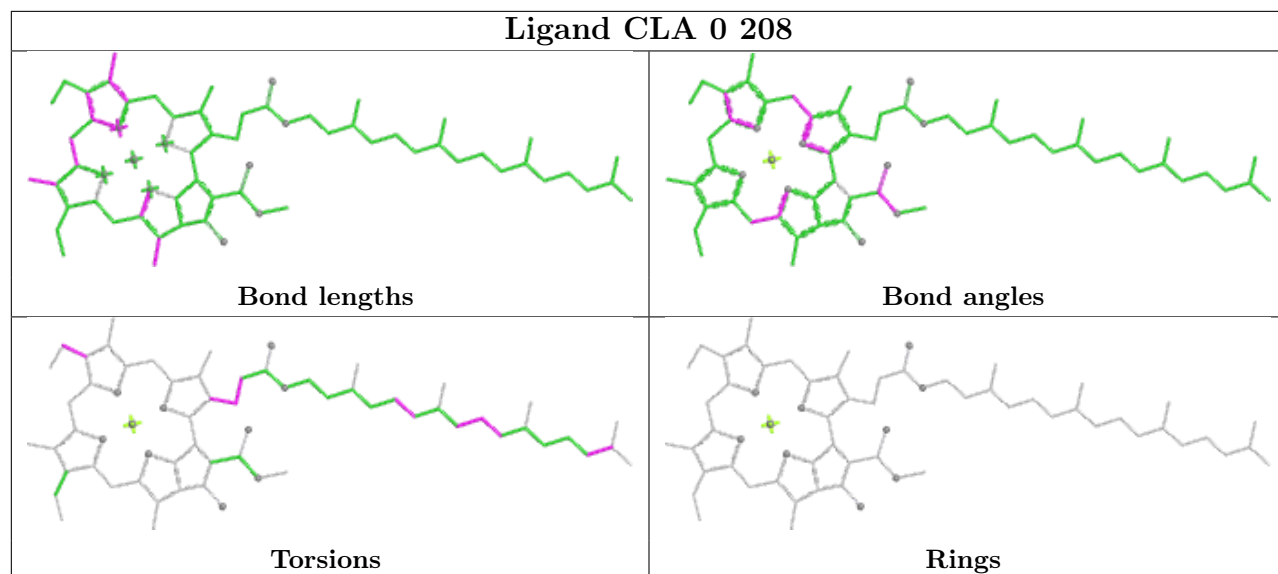
Rings



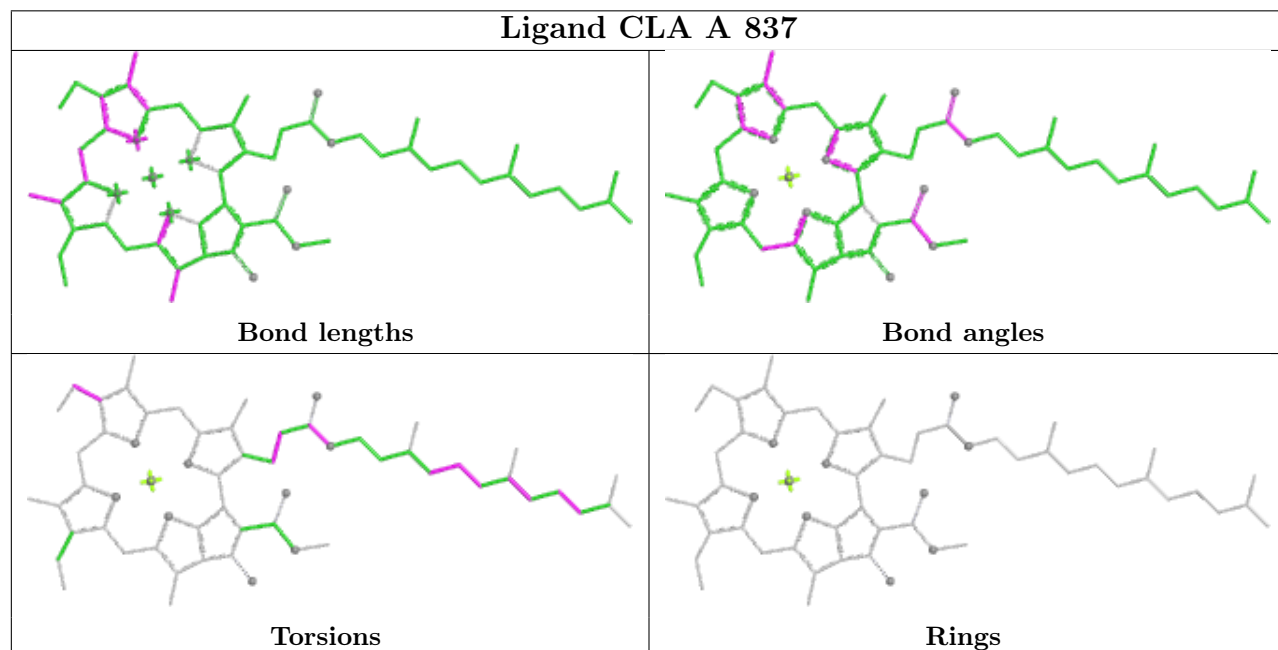


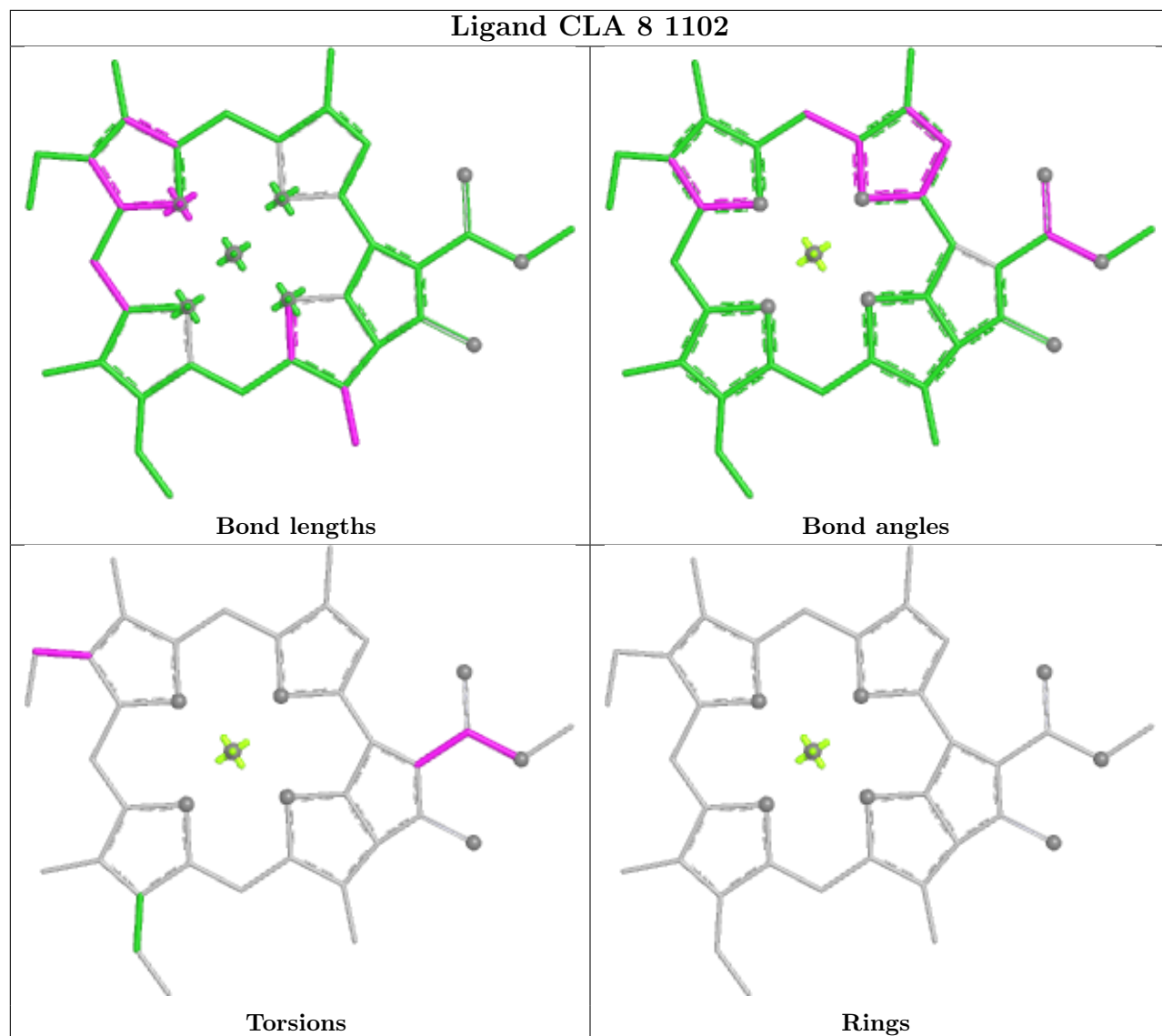


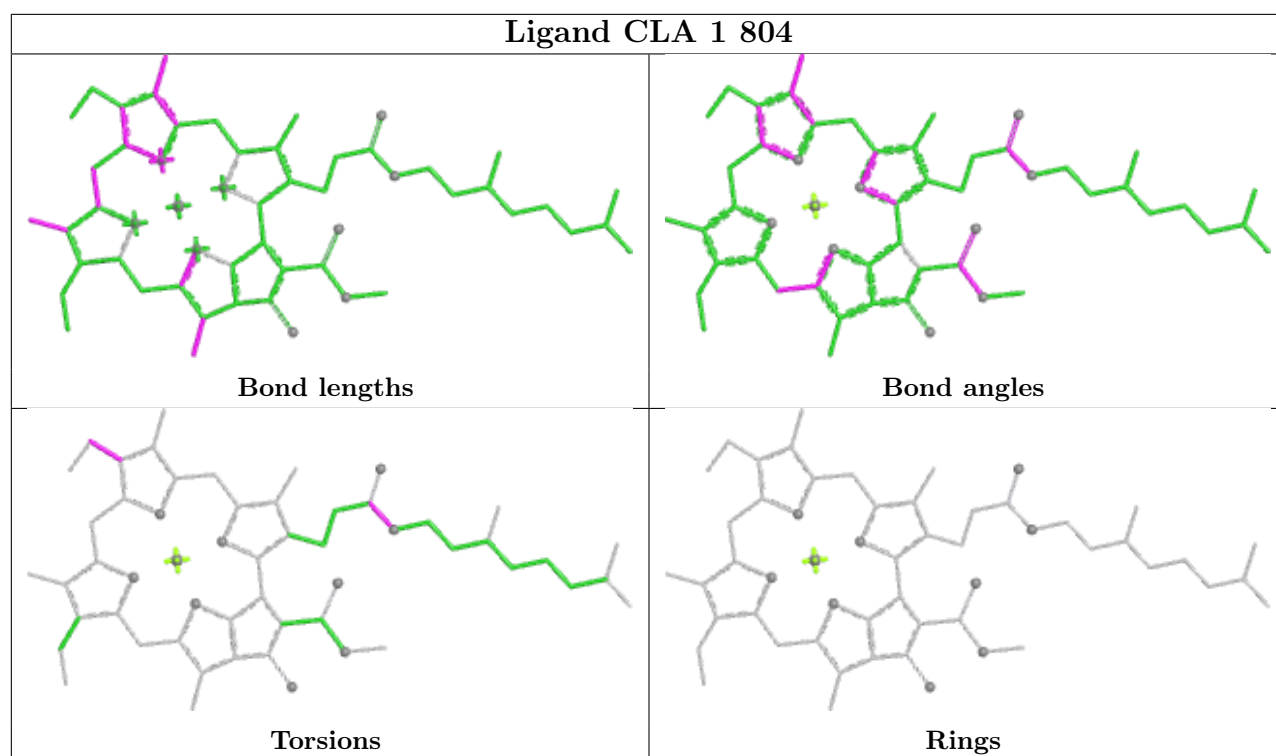
Ligand CLA 0 208

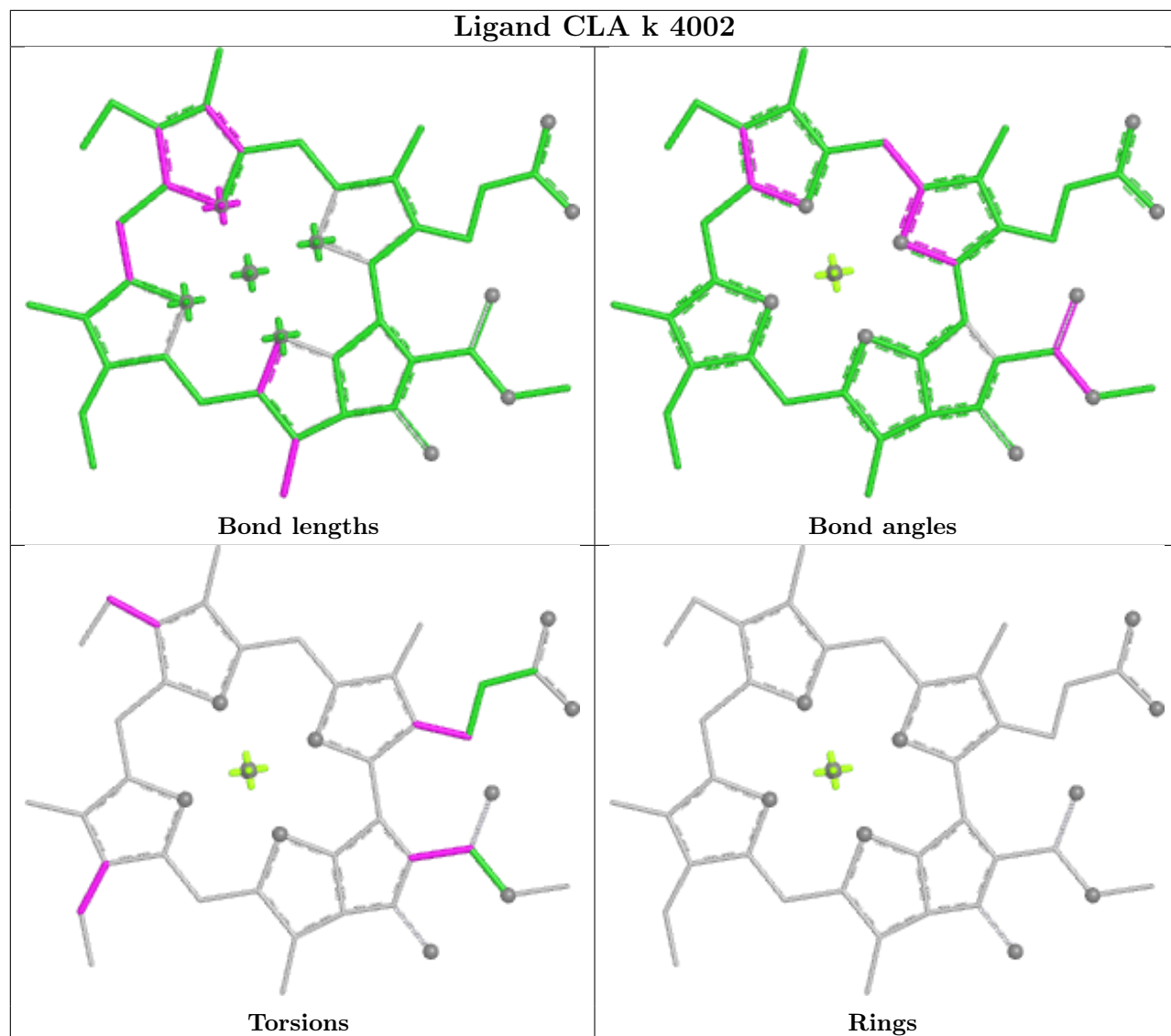


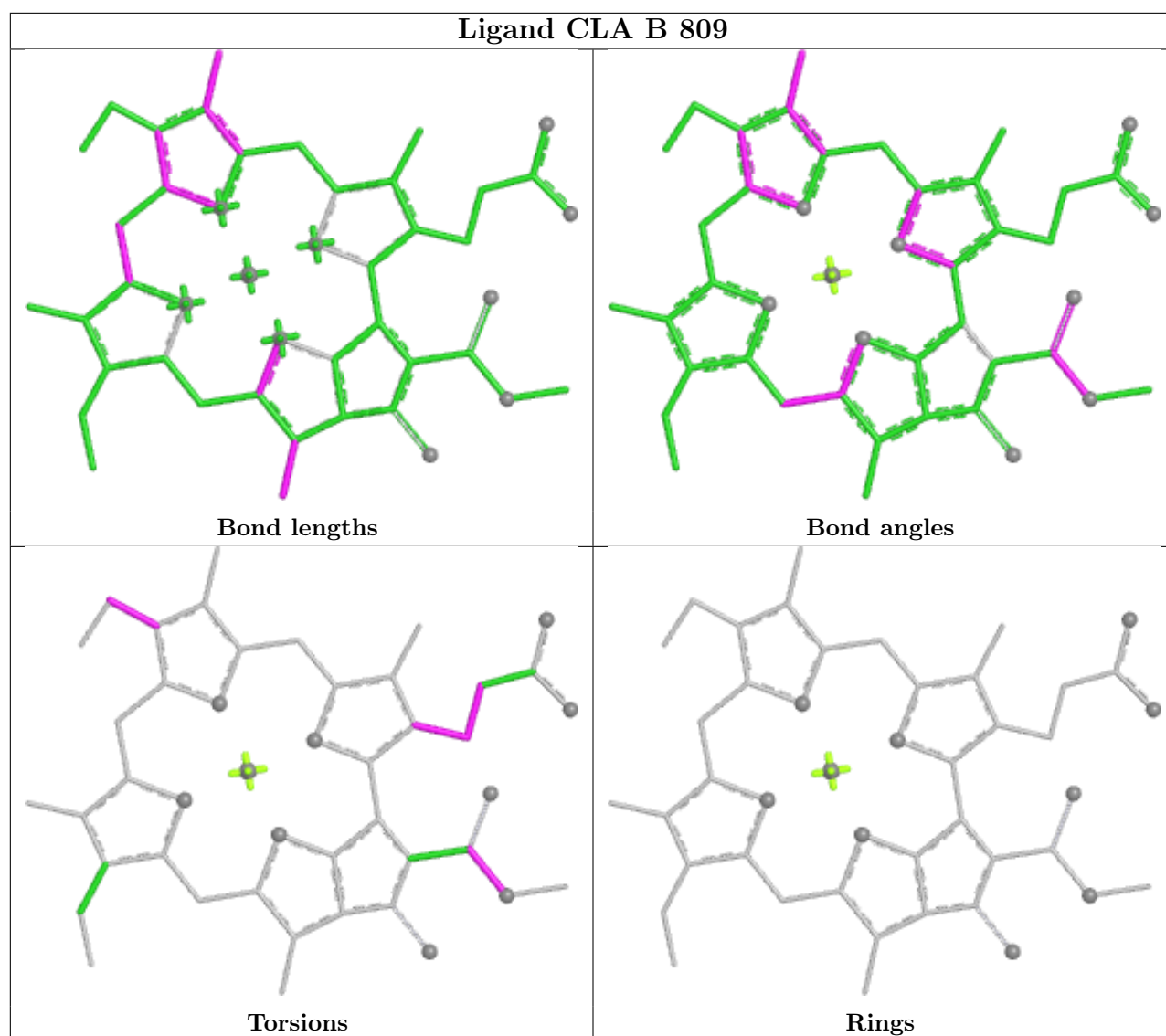
Ligand CLA A 837











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

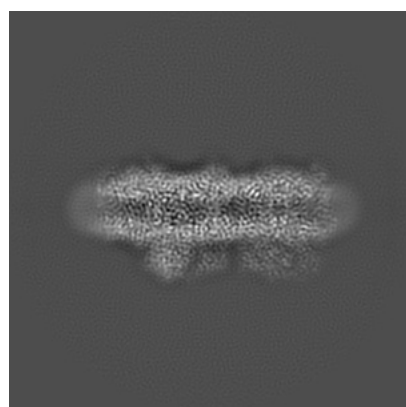
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21320. These allow visual inspection of the internal detail of the map and identification of artifacts.

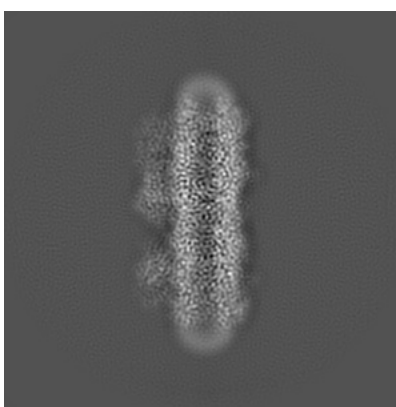
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

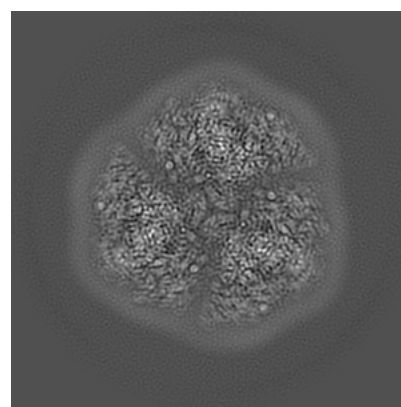
6.1.1 Primary map



X



Y

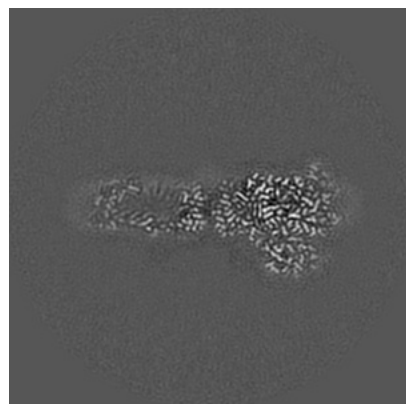


Z

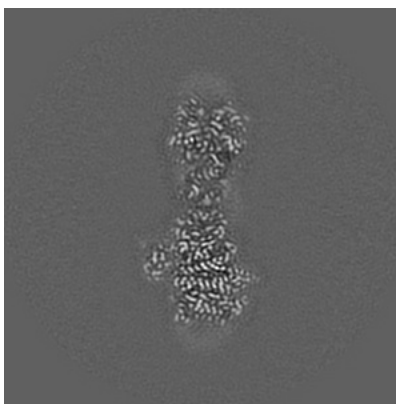
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

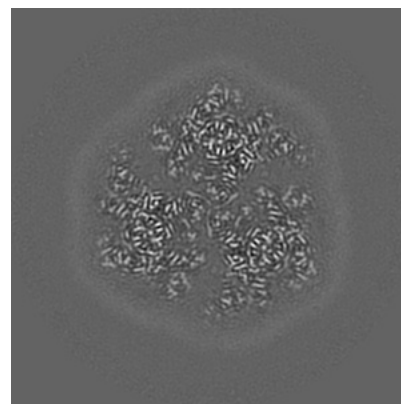
6.2.1 Primary map



X Index: 150



Y Index: 150

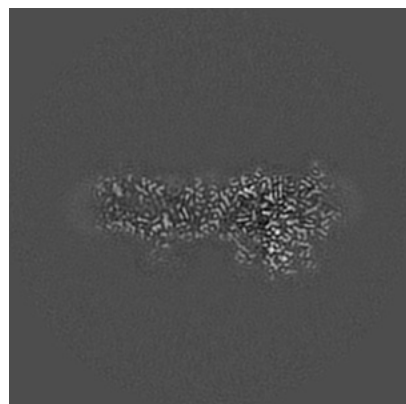


Z Index: 150

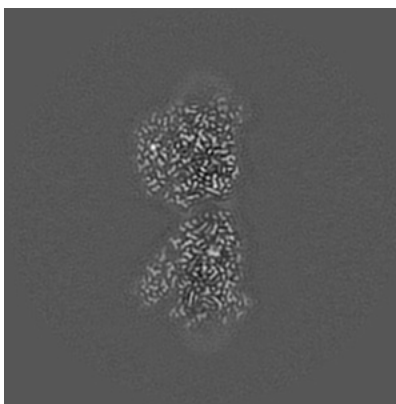
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

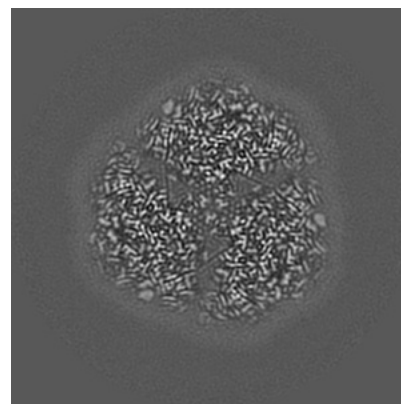
6.3.1 Primary map



X Index: 158



Y Index: 116

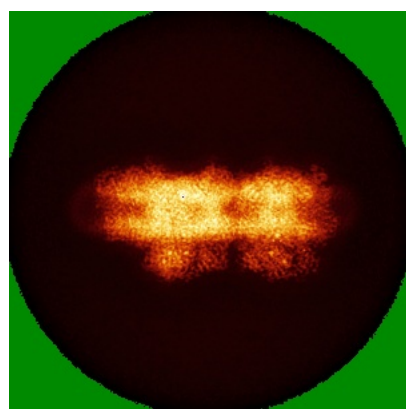


Z Index: 161

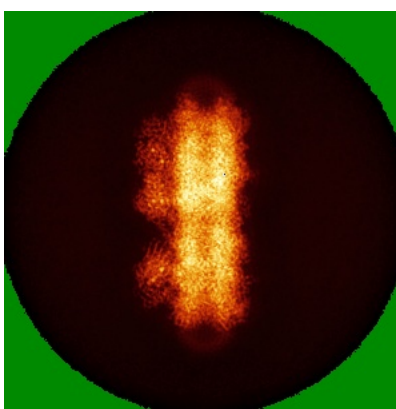
The images above show the largest variance slices of the map in three orthogonal directions.

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

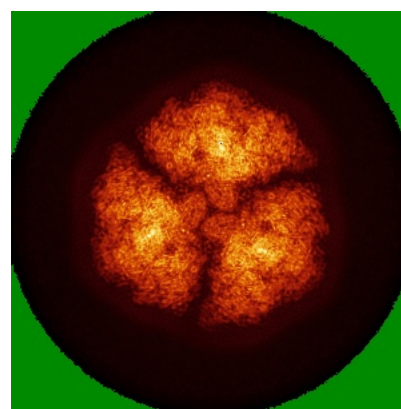
6.4.1 Primary map



X



Y

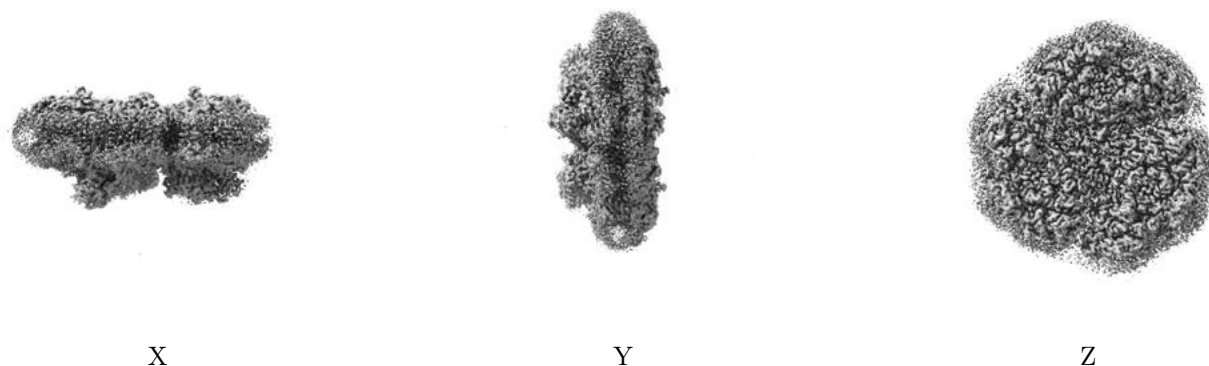


Z

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 2.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

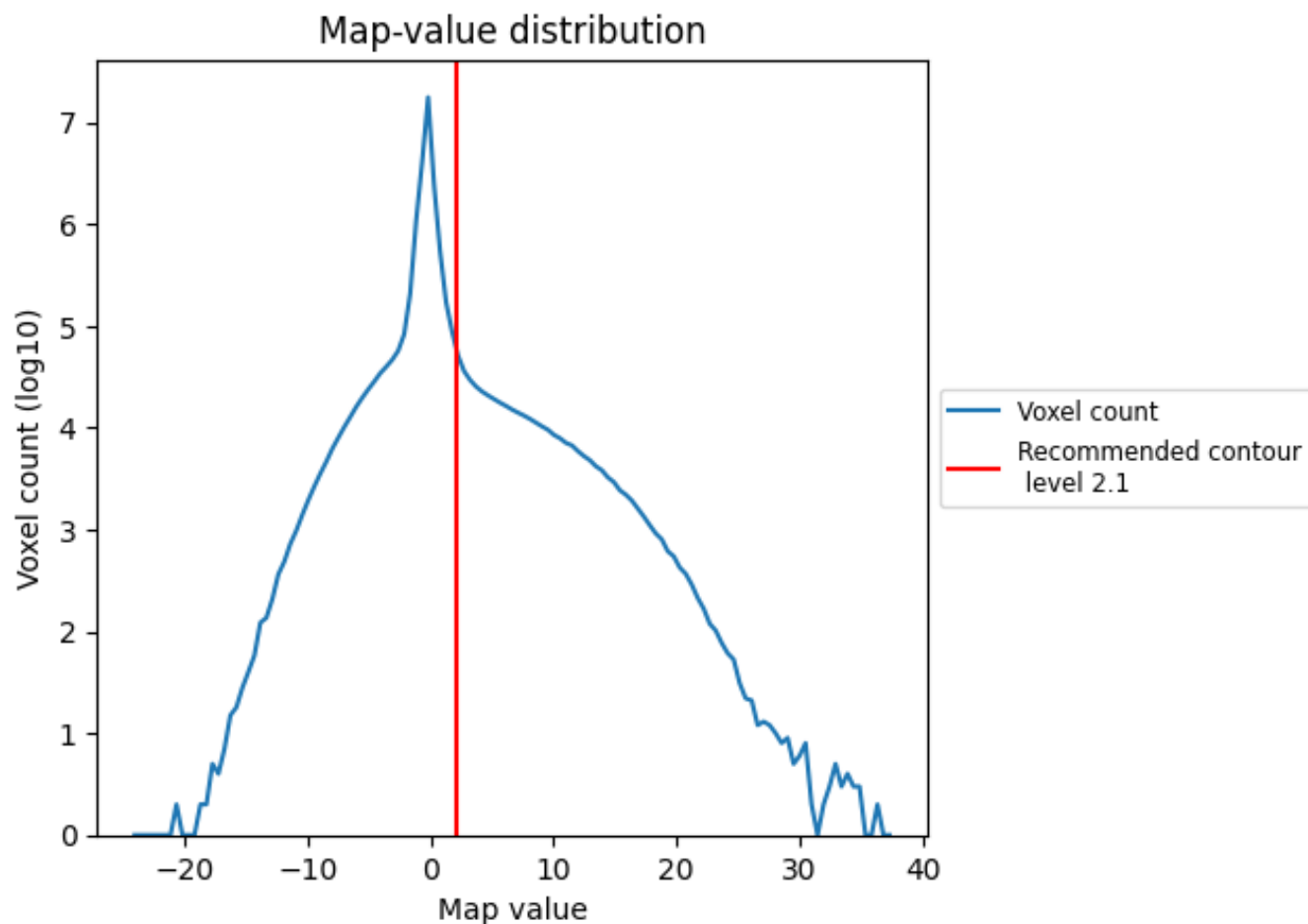
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

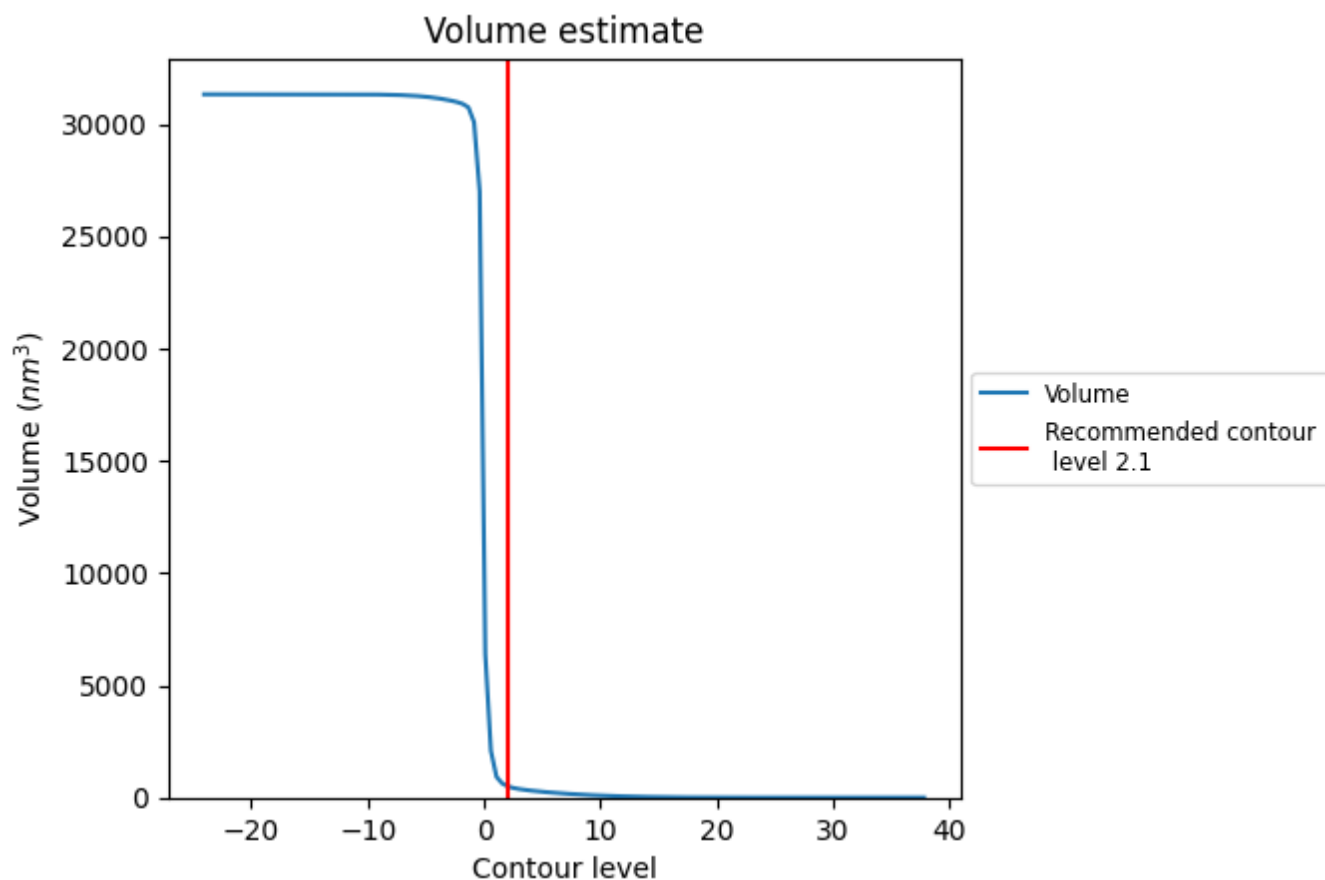
This section contains the results of statistical analysis of the map.

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.

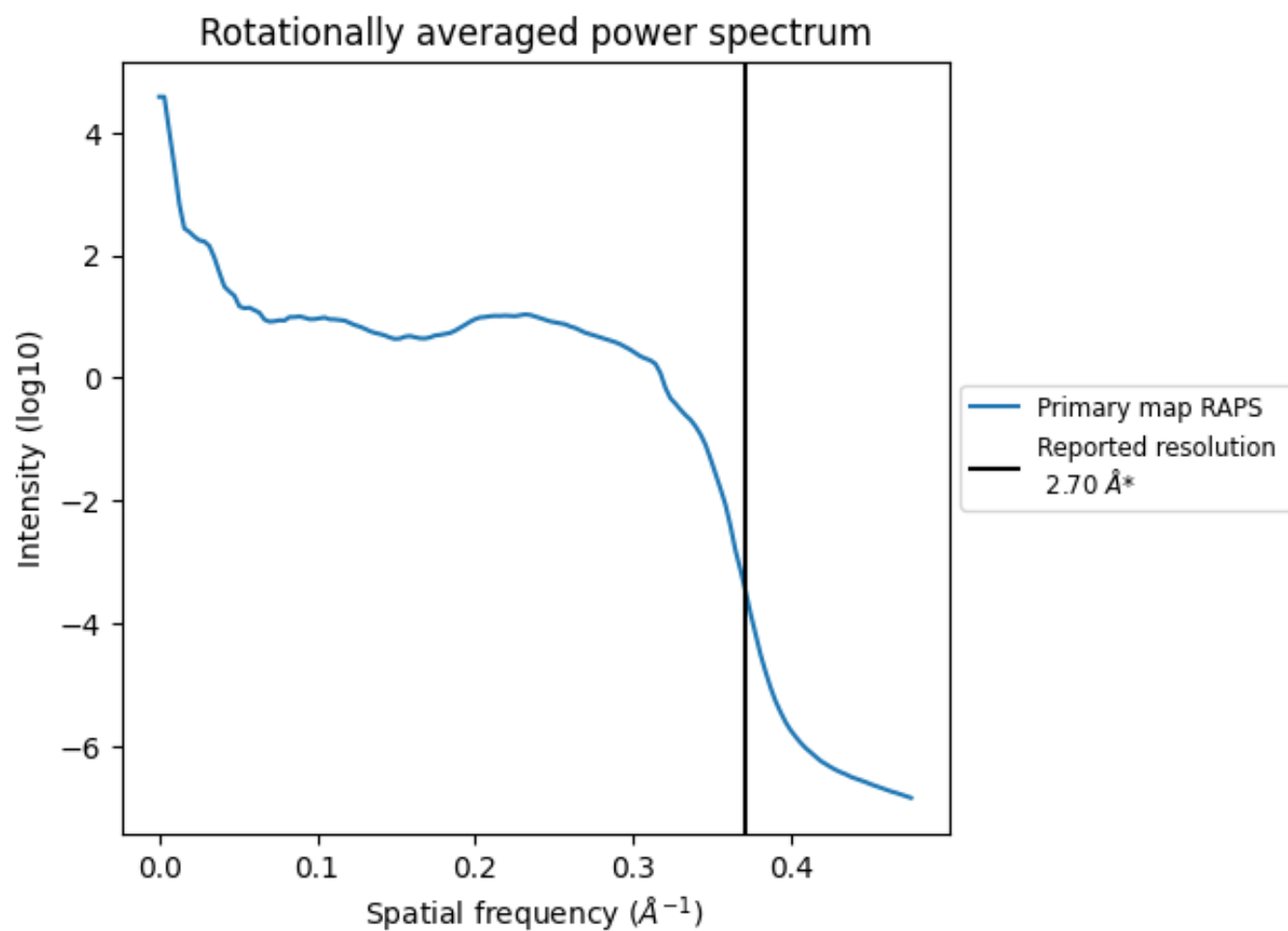
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 492 nm^3 ; this corresponds to an approximate mass of 445 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 ⓘ

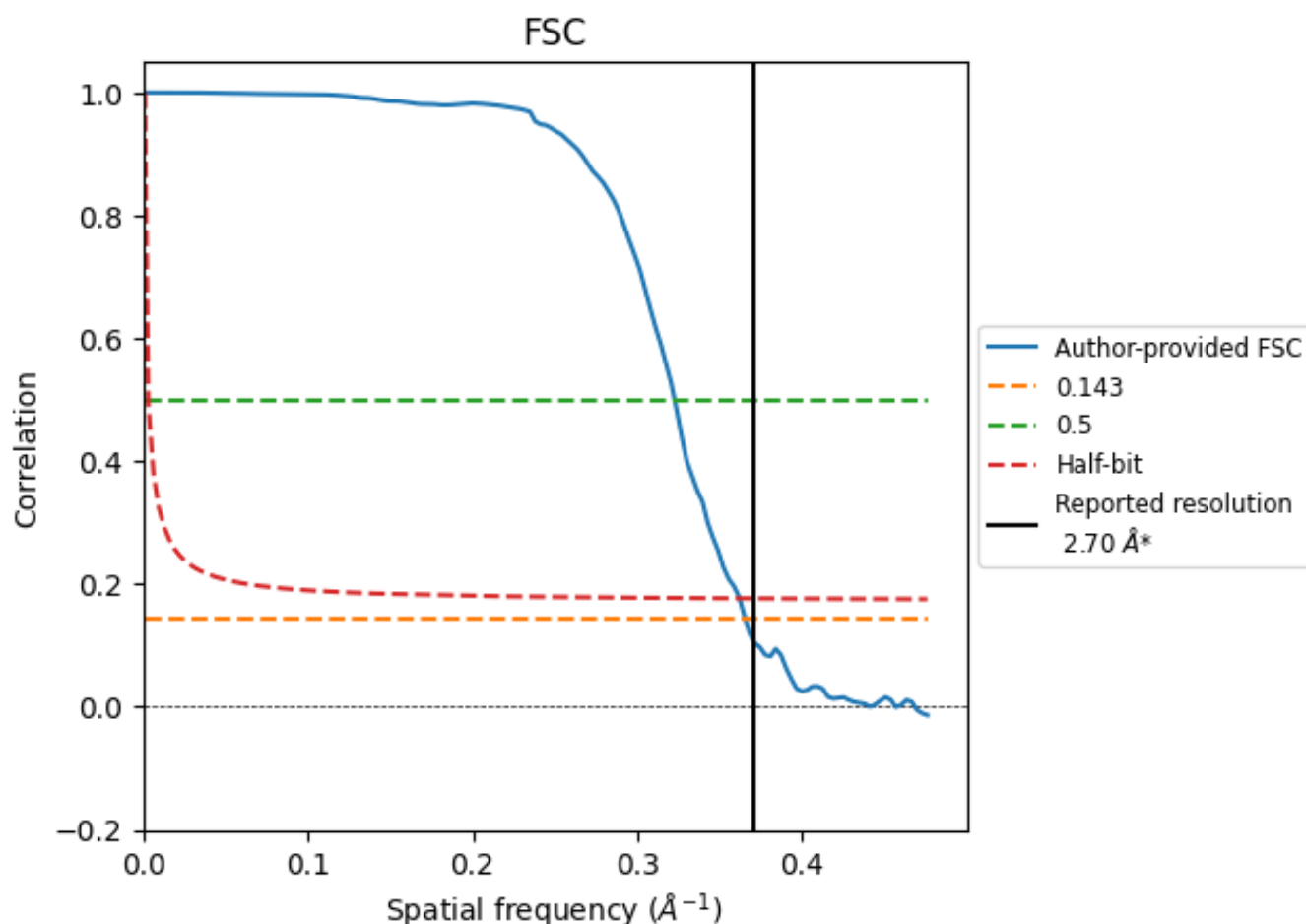


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 Å⁻¹

8.2 Resolution estimates [i](#)

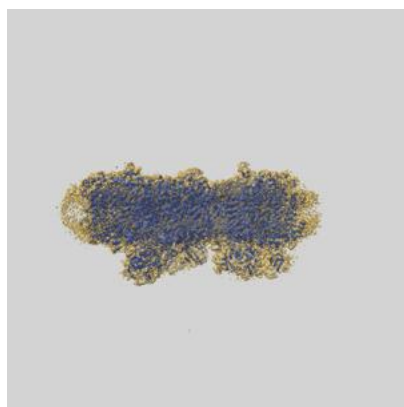
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.73	3.10	2.76
Unmasked-calculated*	-	-	-

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

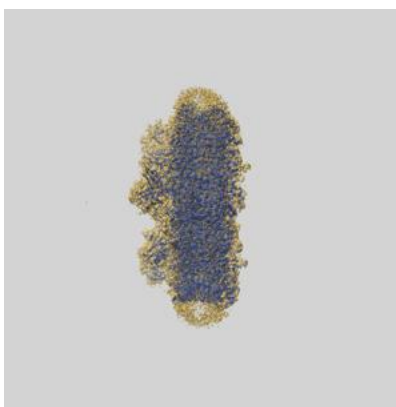
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21320 and PDB model 6VPV. Per-residue inclusion information can be found in section 3 on page 31.

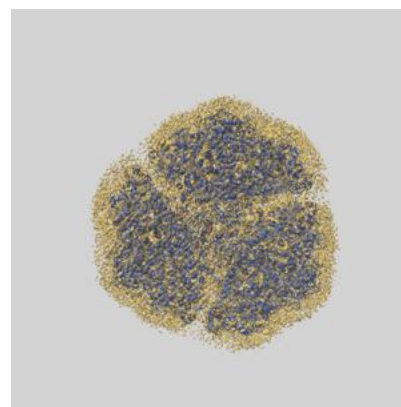
9.1 Map-model overlay [i](#)



X



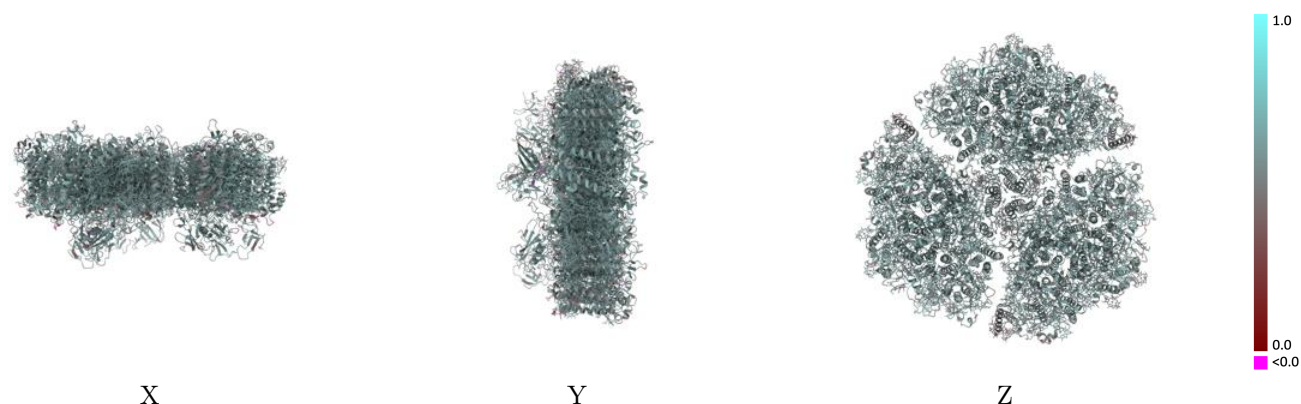
Y



Z

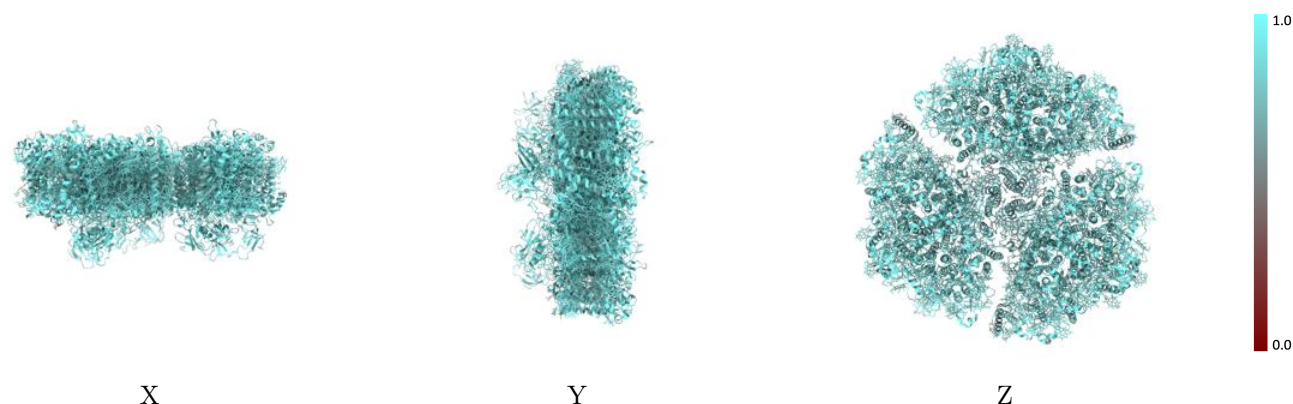
The images above show the 3D surface view of the map at the recommended contour level 2.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



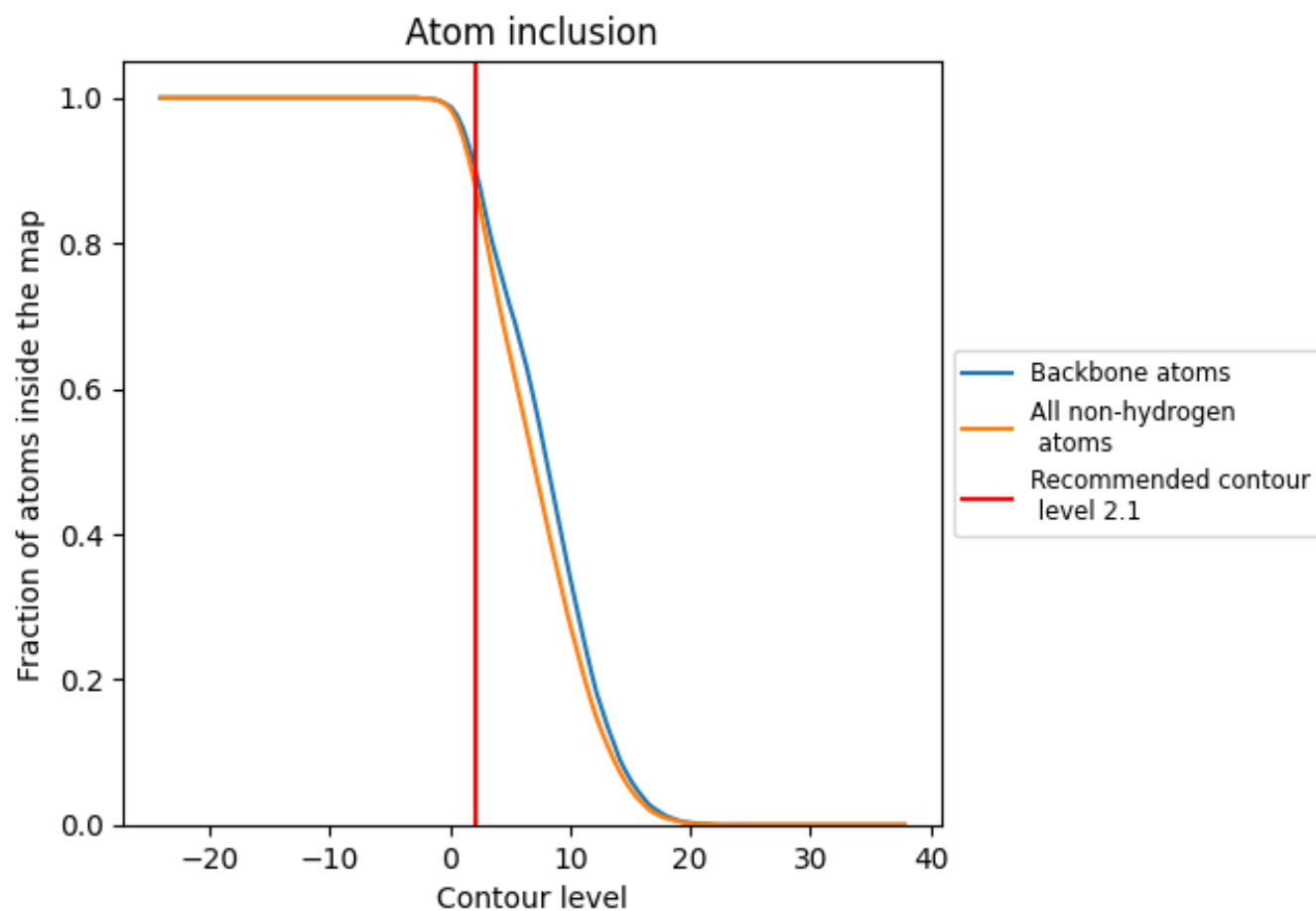
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 88% 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 (2.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8800	 0.5690
0	 0.8310	 0.5540
1	 0.8910	 0.5810
2	 0.8870	 0.5730
3	 0.9220	 0.5680
4	 0.8620	 0.5350
5	 0.8590	 0.5340
6	 0.8340	 0.5290
7	 0.8120	 0.5610
8	 0.8270	 0.5480
9	 0.7340	 0.4740
A	 0.8990	 0.5850
B	 0.8970	 0.5800
C	 0.9430	 0.5710
D	 0.8730	 0.5410
E	 0.8750	 0.5440
F	 0.8380	 0.5340
I	 0.8290	 0.5630
J	 0.8370	 0.5650
K	 0.7620	 0.4920
L	 0.8420	 0.5560
M	 0.8220	 0.5660
a	 0.9020	 0.5830
b	 0.9020	 0.5810
c	 0.9430	 0.5770
d	 0.8700	 0.5410
e	 0.8710	 0.5430
f	 0.8410	 0.5370
i	 0.8290	 0.5690
j	 0.8410	 0.5610
k	 0.7600	 0.4880
l	 0.8410	 0.5560
m	 0.8250	 0.5650
z	 0.7880	 0.5480

