



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:39 PM UTC

PDB ID : 6TRA / pdb_00006tra
EMDB ID : EMD-10557
Title : Cryo- EM structure of the Thermosynechococcus elongatus photosystem I in the presence of cytochrome c6
Authors : Koelsch, A.; Radon, C.; Baumert, A.; Buerger, J.; Miehke, T.; Lisdat, F.; Zouni, A.; Wendler, P.
Deposited on : 2019-12-18
Resolution : 2.85 Å(reported)
Based on initial model : 1JB0

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

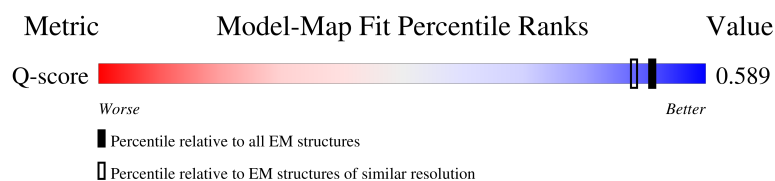
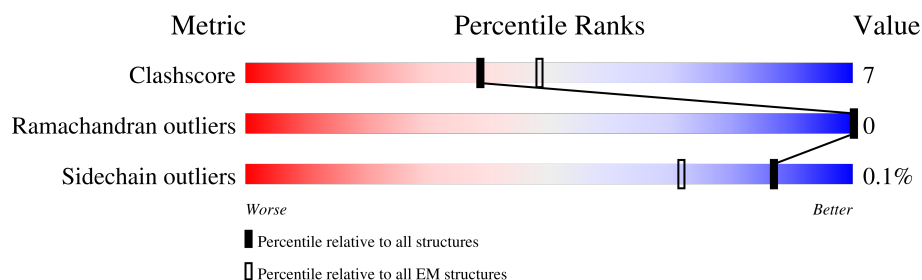
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.85 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	11965 (2.35 - 3.35)

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

Mol	Chain	Length	Quality of chain
1	A	755	9% 83% 16%
2	B	741	11% 85% 15%
3	C	81	11% 79% 20%

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Mol	Chain	Length	Quality of chain
4	D	139	
5	E	76	
6	F	141	
7	I	38	
8	J	41	
9	K	83	
10	L	155	
11	M	31	
12	X	36	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CL0	A	801	X	-	-	-
14	CLA	A	802	X	-	-	-
14	CLA	A	803	X	-	-	-
14	CLA	A	804	X	-	-	-
14	CLA	A	805	X	-	-	-
14	CLA	A	806	X	-	-	-
14	CLA	A	807	X	-	-	-
14	CLA	A	808	X	-	-	-
14	CLA	A	809	X	-	-	-
14	CLA	A	810	X	-	-	-
14	CLA	A	811	X	-	-	-
14	CLA	A	812	X	-	-	-
14	CLA	A	813	X	-	-	-
14	CLA	A	814	X	-	-	-
14	CLA	A	815	X	-	-	-
14	CLA	A	816	X	-	-	-
14	CLA	A	817	X	-	-	-
14	CLA	A	818	X	-	-	-
14	CLA	A	819	X	-	-	-
14	CLA	A	820	X	-	-	-
14	CLA	A	821	X	-	-	-
14	CLA	A	822	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A	823	X	-	-	-
14	CLA	A	824	X	-	-	-
14	CLA	A	825	X	-	-	-
14	CLA	A	826	X	-	-	-
14	CLA	A	827	X	-	-	-
14	CLA	A	828	X	-	-	-
14	CLA	A	829	X	-	-	-
14	CLA	A	830	X	-	-	-
14	CLA	A	831	X	-	-	-
14	CLA	A	832	X	-	-	-
14	CLA	A	833	X	-	-	-
14	CLA	A	834	X	-	-	-
14	CLA	A	835	X	-	-	-
14	CLA	A	836	X	-	-	-
14	CLA	A	837	X	-	-	-
14	CLA	A	838	X	-	-	-
14	CLA	A	839	X	-	-	-
14	CLA	A	840	X	-	-	-
14	CLA	A	841	X	-	-	-
14	CLA	A	842	X	-	-	-
14	CLA	A	843	X	-	-	-
14	CLA	A	854	X	-	-	-
14	CLA	B	801	X	-	-	-
14	CLA	B	804	X	-	-	-
14	CLA	B	805	X	-	-	-
14	CLA	B	806	X	-	-	-
14	CLA	B	807	X	-	-	-
14	CLA	B	808	X	-	-	-
14	CLA	B	809	X	-	-	-
14	CLA	B	810	X	-	-	-
14	CLA	B	811	X	-	-	-
14	CLA	B	812	X	-	-	-
14	CLA	B	813	X	-	-	-
14	CLA	B	814	X	-	-	-
14	CLA	B	815	X	-	-	-
14	CLA	B	816	X	-	-	-
14	CLA	B	817	X	-	-	-
14	CLA	B	818	X	-	-	-
14	CLA	B	819	X	-	-	-
14	CLA	B	820	X	-	-	-
14	CLA	B	821	X	-	-	-
14	CLA	B	822	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B	823	X	-	-	-
14	CLA	B	824	X	-	-	-
14	CLA	B	825	X	-	-	-
14	CLA	B	826	X	-	-	-
14	CLA	B	827	X	-	-	-
14	CLA	B	828	X	-	-	-
14	CLA	B	829	X	-	-	-
14	CLA	B	830	X	-	-	-
14	CLA	B	831	X	-	-	-
14	CLA	B	832	X	-	-	-
14	CLA	B	833	X	-	-	-
14	CLA	B	834	X	-	-	-
14	CLA	B	835	X	-	-	-
14	CLA	B	836	X	-	-	-
14	CLA	B	837	X	-	-	-
14	CLA	B	838	X	-	-	-
14	CLA	B	839	X	-	-	-
14	CLA	B	840	X	-	-	-
14	CLA	B	841	X	-	-	-
14	CLA	B	842	X	-	-	-
14	CLA	F	201	X	-	-	-
14	CLA	F	203	X	-	-	-
14	CLA	F	204	X	-	-	-
14	CLA	J	101	X	-	-	-
14	CLA	J	102	X	-	-	-
14	CLA	K	101	X	-	-	-
14	CLA	K	102	X	-	-	-
14	CLA	L	201	X	-	-	-
14	CLA	L	204	X	-	-	-
14	CLA	L	205	X	-	-	-
14	CLA	L	206	X	-	-	-
14	CLA	M	102	X	-	-	-
14	CLA	X	1701	X	-	-	-

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 25197 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	746	Total	C	N	O	S	0	0
			5826	3823	995	982	26		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	740	Total	C	N	O	S	0	0
			5894	3878	988	1007	21		

- 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
			598	367	103	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	138	Total	C	N	O	S	0	0
			1075	682	186	204	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	70	Total	C	N	O	0	0
			546	347	94	105		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		

- 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
			303	209	40	49	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	41	Total	C	N	O	S	0	0
			340	232	51	55	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	79	Total	C	N	O	S	0	0
			571	377	92	101	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	152	Total	C	N	O	S	0	0
			1124	738	180	202	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	143	LEU	SER	conflict	UNP Q8DGB4

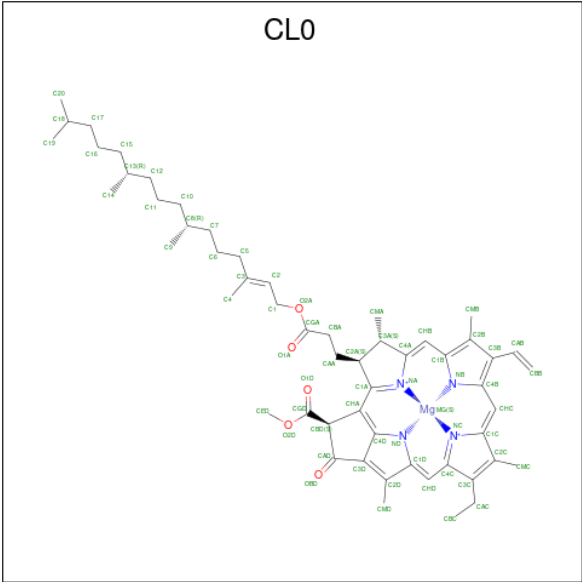
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total	C	N	O	S	0	0
			241	161	36	43	1		

- Molecule 12 is a protein called Photosystem I 4.8K protein.

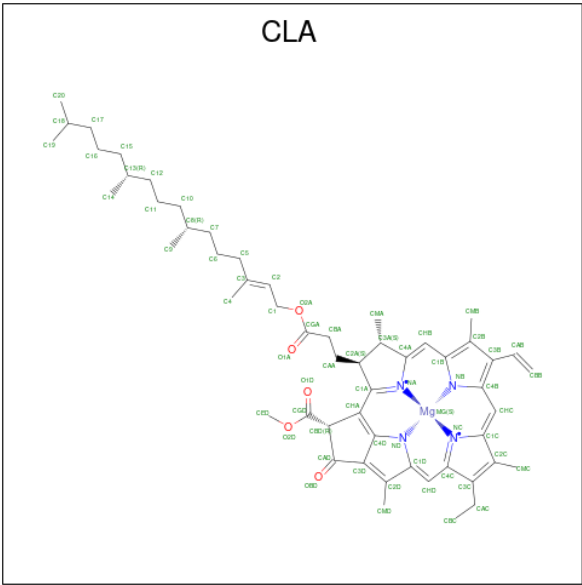
Mol	Chain	Residues	Atoms				AltConf	Trace
12	X	27	Total	C	N	O	0	0
			228	163	33	32		

- Molecule 13 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

- Molecule 14 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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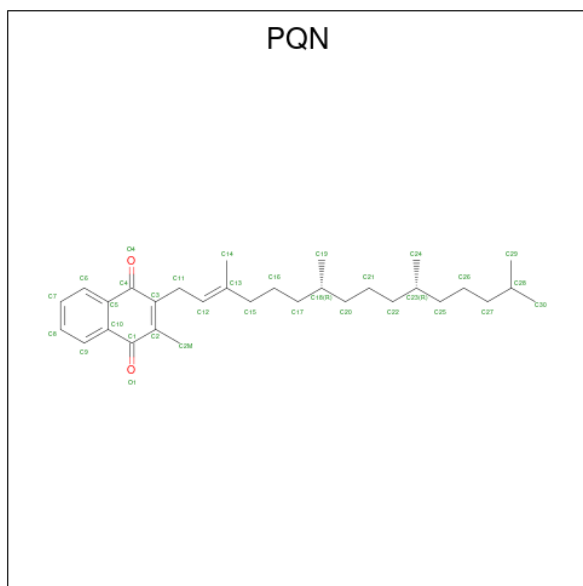
Mol	Chain	Residues	Atoms					AltConf
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14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	B	1	Total 49	C 39	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	F	1	Total 58	C 48	Mg 1	N 4	O 5	0
14	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	F	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	J	1	Total 45	C 35	Mg 1	N 4	O 5	0

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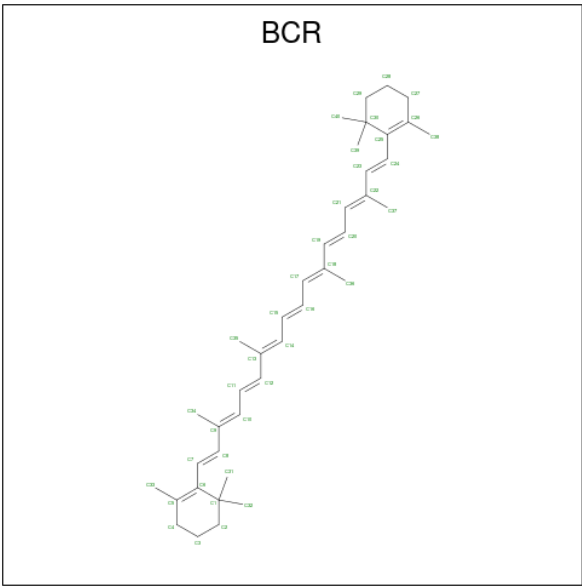
Mol	Chain	Residues	Atoms					AltConf
14	J	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
14	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	K	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	M	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
14	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 15 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	C	O	0
			33	31	2	
15	B	1	Total	C	O	0
			33	31	2	

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



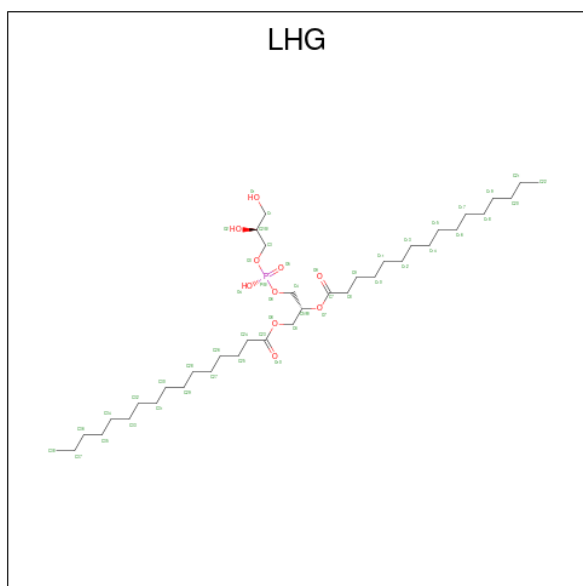
Mol	Chain	Residues	Atoms		AltConf
16	A	1	Total	C	0
			40	40	
16	A	1	Total	C	0
			40	40	
16	A	1	Total	C	0
			40	40	
16	A	1	Total	C	0
			40	40	
16	A	1	Total	C	0
			40	40	
16	A	1	Total	C	0
			40	40	
16	A	1	Total	C	0
			25	25	
16	B	1	Total	C	0
			40	40	
16	B	1	Total	C	0
			40	40	
16	B	1	Total	C	0
			40	40	
16	B	1	Total	C	0
			40	40	
16	B	1	Total	C	0
			40	40	

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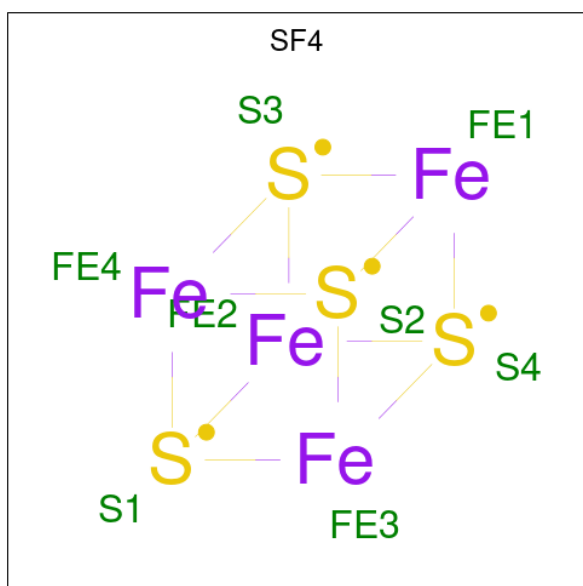
Mol	Chain	Residues	Atoms	AltConf
16	B	1	Total C 40 40	0
16	B	1	Total C 40 40	0
16	F	1	Total C 40 40	0
16	F	1	Total C 40 40	0
16	I	1	Total C 40 40	0
16	I	1	Total C 40 40	0
16	J	1	Total C 40 40	0
16	J	1	Total C 40 40	0
16	K	1	Total C 25 25	0
16	L	1	Total C 40 40	0
16	L	1	Total C 40 40	0

- 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
			49	38	10	1	
17	A	1	Total	C	O	P	0
			41	30	10	1	
17	B	1	Total	C	O	P	0
			49	38	10	1	
17	I	1	Total	C	O	P	0
			39	28	10	1	
17	M	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 18 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).

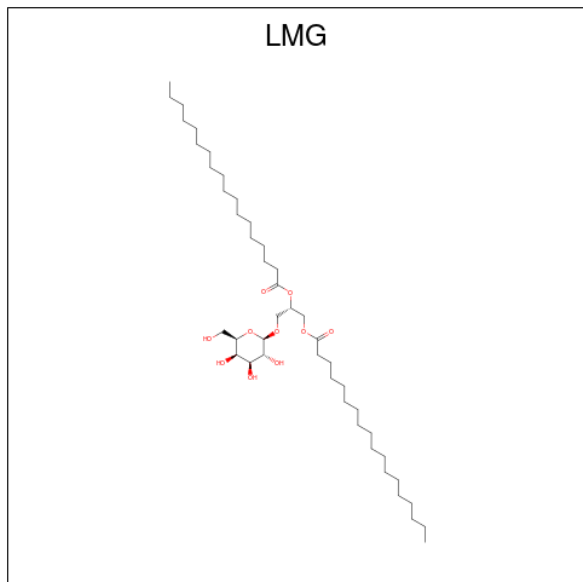


Mol	Chain	Residues	Atoms			AltConf
18	B	1	Total	Fe	S	0
			8	4	4	
18	C	1	Total	Fe	S	0
			8	4	4	
18	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 19 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
19	B	1	Total	Ca	0
			1	1	
19	L	1	Total	Ca	0
			1	1	

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
20	B	1	Total	C	O	0
			55	45	10	

- Molecule 21 is water.

Mol	Chain	Residues	Atoms		AltConf
21	A	65	Total	O	0
			65	65	
21	B	77	Total	O	0
			77	77	
21	C	25	Total	O	0
			25	25	
21	D	23	Total	O	0
			23	23	
21	E	9	Total	O	0
			9	9	
21	F	4	Total	O	0
			4	4	
21	I	1	Total	O	0
			1	1	
21	J	1	Total	O	0
			1	1	
21	K	1	Total	O	0
			1	1	

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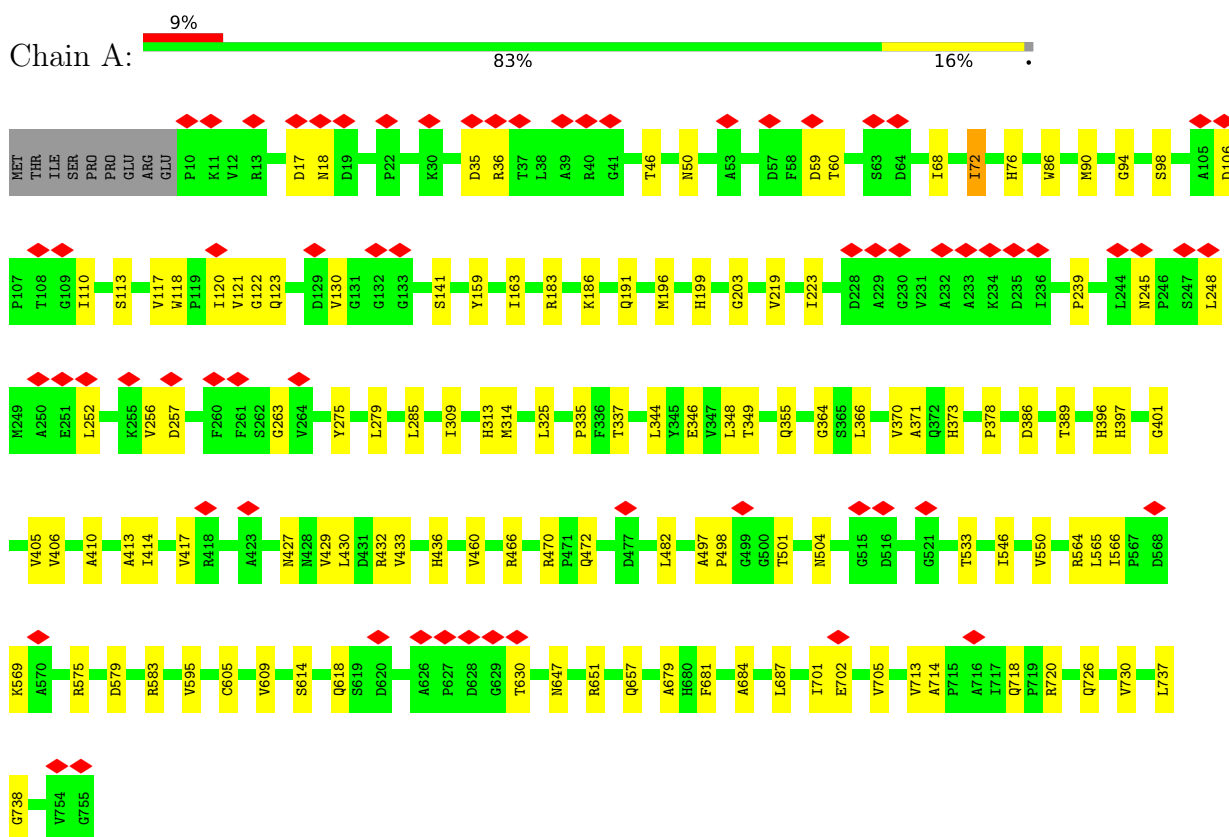
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Mol	Chain	Residues	Atoms		AltConf
21	L	10	Total	O	0
			10	10	
21	M	1	Total	O	0
			1	1	

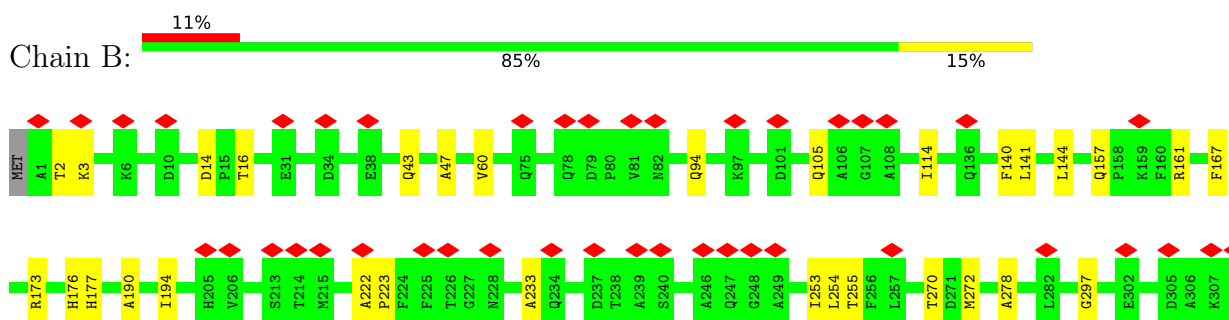
3 Residue-property plots [i](#)

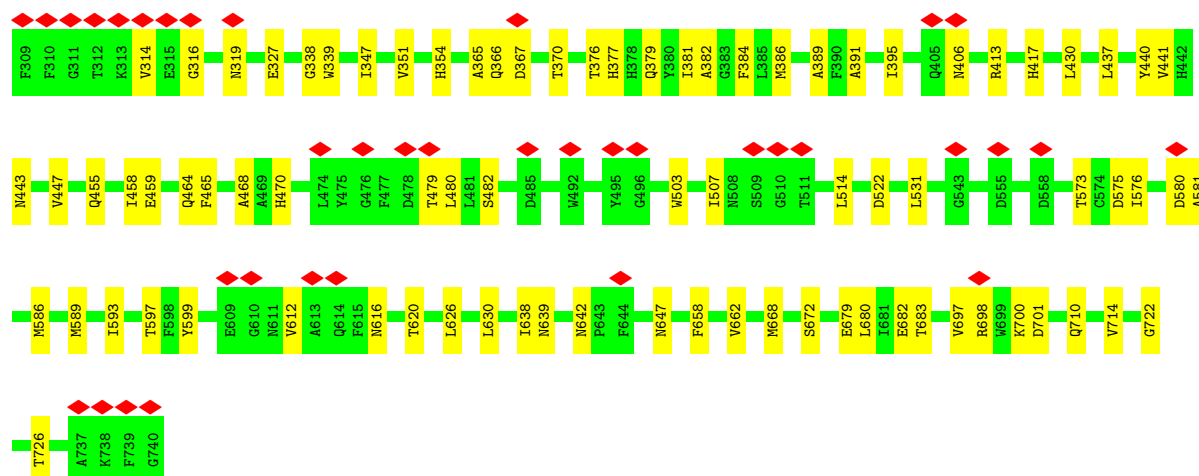
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

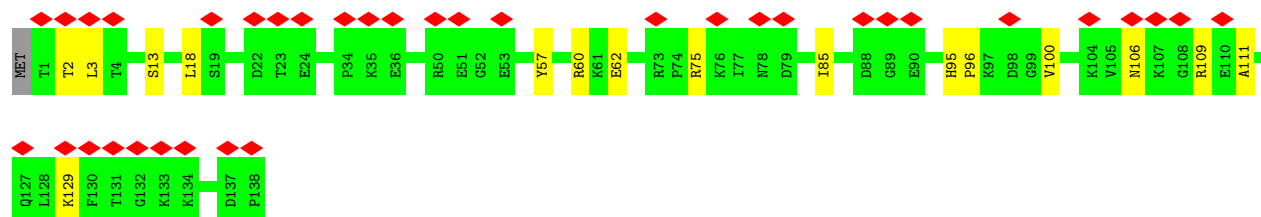
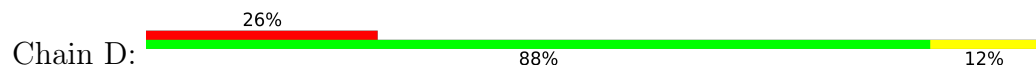




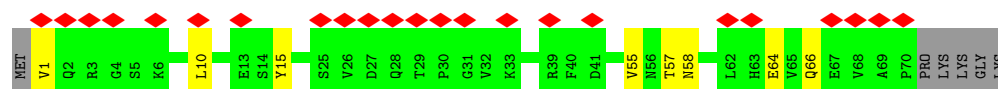
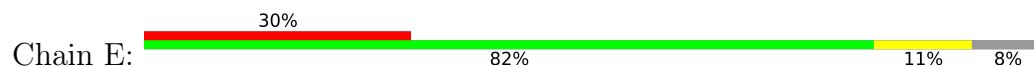
- Molecule 3: Photosystem I iron-sulfur center



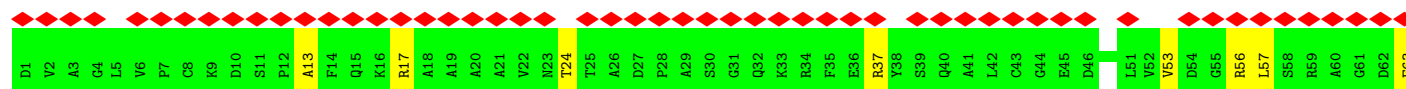
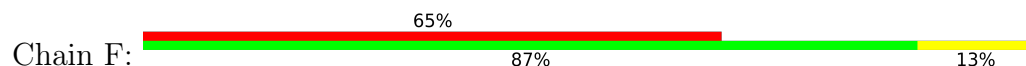
- Molecule 4: Photosystem I reaction center subunit II

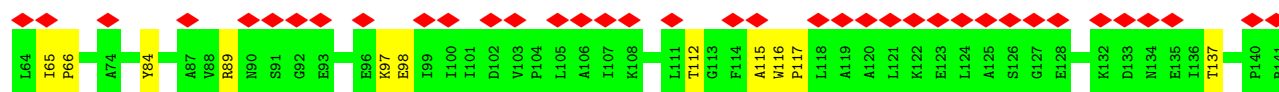


- Molecule 5: Photosystem I reaction center subunit IV



- Molecule 6: Photosystem I reaction center subunit III





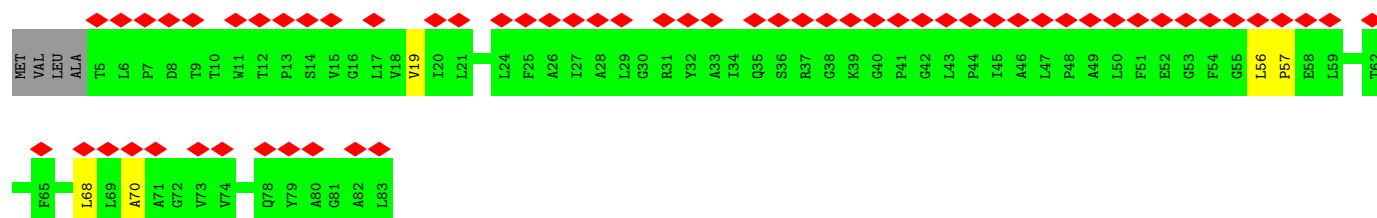
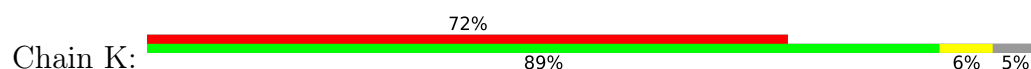
• Molecule 7: Photosystem I reaction center subunit VIII



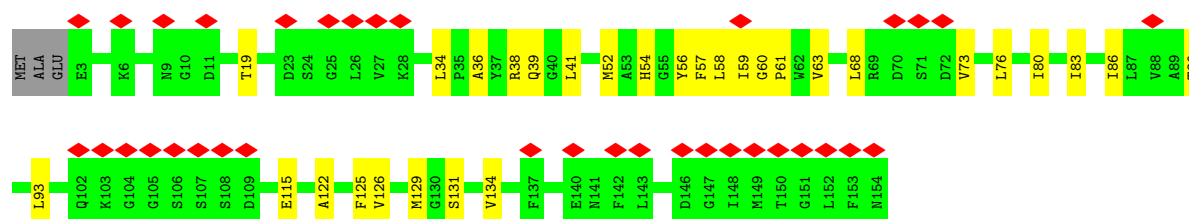
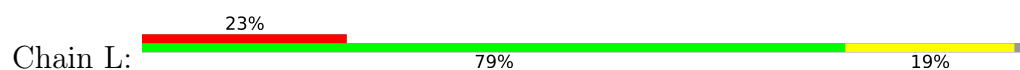
• Molecule 8: Photosystem I reaction center subunit IX



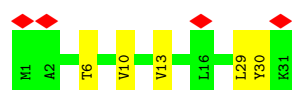
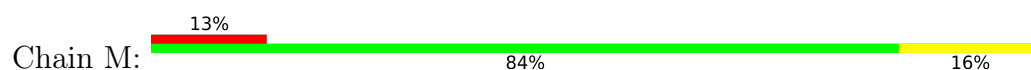
• Molecule 9: Photosystem I reaction center subunit PsaK



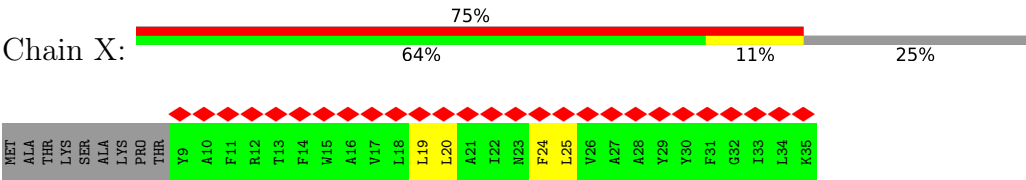
• Molecule 10: Photosystem I reaction center subunit XI



• Molecule 11: Photosystem I reaction center subunit XII



• Molecule 12: Photosystem I 4.8K protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	175999	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTFFIND4 was used to estimate contrast transfer function parameters. CTF correction was done in Relion 3.0.	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32	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	0.071	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.017	Depositor
Map size ($\text{\AA}$)	351.68002, 351.68002, 351.68002	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.628, 0.628, 0.628	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.21	0/6027	0.35	0/8220
2	B	0.21	0/6112	0.37	0/8350
3	C	0.24	0/608	0.39	0/824
4	D	0.20	0/1101	0.38	0/1492
5	E	0.19	0/559	0.35	0/762
6	F	0.17	0/1087	0.35	0/1476
7	I	0.22	0/304	0.51	0/415
8	J	0.14	0/342	0.29	0/467
9	K	0.17	0/585	0.35	0/800
10	L	0.19	0/1153	0.35	0/1565
11	M	0.23	0/244	0.36	0/332
12	X	0.13	0/236	0.28	0/321
All	All	0.21	0/18358	0.36	0/25024

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5826	0	5692	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5894	0	5653	95	0
3	C	598	0	580	13	0
4	D	1075	0	1077	19	0
5	E	546	0	535	7	0
6	F	1065	0	1077	14	0
7	I	303	0	305	8	0
8	J	340	0	346	1	0
9	K	571	0	593	3	0
10	L	1124	0	1127	23	0
11	M	241	0	264	4	0
12	X	228	0	234	4	0
13	A	65	0	72	1	0
14	A	2674	0	2849	56	0
14	B	2446	0	2562	40	0
14	F	153	0	127	1	0
14	J	82	0	58	0	0
14	K	104	0	88	2	0
14	L	260	0	288	6	0
14	M	36	0	24	0	0
14	X	45	0	33	1	0
15	A	33	0	46	2	0
15	B	33	0	46	0	0
16	A	265	0	369	18	0
16	B	320	0	448	13	0
16	F	80	0	112	1	0
16	I	80	0	112	3	0
16	J	80	0	112	5	0
16	K	25	0	33	4	0
16	L	80	0	112	1	0
17	A	90	0	129	4	0
17	B	49	0	74	1	0
17	I	39	0	51	2	0
17	M	49	0	74	1	0
18	B	8	0	0	0	0
18	C	16	0	0	0	0
19	B	1	0	0	0	0
19	L	1	0	0	0	0
20	B	55	0	86	3	0
21	A	65	0	0	21	0
21	B	77	0	0	11	0
21	C	25	0	0	5	0
21	D	23	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	E	9	0	0	5	0
21	F	4	0	0	1	0
21	I	1	0	0	1	0
21	J	1	0	0	0	0
21	K	1	0	0	0	0
21	L	10	0	0	6	0
21	M	1	0	0	0	0
All	All	25197	0	25388	369	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 7.

All (369) 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)
1:A:18:ASN:OD1	1:A:183:ARG:NH1	2.08	0.87
4:D:95:HIS:O	21:D:201:HOH:O	1.96	0.84
7:I:33:TYR:OH	11:M:30:TYR:OH	1.92	0.84
4:D:60:ARG:NH2	4:D:62:GLU:OE1	2.11	0.82
1:A:569:LYS:NZ	2:B:679:GLU:OE2	2.13	0.82
1:A:579:ASP:O	21:A:901:HOH:O	1.98	0.81
1:A:460:VAL:HG12	14:A:835:CLA:HBC2	1.61	0.81
2:B:698:ARG:NH1	21:B:906:HOH:O	2.13	0.81
2:B:43:GLN:OE1	2:B:161:ARG:NH2	2.16	0.79
6:F:98:GLU:OE2	21:F:301:HOH:O	2.01	0.79
2:B:167:PHE:O	2:B:173:ARG:NH2	2.16	0.78
1:A:263:GLY:O	1:A:275:TYR:OH	2.02	0.78
2:B:580:ASP:OD1	2:B:581:ALA:N	2.17	0.77
1:A:657:GLN:OE1	21:A:902:HOH:O	2.03	0.76
10:L:63:VAL:O	21:L:301:HOH:O	2.03	0.76
1:A:94:GLY:O	1:A:98:SER:OG	2.02	0.76
4:D:75:ARG:NH1	21:D:205:HOH:O	2.18	0.76
3:C:13:CYS:O	3:C:14:THR:OG1	2.02	0.75
3:C:46:ASP:OD1	21:C:201:HOH:O	2.03	0.75
1:A:472:GLN:OE1	21:A:904:HOH:O	2.05	0.74
1:A:564:ARG:O	4:D:60:ARG:NH1	2.20	0.74
11:M:6:THR:O	11:M:10:VAL:HG23	1.88	0.74
5:E:58:ASN:OD1	21:E:101:HOH:O	2.06	0.74
14:B:815:CLA:HBC3	14:B:815:CLA:HHD	1.70	0.73
4:D:129:LYS:NZ	21:D:206:HOH:O	2.20	0.73
1:A:647:ASN:OD1	21:A:903:HOH:O	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:616:ASN:OD1	21:B:901:HOH:O	2.06	0.73
6:F:84:TYR:OH	6:F:97:LYS:O	2.07	0.73
2:B:443:ASN:O	2:B:447:VAL:HG12	1.89	0.73
1:A:314:MET:SD	21:A:945:HOH:O	2.46	0.72
2:B:367:ASP:OD2	2:B:370:THR:OG1	2.06	0.72
4:D:57:TYR:OH	21:D:202:HOH:O	2.07	0.72
14:A:805:CLA:OBD	21:A:907:HOH:O	2.07	0.72
10:L:36:ALA:O	21:L:302:HOH:O	2.07	0.72
14:A:809:CLA:H91	14:A:812:CLA:H191	1.71	0.72
2:B:701:ASP:OD1	21:B:902:HOH:O	2.07	0.72
1:A:120:ILE:O	21:A:908:HOH:O	2.08	0.72
17:A:852:LHG:O5	21:A:905:HOH:O	2.06	0.72
2:B:573:THR:HG22	2:B:576:ILE:HG21	1.72	0.71
14:L:205:CLA:HBC2	14:L:205:CLA:HHD	1.72	0.71
14:A:833:CLA:O1A	21:A:906:HOH:O	2.07	0.71
3:C:57:CYS:O	21:C:202:HOH:O	2.08	0.70
7:I:1:FME:O	21:I:201:HOH:O	2.08	0.70
1:A:219:VAL:HG13	1:A:239:PRO:HB3	1.74	0.70
5:E:1:VAL:N	21:E:105:HOH:O	2.25	0.70
1:A:501:THR:OG1	14:A:836:CLA:OBD	2.07	0.70
2:B:406:ASN:ND2	21:B:909:HOH:O	2.25	0.70
2:B:365:ALA:O	21:B:904:HOH:O	2.10	0.69
10:L:41:LEU:O	21:L:303:HOH:O	2.09	0.69
1:A:68:ILE:O	1:A:72:ILE:HD12	1.93	0.69
2:B:658:PHE:O	2:B:662:VAL:HG23	1.93	0.69
3:C:80:TYR:O	21:C:203:HOH:O	2.09	0.69
1:A:366:LEU:O	1:A:370:VAL:HG23	1.92	0.68
16:B:853:BCR:H23C	16:B:853:BCR:H392	1.75	0.68
14:A:819:CLA:HBC2	14:A:836:CLA:H42	1.76	0.68
7:I:20:TRP:O	7:I:24:THR:OG1	2.09	0.68
1:A:196:MET:HE1	14:A:826:CLA:H142	1.76	0.68
1:A:657:GLN:O	21:A:911:HOH:O	2.12	0.68
1:A:718:GLN:OE1	21:A:909:HOH:O	2.10	0.68
10:L:39:GLN:NE2	21:L:305:HOH:O	2.26	0.68
2:B:682:GLU:OE2	21:B:905:HOH:O	2.11	0.68
2:B:255:THR:OG1	2:B:270:THR:OG1	1.93	0.68
1:A:335:PRO:O	21:A:910:HOH:O	2.10	0.67
2:B:514:LEU:O	21:B:903:HOH:O	2.10	0.67
1:A:121:VAL:HG23	1:A:122:GLY:H	1.58	0.67
1:A:373:HIS:ND1	14:A:819:CLA:OBD	2.28	0.67
16:A:850:BCR:H362	14:A:854:CLA:C4	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:836:CLA:O1D	21:A:912:HOH:O	2.12	0.66
14:A:821:CLA:HBC2	14:A:821:CLA:HHD	1.78	0.66
4:D:18:LEU:O	21:D:203:HOH:O	2.14	0.66
2:B:278:ALA:HA	14:B:817:CLA:HMC2	1.78	0.65
2:B:468:ALA:O	2:B:482:SER:OG	2.15	0.65
14:B:805:CLA:HBC3	14:B:805:CLA:HHD	1.78	0.65
16:I:103:BCR:H23C	16:I:103:BCR:H403	1.78	0.65
1:A:386:ASP:OD2	1:A:389:THR:OG1	2.13	0.65
2:B:354:HIS:ND1	14:B:818:CLA:OBD	2.29	0.65
4:D:13:SER:OG	21:D:204:HOH:O	2.15	0.65
6:F:53:VAL:HG12	6:F:63:PHE:HB2	1.78	0.65
2:B:384:PHE:CE1	2:B:586:MET:HE1	2.33	0.64
2:B:700:LYS:O	21:B:907:HOH:O	2.14	0.64
14:A:838:CLA:HBC2	14:A:838:CLA:HHD	1.80	0.64
2:B:14:ASP:OD2	2:B:16:THR:OG1	2.16	0.64
1:A:17:ASP:OD2	1:A:186:LYS:NZ	2.31	0.64
1:A:50:ASN:ND2	21:A:920:HOH:O	2.27	0.63
1:A:219:VAL:O	1:A:223:ILE:HD12	1.98	0.63
2:B:222:ALA:HB3	2:B:223:PRO:HD3	1.81	0.62
16:J:103:BCR:HC8	16:J:103:BCR:H311	1.82	0.62
1:A:429:VAL:HG23	14:A:825:CLA:HBC2	1.80	0.62
14:B:814:CLA:HBC2	14:B:814:CLA:HHD	1.80	0.61
1:A:720:ARG:NH1	21:A:921:HOH:O	2.33	0.61
1:A:702:GLU:OE2	21:A:913:HOH:O	2.17	0.61
2:B:377:HIS:CE1	2:B:381:ILE:HD11	2.35	0.61
1:A:583:ARG:NH2	4:D:62:GLU:OE2	2.34	0.60
14:A:822:CLA:HMB2	14:A:826:CLA:HMA3	1.82	0.60
2:B:327:GLU:OE1	2:B:327:GLU:N	2.33	0.60
6:F:37:ARG:NH2	8:J:34:PRO:O	2.35	0.60
1:A:713:VAL:HG12	1:A:713:VAL:O	2.01	0.59
2:B:413:ARG:NH2	14:B:831:CLA:OBD	2.33	0.59
14:A:825:CLA:H141	17:A:853:LHG:H342	1.84	0.59
10:L:90:THR:HA	10:L:93:LEU:HD12	1.84	0.59
2:B:105:GLN:NE2	21:B:912:HOH:O	2.31	0.59
2:B:480:LEU:HD23	14:B:836:CLA:HBC2	1.83	0.59
14:A:833:CLA:OBD	10:L:19:THR:HG21	2.03	0.58
14:B:834:CLA:HBB1	14:B:834:CLA:HMB3	1.84	0.58
2:B:710:GLN:O	2:B:714:VAL:HG23	2.03	0.58
6:F:53:VAL:O	6:F:53:VAL:HG23	2.01	0.58
2:B:668:MET:O	2:B:672:SER:OG	2.20	0.57
1:A:219:VAL:HG13	1:A:239:PRO:CB	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:314:VAL:HG13	2:B:316:GLY:H	1.69	0.57
14:K:101:CLA:HMC3	16:K:103:BCR:H332	1.87	0.56
1:A:687:LEU:HB2	14:A:802:CLA:HMC2	1.86	0.56
14:B:828:CLA:H202	20:B:850:LMG:H273	1.85	0.56
1:A:427:ASN:OD1	1:A:432:ARG:NH1	2.39	0.56
14:A:803:CLA:OBD	14:B:804:CLA:HMB3	2.05	0.56
14:B:827:CLA:HBB1	14:B:827:CLA:HMB1	1.88	0.56
1:A:466:ARG:NE	21:A:923:HOH:O	2.37	0.55
14:A:802:CLA:HBA2	2:B:430:LEU:HD23	1.88	0.55
9:K:68:LEU:CD2	16:K:103:BCR:H311	2.37	0.55
1:A:118:TRP:HE1	16:A:851:BCR:H332	1.72	0.55
2:B:177:HIS:ND1	14:B:825:CLA:O1D	2.37	0.55
2:B:647:ASN:ND2	21:B:917:HOH:O	2.40	0.54
7:I:26:VAL:HG13	17:I:102:LHG:H152	1.88	0.54
1:A:344:LEU:HD23	14:A:825:CLA:HMD2	1.89	0.54
2:B:465:PHE:CE1	2:B:479:THR:HG21	2.43	0.54
4:D:95:HIS:HB3	4:D:96:PRO:HD3	1.89	0.54
2:B:384:PHE:HE1	2:B:586:MET:HE1	1.73	0.54
16:A:848:BCR:C8	16:A:848:BCR:H331	2.37	0.53
14:L:201:CLA:H2A	14:L:201:CLA:O2A	2.08	0.53
14:B:833:CLA:HBC2	14:B:833:CLA:HHD	1.89	0.53
1:A:726:GLN:O	1:A:730:VAL:HG23	2.09	0.53
10:L:68:LEU:HD23	10:L:73:VAL:HG23	1.89	0.53
1:A:346:GLU:OE1	1:A:346:GLU:N	2.39	0.53
2:B:697:VAL:HG11	14:B:801:CLA:HAB	1.91	0.53
1:A:565:LEU:HB3	1:A:566:ILE:HD12	1.91	0.52
16:B:853:BCR:H321	16:B:853:BCR:HC8	1.91	0.52
1:A:714:ALA:O	6:F:89:ARG:NH1	2.40	0.52
14:A:842:CLA:H41	15:A:844:PQN:H18	1.89	0.52
1:A:325:LEU:HD12	14:A:822:CLA:HED3	1.91	0.52
2:B:480:LEU:CD2	14:B:836:CLA:HBC2	2.40	0.52
10:L:54:HIS:HA	10:L:57:PHE:CE1	2.43	0.52
16:A:845:BCR:H332	16:A:846:BCR:H21C	1.90	0.52
16:A:850:BCR:H393	16:J:103:BCR:H322	1.92	0.52
10:L:59:ILE:HG13	10:L:59:ILE:O	2.08	0.52
3:C:28:VAL:HG12	4:D:109:ARG:HB3	1.92	0.52
14:A:833:CLA:HMB1	14:A:833:CLA:HBB1	1.91	0.52
3:C:52:ARG:NH2	21:C:207:HOH:O	2.42	0.51
4:D:3:LEU:HD11	4:D:85:ILE:HD11	1.91	0.51
17:A:852:LHG:O1	21:A:914:HOH:O	2.19	0.51
1:A:309:ILE:O	1:A:313:HIS:ND1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:573:THR:HG22	2:B:576:ILE:CG2	2.39	0.51
1:A:647:ASN:ND2	2:B:638:ILE:O	2.44	0.51
2:B:573:THR:CG2	2:B:576:ILE:HG21	2.40	0.51
14:B:826:CLA:H191	12:X:25:LEU:HD23	1.93	0.51
10:L:125:PHE:O	10:L:129:MET:HG2	2.11	0.51
14:L:204:CLA:CBC	14:L:204:CLA:HHD	2.41	0.51
9:K:19:VAL:HG22	9:K:70:ALA:HB1	1.92	0.51
14:A:819:CLA:H42	14:A:828:CLA:HBB2	1.93	0.51
4:D:3:LEU:CD1	4:D:85:ILE:HD11	2.40	0.51
5:E:64:GLU:OE2	21:E:103:HOH:O	2.19	0.51
14:A:816:CLA:H101	16:A:846:BCR:H402	1.93	0.50
1:A:120:ILE:HG12	16:J:104:BCR:H322	1.92	0.50
1:A:737:LEU:HD11	16:A:850:BCR:HC8	1.93	0.50
5:E:57:THR:O	21:E:102:HOH:O	2.18	0.50
6:F:65:ILE:HB	6:F:66:PRO:HD3	1.93	0.50
1:A:344:LEU:HD21	14:A:825:CLA:HBC3	1.93	0.50
13:A:801:CL0:H13	14:A:854:CLA:OBD	2.12	0.50
2:B:297:GLY:O	14:B:822:CLA:HED3	2.11	0.50
10:L:60:GLY:H	10:L:61:PRO:CD	2.25	0.50
14:B:827:CLA:H122	16:B:847:BCR:H373	1.93	0.49
1:A:113:SER:OG	1:A:130:VAL:HG11	2.12	0.49
7:I:28:GLY:O	7:I:32:LEU:HD23	2.12	0.49
1:A:470:ARG:NH2	14:A:835:CLA:OBD	2.44	0.49
1:A:432:ARG:O	1:A:436:HIS:ND1	2.42	0.49
2:B:194:ILE:HD12	2:B:253:ILE:HB	1.93	0.49
2:B:630:LEU:HD22	14:B:804:CLA:HMD3	1.94	0.49
1:A:718:GLN:NE2	5:E:15:TYR:OH	2.46	0.49
1:A:120:ILE:CG1	16:J:104:BCR:H322	2.42	0.49
1:A:460:VAL:CG1	14:A:835:CLA:HBC2	2.40	0.49
2:B:726:THR:HG23	14:B:804:CLA:O1D	2.13	0.49
1:A:504:ASN:HB2	14:A:837:CLA:HED2	1.95	0.49
1:A:432:ARG:NE	14:A:832:CLA:OBD	2.45	0.48
10:L:76:LEU:O	10:L:80:ILE:HG12	2.14	0.48
14:A:825:CLA:H91	14:A:825:CLA:H193	1.95	0.48
16:B:847:BCR:C8	16:B:847:BCR:H331	2.43	0.48
1:A:121:VAL:HG23	1:A:122:GLY:N	2.27	0.48
2:B:522:ASP:OD1	2:B:599:TYR:OH	2.25	0.48
2:B:593:ILE:O	2:B:597:THR:HG23	2.14	0.48
2:B:722:GLY:O	2:B:726:THR:HG22	2.12	0.48
1:A:285:LEU:HD21	1:A:378:PRO:HD2	1.96	0.48
1:A:501:THR:O	14:A:837:CLA:ND	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:116:TRP:N	6:F:117:PRO:CD	2.77	0.48
10:L:115:GLU:OE1	10:L:115:GLU:N	2.44	0.48
1:A:482:LEU:HB2	1:A:533:THR:HG23	1.96	0.48
1:A:575:ARG:O	21:A:905:HOH:O	2.20	0.48
2:B:140:PHE:CZ	2:B:144:LEU:HD11	2.49	0.48
10:L:39:GLN:NE2	21:L:307:HOH:O	2.47	0.47
1:A:630:THR:HG23	1:A:630:THR:O	2.14	0.47
14:A:825:CLA:H202	17:A:853:LHG:H242	1.96	0.47
2:B:626:LEU:HD12	2:B:630:LEU:HD12	1.96	0.47
1:A:470:ARG:NH1	2:B:94:GLN:O	2.41	0.47
17:M:101:LHG:O3	17:M:101:LHG:O1	2.16	0.47
10:L:131:SER:HA	10:L:134:VAL:HG12	1.95	0.47
14:A:825:CLA:HED3	14:A:825:CLA:H2A	1.96	0.47
2:B:612:VAL:O	2:B:616:ASN:ND2	2.47	0.47
5:E:10:LEU:HD11	5:E:66:GLN:HB2	1.95	0.47
1:A:605:CYS:O	1:A:609:VAL:HG23	2.15	0.47
1:A:651:ARG:HG3	2:B:638:ILE:HD12	1.97	0.47
1:A:679:ALA:HB1	1:A:738:GLY:O	2.14	0.47
15:A:844:PQN:H241	15:A:844:PQN:C27	2.45	0.47
4:D:100:VAL:HG21	4:D:106:ASN:ND2	2.29	0.47
16:I:101:BCR:H382	16:I:101:BCR:H23C	1.97	0.47
9:K:56:LEU:N	9:K:57:PRO:CD	2.78	0.47
14:A:829:CLA:H93	16:J:103:BCR:H361	1.95	0.47
7:I:21:LEU:O	7:I:25:VAL:HG23	2.15	0.47
1:A:199:HIS:O	1:A:203:GLY:N	2.47	0.47
2:B:60:VAL:HG13	2:B:141:LEU:HD13	1.96	0.47
16:B:852:BCR:H331	16:B:852:BCR:C8	2.44	0.46
16:A:846:BCR:H362	16:A:847:BCR:H10C	1.96	0.46
14:A:807:CLA:H193	14:A:807:CLA:H151	1.97	0.46
10:L:34:LEU:O	10:L:38:ARG:N	2.45	0.46
5:E:55:VAL:HG11	21:E:102:HOH:O	2.15	0.46
2:B:391:ALA:O	2:B:395:ILE:HG13	2.16	0.46
6:F:115:ALA:HB2	14:F:204:CLA:HMB3	1.97	0.46
1:A:614:SER:OG	1:A:618:GLN:OE1	2.33	0.46
3:C:28:VAL:HG21	4:D:111:ALA:HB2	1.98	0.46
14:B:829:CLA:HHC	14:B:829:CLA:HBB1	1.98	0.46
3:C:57:CYS:SG	3:C:63:SER:OG	2.73	0.46
2:B:233:ALA:HB2	2:B:254:LEU:O	2.16	0.46
14:B:826:CLA:H111	14:B:835:CLA:H193	1.97	0.46
14:K:101:CLA:CMC	16:K:103:BCR:H332	2.46	0.46
10:L:52:MET:HA	10:L:131:SER:OG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:851:BCR:C8	16:A:851:BCR:H331	2.46	0.45
6:F:112:THR:O	6:F:112:THR:HG22	2.17	0.45
1:A:702:GLU:O	21:A:915:HOH:O	2.21	0.45
14:B:810:CLA:C1A	14:B:810:CLA:CGA	2.94	0.45
11:M:10:VAL:HA	11:M:13:VAL:HG22	1.98	0.45
2:B:458:ILE:HD11	16:B:852:BCR:C34	2.47	0.45
10:L:57:PHE:CD2	10:L:57:PHE:C	2.95	0.45
1:A:406:VAL:HG12	1:A:595:VAL:HG13	1.98	0.45
1:A:86:TRP:NE1	14:A:829:CLA:OBD	2.49	0.45
2:B:381:ILE:HG23	14:B:808:CLA:H143	1.99	0.45
4:D:109:ARG:NH2	21:D:209:HOH:O	2.50	0.45
1:A:141:SER:OG	14:A:829:CLA:HED2	2.17	0.44
1:A:256:VAL:HG12	1:A:257:ASP:N	2.32	0.44
14:A:802:CLA:O1A	2:B:531:LEU:HD11	2.17	0.44
14:A:821:CLA:H192	16:A:847:BCR:C31	2.47	0.44
16:L:202:BCR:H20C	16:L:202:BCR:H361	1.87	0.44
14:A:854:CLA:O1D	14:A:854:CLA:H2A	2.17	0.44
1:A:405:VAL:HG13	16:A:849:BCR:H343	2.00	0.44
2:B:339:TRP:HE1	14:B:825:CLA:C2B	2.30	0.44
1:A:46:THR:HG22	21:A:922:HOH:O	2.17	0.44
1:A:364:GLY:HA2	1:A:401:GLY:HA2	2.00	0.44
2:B:680:LEU:O	2:B:683:THR:OG1	2.34	0.44
10:L:54:HIS:O	10:L:58:LEU:HB2	2.18	0.44
1:A:396:HIS:CE1	14:A:829:CLA:ND	2.85	0.44
2:B:465:PHE:HE1	2:B:479:THR:HG21	1.83	0.44
16:B:844:BCR:H392	16:B:844:BCR:H371	1.99	0.44
3:C:78:LEU:HD22	3:C:80:TYR:CZ	2.52	0.44
10:L:122:ALA:O	10:L:126:VAL:HG23	2.17	0.44
1:A:106:ASP:HB3	1:A:110:ILE:HD12	2.00	0.44
1:A:413:ALA:O	1:A:417:VAL:HG23	2.18	0.44
1:A:713:VAL:HG11	14:A:841:CLA:HMB2	1.99	0.44
14:A:820:CLA:H92	14:A:830:CLA:H91	1.98	0.44
2:B:503:TRP:O	2:B:507:ILE:HG22	2.16	0.44
16:K:103:BCR:H15C	16:K:103:BCR:H351	1.84	0.43
1:A:59:ASP:OD1	1:A:60:THR:N	2.52	0.43
1:A:121:VAL:O	6:F:24:THR:HG22	2.18	0.43
1:A:501:THR:HG21	14:A:836:CLA:HMD1	1.99	0.43
14:B:814:CLA:H203	14:B:829:CLA:CAD	2.48	0.43
1:A:701:ILE:O	1:A:705:VAL:HG23	2.18	0.43
16:A:849:BCR:H20C	16:A:849:BCR:H361	1.91	0.43
2:B:377:HIS:ND1	14:B:828:CLA:NB	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:825:CLA:CGA	14:B:825:CLA:HMA2	2.49	0.43
1:A:159:TYR:CE2	1:A:163:ILE:HD11	2.54	0.42
2:B:190:ALA:O	2:B:194:ILE:HG12	2.18	0.42
3:C:75:SER:O	21:C:204:HOH:O	2.22	0.42
1:A:117:VAL:HG11	1:A:123:GLN:HB3	2.00	0.42
1:A:429:VAL:O	1:A:433:VAL:HG13	2.18	0.42
2:B:140:PHE:O	2:B:144:LEU:HD13	2.19	0.42
2:B:338:GLY:HA2	2:B:389:ALA:HA	2.01	0.42
2:B:455:GLN:NE2	2:B:620:THR:OG1	2.52	0.42
2:B:580:ASP:OD1	2:B:580:ASP:C	2.61	0.42
14:B:826:CLA:HMA1	16:B:848:BCR:H14C	2.00	0.42
14:B:828:CLA:C20	20:B:850:LMG:H273	2.50	0.42
16:B:849:BCR:H24C	16:B:849:BCR:H371	1.86	0.42
3:C:22:THR:OG1	3:C:24:VAL:HG23	2.18	0.42
2:B:589:MET:O	2:B:593:ILE:HG12	2.19	0.42
14:B:830:CLA:H142	14:B:842:CLA:HAA2	2.00	0.42
16:B:846:BCR:H371	16:B:846:BCR:H24C	1.79	0.42
1:A:410:ALA:O	1:A:414:ILE:HG13	2.19	0.42
2:B:377:HIS:CE1	14:B:828:CLA:ND	2.87	0.42
14:B:828:CLA:HHC	14:B:828:CLA:HBB1	2.02	0.42
16:B:848:BCR:C8	16:B:848:BCR:H331	2.50	0.42
1:A:252:LEU:HD23	1:A:252:LEU:H	1.83	0.42
2:B:459:GLU:OE1	2:B:464:GLN:NE2	2.42	0.42
2:B:573:THR:HG23	2:B:576:ILE:HD13	2.02	0.42
14:B:801:CLA:H192	14:B:801:CLA:H162	1.94	0.42
14:B:838:CLA:H143	12:X:19:LEU:HB3	2.01	0.42
1:A:348:LEU:HD22	1:A:355:GLN:OE1	2.20	0.42
2:B:2:THR:HG22	2:B:3:LYS:H	1.84	0.42
2:B:114:ILE:O	14:B:810:CLA:HMD1	2.19	0.42
1:A:191:GLN:OE1	1:A:349:THR:O	2.38	0.42
14:A:811:CLA:HHC	14:A:811:CLA:HBB1	2.02	0.42
10:L:83:ILE:HA	10:L:129:MET:HE1	2.01	0.42
10:L:86:ILE:HG21	10:L:129:MET:SD	2.60	0.42
1:A:275:TYR:O	1:A:279:LEU:HB2	2.20	0.42
14:A:816:CLA:C4	14:A:816:CLA:O2A	2.68	0.42
2:B:575:ASP:O	2:B:580:ASP:OD2	2.38	0.42
4:D:2:THR:O	4:D:2:THR:HG22	2.20	0.42
10:L:56:TYR:O	21:L:304:HOH:O	2.21	0.42
2:B:366:GLN:OE1	2:B:366:GLN:N	2.48	0.42
3:C:48:VAL:HG12	3:C:74:ARG:O	2.19	0.42
14:A:813:CLA:HHC	14:A:813:CLA:HBB1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:ALA:HB3	11:M:29:LEU:HD21	2.02	0.41
16:B:847:BCR:H24C	16:B:847:BCR:H371	1.83	0.41
16:B:853:BCR:H15C	16:B:853:BCR:H351	1.90	0.41
16:A:846:BCR:H362	16:A:847:BCR:C10	2.50	0.41
14:L:201:CLA:CBB	14:L:201:CLA:HHC	2.50	0.41
1:A:72:ILE:HG23	1:A:76:HIS:NE2	2.35	0.41
1:A:430:LEU:O	1:A:433:VAL:HG22	2.21	0.41
2:B:272:MET:SD	14:B:819:CLA:HED2	2.61	0.41
14:B:830:CLA:H143	20:B:850:LMG:H212	2.02	0.41
7:I:22:MET:N	7:I:23:PRO:HD2	2.34	0.41
14:B:839:CLA:C1A	14:B:839:CLA:CGA	2.98	0.41
3:C:33:CYS:SG	3:C:34:LYS:N	2.93	0.41
7:I:19:CYS:HB3	14:L:201:CLA:CBB	2.50	0.41
14:L:204:CLA:HHC	14:L:204:CLA:HBB1	2.02	0.41
2:B:176:HIS:O	2:B:177:HIS:C	2.63	0.41
1:A:35:ASP:OD1	1:A:36:ARG:N	2.53	0.41
1:A:684:ALA:HB3	14:A:802:CLA:HBB2	2.03	0.41
2:B:319:ASN:HB3	17:B:851:LHG:H112	2.03	0.41
2:B:440:TYR:OH	21:B:908:HOH:O	2.19	0.41
16:F:205:BCR:H20C	16:F:205:BCR:H361	1.88	0.41
1:A:245:ASN:O	1:A:248:LEU:HD23	2.20	0.41
14:A:821:CLA:H141	16:A:846:BCR:H393	2.03	0.41
2:B:437:LEU:O	2:B:441:VAL:HG23	2.20	0.41
2:B:470:HIS:NE2	14:B:835:CLA:NA	2.68	0.41
6:F:56:ARG:HG2	6:F:57:LEU:O	2.21	0.41
14:X:1701:CLA:O1D	14:X:1701:CLA:H2A	2.21	0.41
1:A:86:TRP:CD1	1:A:90:MET:HE3	2.56	0.41
1:A:546:ILE:O	1:A:550:VAL:HG23	2.20	0.41
14:A:802:CLA:HBB1	14:A:802:CLA:HMB1	2.02	0.41
14:A:804:CLA:CGA	14:A:842:CLA:H43	2.51	0.41
16:A:850:BCR:H20C	16:A:850:BCR:H361	1.90	0.41
2:B:347:ILE:O	2:B:351:VAL:HG23	2.20	0.41
2:B:376:THR:HG23	2:B:597:THR:HG21	2.02	0.41
2:B:382:ALA:O	2:B:386:MET:HG2	2.20	0.41
2:B:417:HIS:O	2:B:417:HIS:CD2	2.74	0.41
4:D:2:THR:O	4:D:3:LEU:C	2.64	0.41
6:F:137:THR:O	6:F:137:THR:HG23	2.21	0.41
1:A:681:PHE:CD1	16:A:850:BCR:H363	2.56	0.41
2:B:639:ASN:OD1	2:B:642:ASN:ND2	2.49	0.41
6:F:13:ALA:O	6:F:17:ARG:HG2	2.21	0.41
12:X:20:LEU:HD11	12:X:24:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:X:20:LEU:HD11	12:X:24:PHE:CZ	2.56	0.41
1:A:337:THR:O	1:A:337:THR:HG22	2.19	0.40
1:A:497:ALA:HB3	1:A:498:PRO:HD3	2.03	0.40
16:A:850:BCR:H362	14:A:854:CLA:H41	2.01	0.40
2:B:2:THR:HG22	2:B:3:LYS:N	2.36	0.40
2:B:314:VAL:O	2:B:319:ASN:HA	2.21	0.40
16:I:101:BCR:H332	17:I:102:LHG:H223	2.03	0.40
14:A:840:CLA:O1A	14:A:840:CLA:C2	2.69	0.40
16:A:848:BCR:H15C	16:A:848:BCR:H351	1.89	0.40
2:B:573:THR:HG22	2:B:573:THR:O	2.22	0.40
4:D:95:HIS:CB	4:D:96:PRO:HD3	2.51	0.40
1:A:371:ALA:HB2	1:A:397:HIS:HB2	2.03	0.40
14:A:802:CLA:CBA	2:B:430:LEU:HD23	2.52	0.40
2:B:157:GLN:O	2:B:161:ARG:HG3	2.20	0.40
2:B:379:GLN:OE1	2:B:379:GLN:HA	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	744/755 (98%)	712 (96%)	32 (4%)	0	100	100
2	B	738/741 (100%)	706 (96%)	32 (4%)	0	100	100
3	C	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
4	D	136/139 (98%)	124 (91%)	12 (9%)	0	100	100
5	E	68/76 (90%)	68 (100%)	0	0	100	100
6	F	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
7	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	J	39/41 (95%)	39 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	K	77/83 (93%)	72 (94%)	5 (6%)	0	100	100
10	L	150/155 (97%)	145 (97%)	5 (3%)	0	100	100
11	M	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
12	X	25/36 (69%)	25 (100%)	0	0	100	100
All	All	2259/2317 (98%)	2154 (95%)	105 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	594/603 (98%)	593 (100%)	1 (0%)	87	95
2	B	597/598 (100%)	597 (100%)	0	100	100
3	C	67/68 (98%)	67 (100%)	0	100	100
4	D	115/116 (99%)	115 (100%)	0	100	100
5	E	60/65 (92%)	60 (100%)	0	100	100
6	F	109/109 (100%)	109 (100%)	0	100	100
7	I	31/31 (100%)	31 (100%)	0	100	100
8	J	35/35 (100%)	35 (100%)	0	100	100
9	K	58/61 (95%)	58 (100%)	0	100	100
10	L	117/120 (98%)	117 (100%)	0	100	100
11	M	26/26 (100%)	26 (100%)	0	100	100
12	X	21/28 (75%)	21 (100%)	0	100	100
All	All	1830/1860 (98%)	1829 (100%)	1 (0%)	87	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	HIS
1	A	93	HIS
1	A	115	GLN
1	A	192	ASN
1	A	397	HIS
1	A	504	ASN
1	A	641	GLN
1	A	718	GLN
2	B	13	GLN
2	B	155	HIS
2	B	210	ASN
2	B	261	HIS
2	B	455	GLN
2	B	604	HIS
2	B	611	ASN
2	B	616	ASN
3	C	15	GLN
4	D	106	ASN
5	E	58	ASN
5	E	59	ASN
8	J	3	HIS
9	K	23	ASN
9	K	78	GLN
10	L	33	ASN
10	L	39	GLN
10	L	75	ASN
10	L	141	ASN
11	M	7	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
8	FME	J	1	8	8,9,10	0.97	0	8,9,11	0.92	0
7	FME	I	1	7	8,9,10	1.01	0	8,9,11	0.82	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	J	1	8	-	1/7/9/11	-
7	FME	I	1	7	-	0/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	J	1	FME	CB-CG-SD-CE

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 134 ligands modelled in this entry, 2 are monoatomic - leaving 132 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
17	LHG	B	851	-	48,48,48	0.68	2 (4%)	51,54,54	1.22	5 (9%)
14	CLA	B	819	-	69,73,73	1.15	9 (13%)	82,113,113	1.26	6 (7%)
14	CLA	K	102	21	62,66,73	1.23	8 (12%)	73,104,113	1.28	6 (8%)
14	CLA	B	821	-	69,73,73	1.18	9 (13%)	82,113,113	1.19	5 (6%)
14	CLA	B	842	-	69,73,73	1.17	9 (13%)	82,113,113	1.26	5 (6%)
14	CLA	A	831	-	69,73,73	1.17	8 (11%)	82,113,113	1.28	7 (8%)
14	CLA	B	830	-	69,73,73	1.16	7 (10%)	82,113,113	1.30	6 (7%)
14	CLA	B	832	-	53,57,73	1.31	8 (15%)	61,93,113	1.34	4 (6%)
14	CLA	B	816	-	69,73,73	1.14	9 (13%)	82,113,113	1.24	5 (6%)
14	CLA	A	837	1	49,53,73	1.37	9 (18%)	58,89,113	1.43	5 (8%)
14	CLA	B	827	-	69,73,73	1.16	8 (11%)	82,113,113	1.24	5 (6%)
14	CLA	A	841	-	69,73,73	1.16	8 (11%)	82,113,113	1.24	5 (6%)
14	CLA	B	836	21	54,58,73	1.33	8 (14%)	64,95,113	1.40	7 (10%)
14	CLA	A	821	-	69,73,73	1.16	7 (10%)	82,113,113	1.23	6 (7%)
14	CLA	L	201	2	69,73,73	1.16	8 (11%)	82,113,113	1.28	6 (7%)
14	CLA	B	811	2	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
16	BCR	B	847	-	41,41,41	1.20	2 (4%)	56,56,56	1.24	8 (14%)
14	CLA	L	205	-	69,73,73	1.14	8 (11%)	82,113,113	1.28	6 (7%)
14	CLA	B	838	-	64,68,73	1.22	9 (14%)	76,107,113	1.27	5 (6%)
14	CLA	A	817	21	69,73,73	1.17	8 (11%)	82,113,113	1.25	5 (6%)
14	CLA	B	841	21	69,73,73	1.17	9 (13%)	82,113,113	1.22	5 (6%)
14	CLA	B	815	-	69,73,73	1.16	9 (13%)	82,113,113	1.24	6 (7%)
14	CLA	A	826	21	69,73,73	1.16	8 (11%)	82,113,113	1.23	4 (4%)
14	CLA	A	836	-	69,73,73	1.16	9 (13%)	82,113,113	1.26	5 (6%)
14	CLA	B	801	21	69,73,73	1.17	9 (13%)	82,113,113	1.24	4 (4%)
14	CLA	M	102	-	39,44,73	1.51	9 (23%)	47,76,113	1.45	4 (8%)
14	CLA	A	833	-	69,73,73	1.15	8 (11%)	82,113,113	1.21	5 (6%)
14	CLA	B	814	-	69,73,73	1.16	9 (13%)	82,113,113	1.40	8 (9%)
14	CLA	A	816	-	69,73,73	1.16	9 (13%)	82,113,113	1.25	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A	829	-	69,73,73	1.14	9 (13%)	82,113,113	1.21	7 (8%)
14	CLA	B	820	21	69,73,73	1.17	9 (13%)	82,113,113	1.29	7 (8%)
14	CLA	A	812	14	69,73,73	1.15	8 (11%)	82,113,113	1.22	4 (4%)
14	CLA	B	837	21	49,53,73	1.40	7 (14%)	58,89,113	1.40	4 (6%)
17	LHG	I	102	-	38,38,48	0.71	0	41,44,54	1.29	4 (9%)
14	CLA	A	825	-	69,73,73	1.16	9 (13%)	82,113,113	1.23	6 (7%)
16	BCR	I	103	-	41,41,41	1.13	3 (7%)	56,56,56	1.32	8 (14%)
14	CLA	A	835	-	69,73,73	1.14	8 (11%)	82,113,113	1.31	5 (6%)
14	CLA	B	806	-	69,73,73	1.16	9 (13%)	82,113,113	1.24	6 (7%)
14	CLA	A	814	-	69,73,73	1.17	9 (13%)	82,113,113	1.23	4 (4%)
14	CLA	A	822	21	69,73,73	1.15	9 (13%)	82,113,113	1.22	4 (4%)
18	SF4	C	102	3	0,12,12	-	-	-	-	-
14	CLA	B	817	-	69,73,73	1.17	8 (11%)	82,113,113	1.23	6 (7%)
14	CLA	A	808	-	55,59,73	1.29	8 (14%)	64,96,113	1.32	5 (7%)
16	BCR	A	848	-	41,41,41	1.14	3 (7%)	56,56,56	1.18	5 (8%)
14	CLA	A	819	-	69,73,73	1.17	9 (13%)	82,113,113	1.20	5 (6%)
14	CLA	B	823	21	59,63,73	1.26	8 (13%)	70,101,113	1.28	5 (7%)
14	CLA	B	810	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	7 (8%)
16	BCR	J	103	-	41,41,41	1.19	3 (7%)	56,56,56	1.26	6 (10%)
14	CLA	A	807	-	69,73,73	1.17	9 (13%)	82,113,113	1.19	5 (6%)
14	CLA	B	805	-	69,73,73	1.14	8 (11%)	82,113,113	1.31	5 (6%)
14	CLA	A	834	-	69,73,73	1.15	8 (11%)	82,113,113	1.29	8 (9%)
16	BCR	A	849	-	41,41,41	1.19	3 (7%)	56,56,56	1.23	5 (8%)
16	BCR	K	103	-	25,25,41	1.17	1 (4%)	33,33,56	1.35	5 (15%)
16	BCR	A	846	-	41,41,41	1.17	2 (4%)	56,56,56	1.27	8 (14%)
16	BCR	L	207	-	41,41,41	1.16	2 (4%)	56,56,56	1.21	7 (12%)
14	CLA	B	809	-	69,73,73	1.16	9 (13%)	82,113,113	1.24	6 (7%)
14	CLA	A	842	-	69,73,73	1.16	9 (13%)	82,113,113	1.22	5 (6%)
13	CL0	A	801	-	58,73,73	2.20	10 (17%)	60,113,113	1.64	14 (23%)
14	CLA	A	805	14	63,67,73	1.21	8 (12%)	74,105,113	1.30	7 (9%)
14	CLA	A	830	-	69,73,73	1.17	9 (13%)	82,113,113	1.20	5 (6%)
16	BCR	A	851	-	25,25,41	1.19	2 (8%)	33,33,56	1.46	6 (18%)
14	CLA	X	1701	12	49,53,73	1.39	8 (16%)	58,89,113	1.41	5 (8%)
14	CLA	B	808	-	69,73,73	1.17	9 (13%)	82,113,113	1.23	4 (4%)
14	CLA	L	206	21	69,73,73	1.16	9 (13%)	82,113,113	1.27	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A	818	-	69,73,73	1.16	9 (13%)	82,113,113	1.25	6 (7%)
14	CLA	B	812	-	69,73,73	1.16	9 (13%)	82,113,113	1.24	5 (6%)
15	PQN	A	844	-	34,34,34	0.42	0	43,45,45	0.52	1 (2%)
14	CLA	A	827	21	69,73,73	1.15	9 (13%)	82,113,113	1.30	8 (9%)
14	CLA	K	101	-	50,54,73	1.36	9 (18%)	59,90,113	1.39	4 (6%)
16	BCR	B	852	-	41,41,41	1.21	2 (4%)	56,56,56	1.36	8 (14%)
14	CLA	B	807	-	69,73,73	1.16	9 (13%)	82,113,113	1.25	5 (6%)
16	BCR	B	849	-	41,41,41	1.18	2 (4%)	56,56,56	1.21	7 (12%)
16	BCR	L	202	-	41,41,41	1.22	3 (7%)	56,56,56	1.31	8 (14%)
16	BCR	B	844	-	41,41,41	1.19	2 (4%)	56,56,56	1.24	7 (12%)
14	CLA	F	204	-	54,58,73	1.31	8 (14%)	64,95,113	1.37	6 (9%)
16	BCR	B	853	-	41,41,41	1.17	3 (7%)	56,56,56	1.21	4 (7%)
14	CLA	B	829	-	69,73,73	1.17	9 (13%)	82,113,113	1.24	6 (7%)
16	BCR	B	845	-	41,41,41	1.15	3 (7%)	56,56,56	1.19	5 (8%)
14	CLA	B	833	-	69,73,73	1.17	9 (13%)	82,113,113	1.23	5 (6%)
14	CLA	A	815	-	69,73,73	1.16	8 (11%)	82,113,113	1.23	4 (4%)
14	CLA	A	854	21	69,73,73	1.15	9 (13%)	82,113,113	1.30	6 (7%)
20	LMG	B	850	-	55,55,55	0.71	1 (1%)	63,63,63	1.34	8 (12%)
14	CLA	A	828	-	69,73,73	1.16	9 (13%)	82,113,113	1.26	6 (7%)
17	LHG	M	101	-	48,48,48	0.61	1 (2%)	51,54,54	1.20	5 (9%)
14	CLA	B	831	-	59,63,73	1.25	9 (15%)	70,101,113	1.30	4 (5%)
14	CLA	A	811	-	53,57,73	1.32	8 (15%)	61,93,113	1.31	5 (8%)
15	PQN	B	843	-	34,34,34	0.43	0	43,45,45	0.53	1 (2%)
14	CLA	A	804	-	69,73,73	1.15	8 (11%)	82,113,113	1.26	5 (6%)
14	CLA	B	818	-	69,73,73	1.15	9 (13%)	82,113,113	1.33	8 (9%)
14	CLA	F	203	21	49,53,73	1.38	8 (16%)	58,89,113	1.43	4 (6%)
16	BCR	A	850	-	41,41,41	1.21	2 (4%)	56,56,56	1.47	11 (19%)
17	LHG	A	853	14	40,40,48	0.73	1 (2%)	43,46,54	1.22	4 (9%)
14	CLA	B	824	-	49,53,73	1.39	5 (10%)	58,89,113	1.38	4 (6%)
16	BCR	F	202	-	41,41,41	1.22	3 (7%)	56,56,56	1.28	9 (16%)
14	CLA	A	820	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	6 (7%)
16	BCR	J	104	-	41,41,41	1.23	3 (7%)	56,56,56	1.40	10 (17%)
14	CLA	B	834	-	69,73,73	1.16	9 (13%)	82,113,113	1.20	4 (4%)
18	SF4	C	101	3	0,12,12	-	-	-	-	-
14	CLA	A	832	-	64,68,73	1.21	9 (14%)	76,107,113	1.27	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	822	-	49,53,73	1.38	9 (18%)	58,89,113	1.42	4 (6%)
14	CLA	B	828	-	69,73,73	1.16	8 (11%)	82,113,113	1.15	5 (6%)
14	CLA	A	810	1	69,73,73	1.17	9 (13%)	82,113,113	1.27	5 (6%)
14	CLA	B	825	2	69,73,73	1.17	8 (11%)	82,113,113	1.17	5 (6%)
17	LHG	A	852	-	48,48,48	0.67	1 (2%)	51,54,54	1.23	5 (9%)
14	CLA	A	806	-	69,73,73	1.15	8 (11%)	82,113,113	1.26	5 (6%)
14	CLA	A	809	1	69,73,73	1.15	9 (13%)	82,113,113	1.26	4 (4%)
14	CLA	B	826	21	69,73,73	1.16	9 (13%)	82,113,113	1.31	7 (8%)
16	BCR	A	845	-	41,41,41	1.15	3 (7%)	56,56,56	1.31	7 (12%)
16	BCR	F	205	-	41,41,41	1.15	3 (7%)	56,56,56	1.30	8 (14%)
14	CLA	A	823	-	49,53,73	1.37	9 (18%)	58,89,113	1.42	5 (8%)
14	CLA	A	840	-	69,73,73	1.17	8 (11%)	82,113,113	1.23	4 (4%)
14	CLA	J	101	8	49,53,73	1.38	9 (18%)	58,89,113	1.38	5 (8%)
14	CLA	A	802	-	69,73,73	1.15	9 (13%)	82,113,113	1.24	6 (7%)
14	CLA	J	102	-	41,45,73	1.48	7 (17%)	50,78,113	1.37	3 (6%)
14	CLA	A	803	21	69,73,73	1.18	9 (13%)	82,113,113	1.14	5 (6%)
14	CLA	A	843	17	49,53,73	1.38	9 (18%)	58,89,113	1.40	4 (6%)
16	BCR	B	848	-	41,41,41	1.21	3 (7%)	56,56,56	1.29	6 (10%)
14	CLA	B	839	-	69,73,73	1.16	9 (13%)	82,113,113	1.25	5 (6%)
14	CLA	A	824	-	69,73,73	1.18	7 (10%)	82,113,113	1.16	4 (4%)
16	BCR	B	846	-	41,41,41	1.19	2 (4%)	56,56,56	1.30	7 (12%)
14	CLA	L	204	10	69,73,73	1.18	8 (11%)	82,113,113	1.41	9 (10%)
14	CLA	B	813	-	49,53,73	1.37	9 (18%)	58,89,113	1.41	4 (6%)
14	CLA	B	835	-	69,73,73	1.16	9 (13%)	82,113,113	1.26	4 (4%)
14	CLA	B	840	-	51,55,73	1.34	9 (17%)	60,91,113	1.38	6 (10%)
18	SF4	B	802	1,2	0,12,12	-	-	-	-	-
14	CLA	B	804	-	69,73,73	1.15	9 (13%)	82,113,113	1.21	4 (4%)
16	BCR	I	101	-	41,41,41	1.22	3 (7%)	56,56,56	1.26	7 (12%)
16	BCR	A	847	-	41,41,41	1.19	4 (9%)	56,56,56	1.36	8 (14%)
14	CLA	A	839	-	69,73,73	1.15	9 (13%)	82,113,113	1.28	6 (7%)
14	CLA	A	838	-	69,73,73	1.17	8 (11%)	82,113,113	1.28	6 (7%)
14	CLA	F	201	21	62,66,73	1.24	8 (12%)	73,104,113	1.25	5 (6%)
14	CLA	A	813	-	49,53,73	1.40	9 (18%)	58,89,113	1.36	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
17	LHG	B	851	-	-	27/53/53/53	-
14	CLA	B	819	-	1/1/15/20	14/39/115/115	-
14	CLA	K	102	21	1/1/13/20	13/31/107/115	-
14	CLA	B	821	-	1/1/15/20	12/39/115/115	-
14	CLA	B	842	-	1/1/15/20	8/39/115/115	-
14	CLA	A	831	-	1/1/15/20	7/39/115/115	-
14	CLA	B	830	-	1/1/15/20	7/39/115/115	-
14	CLA	B	832	-	1/1/11/20	5/20/96/115	-
14	CLA	B	816	-	1/1/15/20	12/39/115/115	-
14	CLA	A	837	1	1/1/11/20	5/15/91/115	-
14	CLA	B	827	-	1/1/15/20	7/39/115/115	-
14	CLA	A	841	-	1/1/15/20	13/39/115/115	-
14	CLA	B	836	21	1/1/12/20	5/21/97/115	-
14	CLA	A	821	-	1/1/15/20	12/39/115/115	-
14	CLA	L	201	2	1/1/15/20	11/39/115/115	-
14	CLA	B	811	2	1/1/15/20	9/39/115/115	-
16	BCR	B	847	-	-	10/29/63/63	0/2/2/2
14	CLA	L	205	-	1/1/15/20	10/39/115/115	-
14	CLA	B	838	-	1/1/14/20	8/33/109/115	-
14	CLA	A	817	21	1/1/15/20	9/39/115/115	-
14	CLA	B	841	21	1/1/15/20	11/39/115/115	-
14	CLA	B	815	-	1/1/15/20	20/39/115/115	-
14	CLA	A	826	21	1/1/15/20	14/39/115/115	-
14	CLA	A	836	-	1/1/15/20	13/39/115/115	-
14	CLA	B	801	21	1/1/15/20	15/39/115/115	-
14	CLA	M	102	-	1/1/7/20	2/4/72/115	-
14	CLA	A	833	-	1/1/15/20	12/39/115/115	-
14	CLA	B	814	-	1/1/15/20	18/39/115/115	-
14	CLA	A	816	-	1/1/15/20	16/39/115/115	-
14	CLA	A	829	-	1/1/15/20	13/39/115/115	-
14	CLA	B	820	21	1/1/15/20	17/39/115/115	-
14	CLA	A	812	14	1/1/15/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	837	21	1/1/11/20	6/15/91/115	-
17	LHG	I	102	-	-	23/43/43/53	-
14	CLA	A	825	-	1/1/15/20	13/39/115/115	-
16	BCR	I	103	-	-	9/29/63/63	0/2/2/2
14	CLA	A	835	-	1/1/15/20	7/39/115/115	-
14	CLA	B	806	-	1/1/15/20	10/39/115/115	-
14	CLA	A	814	-	1/1/15/20	13/39/115/115	-
14	CLA	A	822	21	1/1/15/20	5/39/115/115	-
18	SF4	C	102	3	-	-	0/6/5/5
14	CLA	B	817	-	1/1/15/20	17/39/115/115	-
14	CLA	A	808	-	1/1/12/20	3/23/99/115	-
16	BCR	A	848	-	-	7/29/63/63	0/2/2/2
14	CLA	A	819	-	1/1/15/20	12/39/115/115	-
14	CLA	B	823	21	1/1/13/20	4/27/103/115	-
14	CLA	B	810	-	1/1/15/20	5/39/115/115	-
16	BCR	J	103	-	-	13/29/63/63	0/2/2/2
14	CLA	A	807	-	1/1/15/20	14/39/115/115	-
14	CLA	B	805	-	1/1/15/20	12/39/115/115	-
14	CLA	A	834	-	1/1/15/20	12/39/115/115	-
16	BCR	A	849	-	-	5/29/63/63	0/2/2/2
16	BCR	K	103	-	-	4/18/35/63	0/1/1/2
16	BCR	A	846	-	-	11/29/63/63	0/2/2/2
16	BCR	L	207	-	-	17/29/63/63	0/2/2/2
14	CLA	B	809	-	1/1/15/20	9/39/115/115	-
14	CLA	A	842	-	1/1/15/20	4/39/115/115	-
13	CL0	A	801	-	3/3/20/25	7/37/135/135	-
14	CLA	A	805	14	1/1/13/20	9/32/108/115	-
14	CLA	A	830	-	1/1/15/20	9/39/115/115	-
16	BCR	A	851	-	-	13/18/35/63	0/1/1/2
14	CLA	X	1701	12	1/1/11/20	4/15/91/115	-
14	CLA	B	808	-	1/1/15/20	8/39/115/115	-
14	CLA	L	206	21	1/1/15/20	5/39/115/115	-
14	CLA	A	818	-	1/1/15/20	11/39/115/115	-
14	CLA	B	812	-	1/1/15/20	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	PQN	A	844	-	-	1/23/43/43	0/2/2/2
14	CLA	A	827	21	1/1/15/20	10/39/115/115	-
14	CLA	K	101	-	1/1/11/20	8/17/93/115	-
16	BCR	B	852	-	-	12/29/63/63	0/2/2/2
14	CLA	B	807	-	1/1/15/20	16/39/115/115	-
16	BCR	B	849	-	-	4/29/63/63	0/2/2/2
16	BCR	L	202	-	-	12/29/63/63	0/2/2/2
16	BCR	B	844	-	-	11/29/63/63	0/2/2/2
14	CLA	F	204	-	1/1/12/20	8/21/97/115	-
16	BCR	B	853	-	-	13/29/63/63	0/2/2/2
14	CLA	B	829	-	1/1/15/20	14/39/115/115	-
16	BCR	B	845	-	-	14/29/63/63	0/2/2/2
14	CLA	B	833	-	1/1/15/20	12/39/115/115	-
14	CLA	A	815	-	1/1/15/20	12/39/115/115	-
14	CLA	A	854	21	1/1/15/20	15/39/115/115	-
20	LMG	B	850	-	-	23/50/70/70	0/1/1/1
14	CLA	A	828	-	1/1/15/20	6/39/115/115	-
17	LHG	M	101	-	-	20/53/53/53	-
14	CLA	B	831	-	1/1/13/20	7/27/103/115	-
14	CLA	A	811	-	1/1/11/20	5/20/96/115	-
15	PQN	B	843	-	-	2/23/43/43	0/2/2/2
14	CLA	A	804	-	1/1/15/20	10/39/115/115	-
14	CLA	B	818	-	1/1/15/20	12/39/115/115	-
14	CLA	F	203	21	1/1/11/20	4/15/91/115	-
16	BCR	A	850	-	-	18/29/63/63	0/2/2/2
17	LHG	A	853	14	-	13/45/45/53	-
14	CLA	B	824	-	1/1/11/20	6/15/91/115	-
16	BCR	F	202	-	-	8/29/63/63	0/2/2/2
14	CLA	A	820	-	1/1/15/20	6/39/115/115	-
16	BCR	J	104	-	-	10/29/63/63	0/2/2/2
14	CLA	B	834	-	1/1/15/20	9/39/115/115	-
18	SF4	C	101	3	-	-	0/6/5/5
14	CLA	A	832	-	1/1/14/20	8/33/109/115	-
14	CLA	B	822	-	1/1/11/20	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	828	-	1/1/15/20	17/39/115/115	-
14	CLA	A	810	1	1/1/15/20	13/39/115/115	-
14	CLA	B	825	2	1/1/15/20	12/39/115/115	-
17	LHG	A	852	-	-	22/53/53/53	-
14	CLA	A	806	-	1/1/15/20	24/39/115/115	-
14	CLA	A	809	1	1/1/15/20	9/39/115/115	-
14	CLA	B	826	21	1/1/15/20	15/39/115/115	-
16	BCR	A	845	-	-	4/29/63/63	0/2/2/2
16	BCR	F	205	-	-	10/29/63/63	0/2/2/2
14	CLA	A	823	-	1/1/11/20	6/15/91/115	-
14	CLA	A	840	-	1/1/15/20	6/39/115/115	-
14	CLA	J	101	8	1/1/11/20	2/15/91/115	-
14	CLA	A	802	-	1/1/15/20	11/39/115/115	-
14	CLA	J	102	-	1/1/8/20	0/4/76/115	-
14	CLA	A	803	21	1/1/15/20	11/39/115/115	-
14	CLA	A	843	17	1/1/11/20	3/15/91/115	-
16	BCR	B	848	-	-	6/29/63/63	0/2/2/2
14	CLA	B	839	-	1/1/15/20	10/39/115/115	-
14	CLA	A	824	-	1/1/15/20	7/39/115/115	-
16	BCR	B	846	-	-	8/29/63/63	0/2/2/2
14	CLA	L	204	10	1/1/15/20	15/39/115/115	-
14	CLA	B	813	-	1/1/11/20	5/15/91/115	-
14	CLA	B	835	-	1/1/15/20	10/39/115/115	-
14	CLA	B	840	-	1/1/11/20	4/18/94/115	-
18	SF4	B	802	1,2	-	-	0/6/5/5
14	CLA	B	804	-	1/1/15/20	11/39/115/115	-
16	BCR	I	101	-	-	11/29/63/63	0/2/2/2
16	BCR	A	847	-	-	12/29/63/63	0/2/2/2
14	CLA	A	839	-	1/1/15/20	14/39/115/115	-
14	CLA	A	838	-	1/1/15/20	13/39/115/115	-
14	CLA	F	201	21	1/1/13/20	8/31/107/115	-
14	CLA	A	813	-	1/1/11/20	2/15/91/115	-

All (895) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	801	CL0	C1B-C2B	9.07	1.49	1.39
13	A	801	CL0	C3B-C4B	7.40	1.48	1.41
13	A	801	CL0	C1D-C2D	7.18	1.47	1.39
16	B	847	BCR	C30-C25	-4.33	1.48	1.53
13	A	801	CL0	C3D-C4D	4.32	1.48	1.41
16	J	104	BCR	C1-C6	-4.24	1.48	1.53
16	B	848	BCR	C1-C6	-4.14	1.48	1.53
16	A	847	BCR	C1-C6	-4.10	1.48	1.53
16	B	844	BCR	C1-C6	-4.05	1.48	1.53
16	F	202	BCR	C1-C6	-4.03	1.48	1.53
16	J	103	BCR	C1-C6	-3.98	1.48	1.53
16	I	101	BCR	C1-C6	-3.98	1.48	1.53
16	A	849	BCR	C1-C6	-3.96	1.48	1.53
16	A	850	BCR	C1-C6	-3.95	1.48	1.53
16	A	846	BCR	C1-C6	-3.92	1.48	1.53
16	B	845	BCR	C1-C6	-3.91	1.48	1.53
16	B	846	BCR	C1-C6	-3.90	1.48	1.53
16	B	852	BCR	C1-C6	-3.90	1.48	1.53
16	B	853	BCR	C1-C6	-3.87	1.48	1.53
16	L	202	BCR	C1-C6	-3.86	1.48	1.53
16	A	851	BCR	C1-C6	-3.78	1.48	1.53
16	L	207	BCR	C1-C6	-3.76	1.49	1.53
16	I	103	BCR	C1-C6	-3.75	1.49	1.53
16	A	848	BCR	C1-C6	-3.72	1.49	1.53
16	F	205	BCR	C1-C6	-3.69	1.49	1.53
16	B	849	BCR	C1-C6	-3.67	1.49	1.53
16	L	202	BCR	C30-C25	-3.63	1.49	1.53
16	B	849	BCR	C30-C25	-3.62	1.49	1.53
16	A	845	BCR	C1-C6	-3.62	1.49	1.53
16	F	202	BCR	C30-C25	-3.60	1.49	1.53
14	X	1701	CLA	C1D-ND	3.59	1.42	1.37
14	B	837	CLA	C1D-ND	3.56	1.42	1.37
16	J	104	BCR	C30-C25	-3.55	1.49	1.53
14	J	102	CLA	C1D-ND	3.54	1.42	1.37
14	K	101	CLA	C1D-ND	3.54	1.42	1.37
16	B	847	BCR	C1-C6	-3.53	1.49	1.53
16	B	846	BCR	C30-C25	-3.53	1.49	1.53
14	B	824	CLA	C1D-ND	3.52	1.42	1.37
16	B	844	BCR	C30-C25	-3.52	1.49	1.53
16	K	103	BCR	C1-C6	-3.52	1.49	1.53
16	B	852	BCR	C30-C25	-3.52	1.49	1.53
14	K	102	CLA	C1D-ND	3.50	1.42	1.37
16	B	848	BCR	C30-C25	-3.49	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	817	CLA	C1D-ND	3.47	1.42	1.37
14	A	824	CLA	C1D-ND	3.46	1.42	1.37
14	M	102	CLA	C1D-ND	3.46	1.42	1.37
14	B	806	CLA	C1D-ND	3.46	1.42	1.37
14	A	839	CLA	C1D-ND	3.46	1.42	1.37
14	A	837	CLA	C1D-ND	3.46	1.42	1.37
14	A	825	CLA	C1D-ND	3.44	1.42	1.37
14	B	832	CLA	C1D-ND	3.44	1.42	1.37
14	J	101	CLA	C1D-ND	3.43	1.42	1.37
16	I	101	BCR	C30-C25	-3.42	1.49	1.53
14	B	828	CLA	C1D-ND	3.42	1.42	1.37
14	F	203	CLA	C1D-ND	3.42	1.42	1.37
14	B	808	CLA	C1D-ND	3.41	1.42	1.37
14	B	813	CLA	C1D-ND	3.41	1.42	1.37
14	B	836	CLA	C1D-ND	3.41	1.42	1.37
14	B	840	CLA	C1D-ND	3.40	1.42	1.37
14	B	809	CLA	C1D-ND	3.39	1.42	1.37
14	A	820	CLA	C1D-ND	3.37	1.42	1.37
14	B	820	CLA	C1D-ND	3.37	1.42	1.37
14	A	804	CLA	C1D-ND	3.37	1.42	1.37
14	A	841	CLA	C1D-ND	3.37	1.42	1.37
14	F	204	CLA	C1D-ND	3.37	1.42	1.37
14	B	823	CLA	C1D-ND	3.36	1.42	1.37
14	B	841	CLA	C1D-ND	3.36	1.42	1.37
16	B	853	BCR	C30-C25	-3.36	1.49	1.53
14	L	201	CLA	C1D-ND	3.36	1.42	1.37
14	A	833	CLA	C1D-ND	3.35	1.42	1.37
14	B	821	CLA	C1D-ND	3.35	1.42	1.37
14	L	206	CLA	C1D-ND	3.35	1.42	1.37
14	B	839	CLA	C1D-ND	3.35	1.42	1.37
14	F	201	CLA	C1D-ND	3.35	1.42	1.37
14	A	813	CLA	C1D-ND	3.35	1.42	1.37
14	A	834	CLA	C1D-ND	3.34	1.42	1.37
14	A	828	CLA	C1D-ND	3.34	1.42	1.37
14	B	818	CLA	C1D-ND	3.34	1.42	1.37
14	B	842	CLA	C1D-ND	3.34	1.42	1.37
14	A	838	CLA	C1D-ND	3.33	1.42	1.37
14	A	843	CLA	C1D-ND	3.33	1.42	1.37
14	A	815	CLA	C1D-ND	3.33	1.42	1.37
14	A	842	CLA	C1D-ND	3.33	1.42	1.37
14	B	827	CLA	C1D-ND	3.32	1.42	1.37
14	A	814	CLA	C1D-ND	3.32	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	846	BCR	C30-C25	-3.32	1.49	1.53
14	A	812	CLA	C1D-ND	3.32	1.42	1.37
14	A	823	CLA	C1D-ND	3.32	1.42	1.37
14	A	811	CLA	C1D-ND	3.32	1.42	1.37
16	A	849	BCR	C30-C25	-3.32	1.49	1.53
14	A	835	CLA	C1D-ND	3.32	1.42	1.37
14	A	819	CLA	C1D-ND	3.31	1.42	1.37
14	B	831	CLA	C1D-ND	3.31	1.42	1.37
14	B	822	CLA	C1D-ND	3.31	1.42	1.37
14	B	825	CLA	C1D-ND	3.31	1.42	1.37
16	L	207	BCR	C30-C25	-3.30	1.49	1.53
14	A	826	CLA	C1D-ND	3.30	1.42	1.37
14	A	840	CLA	C1D-ND	3.30	1.42	1.37
14	B	817	CLA	C1D-ND	3.30	1.42	1.37
14	B	811	CLA	C1D-ND	3.30	1.42	1.37
14	A	824	CLA	C4B-NB	3.29	1.42	1.37
14	A	829	CLA	C1D-ND	3.28	1.42	1.37
14	A	802	CLA	C1D-ND	3.28	1.42	1.37
16	A	848	BCR	C30-C25	-3.28	1.49	1.53
14	A	803	CLA	C1D-ND	3.28	1.42	1.37
14	A	807	CLA	C1D-ND	3.28	1.42	1.37
14	A	836	CLA	C1D-ND	3.28	1.42	1.37
14	A	808	CLA	C1D-ND	3.28	1.42	1.37
14	B	830	CLA	C1D-ND	3.27	1.42	1.37
14	B	807	CLA	C1D-ND	3.27	1.42	1.37
14	B	834	CLA	C1D-ND	3.26	1.42	1.37
14	A	810	CLA	C1D-ND	3.26	1.42	1.37
14	B	833	CLA	C1D-ND	3.26	1.42	1.37
16	F	205	BCR	C30-C25	-3.26	1.49	1.53
14	B	816	CLA	C1D-ND	3.26	1.42	1.37
14	B	812	CLA	C1D-ND	3.26	1.42	1.37
14	A	854	CLA	C1D-ND	3.25	1.42	1.37
14	A	818	CLA	C1D-ND	3.25	1.42	1.37
14	B	801	CLA	C1D-ND	3.25	1.42	1.37
14	B	826	CLA	C1D-ND	3.25	1.42	1.37
14	A	809	CLA	C1D-ND	3.24	1.42	1.37
14	A	832	CLA	C1D-ND	3.24	1.42	1.37
14	B	838	CLA	C1D-ND	3.24	1.42	1.37
14	A	821	CLA	C1D-ND	3.24	1.42	1.37
14	B	819	CLA	C1D-ND	3.23	1.42	1.37
14	A	811	CLA	C4B-NB	3.22	1.42	1.37
14	A	831	CLA	C1D-ND	3.22	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	810	CLA	C1D-ND	3.22	1.42	1.37
14	B	828	CLA	C4B-NB	3.22	1.42	1.37
14	L	204	CLA	C4B-NB	3.21	1.42	1.37
14	A	822	CLA	C1D-ND	3.20	1.42	1.37
14	B	835	CLA	C1D-ND	3.20	1.42	1.37
14	L	205	CLA	C1D-ND	3.19	1.42	1.37
14	A	816	CLA	C1D-ND	3.18	1.42	1.37
14	A	827	CLA	C1D-ND	3.18	1.42	1.37
14	A	805	CLA	C1D-ND	3.18	1.42	1.37
14	L	204	CLA	C1D-ND	3.17	1.42	1.37
14	A	806	CLA	C1D-ND	3.17	1.42	1.37
14	A	803	CLA	C4B-NB	3.17	1.42	1.37
16	J	103	BCR	C30-C25	-3.16	1.49	1.53
16	A	850	BCR	C30-C25	-3.15	1.49	1.53
14	B	821	CLA	C4B-NB	3.15	1.42	1.37
14	B	814	CLA	C1D-ND	3.15	1.42	1.37
14	B	805	CLA	C1D-ND	3.15	1.42	1.37
14	B	837	CLA	C4B-NB	3.15	1.42	1.37
14	A	817	CLA	C4B-NB	3.15	1.42	1.37
14	J	102	CLA	C4B-NB	3.15	1.42	1.37
14	B	838	CLA	C4B-NB	3.14	1.42	1.37
14	B	829	CLA	C4B-NB	3.13	1.42	1.37
14	B	815	CLA	C1D-ND	3.13	1.42	1.37
14	A	830	CLA	C1D-ND	3.12	1.42	1.37
14	B	833	CLA	C4B-NB	3.12	1.42	1.37
14	B	842	CLA	C4B-NB	3.11	1.42	1.37
14	B	829	CLA	C1D-ND	3.11	1.41	1.37
14	A	813	CLA	C4B-NB	3.10	1.41	1.37
14	B	804	CLA	C1D-ND	3.10	1.41	1.37
14	J	101	CLA	C4B-NB	3.08	1.41	1.37
16	B	845	BCR	C30-C25	-3.07	1.49	1.53
14	M	102	CLA	C4B-NB	3.06	1.41	1.37
16	A	847	BCR	C30-C25	-3.05	1.49	1.53
14	F	201	CLA	C4B-NB	3.05	1.41	1.37
14	K	101	CLA	C4B-NB	3.04	1.41	1.37
14	A	842	CLA	C4B-NB	3.04	1.41	1.37
14	B	801	CLA	C4B-NB	3.04	1.41	1.37
14	F	204	CLA	C4B-NB	3.04	1.41	1.37
14	B	810	CLA	C4B-NB	3.03	1.41	1.37
14	B	824	CLA	C4B-NB	3.03	1.41	1.37
14	B	836	CLA	C4B-NB	3.02	1.41	1.37
14	K	102	CLA	C4B-NB	3.02	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	X	1701	CLA	C4B-NB	3.01	1.41	1.37
14	A	840	CLA	C4B-NB	3.01	1.41	1.37
14	B	823	CLA	C4B-NB	3.01	1.41	1.37
14	B	840	CLA	C4B-NB	3.00	1.41	1.37
14	B	834	CLA	C4B-NB	3.00	1.41	1.37
16	A	845	BCR	C30-C25	-2.99	1.49	1.53
14	A	843	CLA	C4B-NB	2.98	1.41	1.37
14	A	819	CLA	C4B-NB	2.96	1.41	1.37
14	B	817	CLA	C4B-NB	2.96	1.41	1.37
14	B	832	CLA	C4B-NB	2.96	1.41	1.37
14	B	820	CLA	C4B-NB	2.96	1.41	1.37
14	B	835	CLA	C4B-NB	2.94	1.41	1.37
14	A	808	CLA	C4B-NB	2.93	1.41	1.37
14	B	826	CLA	C4B-NB	2.92	1.41	1.37
14	B	841	CLA	C4B-NB	2.92	1.41	1.37
14	A	837	CLA	C4B-NB	2.92	1.41	1.37
14	B	818	CLA	C4B-NB	2.92	1.41	1.37
14	B	813	CLA	C4B-NB	2.91	1.41	1.37
14	A	815	CLA	C4B-NB	2.91	1.41	1.37
14	F	203	CLA	C4B-NB	2.90	1.41	1.37
14	A	823	CLA	C4B-NB	2.88	1.41	1.37
14	A	812	CLA	C4B-NB	2.88	1.41	1.37
14	A	836	CLA	C4B-NB	2.88	1.41	1.37
14	B	839	CLA	C4B-NB	2.88	1.41	1.37
14	A	841	CLA	C4B-NB	2.88	1.41	1.37
14	A	825	CLA	C4B-NB	2.88	1.41	1.37
14	A	808	CLA	C1B-C2B	2.88	1.49	1.43
14	B	837	CLA	C1B-C2B	2.87	1.49	1.43
14	B	830	CLA	C4B-NB	2.87	1.41	1.37
14	A	820	CLA	C4B-NB	2.87	1.41	1.37
14	B	812	CLA	C4B-NB	2.87	1.41	1.37
14	A	804	CLA	C1B-C2B	2.87	1.49	1.43
14	B	806	CLA	C4B-NB	2.86	1.41	1.37
14	A	810	CLA	C4B-NB	2.86	1.41	1.37
14	B	808	CLA	C4B-NB	2.86	1.41	1.37
14	A	805	CLA	C4B-NB	2.85	1.41	1.37
14	B	822	CLA	C4B-NB	2.84	1.41	1.37
14	B	807	CLA	C4B-NB	2.84	1.41	1.37
14	B	809	CLA	C4B-NB	2.83	1.41	1.37
14	A	818	CLA	C4B-NB	2.83	1.41	1.37
14	A	841	CLA	C1B-C2B	2.83	1.49	1.43
14	A	814	CLA	C4B-NB	2.83	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	828	CLA	C4B-NB	2.82	1.41	1.37
14	B	834	CLA	C1B-C2B	2.82	1.49	1.43
14	J	102	CLA	C1B-C2B	2.82	1.49	1.43
14	A	843	CLA	C1B-C2B	2.81	1.49	1.43
17	B	851	LHG	O7-C5	-2.81	1.40	1.46
14	B	823	CLA	C1B-C2B	2.81	1.49	1.43
14	A	821	CLA	C4B-NB	2.81	1.41	1.37
14	M	102	CLA	C1B-C2B	2.80	1.49	1.43
13	A	801	CL0	CMD-C2D	-2.80	1.46	1.51
14	B	815	CLA	C4B-NB	2.80	1.41	1.37
14	B	804	CLA	C1B-C2B	2.80	1.49	1.43
14	B	825	CLA	C4B-NB	2.80	1.41	1.37
14	A	821	CLA	C1B-C2B	2.80	1.49	1.43
14	A	823	CLA	C1B-C2B	2.80	1.49	1.43
14	B	831	CLA	C4B-NB	2.79	1.41	1.37
14	F	203	CLA	C1B-C2B	2.79	1.49	1.43
14	B	827	CLA	C4B-NB	2.79	1.41	1.37
14	A	835	CLA	C1B-C2B	2.78	1.49	1.43
14	L	206	CLA	C4B-NB	2.78	1.41	1.37
14	A	827	CLA	C4B-NB	2.78	1.41	1.37
14	B	824	CLA	C1B-C2B	2.77	1.49	1.43
14	A	854	CLA	C1B-C2B	2.77	1.49	1.43
14	A	815	CLA	C1B-C2B	2.77	1.49	1.43
14	A	807	CLA	C4B-NB	2.77	1.41	1.37
14	B	816	CLA	C4B-NB	2.77	1.41	1.37
14	A	812	CLA	C1B-C2B	2.77	1.49	1.43
14	B	801	CLA	C1B-C2B	2.77	1.49	1.43
14	B	808	CLA	C1B-C2B	2.77	1.49	1.43
14	A	816	CLA	C4B-NB	2.77	1.41	1.37
14	A	833	CLA	C4B-NB	2.76	1.41	1.37
14	A	831	CLA	CMB-C2B	-2.76	1.45	1.50
14	A	835	CLA	C4B-NB	2.76	1.41	1.37
14	A	825	CLA	C1B-C2B	2.75	1.49	1.43
14	A	838	CLA	C4B-NB	2.75	1.41	1.37
14	J	101	CLA	C1B-C2B	2.74	1.49	1.43
14	B	839	CLA	C1B-C2B	2.74	1.49	1.43
14	A	854	CLA	C4B-NB	2.74	1.41	1.37
14	B	805	CLA	C1B-C2B	2.74	1.49	1.43
14	A	822	CLA	C4B-NB	2.74	1.41	1.37
14	A	830	CLA	C4B-NB	2.74	1.41	1.37
14	B	841	CLA	C1B-C2B	2.73	1.49	1.43
14	A	834	CLA	C4B-NB	2.73	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	K	102	CLA	C1B-C2B	2.73	1.49	1.43
14	A	802	CLA	C4B-NB	2.72	1.41	1.37
14	B	819	CLA	C4B-NB	2.72	1.41	1.37
14	F	204	CLA	C1B-C2B	2.72	1.49	1.43
14	A	829	CLA	C4B-NB	2.72	1.41	1.37
14	B	816	CLA	C1B-C2B	2.72	1.49	1.43
14	L	205	CLA	C1B-C2B	2.72	1.49	1.43
14	B	818	CLA	C1B-C2B	2.72	1.49	1.43
14	A	831	CLA	C4B-NB	2.72	1.41	1.37
14	A	827	CLA	C1B-C2B	2.71	1.49	1.43
14	B	840	CLA	C1B-C2B	2.71	1.49	1.43
14	A	816	CLA	C1B-C2B	2.71	1.49	1.43
14	A	838	CLA	C1B-C2B	2.71	1.49	1.43
14	A	806	CLA	C1B-C2B	2.71	1.49	1.43
14	A	824	CLA	C1B-C2B	2.71	1.49	1.43
14	A	826	CLA	C4B-NB	2.71	1.41	1.37
14	L	201	CLA	C1B-C2B	2.70	1.49	1.43
14	B	821	CLA	C1B-C2B	2.70	1.49	1.43
14	A	833	CLA	C1B-C2B	2.70	1.49	1.43
14	A	832	CLA	C4B-NB	2.70	1.41	1.37
14	L	201	CLA	C4B-NB	2.69	1.41	1.37
14	B	835	CLA	C1B-C2B	2.69	1.49	1.43
14	B	811	CLA	C4B-NB	2.69	1.41	1.37
14	A	807	CLA	C1B-C2B	2.69	1.49	1.43
14	X	1701	CLA	C1B-C2B	2.68	1.49	1.43
14	B	832	CLA	C1B-C2B	2.68	1.49	1.43
14	B	814	CLA	C1B-C2B	2.68	1.49	1.43
14	B	827	CLA	C1B-C2B	2.68	1.49	1.43
14	B	825	CLA	C1B-C2B	2.68	1.49	1.43
14	A	830	CLA	C1B-C2B	2.67	1.49	1.43
14	K	101	CLA	C1B-C2B	2.67	1.49	1.43
14	A	839	CLA	C1B-C2B	2.67	1.49	1.43
14	B	815	CLA	C1B-C2B	2.66	1.49	1.43
14	B	842	CLA	C1B-C2B	2.66	1.49	1.43
14	B	806	CLA	C1B-C2B	2.65	1.49	1.43
14	B	807	CLA	C1B-C2B	2.65	1.49	1.43
14	A	837	CLA	C1B-C2B	2.65	1.49	1.43
14	B	809	CLA	C1B-C2B	2.65	1.49	1.43
14	B	822	CLA	C1B-C2B	2.65	1.49	1.43
14	B	811	CLA	C1B-C2B	2.64	1.49	1.43
14	A	805	CLA	C1B-C2B	2.64	1.49	1.43
14	A	802	CLA	C1B-C2B	2.63	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	820	CLA	C1B-C2B	2.63	1.49	1.43
14	B	804	CLA	C4B-NB	2.63	1.41	1.37
14	A	810	CLA	C1B-C2B	2.63	1.49	1.43
14	B	838	CLA	C1B-C2B	2.63	1.49	1.43
14	L	205	CLA	C4B-NB	2.62	1.41	1.37
14	B	814	CLA	C4B-NB	2.62	1.41	1.37
14	F	201	CLA	C1B-C2B	2.62	1.49	1.43
14	A	839	CLA	C4B-NB	2.62	1.41	1.37
14	A	809	CLA	C4B-NB	2.61	1.41	1.37
14	A	809	CLA	C1B-C2B	2.61	1.49	1.43
17	A	852	LHG	O7-C5	-2.61	1.40	1.46
14	B	830	CLA	C1B-C2B	2.61	1.49	1.43
14	L	206	CLA	C1B-C2B	2.60	1.49	1.43
14	A	814	CLA	C1B-C2B	2.60	1.49	1.43
14	B	813	CLA	C1B-C2B	2.60	1.49	1.43
14	B	833	CLA	C1B-C2B	2.60	1.49	1.43
14	A	817	CLA	C1B-C2B	2.60	1.49	1.43
13	A	801	CL0	CMC-C2C	-2.60	1.46	1.50
14	A	811	CLA	C3B-C4B	2.59	1.50	1.42
14	A	806	CLA	C4B-NB	2.59	1.41	1.37
17	A	853	LHG	O7-C5	-2.59	1.40	1.46
14	B	831	CLA	C1B-C2B	2.58	1.49	1.43
14	A	828	CLA	C1B-C2B	2.58	1.49	1.43
14	A	813	CLA	C3B-C4B	2.58	1.50	1.42
14	B	829	CLA	C3B-C4B	2.57	1.50	1.42
14	A	804	CLA	C4B-NB	2.56	1.41	1.37
13	A	801	CL0	CMB-C2B	-2.56	1.46	1.51
14	A	840	CLA	C1B-C2B	2.56	1.49	1.43
14	L	204	CLA	C3B-C4B	2.56	1.50	1.42
14	A	819	CLA	C3B-C4B	2.55	1.50	1.42
14	A	826	CLA	C1B-C2B	2.55	1.49	1.43
14	B	812	CLA	C1B-C2B	2.55	1.49	1.43
14	B	805	CLA	C4B-NB	2.54	1.41	1.37
14	A	830	CLA	CMD-C2D	-2.53	1.45	1.50
14	B	828	CLA	C3B-C4B	2.53	1.50	1.42
14	A	803	CLA	C3B-C4B	2.53	1.50	1.42
14	B	817	CLA	C1B-C2B	2.53	1.49	1.43
14	A	818	CLA	C1B-C2B	2.53	1.49	1.43
14	B	833	CLA	C3B-C4B	2.52	1.50	1.42
14	A	834	CLA	C1B-C2B	2.52	1.49	1.43
14	A	831	CLA	C1B-C2B	2.51	1.49	1.43
14	B	836	CLA	C1B-C2B	2.51	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	810	CLA	C3B-C4B	2.51	1.50	1.42
14	A	842	CLA	C1B-C2B	2.50	1.49	1.43
14	A	842	CLA	C3B-C4B	2.50	1.50	1.42
14	B	826	CLA	C1B-C2B	2.49	1.49	1.43
14	B	830	CLA	CMB-C2B	-2.49	1.45	1.50
14	A	811	CLA	C1B-C2B	2.48	1.49	1.43
14	B	836	CLA	C3B-C4B	2.48	1.49	1.42
14	B	817	CLA	C3B-C4B	2.47	1.49	1.42
14	B	829	CLA	CMD-C2D	-2.47	1.45	1.50
14	L	204	CLA	C1B-C2B	2.47	1.48	1.43
14	B	820	CLA	C1B-C2B	2.46	1.48	1.43
14	A	803	CLA	C1B-C2B	2.46	1.48	1.43
14	A	826	CLA	CMD-C2D	-2.46	1.45	1.50
14	B	819	CLA	C1B-C2B	2.45	1.48	1.43
14	A	832	CLA	C1B-C2B	2.44	1.48	1.43
14	A	822	CLA	C1B-C2B	2.44	1.48	1.43
14	A	836	CLA	C1B-C2B	2.43	1.48	1.43
14	A	814	CLA	CMC-C2C	-2.43	1.45	1.50
14	A	829	CLA	C3B-C4B	2.43	1.49	1.42
14	B	821	CLA	C3B-C4B	2.43	1.49	1.42
14	A	824	CLA	C3B-C4B	2.42	1.49	1.42
14	A	802	CLA	C3B-C4B	2.42	1.49	1.42
14	J	101	CLA	C3B-C4B	2.42	1.49	1.42
14	B	804	CLA	CMD-C2D	-2.42	1.45	1.50
14	B	830	CLA	CMD-C2D	-2.42	1.45	1.50
14	B	828	CLA	C1B-C2B	2.41	1.48	1.43
14	A	817	CLA	C3B-C4B	2.41	1.49	1.42
14	A	832	CLA	CMB-C2B	-2.41	1.45	1.50
14	A	816	CLA	CMD-C2D	-2.40	1.45	1.50
14	F	201	CLA	C3B-C4B	2.40	1.49	1.42
14	B	836	CLA	CHC-C1C	2.40	1.43	1.38
13	A	801	CL0	CAC-C3C	-2.40	1.47	1.51
14	B	842	CLA	C3B-C4B	2.40	1.49	1.42
14	A	803	CLA	CMC-C2C	-2.40	1.45	1.50
14	A	836	CLA	CMB-C2B	-2.40	1.45	1.50
14	B	817	CLA	CHC-C1C	2.39	1.43	1.38
14	J	102	CLA	C3B-C4B	2.39	1.49	1.42
16	I	103	BCR	C30-C25	-2.39	1.50	1.53
14	B	832	CLA	C3B-C4B	2.39	1.49	1.42
14	B	838	CLA	C3B-C4B	2.39	1.49	1.42
14	A	831	CLA	CMD-C2D	-2.38	1.45	1.50
14	B	813	CLA	C3B-C4B	2.38	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	802	CLA	CHC-C1C	2.38	1.43	1.38
14	A	840	CLA	C3B-C4B	2.38	1.49	1.42
14	B	811	CLA	CMB-C2B	-2.37	1.45	1.50
14	B	821	CLA	CMD-C2D	-2.37	1.45	1.50
14	A	829	CLA	C1B-C2B	2.37	1.48	1.43
14	A	819	CLA	CHC-C1C	2.37	1.43	1.38
14	A	810	CLA	CMD-C2D	-2.37	1.45	1.50
14	F	204	CLA	C3B-C4B	2.36	1.49	1.42
14	K	101	CLA	C3B-C4B	2.36	1.49	1.42
14	B	834	CLA	C3B-C4B	2.36	1.49	1.42
14	J	102	CLA	CHC-C1C	2.35	1.43	1.38
14	A	832	CLA	CMD-C2D	-2.35	1.46	1.50
14	B	826	CLA	C3B-C4B	2.35	1.49	1.42
14	A	813	CLA	C1B-C2B	2.35	1.48	1.43
14	B	829	CLA	C1B-C2B	2.35	1.48	1.43
14	A	821	CLA	C3B-C4B	2.35	1.49	1.42
14	A	842	CLA	CMC-C2C	-2.35	1.46	1.50
14	B	801	CLA	C3B-C4B	2.34	1.49	1.42
14	B	812	CLA	CMB-C2B	-2.34	1.46	1.50
14	A	822	CLA	CMD-C2D	-2.34	1.46	1.50
14	X	1701	CLA	C3B-C4B	2.34	1.49	1.42
14	A	843	CLA	C3B-C4B	2.34	1.49	1.42
14	A	822	CLA	CMB-C2B	-2.33	1.46	1.50
14	A	813	CLA	CHC-C1C	2.33	1.43	1.38
14	A	814	CLA	C3B-C4B	2.33	1.49	1.42
14	B	818	CLA	C3B-C4B	2.33	1.49	1.42
14	B	820	CLA	C3B-C4B	2.33	1.49	1.42
14	B	810	CLA	CMC-C2C	-2.33	1.46	1.50
14	B	827	CLA	C3B-C4B	2.33	1.49	1.42
14	M	102	CLA	C3B-C4B	2.32	1.49	1.42
14	B	810	CLA	CMB-C2B	-2.32	1.46	1.50
14	B	809	CLA	CMD-C2D	-2.32	1.46	1.50
14	A	833	CLA	C3B-C4B	2.32	1.49	1.42
14	B	837	CLA	C3B-C4B	2.32	1.49	1.42
14	B	814	CLA	C3B-C4B	2.32	1.49	1.42
14	B	810	CLA	CMD-C2D	-2.32	1.46	1.50
14	B	801	CLA	CMD-C2D	-2.31	1.46	1.50
14	B	823	CLA	C3B-C4B	2.31	1.49	1.42
14	X	1701	CLA	CHC-C1C	2.31	1.43	1.38
14	K	102	CLA	C3B-C4B	2.31	1.49	1.42
14	A	832	CLA	MG-NB	-2.31	2.01	2.05
14	B	815	CLA	CMD-C2D	-2.31	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	831	CLA	CMB-C2B	-2.31	1.46	1.50
14	A	821	CLA	CHC-C1C	2.31	1.43	1.38
14	A	827	CLA	C3B-C4B	2.30	1.49	1.42
14	A	830	CLA	MG-NB	-2.30	2.01	2.05
14	A	837	CLA	C3B-C4B	2.30	1.49	1.42
14	A	838	CLA	C3B-C4B	2.30	1.49	1.42
14	B	841	CLA	C3B-C4B	2.30	1.49	1.42
14	A	820	CLA	C3B-C4B	2.30	1.49	1.42
14	L	206	CLA	C3B-C4B	2.30	1.49	1.42
14	A	804	CLA	MG-NB	-2.29	2.01	2.05
14	A	842	CLA	CHC-C1C	2.29	1.43	1.38
14	A	822	CLA	C3B-C4B	2.29	1.49	1.42
14	A	840	CLA	CHC-C1C	2.29	1.43	1.38
14	A	831	CLA	MG-NB	-2.29	2.01	2.05
14	B	819	CLA	CMB-C2B	-2.29	1.46	1.50
14	B	816	CLA	C3B-C4B	2.29	1.49	1.42
14	M	102	CLA	CHC-C1C	2.29	1.43	1.38
14	B	810	CLA	CHC-C1C	2.28	1.43	1.38
14	L	201	CLA	C3B-C4B	2.28	1.49	1.42
14	A	809	CLA	CMB-C2B	-2.28	1.46	1.50
14	B	807	CLA	C3B-C4B	2.28	1.49	1.42
14	F	203	CLA	C3B-C4B	2.28	1.49	1.42
14	A	815	CLA	C3B-C4B	2.28	1.49	1.42
14	B	825	CLA	CMD-C2D	-2.28	1.46	1.50
14	B	829	CLA	CMB-C2B	-2.28	1.46	1.50
14	B	822	CLA	C3B-C4B	2.28	1.49	1.42
14	A	812	CLA	C3B-C4B	2.27	1.49	1.42
14	B	831	CLA	MG-NB	-2.27	2.01	2.05
14	A	854	CLA	C3B-C4B	2.27	1.49	1.42
14	B	812	CLA	MG-NB	-2.27	2.01	2.05
14	B	820	CLA	CMB-C2B	-2.27	1.46	1.50
14	A	811	CLA	CHC-C1C	2.27	1.43	1.38
14	A	825	CLA	C3B-C4B	2.27	1.49	1.42
14	B	835	CLA	C3B-C4B	2.27	1.49	1.42
14	A	840	CLA	CMD-C2D	-2.27	1.46	1.50
14	A	805	CLA	CMB-C2B	-2.27	1.46	1.50
14	A	803	CLA	CHC-C1C	2.27	1.43	1.38
14	A	805	CLA	C3B-C4B	2.27	1.49	1.42
14	B	824	CLA	C3B-C4B	2.27	1.49	1.42
14	A	817	CLA	CMB-C2B	-2.27	1.46	1.50
14	B	827	CLA	CMD-C2D	-2.27	1.46	1.50
14	A	842	CLA	CMD-C2D	-2.26	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	828	CLA	CHC-C1C	2.26	1.43	1.38
14	A	815	CLA	CMC-C2C	-2.26	1.46	1.50
14	A	818	CLA	CMD-C2D	-2.26	1.46	1.50
14	B	840	CLA	C3B-C4B	2.26	1.49	1.42
14	A	823	CLA	C3B-C4B	2.26	1.49	1.42
14	B	815	CLA	C3B-C4B	2.26	1.49	1.42
14	B	833	CLA	CHC-C1C	2.26	1.43	1.38
14	A	819	CLA	CMD-C2D	-2.26	1.46	1.50
14	A	820	CLA	CMD-C2D	-2.26	1.46	1.50
14	A	826	CLA	MG-NB	-2.26	2.01	2.05
14	A	816	CLA	C3B-C4B	2.26	1.49	1.42
14	A	837	CLA	CHC-C1C	2.26	1.43	1.38
14	A	807	CLA	CMD-C2D	-2.25	1.46	1.50
14	A	814	CLA	CMD-C2D	-2.25	1.46	1.50
14	B	806	CLA	C3B-C4B	2.25	1.49	1.42
14	A	810	CLA	CMB-C2B	-2.25	1.46	1.50
14	B	835	CLA	CMB-C2B	-2.25	1.46	1.50
14	B	835	CLA	CMD-C2D	-2.25	1.46	1.50
14	B	842	CLA	CMB-C2B	-2.25	1.46	1.50
14	B	808	CLA	C3B-C4B	2.25	1.49	1.42
14	B	806	CLA	CHC-C1C	2.25	1.43	1.38
14	A	828	CLA	C3B-C4B	2.25	1.49	1.42
14	A	813	CLA	CMB-C2B	-2.25	1.46	1.50
14	A	819	CLA	CMB-C2B	-2.25	1.46	1.50
14	J	101	CLA	CMD-C2D	-2.25	1.46	1.50
14	A	828	CLA	CMB-C2B	-2.24	1.46	1.50
14	B	824	CLA	CHC-C1C	2.24	1.43	1.38
14	A	806	CLA	CMD-C2D	-2.24	1.46	1.50
14	B	819	CLA	CMD-C2D	-2.24	1.46	1.50
14	A	812	CLA	CMC-C2C	-2.24	1.46	1.50
14	A	841	CLA	CHC-C1C	2.24	1.43	1.38
14	B	841	CLA	CHC-C1C	2.24	1.43	1.38
14	A	805	CLA	MG-NB	-2.24	2.01	2.05
14	A	836	CLA	CMD-C2D	-2.24	1.46	1.50
14	F	201	CLA	CHC-C1C	2.23	1.43	1.38
14	A	841	CLA	C3B-C4B	2.23	1.49	1.42
14	A	830	CLA	CMB-C2B	-2.23	1.46	1.50
14	A	819	CLA	C1B-C2B	2.23	1.48	1.43
14	A	838	CLA	CMD-C2D	-2.23	1.46	1.50
13	A	801	CL0	MG-NB	-2.23	2.01	2.05
14	F	201	CLA	CMD-C2D	-2.23	1.46	1.50
14	A	818	CLA	MG-NB	-2.23	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	820	CLA	CMC-C2C	-2.23	1.46	1.50
14	B	826	CLA	CHC-C1C	2.23	1.43	1.38
14	A	834	CLA	CMD-C2D	-2.23	1.46	1.50
14	B	819	CLA	C3B-C4B	2.23	1.49	1.42
14	A	839	CLA	CMD-C2D	-2.23	1.46	1.50
14	A	836	CLA	C3B-C4B	2.23	1.49	1.42
14	L	204	CLA	CMB-C2B	-2.23	1.46	1.50
14	A	822	CLA	MG-NB	-2.23	2.01	2.05
14	B	807	CLA	CMD-C2D	-2.23	1.46	1.50
14	A	835	CLA	CMD-C2D	-2.22	1.46	1.50
14	A	818	CLA	C3B-C4B	2.22	1.49	1.42
14	A	815	CLA	CMD-C2D	-2.22	1.46	1.50
14	B	838	CLA	CMB-C2B	-2.22	1.46	1.50
14	A	804	CLA	CMD-C2D	-2.22	1.46	1.50
14	K	102	CLA	CHC-C1C	2.22	1.42	1.38
14	A	841	CLA	CMD-C2D	-2.22	1.46	1.50
14	J	101	CLA	CHC-C1C	2.22	1.42	1.38
14	A	821	CLA	CMD-C2D	-2.22	1.46	1.50
14	B	804	CLA	CMC-C2C	-2.22	1.46	1.50
14	A	802	CLA	CMD-C2D	-2.22	1.46	1.50
14	A	828	CLA	MG-NB	-2.22	2.01	2.05
14	F	204	CLA	CMD-C2D	-2.22	1.46	1.50
14	B	841	CLA	CMD-C2D	-2.22	1.46	1.50
14	B	836	CLA	CMD-C2D	-2.22	1.46	1.50
14	A	829	CLA	CMD-C2D	-2.22	1.46	1.50
14	B	813	CLA	CMD-C2D	-2.22	1.46	1.50
14	B	809	CLA	C3B-C4B	2.22	1.49	1.42
14	A	827	CLA	CMD-C2D	-2.22	1.46	1.50
14	B	838	CLA	CMD-C2D	-2.22	1.46	1.50
14	L	204	CLA	CMD-C2D	-2.22	1.46	1.50
14	B	839	CLA	C3B-C4B	2.22	1.49	1.42
14	B	811	CLA	MG-NB	-2.21	2.01	2.05
14	B	819	CLA	MG-NB	-2.21	2.01	2.05
14	A	814	CLA	CHC-C1C	2.21	1.42	1.38
14	A	828	CLA	CHC-C1C	2.21	1.42	1.38
14	A	834	CLA	MG-NB	-2.21	2.01	2.05
14	L	205	CLA	CMD-C2D	-2.21	1.46	1.50
14	B	810	CLA	C1B-C2B	2.21	1.48	1.43
14	B	817	CLA	CMB-C2B	-2.21	1.46	1.50
14	A	811	CLA	CMB-C2B	-2.21	1.46	1.50
14	A	810	CLA	MG-NB	-2.21	2.01	2.05
14	L	205	CLA	C3B-C4B	2.20	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	808	CLA	C3B-C4B	2.20	1.49	1.42
14	A	833	CLA	CMD-C2D	-2.20	1.46	1.50
14	B	823	CLA	CHC-C1C	2.20	1.42	1.38
14	B	829	CLA	CHC-C1C	2.20	1.42	1.38
14	B	816	CLA	CMD-C2D	-2.20	1.46	1.50
14	A	838	CLA	CMB-C2B	-2.20	1.46	1.50
14	A	806	CLA	CMB-C2B	-2.20	1.46	1.50
14	A	813	CLA	MG-NB	-2.20	2.01	2.05
14	A	803	CLA	CMD-C2D	-2.20	1.46	1.50
14	B	842	CLA	CMD-C2D	-2.20	1.46	1.50
14	B	804	CLA	MG-NB	-2.20	2.01	2.05
14	B	814	CLA	CMC-C2C	-2.20	1.46	1.50
14	A	835	CLA	C3B-C4B	2.20	1.49	1.42
14	A	813	CLA	CMD-C2D	-2.19	1.46	1.50
14	B	832	CLA	CHC-C1C	2.19	1.42	1.38
14	A	826	CLA	C3B-C4B	2.19	1.49	1.42
14	B	830	CLA	MG-NB	-2.19	2.01	2.05
14	A	819	CLA	CMC-C2C	-2.19	1.46	1.50
14	B	833	CLA	CMD-C2D	-2.19	1.46	1.50
14	B	822	CLA	MG-NB	-2.19	2.01	2.05
14	A	854	CLA	CMD-C2D	-2.19	1.46	1.50
14	B	806	CLA	CMD-C2D	-2.19	1.46	1.50
14	B	820	CLA	CHC-C1C	2.19	1.42	1.38
14	B	838	CLA	CHC-C1C	2.19	1.42	1.38
14	A	842	CLA	CMB-C2B	-2.19	1.46	1.50
14	A	807	CLA	C3B-C4B	2.19	1.49	1.42
14	A	805	CLA	CMD-C2D	-2.19	1.46	1.50
14	B	826	CLA	CMD-C2D	-2.19	1.46	1.50
14	B	822	CLA	CHC-C1C	2.19	1.42	1.38
14	B	820	CLA	MG-NB	-2.19	2.01	2.05
14	B	834	CLA	CHC-C1C	2.19	1.42	1.38
14	B	805	CLA	CMD-C2D	-2.19	1.46	1.50
14	L	201	CLA	CMD-C2D	-2.18	1.46	1.50
14	B	806	CLA	CMC-C2C	-2.18	1.46	1.50
14	L	205	CLA	CHC-C1C	2.18	1.42	1.38
14	A	812	CLA	CMD-C2D	-2.18	1.46	1.50
14	A	805	CLA	CHC-C1C	2.18	1.42	1.38
14	B	822	CLA	CMB-C2B	-2.18	1.46	1.50
14	B	840	CLA	CHC-C1C	2.18	1.42	1.38
14	A	834	CLA	C3B-C4B	2.18	1.49	1.42
14	A	816	CLA	CMB-C2B	-2.18	1.46	1.50
14	B	817	CLA	CMD-C2D	-2.18	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	L	201	CLA	CMC-C2C	-2.18	1.46	1.50
14	B	814	CLA	CHC-C1C	2.18	1.42	1.38
14	A	822	CLA	CMC-C2C	-2.18	1.46	1.50
14	L	206	CLA	CMD-C2D	-2.18	1.46	1.50
14	A	815	CLA	CHC-C1C	2.18	1.42	1.38
14	B	837	CLA	CHC-C1C	2.18	1.42	1.38
14	A	832	CLA	C3B-C4B	2.18	1.49	1.42
14	A	843	CLA	CHC-C1C	2.18	1.42	1.38
14	B	814	CLA	CMD-C2D	-2.18	1.46	1.50
14	A	810	CLA	C3B-C4B	2.17	1.49	1.42
14	B	813	CLA	CHC-C1C	2.17	1.42	1.38
14	B	811	CLA	CMD-C2D	-2.17	1.46	1.50
14	B	825	CLA	CHC-C1C	2.17	1.42	1.38
14	J	102	CLA	CBD-CAD	2.17	1.56	1.51
14	B	809	CLA	CHC-C1C	2.17	1.42	1.38
14	A	830	CLA	C3B-C4B	2.17	1.49	1.42
14	A	806	CLA	MG-NB	-2.17	2.01	2.05
14	A	808	CLA	CMD-C2D	-2.17	1.46	1.50
14	B	821	CLA	CHC-C1C	2.17	1.42	1.38
14	A	839	CLA	MG-NB	-2.17	2.01	2.05
14	B	825	CLA	C3B-C4B	2.17	1.49	1.42
14	A	826	CLA	CMB-C2B	-2.17	1.46	1.50
14	B	805	CLA	CMC-C2C	-2.17	1.46	1.50
14	A	824	CLA	CMB-C2B	-2.17	1.46	1.50
14	L	201	CLA	MG-NB	-2.17	2.01	2.05
14	B	809	CLA	MG-NB	-2.17	2.01	2.05
14	B	826	CLA	CMC-C2C	-2.17	1.46	1.50
14	L	204	CLA	CHC-C1C	2.17	1.42	1.38
14	B	804	CLA	CHC-C1C	2.17	1.42	1.38
14	B	836	CLA	CMB-C2B	-2.16	1.46	1.50
14	B	813	CLA	CMC-C2C	-2.16	1.46	1.50
14	F	203	CLA	CHC-C1C	2.16	1.42	1.38
14	B	825	CLA	CMC-C2C	-2.16	1.46	1.50
14	B	822	CLA	CMD-C2D	-2.16	1.46	1.50
14	M	102	CLA	CBD-CAD	2.16	1.56	1.51
14	A	823	CLA	CMB-C2B	-2.16	1.46	1.50
14	A	809	CLA	CHC-C1C	2.16	1.42	1.38
14	A	809	CLA	CMD-C2D	-2.16	1.46	1.50
14	B	808	CLA	CMC-C2C	-2.16	1.46	1.50
14	A	836	CLA	MG-NB	-2.16	2.01	2.05
14	A	811	CLA	CMD-C2D	-2.16	1.46	1.50
14	A	828	CLA	CMD-C2D	-2.16	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	814	CLA	MG-NB	-2.16	2.01	2.05
14	B	834	CLA	CMD-C2D	-2.16	1.46	1.50
14	A	807	CLA	MG-NB	-2.16	2.01	2.05
14	B	832	CLA	CMD-C2D	-2.16	1.46	1.50
13	A	801	CL0	CHC-C4B	-2.16	1.36	1.39
14	A	836	CLA	CMC-C2C	-2.16	1.46	1.50
14	K	101	CLA	CHC-C1C	2.16	1.42	1.38
14	B	823	CLA	CMD-C2D	-2.15	1.46	1.50
14	B	839	CLA	CMB-C2B	-2.15	1.46	1.50
14	A	824	CLA	CHC-C1C	2.15	1.42	1.38
14	B	812	CLA	C3B-C4B	2.15	1.49	1.42
14	B	807	CLA	CMB-C2B	-2.15	1.46	1.50
14	B	828	CLA	CMC-C2C	-2.15	1.46	1.50
14	B	810	CLA	MG-NB	-2.15	2.01	2.05
14	B	838	CLA	CMC-C2C	-2.15	1.46	1.50
14	A	808	CLA	CHC-C1C	2.15	1.42	1.38
14	A	809	CLA	C3B-C4B	2.15	1.49	1.42
14	B	827	CLA	MG-NB	-2.15	2.01	2.05
14	B	831	CLA	C3B-C4B	2.15	1.49	1.42
14	A	820	CLA	CMB-C2B	-2.15	1.46	1.50
14	K	101	CLA	CMD-C2D	-2.15	1.46	1.50
14	B	815	CLA	CHC-C1C	2.15	1.42	1.38
14	A	835	CLA	CMC-C2C	-2.15	1.46	1.50
14	B	820	CLA	CMD-C2D	-2.15	1.46	1.50
14	L	206	CLA	CHC-C1C	2.15	1.42	1.38
14	A	803	CLA	CMB-C2B	-2.15	1.46	1.50
14	A	824	CLA	CMD-C2D	-2.15	1.46	1.50
14	B	818	CLA	CMD-C2D	-2.15	1.46	1.50
14	A	812	CLA	CHC-C1C	2.14	1.42	1.38
14	B	842	CLA	CHC-C1C	2.14	1.42	1.38
14	A	818	CLA	CMB-C2B	-2.14	1.46	1.50
14	A	816	CLA	MG-NB	-2.14	2.01	2.05
14	A	843	CLA	CMC-C2C	-2.14	1.46	1.50
14	B	801	CLA	CMB-C2B	-2.14	1.46	1.50
14	L	206	CLA	MG-NB	-2.14	2.01	2.05
14	B	805	CLA	C3B-C4B	2.14	1.49	1.42
14	B	815	CLA	CMB-C2B	-2.14	1.46	1.50
14	B	840	CLA	CMC-C2C	-2.14	1.46	1.50
14	A	826	CLA	CHC-C1C	2.14	1.42	1.38
14	A	829	CLA	CHC-C1C	2.14	1.42	1.38
14	A	825	CLA	CHC-C1C	2.14	1.42	1.38
14	A	820	CLA	CHC-C1C	2.14	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	809	CLA	MG-NB	-2.14	2.01	2.05
16	I	101	BCR	C33-C5	-2.14	1.47	1.50
14	B	825	CLA	MG-NB	-2.14	2.01	2.05
14	A	839	CLA	C3B-C4B	2.13	1.49	1.42
14	A	843	CLA	CMD-C2D	-2.13	1.46	1.50
14	B	840	CLA	CMD-C2D	-2.13	1.46	1.50
16	J	103	BCR	C33-C5	-2.13	1.47	1.50
14	B	828	CLA	CMB-C2B	-2.13	1.46	1.50
14	F	203	CLA	CMD-C2D	-2.13	1.46	1.50
14	A	834	CLA	CMB-C2B	-2.13	1.46	1.50
14	B	816	CLA	CHC-C1C	2.13	1.42	1.38
14	B	805	CLA	MG-NB	-2.13	2.01	2.05
14	B	839	CLA	CMD-C2D	-2.13	1.46	1.50
14	K	101	CLA	CMB-C2B	-2.13	1.46	1.50
14	A	804	CLA	CMB-C2B	-2.12	1.46	1.50
14	A	815	CLA	MG-NB	-2.12	2.01	2.05
14	B	809	CLA	CMB-C2B	-2.12	1.46	1.50
14	A	810	CLA	CHC-C1C	2.12	1.42	1.38
14	A	808	CLA	MG-NB	-2.12	2.01	2.05
14	B	807	CLA	CHC-C1C	2.12	1.42	1.38
14	B	815	CLA	MG-NB	-2.12	2.01	2.05
14	A	836	CLA	CHC-C1C	2.12	1.42	1.38
14	A	818	CLA	CHC-C1C	2.12	1.42	1.38
14	B	831	CLA	CMD-C2D	-2.12	1.46	1.50
14	B	807	CLA	MG-NB	-2.12	2.01	2.05
14	B	834	CLA	CMB-C2B	-2.12	1.46	1.50
14	A	833	CLA	MG-NB	-2.12	2.01	2.05
14	B	831	CLA	CHC-C1C	2.12	1.42	1.38
14	A	823	CLA	CHC-C1C	2.12	1.42	1.38
14	B	818	CLA	CMB-C2B	-2.12	1.46	1.50
14	B	811	CLA	C3B-C4B	2.12	1.48	1.42
14	A	825	CLA	MG-NB	-2.12	2.01	2.05
14	A	823	CLA	CMD-C2D	-2.12	1.46	1.50
14	B	812	CLA	CMC-C2C	-2.12	1.46	1.50
14	F	204	CLA	MG-NB	-2.12	2.01	2.05
14	B	805	CLA	CMB-C2B	-2.11	1.46	1.50
14	B	833	CLA	CMC-C2C	-2.11	1.46	1.50
14	A	828	CLA	CMC-C2C	-2.11	1.46	1.50
14	F	204	CLA	CHC-C1C	2.11	1.42	1.38
14	A	808	CLA	CMC-C2C	-2.11	1.46	1.50
14	B	826	CLA	CMB-C2B	-2.11	1.46	1.50
14	L	201	CLA	CMB-C2B	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	802	CLA	MG-NB	-2.11	2.01	2.05
14	B	837	CLA	CMB-C2B	-2.11	1.46	1.50
14	A	817	CLA	CMD-C2D	-2.11	1.46	1.50
14	B	820	CLA	CMC-C2C	-2.11	1.46	1.50
14	A	817	CLA	CHC-C1C	2.11	1.42	1.38
17	M	101	LHG	O7-C5	-2.11	1.41	1.46
14	B	842	CLA	CMC-C2C	-2.11	1.46	1.50
14	A	839	CLA	CHC-C1C	2.11	1.42	1.38
14	B	808	CLA	CMD-C2D	-2.11	1.46	1.50
14	A	831	CLA	CMC-C2C	-2.10	1.46	1.50
14	B	827	CLA	CMC-C2C	-2.10	1.46	1.50
14	A	829	CLA	CMC-C2C	-2.10	1.46	1.50
14	A	832	CLA	CMC-C2C	-2.10	1.46	1.50
14	A	816	CLA	CMC-C2C	-2.10	1.46	1.50
14	A	814	CLA	CMB-C2B	-2.10	1.46	1.50
14	A	827	CLA	CHC-C1C	2.10	1.42	1.38
14	A	827	CLA	CMB-C2B	-2.10	1.46	1.50
14	A	806	CLA	CMC-C2C	-2.10	1.46	1.50
14	B	829	CLA	MG-NB	-2.10	2.01	2.05
14	A	833	CLA	CHC-C1C	2.10	1.42	1.38
14	L	205	CLA	MG-NB	-2.10	2.01	2.05
14	A	837	CLA	CMB-C2B	-2.10	1.46	1.50
14	L	204	CLA	MG-NB	-2.10	2.01	2.05
14	B	835	CLA	CMC-C2C	-2.10	1.46	1.50
14	A	829	CLA	CMB-C2B	-2.10	1.46	1.50
16	A	847	BCR	C33-C5	-2.10	1.47	1.50
14	B	807	CLA	CMC-C2C	-2.10	1.46	1.50
14	B	808	CLA	MG-NB	-2.10	2.01	2.05
14	A	840	CLA	CMB-C2B	-2.10	1.46	1.50
14	A	854	CLA	CMC-C2C	-2.09	1.46	1.50
14	B	839	CLA	CMC-C2C	-2.09	1.46	1.50
14	B	808	CLA	CHC-C1C	2.09	1.42	1.38
14	B	835	CLA	MG-NB	-2.09	2.01	2.05
14	A	832	CLA	CHC-C1C	2.09	1.42	1.38
14	A	830	CLA	CMC-C2C	-2.09	1.46	1.50
14	A	843	CLA	MG-NB	-2.09	2.01	2.05
14	B	816	CLA	CMC-C2C	-2.09	1.46	1.50
14	B	804	CLA	CMB-C2B	-2.09	1.46	1.50
14	B	829	CLA	CMC-C2C	-2.09	1.46	1.50
14	A	812	CLA	CMB-C2B	-2.09	1.46	1.50
16	A	847	BCR	C38-C26	-2.09	1.47	1.50
14	B	827	CLA	CHC-C1C	2.09	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	813	CLA	CMC-C2C	-2.09	1.46	1.50
14	B	837	CLA	CMD-C2D	-2.09	1.46	1.50
14	J	102	CLA	MG-NB	-2.08	2.01	2.05
14	A	842	CLA	MG-NB	-2.08	2.01	2.05
14	B	812	CLA	CMD-C2D	-2.08	1.46	1.50
14	A	822	CLA	CHC-C1C	2.08	1.42	1.38
14	B	813	CLA	CMB-C2B	-2.08	1.46	1.50
14	F	201	CLA	CMB-C2B	-2.08	1.46	1.50
14	B	821	CLA	CMB-C2B	-2.08	1.46	1.50
14	B	830	CLA	C3B-C4B	2.08	1.48	1.42
14	B	816	CLA	CMB-C2B	-2.08	1.46	1.50
14	X	1701	CLA	CMD-C2D	-2.08	1.46	1.50
14	L	206	CLA	CMC-C2C	-2.08	1.46	1.50
14	A	839	CLA	CMB-C2B	-2.08	1.46	1.50
16	B	845	BCR	C33-C5	-2.08	1.47	1.50
14	B	801	CLA	CMC-C2C	-2.07	1.46	1.50
14	A	825	CLA	CMD-C2D	-2.07	1.46	1.50
14	F	203	CLA	CMC-C2C	-2.07	1.46	1.50
14	B	819	CLA	CHC-C1C	2.07	1.42	1.38
14	A	819	CLA	MG-NB	-2.07	2.01	2.05
14	F	201	CLA	MG-NB	-2.07	2.01	2.05
14	B	814	CLA	CMB-C2B	-2.07	1.46	1.50
14	B	804	CLA	C3B-C4B	2.07	1.48	1.42
14	A	838	CLA	MG-NB	-2.07	2.01	2.05
14	B	801	CLA	CHC-C1C	2.07	1.42	1.38
14	K	102	CLA	MG-NB	-2.07	2.01	2.05
14	A	840	CLA	MG-NB	-2.07	2.01	2.05
14	B	832	CLA	CMB-C2B	-2.07	1.46	1.50
14	B	801	CLA	MG-NB	-2.07	2.01	2.05
14	B	838	CLA	MG-NB	-2.07	2.01	2.05
14	B	834	CLA	CMC-C2C	-2.07	1.46	1.50
14	M	102	CLA	CMD-C2D	-2.07	1.46	1.50
14	A	833	CLA	CMC-C2C	-2.07	1.46	1.50
14	B	826	CLA	MG-NB	-2.06	2.01	2.05
14	A	803	CLA	MG-NB	-2.06	2.01	2.05
14	B	816	CLA	MG-NB	-2.06	2.01	2.05
14	L	206	CLA	CMB-C2B	-2.06	1.46	1.50
14	B	806	CLA	CMB-C2B	-2.06	1.46	1.50
14	A	818	CLA	CMC-C2C	-2.06	1.46	1.50
14	A	854	CLA	CHC-C1C	2.06	1.42	1.38
14	B	806	CLA	MG-NB	-2.06	2.01	2.05
16	B	853	BCR	C33-C5	-2.06	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	851	BCR	C33-C5	-2.06	1.47	1.50
14	A	810	CLA	CMC-C2C	-2.06	1.46	1.50
14	K	101	CLA	MG-NB	-2.06	2.01	2.05
14	A	837	CLA	CMD-C2D	-2.06	1.46	1.50
14	A	854	CLA	CMB-C2B	-2.06	1.46	1.50
14	B	809	CLA	CMC-C2C	-2.06	1.46	1.50
14	B	813	CLA	MG-NB	-2.06	2.01	2.05
14	B	812	CLA	CHC-C1C	2.05	1.42	1.38
14	B	817	CLA	MG-NB	-2.05	2.01	2.05
14	A	817	CLA	CMC-C2C	-2.05	1.46	1.50
14	B	840	CLA	CMB-C2B	-2.05	1.46	1.50
16	A	845	BCR	C33-C5	-2.05	1.47	1.50
14	B	819	CLA	CMC-C2C	-2.05	1.46	1.50
14	B	832	CLA	MG-NB	-2.05	2.01	2.05
14	B	822	CLA	CMC-C2C	-2.05	1.46	1.50
14	B	841	CLA	CMB-C2B	-2.05	1.46	1.50
14	A	816	CLA	CHC-C1C	2.05	1.42	1.38
14	B	811	CLA	CMC-C2C	-2.05	1.46	1.50
14	B	823	CLA	CMB-C2B	-2.05	1.46	1.50
20	B	850	LMG	O7-C8	-2.05	1.41	1.46
14	A	827	CLA	CMC-C2C	-2.05	1.46	1.50
14	B	833	CLA	CMB-C2B	-2.05	1.46	1.50
14	K	102	CLA	CMD-C2D	-2.05	1.46	1.50
14	A	814	CLA	MG-NB	-2.05	2.01	2.05
14	B	808	CLA	CMB-C2B	-2.05	1.46	1.50
14	B	821	CLA	MG-NB	-2.05	2.01	2.05
14	A	807	CLA	CMB-C2B	-2.05	1.46	1.50
14	A	841	CLA	CMC-C2C	-2.05	1.46	1.50
16	A	849	BCR	C33-C5	-2.05	1.47	1.50
14	A	804	CLA	CMC-C2C	-2.05	1.46	1.50
14	B	834	CLA	MG-NB	-2.05	2.01	2.05
14	B	842	CLA	MG-NB	-2.05	2.01	2.05
14	A	807	CLA	CHC-C1C	2.05	1.42	1.38
14	A	835	CLA	CHC-C1C	2.05	1.42	1.38
14	A	835	CLA	MG-NB	-2.04	2.01	2.05
14	B	835	CLA	CHC-C1C	2.04	1.42	1.38
14	A	823	CLA	MG-NB	-2.04	2.01	2.05
14	B	836	CLA	MG-NB	-2.04	2.01	2.05
16	F	202	BCR	C38-C26	-2.04	1.47	1.50
14	A	843	CLA	CMB-C2B	-2.04	1.46	1.50
14	B	818	CLA	CHC-C1C	2.04	1.42	1.38
14	F	203	CLA	MG-NB	-2.04	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	J	104	BCR	C33-C5	-2.04	1.47	1.50
14	A	841	CLA	MG-NB	-2.04	2.01	2.05
14	A	834	CLA	CMC-C2C	-2.04	1.46	1.50
14	A	830	CLA	CHC-C1C	2.04	1.42	1.38
14	A	825	CLA	CMC-C2C	-2.04	1.46	1.50
14	X	1701	CLA	CMB-C2B	-2.04	1.46	1.50
14	X	1701	CLA	MG-NB	-2.04	2.01	2.05
14	A	811	CLA	CMC-C2C	-2.03	1.46	1.50
14	A	837	CLA	CMC-C2C	-2.03	1.46	1.50
14	J	101	CLA	CMB-C2B	-2.03	1.46	1.50
14	B	839	CLA	MG-NB	-2.03	2.01	2.05
14	B	821	CLA	CMC-C2C	-2.03	1.46	1.50
14	B	823	CLA	CMC-C2C	-2.03	1.46	1.50
14	B	840	CLA	MG-NB	-2.03	2.01	2.05
14	A	829	CLA	MG-NB	-2.03	2.01	2.05
14	A	837	CLA	MG-NB	-2.03	2.01	2.05
14	M	102	CLA	MG-NB	-2.03	2.01	2.05
14	A	838	CLA	CHC-C1C	2.03	1.42	1.38
14	A	809	CLA	CMC-C2C	-2.03	1.46	1.50
14	B	818	CLA	MG-NB	-2.02	2.01	2.05
14	A	831	CLA	C3B-C4B	2.02	1.48	1.42
14	B	831	CLA	CMC-C2C	-2.02	1.46	1.50
14	L	205	CLA	CMC-C2C	-2.02	1.46	1.50
14	B	828	CLA	CMD-C2D	-2.02	1.46	1.50
16	A	848	BCR	C33-C5	-2.02	1.47	1.50
16	L	202	BCR	C38-C26	-2.02	1.47	1.50
14	B	818	CLA	CMC-C2C	-2.02	1.46	1.50
14	B	841	CLA	CMC-C2C	-2.02	1.46	1.50
17	B	851	LHG	P-O6	2.02	1.67	1.59
16	F	205	BCR	C33-C5	-2.02	1.47	1.50
14	J	101	CLA	CMC-C2C	-2.02	1.46	1.50
14	A	839	CLA	CMC-C2C	-2.02	1.46	1.50
14	K	101	CLA	CMC-C2C	-2.02	1.46	1.50
16	I	103	BCR	C33-C5	-2.02	1.47	1.50
14	A	823	CLA	CMC-C2C	-2.02	1.46	1.50
14	A	825	CLA	CMB-C2B	-2.02	1.46	1.50
14	A	806	CLA	C3B-C4B	2.02	1.48	1.42
14	K	102	CLA	CMC-C2C	-2.01	1.46	1.50
14	A	854	CLA	MG-NB	-2.01	2.01	2.05
14	A	827	CLA	MG-NB	-2.01	2.01	2.05
14	A	802	CLA	CMC-C2C	-2.01	1.46	1.50
14	F	204	CLA	CMB-C2B	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	815	CLA	CMC-C2C	-2.01	1.46	1.50
14	B	841	CLA	MG-NB	-2.01	2.01	2.05
14	A	821	CLA	MG-NB	-2.01	2.01	2.05
14	A	802	CLA	CMB-C2B	-2.01	1.46	1.50
14	J	101	CLA	MG-NB	-2.01	2.01	2.05
16	B	848	BCR	C33-C5	-2.01	1.47	1.50
14	B	839	CLA	CHC-C1C	2.01	1.42	1.38
14	M	102	CLA	CMB-C2B	-2.00	1.46	1.50
14	A	807	CLA	CMC-C2C	-2.00	1.46	1.50
14	A	804	CLA	C3B-C4B	2.00	1.48	1.42
14	A	820	CLA	MG-NB	-2.00	2.01	2.05
14	B	833	CLA	MG-NB	-2.00	2.01	2.05

All (724) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	835	CLA	C4A-NA-C1A	7.41	110.06	106.68
14	L	201	CLA	C4A-NA-C1A	7.29	110.01	106.68
14	B	805	CLA	C4A-NA-C1A	7.02	109.88	106.68
14	A	837	CLA	C4A-NA-C1A	6.94	109.85	106.68
14	B	839	CLA	C4A-NA-C1A	6.93	109.84	106.68
14	B	801	CLA	C4A-NA-C1A	6.92	109.83	106.68
14	A	831	CLA	C4A-NA-C1A	6.87	109.81	106.68
14	A	816	CLA	C4A-NA-C1A	6.85	109.81	106.68
14	B	804	CLA	C4A-NA-C1A	6.84	109.80	106.68
14	A	841	CLA	C4A-NA-C1A	6.83	109.80	106.68
14	B	806	CLA	C4A-NA-C1A	6.83	109.80	106.68
14	B	837	CLA	C4A-NA-C1A	6.82	109.79	106.68
13	A	801	CL0	C1B-CHB-C4A	6.82	125.71	121.32
14	A	817	CLA	C4A-NA-C1A	6.81	109.79	106.68
14	A	843	CLA	C4A-NA-C1A	6.74	109.75	106.68
14	A	804	CLA	C4A-NA-C1A	6.73	109.75	106.68
14	F	203	CLA	C4A-NA-C1A	6.73	109.75	106.68
14	B	835	CLA	C4A-NA-C1A	6.71	109.74	106.68
14	A	834	CLA	C4A-NA-C1A	6.71	109.74	106.68
14	A	809	CLA	C4A-NA-C1A	6.70	109.73	106.68
14	B	838	CLA	C4A-NA-C1A	6.67	109.72	106.68
14	B	808	CLA	C4A-NA-C1A	6.65	109.71	106.68
14	A	842	CLA	C4A-NA-C1A	6.61	109.69	106.68
14	A	828	CLA	C4A-NA-C1A	6.60	109.69	106.68
14	B	816	CLA	C4A-NA-C1A	6.59	109.69	106.68
14	A	827	CLA	C4A-NA-C1A	6.59	109.68	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	811	CLA	C4A-NA-C1A	6.57	109.68	106.68
14	A	806	CLA	C4A-NA-C1A	6.57	109.68	106.68
14	L	205	CLA	C4A-NA-C1A	6.57	109.68	106.68
14	A	810	CLA	C4A-NA-C1A	6.56	109.67	106.68
14	B	820	CLA	C4A-NA-C1A	6.56	109.67	106.68
14	A	815	CLA	C4A-NA-C1A	6.56	109.67	106.68
14	B	842	CLA	C4A-NA-C1A	6.55	109.67	106.68
14	A	812	CLA	C4A-NA-C1A	6.55	109.67	106.68
14	B	841	CLA	C4A-NA-C1A	6.55	109.67	106.68
14	B	813	CLA	C4A-NA-C1A	6.55	109.67	106.68
14	A	807	CLA	C4A-NA-C1A	6.54	109.66	106.68
14	B	822	CLA	C4A-NA-C1A	6.54	109.66	106.68
14	B	823	CLA	C4A-NA-C1A	6.52	109.65	106.68
14	B	818	CLA	C4A-NA-C1A	6.51	109.65	106.68
14	B	809	CLA	C4A-NA-C1A	6.50	109.64	106.68
14	B	815	CLA	C4A-NA-C1A	6.49	109.64	106.68
14	A	820	CLA	C4A-NA-C1A	6.48	109.64	106.68
14	J	101	CLA	C4A-NA-C1A	6.48	109.64	106.68
14	B	807	CLA	C4A-NA-C1A	6.47	109.63	106.68
14	A	823	CLA	C4A-NA-C1A	6.47	109.63	106.68
14	B	833	CLA	C4A-NA-C1A	6.47	109.63	106.68
14	A	802	CLA	C4A-NA-C1A	6.46	109.62	106.68
14	A	836	CLA	C4A-NA-C1A	6.44	109.62	106.68
14	A	818	CLA	C4A-NA-C1A	6.42	109.61	106.68
14	B	824	CLA	C4A-NA-C1A	6.42	109.61	106.68
14	B	834	CLA	C4A-NA-C1A	6.42	109.61	106.68
14	A	838	CLA	C4A-NA-C1A	6.42	109.61	106.68
14	A	805	CLA	C4A-NA-C1A	6.41	109.60	106.68
14	A	840	CLA	C4A-NA-C1A	6.40	109.60	106.68
14	A	825	CLA	C4A-NA-C1A	6.39	109.59	106.68
14	K	101	CLA	C4A-NA-C1A	6.39	109.59	106.68
14	B	840	CLA	C4A-NA-C1A	6.39	109.59	106.68
14	A	839	CLA	C4A-NA-C1A	6.38	109.59	106.68
14	A	814	CLA	C4A-NA-C1A	6.36	109.58	106.68
14	B	812	CLA	C4A-NA-C1A	6.35	109.58	106.68
14	A	854	CLA	C4A-NA-C1A	6.33	109.57	106.68
14	B	830	CLA	C4A-NA-C1A	6.30	109.55	106.68
14	A	808	CLA	C4A-NA-C1A	6.28	109.55	106.68
14	M	102	CLA	C4A-NA-C1A	6.27	109.54	106.68
14	A	832	CLA	C4A-NA-C1A	6.24	109.53	106.68
14	F	201	CLA	C4A-NA-C1A	6.24	109.52	106.68
14	B	827	CLA	C4A-NA-C1A	6.22	109.52	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	822	CLA	C4A-NA-C1A	6.21	109.51	106.68
14	B	832	CLA	C4A-NA-C1A	6.21	109.51	106.68
14	F	204	CLA	C4A-NA-C1A	6.21	109.51	106.68
14	K	102	CLA	C4A-NA-C1A	6.19	109.50	106.68
14	L	206	CLA	C4A-NA-C1A	6.19	109.50	106.68
14	B	826	CLA	C4A-NA-C1A	6.18	109.50	106.68
14	A	826	CLA	C4A-NA-C1A	6.18	109.50	106.68
14	A	829	CLA	C4A-NA-C1A	6.17	109.49	106.68
14	A	833	CLA	C4A-NA-C1A	6.16	109.49	106.68
14	B	825	CLA	C4A-NA-C1A	6.15	109.49	106.68
14	A	830	CLA	C4A-NA-C1A	6.15	109.49	106.68
14	B	821	CLA	C4A-NA-C1A	6.15	109.48	106.68
14	J	102	CLA	C4A-NA-C1A	6.12	109.47	106.68
14	B	831	CLA	C4A-NA-C1A	6.10	109.46	106.68
14	A	824	CLA	C4A-NA-C1A	6.09	109.46	106.68
14	A	821	CLA	C4A-NA-C1A	6.08	109.45	106.68
14	B	829	CLA	C4A-NA-C1A	6.07	109.45	106.68
14	B	836	CLA	C4A-NA-C1A	6.07	109.45	106.68
14	B	819	CLA	C4A-NA-C1A	6.06	109.44	106.68
14	B	814	CLA	C4A-NA-C1A	6.06	109.44	106.68
14	B	810	CLA	C4A-NA-C1A	5.99	109.41	106.68
14	X	1701	CLA	C4A-NA-C1A	5.99	109.41	106.68
14	A	811	CLA	C4A-NA-C1A	5.94	109.39	106.68
14	B	828	CLA	C4A-NA-C1A	5.87	109.36	106.68
14	B	817	CLA	C4A-NA-C1A	5.87	109.36	106.68
14	A	813	CLA	C4A-NA-C1A	5.77	109.31	106.68
14	L	204	CLA	C4A-NA-C1A	5.75	109.30	106.68
14	A	803	CLA	C4A-NA-C1A	5.64	109.25	106.68
14	A	819	CLA	C4A-NA-C1A	5.63	109.25	106.68
14	L	204	CLA	CAC-C3C-C4C	4.86	131.11	124.79
17	A	853	LHG	O4-P-O5	4.50	133.37	112.44
17	A	852	LHG	O4-P-O5	4.47	133.23	112.44
17	M	101	LHG	O4-P-O5	4.45	133.12	112.44
17	I	102	LHG	O4-P-O5	4.43	133.05	112.44
16	A	845	BCR	C2-C1-C6	4.42	116.86	110.44
17	B	851	LHG	O4-P-O5	4.41	132.96	112.44
14	B	814	CLA	CAC-C3C-C4C	4.26	130.33	124.79
16	A	851	BCR	C15-C14-C13	-3.94	121.75	127.28
14	B	818	CLA	C4-C3-C5	3.85	121.92	115.23
16	B	848	BCR	C15-C16-C17	-3.72	115.91	123.52
16	A	850	BCR	C2-C1-C6	3.70	115.81	110.44
14	B	826	CLA	O2D-CGD-O1D	-3.65	116.75	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	839	CLA	O2D-CGD-O1D	-3.64	116.75	123.85
14	A	854	CLA	C4-C3-C5	3.60	121.48	115.23
14	B	830	CLA	O2D-CGD-O1D	-3.59	116.87	123.85
16	F	205	BCR	C2-C1-C6	3.58	115.64	110.44
13	A	801	CL0	C4D-CHA-CBD	-3.57	105.37	108.97
14	A	813	CLA	C3B-C4B-NB	-3.53	107.38	110.53
14	X	1701	CLA	O2D-CGD-O1D	-3.49	117.06	123.85
14	A	854	CLA	O2D-CGD-O1D	-3.47	117.10	123.85
16	A	847	BCR	C15-C14-C13	-3.43	122.47	127.28
14	B	810	CLA	C3B-C4B-NB	-3.42	107.48	110.53
16	B	848	BCR	C15-C14-C13	-3.41	122.50	127.28
14	B	840	CLA	O2D-CGD-O1D	-3.41	117.22	123.85
14	B	827	CLA	O2D-CGD-O1D	-3.38	117.26	123.85
14	B	817	CLA	O2D-CGD-O1D	-3.38	117.27	123.85
16	L	202	BCR	C15-C16-C17	-3.36	116.65	123.52
14	A	836	CLA	C3B-C4B-NB	-3.33	107.56	110.53
14	B	836	CLA	C3B-C4B-NB	-3.28	107.60	110.53
16	F	202	BCR	C2-C1-C6	3.27	115.20	110.44
14	B	829	CLA	C3B-C4B-NB	-3.27	107.61	110.53
14	B	825	CLA	O2D-CGD-O1D	-3.27	117.49	123.85
16	B	844	BCR	C24-C23-C22	-3.27	121.40	126.23
14	B	812	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
14	B	816	CLA	O2D-CGD-O1D	-3.25	117.51	123.85
16	B	852	BCR	C11-C10-C9	-3.24	122.73	127.28
16	K	103	BCR	C2-C1-C6	3.22	115.12	110.44
14	A	835	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
14	L	204	CLA	C3B-C4B-NB	-3.20	107.67	110.53
14	A	804	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
14	B	833	CLA	O2D-CGD-O1D	-3.20	117.63	123.85
14	B	807	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
14	B	817	CLA	C3B-C4B-NB	-3.19	107.69	110.53
16	J	104	BCR	C15-C16-C17	-3.19	117.00	123.52
14	B	820	CLA	O2D-CGD-O1D	-3.18	117.65	123.85
14	F	201	CLA	C3B-C4B-NB	-3.18	107.69	110.53
14	B	814	CLA	C1-C2-C3	-3.18	120.99	126.20
14	B	809	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
14	B	813	CLA	C3B-C4B-NB	-3.16	107.71	110.53
14	L	205	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
14	A	828	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
14	B	835	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
14	B	830	CLA	O2D-CGD-CBD	3.15	116.74	111.23
14	B	813	CLA	O2D-CGD-O1D	-3.15	117.72	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	819	CLA	C3B-C4B-NB	-3.14	107.72	110.53
16	L	202	BCR	C2-C1-C6	3.14	115.00	110.44
14	K	102	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
16	J	104	BCR	C33-C5-C6	-3.13	121.07	124.48
14	A	811	CLA	C3B-C4B-NB	-3.12	107.75	110.53
14	A	805	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
14	A	820	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
14	A	803	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
14	B	805	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
14	A	839	CLA	C3B-C4B-NB	-3.10	107.76	110.53
14	A	826	CLA	O2D-CGD-O1D	-3.09	117.82	123.85
14	A	825	CLA	C3B-C4B-NB	-3.08	107.78	110.53
14	A	831	CLA	O2D-CGD-O1D	-3.07	117.86	123.85
14	A	840	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
14	A	809	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
14	B	810	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
16	A	849	BCR	C33-C5-C6	-3.04	121.16	124.48
14	A	832	CLA	C3B-C4B-NB	-3.04	107.81	110.53
14	K	101	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
14	B	821	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
14	B	815	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
14	B	827	CLA	C3B-C4B-NB	-3.03	107.83	110.53
14	A	816	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
14	B	839	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
16	K	103	BCR	C15-C16-C17	-3.02	117.33	123.52
14	B	801	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
14	B	807	CLA	C3B-C4B-NB	-3.02	107.83	110.53
14	L	204	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
14	B	838	CLA	C3B-C4B-NB	-3.01	107.84	110.53
14	A	841	CLA	C3B-C4B-NB	-3.01	107.84	110.53
14	B	823	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
14	A	827	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
14	A	802	CLA	C3B-C4B-NB	-3.01	107.84	110.53
14	B	832	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
14	B	826	CLA	CAA-C2A-C1A	-3.00	102.14	111.97
14	X	1701	CLA	C3B-C4B-NB	-3.00	107.86	110.53
14	M	102	CLA	C3A-C2A-C1A	-2.99	103.24	106.30
14	A	818	CLA	C3B-C4B-NB	-2.98	107.87	110.53
14	F	204	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
16	A	849	BCR	C15-C16-C17	-2.98	117.43	123.52
14	A	821	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
14	B	833	CLA	C3B-C4B-NB	-2.97	107.88	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	842	CLA	C3B-C4B-NB	-2.97	107.88	110.53
16	B	847	BCR	C30-C25-C26	-2.97	118.58	122.64
16	A	850	BCR	C15-C16-C17	-2.96	117.45	123.52
14	A	829	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
14	B	808	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
14	L	205	CLA	C3B-C4B-NB	-2.95	107.90	110.53
14	B	801	CLA	C3B-C4B-NB	-2.95	107.90	110.53
14	B	806	CLA	C3B-C4B-NB	-2.95	107.90	110.53
13	A	801	CL0	O2D-CGD-O1D	-2.94	118.13	123.85
14	A	808	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
14	F	204	CLA	C3B-C4B-NB	-2.93	107.91	110.53
14	B	819	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
14	A	828	CLA	C3B-C4B-NB	-2.93	107.92	110.53
16	A	847	BCR	C15-C16-C17	-2.92	117.53	123.52
14	B	831	CLA	C3B-C4B-NB	-2.92	107.92	110.53
16	I	103	BCR	C24-C23-C22	-2.92	121.91	126.23
14	B	841	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
14	A	842	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
14	A	835	CLA	CHB-C4A-NA	2.92	128.61	124.40
14	K	102	CLA	C3B-C4B-NB	-2.91	107.93	110.53
14	A	833	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
14	B	821	CLA	C3B-C4B-NB	-2.91	107.94	110.53
14	A	834	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
14	A	840	CLA	C3B-C4B-NB	-2.90	107.94	110.53
14	F	203	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
16	J	104	BCR	C15-C14-C13	-2.89	123.22	127.28
14	A	815	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
14	A	833	CLA	C3B-C4B-NB	-2.89	107.95	110.53
14	B	815	CLA	C3B-C4B-NB	-2.89	107.95	110.53
14	K	101	CLA	C3B-C4B-NB	-2.89	107.95	110.53
14	B	829	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
13	A	801	CL0	C3D-C4D-CHA	2.88	112.91	108.54
14	A	825	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
14	J	101	CLA	C3B-C4B-NB	-2.88	107.96	110.53
14	B	837	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
14	A	814	CLA	C3B-C4B-NB	-2.87	107.97	110.53
14	A	822	CLA	C3B-C4B-NB	-2.87	107.97	110.53
14	L	206	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
16	F	205	BCR	C16-C15-C14	-2.86	117.66	123.52
16	J	103	BCR	C7-C8-C9	-2.86	122.01	126.23
14	A	823	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
16	A	850	BCR	C2-C3-C4	2.86	117.56	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	853	BCR	C27-C26-C25	2.85	126.56	122.70
14	A	811	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
13	A	801	CL0	C1C-CHC-C4B	2.85	126.27	116.07
14	B	841	CLA	C3B-C4B-NB	-2.85	107.99	110.53
14	A	806	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
14	M	102	CLA	C3B-C4B-NB	-2.84	107.99	110.53
14	B	804	CLA	C3B-C4B-NB	-2.84	107.99	110.53
14	A	817	CLA	C3B-C4B-NB	-2.84	107.99	110.53
14	B	814	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
16	L	207	BCR	C15-C16-C17	-2.83	117.72	123.52
14	B	814	CLA	C3B-C4B-NB	-2.83	108.00	110.53
14	A	838	CLA	CHB-C4A-NA	2.83	128.49	124.40
14	A	824	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
14	A	810	CLA	C3B-C4B-NB	-2.83	108.00	110.53
14	A	826	CLA	C3B-C4B-NB	-2.83	108.00	110.53
14	A	810	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
14	A	841	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
14	A	822	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
14	B	822	CLA	C3B-C4B-NB	-2.82	108.01	110.53
16	A	847	BCR	C33-C5-C6	-2.82	121.41	124.48
14	B	834	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
16	I	103	BCR	C2-C1-C6	2.81	114.53	110.44
14	B	818	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
14	A	805	CLA	C3B-C4B-NB	-2.81	108.02	110.53
16	A	850	BCR	C28-C27-C26	-2.81	109.04	114.06
14	J	102	CLA	C3B-C4B-NB	-2.81	108.02	110.53
16	B	846	BCR	C15-C16-C17	-2.81	117.78	123.52
16	A	846	BCR	C33-C5-C6	-2.81	121.42	124.48
16	A	848	BCR	C15-C16-C17	-2.80	117.78	123.52
14	J	101	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
14	A	838	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
14	B	842	CLA	C3B-C4B-NB	-2.79	108.03	110.53
14	B	806	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
14	B	810	CLA	O2A-CGA-O1A	-2.79	116.66	123.63
14	A	812	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
14	L	201	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
16	B	852	BCR	C15-C16-C17	-2.78	117.84	123.52
14	A	835	CLA	C3B-C4B-NB	-2.77	108.05	110.53
14	B	835	CLA	C3B-C4B-NB	-2.77	108.06	110.53
14	A	819	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
14	A	839	CLA	O2D-CGD-CBD	2.77	116.07	111.23
14	A	812	CLA	C3B-C4B-NB	-2.77	108.06	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	830	CLA	C3B-C4B-NB	-2.76	108.06	110.53
14	B	812	CLA	C3B-C4B-NB	-2.76	108.06	110.53
14	B	805	CLA	CHB-C4A-NA	2.76	128.39	124.40
14	A	830	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
14	A	814	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
14	A	813	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
16	A	847	BCR	C27-C26-C25	2.76	126.43	122.70
16	B	853	BCR	C33-C5-C6	-2.75	121.48	124.48
16	A	845	BCR	C24-C23-C22	-2.75	122.16	126.23
17	B	851	LHG	O8-C23-C24	2.75	120.22	111.83
16	B	844	BCR	C33-C5-C6	-2.75	121.48	124.48
14	B	828	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
14	B	837	CLA	C3B-C4B-NB	-2.75	108.08	110.53
16	B	845	BCR	C11-C10-C9	-2.74	123.43	127.28
14	A	809	CLA	C3B-C4B-NB	-2.74	108.08	110.53
16	J	104	BCR	C29-C30-C25	2.74	114.42	110.44
16	B	844	BCR	C15-C16-C17	-2.74	117.91	123.52
14	A	823	CLA	C3B-C4B-NB	-2.74	108.09	110.53
14	B	831	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
14	F	201	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
14	B	816	CLA	C3B-C4B-NB	-2.74	108.09	110.53
16	B	846	BCR	C27-C26-C25	2.73	126.40	122.70
14	L	204	CLA	CAC-C3C-C2C	-2.73	122.54	127.56
14	A	802	CLA	CHB-C4A-NA	2.73	128.34	124.40
14	L	201	CLA	CHB-C4A-NA	2.73	128.34	124.40
14	B	842	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
16	B	846	BCR	C24-C23-C22	-2.73	122.20	126.23
14	B	826	CLA	O2D-CGD-CBD	2.73	116.00	111.23
20	B	850	LMG	O6-C1-O1	-2.73	103.60	110.04
14	A	837	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
14	B	836	CLA	O2D-CGD-O1D	-2.72	118.54	123.85
14	A	818	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
14	A	803	CLA	C3B-C4B-NB	-2.72	108.10	110.53
16	I	103	BCR	C15-C16-C17	-2.72	117.95	123.52
14	A	802	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
14	B	838	CLA	O2D-CGD-O1D	-2.71	118.56	123.85
16	B	847	BCR	C27-C26-C25	2.71	126.37	122.70
14	A	807	CLA	C3B-C4B-NB	-2.71	108.11	110.53
14	A	817	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
14	B	804	CLA	O2D-CGD-O1D	-2.70	118.58	123.85
14	A	820	CLA	C3B-C4B-NB	-2.70	108.12	110.53
14	B	826	CLA	C3B-C4B-NB	-2.70	108.12	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	836	CLA	CHB-C4A-NA	2.70	128.29	124.40
14	A	837	CLA	C3B-C4B-NB	-2.70	108.12	110.53
14	B	825	CLA	C3B-C4B-NB	-2.70	108.12	110.53
14	A	815	CLA	C3B-C4B-NB	-2.69	108.13	110.53
16	J	103	BCR	C33-C5-C6	-2.68	121.56	124.48
14	A	816	CLA	C3B-C4B-NB	-2.68	108.14	110.53
14	A	836	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
14	A	827	CLA	C3B-C4B-NB	-2.67	108.14	110.53
14	L	201	CLA	C3B-C4B-NB	-2.67	108.15	110.53
14	A	808	CLA	C3B-C4B-NB	-2.67	108.15	110.53
14	B	806	CLA	CHB-C4A-NA	2.67	128.25	124.40
16	B	845	BCR	C33-C5-C6	-2.66	121.58	124.48
14	F	203	CLA	C3B-C4B-NB	-2.66	108.16	110.53
14	A	834	CLA	CHB-C4A-NA	2.66	128.24	124.40
13	A	801	CL0	CMD-C2D-C3D	2.66	129.99	124.68
16	F	202	BCR	C15-C16-C17	-2.65	118.09	123.52
16	A	850	BCR	C24-C23-C22	-2.65	122.32	126.23
14	A	835	CLA	O2D-CGD-CBD	2.65	115.86	111.23
16	B	849	BCR	C27-C26-C25	2.64	126.28	122.70
14	A	824	CLA	C3B-C4B-NB	-2.64	108.17	110.53
14	A	806	CLA	C3B-C4B-NB	-2.64	108.18	110.53
14	B	839	CLA	C3B-C4B-NB	-2.63	108.18	110.53
16	L	207	BCR	C24-C23-C22	-2.63	122.34	126.23
14	A	843	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
16	B	847	BCR	C24-C23-C22	-2.63	122.34	126.23
16	F	202	BCR	C33-C5-C6	-2.63	121.61	124.48
16	B	852	BCR	C7-C8-C9	-2.63	122.35	126.23
14	B	824	CLA	C3B-C4B-NB	-2.62	108.19	110.53
14	B	808	CLA	CHB-C4A-NA	2.62	128.18	124.40
17	A	852	LHG	O8-C23-C24	2.62	119.82	111.83
14	B	817	CLA	O2D-CGD-CBD	2.62	115.81	111.23
16	B	848	BCR	C27-C26-C25	2.61	126.23	122.70
14	A	804	CLA	C3B-C4B-NB	-2.61	108.20	110.53
14	B	820	CLA	C3B-C4B-NB	-2.61	108.20	110.53
14	B	811	CLA	CHB-C4A-NA	2.60	128.15	124.40
14	B	808	CLA	C3B-C4B-NB	-2.60	108.21	110.53
16	L	202	BCR	C8-C7-C6	-2.60	120.06	127.00
14	F	204	CLA	C1-C2-C3	-2.60	122.56	126.76
13	A	801	CL0	O2D-CGD-CBD	2.59	113.79	110.95
14	B	835	CLA	CHB-C4A-NA	2.59	128.14	124.40
14	B	832	CLA	C3B-C4B-NB	-2.59	108.22	110.53
14	A	843	CLA	C3B-C4B-NB	-2.58	108.22	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	850	BCR	C29-C30-C25	2.58	114.19	110.44
14	B	822	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
14	A	806	CLA	CHB-C4A-NA	2.58	128.12	124.40
14	A	814	CLA	CHB-C4A-NA	2.58	128.12	124.40
16	A	846	BCR	C27-C26-C25	2.57	126.17	122.70
16	J	103	BCR	C15-C14-C13	-2.57	123.68	127.28
14	B	811	CLA	C3B-C4B-NB	-2.56	108.25	110.53
13	A	801	CL0	C4C-CHD-C1D	2.56	125.21	116.07
14	F	203	CLA	CHB-C4A-NA	2.55	128.09	124.40
14	A	827	CLA	C1-C2-C3	-2.55	122.01	126.20
16	A	851	BCR	C15-C16-C17	-2.55	118.29	123.52
14	A	820	CLA	CHB-C4A-NA	2.55	128.09	124.40
14	A	827	CLA	CHB-C4A-NA	2.55	128.09	124.40
14	B	823	CLA	C3B-C4B-NB	-2.55	108.25	110.53
14	A	837	CLA	CHB-C4A-NA	2.55	128.08	124.40
17	A	853	LHG	O8-C23-C24	2.55	119.60	111.83
16	F	202	BCR	C27-C26-C25	2.55	126.14	122.70
17	I	102	LHG	O8-C23-C24	2.54	119.59	111.83
14	A	804	CLA	CHB-C4A-NA	2.54	128.07	124.40
14	A	807	CLA	CHB-C4A-NA	2.54	128.07	124.40
14	B	805	CLA	C3B-C4B-NB	-2.54	108.26	110.53
14	B	809	CLA	C3B-C4B-NB	-2.54	108.26	110.53
14	B	823	CLA	CHB-C4A-NA	2.53	128.05	124.40
14	A	822	CLA	CHB-C4A-NA	2.53	128.05	124.40
14	A	838	CLA	C3B-C4B-NB	-2.53	108.28	110.53
14	B	828	CLA	C3B-C4B-NB	-2.53	108.28	110.53
14	B	804	CLA	CHB-C4A-NA	2.52	128.04	124.40
14	B	810	CLA	C1-C2-C3	-2.52	122.06	126.20
14	A	839	CLA	CHB-C4A-NA	2.52	128.04	124.40
14	A	816	CLA	CHB-C4A-NA	2.52	128.04	124.40
16	B	852	BCR	C27-C26-C25	2.52	126.11	122.70
14	B	824	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
16	L	202	BCR	C15-C14-C13	-2.52	123.75	127.28
14	B	814	CLA	CHB-C4A-NA	2.51	128.03	124.40
16	J	103	BCR	C15-C16-C17	-2.51	118.38	123.52
14	A	827	CLA	CAA-C2A-C1A	-2.51	103.74	111.97
14	L	206	CLA	C3B-C4B-NB	-2.51	108.29	110.53
14	A	841	CLA	CHB-C4A-NA	2.51	128.02	124.40
14	B	834	CLA	C3B-C4B-NB	-2.51	108.29	110.53
14	B	816	CLA	CHB-C4A-NA	2.50	128.01	124.40
14	L	205	CLA	CHB-C4A-NA	2.50	128.01	124.40
16	B	852	BCR	C33-C5-C6	-2.50	121.75	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	807	CLA	CHB-C4A-NA	2.50	128.01	124.40
14	A	843	CLA	CHB-C4A-NA	2.50	128.01	124.40
14	A	810	CLA	O2A-CGA-O1A	-2.50	117.38	123.63
16	I	103	BCR	C33-C5-C6	-2.50	121.76	124.48
14	A	821	CLA	CHB-C4A-NA	2.50	128.00	124.40
14	B	824	CLA	CHB-C4A-NA	2.50	128.00	124.40
14	B	840	CLA	O2D-CGD-CBD	2.49	115.59	111.23
14	A	836	CLA	CHB-C4A-NA	2.49	128.00	124.40
14	A	831	CLA	CHB-C4A-NA	2.49	127.99	124.40
14	J	101	CLA	CHB-C4A-NA	2.49	127.99	124.40
14	A	812	CLA	CHB-C4A-NA	2.49	127.99	124.40
16	B	849	BCR	C33-C5-C6	-2.49	121.77	124.48
16	B	846	BCR	C33-C5-C6	-2.48	121.77	124.48
14	A	805	CLA	CHB-C4A-NA	2.48	127.98	124.40
14	A	809	CLA	CHB-C4A-NA	2.48	127.98	124.40
14	B	827	CLA	CHB-C4A-NA	2.48	127.98	124.40
14	A	829	CLA	C3B-C4B-NB	-2.48	108.32	110.53
14	L	204	CLA	CHB-C4A-NA	2.48	127.97	124.40
16	I	101	BCR	C15-C16-C17	-2.47	118.45	123.52
16	B	852	BCR	C38-C26-C25	-2.47	121.79	124.48
16	I	101	BCR	C16-C15-C14	-2.47	118.47	123.52
14	B	813	CLA	CHB-C4A-NA	2.46	127.96	124.40
16	I	101	BCR	C33-C5-C6	-2.46	121.80	124.48
14	A	833	CLA	CHB-C4A-NA	2.46	127.95	124.40
16	A	845	BCR	C15-C16-C17	-2.46	118.48	123.52
16	A	846	BCR	C15-C16-C17	-2.46	118.48	123.52
16	B	852	BCR	C15-C14-C13	-2.46	123.83	127.28
14	B	829	CLA	CHB-C4A-NA	2.46	127.95	124.40
16	F	205	BCR	C35-C13-C14	-2.46	118.83	122.82
16	I	101	BCR	C2-C1-C6	2.46	114.01	110.44
16	B	849	BCR	C15-C16-C17	-2.46	118.50	123.52
16	B	852	BCR	C2-C1-C6	2.45	114.00	110.44
14	B	842	CLA	CHB-C4A-NA	2.45	127.94	124.40
16	B	844	BCR	C27-C26-C25	2.45	126.02	122.70
14	B	811	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
14	B	840	CLA	C3B-C4B-NB	-2.45	108.34	110.53
14	X	1701	CLA	O2D-CGD-CBD	2.45	115.51	111.23
14	B	837	CLA	CHB-C4A-NA	2.45	127.93	124.40
16	A	851	BCR	C35-C13-C14	-2.44	118.86	122.82
14	B	815	CLA	CHB-C4A-NA	2.44	127.92	124.40
14	B	836	CLA	O2A-CGA-O1A	-2.44	117.52	123.63
14	B	838	CLA	CHB-C4A-NA	2.44	127.92	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	848	BCR	C27-C26-C25	2.44	126.00	122.70
14	A	830	CLA	CHB-C4A-NA	2.44	127.91	124.40
14	B	818	CLA	C3B-C4B-NB	-2.43	108.36	110.53
14	A	825	CLA	CHB-C4A-NA	2.43	127.91	124.40
14	B	828	CLA	O2A-CGA-O1A	-2.43	117.55	123.63
13	A	801	CL0	CHA-C1A-C2A	-2.43	127.61	133.31
16	B	847	BCR	C33-C5-C6	-2.43	121.84	124.48
16	I	101	BCR	C27-C26-C25	2.43	125.98	122.70
14	B	839	CLA	CHB-C4A-NA	2.42	127.90	124.40
16	F	205	BCR	C38-C26-C25	-2.42	121.84	124.48
16	B	845	BCR	C15-C16-C17	-2.42	118.56	123.52
16	B	846	BCR	C38-C26-C25	-2.42	121.84	124.48
14	A	832	CLA	CHB-C4A-NA	2.42	127.89	124.40
14	L	205	CLA	CAC-C3C-C4C	2.42	127.94	124.79
16	K	103	BCR	C15-C14-C13	-2.42	123.89	127.28
14	A	829	CLA	CMB-C2B-C1B	-2.41	121.75	125.42
14	B	801	CLA	CHB-C4A-NA	2.41	127.88	124.40
14	B	826	CLA	C1-C2-C3	-2.41	122.25	126.20
16	B	846	BCR	C7-C8-C9	-2.41	122.67	126.23
14	A	821	CLA	C3B-C4B-NB	-2.41	108.38	110.53
14	A	838	CLA	CAC-C3C-C4C	2.41	127.93	124.79
15	B	843	PQN	C11-C3-C2	-2.41	120.76	124.89
15	A	844	PQN	C11-C3-C2	-2.41	120.76	124.89
16	F	202	BCR	C8-C7-C6	-2.41	120.56	127.00
14	A	819	CLA	CHB-C4A-NA	2.41	127.87	124.40
14	A	820	CLA	O2A-CGA-O1A	-2.41	117.61	123.63
14	A	828	CLA	CHB-C4A-NA	2.40	127.87	124.40
14	A	815	CLA	CHB-C4A-NA	2.40	127.87	124.40
14	B	809	CLA	CHB-C4A-NA	2.40	127.87	124.40
14	L	204	CLA	C1-C2-C3	-2.40	122.26	126.20
14	B	822	CLA	CHB-C4A-NA	2.40	127.86	124.40
14	B	819	CLA	CHB-C4A-NA	2.40	127.86	124.40
14	A	805	CLA	O2D-CGD-CBD	2.40	115.42	111.23
14	B	831	CLA	CHB-C4A-NA	2.40	127.86	124.40
14	A	832	CLA	O2D-CGD-O1D	-2.39	119.19	123.85
17	I	102	LHG	C20-C19-C18	-2.39	102.28	114.37
14	B	817	CLA	CHB-C4A-NA	2.39	127.85	124.40
14	A	834	CLA	C3B-C4B-NB	-2.39	108.40	110.53
14	B	832	CLA	CHB-C4A-NA	2.39	127.85	124.40
14	A	823	CLA	CHB-C4A-NA	2.39	127.84	124.40
14	A	806	CLA	O2A-CGA-O1A	-2.38	117.66	123.63
14	B	821	CLA	CHB-C4A-NA	2.38	127.84	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	804	CLA	O2D-CGD-CBD	2.38	115.39	111.23
16	A	847	BCR	C37-C22-C21	-2.38	118.96	122.82
16	F	205	BCR	C27-C26-C25	2.38	125.92	122.70
16	I	103	BCR	C28-C27-C26	-2.38	109.82	114.06
16	B	848	BCR	C2-C1-C6	2.38	113.89	110.44
16	F	202	BCR	C38-C26-C25	-2.38	121.89	124.48
14	M	102	CLA	CHB-C4A-NA	2.37	127.83	124.40
14	B	827	CLA	O2D-CGD-CBD	2.37	115.38	111.23
16	I	101	BCR	C8-C7-C6	-2.37	120.66	127.00
16	A	850	BCR	C15-C14-C13	-2.37	123.95	127.28
16	A	846	BCR	C24-C23-C22	-2.37	122.73	126.23
16	B	848	BCR	C8-C7-C6	-2.36	120.68	127.00
14	K	101	CLA	CHB-C4A-NA	2.36	127.81	124.40
16	A	847	BCR	C8-C7-C6	-2.36	120.69	127.00
14	A	819	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
14	B	818	CLA	CMB-C2B-C1B	-2.36	121.83	125.42
16	A	846	BCR	C15-C14-C13	-2.35	123.98	127.28
14	A	817	CLA	CHB-C4A-NA	2.35	127.80	124.40
14	A	802	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
14	X	1701	CLA	CHB-C4A-NA	2.35	127.79	124.40
14	A	807	CLA	O1D-CGD-CBD	2.34	129.14	124.52
16	L	207	BCR	C27-C26-C25	2.34	125.87	122.70
14	A	811	CLA	CHB-C4A-NA	2.34	127.78	124.40
14	A	840	CLA	CHB-C4A-NA	2.34	127.78	124.40
16	F	205	BCR	C24-C23-C22	-2.34	122.77	126.23
14	A	818	CLA	CHB-C4A-NA	2.33	127.76	124.40
14	A	831	CLA	C3B-C4B-NB	-2.32	108.46	110.53
14	B	833	CLA	CHB-C4A-NA	2.32	127.75	124.40
16	A	847	BCR	C35-C13-C14	-2.32	119.05	122.82
16	A	846	BCR	C8-C7-C6	-2.32	120.80	127.00
20	B	850	LMG	O1-C7-C8	-2.32	105.18	110.82
14	B	820	CLA	CHB-C4A-NA	2.32	127.75	124.40
14	B	821	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
14	B	819	CLA	C3B-C4B-NB	-2.31	108.47	110.53
16	A	851	BCR	C33-C5-C6	-2.31	121.97	124.48
16	F	205	BCR	C33-C5-C6	-2.31	121.97	124.48
14	B	829	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
14	B	834	CLA	CHB-C4A-NA	2.31	127.73	124.40
16	A	848	BCR	C33-C5-C6	-2.30	121.97	124.48
14	L	201	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
14	A	808	CLA	CHB-C4A-NA	2.29	127.71	124.40
16	A	845	BCR	C15-C14-C13	-2.29	124.06	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	829	CLA	CMB-C2B-C3B	2.29	131.94	126.55
14	A	842	CLA	CHB-C4A-NA	2.29	127.70	124.40
16	A	850	BCR	C11-C10-C9	-2.29	124.07	127.28
14	L	206	CLA	C6-C5-C3	2.28	119.03	113.47
14	B	840	CLA	CHB-C4A-NA	2.28	127.69	124.40
14	B	825	CLA	O2D-CGD-CBD	2.28	115.21	111.23
14	A	808	CLA	O2A-CGA-O1A	-2.28	117.94	123.63
13	A	801	CL0	CMB-C2B-C3B	2.27	129.23	124.68
16	B	849	BCR	C24-C23-C22	-2.27	122.87	126.23
14	B	830	CLA	C3B-C4B-NB	-2.27	108.50	110.53
14	B	830	CLA	CHB-C4A-NA	2.27	127.68	124.40
14	B	826	CLA	CHB-C4A-NA	2.27	127.67	124.40
14	L	206	CLA	CHB-C4A-NA	2.27	127.67	124.40
14	B	806	CLA	O2A-CGA-O1A	-2.26	117.96	123.63
16	K	103	BCR	C35-C13-C14	-2.26	119.15	122.82
17	A	853	LHG	C11-C10-C9	-2.26	102.93	114.37
16	F	205	BCR	C8-C7-C6	-2.26	120.95	127.00
14	B	842	CLA	C1-C2-C3	-2.26	122.49	126.20
16	A	849	BCR	C8-C7-C6	-2.26	120.96	127.00
16	B	853	BCR	C15-C16-C17	-2.26	118.89	123.52
14	B	840	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
16	A	848	BCR	C2-C1-C6	2.26	113.72	110.44
16	A	849	BCR	C2-C1-C6	2.26	113.72	110.44
14	A	827	CLA	O2D-CGD-CBD	2.25	115.17	111.23
16	K	103	BCR	C8-C7-C6	-2.25	120.98	127.00
16	B	847	BCR	C38-C26-C25	-2.25	122.03	124.48
14	A	854	CLA	O2D-CGD-CBD	2.25	115.16	111.23
14	B	828	CLA	CHB-C4A-NA	2.25	127.64	124.40
14	B	818	CLA	CHB-C4A-NA	2.25	127.64	124.40
14	A	825	CLA	C1-C2-C3	-2.25	122.52	126.20
14	B	841	CLA	CHB-C4A-NA	2.24	127.64	124.40
14	A	854	CLA	C3B-C4B-NB	-2.24	108.53	110.53
17	M	101	LHG	C11-C10-C9	-2.24	103.06	114.37
16	I	103	BCR	C29-C30-C25	2.24	113.69	110.44
14	A	810	CLA	CHB-C4A-NA	2.24	127.63	124.40
16	L	207	BCR	C33-C5-C6	-2.24	122.05	124.48
14	L	204	CLA	CBC-CAC-C3C	2.23	118.48	112.42
20	B	850	LMG	C40-C39-C38	-2.23	103.08	114.37
17	M	101	LHG	C20-C19-C18	-2.23	103.09	114.37
14	J	102	CLA	CHB-C4A-NA	2.23	127.62	124.40
14	A	805	CLA	C1-C2-C3	-2.23	122.54	126.20
14	B	805	CLA	CAC-C3C-C4C	2.23	127.69	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	F	204	CLA	CHB-C4A-NA	2.23	127.62	124.40
14	B	815	CLA	CAC-C3C-C4C	2.23	127.69	124.79
14	A	831	CLA	O2D-CGD-CBD	2.23	115.13	111.23
14	B	841	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
16	A	850	BCR	C33-C5-C6	-2.23	122.05	124.48
17	M	101	LHG	O8-C23-C24	2.22	118.61	111.83
14	B	818	CLA	C6-C5-C3	2.22	118.88	113.47
14	A	854	CLA	CHB-C4A-NA	2.22	127.60	124.40
14	A	824	CLA	CHB-C4A-NA	2.22	127.60	124.40
16	F	202	BCR	C16-C15-C14	-2.22	118.98	123.52
16	J	104	BCR	C28-C27-C26	-2.22	110.10	114.06
14	F	201	CLA	CHB-C4A-NA	2.21	127.59	124.40
13	A	801	CL0	O1D-CGD-CBD	2.21	128.08	124.72
16	J	104	BCR	C35-C13-C12	2.21	121.47	118.09
16	B	849	BCR	C8-C7-C6	-2.21	121.09	127.00
14	B	819	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
14	A	839	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
14	B	812	CLA	O2D-CGD-CBD	2.21	115.09	111.23
14	A	832	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
14	B	812	CLA	CHB-C4A-NA	2.20	127.58	124.40
14	A	838	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
13	A	801	CL0	O2A-CGA-O1A	-2.20	118.13	123.63
16	B	845	BCR	C8-C7-C6	-2.20	121.13	127.00
14	A	805	CLA	O2A-CGA-O1A	-2.20	118.14	123.63
16	J	103	BCR	C27-C26-C25	2.19	125.67	122.70
16	A	850	BCR	C7-C8-C9	-2.19	122.99	126.23
14	B	807	CLA	O1D-CGD-CBD	2.19	128.84	124.52
16	B	847	BCR	C8-C7-C6	-2.19	121.15	127.00
20	B	850	LMG	O3-C3-C2	-2.19	105.22	110.38
14	B	825	CLA	CHB-C4A-NA	2.19	127.56	124.40
17	A	852	LHG	C20-C19-C18	-2.19	103.31	114.37
16	J	104	BCR	C11-C10-C9	-2.19	124.21	127.28
14	B	814	CLA	CAC-C3C-C2C	-2.19	123.54	127.56
16	L	202	BCR	C27-C26-C25	2.19	125.66	122.70
14	A	813	CLA	CHB-C4A-NA	2.18	127.55	124.40
14	B	814	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
14	K	102	CLA	CHB-C4A-NA	2.18	127.54	124.40
14	A	834	CLA	CMB-C2B-C1B	-2.18	122.10	125.42
14	A	829	CLA	CHB-C4A-NA	2.18	127.54	124.40
14	B	829	CLA	C1-C2-C3	-2.18	122.63	126.20
16	B	847	BCR	C15-C14-C13	-2.17	124.23	127.28
14	B	818	CLA	C5-C3-C2	-2.17	116.30	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	I	103	BCR	C8-C7-C6	-2.16	121.22	127.00
14	A	834	CLA	CMB-C2B-C3B	2.16	131.63	126.55
14	A	811	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
14	B	819	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
14	F	204	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
16	J	103	BCR	C11-C10-C9	-2.16	124.25	127.28
16	A	848	BCR	C38-C26-C25	-2.15	122.13	124.48
14	B	817	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
14	A	827	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
20	B	850	LMG	O2-C2-C1	-2.15	104.95	110.08
16	L	207	BCR	C15-C14-C13	-2.15	124.26	127.28
14	B	839	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
14	B	820	CLA	CMB-C2B-C1B	-2.15	122.15	125.42
16	A	846	BCR	C11-C10-C9	-2.14	124.27	127.28
16	A	845	BCR	C8-C7-C6	-2.14	121.28	127.00
16	A	851	BCR	C2-C1-C6	2.14	113.55	110.44
17	B	851	LHG	C27-C26-C25	-2.14	103.56	114.37
14	B	810	CLA	CHB-C4A-NA	2.14	127.48	124.40
14	L	205	CLA	O2D-CGD-CBD	2.14	114.97	111.23
20	B	850	LMG	O1-C1-C2	-2.14	105.03	108.27
14	L	204	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
16	A	845	BCR	C33-C5-C6	-2.13	122.16	124.48
16	L	207	BCR	C8-C7-C6	-2.13	121.31	127.00
16	B	844	BCR	C15-C14-C13	-2.13	124.30	127.28
13	A	801	CL0	C3C-C4C-NC	-2.12	109.46	114.65
16	I	101	BCR	C15-C14-C13	-2.12	124.31	127.28
16	A	846	BCR	C38-C26-C25	-2.12	122.17	124.48
14	A	802	CLA	O1D-CGD-CBD	2.11	128.68	124.52
14	A	820	CLA	O2D-CGD-CBD	2.11	114.91	111.23
14	A	842	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
16	B	847	BCR	C2-C1-C6	2.10	113.49	110.44
14	A	831	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
14	A	834	CLA	C1-C2-C3	-2.10	122.76	126.20
14	B	811	CLA	CBA-CAA-C2A	-2.10	107.55	113.79
16	B	853	BCR	C38-C26-C25	-2.10	122.20	124.48
14	A	817	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
14	B	809	CLA	C1-C2-C3	-2.09	122.77	126.20
16	F	202	BCR	C24-C23-C22	-2.09	123.14	126.23
14	A	834	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
14	K	102	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
14	A	836	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
14	B	815	CLA	O2A-CGA-O1A	-2.09	118.41	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	818	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
16	B	844	BCR	C2-C1-C6	2.09	113.47	110.44
16	B	849	BCR	C16-C15-C14	-2.08	119.26	123.52
14	B	833	CLA	O2D-CGD-CBD	2.08	114.87	111.23
16	A	851	BCR	C8-C7-C6	-2.08	121.44	127.00
14	B	836	CLA	CBA-CAA-C2A	2.08	119.98	113.79
14	A	828	CLA	O2D-CGD-CBD	2.08	114.86	111.23
14	B	838	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
14	B	811	CLA	O1D-CGD-CBD	2.08	128.61	124.52
16	B	844	BCR	C8-C7-C6	-2.08	121.45	127.00
14	F	201	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
17	A	852	LHG	C27-C26-C25	-2.07	103.91	114.37
14	A	823	CLA	O2A-CGA-O1A	-2.07	118.02	123.33
17	A	853	LHG	C27-C26-C25	-2.07	103.92	114.37
16	L	202	BCR	C20-C21-C22	-2.07	124.38	127.28
16	L	202	BCR	C10-C11-C12	-2.06	117.22	123.20
14	A	818	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
16	B	848	BCR	C33-C5-C6	-2.06	122.23	124.48
14	B	820	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
16	A	850	BCR	C8-C7-C6	-2.06	121.50	127.00
16	B	849	BCR	C10-C11-C12	-2.06	117.23	123.20
16	L	202	BCR	C37-C22-C21	-2.06	119.48	122.82
14	A	821	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
16	B	846	BCR	C16-C15-C14	-2.06	119.31	123.52
16	L	207	BCR	C7-C8-C9	-2.06	123.19	126.23
16	J	104	BCR	C8-C7-C6	-2.06	121.51	127.00
14	B	836	CLA	CAA-C2A-C3A	-2.05	107.45	113.00
13	A	801	CL0	C4D-ND-C1D	2.05	106.78	105.22
16	B	845	BCR	C27-C26-C25	2.05	125.48	122.70
14	A	826	CLA	CHB-C4A-NA	2.05	127.36	124.40
14	B	810	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
20	B	850	LMG	O7-C10-O9	-2.05	118.92	123.70
16	J	104	BCR	C30-C25-C26	-2.05	119.84	122.64
16	F	202	BCR	C10-C11-C12	-2.04	117.28	123.20
14	A	803	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
14	A	807	CLA	O2D-CGD-O1D	-2.04	119.88	123.85
20	B	850	LMG	C38-C37-C36	-2.04	104.08	114.37
14	A	829	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
14	A	841	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
14	B	806	CLA	O1D-CGD-CBD	2.03	128.51	124.52
17	M	101	LHG	C27-C26-C25	-2.02	104.14	114.37
16	J	104	BCR	C37-C22-C23	2.02	121.18	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	828	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
14	B	809	CLA	O2D-CGD-CBD	2.02	114.76	111.23
14	A	803	CLA	CHB-C4A-NA	2.02	127.31	124.40
17	A	852	LHG	C18-C17-C16	-2.02	104.16	114.37
14	A	813	CLA	CHB-C1B-NB	2.02	127.08	124.05
16	A	845	BCR	C28-C27-C26	-2.02	110.45	114.06
16	I	103	BCR	C7-C8-C9	-2.02	123.25	126.23
17	B	851	LHG	C20-C19-C18	-2.02	104.16	114.37
14	K	102	CLA	O2D-CGD-CBD	2.02	114.76	111.23
17	B	851	LHG	C11-C10-C9	-2.02	104.17	114.37
14	L	206	CLA	C5-C3-C2	2.02	125.69	121.17
17	I	102	LHG	C11-C10-C9	-2.02	104.18	114.37
14	B	830	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
14	B	823	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
14	B	820	CLA	C1-C2-C3	-2.01	122.90	126.20
16	A	847	BCR	C36-C18-C17	-2.01	119.56	122.82
14	A	821	CLA	C1-C2-C3	-2.01	122.91	126.20
14	A	833	CLA	C1-C2-C3	-2.01	122.91	126.20
14	A	831	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
14	A	830	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
16	A	849	BCR	C28-C27-C26	-2.01	110.48	114.06
14	L	201	CLA	CAC-C3C-C4C	2.01	127.40	124.79
14	A	837	CLA	O2A-CGA-O1A	-2.00	118.18	123.33
14	A	825	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
14	B	816	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
14	J	101	CLA	O2A-CGA-O1A	-2.00	118.19	123.33

All (99) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	801	CL0	NC
13	A	801	CL0	ND
13	A	801	CL0	NA
14	A	802	CLA	ND
14	A	803	CLA	ND
14	A	804	CLA	ND
14	A	805	CLA	ND
14	A	806	CLA	ND
14	A	807	CLA	ND
14	A	808	CLA	ND
14	A	809	CLA	ND
14	A	810	CLA	ND

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Mol	Chain	Res	Type	Atom
14	A	811	CLA	ND
14	A	812	CLA	ND
14	A	813	CLA	ND
14	A	814	CLA	ND
14	A	815	CLA	ND
14	A	816	CLA	ND
14	A	817	CLA	ND
14	A	818	CLA	ND
14	A	819	CLA	ND
14	A	820	CLA	ND
14	A	821	CLA	ND
14	A	822	CLA	ND
14	A	823	CLA	ND
14	A	824	CLA	ND
14	A	825	CLA	ND
14	A	826	CLA	ND
14	A	827	CLA	ND
14	A	828	CLA	ND
14	A	829	CLA	ND
14	A	830	CLA	ND
14	A	831	CLA	ND
14	A	832	CLA	ND
14	A	833	CLA	ND
14	A	834	CLA	ND
14	A	835	CLA	ND
14	A	836	CLA	ND
14	A	837	CLA	ND
14	A	838	CLA	ND
14	A	839	CLA	ND
14	A	840	CLA	ND
14	A	841	CLA	ND
14	A	842	CLA	ND
14	A	843	CLA	ND
14	A	854	CLA	ND
14	B	801	CLA	ND
14	B	804	CLA	ND
14	B	805	CLA	ND
14	B	806	CLA	ND
14	B	807	CLA	ND
14	B	808	CLA	ND
14	B	809	CLA	ND
14	B	810	CLA	ND

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Mol	Chain	Res	Type	Atom
14	B	811	CLA	ND
14	B	812	CLA	ND
14	B	813	CLA	ND
14	B	814	CLA	ND
14	B	815	CLA	ND
14	B	816	CLA	ND
14	B	817	CLA	ND
14	B	818	CLA	ND
14	B	819	CLA	ND
14	B	820	CLA	ND
14	B	821	CLA	ND
14	B	822	CLA	ND
14	B	823	CLA	ND
14	B	824	CLA	ND
14	B	825	CLA	ND
14	B	826	CLA	ND
14	B	827	CLA	ND
14	B	828	CLA	ND
14	B	829	CLA	ND
14	B	830	CLA	ND
14	B	831	CLA	ND
14	B	832	CLA	ND
14	B	833	CLA	ND
14	B	834	CLA	ND
14	B	835	CLA	ND
14	B	836	CLA	ND
14	B	837	CLA	ND
14	B	838	CLA	ND
14	B	839	CLA	ND
14	B	840	CLA	ND
14	B	841	CLA	ND
14	B	842	CLA	ND
14	F	201	CLA	ND
14	F	203	CLA	ND
14	F	204	CLA	ND
14	J	101	CLA	ND
14	J	102	CLA	ND
14	K	101	CLA	ND
14	K	102	CLA	ND
14	L	201	CLA	ND
14	L	204	CLA	ND
14	L	205	CLA	ND

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Mol	Chain	Res	Type	Atom
14	L	206	CLA	ND
14	M	102	CLA	ND
14	X	1701	CLA	ND

All (1311) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	804	CLA	C1A-C2A-CAA-CBA
14	A	804	CLA	C3A-C2A-CAA-CBA
14	A	804	CLA	CHA-CBD-CGD-O1D
14	A	804	CLA	CHA-CBD-CGD-O2D
14	A	805	CLA	C1A-C2A-CAA-CBA
14	A	805	CLA	C3A-C2A-CAA-CBA
14	A	805	CLA	CHA-CBD-CGD-O1D
14	A	805	CLA	CHA-CBD-CGD-O2D
14	A	807	CLA	C1A-C2A-CAA-CBA
14	A	809	CLA	C1A-C2A-CAA-CBA
14	A	809	CLA	C3A-C2A-CAA-CBA
14	A	809	CLA	CHA-CBD-CGD-O2D
14	A	810	CLA	CBD-CGD-O2D-CED
14	A	811	CLA	CBD-CGD-O2D-CED
14	A	812	CLA	CBD-CGD-O2D-CED
14	A	814	CLA	CAD-CBD-CGD-O1D
14	A	814	CLA	CAD-CBD-CGD-O2D
14	A	816	CLA	C1A-C2A-CAA-CBA
14	A	816	CLA	O2A-C1-C2-C3
14	A	819	CLA	C1A-C2A-CAA-CBA
14	A	819	CLA	C3A-C2A-CAA-CBA
14	A	819	CLA	C11-C10-C8-C9
14	A	820	CLA	C1A-C2A-CAA-CBA
14	A	820	CLA	C3A-C2A-CAA-CBA
14	A	821	CLA	C1A-C2A-CAA-CBA
14	A	821	CLA	C3A-C2A-CAA-CBA
14	A	823	CLA	C3A-C2A-CAA-CBA
14	A	823	CLA	CBD-CGD-O2D-CED
14	A	826	CLA	CBD-CGD-O2D-CED
14	A	829	CLA	CBD-CGD-O2D-CED
14	A	829	CLA	O2A-C1-C2-C3
14	A	831	CLA	CHA-CBD-CGD-O1D
14	A	831	CLA	CHA-CBD-CGD-O2D
14	A	834	CLA	CBD-CGD-O2D-CED
14	A	835	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
14	A	835	CLA	CHA-CBD-CGD-O2D
14	A	838	CLA	CHA-CBD-CGD-O1D
14	A	838	CLA	CHA-CBD-CGD-O2D
14	A	839	CLA	CAD-CBD-CGD-O1D
14	A	839	CLA	CAD-CBD-CGD-O2D
14	A	843	CLA	CAD-CBD-CGD-O1D
14	A	843	CLA	CAD-CBD-CGD-O2D
14	A	854	CLA	CAD-CBD-CGD-O1D
14	A	854	CLA	CAD-CBD-CGD-O2D
14	B	804	CLA	CBD-CGD-O2D-CED
14	B	805	CLA	CBD-CGD-O2D-CED
14	B	806	CLA	CHA-CBD-CGD-O1D
14	B	806	CLA	CHA-CBD-CGD-O2D
14	B	807	CLA	C3A-C2A-CAA-CBA
14	B	807	CLA	CAD-CBD-CGD-O1D
14	B	807	CLA	CAD-CBD-CGD-O2D
14	B	815	CLA	CHA-CBD-CGD-O1D
14	B	815	CLA	CHA-CBD-CGD-O2D
14	B	819	CLA	C1A-C2A-CAA-CBA
14	B	819	CLA	C3A-C2A-CAA-CBA
14	B	820	CLA	C1A-C2A-CAA-CBA
14	B	820	CLA	C4B-C3B-CAB-CBB
14	B	822	CLA	CHA-CBD-CGD-O1D
14	B	822	CLA	CHA-CBD-CGD-O2D
14	B	825	CLA	CHA-CBD-CGD-O1D
14	B	825	CLA	CHA-CBD-CGD-O2D
14	B	825	CLA	CBD-CGD-O2D-CED
14	B	828	CLA	C1A-C2A-CAA-CBA
14	B	828	CLA	C3A-C2A-CAA-CBA
14	B	831	CLA	CBD-CGD-O2D-CED
14	B	835	CLA	CHA-CBD-CGD-O1D
14	B	835	CLA	CHA-CBD-CGD-O2D
14	B	835	CLA	CBD-CGD-O2D-CED
14	B	836	CLA	C1A-C2A-CAA-CBA
14	B	842	CLA	C1A-C2A-CAA-CBA
14	B	842	CLA	C3A-C2A-CAA-CBA
14	L	204	CLA	C1A-C2A-CAA-CBA
14	L	204	CLA	C3A-C2A-CAA-CBA
14	L	204	CLA	C2C-C3C-CAC-CBC
14	L	204	CLA	C4C-C3C-CAC-CBC
14	X	1701	CLA	CAD-CBD-CGD-O1D
14	X	1701	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
16	A	846	BCR	C18-C19-C20-C21
16	A	846	BCR	C20-C21-C22-C23
16	A	846	BCR	C20-C21-C22-C37
16	A	847	BCR	C7-C8-C9-C34
16	A	847	BCR	C35-C13-C14-C15
16	A	847	BCR	C13-C14-C15-C16
16	A	847	BCR	C14-C15-C16-C17
16	A	847	BCR	C16-C17-C18-C19
16	A	847	BCR	C16-C17-C18-C36
16	A	848	BCR	C21-C22-C23-C24
16	A	849	BCR	C20-C21-C22-C37
16	A	850	BCR	C7-C8-C9-C10
16	A	850	BCR	C11-C10-C9-C8
16	A	850	BCR	C12-C13-C14-C15
16	A	850	BCR	C35-C13-C14-C15
16	A	850	BCR	C14-C15-C16-C17
16	A	850	BCR	C16-C17-C18-C36
16	A	850	BCR	C21-C22-C23-C24
16	A	851	BCR	C7-C8-C9-C10
16	A	851	BCR	C9-C10-C11-C12
16	A	851	BCR	C11-C12-C13-C35
16	A	851	BCR	C12-C13-C14-C15
16	A	851	BCR	C14-C15-C16-C17
16	A	851	BCR	C16-C17-C18-C19
16	A	851	BCR	C16-C17-C18-C36
16	B	844	BCR	C7-C8-C9-C10
16	B	844	BCR	C7-C8-C9-C34
16	B	844	BCR	C35-C13-C14-C15
16	B	844	BCR	C21-C22-C23-C24
16	B	844	BCR	C37-C22-C23-C24
16	B	844	BCR	C22-C23-C24-C25
16	B	845	BCR	C7-C8-C9-C10
16	B	845	BCR	C7-C8-C9-C34
16	B	845	BCR	C11-C10-C9-C8
16	B	845	BCR	C11-C10-C9-C34
16	B	845	BCR	C21-C22-C23-C24
16	B	845	BCR	C37-C22-C23-C24
16	B	846	BCR	C7-C8-C9-C10
16	B	846	BCR	C7-C8-C9-C34
16	B	847	BCR	C12-C13-C14-C15
16	B	847	BCR	C14-C15-C16-C17
16	B	852	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
16	B	852	BCR	C11-C12-C13-C35
16	B	852	BCR	C35-C13-C14-C15
16	B	852	BCR	C16-C17-C18-C19
16	B	852	BCR	C16-C17-C18-C36
16	B	852	BCR	C18-C19-C20-C21
16	B	853	BCR	C5-C6-C7-C8
16	B	853	BCR	C23-C24-C25-C26
16	B	853	BCR	C23-C24-C25-C30
16	F	202	BCR	C7-C8-C9-C34
16	I	101	BCR	C16-C17-C18-C19
16	I	101	BCR	C16-C17-C18-C36
16	I	103	BCR	C7-C8-C9-C10
16	I	103	BCR	C16-C17-C18-C36
16	I	103	BCR	C21-C22-C23-C24
16	J	103	BCR	C1-C6-C7-C8
16	J	103	BCR	C5-C6-C7-C8
16	J	103	BCR	C6-C7-C8-C9
16	J	103	BCR	C7-C8-C9-C10
16	J	103	BCR	C7-C8-C9-C34
16	J	103	BCR	C35-C13-C14-C15
16	J	103	BCR	C16-C17-C18-C36
16	J	104	BCR	C1-C6-C7-C8
16	J	104	BCR	C5-C6-C7-C8
16	J	104	BCR	C7-C8-C9-C34
16	J	104	BCR	C22-C23-C24-C25
16	J	104	BCR	C23-C24-C25-C26
16	K	103	BCR	C6-C7-C8-C9
16	K	103	BCR	C16-C17-C18-C19
16	K	103	BCR	C16-C17-C18-C36
16	L	202	BCR	C11-C10-C9-C34
16	L	202	BCR	C11-C12-C13-C35
16	L	202	BCR	C20-C21-C22-C23
16	L	202	BCR	C20-C21-C22-C37
16	L	207	BCR	C6-C7-C8-C9
16	L	207	BCR	C7-C8-C9-C34
16	L	207	BCR	C11-C10-C9-C34
16	L	207	BCR	C11-C12-C13-C14
16	L	207	BCR	C11-C12-C13-C35
16	L	207	BCR	C16-C17-C18-C36
16	L	207	BCR	C17-C18-C19-C20
16	L	207	BCR	C20-C21-C22-C37
16	L	207	BCR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
17	A	852	LHG	C3-O3-P-O5
17	A	852	LHG	C3-O3-P-O6
17	B	851	LHG	C1-C2-C3-O3
17	B	851	LHG	C3-O3-P-O5
17	B	851	LHG	C4-O6-P-O3
17	B	851	LHG	C4-O6-P-O5
17	I	102	LHG	O1-C1-C2-C3
17	I	102	LHG	C1-C2-C3-O3
17	I	102	LHG	C3-O3-P-O6
17	I	102	LHG	C4-O6-P-O4
17	M	101	LHG	C3-O3-P-O6
17	M	101	LHG	C24-C23-O8-C6
14	A	814	CLA	O1D-CGD-O2D-CED
14	A	830	CLA	O1D-CGD-O2D-CED
14	B	804	CLA	O1D-CGD-O2D-CED
14	B	805	CLA	O1D-CGD-O2D-CED
14	B	814	CLA	C2C-C3C-CAC-CBC
14	B	835	CLA	O1D-CGD-O2D-CED
14	F	201	CLA	O1D-CGD-O2D-CED
14	A	814	CLA	CBD-CGD-O2D-CED
14	A	821	CLA	CBD-CGD-O2D-CED
14	A	822	CLA	CBD-CGD-O2D-CED
14	A	830	CLA	CBD-CGD-O2D-CED
14	B	808	CLA	CBD-CGD-O2D-CED
14	B	814	CLA	CBD-CGD-O2D-CED
14	B	836	CLA	CBD-CGD-O2D-CED
14	F	201	CLA	CBD-CGD-O2D-CED
14	F	203	CLA	CBD-CGD-O2D-CED
14	J	101	CLA	CBD-CGD-O2D-CED
14	K	101	CLA	CBD-CGD-O2D-CED
14	L	201	CLA	CBD-CGD-O2D-CED
14	A	809	CLA	O1A-CGA-O2A-C1
17	M	101	LHG	O10-C23-O8-C6
14	B	814	CLA	C4C-C3C-CAC-CBC
14	F	203	CLA	O1D-CGD-O2D-CED
14	A	809	CLA	CBA-CGA-O2A-C1
14	B	828	CLA	CBD-CGD-O2D-CED
14	A	802	CLA	O1A-CGA-O2A-C1
14	A	806	CLA	O1A-CGA-O2A-C1
14	A	820	CLA	O1A-CGA-O2A-C1
14	B	819	CLA	O1A-CGA-O2A-C1
14	B	820	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	B	821	CLA	O1A-CGA-O2A-C1
14	A	834	CLA	O1D-CGD-O2D-CED
14	A	812	CLA	O1D-CGD-O2D-CED
14	A	823	CLA	O1D-CGD-O2D-CED
14	B	825	CLA	O1D-CGD-O2D-CED
14	B	831	CLA	O1D-CGD-O2D-CED
14	A	833	CLA	O1A-CGA-O2A-C1
14	B	815	CLA	C2C-C3C-CAC-CBC
17	B	851	LHG	O9-C7-O7-C5
14	A	802	CLA	C3-C5-C6-C7
14	A	809	CLA	C3-C5-C6-C7
14	A	827	CLA	C3-C5-C6-C7
14	A	839	CLA	C3-C5-C6-C7
14	B	806	CLA	C3-C5-C6-C7
14	B	815	CLA	C3-C5-C6-C7
14	B	816	CLA	C3-C5-C6-C7
14	B	819	CLA	C3-C5-C6-C7
14	B	821	CLA	C3-C5-C6-C7
14	L	205	CLA	C2C-C3C-CAC-CBC
14	A	806	CLA	CBA-CGA-O2A-C1
14	A	811	CLA	CBA-CGA-O2A-C1
14	A	825	CLA	CBA-CGA-O2A-C1
14	A	836	CLA	CBA-CGA-O2A-C1
14	B	820	CLA	CBA-CGA-O2A-C1
14	B	821	CLA	CBA-CGA-O2A-C1
17	B	851	LHG	C24-C23-O8-C6
14	A	825	CLA	CBD-CGD-O2D-CED
14	A	841	CLA	CBD-CGD-O2D-CED
14	B	801	CLA	CBD-CGD-O2D-CED
14	B	807	CLA	CBD-CGD-O2D-CED
14	B	815	CLA	CBD-CGD-O2D-CED
14	B	819	CLA	CBD-CGD-O2D-CED
14	B	820	CLA	CBD-CGD-O2D-CED
14	B	822	CLA	CBD-CGD-O2D-CED
14	B	823	CLA	CBD-CGD-O2D-CED
14	X	1701	CLA	CBD-CGD-O2D-CED
14	A	810	CLA	O1D-CGD-O2D-CED
14	A	826	CLA	O1D-CGD-O2D-CED
14	A	829	CLA	O1D-CGD-O2D-CED
14	B	808	CLA	O1D-CGD-O2D-CED
14	B	818	CLA	O1A-CGA-O2A-C1
14	A	838	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
14	B	805	CLA	C2C-C3C-CAC-CBC
14	A	811	CLA	O1D-CGD-O2D-CED
14	A	818	CLA	C4-C3-C5-C6
14	A	836	CLA	C4-C3-C5-C6
14	B	818	CLA	C4-C3-C5-C6
14	A	836	CLA	C2-C3-C5-C6
14	B	818	CLA	C2-C3-C5-C6
14	L	205	CLA	C4C-C3C-CAC-CBC
14	B	841	CLA	CBD-CGD-O2D-CED
14	B	822	CLA	C2A-CAA-CBA-CGA
14	A	817	CLA	O1A-CGA-O2A-C1
14	A	810	CLA	C3-C5-C6-C7
14	A	824	CLA	C3-C5-C6-C7
14	B	811	CLA	C3-C5-C6-C7
14	L	206	CLA	C3-C5-C6-C7
14	A	802	CLA	CBA-CGA-O2A-C1
14	A	820	CLA	CBA-CGA-O2A-C1
14	A	833	CLA	CBA-CGA-O2A-C1
14	B	818	CLA	CBA-CGA-O2A-C1
14	B	819	CLA	CBA-CGA-O2A-C1
14	B	829	CLA	CBA-CGA-O2A-C1
14	B	832	CLA	CBA-CGA-O2A-C1
16	A	847	BCR	C15-C16-C17-C18
14	A	805	CLA	O1A-CGA-O2A-C1
14	A	811	CLA	O1A-CGA-O2A-C1
14	A	836	CLA	O1A-CGA-O2A-C1
14	A	838	CLA	O1A-CGA-O2A-C1
14	B	832	CLA	O1A-CGA-O2A-C1
17	B	851	LHG	O10-C23-O8-C6
14	A	821	CLA	C2C-C3C-CAC-CBC
14	B	815	CLA	C4C-C3C-CAC-CBC
14	J	101	CLA	O1D-CGD-O2D-CED
14	A	819	CLA	C3-C5-C6-C7
14	A	833	CLA	C3-C5-C6-C7
14	B	810	CLA	C3-C5-C6-C7
14	B	818	CLA	C3-C5-C6-C7
14	B	821	CLA	CBD-CGD-O2D-CED
17	A	852	LHG	O2-C2-C3-O3
17	A	853	LHG	O2-C2-C3-O3
17	B	851	LHG	O2-C2-C3-O3
17	I	102	LHG	O2-C2-C3-O3
17	M	101	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
14	B	814	CLA	O1D-CGD-O2D-CED
14	L	201	CLA	O1D-CGD-O2D-CED
14	A	805	CLA	CBA-CGA-O2A-C1
14	A	817	CLA	CBA-CGA-O2A-C1
14	B	817	CLA	CBA-CGA-O2A-C1
20	B	850	LMG	O6-C5-C6-O5
14	A	825	CLA	O1A-CGA-O2A-C1
14	B	817	CLA	O1A-CGA-O2A-C1
14	B	829	CLA	O1A-CGA-O2A-C1
14	A	821	CLA	O1D-CGD-O2D-CED
14	A	807	CLA	CBD-CGD-O2D-CED
14	K	101	CLA	O1D-CGD-O2D-CED
14	A	838	CLA	CBA-CGA-O2A-C1
14	A	817	CLA	C4-C3-C5-C6
14	A	817	CLA	C2-C3-C5-C6
14	A	818	CLA	C2-C3-C5-C6
14	L	204	CLA	CBD-CGD-O2D-CED
14	A	822	CLA	O1D-CGD-O2D-CED
14	B	828	CLA	O1D-CGD-O2D-CED
14	B	836	CLA	O1D-CGD-O2D-CED
14	A	818	CLA	O1A-CGA-O2A-C1
14	A	818	CLA	CBA-CGA-O2A-C1
14	B	801	CLA	CBA-CGA-O2A-C1
14	A	806	CLA	CBD-CGD-O2D-CED
14	A	816	CLA	CBD-CGD-O2D-CED
14	A	833	CLA	CBD-CGD-O2D-CED
14	A	836	CLA	CBD-CGD-O2D-CED
14	A	854	CLA	CBD-CGD-O2D-CED
14	B	824	CLA	CBD-CGD-O2D-CED
14	B	837	CLA	CBD-CGD-O2D-CED
16	B	852	BCR	C9-C10-C11-C12
17	A	853	LHG	C1-C2-C3-O3
14	A	827	CLA	CBA-CGA-O2A-C1
14	B	831	CLA	CBA-CGA-O2A-C1
14	L	204	CLA	CBA-CGA-O2A-C1
14	A	815	CLA	CBD-CGD-O2D-CED
14	A	854	CLA	C4-C3-C5-C6
14	A	854	CLA	C2-C3-C5-C6
14	B	805	CLA	C4C-C3C-CAC-CBC
13	A	801	CL0	C3-C5-C6-C7
14	A	803	CLA	C6-C7-C8-C9
14	A	812	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
14	A	817	CLA	C11-C10-C8-C9
14	A	824	CLA	C11-C12-C13-C14
14	A	842	CLA	C14-C13-C15-C16
14	B	805	CLA	C11-C12-C13-C14
14	B	806	CLA	C14-C13-C15-C16
14	B	814	CLA	C14-C13-C15-C16
14	B	817	CLA	C14-C13-C15-C16
14	B	835	CLA	C14-C13-C15-C16
14	B	841	CLA	C6-C7-C8-C9
14	L	205	CLA	C6-C7-C8-C9
14	B	823	CLA	O1D-CGD-O2D-CED
14	A	834	CLA	CBA-CGA-O2A-C1
14	A	803	CLA	CBD-CGD-O2D-CED
14	A	825	CLA	O1D-CGD-O2D-CED
16	A	850	BCR	C7-C8-C9-C34
16	A	850	BCR	C11-C12-C13-C35
16	A	850	BCR	C37-C22-C23-C24
16	A	851	BCR	C7-C8-C9-C34
16	B	845	BCR	C36-C18-C19-C20
16	B	847	BCR	C11-C12-C13-C35
16	B	848	BCR	C7-C8-C9-C34
16	F	202	BCR	C37-C22-C23-C24
16	I	103	BCR	C7-C8-C9-C34
16	J	103	BCR	C36-C18-C19-C20
16	J	103	BCR	C37-C22-C23-C24
16	L	202	BCR	C7-C8-C9-C34
14	B	813	CLA	C2A-CAA-CBA-CGA
14	B	831	CLA	O1A-CGA-O2A-C1
14	L	204	CLA	O1A-CGA-O2A-C1
17	M	101	LHG	C8-C7-O7-C5
14	B	807	CLA	O1D-CGD-O2D-CED
14	A	829	CLA	CBA-CGA-O2A-C1
17	I	102	LHG	C24-C23-O8-C6
14	A	815	CLA	C10-C11-C12-C13
14	B	815	CLA	O1D-CGD-O2D-CED
14	B	820	CLA	O1D-CGD-O2D-CED
14	B	822	CLA	O1D-CGD-O2D-CED
14	A	831	CLA	C5-C6-C7-C8
14	B	801	CLA	C5-C6-C7-C8
17	B	851	LHG	O1-C1-C2-O2
17	B	851	LHG	C23-C24-C25-C26
14	A	838	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
14	A	812	CLA	C11-C12-C13-C15
14	A	816	CLA	C12-C13-C15-C16
14	A	833	CLA	C6-C7-C8-C10
14	B	805	CLA	C11-C10-C8-C7
14	A	816	CLA	CBA-CGA-O2A-C1
20	B	850	LMG	C4-C5-C6-O5
16	A	851	BCR	C13-C14-C15-C16
14	A	834	CLA	C3-C5-C6-C7
14	A	828	CLA	C8-C10-C11-C12
14	B	834	CLA	C13-C15-C16-C17
14	L	204	CLA	C10-C11-C12-C13
17	I	102	LHG	C23-C24-C25-C26
14	A	827	CLA	O1A-CGA-O2A-C1
14	B	801	CLA	O1D-CGD-O2D-CED
14	B	835	CLA	CBA-CGA-O2A-C1
14	K	102	CLA	CBA-CGA-O2A-C1
14	B	815	CLA	C8-C10-C11-C12
14	B	817	CLA	C5-C6-C7-C8
14	B	835	CLA	C8-C10-C11-C12
17	I	102	LHG	C2-C3-O3-P
14	A	802	CLA	C2A-CAA-CBA-CGA
14	A	809	CLA	C2A-CAA-CBA-CGA
14	A	843	CLA	C2A-CAA-CBA-CGA
14	A	854	CLA	C2A-CAA-CBA-CGA
14	B	801	CLA	C2A-CAA-CBA-CGA
14	B	815	CLA	C2A-CAA-CBA-CGA
14	B	818	CLA	C2A-CAA-CBA-CGA
14	B	841	CLA	C2A-CAA-CBA-CGA
16	A	845	BCR	C18-C19-C20-C21
16	A	851	BCR	C10-C11-C12-C13
14	A	819	CLA	C13-C15-C16-C17
14	A	824	CLA	C10-C11-C12-C13
14	B	819	CLA	C5-C6-C7-C8
14	B	826	CLA	C10-C11-C12-C13
14	L	204	CLA	C13-C15-C16-C17
20	B	850	LMG	C28-C29-C30-C31
14	A	841	CLA	O1D-CGD-O2D-CED
14	A	838	CLA	CBD-CGD-O2D-CED
16	I	103	BCR	C22-C23-C24-C25
14	A	821	CLA	C5-C6-C7-C8
14	A	825	CLA	C8-C10-C11-C12
14	B	804	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
14	B	805	CLA	C15-C16-C17-C18
14	B	807	CLA	C13-C15-C16-C17
14	B	809	CLA	C13-C15-C16-C17
14	B	828	CLA	C10-C11-C12-C13
14	B	801	CLA	O1A-CGA-O2A-C1
14	A	807	CLA	C13-C15-C16-C17
14	A	838	CLA	C13-C15-C16-C17
17	A	853	LHG	C29-C30-C31-C32
14	B	840	CLA	C2-C1-O2A-CGA
14	A	821	CLA	C4C-C3C-CAC-CBC
14	B	819	CLA	O1D-CGD-O2D-CED
14	B	821	CLA	O1D-CGD-O2D-CED
14	X	1701	CLA	O1D-CGD-O2D-CED
13	A	801	CL0	C8-C10-C11-C12
14	A	806	CLA	C13-C15-C16-C17
14	A	839	CLA	C8-C10-C11-C12
14	A	834	CLA	O1A-CGA-O2A-C1
14	B	841	CLA	O1D-CGD-O2D-CED
14	B	806	CLA	C10-C11-C12-C13
14	L	205	CLA	C8-C10-C11-C12
17	B	851	LHG	C8-C7-O7-C5
14	B	814	CLA	C3-C5-C6-C7
14	A	828	CLA	C5-C6-C7-C8
14	B	835	CLA	C15-C16-C17-C18
17	M	101	LHG	C1-C2-C3-O3
14	A	830	CLA	C2A-CAA-CBA-CGA
14	L	206	CLA	C2A-CAA-CBA-CGA
14	A	831	CLA	CBA-CGA-O2A-C1
14	B	830	CLA	CBA-CGA-O2A-C1
14	A	826	CLA	C8-C10-C11-C12
14	B	807	CLA	C10-C11-C12-C13
14	B	821	CLA	C10-C11-C12-C13
14	B	839	CLA	C13-C15-C16-C17
14	B	816	CLA	CBD-CGD-O2D-CED
14	A	803	CLA	C3-C5-C6-C7
14	A	807	CLA	O1D-CGD-O2D-CED
14	A	810	CLA	C15-C16-C17-C18
14	A	825	CLA	C15-C16-C17-C18
14	B	810	CLA	C13-C15-C16-C17
14	B	825	CLA	C13-C15-C16-C17
14	B	827	CLA	C8-C10-C11-C12
14	B	829	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
14	B	830	CLA	C13-C15-C16-C17
14	K	102	CLA	C5-C6-C7-C8
14	A	828	CLA	C15-C16-C17-C18
14	B	812	CLA	C13-C15-C16-C17
14	B	830	CLA	C5-C6-C7-C8
14	B	825	CLA	C8-C10-C11-C12
14	B	829	CLA	C13-C15-C16-C17
14	B	833	CLA	C15-C16-C17-C18
14	A	840	CLA	C3-C5-C6-C7
14	B	823	CLA	C3-C5-C6-C7
20	B	850	LMG	C11-C10-O7-C8
14	A	802	CLA	C11-C12-C13-C14
14	B	811	CLA	C14-C13-C15-C16
14	A	816	CLA	C16-C17-C18-C19
14	A	836	CLA	C16-C17-C18-C19
14	B	806	CLA	C8-C10-C11-C12
14	A	829	CLA	O1A-CGA-O2A-C1
16	A	848	BCR	C20-C21-C22-C37
16	A	850	BCR	C11-C10-C9-C34
16	B	844	BCR	C11-C10-C9-C34
16	B	844	BCR	C16-C17-C18-C36
16	B	844	BCR	C20-C21-C22-C37
16	B	845	BCR	C20-C21-C22-C37
16	B	847	BCR	C35-C13-C14-C15
16	B	847	BCR	C20-C21-C22-C37
16	B	848	BCR	C20-C21-C22-C37
16	B	849	BCR	C35-C13-C14-C15
16	B	849	BCR	C16-C17-C18-C36
16	B	852	BCR	C11-C10-C9-C34
16	B	852	BCR	C20-C21-C22-C37
16	B	853	BCR	C11-C10-C9-C34
16	B	853	BCR	C16-C17-C18-C36
16	B	853	BCR	C20-C21-C22-C37
16	F	202	BCR	C35-C13-C14-C15
16	F	202	BCR	C20-C21-C22-C37
16	F	205	BCR	C16-C17-C18-C36
16	I	101	BCR	C11-C10-C9-C34
16	I	103	BCR	C35-C13-C14-C15
16	J	103	BCR	C20-C21-C22-C37
16	L	202	BCR	C35-C13-C14-C15
14	A	817	CLA	C13-C15-C16-C17
14	B	834	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
16	A	845	BCR	C37-C22-C23-C24
16	A	846	BCR	C11-C12-C13-C35
16	A	846	BCR	C37-C22-C23-C24
16	B	845	BCR	C11-C12-C13-C35
16	B	853	BCR	C37-C22-C23-C24
16	F	205	BCR	C37-C22-C23-C24
16	I	101	BCR	C11-C12-C13-C35
16	B	852	BCR	C11-C12-C13-C14
16	L	207	BCR	C21-C22-C23-C24
14	A	832	CLA	C2A-CAA-CBA-CGA
14	B	836	CLA	C2A-CAA-CBA-CGA
14	A	840	CLA	C10-C11-C12-C13
14	B	827	CLA	C13-C15-C16-C17
17	B	851	LHG	O1-C1-C2-C3
14	A	833	CLA	C16-C17-C18-C19
14	A	833	CLA	C16-C17-C18-C20
14	B	839	CLA	C16-C17-C18-C20
14	L	205	CLA	C16-C17-C18-C20
14	A	816	CLA	O1A-CGA-O2A-C1
14	B	835	CLA	O1A-CGA-O2A-C1
14	K	102	CLA	O1A-CGA-O2A-C1
16	A	846	BCR	C11-C10-C9-C8
16	A	847	BCR	C12-C13-C14-C15
16	A	849	BCR	C20-C21-C22-C23
16	A	850	BCR	C16-C17-C18-C19
16	B	845	BCR	C12-C13-C14-C15
16	B	847	BCR	C16-C17-C18-C19
16	B	848	BCR	C11-C10-C9-C8
16	B	853	BCR	C11-C10-C9-C8
16	F	205	BCR	C16-C17-C18-C19
16	I	101	BCR	C20-C21-C22-C23
16	J	103	BCR	C12-C13-C14-C15
16	L	207	BCR	C16-C17-C18-C19
16	L	207	BCR	C20-C21-C22-C23
14	B	816	CLA	C13-C15-C16-C17
14	L	204	CLA	O1D-CGD-O2D-CED
14	A	821	CLA	CBA-CGA-O2A-C1
14	B	806	CLA	CBA-CGA-O2A-C1
14	A	816	CLA	O1D-CGD-O2D-CED
14	A	806	CLA	C2-C1-O2A-CGA
14	A	806	CLA	C16-C17-C18-C19
14	A	829	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
14	B	817	CLA	C16-C17-C18-C20
14	B	839	CLA	C16-C17-C18-C19
14	A	818	CLA	C10-C11-C12-C13
14	A	836	CLA	C5-C6-C7-C8
17	M	101	LHG	C30-C31-C32-C33
14	A	806	CLA	O1D-CGD-O2D-CED
14	A	854	CLA	C13-C15-C16-C17
17	A	853	LHG	C27-C28-C29-C30
20	B	850	LMG	C29-C30-C31-C32
17	I	102	LHG	O1-C1-C2-O2
17	A	852	LHG	C9-C10-C11-C12
20	B	850	LMG	C39-C40-C41-C42
14	A	833	CLA	O1D-CGD-O2D-CED
14	A	825	CLA	C4B-C3B-CAB-CBB
14	K	102	CLA	C4B-C3B-CAB-CBB
17	M	101	LHG	C7-C8-C9-C10
20	B	850	LMG	C16-C17-C18-C19
14	A	806	CLA	C16-C17-C18-C20
14	A	829	CLA	C16-C17-C18-C20
14	B	817	CLA	C16-C17-C18-C19
14	B	825	CLA	C16-C17-C18-C19
14	B	825	CLA	C16-C17-C18-C20
14	B	829	CLA	C16-C17-C18-C20
14	L	205	CLA	C16-C17-C18-C19
14	A	836	CLA	O1D-CGD-O2D-CED
14	B	839	CLA	C8-C10-C11-C12
14	A	807	CLA	C11-C12-C13-C15
14	B	839	CLA	C12-C13-C15-C16
14	B	841	CLA	C11-C12-C13-C15
17	A	852	LHG	C33-C34-C35-C36
14	L	201	CLA	CBA-CGA-O2A-C1
14	B	826	CLA	C8-C10-C11-C12
14	B	831	CLA	C5-C6-C7-C8
14	B	830	CLA	O1A-CGA-O2A-C1
14	A	806	CLA	C3A-C2A-CAA-CBA
14	A	807	CLA	C3A-C2A-CAA-CBA
14	B	836	CLA	C3A-C2A-CAA-CBA
14	B	837	CLA	C3A-C2A-CAA-CBA
14	A	810	CLA	C13-C15-C16-C17
14	A	815	CLA	C15-C16-C17-C18
14	A	832	CLA	C5-C6-C7-C8
14	B	829	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
14	A	831	CLA	O1A-CGA-O2A-C1
14	B	807	CLA	CBA-CGA-O2A-C1
14	F	201	CLA	CBA-CGA-O2A-C1
17	A	852	LHG	C10-C11-C12-C13
14	A	804	CLA	C8-C10-C11-C12
17	B	851	LHG	C13-C14-C15-C16
17	I	102	LHG	C15-C16-C17-C18
14	B	830	CLA	C10-C11-C12-C13
17	A	852	LHG	C27-C28-C29-C30
14	B	812	CLA	C16-C17-C18-C20
14	B	806	CLA	O1A-CGA-O2A-C1
14	A	825	CLA	C2B-C3B-CAB-CBB
14	B	820	CLA	C2B-C3B-CAB-CBB
16	A	846	BCR	C23-C24-C25-C30
16	A	848	BCR	C23-C24-C25-C26
16	A	848	BCR	C23-C24-C25-C30
16	A	850	BCR	C23-C24-C25-C26
16	A	850	BCR	C23-C24-C25-C30
16	B	847	BCR	C23-C24-C25-C30
16	B	848	BCR	C23-C24-C25-C26
16	B	848	BCR	C23-C24-C25-C30
16	B	853	BCR	C1-C6-C7-C8
16	F	205	BCR	C23-C24-C25-C26
16	F	205	BCR	C23-C24-C25-C30
16	I	103	BCR	C23-C24-C25-C26
16	I	103	BCR	C23-C24-C25-C30
16	J	104	BCR	C23-C24-C25-C30
14	A	834	CLA	C2A-CAA-CBA-CGA
14	B	826	CLA	C5-C6-C7-C8
17	M	101	LHG	C26-C27-C28-C29
14	B	807	CLA	O1A-CGA-O2A-C1
17	A	852	LHG	C32-C33-C34-C35
16	B	844	BCR	C10-C11-C12-C13
16	B	845	BCR	C10-C11-C12-C13
16	L	202	BCR	C10-C11-C12-C13
17	I	102	LHG	C16-C17-C18-C19
14	B	824	CLA	O1D-CGD-O2D-CED
17	A	852	LHG	C15-C16-C17-C18
17	A	853	LHG	C32-C33-C34-C35
16	B	845	BCR	C6-C7-C8-C9
16	B	847	BCR	C22-C23-C24-C25
16	L	202	BCR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
14	K	102	CLA	CBD-CGD-O2D-CED
14	B	806	CLA	C5-C6-C7-C8
14	B	818	CLA	C15-C16-C17-C18
14	A	821	CLA	O1A-CGA-O2A-C1
20	B	850	LMG	C11-C12-C13-C14
14	B	812	CLA	C3-C5-C6-C7
14	A	816	CLA	C16-C17-C18-C20
14	L	201	CLA	O1A-CGA-O2A-C1
14	A	816	CLA	C8-C10-C11-C12
14	A	833	CLA	C8-C10-C11-C12
14	B	833	CLA	C2C-C3C-CAC-CBC
16	A	847	BCR	C37-C22-C23-C24
16	K	103	BCR	C11-C12-C13-C35
17	A	852	LHG	C23-C24-C25-C26
16	B	853	BCR	C21-C22-C23-C24
14	L	206	CLA	C13-C15-C16-C17
14	A	836	CLA	C16-C17-C18-C20
14	A	839	CLA	C16-C17-C18-C20
14	B	812	CLA	C16-C17-C18-C19
17	B	851	LHG	C31-C32-C33-C34
14	A	825	CLA	C4-C3-C5-C6
14	B	815	CLA	C4-C3-C5-C6
14	B	815	CLA	C2-C3-C5-C6
17	M	101	LHG	C31-C32-C33-C34
14	A	812	CLA	C8-C10-C11-C12
17	B	851	LHG	C12-C13-C14-C15
15	A	844	PQN	C25-C26-C27-C28
14	F	201	CLA	O1A-CGA-O2A-C1
14	B	837	CLA	O1D-CGD-O2D-CED
14	B	814	CLA	C16-C17-C18-C19
20	B	850	LMG	C22-C23-C24-C25
14	B	819	CLA	C15-C16-C17-C18
14	A	854	CLA	O1D-CGD-O2D-CED
17	B	851	LHG	C32-C33-C34-C35
14	A	812	CLA	C1A-C2A-CAA-CBA
14	A	823	CLA	C1A-C2A-CAA-CBA
14	B	807	CLA	C1A-C2A-CAA-CBA
14	B	817	CLA	C1A-C2A-CAA-CBA
14	B	833	CLA	C1A-C2A-CAA-CBA
14	K	102	CLA	C1A-C2A-CAA-CBA
14	A	814	CLA	C10-C11-C12-C13
14	A	815	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	M	101	LHG	C28-C29-C30-C31
14	A	841	CLA	C8-C10-C11-C12
14	B	821	CLA	C15-C16-C17-C18
17	M	101	LHG	O9-C7-O7-C5
14	A	806	CLA	C11-C10-C8-C7
14	A	818	CLA	C12-C13-C15-C16
14	A	819	CLA	C11-C10-C8-C7
14	A	827	CLA	C11-C12-C13-C15
14	A	828	CLA	C6-C7-C8-C10
14	A	835	CLA	C12-C13-C15-C16
14	A	839	CLA	C11-C12-C13-C15
14	A	841	CLA	C11-C10-C8-C7
14	A	841	CLA	C11-C12-C13-C15
14	B	804	CLA	C11-C10-C8-C7
14	B	812	CLA	C11-C10-C8-C7
14	B	814	CLA	C11-C10-C8-C7
14	B	816	CLA	C6-C7-C8-C10
14	B	820	CLA	C6-C7-C8-C10
14	B	825	CLA	C11-C12-C13-C15
14	B	827	CLA	C12-C13-C15-C16
14	B	828	CLA	C11-C12-C13-C15
14	K	102	CLA	C11-C10-C8-C7
14	L	204	CLA	C12-C13-C15-C16
14	A	807	CLA	C16-C17-C18-C20
17	B	851	LHG	C27-C28-C29-C30
14	A	812	CLA	CBA-CGA-O2A-C1
14	B	804	CLA	C13-C15-C16-C17
14	B	819	CLA	C8-C10-C11-C12
14	A	807	CLA	C8-C10-C11-C12
14	B	808	CLA	C8-C10-C11-C12
14	L	205	CLA	C13-C15-C16-C17
14	A	803	CLA	O1D-CGD-O2D-CED
14	B	828	CLA	C2A-CAA-CBA-CGA
14	A	810	CLA	C11-C12-C13-C14
14	A	826	CLA	C14-C13-C15-C16
14	A	828	CLA	C6-C7-C8-C9
14	A	835	CLA	C14-C13-C15-C16
14	A	838	CLA	C6-C7-C8-C9
14	A	839	CLA	C11-C12-C13-C14
14	B	801	CLA	C6-C7-C8-C9
14	B	804	CLA	C14-C13-C15-C16
14	B	809	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
14	B	814	CLA	C11-C10-C8-C9
14	B	816	CLA	C6-C7-C8-C9
14	B	828	CLA	C11-C12-C13-C14
14	B	829	CLA	C14-C13-C15-C16
16	B	845	BCR	C9-C10-C11-C12
14	B	815	CLA	CBA-CGA-O2A-C1
20	B	850	LMG	O9-C10-O7-C8
17	A	852	LHG	C11-C10-C9-C8
16	A	848	BCR	C16-C17-C18-C36
16	A	850	BCR	C20-C21-C22-C37
16	A	851	BCR	C35-C13-C14-C15
14	B	820	CLA	C3-C5-C6-C7
14	A	825	CLA	C2-C3-C5-C6
14	B	838	CLA	C10-C11-C12-C13
14	B	809	CLA	C16-C17-C18-C20
16	A	847	BCR	C17-C18-C19-C20
16	L	202	BCR	C11-C12-C13-C14
14	L	205	CLA	C2A-CAA-CBA-CGA
17	I	102	LHG	C12-C13-C14-C15
17	A	853	LHG	C23-C24-C25-C26
14	A	814	CLA	CBA-CGA-O2A-C1
14	A	806	CLA	O2A-C1-C2-C3
14	B	817	CLA	O2A-C1-C2-C3
14	B	819	CLA	O2A-C1-C2-C3
17	A	853	LHG	C24-C25-C26-C27
14	L	206	CLA	C5-C6-C7-C8
20	B	850	LMG	C37-C38-C39-C40
16	A	851	BCR	C15-C16-C17-C18
14	A	807	CLA	C16-C17-C18-C19
16	A	848	BCR	C11-C10-C9-C8
16	F	202	BCR	C11-C10-C9-C8
16	J	103	BCR	C11-C10-C9-C8
16	L	207	BCR	C12-C13-C14-C15
14	A	838	CLA	O1D-CGD-O2D-CED
14	A	840	CLA	CBA-CGA-O2A-C1
14	F	204	CLA	CBA-CGA-O2A-C1
13	A	801	CL0	C16-C17-C18-C19
13	A	801	CL0	C16-C17-C18-C20
20	B	850	LMG	C18-C19-C20-C21
14	B	828	CLA	C3-C5-C6-C7
14	B	841	CLA	C3-C5-C6-C7
20	B	850	LMG	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
14	A	812	CLA	O1A-CGA-O2A-C1
17	B	851	LHG	C11-C12-C13-C14
14	B	816	CLA	CBA-CGA-O2A-C1
14	F	201	CLA	C10-C11-C12-C13
14	A	854	CLA	C16-C17-C18-C20
14	A	830	CLA	C4-C3-C5-C6
17	I	102	LHG	C19-C20-C21-C22
14	B	829	CLA	C2-C3-C5-C6
17	B	851	LHG	C9-C10-C11-C12
14	B	812	CLA	C10-C11-C12-C13
14	A	806	CLA	C11-C10-C8-C9
14	A	807	CLA	C11-C12-C13-C14
14	A	815	CLA	C11-C10-C8-C9
14	A	815	CLA	C14-C13-C15-C16
14	A	818	CLA	C14-C13-C15-C16
14	A	827	CLA	C11-C12-C13-C14
14	A	829	CLA	C11-C12-C13-C14
14	A	830	CLA	C14-C13-C15-C16
14	A	839	CLA	C6-C7-C8-C9
14	A	841	CLA	C11-C10-C8-C9
14	A	841	CLA	C11-C12-C13-C14
14	B	804	CLA	C11-C10-C8-C9
14	B	808	CLA	C14-C13-C15-C16
14	B	812	CLA	C11-C10-C8-C9
14	B	815	CLA	C11-C12-C13-C14
14	B	820	CLA	C14-C13-C15-C16
14	B	827	CLA	C14-C13-C15-C16
14	B	834	CLA	C11-C10-C8-C9
14	B	839	CLA	C14-C13-C15-C16
14	B	841	CLA	C11-C12-C13-C14
14	K	102	CLA	C11-C10-C8-C9
14	L	201	CLA	C14-C13-C15-C16
14	L	204	CLA	C14-C13-C15-C16
14	A	807	CLA	C10-C11-C12-C13
14	A	824	CLA	C15-C16-C17-C18
14	A	841	CLA	CBA-CGA-O2A-C1
14	A	816	CLA	C5-C6-C7-C8
17	B	851	LHG	O6-C4-C5-C6
14	A	806	CLA	C11-C12-C13-C15
14	A	810	CLA	C11-C12-C13-C15
14	A	815	CLA	C11-C10-C8-C7
14	A	826	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
14	A	829	CLA	C11-C12-C13-C15
14	A	830	CLA	C12-C13-C15-C16
14	A	833	CLA	C11-C10-C8-C7
14	A	836	CLA	C11-C12-C13-C15
14	A	838	CLA	C6-C7-C8-C10
14	A	839	CLA	C6-C7-C8-C10
14	B	801	CLA	C6-C7-C8-C10
14	B	804	CLA	C12-C13-C15-C16
14	B	807	CLA	C11-C10-C8-C7
14	B	807	CLA	C12-C13-C15-C16
14	B	808	CLA	C12-C13-C15-C16
14	B	815	CLA	C11-C12-C13-C15
14	B	820	CLA	C11-C12-C13-C15
14	B	826	CLA	C11-C10-C8-C7
14	B	829	CLA	C12-C13-C15-C16
14	B	834	CLA	C11-C10-C8-C7
14	L	201	CLA	C12-C13-C15-C16
14	B	841	CLA	C8-C10-C11-C12
14	B	815	CLA	O1A-CGA-O2A-C1
14	B	809	CLA	C16-C17-C18-C19
14	A	805	CLA	C4-C3-C5-C6
14	A	822	CLA	C4-C3-C5-C6
14	B	810	CLA	C4-C3-C5-C6
14	B	820	CLA	C3A-C2A-CAA-CBA
14	B	826	CLA	C3A-C2A-CAA-CBA
14	B	804	CLA	CAA-CBA-CGA-O2A
14	A	805	CLA	C2-C3-C5-C6
14	B	833	CLA	C2-C3-C5-C6
14	B	801	CLA	C3-C5-C6-C7
16	B	853	BCR	C11-C12-C13-C35
14	B	839	CLA	C5-C6-C7-C8
17	A	852	LHG	C14-C15-C16-C17
14	A	837	CLA	C2A-CAA-CBA-CGA
14	B	816	CLA	O1D-CGD-O2D-CED
17	I	102	LHG	C4-C5-C6-O8
17	M	101	LHG	C4-C5-C6-O8
14	L	201	CLA	C16-C17-C18-C20
14	L	201	CLA	C5-C6-C7-C8
14	A	803	CLA	C4-C3-C5-C6
14	B	829	CLA	C4-C3-C5-C6
14	B	833	CLA	C4-C3-C5-C6
14	A	807	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	A	822	CLA	C2-C3-C5-C6
14	B	810	CLA	C2-C3-C5-C6
14	A	840	CLA	O1A-CGA-O2A-C1
14	A	854	CLA	C16-C17-C18-C19
14	A	814	CLA	O1A-CGA-O2A-C1
16	A	846	BCR	C1-C6-C7-C8
16	A	850	BCR	C1-C6-C7-C8
16	B	849	BCR	C1-C6-C7-C8
16	F	205	BCR	C1-C6-C7-C8
16	L	207	BCR	C1-C6-C7-C8
17	A	852	LHG	C8-C7-O7-C5
13	A	801	CL0	CAA-CBA-CGA-O2A
14	A	802	CLA	C15-C16-C17-C18
14	B	814	CLA	C16-C17-C18-C20
14	A	802	CLA	C8-C10-C11-C12
15	B	843	PQN	C18-C20-C21-C22
17	A	852	LHG	C19-C20-C21-C22
14	F	204	CLA	O1A-CGA-O2A-C1
14	A	826	CLA	C4-C3-C5-C6
14	L	204	CLA	C4-C3-C5-C6
17	M	101	LHG	C17-C18-C19-C20
14	A	826	CLA	C2-C3-C5-C6
14	A	830	CLA	C2-C3-C5-C6
14	L	204	CLA	C2-C3-C5-C6
14	L	201	CLA	C16-C17-C18-C19
17	M	101	LHG	C9-C10-C11-C12
14	A	832	CLA	C8-C10-C11-C12
14	A	827	CLA	C11-C10-C8-C9
14	A	854	CLA	C14-C13-C15-C16
14	B	801	CLA	C14-C13-C15-C16
14	B	825	CLA	C11-C10-C8-C9
14	B	820	CLA	C16-C17-C18-C20
14	B	818	CLA	C13-C15-C16-C17
14	L	205	CLA	C3-C5-C6-C7
14	A	839	CLA	CBA-CGA-O2A-C1
14	B	828	CLA	C4-C3-C5-C6
16	L	207	BCR	C15-C16-C17-C18
17	A	852	LHG	C1-C2-C3-O3
16	A	845	BCR	C35-C13-C14-C15
16	B	846	BCR	C16-C17-C18-C36
16	B	847	BCR	C16-C17-C18-C36
16	I	101	BCR	C35-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
16	I	101	BCR	C20-C21-C22-C37
16	I	103	BCR	C20-C21-C22-C37
16	J	104	BCR	C20-C21-C22-C37
14	B	811	CLA	CBA-CGA-O2A-C1
17	A	853	LHG	C24-C23-O8-C6
17	I	102	LHG	C17-C18-C19-C20
14	B	828	CLA	C16-C17-C18-C20
16	A	848	BCR	C7-C8-C9-C34
16	B	846	BCR	C11-C12-C13-C35
14	A	803	CLA	C6-C7-C8-C10
14	A	827	CLA	C11-C10-C8-C7
14	A	831	CLA	C11-C10-C8-C7
14	A	854	CLA	C12-C13-C15-C16
14	B	801	CLA	C12-C13-C15-C16
14	B	814	CLA	C12-C13-C15-C16
14	B	815	CLA	C6-C7-C8-C10
14	B	816	CLA	C11-C12-C13-C15
14	B	819	CLA	C12-C13-C15-C16
14	B	825	CLA	C11-C10-C8-C7
14	B	841	CLA	C6-C7-C8-C10
14	B	842	CLA	C11-C10-C8-C7
14	B	842	CLA	C12-C13-C15-C16
14	A	830	CLA	C8-C10-C11-C12
14	B	801	CLA	C8-C10-C11-C12
16	A	846	BCR	C21-C22-C23-C24
16	A	849	BCR	C21-C22-C23-C24
16	B	852	BCR	C7-C8-C9-C10
16	F	202	BCR	C7-C8-C9-C10
16	J	104	BCR	C7-C8-C9-C10
14	B	839	CLA	CBA-CGA-O2A-C1
14	A	841	CLA	O1A-CGA-O2A-C1
17	I	102	LHG	O10-C23-O8-C6
14	A	803	CLA	C2-C3-C5-C6
14	A	839	CLA	C16-C17-C18-C19
14	B	820	CLA	C16-C17-C18-C19
14	B	811	CLA	O1A-CGA-O2A-C1
14	B	816	CLA	O1A-CGA-O2A-C1
16	B	844	BCR	C20-C21-C22-C23
16	J	103	BCR	C16-C17-C18-C19
14	A	804	CLA	C10-C11-C12-C13
17	A	853	LHG	O6-C4-C5-O7
14	B	832	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
17	A	853	LHG	C11-C10-C9-C8
14	A	812	CLA	C13-C15-C16-C17
14	A	842	CLA	C16-C17-C18-C20
14	B	805	CLA	C2A-CAA-CBA-CGA
14	B	828	CLA	C2-C3-C5-C6
14	B	834	CLA	C8-C10-C11-C12
14	A	839	CLA	O1A-CGA-O2A-C1
17	I	102	LHG	O7-C5-C6-O8
17	M	101	LHG	O7-C5-C6-O8
14	A	831	CLA	C11-C10-C8-C9
14	B	805	CLA	C11-C10-C8-C9
14	B	838	CLA	C6-C7-C8-C9
14	B	828	CLA	C16-C17-C18-C19
14	B	831	CLA	C6-C7-C8-C10
14	A	828	CLA	C10-C11-C12-C13
14	B	828	CLA	C5-C6-C7-C8
14	A	810	CLA	C8-C10-C11-C12
14	B	811	CLA	C10-C11-C12-C13
14	A	829	CLA	C4-C3-C5-C6
14	A	809	CLA	C5-C6-C7-C8
14	F	204	CLA	CBD-CGD-O2D-CED
14	A	807	CLA	O1A-CGA-O2A-C1
14	B	839	CLA	O1A-CGA-O2A-C1
14	B	809	CLA	C15-C16-C17-C18
14	A	826	CLA	C13-C15-C16-C17
14	A	806	CLA	C1A-C2A-CAA-CBA
14	B	826	CLA	C1A-C2A-CAA-CBA
14	B	837	CLA	C1A-C2A-CAA-CBA
14	B	841	CLA	C4B-C3B-CAB-CBB
14	M	102	CLA	C4B-C3B-CAB-CBB
16	A	850	BCR	C22-C23-C24-C25
16	I	101	BCR	C22-C23-C24-C25
16	A	847	BCR	C7-C8-C9-C10
14	K	102	CLA	O1D-CGD-O2D-CED
17	A	853	LHG	O6-C4-C5-C6
17	A	852	LHG	C17-C18-C19-C20
14	A	825	CLA	C11-C10-C8-C7
14	A	827	CLA	C12-C13-C15-C16
14	A	834	CLA	C12-C13-C15-C16
14	B	805	CLA	C12-C13-C15-C16
14	L	205	CLA	C6-C7-C8-C10
14	B	810	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
14	B	838	CLA	CBA-CGA-O2A-C1
17	B	851	LHG	O6-C4-C5-O7
14	A	806	CLA	C11-C12-C13-C14
14	A	833	CLA	C6-C7-C8-C9
14	A	833	CLA	C11-C10-C8-C9
14	A	836	CLA	C11-C12-C13-C14
14	B	815	CLA	C6-C7-C8-C9
14	B	816	CLA	C11-C12-C13-C14
14	B	819	CLA	C14-C13-C15-C16
14	B	820	CLA	C6-C7-C8-C9
14	B	842	CLA	C11-C10-C8-C9
14	B	842	CLA	C14-C13-C15-C16
14	A	804	CLA	C13-C15-C16-C17
14	A	829	CLA	C10-C11-C12-C13
14	B	832	CLA	C1-C2-C3-C4
14	B	827	CLA	C3-C5-C6-C7
17	M	101	LHG	C11-C10-C9-C8
17	M	101	LHG	C33-C34-C35-C36
14	A	806	CLA	CAD-CBD-CGD-O2D
14	A	815	CLA	CAD-CBD-CGD-O2D
14	A	826	CLA	CAD-CBD-CGD-O2D
14	B	814	CLA	CAD-CBD-CGD-O2D
14	B	837	CLA	CAD-CBD-CGD-O2D
14	K	101	CLA	CAD-CBD-CGD-O2D
14	K	102	CLA	CAD-CBD-CGD-O2D
20	B	850	LMG	O6-C1-O1-C7
14	B	831	CLA	C6-C7-C8-C9
14	A	825	CLA	C5-C6-C7-C8
14	B	839	CLA	C15-C16-C17-C18
14	B	838	CLA	O1A-CGA-O2A-C1
20	B	850	LMG	C21-C22-C23-C24
14	A	806	CLA	CAD-CBD-CGD-O1D
14	A	809	CLA	CHA-CBD-CGD-O1D
14	A	815	CLA	CAD-CBD-CGD-O1D
14	A	816	CLA	CHA-CBD-CGD-O1D
14	A	816	CLA	CHA-CBD-CGD-O2D
14	A	826	CLA	CAD-CBD-CGD-O1D
14	B	814	CLA	CAD-CBD-CGD-O1D
14	B	817	CLA	CHA-CBD-CGD-O1D
14	B	817	CLA	CHA-CBD-CGD-O2D
14	B	834	CLA	CHA-CBD-CGD-O1D
14	B	834	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	B	837	CLA	CAD-CBD-CGD-O1D
14	B	838	CLA	CHA-CBD-CGD-O1D
14	B	838	CLA	CHA-CBD-CGD-O2D
14	K	101	CLA	CAD-CBD-CGD-O1D
14	K	102	CLA	CAD-CBD-CGD-O1D
17	B	851	LHG	C4-O6-P-O4
17	I	102	LHG	C3-O3-P-O5
17	M	101	LHG	C3-O3-P-O5
14	B	833	CLA	C10-C11-C12-C13
14	A	821	CLA	C4-C3-C5-C6
14	K	102	CLA	C2B-C3B-CAB-CBB
17	A	852	LHG	C29-C30-C31-C32
14	L	204	CLA	C5-C6-C7-C8
16	A	845	BCR	C7-C8-C9-C34
17	I	102	LHG	C5-C4-O6-P
16	A	851	BCR	C11-C12-C13-C14
14	A	810	CLA	C10-C11-C12-C13
14	L	201	CLA	C15-C16-C17-C18
14	A	816	CLA	C14-C13-C15-C16
14	B	807	CLA	C11-C10-C8-C9
14	B	807	CLA	C14-C13-C15-C16
14	B	820	CLA	C11-C12-C13-C14
14	A	815	CLA	C12-C13-C15-C16
14	B	817	CLA	C12-C13-C15-C16
16	B	846	BCR	C20-C21-C22-C23
16	B	853	BCR	C16-C17-C18-C19
14	F	204	CLA	O1D-CGD-O2D-CED
17	A	852	LHG	O7-C5-C6-O8
14	B	815	CLA	C16-C17-C18-C19
14	A	803	CLA	C2A-CAA-CBA-CGA
14	B	817	CLA	C2C-C3C-CAC-CBC
14	A	841	CLA	C3-C5-C6-C7
14	A	808	CLA	C2A-CAA-CBA-CGA
14	A	819	CLA	C2A-CAA-CBA-CGA
14	B	809	CLA	C2A-CAA-CBA-CGA
17	I	102	LHG	C11-C12-C13-C14
14	A	854	CLA	C3-C5-C6-C7
14	A	812	CLA	C11-C12-C13-C14
14	A	825	CLA	C11-C10-C8-C9
14	A	827	CLA	C14-C13-C15-C16
14	B	834	CLA	C6-C7-C8-C9
14	A	814	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
14	B	801	CLA	C15-C16-C17-C18
14	A	832	CLA	C11-C12-C13-C15
14	B	826	CLA	CBA-CGA-O2A-C1
17	B	851	LHG	C7-C8-C9-C10
14	B	826	CLA	O1A-CGA-O2A-C1
14	A	835	CLA	C2A-CAA-CBA-CGA
14	A	842	CLA	C2A-CAA-CBA-CGA
14	A	821	CLA	C2-C3-C5-C6
14	F	201	CLA	C3-C5-C6-C7
14	A	815	CLA	C13-C15-C16-C17
14	A	802	CLA	C6-C7-C8-C10
14	B	833	CLA	C12-C13-C15-C16
14	B	834	CLA	C6-C7-C8-C10
20	B	850	LMG	C34-C35-C36-C37
14	A	836	CLA	C3A-C2A-CAA-CBA
14	B	816	CLA	C4-C3-C5-C6
14	B	821	CLA	C3A-C2A-CAA-CBA
14	B	828	CLA	CAA-CBA-CGA-O2A
14	B	817	CLA	C4C-C3C-CAC-CBC
16	B	845	BCR	C35-C13-C14-C15
16	B	846	BCR	C20-C21-C22-C37
16	F	205	BCR	C35-C13-C14-C15
14	A	803	CLA	C15-C16-C17-C18
14	B	838	CLA	C8-C10-C11-C12
16	B	852	BCR	C36-C18-C19-C20
14	F	204	CLA	CAA-CBA-CGA-O2A
14	B	821	CLA	C8-C10-C11-C12
14	A	819	CLA	CAA-CBA-CGA-O2A
14	B	833	CLA	C4C-C3C-CAC-CBC
16	I	101	BCR	C14-C15-C16-C17
14	A	835	CLA	C5-C6-C7-C8
14	A	839	CLA	C13-C15-C16-C17
20	B	850	LMG	C32-C33-C34-C35
14	A	806	CLA	C6-C7-C8-C9
14	A	819	CLA	C11-C12-C13-C14
14	A	834	CLA	C11-C12-C13-C14
14	A	841	CLA	C6-C7-C8-C9
14	B	807	CLA	C6-C7-C8-C9
14	B	809	CLA	C11-C10-C8-C9
14	B	817	CLA	C11-C10-C8-C9
14	B	828	CLA	C14-C13-C15-C16
14	B	833	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
14	A	842	CLA	C16-C17-C18-C19
14	B	827	CLA	C16-C17-C18-C20
14	B	801	CLA	C13-C15-C16-C17
14	B	815	CLA	C10-C11-C12-C13
17	A	853	LHG	C10-C11-C12-C13
17	I	102	LHG	C14-C15-C16-C17
20	B	850	LMG	C23-C24-C25-C26
17	A	852	LHG	C31-C32-C33-C34
16	L	202	BCR	C13-C14-C15-C16
17	A	852	LHG	O1-C1-C2-O2
14	B	814	CLA	C1A-C2A-CAA-CBA
14	B	821	CLA	C1A-C2A-CAA-CBA
14	F	201	CLA	C1A-C2A-CAA-CBA
14	F	204	CLA	C1A-C2A-CAA-CBA
16	B	846	BCR	C11-C10-C9-C8
16	F	205	BCR	C12-C13-C14-C15
14	A	837	CLA	C2B-C3B-CAB-CBB
14	B	841	CLA	C2B-C3B-CAB-CBB
14	M	102	CLA	C2B-C3B-CAB-CBB
16	A	846	BCR	C5-C6-C7-C8
16	A	846	BCR	C23-C24-C25-C26
16	A	849	BCR	C1-C6-C7-C8
16	A	850	BCR	C5-C6-C7-C8
16	B	847	BCR	C23-C24-C25-C26
16	F	205	BCR	C5-C6-C7-C8
16	I	101	BCR	C1-C6-C7-C8
16	L	207	BCR	C5-C6-C7-C8
14	B	828	CLA	C8-C10-C11-C12
14	A	823	CLA	CAA-CBA-CGA-O2A
14	B	824	CLA	CAA-CBA-CGA-O2A
14	A	810	CLA	C4-C3-C5-C6
14	B	816	CLA	C2-C3-C5-C6
14	B	822	CLA	CAA-CBA-CGA-O1A
14	A	838	CLA	C11-C10-C8-C7
14	A	839	CLA	C2A-CAA-CBA-CGA
14	A	840	CLA	C13-C15-C16-C17
14	B	829	CLA	C5-C6-C7-C8
16	B	853	BCR	C36-C18-C19-C20
14	F	204	CLA	C2C-C3C-CAC-CBC
17	A	853	LHG	C9-C10-C11-C12
17	B	851	LHG	C15-C16-C17-C18
14	B	826	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
14	B	821	CLA	C5-C6-C7-C8
14	B	826	CLA	C13-C15-C16-C17
14	A	814	CLA	C4-C3-C5-C6
14	A	829	CLA	C2-C3-C5-C6
14	B	824	CLA	CAA-CBA-CGA-O1A
14	F	203	CLA	CAA-CBA-CGA-O2A
14	A	823	CLA	CAA-CBA-CGA-O1A
14	A	824	CLA	O1A-CGA-O2A-C1
14	A	810	CLA	C2A-CAA-CBA-CGA
14	A	836	CLA	C15-C16-C17-C18
14	A	806	CLA	C4-C3-C5-C6
16	F	202	BCR	C15-C16-C17-C18
14	A	837	CLA	C4B-C3B-CAB-CBB
14	B	811	CLA	C4B-C3B-CAB-CBB
14	B	822	CLA	CAA-CBA-CGA-O2A
14	B	804	CLA	CAA-CBA-CGA-O1A
14	B	833	CLA	CAA-CBA-CGA-O2A
14	A	827	CLA	C10-C11-C12-C13
13	A	801	CL0	CHA-CBD-CGD-O2D
16	A	847	BCR	C20-C21-C22-C37
16	B	846	BCR	C11-C10-C9-C34
16	L	202	BCR	C16-C17-C18-C36
14	A	813	CLA	CAA-CBA-CGA-O2A
14	A	804	CLA	C16-C17-C18-C20
14	B	818	CLA	C16-C17-C18-C20
14	A	816	CLA	C4-C3-C5-C6
14	B	813	CLA	CAA-CBA-CGA-O1A
13	A	801	CL0	CAA-CBA-CGA-O1A
14	B	804	CLA	C15-C16-C17-C18
14	A	819	CLA	C11-C12-C13-C15
14	A	824	CLA	C11-C12-C13-C15
14	A	813	CLA	CAA-CBA-CGA-O1A
14	A	832	CLA	C3-C5-C6-C7
14	A	820	CLA	C11-C10-C8-C9
14	A	806	CLA	C15-C16-C17-C18
14	B	829	CLA	C2A-CAA-CBA-CGA
14	A	802	CLA	C2-C1-O2A-CGA
14	A	835	CLA	C2-C1-O2A-CGA
14	B	806	CLA	C2-C1-O2A-CGA
14	A	832	CLA	C11-C12-C13-C14
14	B	827	CLA	C16-C17-C18-C19
14	L	206	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
14	A	822	CLA	C15-C16-C17-C18
14	B	814	CLA	C5-C6-C7-C8
14	A	819	CLA	O1D-CGD-O2D-CED
14	A	824	CLA	CBA-CGA-O2A-C1
14	A	832	CLA	CBA-CGA-O2A-C1
14	A	808	CLA	C3A-C2A-CAA-CBA
14	A	816	CLA	C3A-C2A-CAA-CBA
14	B	814	CLA	C3A-C2A-CAA-CBA
14	B	818	CLA	C3A-C2A-CAA-CBA
14	B	825	CLA	C3A-C2A-CAA-CBA
14	F	201	CLA	C3A-C2A-CAA-CBA
14	A	837	CLA	CAA-CBA-CGA-O2A
20	B	850	LMG	C24-C25-C26-C27
14	A	818	CLA	C16-C17-C18-C20
14	B	842	CLA	C15-C16-C17-C18
16	F	202	BCR	C18-C19-C20-C21
14	F	203	CLA	CAA-CBA-CGA-O1A
14	A	837	CLA	CAA-CBA-CGA-O1A
17	I	102	LHG	O6-C4-C5-O7
14	A	832	CLA	O1A-CGA-O2A-C1
14	B	823	CLA	C2C-C3C-CAC-CBC
14	A	804	CLA	C2A-CAA-CBA-CGA
16	J	104	BCR	C13-C14-C15-C16
14	B	807	CLA	C16-C17-C18-C19
14	B	815	CLA	C16-C17-C18-C20
14	B	818	CLA	C16-C17-C18-C19
20	B	850	LMG	C35-C36-C37-C38
14	A	806	CLA	CAA-CBA-CGA-O2A
14	K	101	CLA	CAA-CBA-CGA-O2A
14	A	804	CLA	C14-C13-C15-C16
14	A	818	CLA	C11-C10-C8-C9
14	B	835	CLA	C10-C11-C12-C13
16	L	207	BCR	C7-C8-C9-C10
14	A	814	CLA	C2C-C3C-CAC-CBC
17	B	851	LHG	C24-C25-C26-C27
14	A	830	CLA	C16-C17-C18-C20
14	A	820	CLA	C11-C10-C8-C7
14	B	805	CLA	C11-C12-C13-C15
14	A	834	CLA	C5-C6-C7-C8
17	A	852	LHG	C35-C36-C37-C38
16	A	849	BCR	C5-C6-C7-C8
16	B	849	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
16	I	101	BCR	C5-C6-C7-C8
14	A	854	CLA	C2-C1-O2A-CGA
14	B	819	CLA	C2-C1-O2A-CGA
14	L	201	CLA	C2-C1-O2A-CGA
14	F	204	CLA	C4C-C3C-CAC-CBC
14	A	819	CLA	CBD-CGD-O2D-CED
14	B	826	CLA	C16-C17-C18-C19
14	B	808	CLA	C3-C5-C6-C7
14	A	814	CLA	CAA-CBA-CGA-O2A
14	B	842	CLA	C3-C5-C6-C7
14	A	802	CLA	CAA-CBA-CGA-O2A
17	B	851	LHG	O7-C7-C8-C9
14	B	814	CLA	C2-C3-C5-C6
14	B	813	CLA	CAA-CBA-CGA-O2A
14	A	803	CLA	C13-C15-C16-C17
14	A	805	CLA	C6-C7-C8-C9
14	B	826	CLA	C11-C12-C13-C14
14	B	811	CLA	CAA-CBA-CGA-O2A
14	A	854	CLA	O1A-CGA-O2A-C1
14	A	834	CLA	C8-C10-C11-C12
14	A	808	CLA	C1A-C2A-CAA-CBA
14	A	838	CLA	C1A-C2A-CAA-CBA
14	A	840	CLA	C4B-C3B-CAB-CBB
14	A	841	CLA	C4B-C3B-CAB-CBB
14	B	818	CLA	C1A-C2A-CAA-CBA
14	B	824	CLA	C1A-C2A-CAA-CBA
14	B	830	CLA	C1A-C2A-CAA-CBA
14	B	840	CLA	C4B-C3B-CAB-CBB
14	K	101	CLA	C4B-C3B-CAB-CBB
14	A	814	CLA	C4C-C3C-CAC-CBC
14	B	813	CLA	O1D-CGD-O2D-CED
14	A	826	CLA	CAA-CBA-CGA-O2A
14	B	817	CLA	CAA-CBA-CGA-O2A
14	B	829	CLA	CAA-CBA-CGA-O2A
14	B	809	CLA	C2-C3-C5-C6
16	F	205	BCR	C21-C22-C23-C24
16	J	104	BCR	C21-C22-C23-C24
20	B	850	LMG	O7-C10-C11-C12
14	A	834	CLA	C15-C16-C17-C18
14	B	833	CLA	C13-C15-C16-C17
14	B	809	CLA	C4-C3-C5-C6
14	B	814	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	B	826	CLA	C2-C1-O2A-CGA
14	B	830	CLA	C2-C1-O2A-CGA
14	B	808	CLA	CAA-CBA-CGA-O2A
14	A	807	CLA	C11-C10-C8-C7
14	A	812	CLA	C6-C7-C8-C10
14	A	817	CLA	C6-C7-C8-C10
14	B	826	CLA	C6-C7-C8-C10
14	B	838	CLA	C11-C10-C8-C7
20	B	850	LMG	C17-C18-C19-C20
14	A	815	CLA	C5-C6-C7-C8
14	A	818	CLA	C2A-CAA-CBA-CGA
14	A	829	CLA	C2A-CAA-CBA-CGA
14	A	841	CLA	C2A-CAA-CBA-CGA
14	K	101	CLA	C2A-CAA-CBA-CGA
14	A	817	CLA	C16-C17-C18-C20
14	B	811	CLA	C16-C17-C18-C19
14	A	811	CLA	C2C-C3C-CAC-CBC
14	B	824	CLA	C3A-C2A-CAA-CBA
14	B	813	CLA	CBD-CGD-O2D-CED
16	L	202	BCR	C11-C10-C9-C8
14	A	802	CLA	CAA-CBA-CGA-O1A
14	B	808	CLA	CAA-CBA-CGA-O1A
14	B	840	CLA	CBA-CGA-O2A-C1
14	A	826	CLA	C6-C7-C8-C9
14	A	834	CLA	C14-C13-C15-C16
14	B	805	CLA	C14-C13-C15-C16
14	B	826	CLA	C11-C10-C8-C9
14	K	101	CLA	CAA-CBA-CGA-O1A
14	B	801	CLA	CAA-CBA-CGA-O2A
16	B	848	BCR	C17-C18-C19-C20
14	A	806	CLA	C2C-C3C-CAC-CBC
14	A	814	CLA	CAA-CBA-CGA-O1A
20	B	850	LMG	O9-C10-C11-C12
14	A	826	CLA	C10-C11-C12-C13
14	A	806	CLA	CAA-CBA-CGA-O1A
14	B	817	CLA	C13-C15-C16-C17
17	A	852	LHG	O10-C23-C24-C25
14	A	803	CLA	C10-C11-C12-C13
14	A	806	CLA	C10-C11-C12-C13
14	A	810	CLA	C2-C3-C5-C6
14	A	817	CLA	CAD-CBD-CGD-O2D
14	A	818	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	B	821	CLA	CAD-CBD-CGD-O2D
14	B	832	CLA	CAD-CBD-CGD-O2D
14	A	821	CLA	CAA-CBA-CGA-O2A
14	B	817	CLA	CAA-CBA-CGA-O1A
14	B	840	CLA	O1A-CGA-O2A-C1
17	B	851	LHG	O9-C7-C8-C9
17	I	102	LHG	O7-C7-C8-C9
14	B	833	CLA	C8-C10-C11-C12
15	B	843	PQN	C13-C15-C16-C17
14	B	811	CLA	CAA-CBA-CGA-O1A
14	B	820	CLA	CAA-CBA-CGA-O2A
14	K	102	CLA	CAA-CBA-CGA-O2A
17	M	101	LHG	C15-C16-C17-C18
14	A	810	CLA	CAA-CBA-CGA-O2A
14	A	826	CLA	CAA-CBA-CGA-O1A
14	B	829	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

89 monomers are involved in 145 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	851	LHG	1	0
14	B	819	CLA	1	0
14	B	842	CLA	1	0
14	B	830	CLA	2	0
14	A	837	CLA	2	0
14	B	827	CLA	2	0
14	A	841	CLA	1	0
14	B	836	CLA	2	0
14	A	821	CLA	3	0
14	L	201	CLA	3	0
16	B	847	BCR	3	0
14	L	205	CLA	1	0
14	B	838	CLA	1	0
14	B	815	CLA	1	0
14	A	826	CLA	2	0
14	A	836	CLA	4	0
14	B	801	CLA	2	0
14	A	833	CLA	3	0
14	B	814	CLA	2	0
14	A	816	CLA	2	0
14	A	829	CLA	4	0

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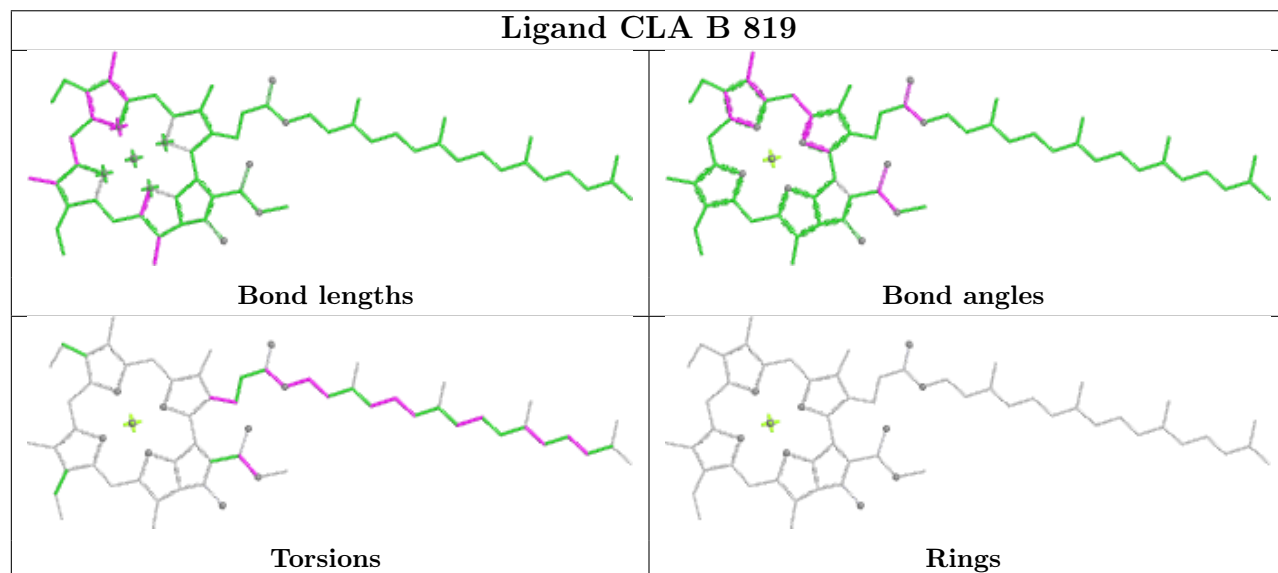
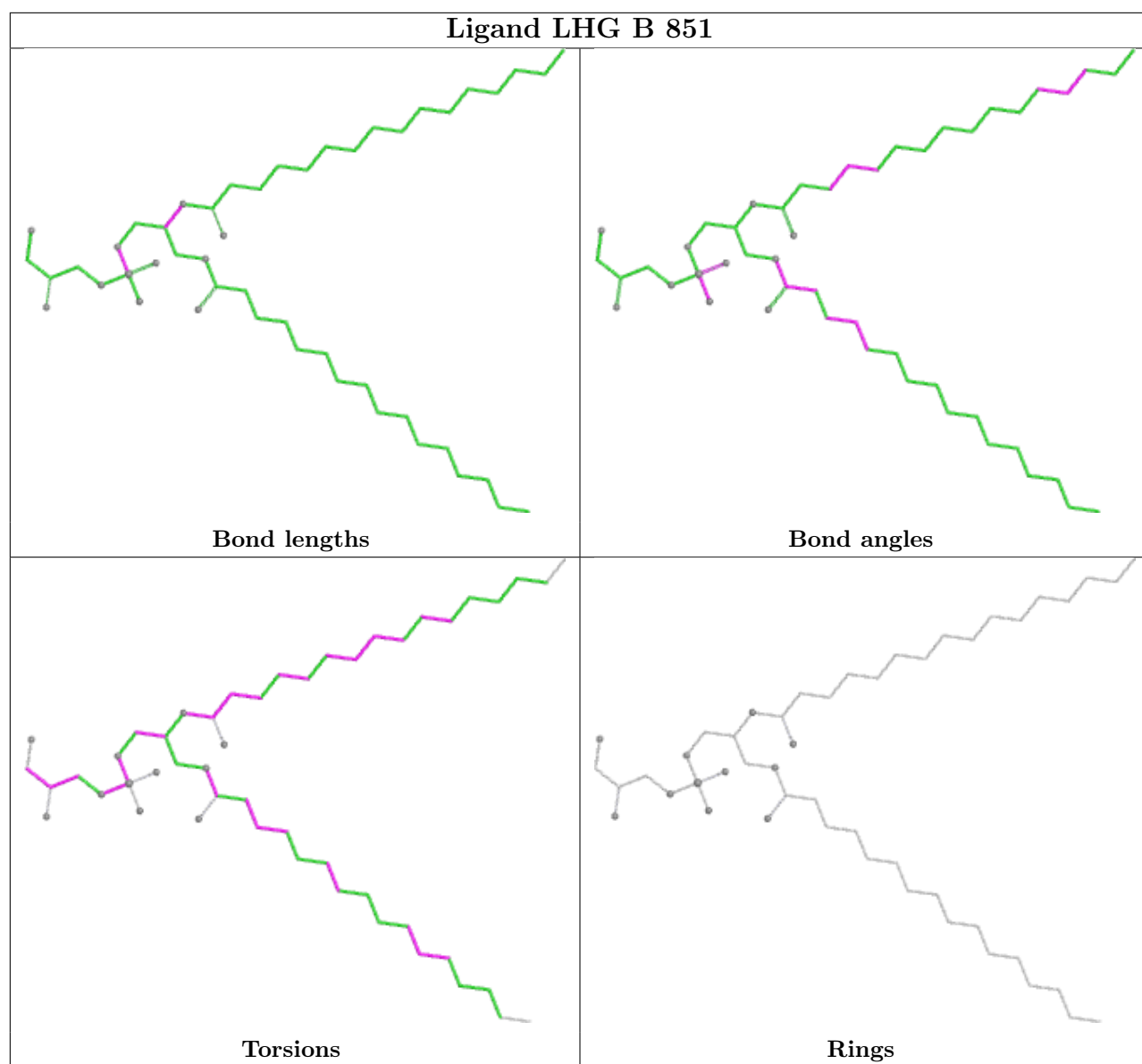
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	812	CLA	1	0
17	I	102	LHG	2	0
14	A	825	CLA	7	0
16	I	103	BCR	1	0
14	A	835	CLA	3	0
14	A	822	CLA	2	0
14	B	817	CLA	1	0
16	A	848	BCR	2	0
14	A	819	CLA	3	0
14	B	810	CLA	2	0
16	J	103	BCR	3	0
14	A	807	CLA	1	0
14	B	805	CLA	1	0
16	A	849	BCR	2	0
16	K	103	BCR	4	0
16	A	846	BCR	5	0
14	A	842	CLA	2	0
13	A	801	CL0	1	0
14	A	805	CLA	1	0
14	A	830	CLA	1	0
16	A	851	BCR	2	0
14	X	1701	CLA	1	0
14	B	808	CLA	1	0
15	A	844	PQN	2	0
14	K	101	CLA	2	0
16	B	852	BCR	2	0
16	B	849	BCR	1	0
16	L	202	BCR	1	0
16	B	844	BCR	1	0
14	F	204	CLA	1	0
16	B	853	BCR	3	0
14	B	829	CLA	2	0
14	B	833	CLA	1	0
14	A	854	CLA	4	0
20	B	850	LMG	3	0
14	A	828	CLA	1	0
17	M	101	LHG	1	0
14	B	831	CLA	1	0
14	A	811	CLA	1	0
14	A	804	CLA	1	0
14	B	818	CLA	1	0
16	A	850	BCR	6	0

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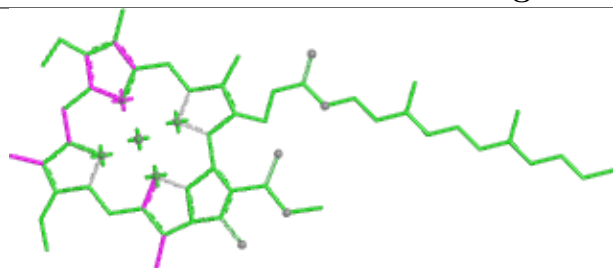
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	853	LHG	2	0
14	A	820	CLA	1	0
16	J	104	BCR	2	0
14	B	834	CLA	1	0
14	A	832	CLA	1	0
14	B	822	CLA	1	0
14	B	828	CLA	5	0
14	B	825	CLA	3	0
17	A	852	LHG	2	0
14	A	809	CLA	1	0
14	B	826	CLA	3	0
16	A	845	BCR	1	0
16	F	205	BCR	1	0
14	A	840	CLA	1	0
14	A	802	CLA	6	0
14	A	803	CLA	1	0
16	B	848	BCR	2	0
14	B	839	CLA	1	0
16	B	846	BCR	1	0
14	L	204	CLA	2	0
14	B	835	CLA	2	0
14	B	804	CLA	3	0
16	I	101	BCR	2	0
16	A	847	BCR	3	0
14	A	838	CLA	1	0
14	A	813	CLA	1	0

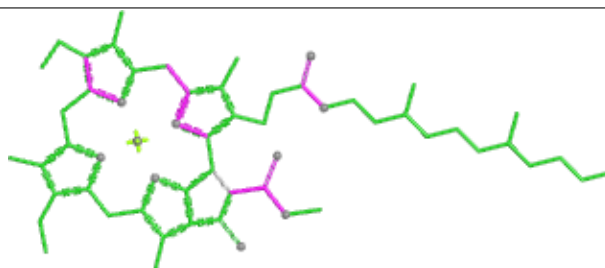
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



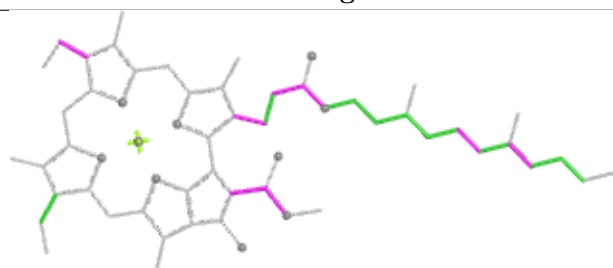
Ligand CLA K 102



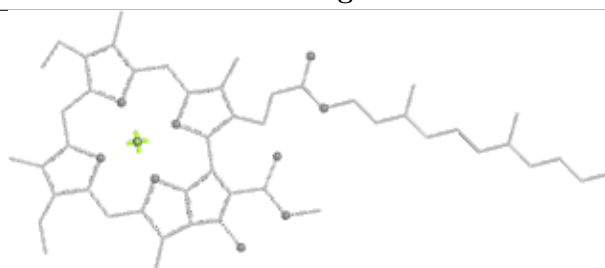
Bond lengths



Bond angles

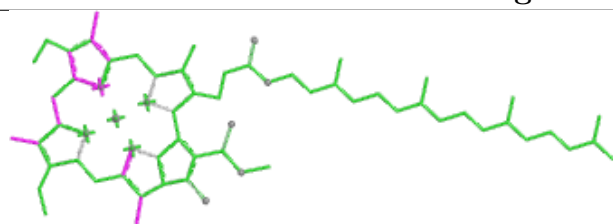


Torsions

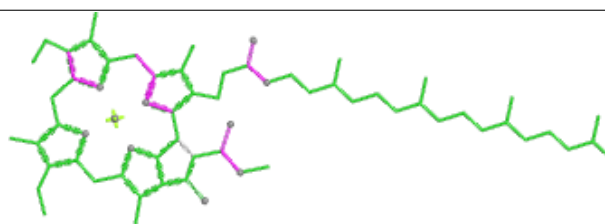


Rings

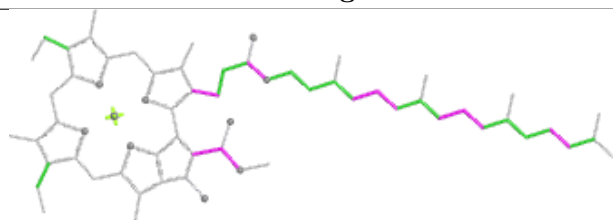
Ligand CLA B 821



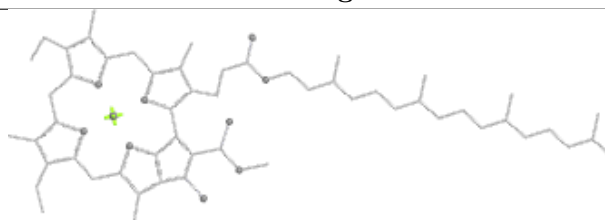
Bond lengths



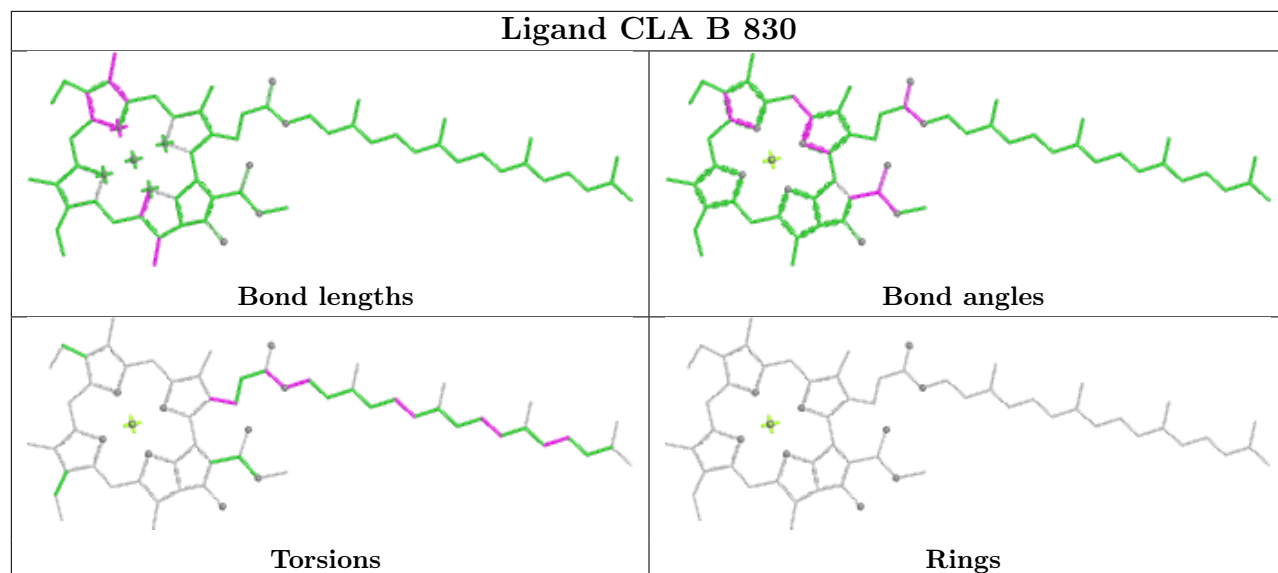
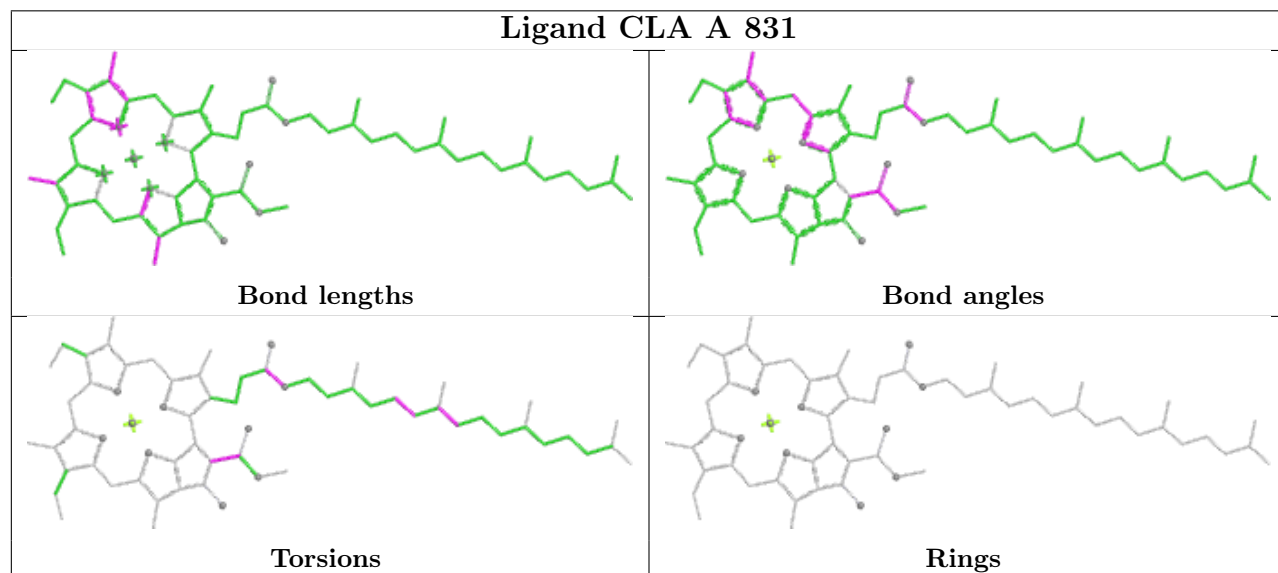
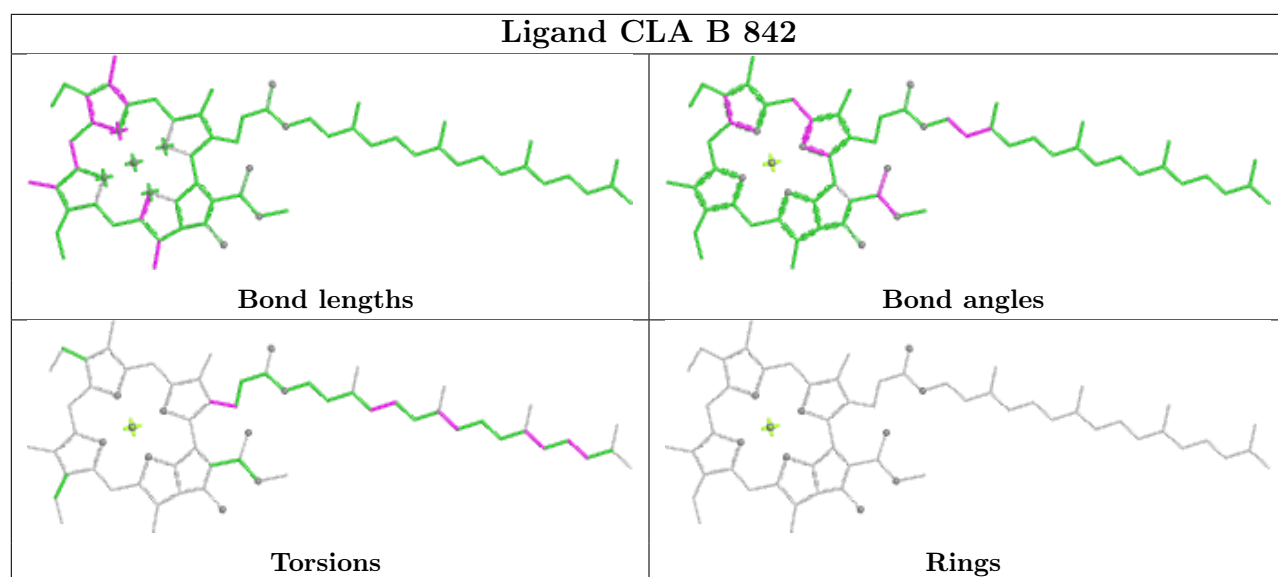
Bond angles



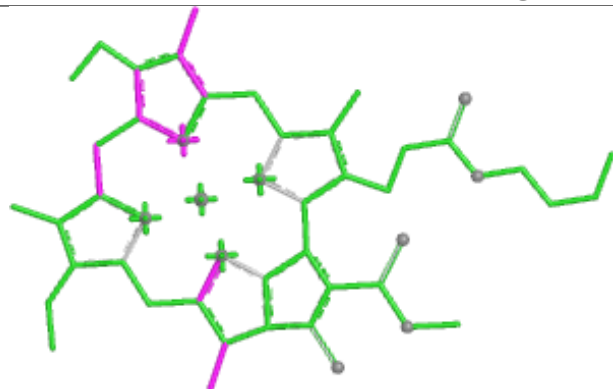
Torsions



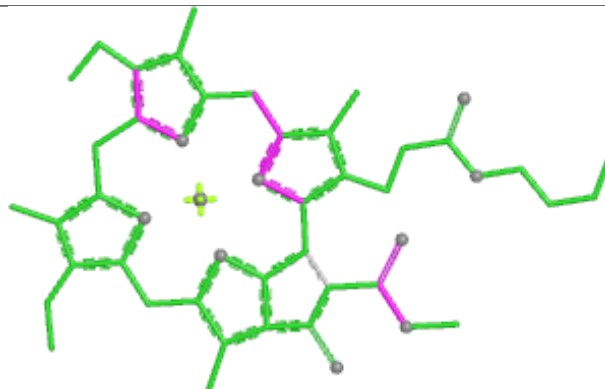
Rings



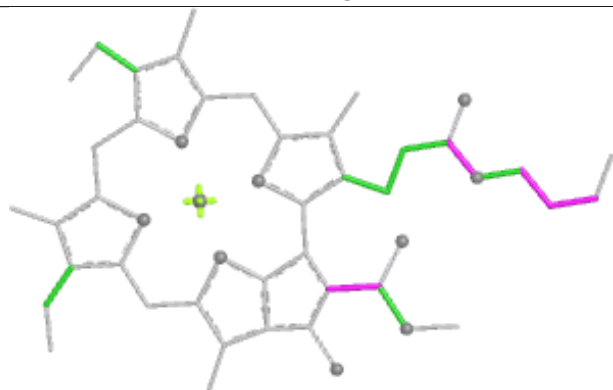
Ligand CLA B 832



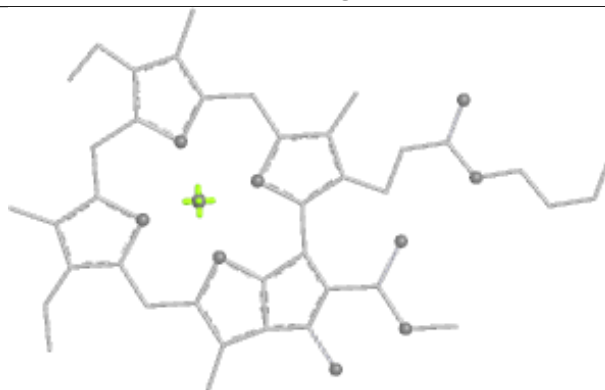
Bond lengths



Bond angles

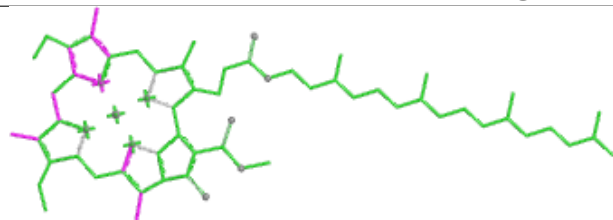


Torsions

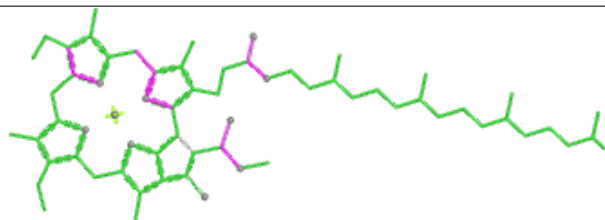


Rings

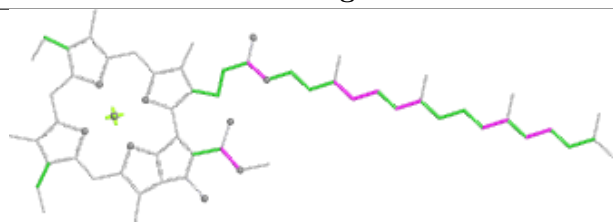
Ligand CLA B 816



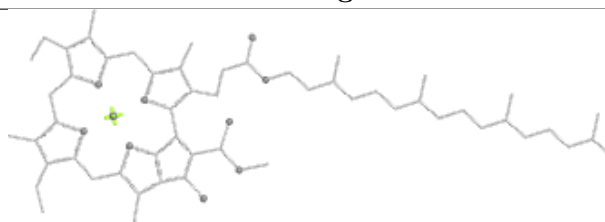
Bond lengths



Bond angles

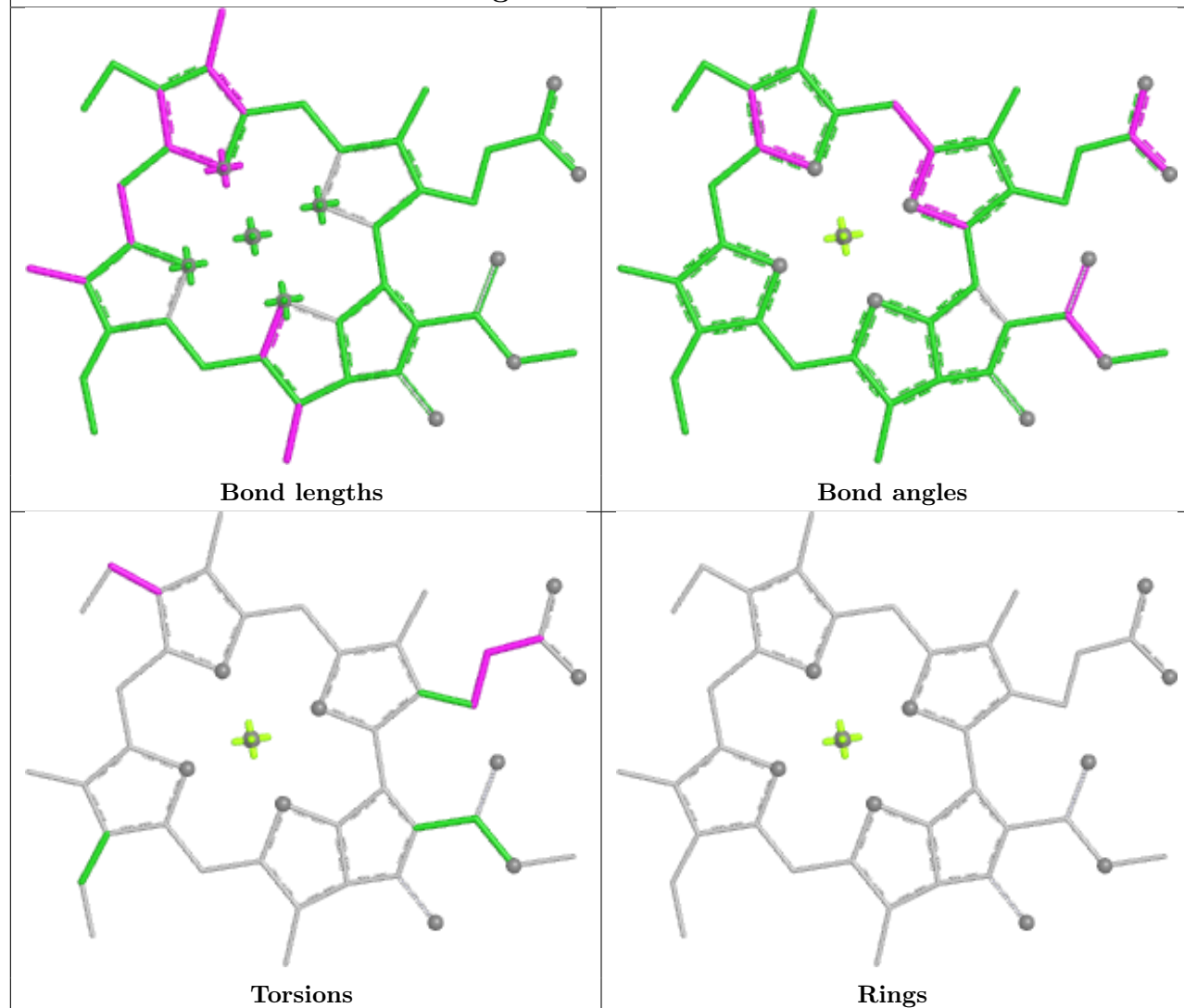


Torsions

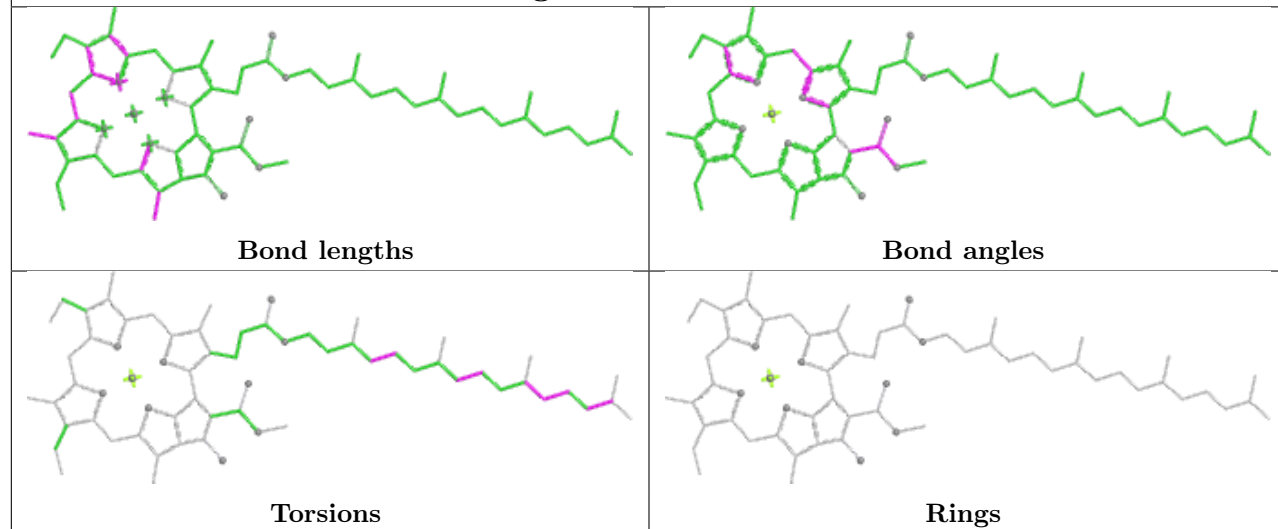


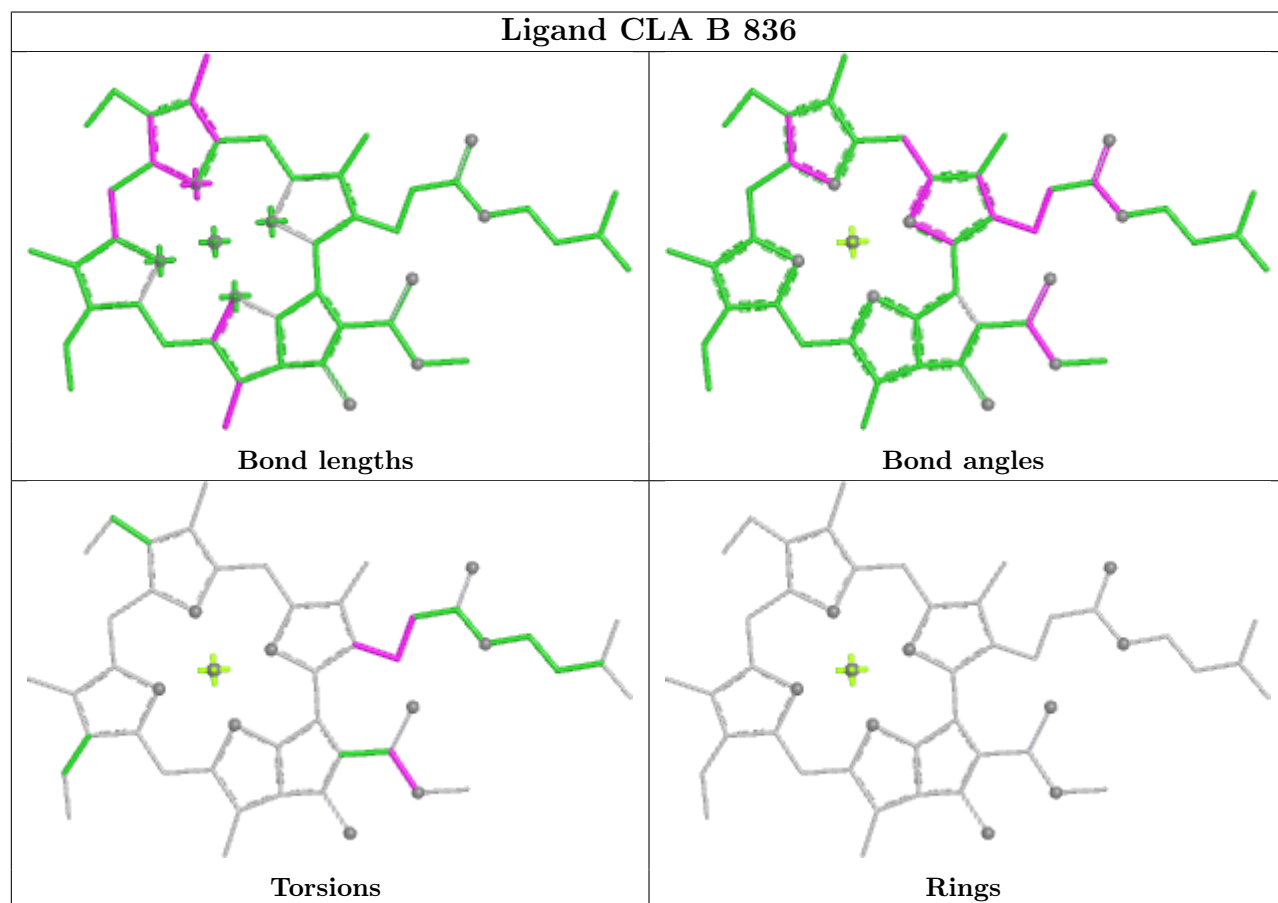
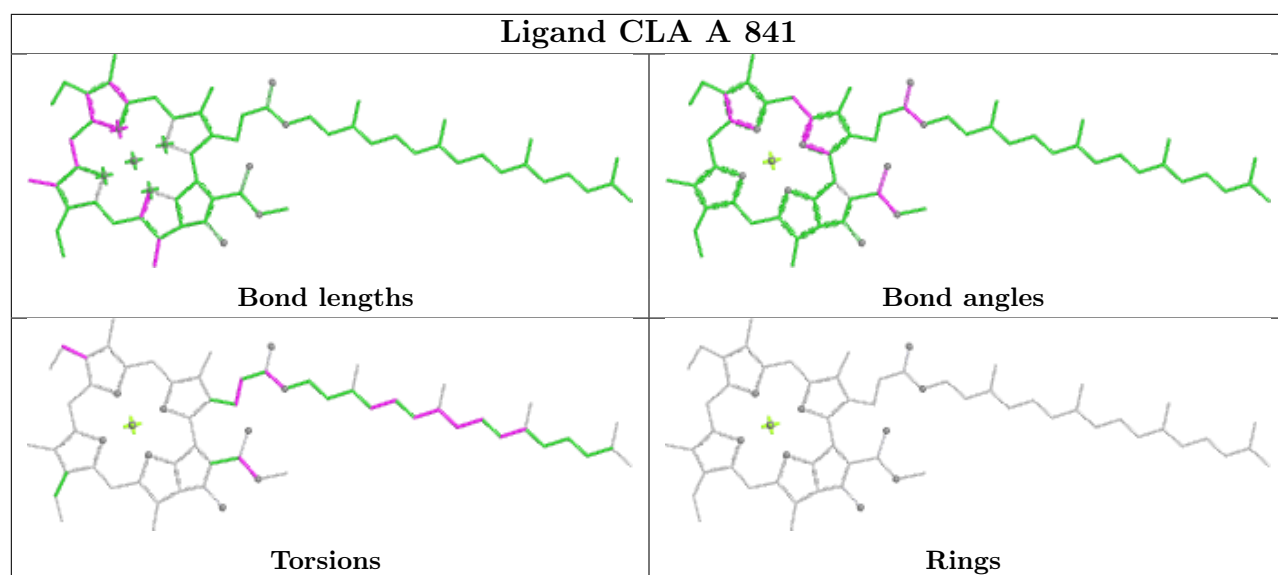
Rings

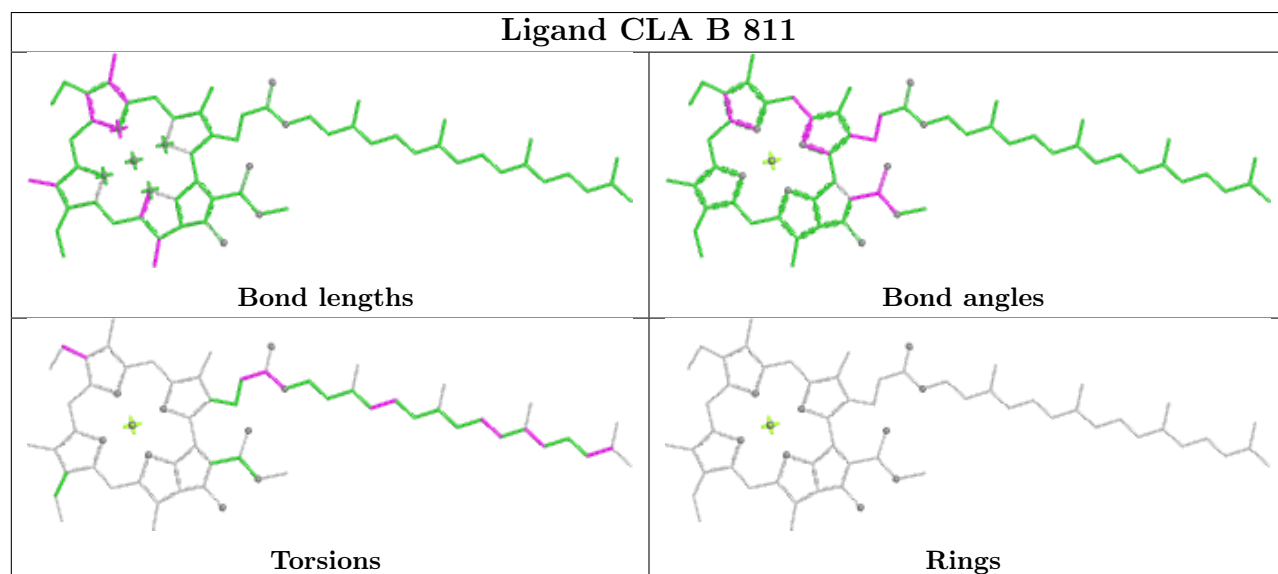
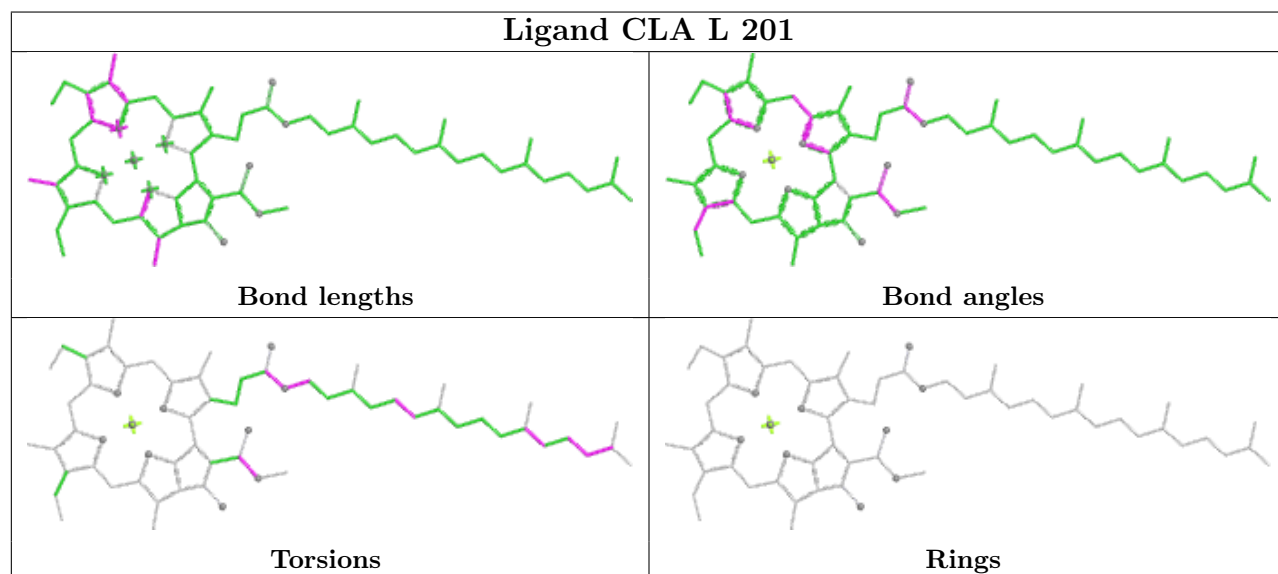
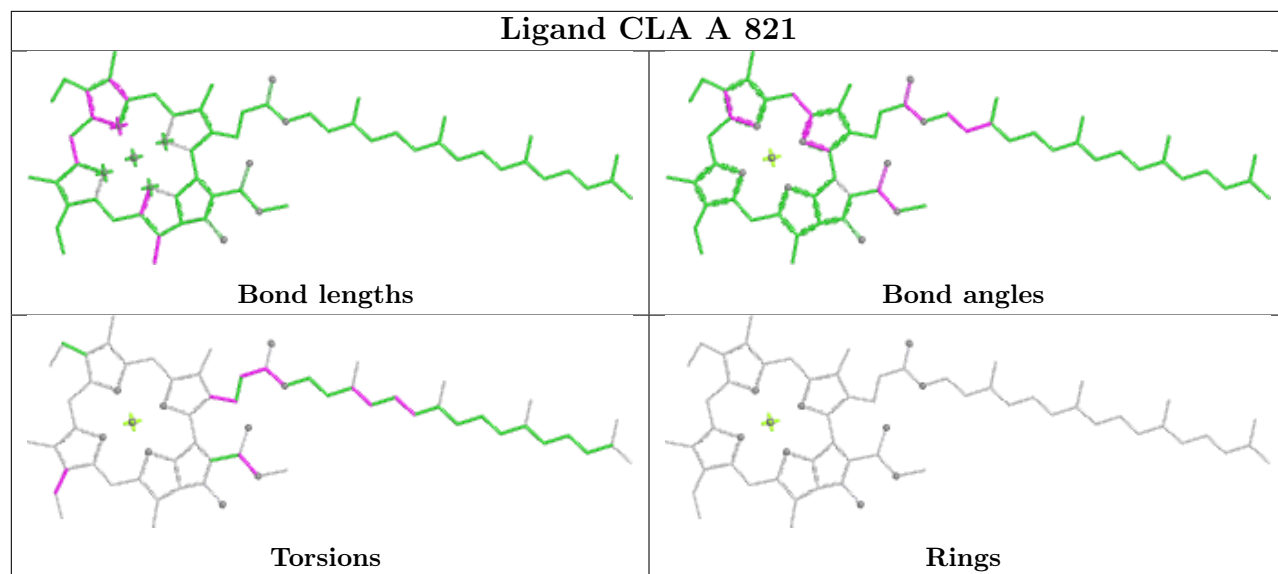
Ligand CLA A 837

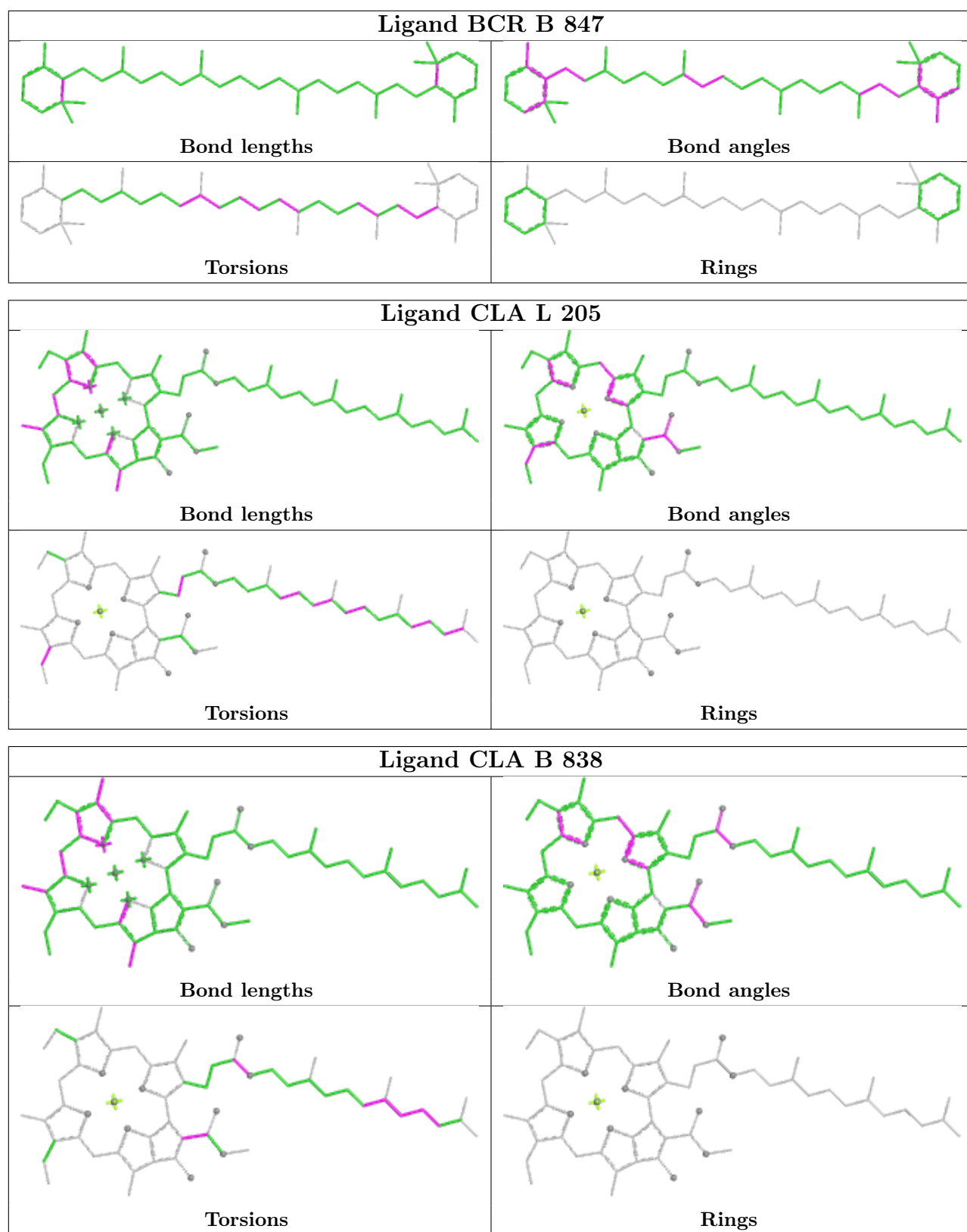


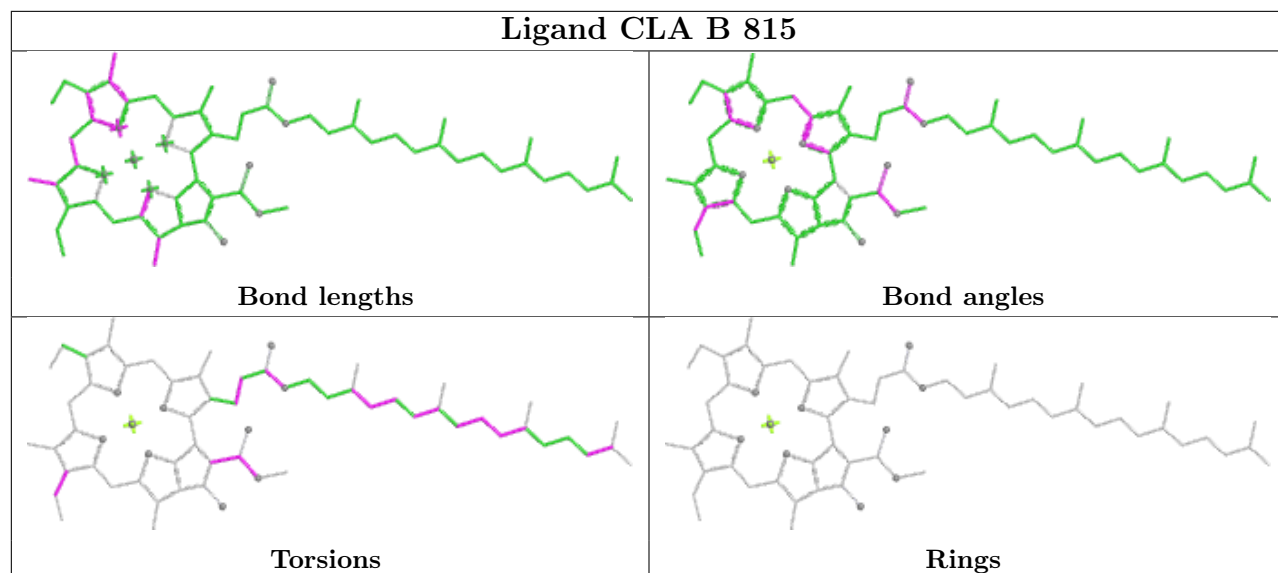
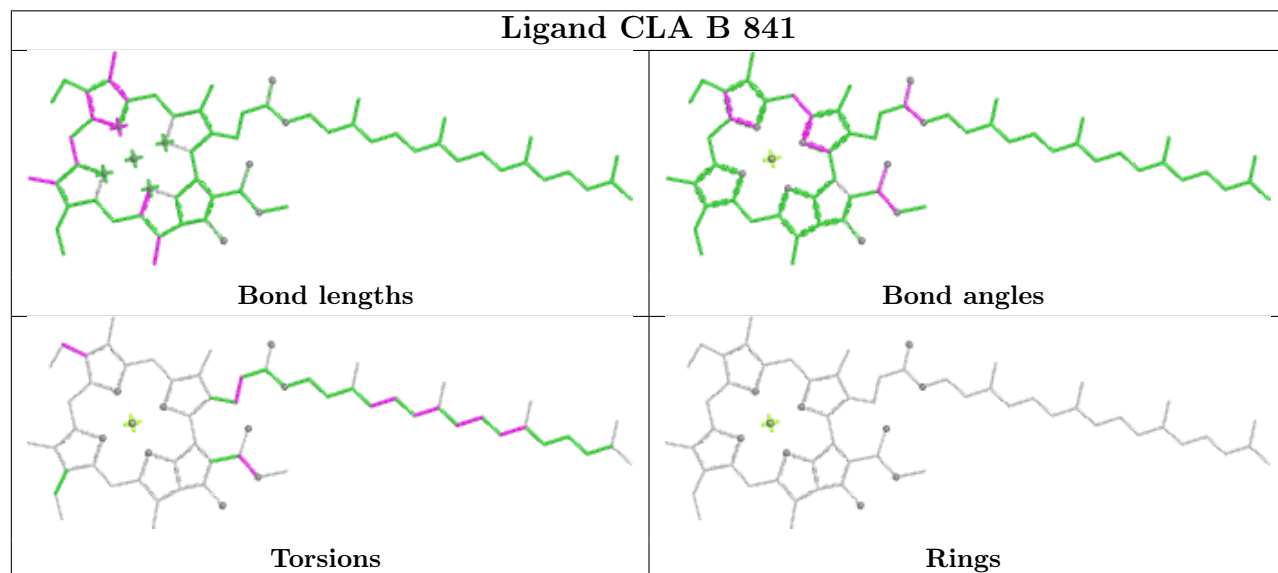
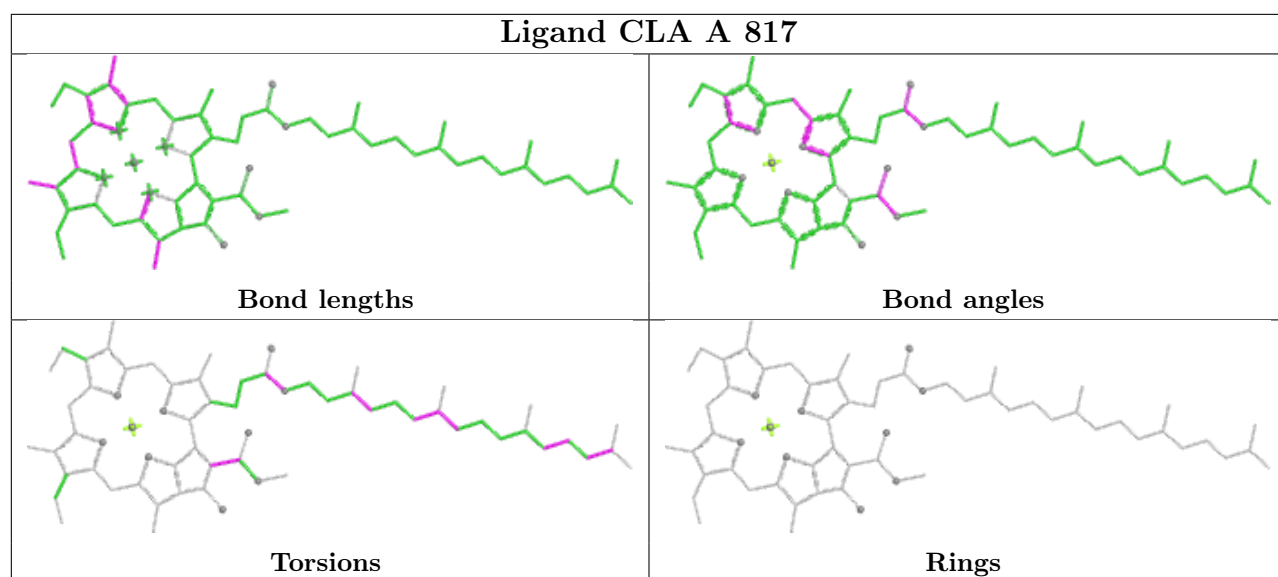
Ligand CLA B 827

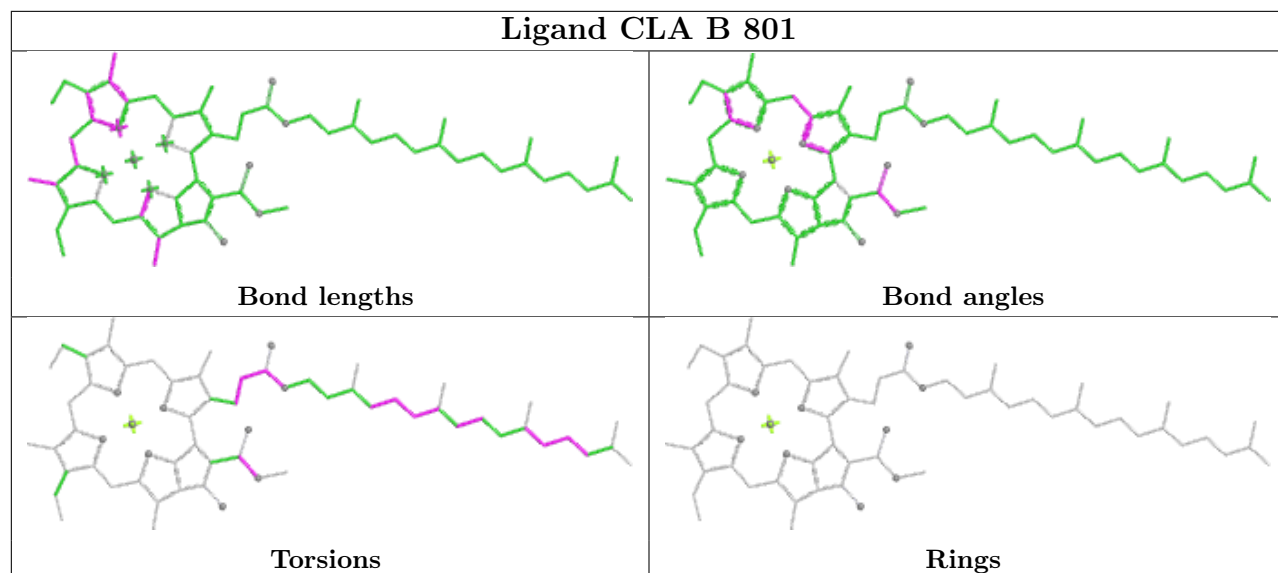
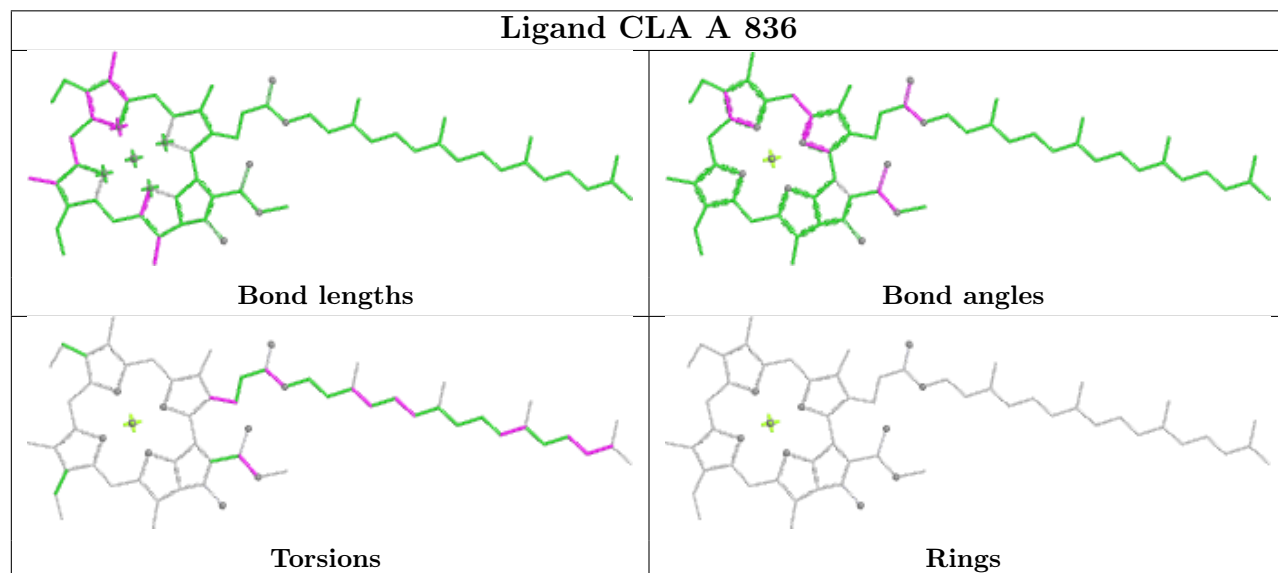
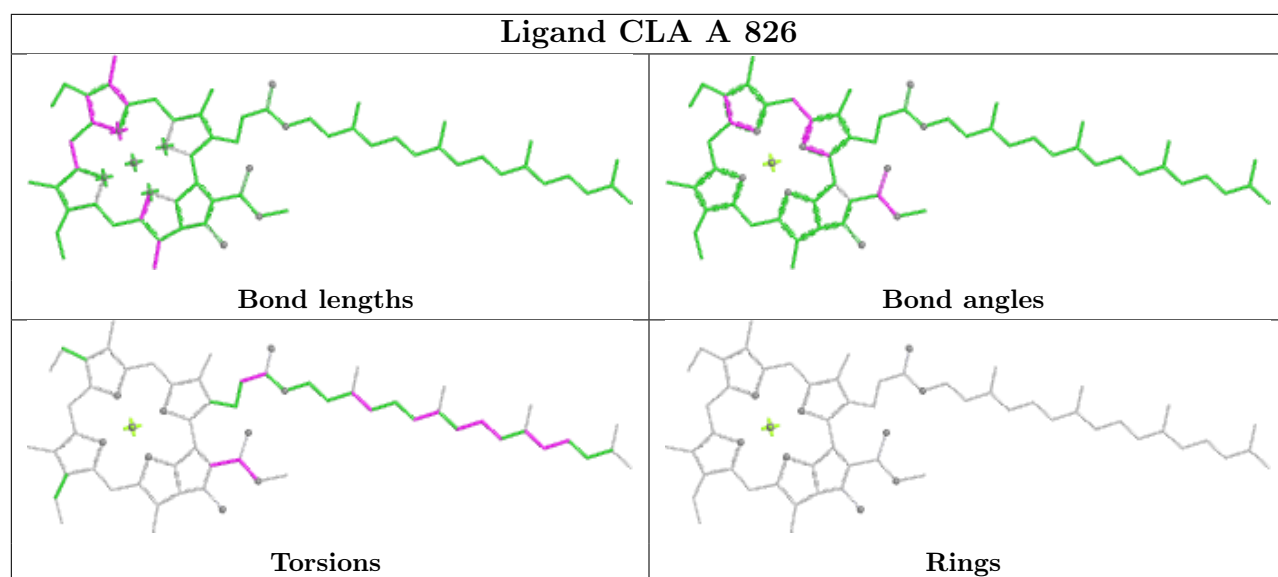


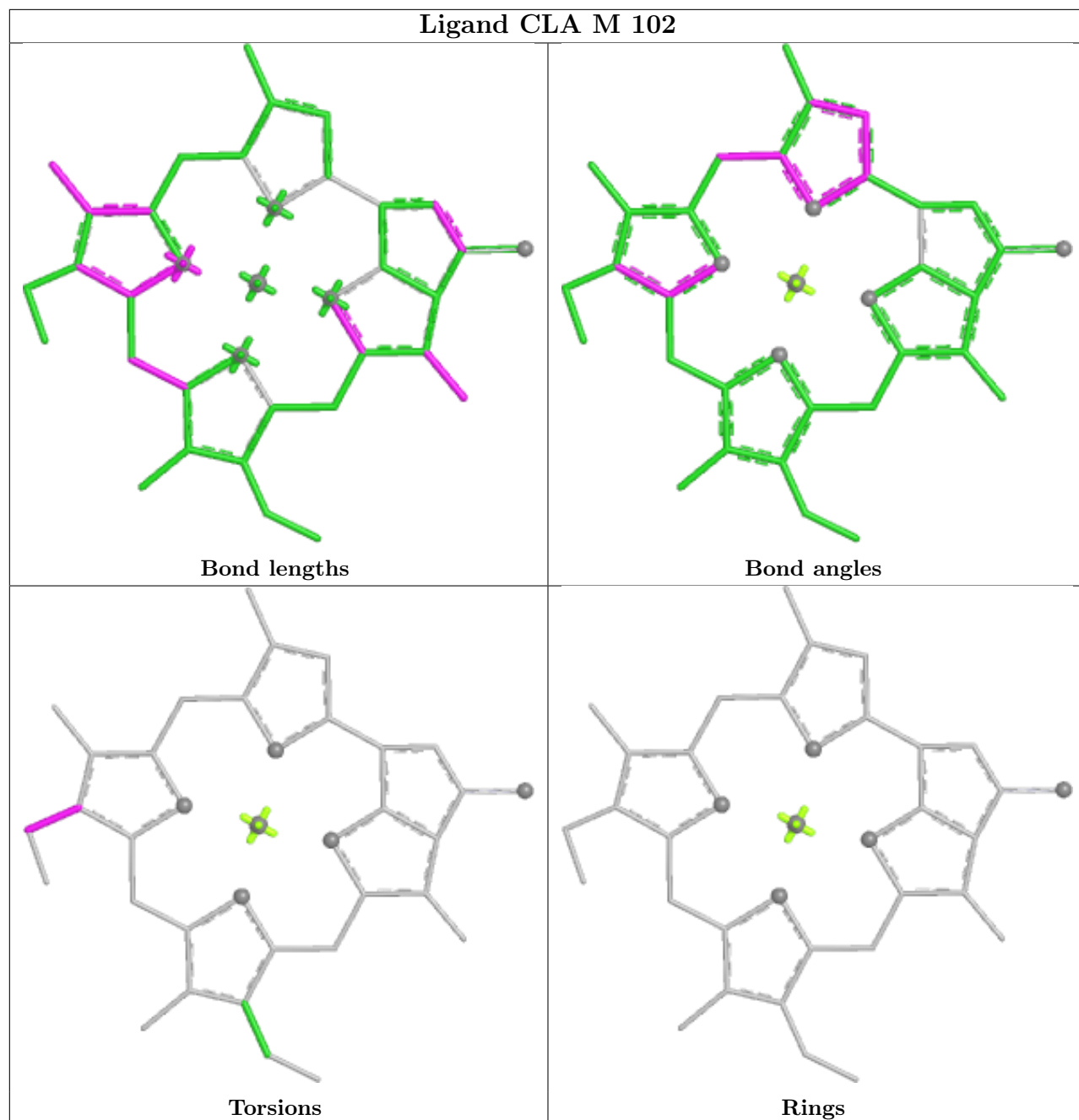


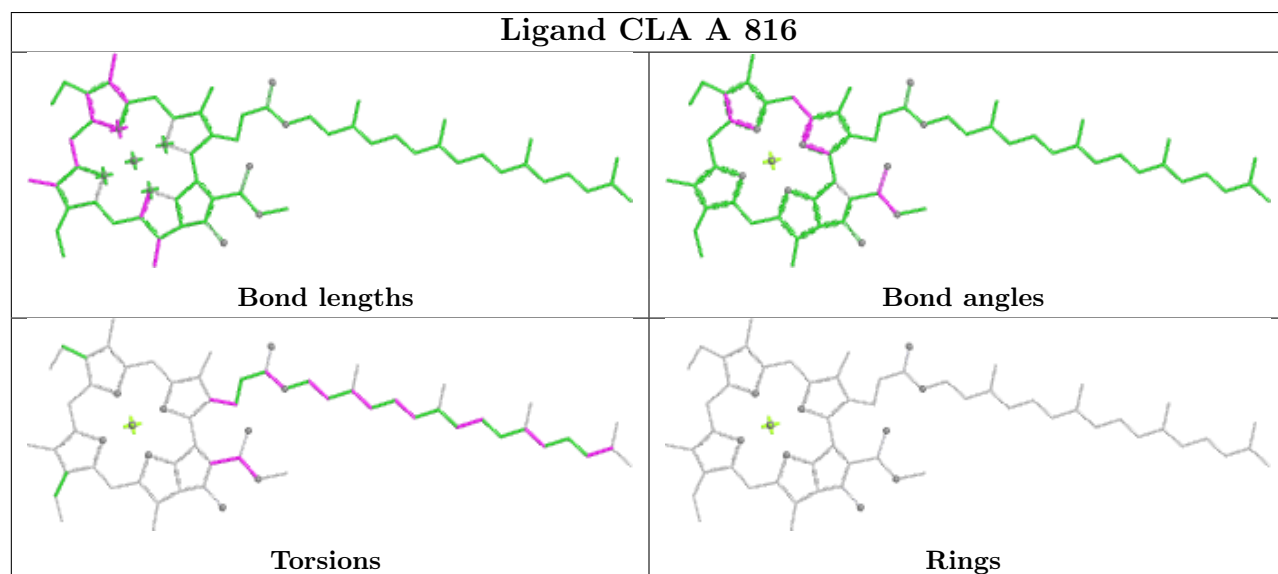
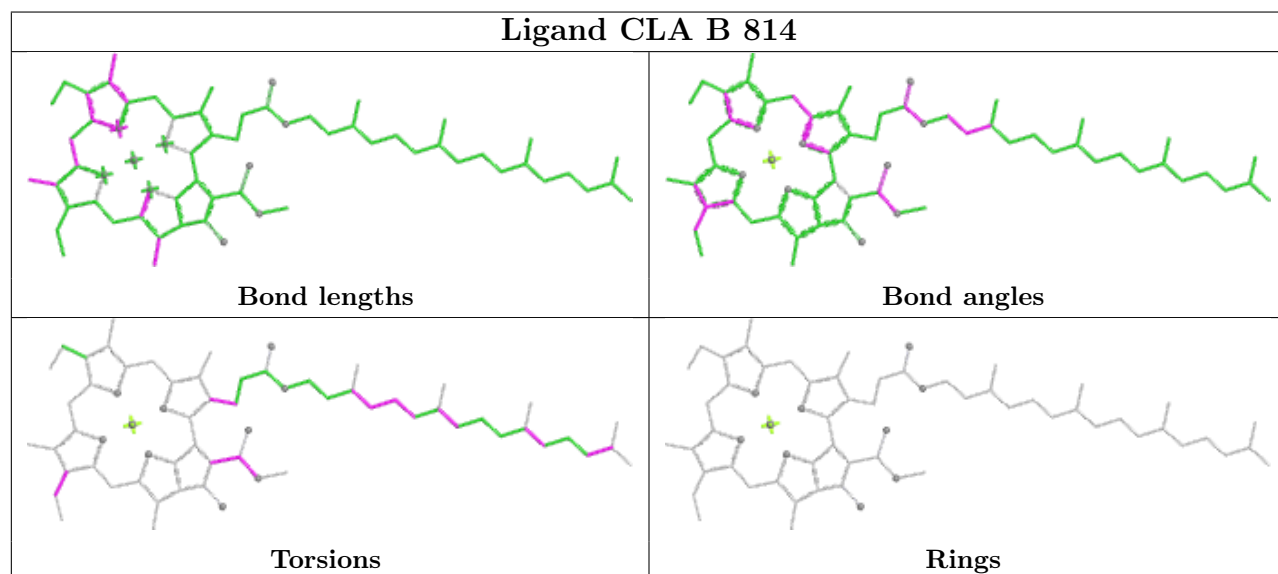
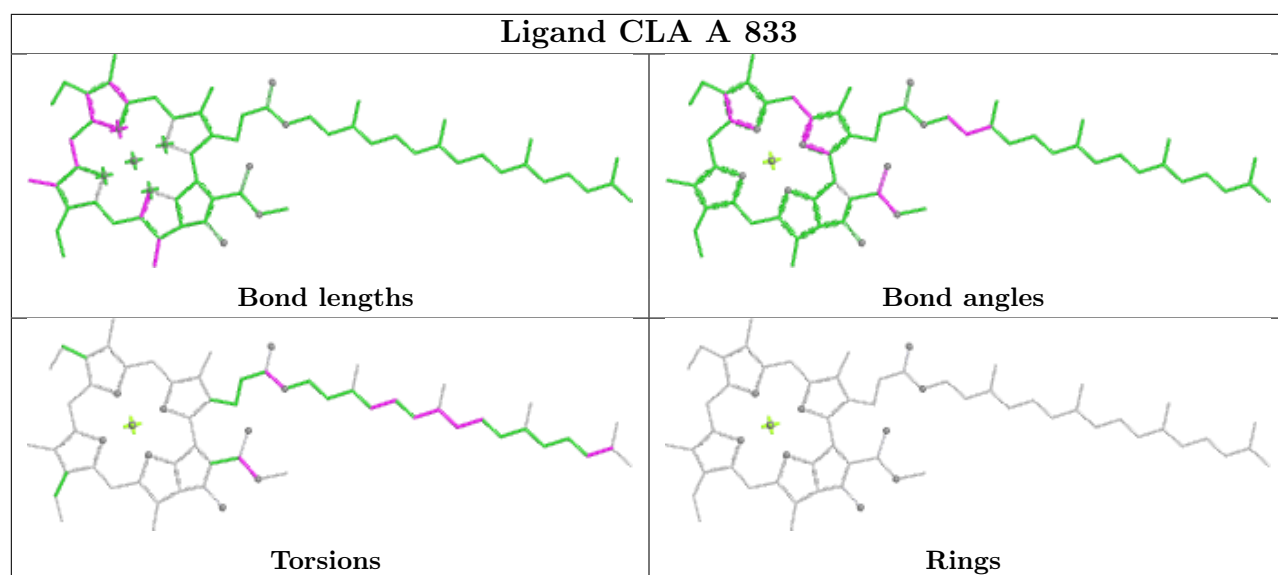


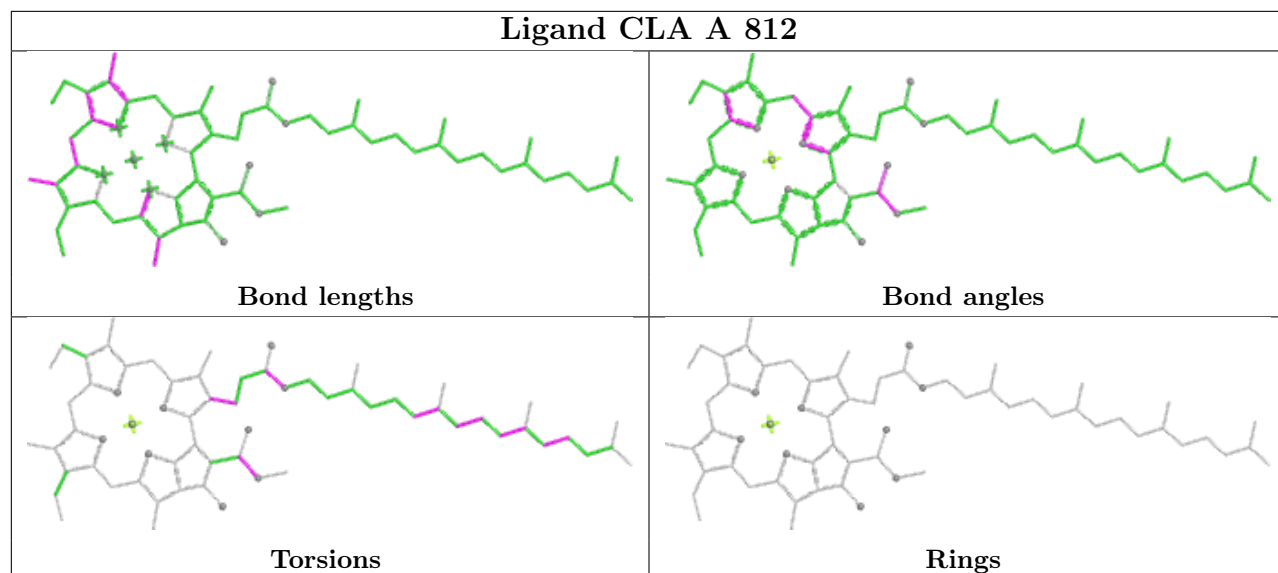
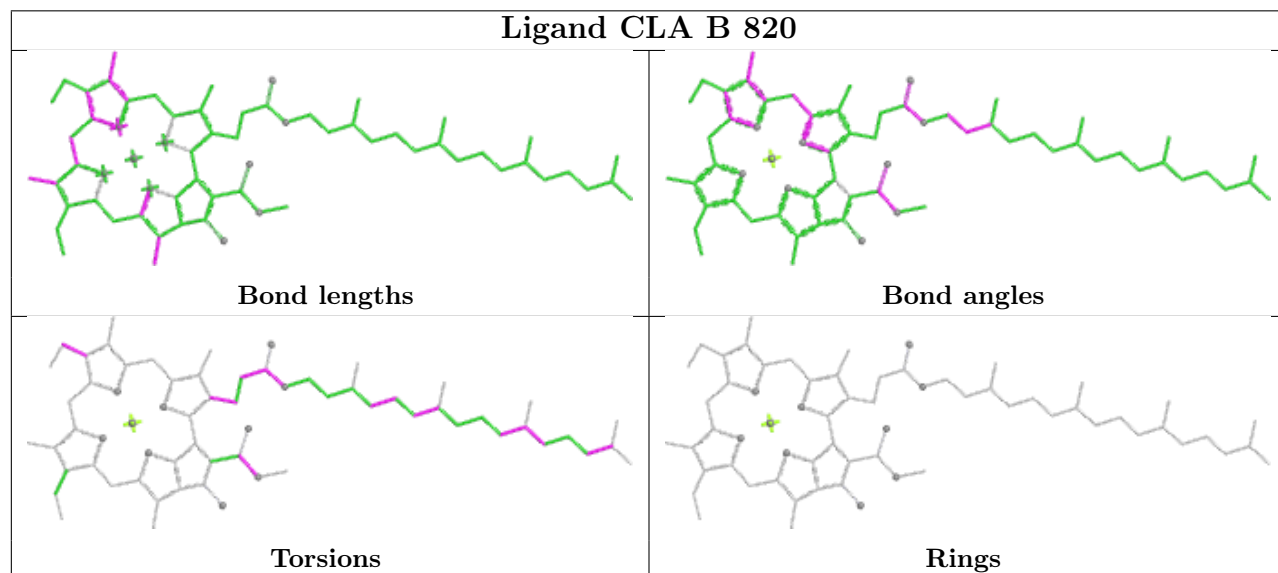
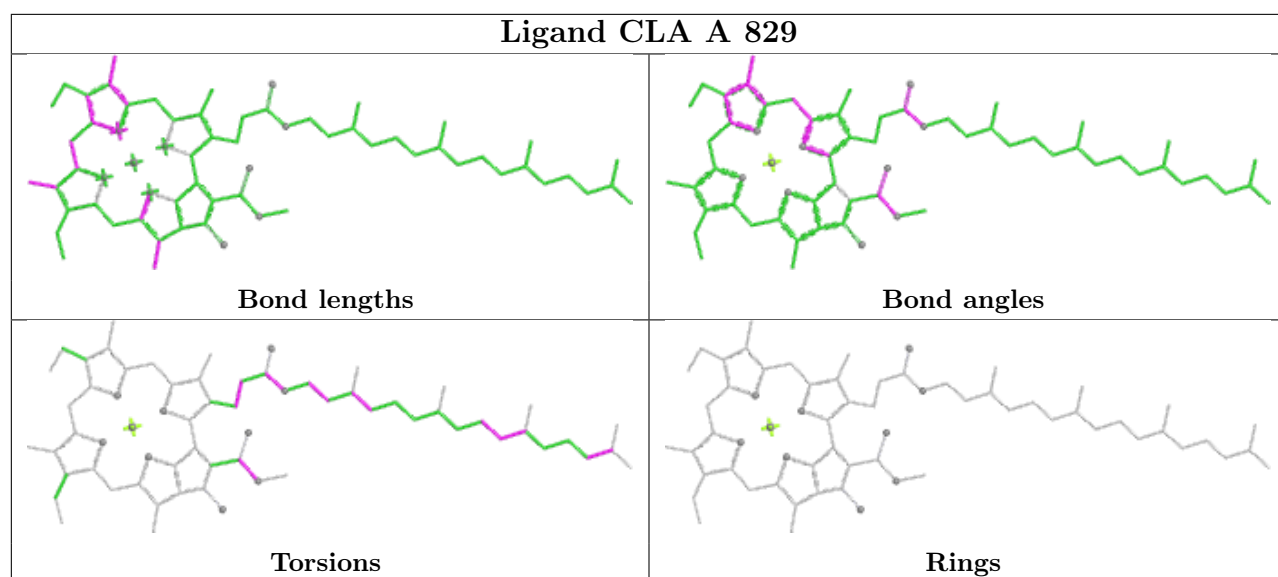




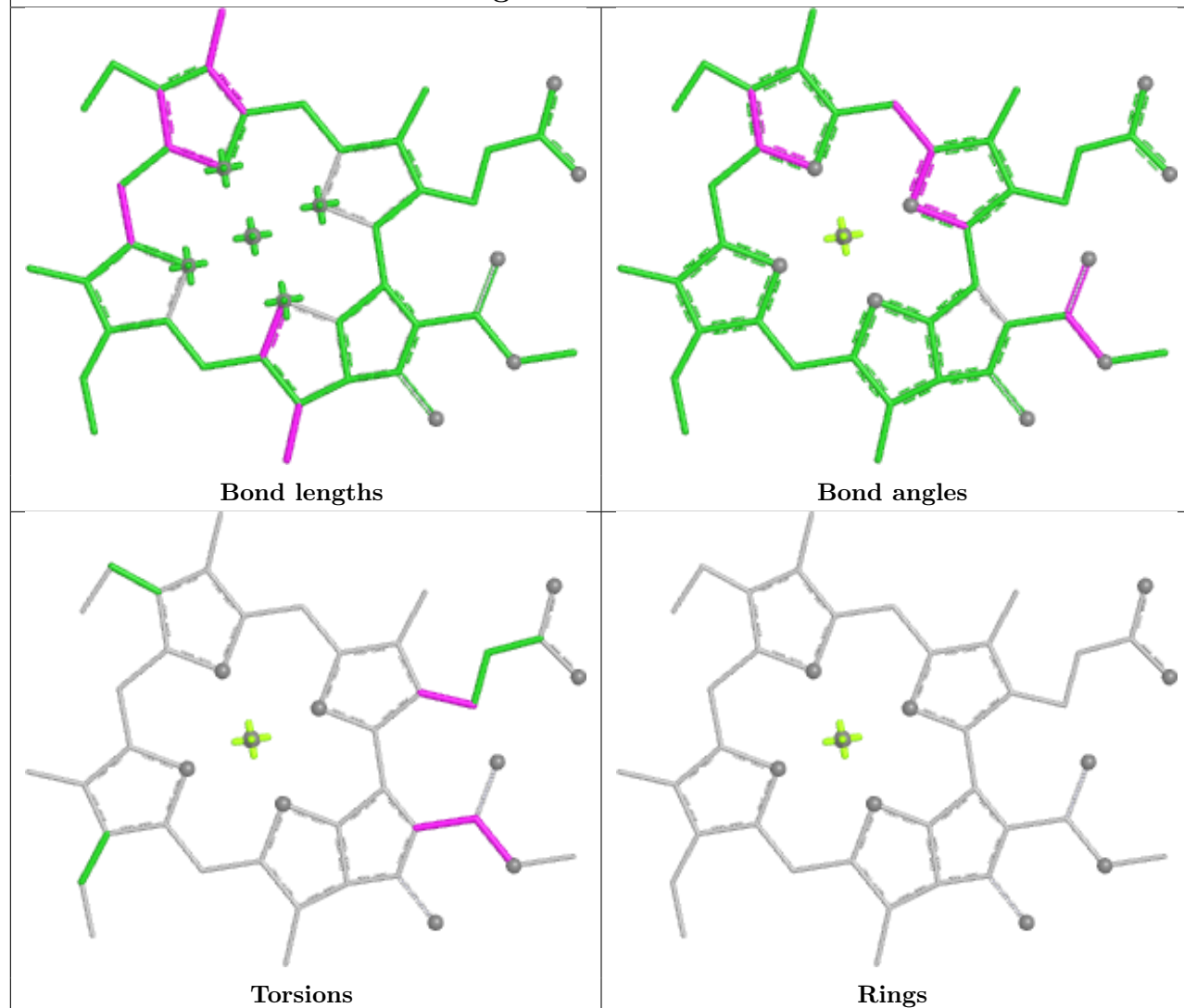




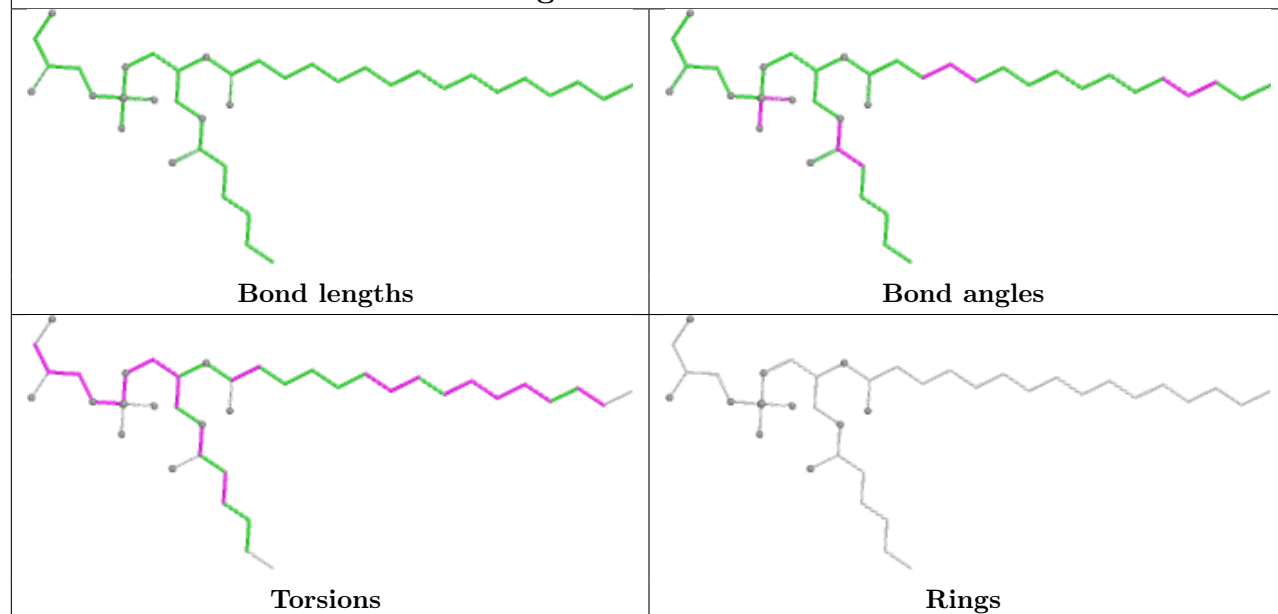




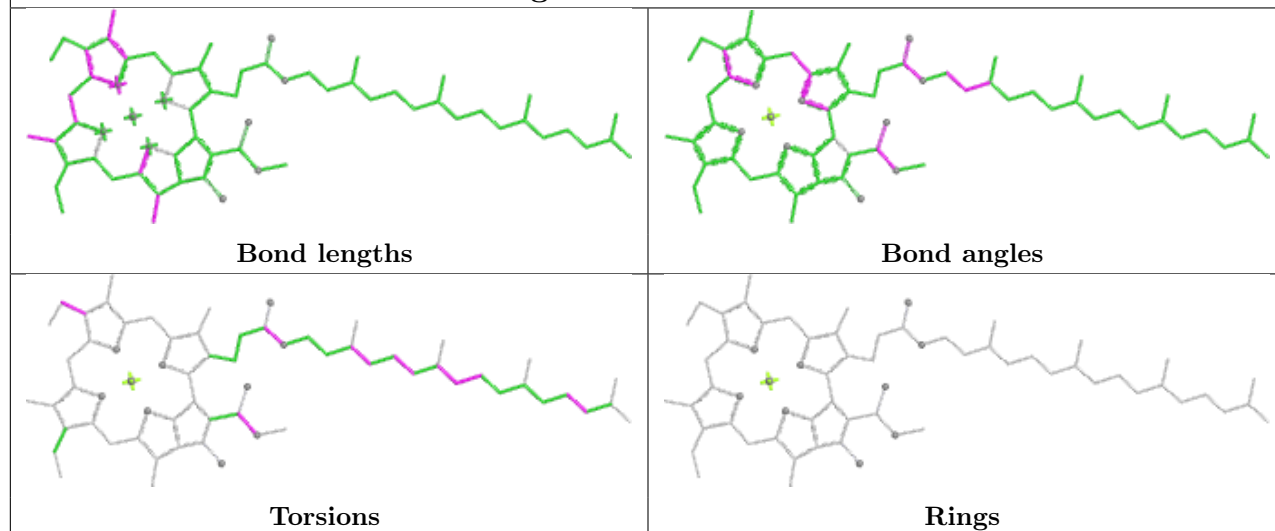
Ligand CLA B 837



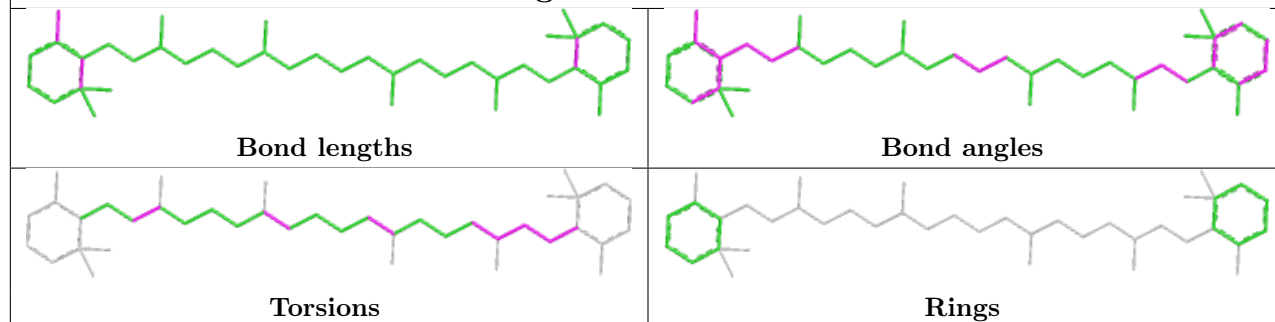
Ligand LHG I 102



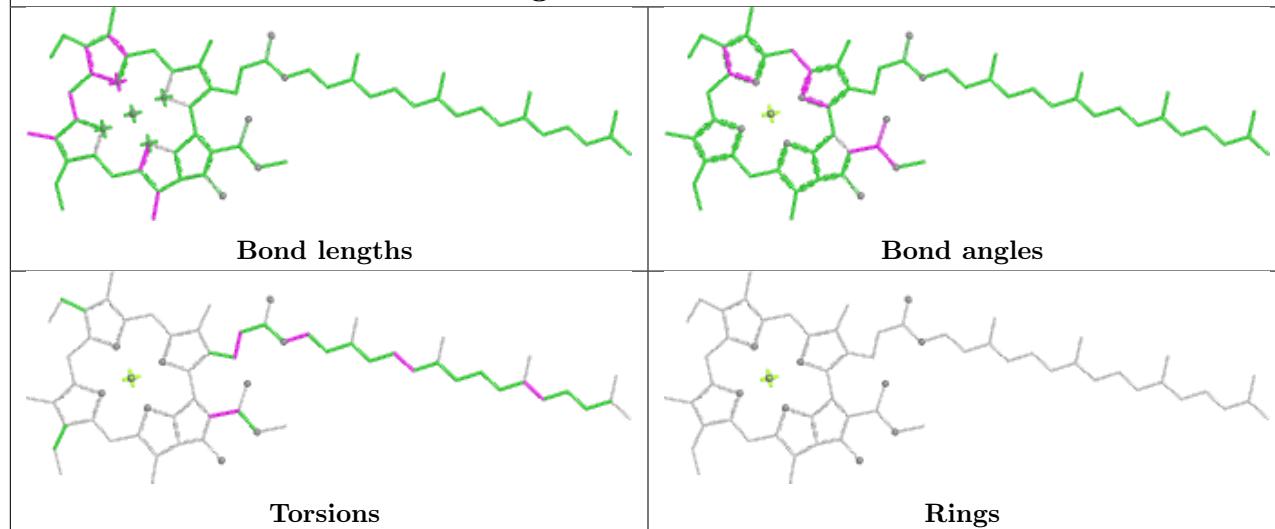
Ligand CLA A 825

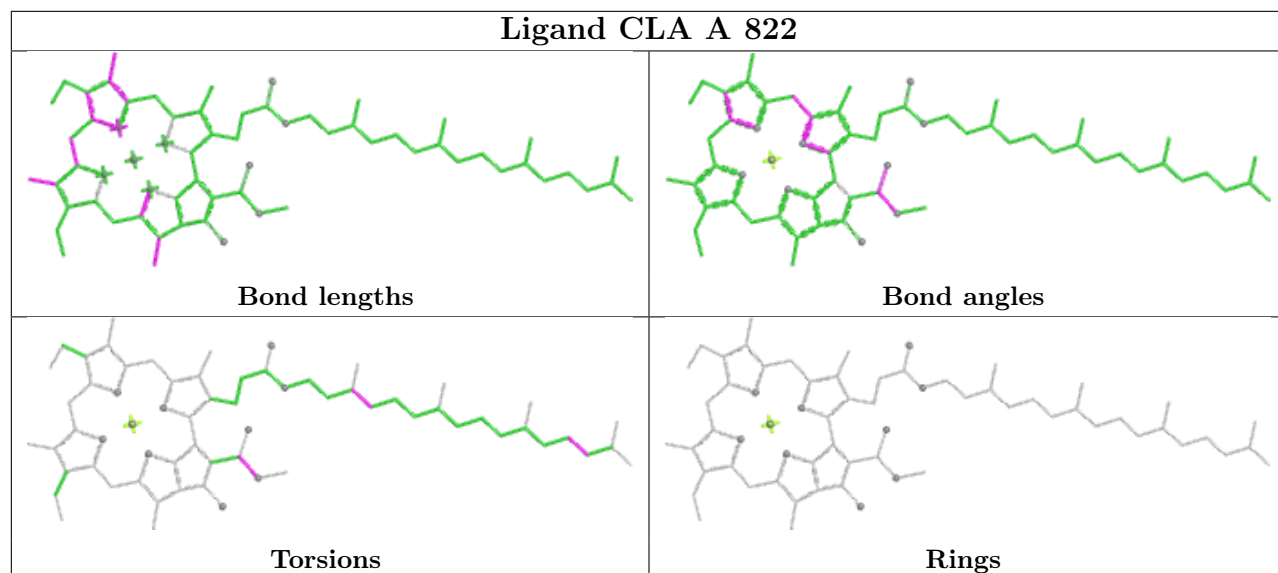
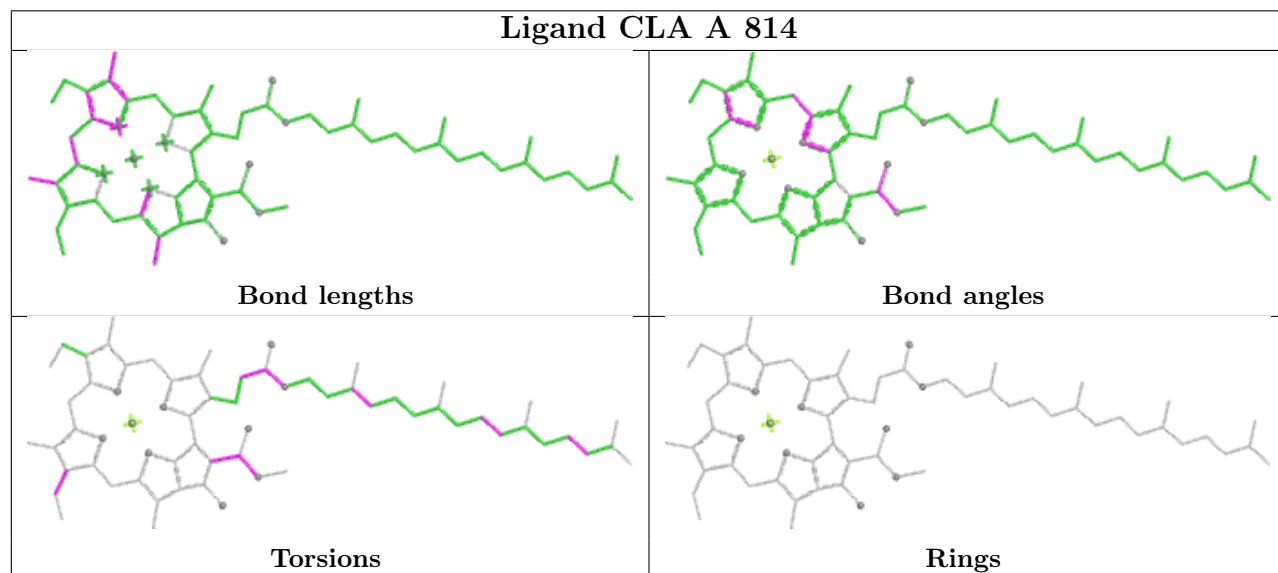
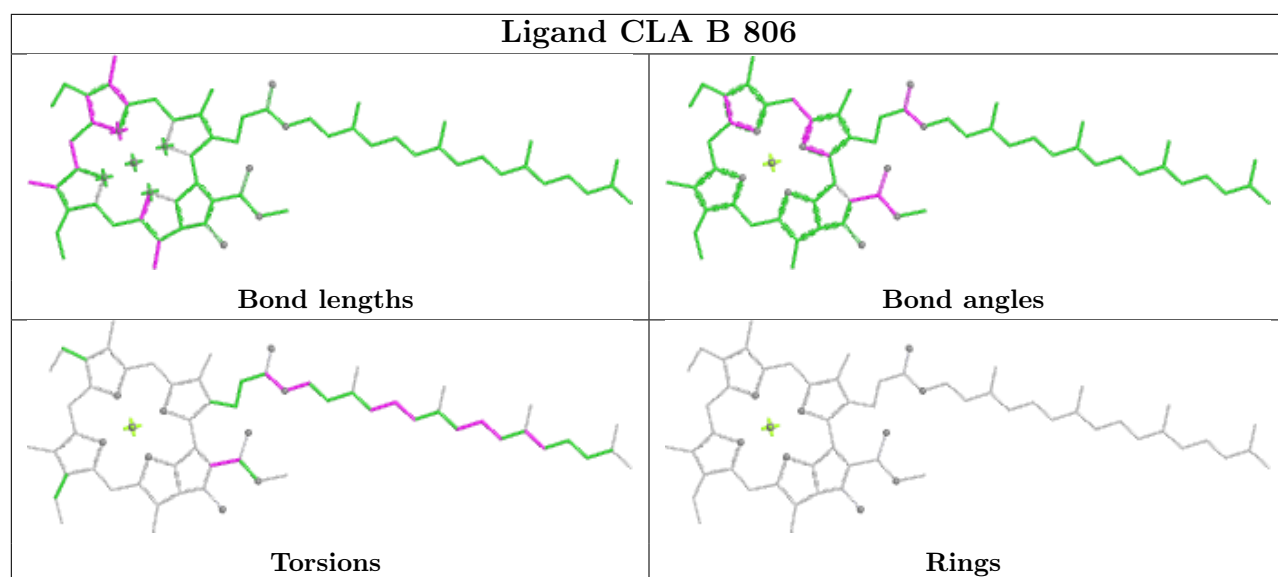


Ligand BCR I 103

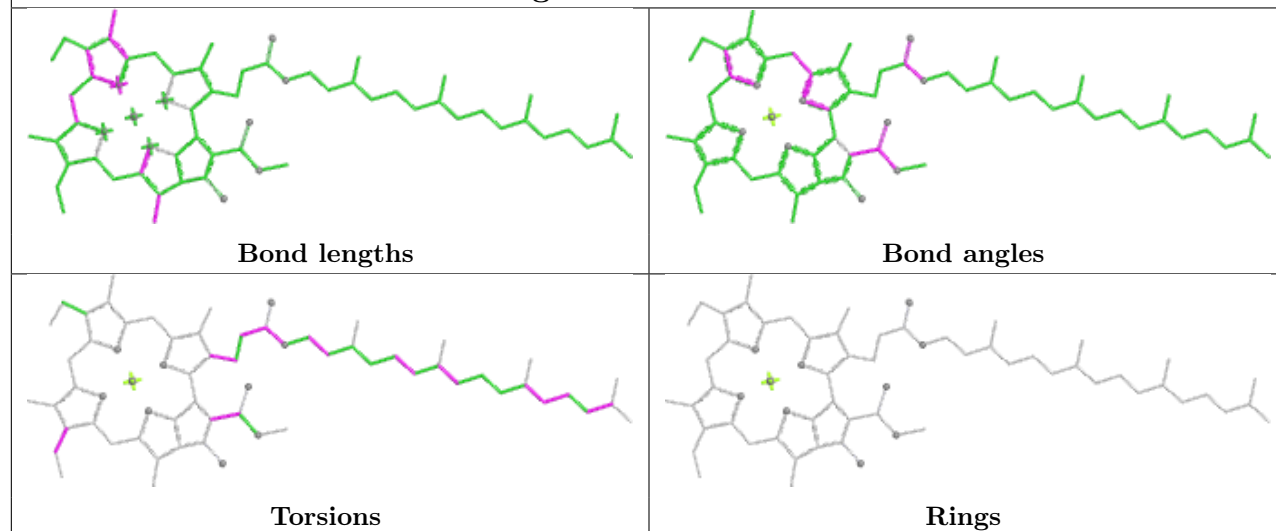


Ligand CLA A 835

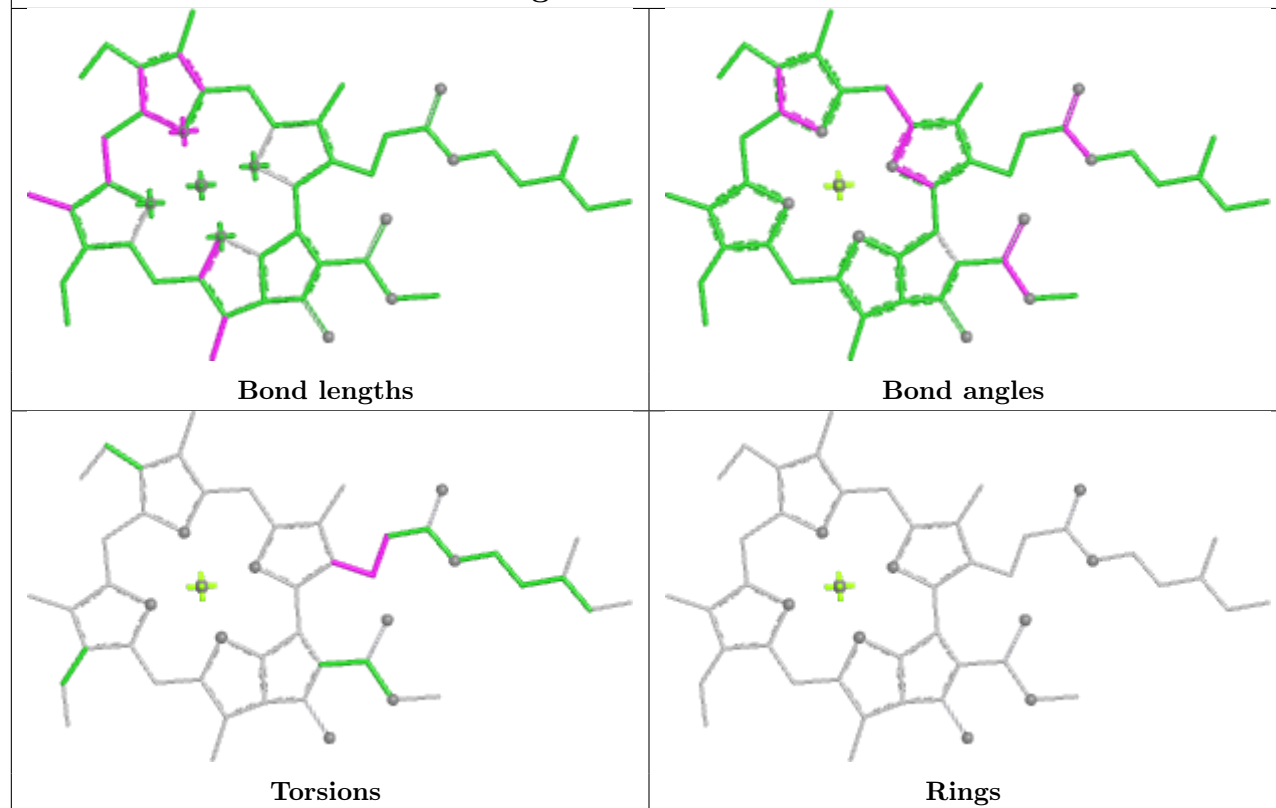


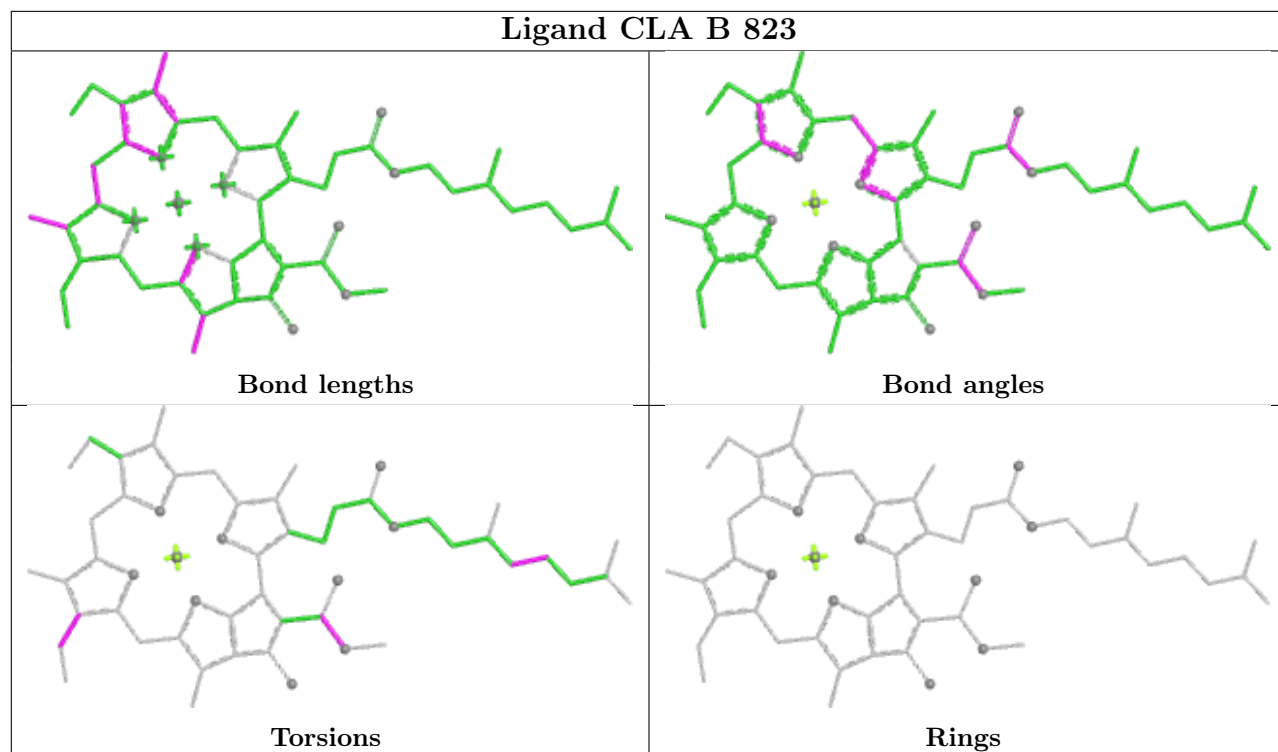
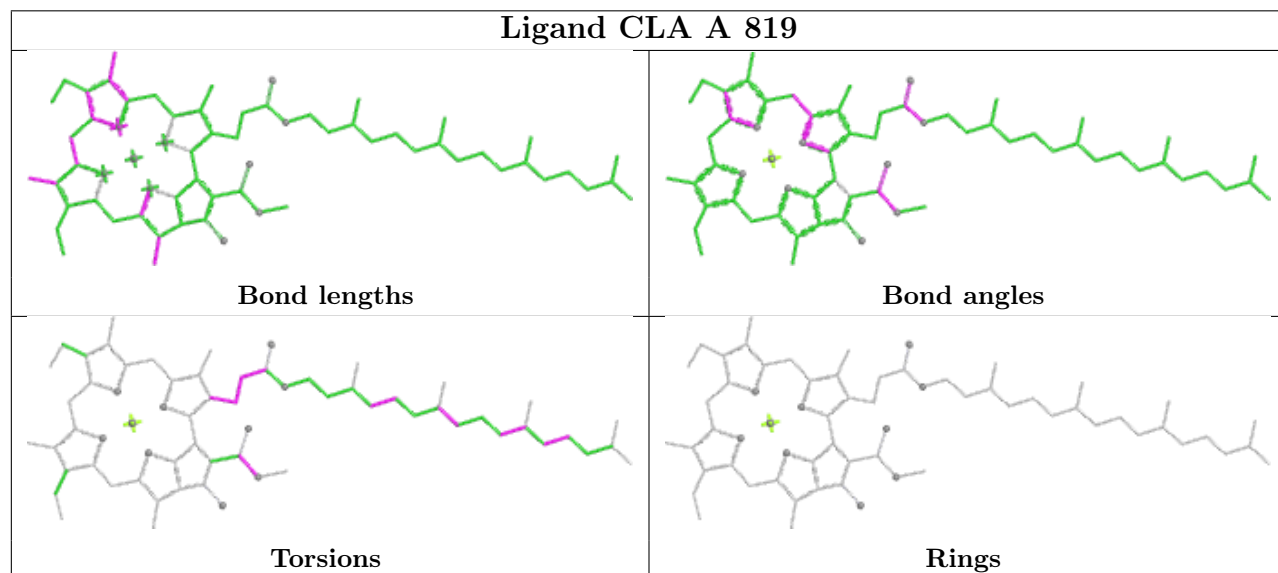
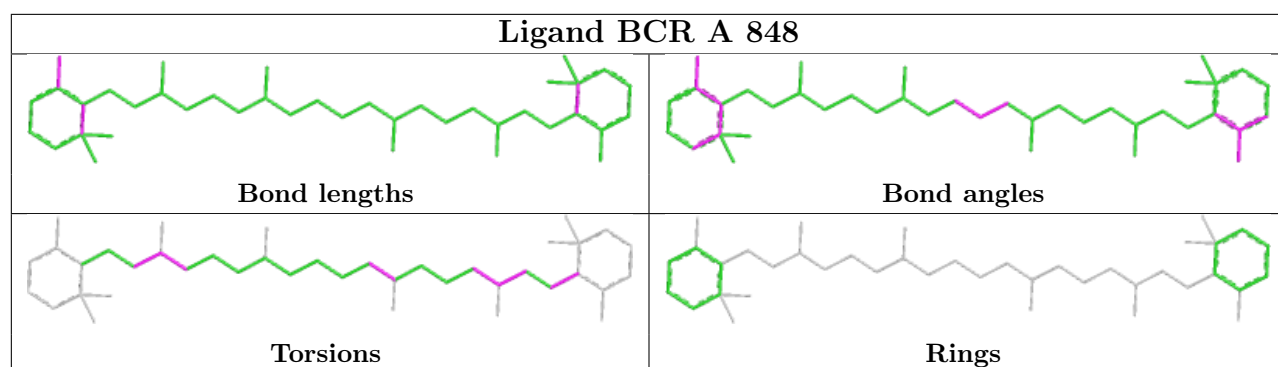


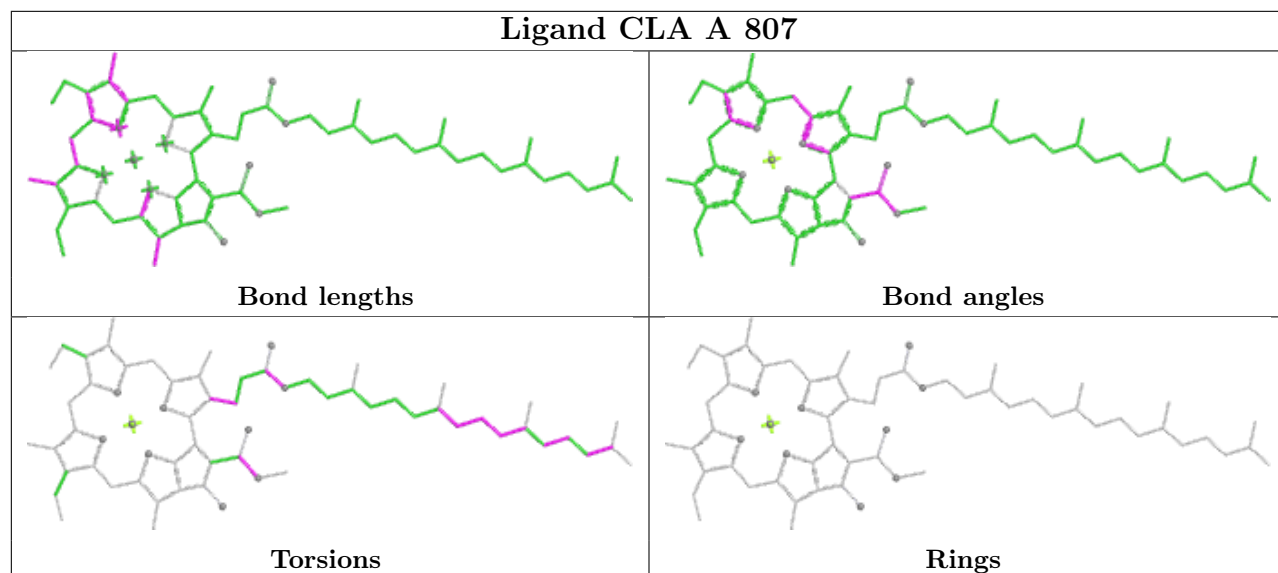
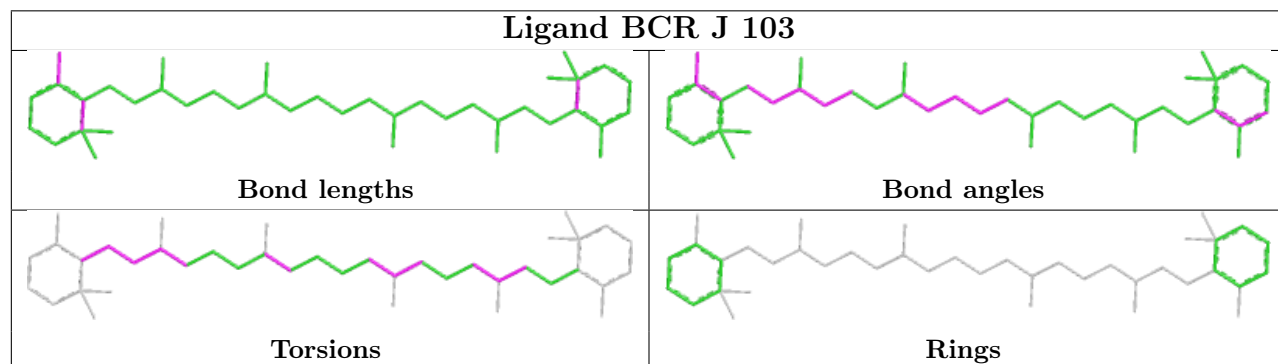
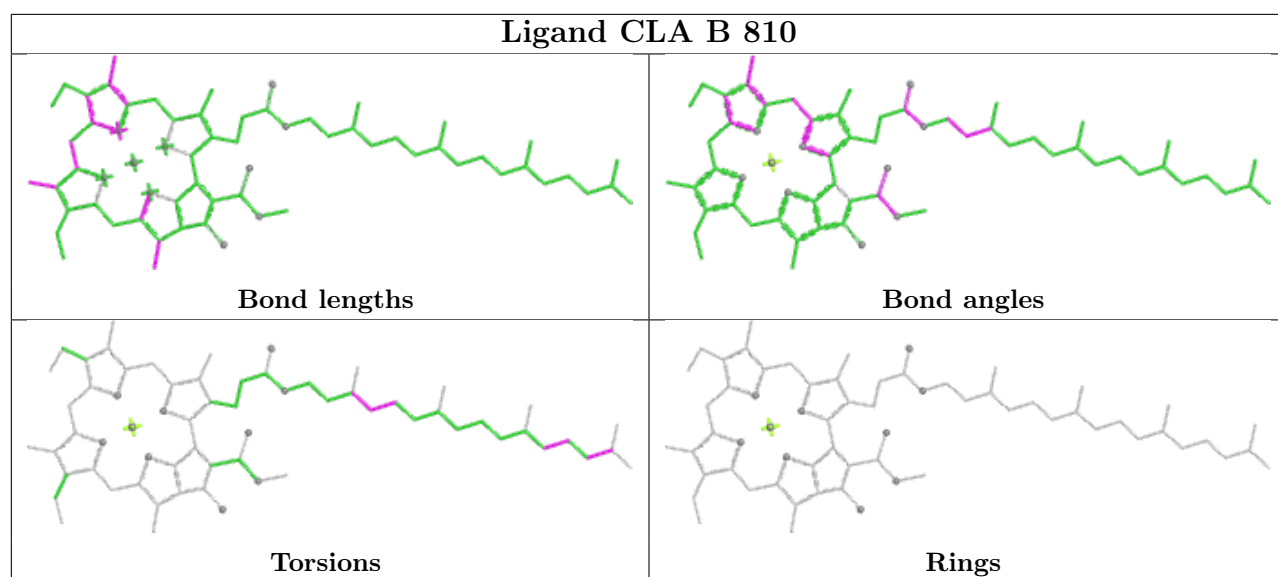
Ligand CLA B 817

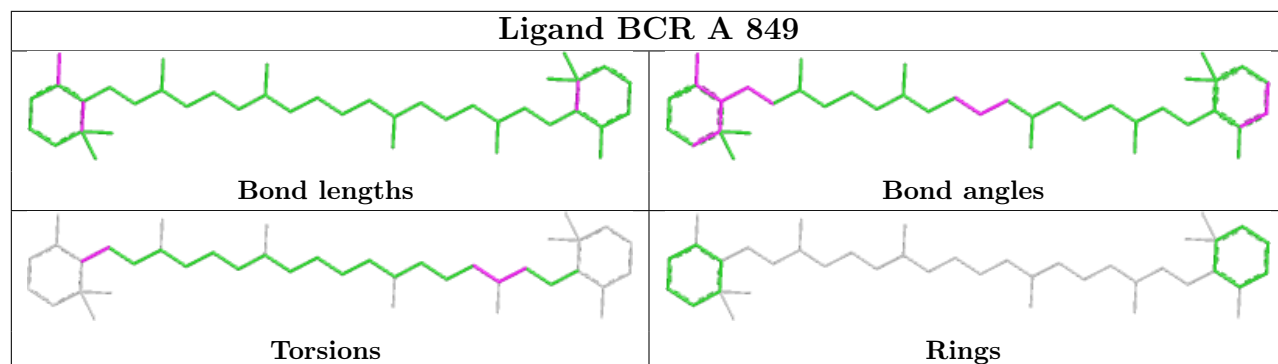
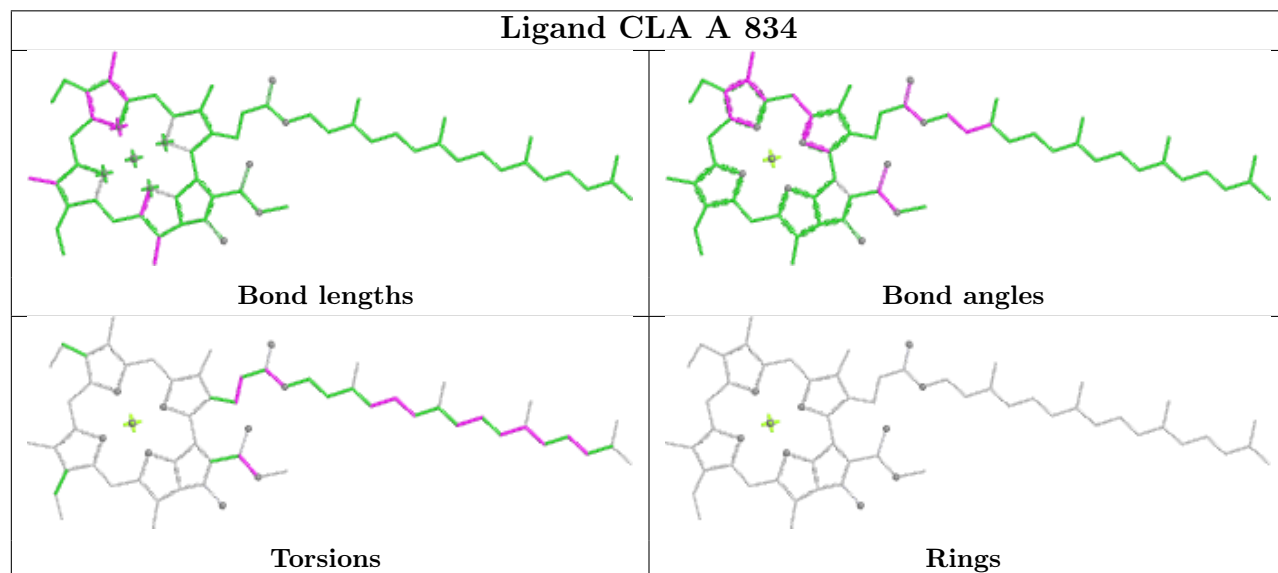
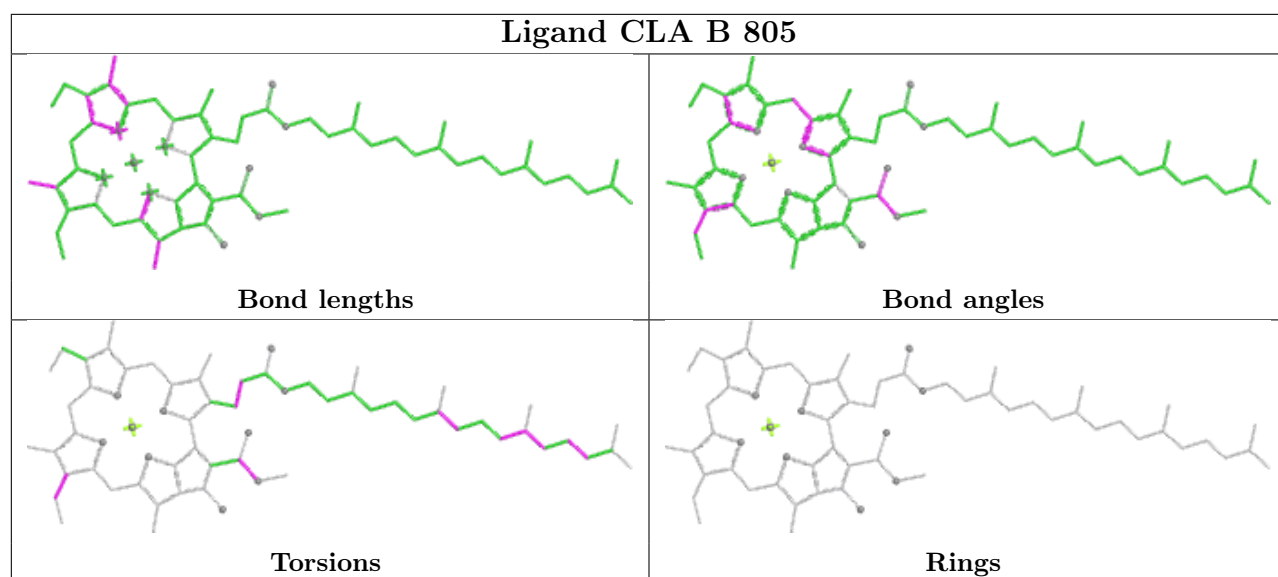


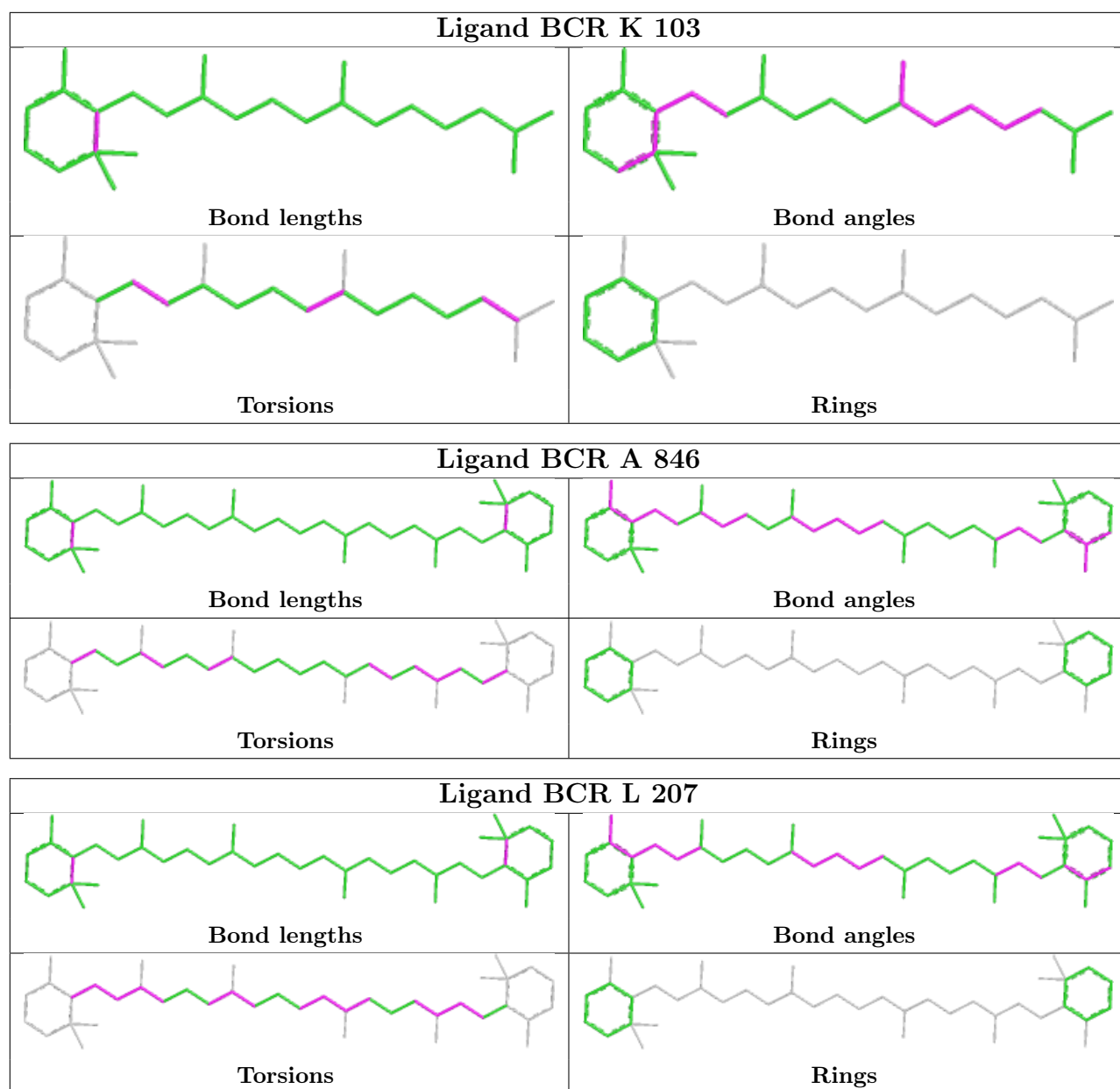
Ligand CLA A 808

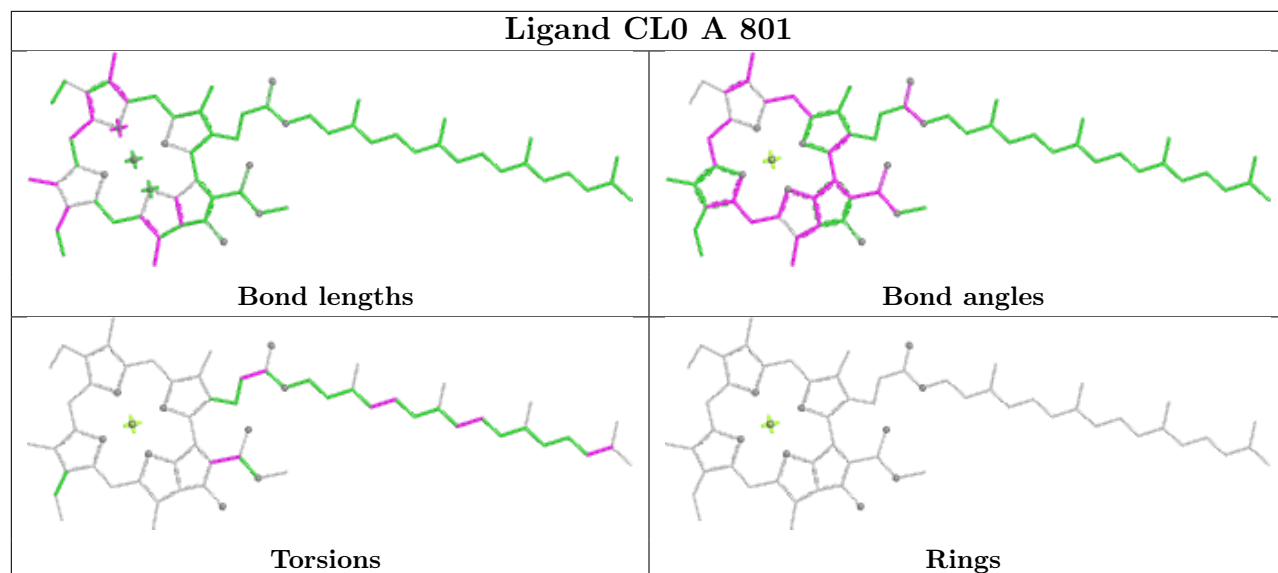
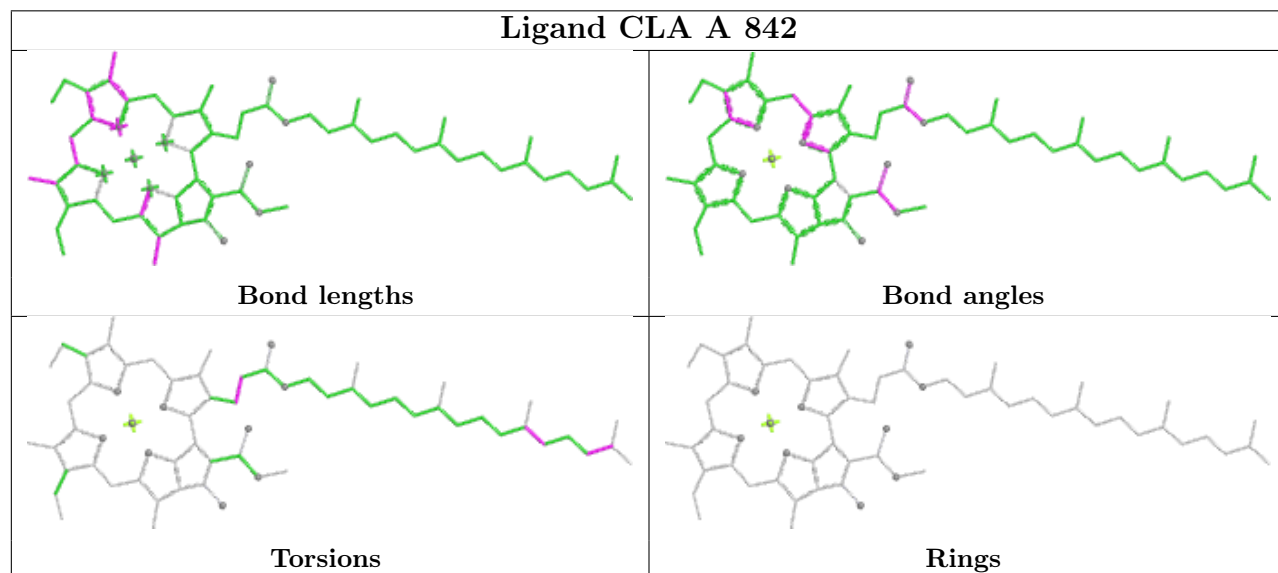
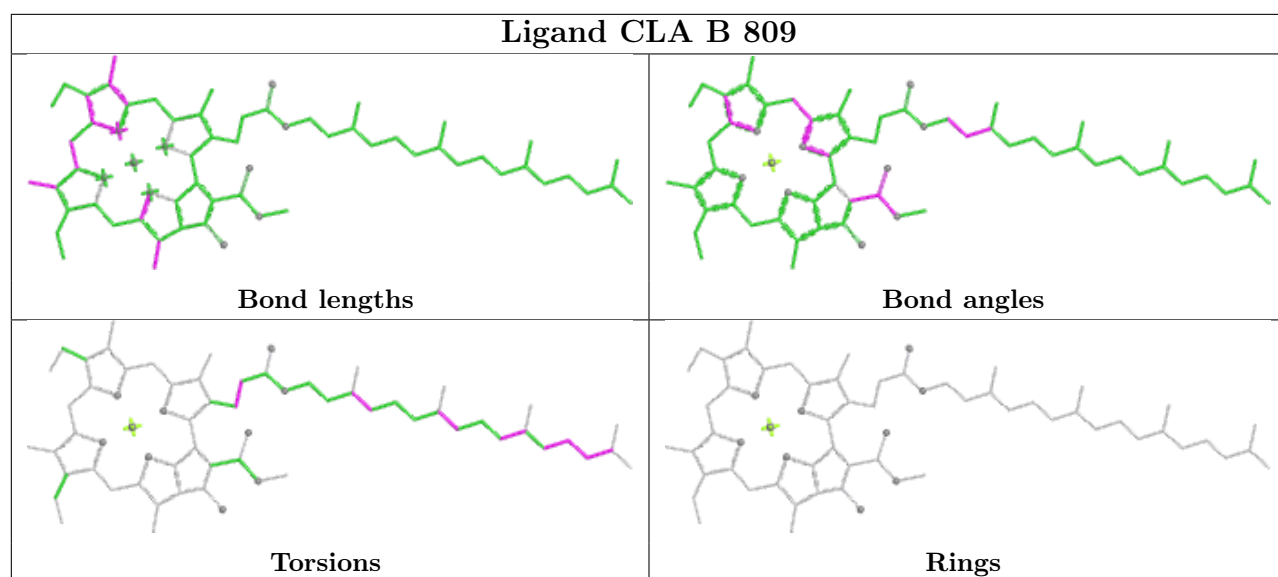


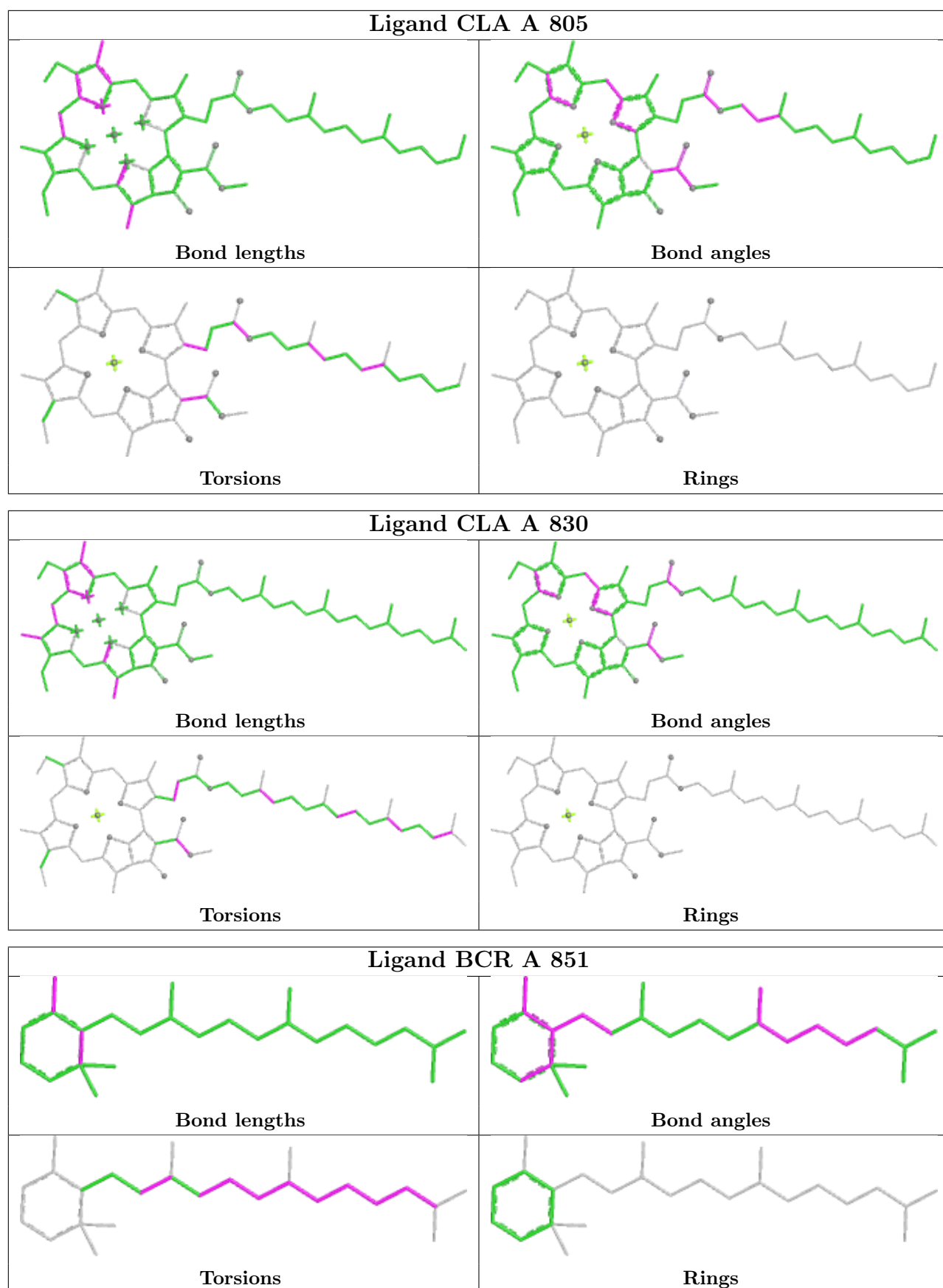




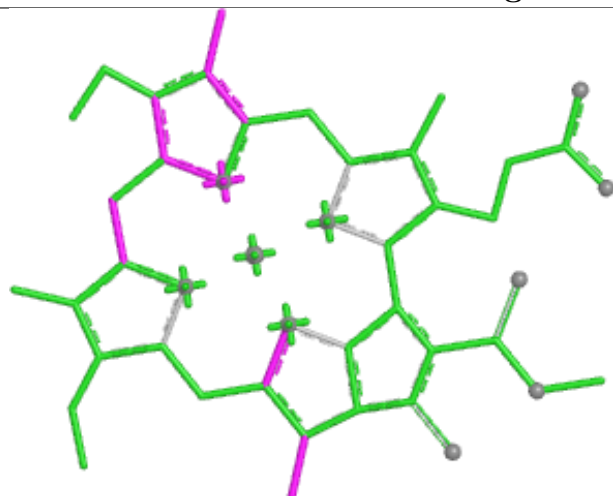




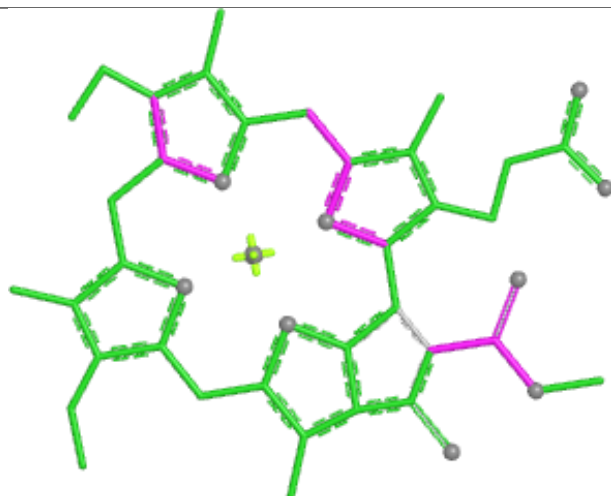




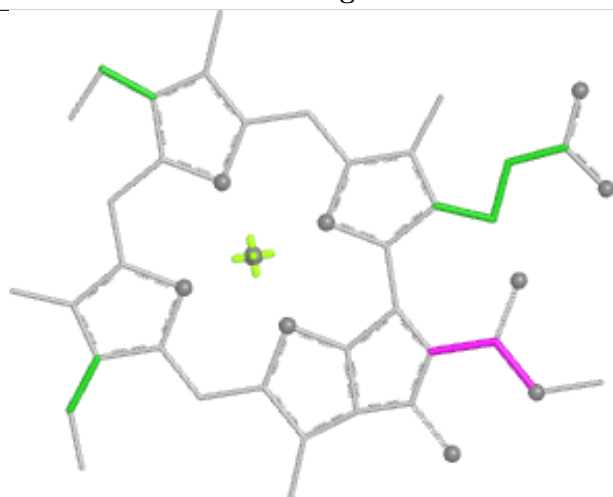
Ligand CLA X 1701



Bond lengths



Bond angles

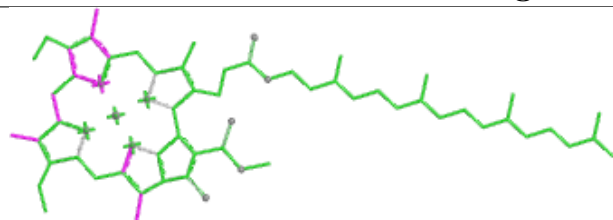


Torsions

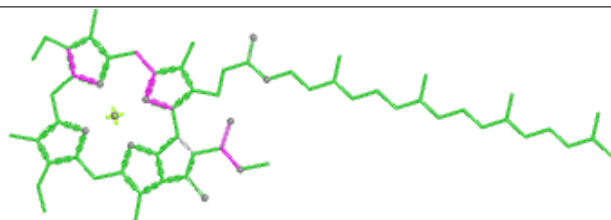


Rings

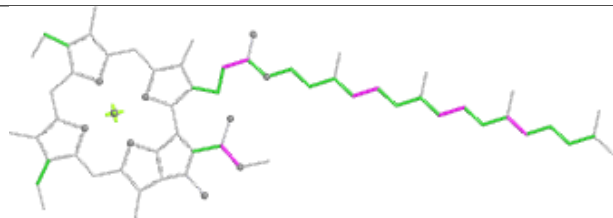
Ligand CLA B 808



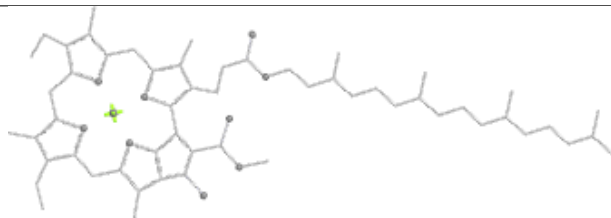
Bond lengths



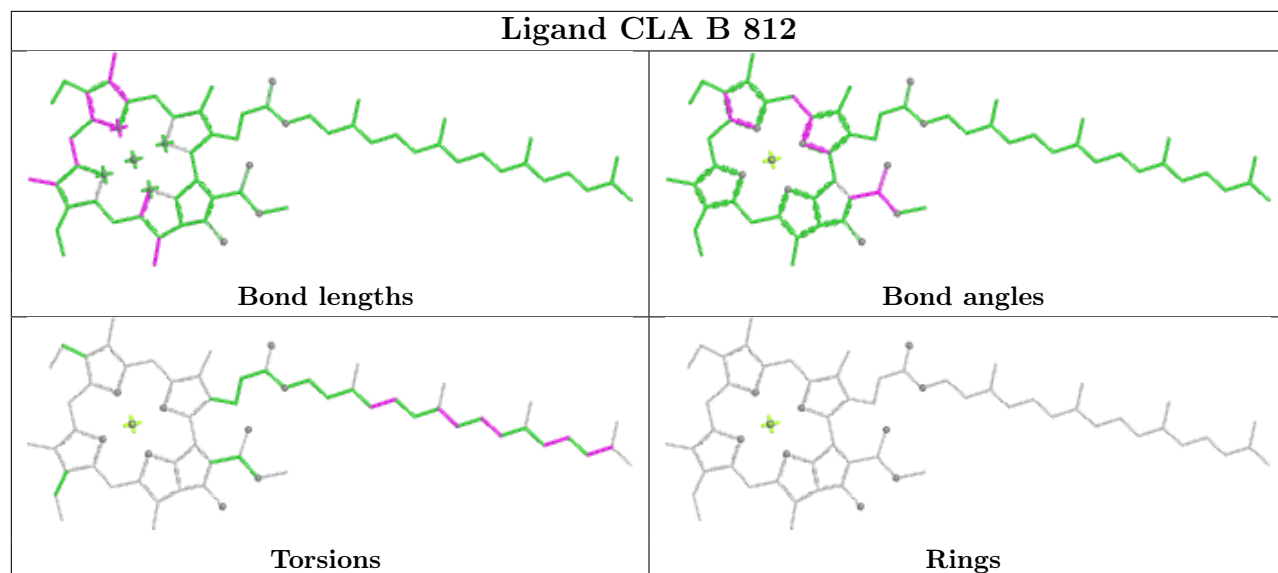
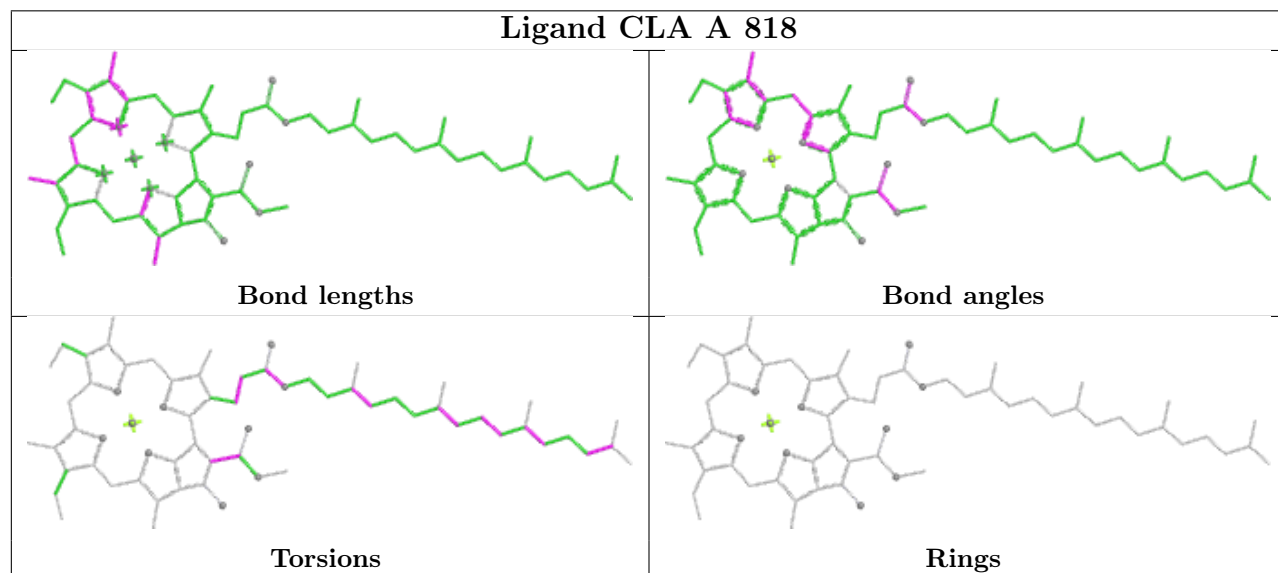
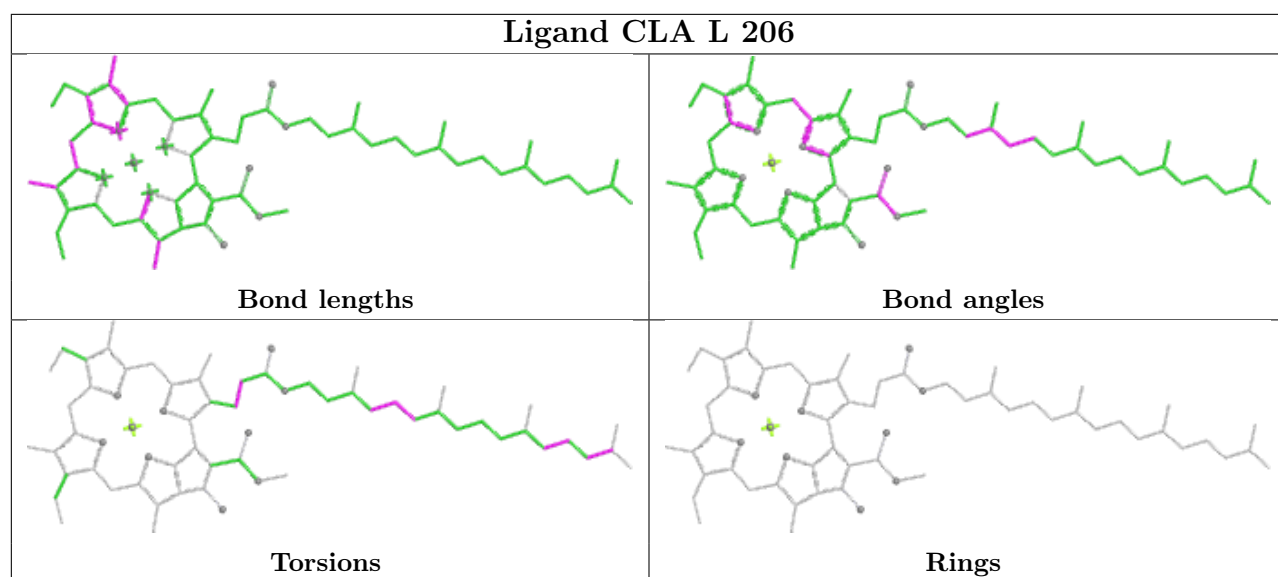
Bond angles

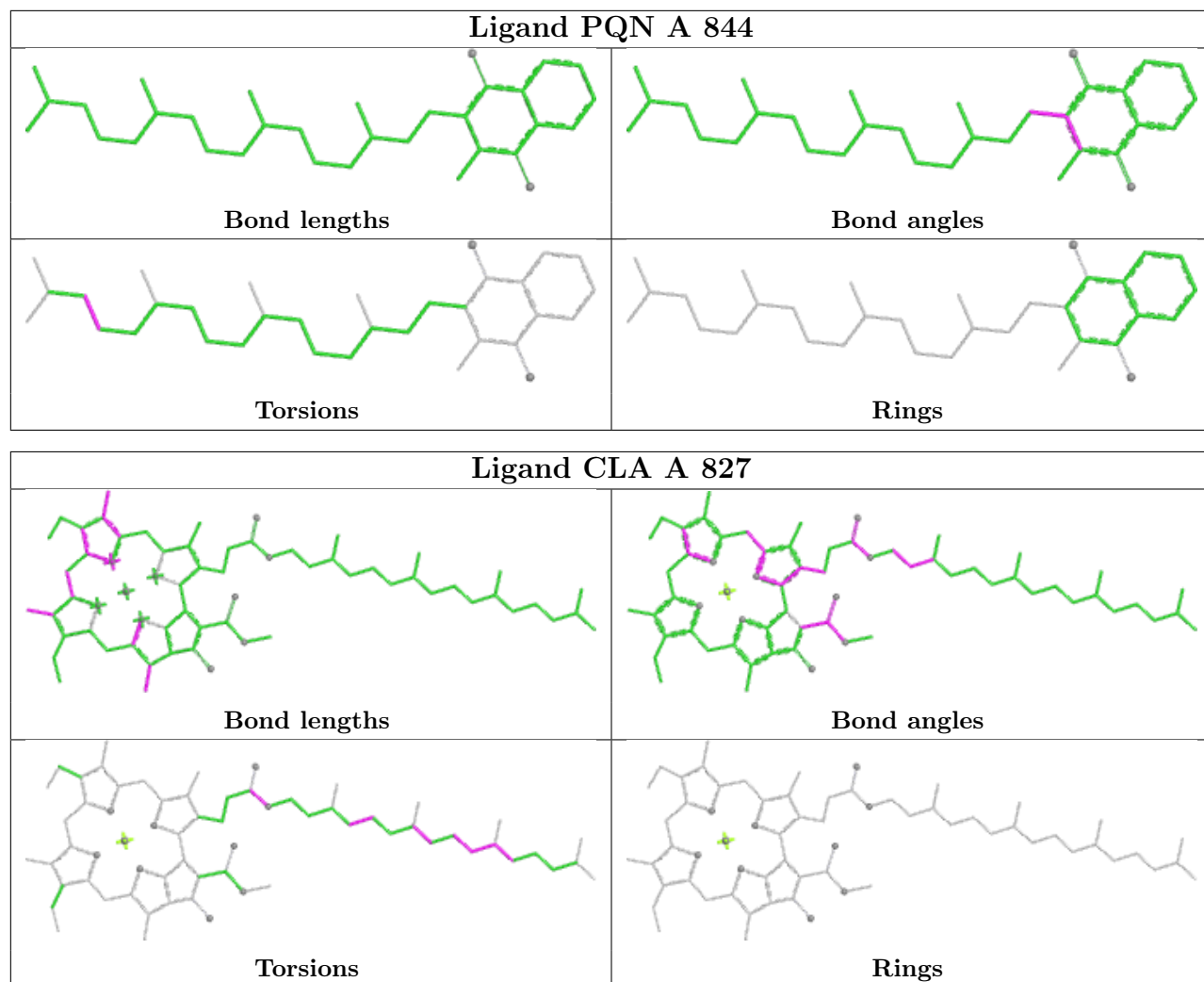


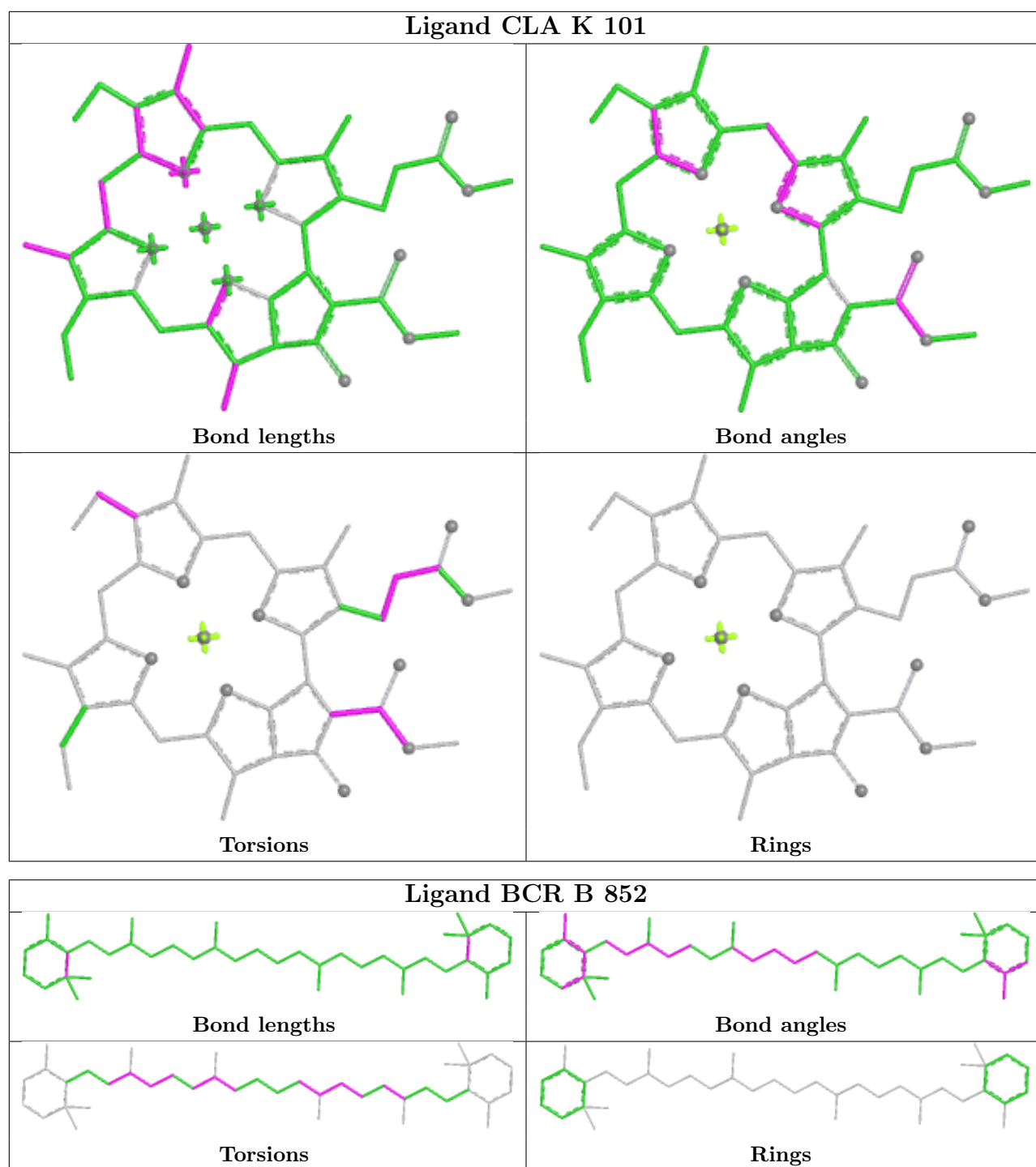
Torsions

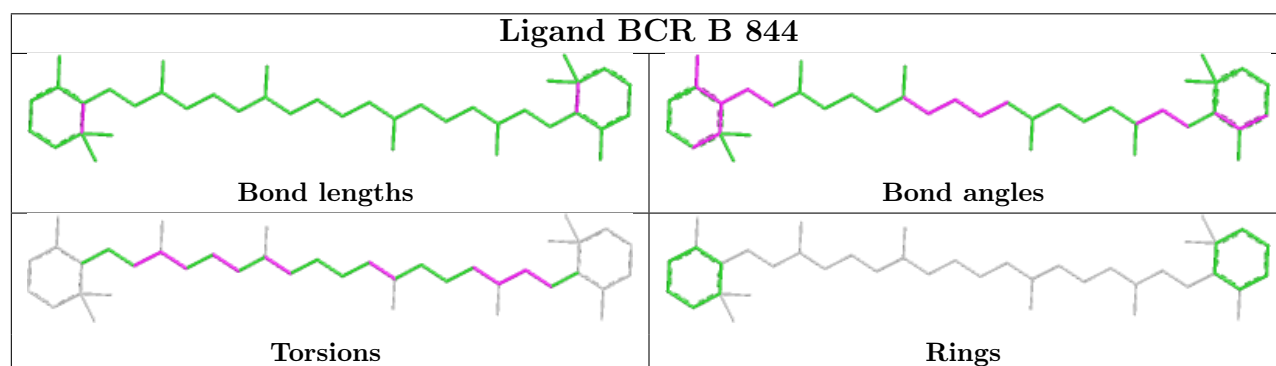
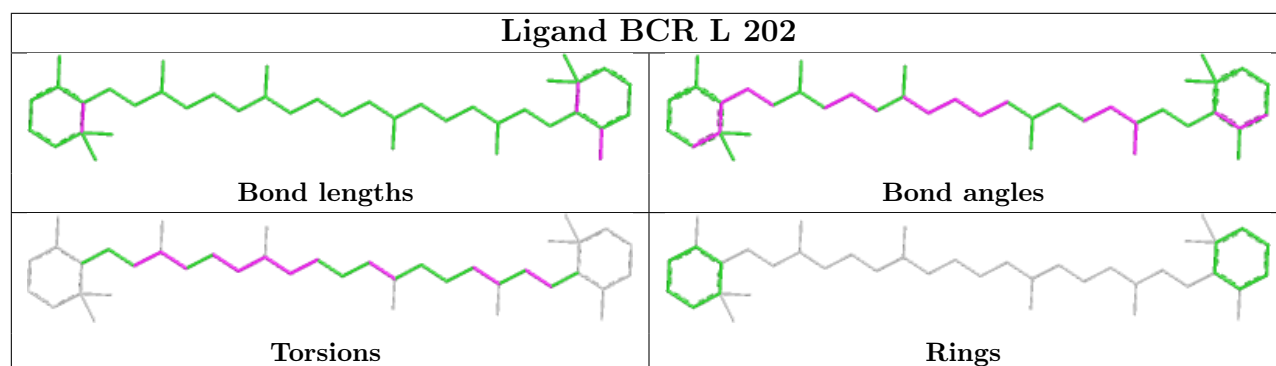
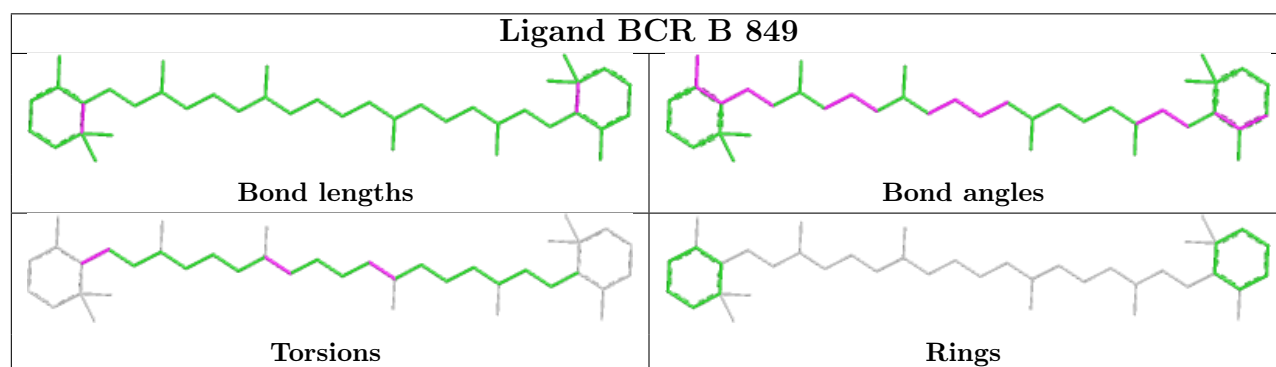
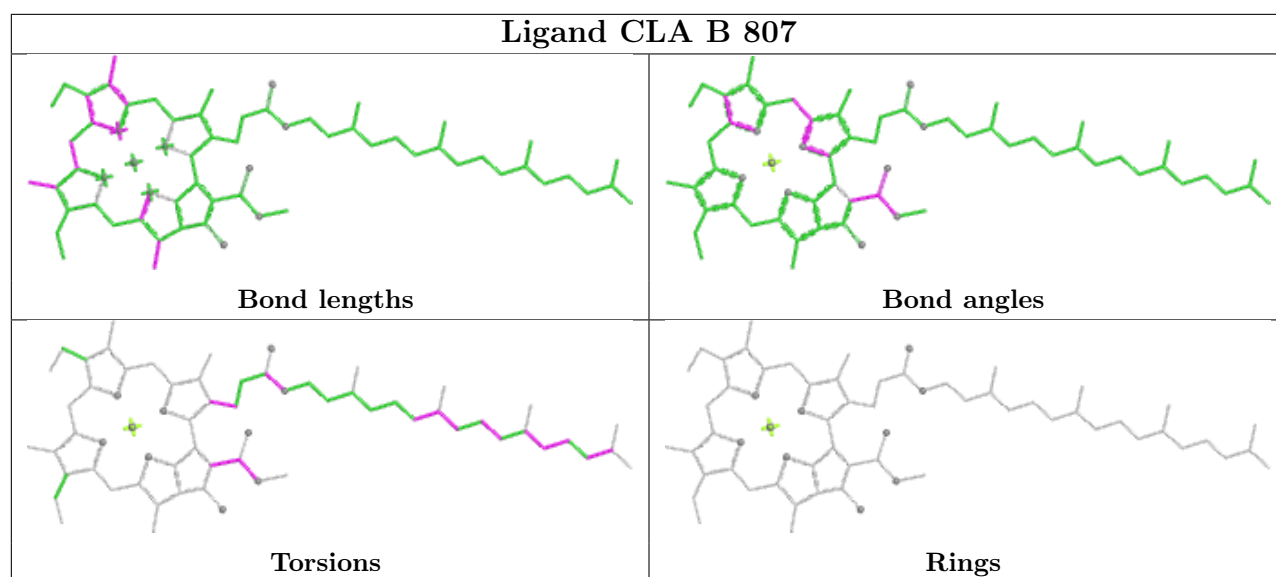


Rings

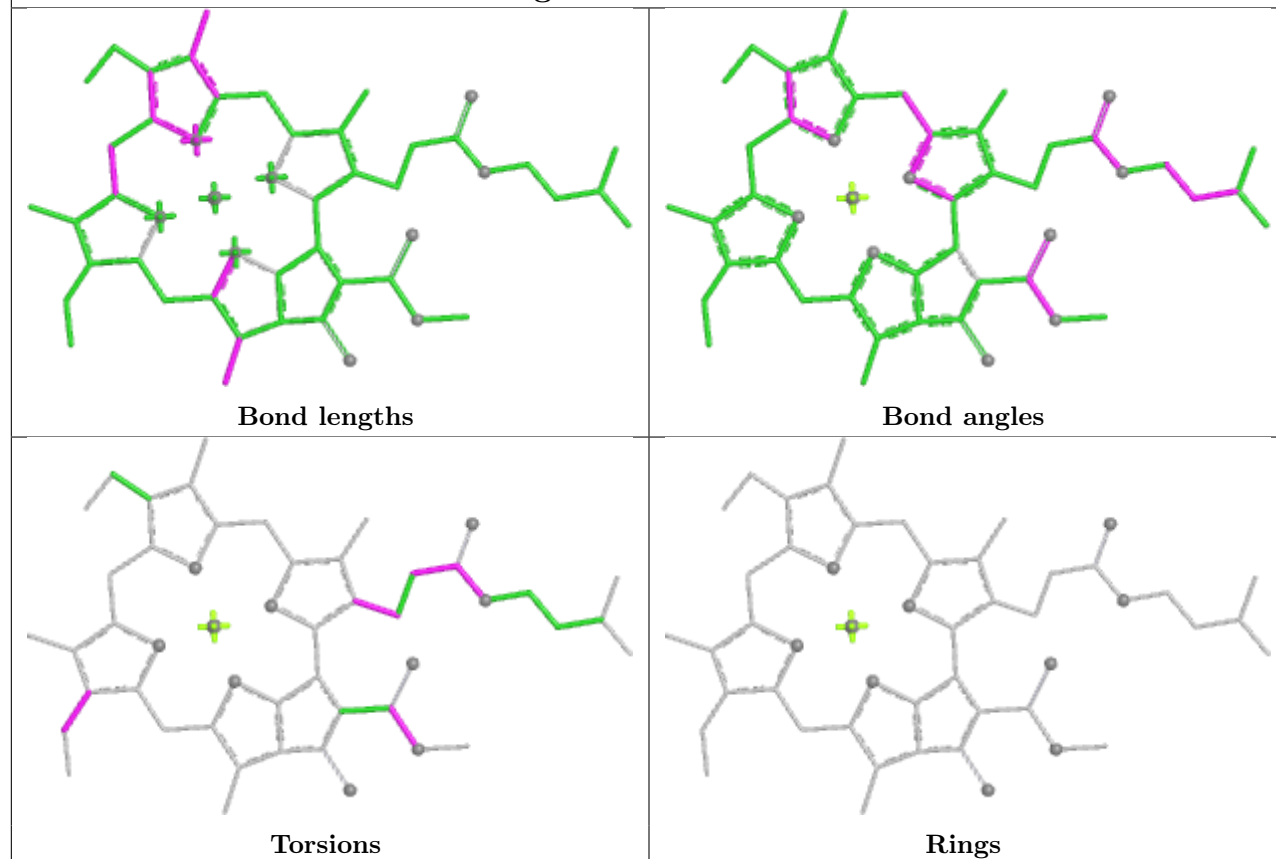




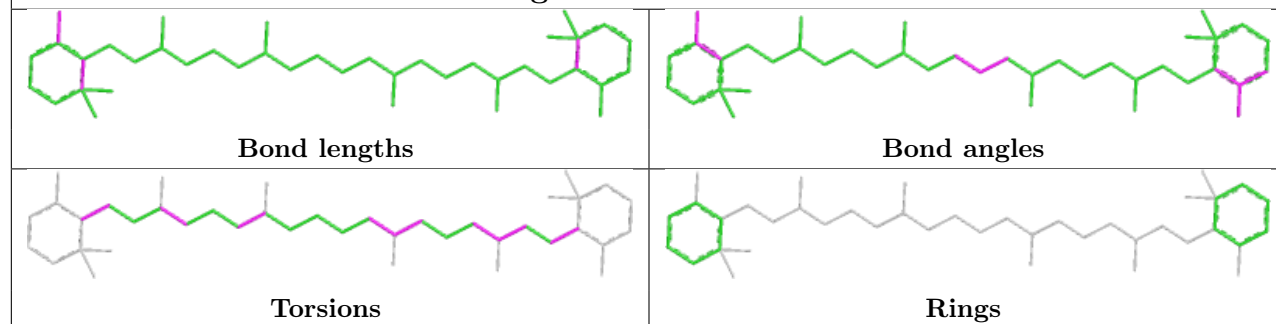


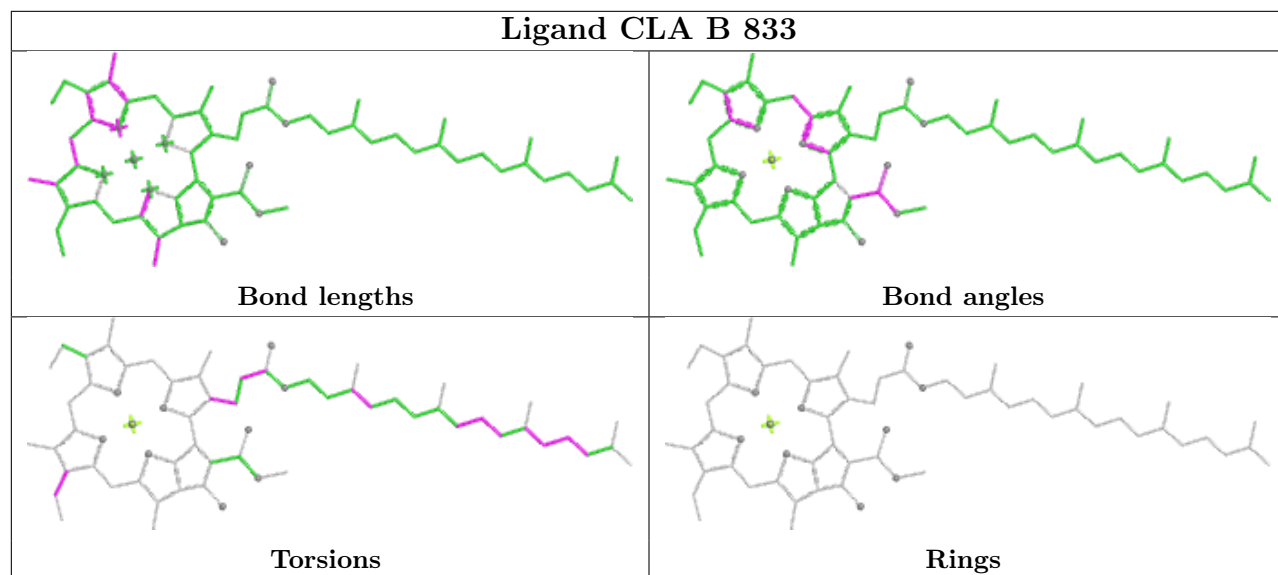
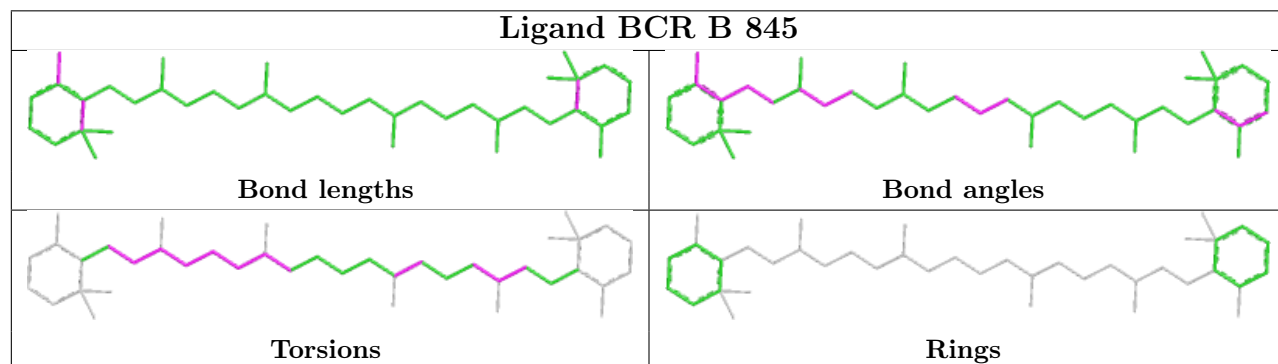
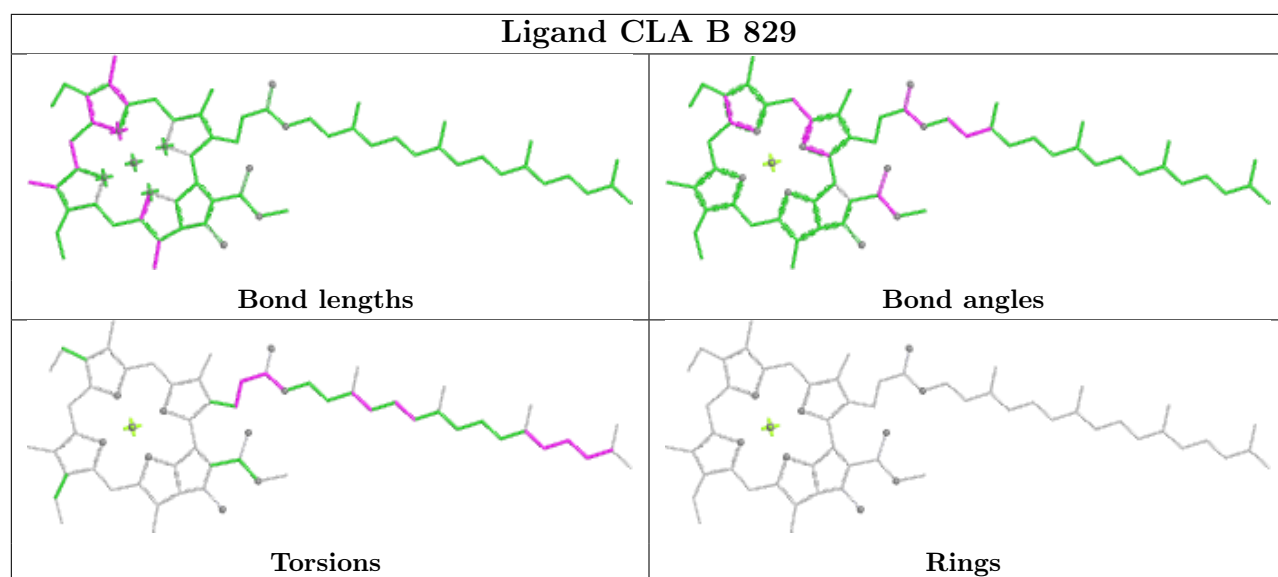


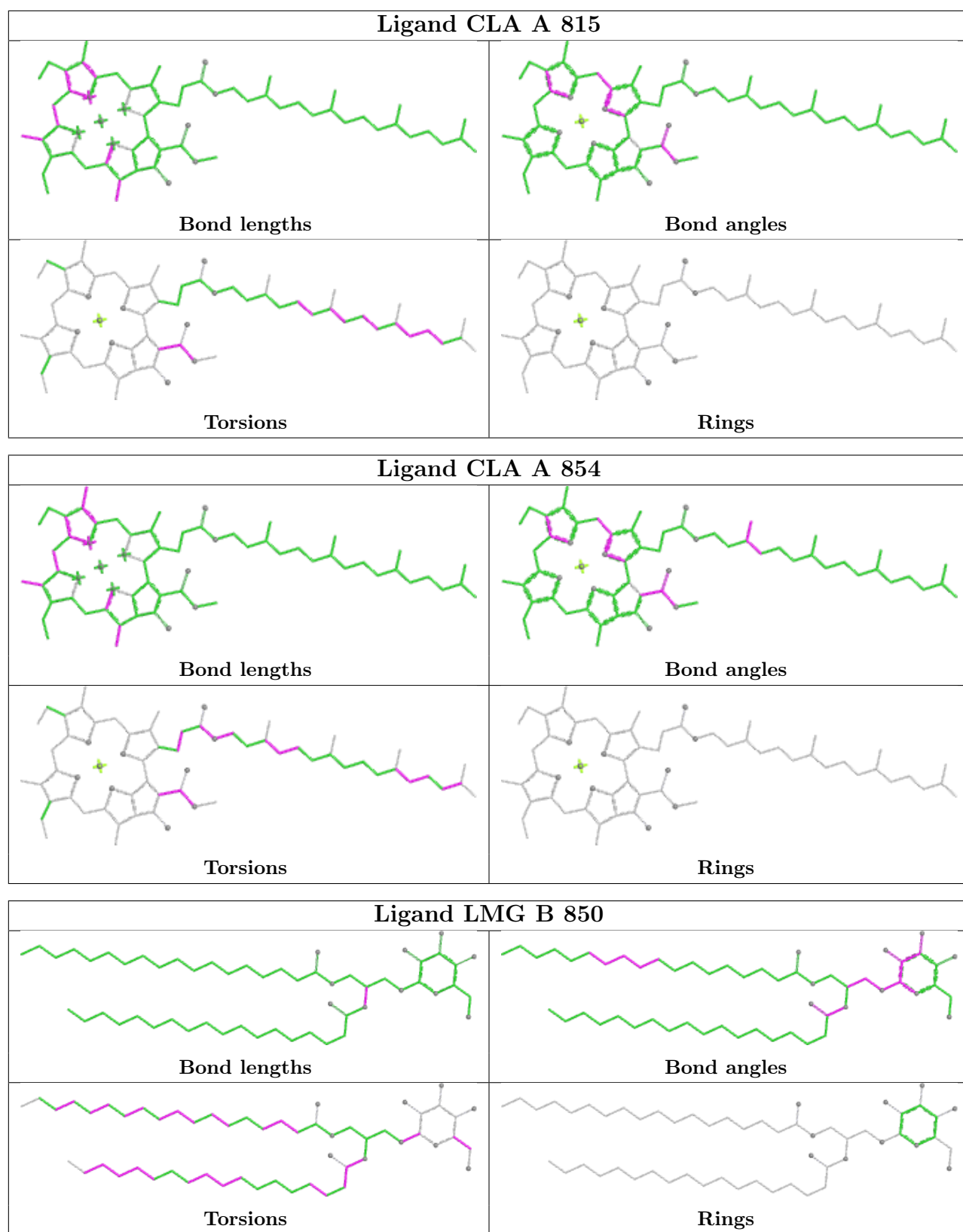
Ligand CLA F 204

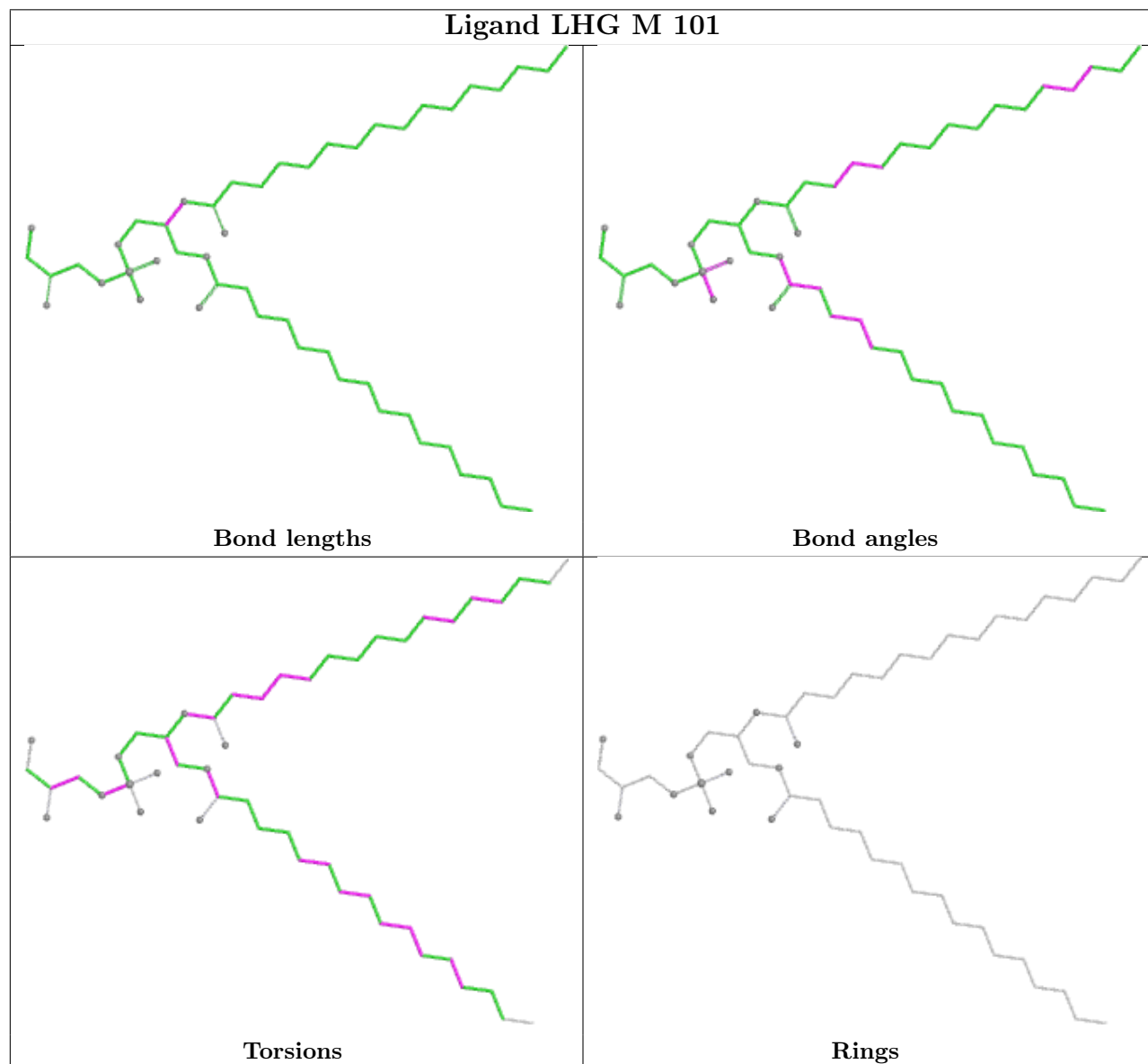
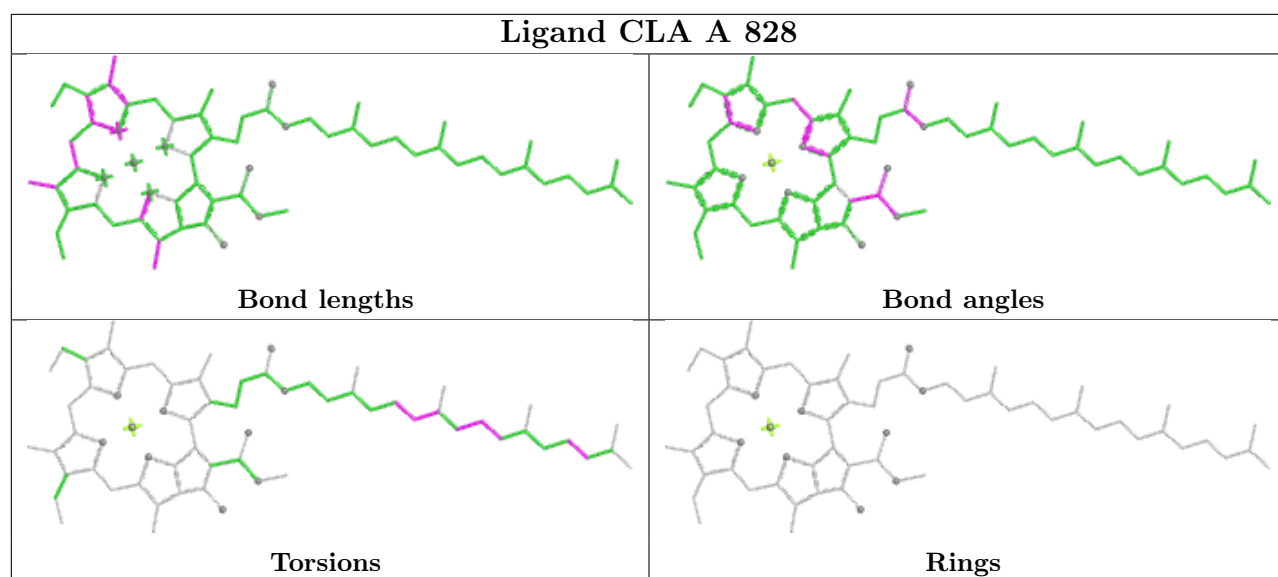


Ligand BCR B 853

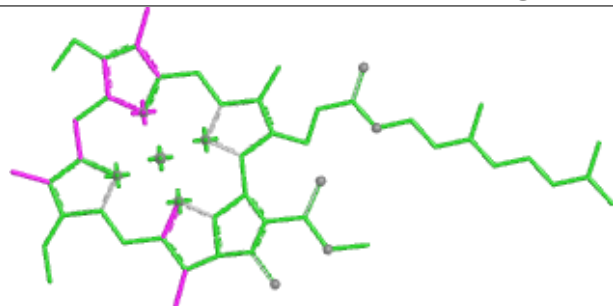




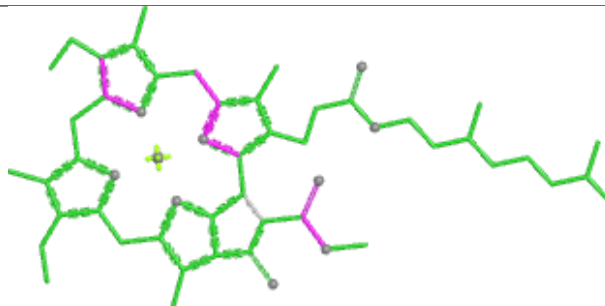




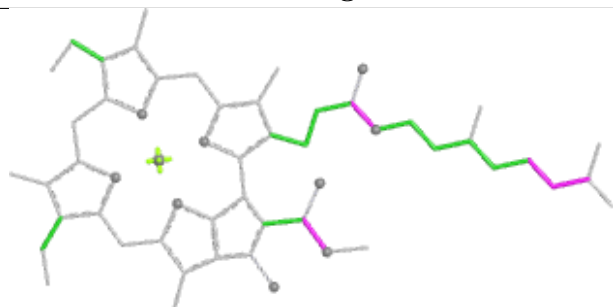
Ligand CLA B 831



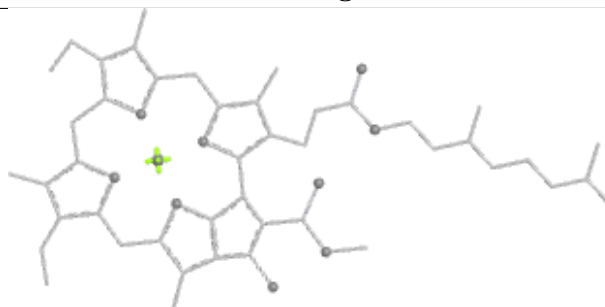
Bond lengths



Bond angles

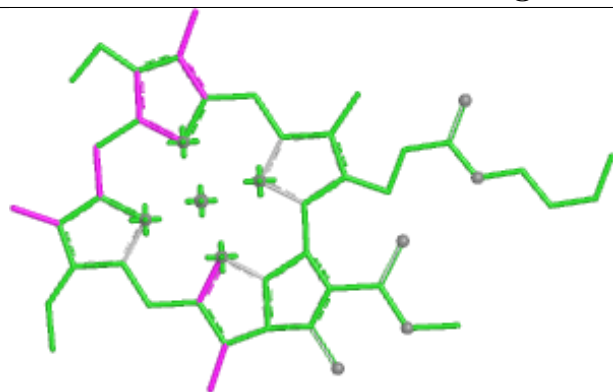


Torsions

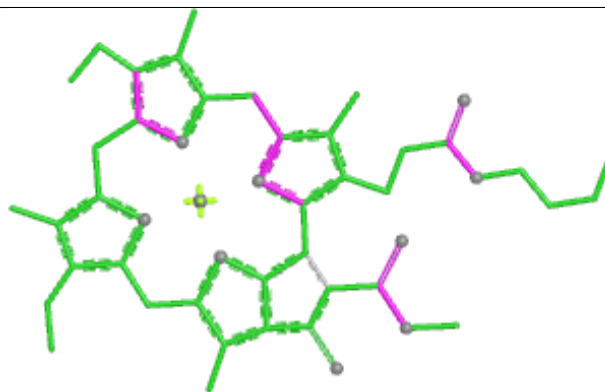


Rings

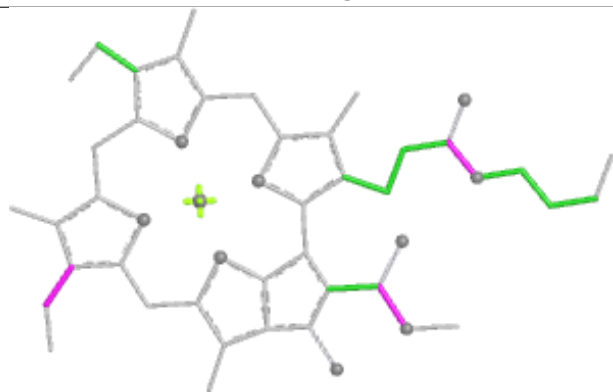
Ligand CLA A 811



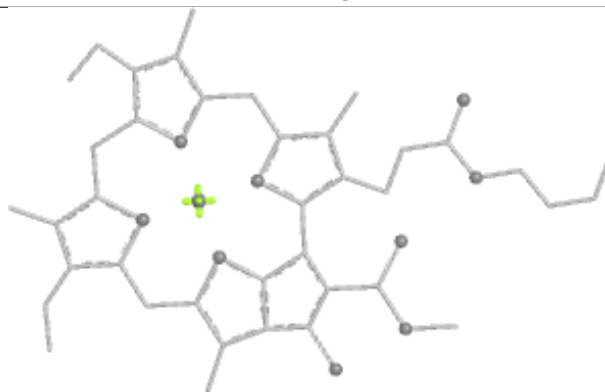
Bond lengths



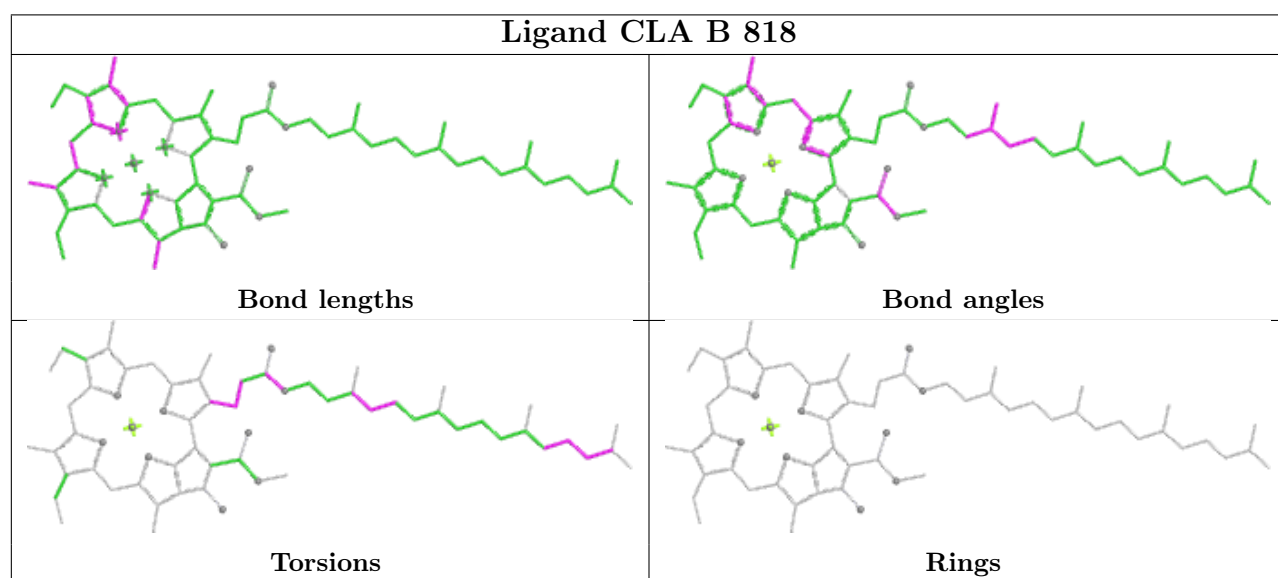
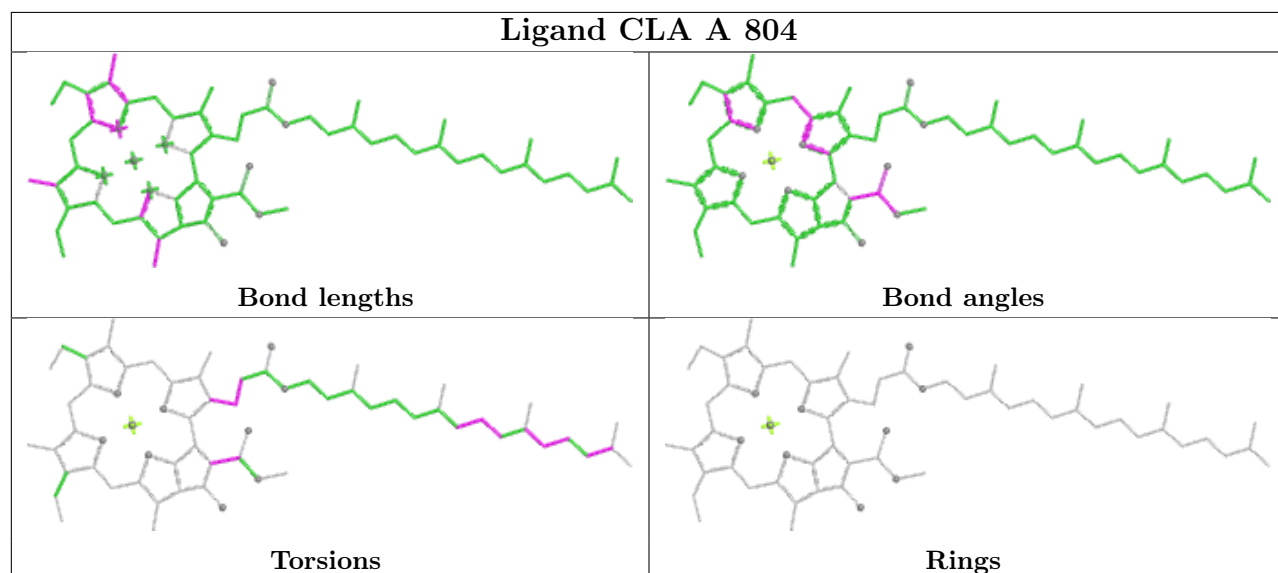
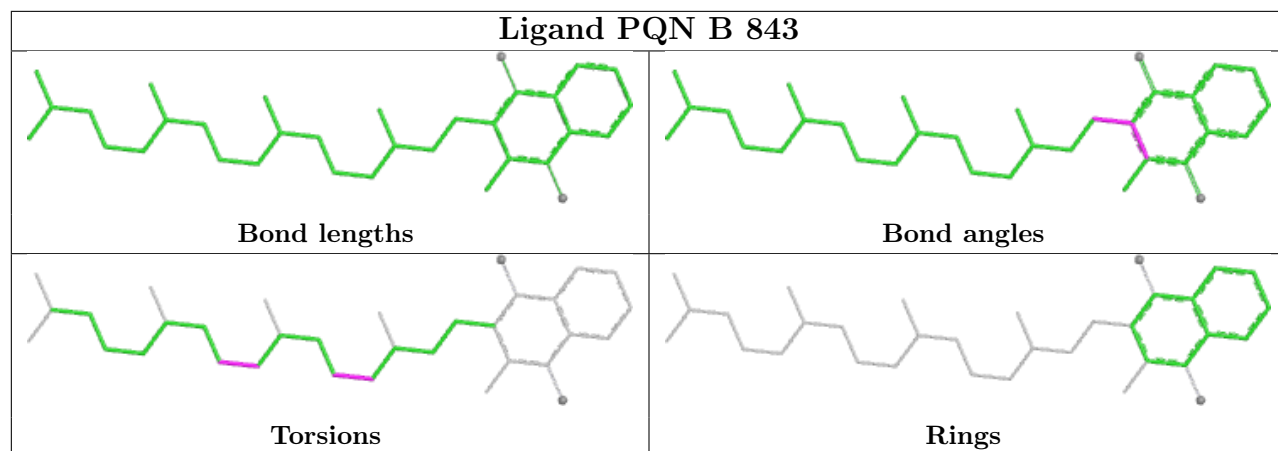
Bond angles



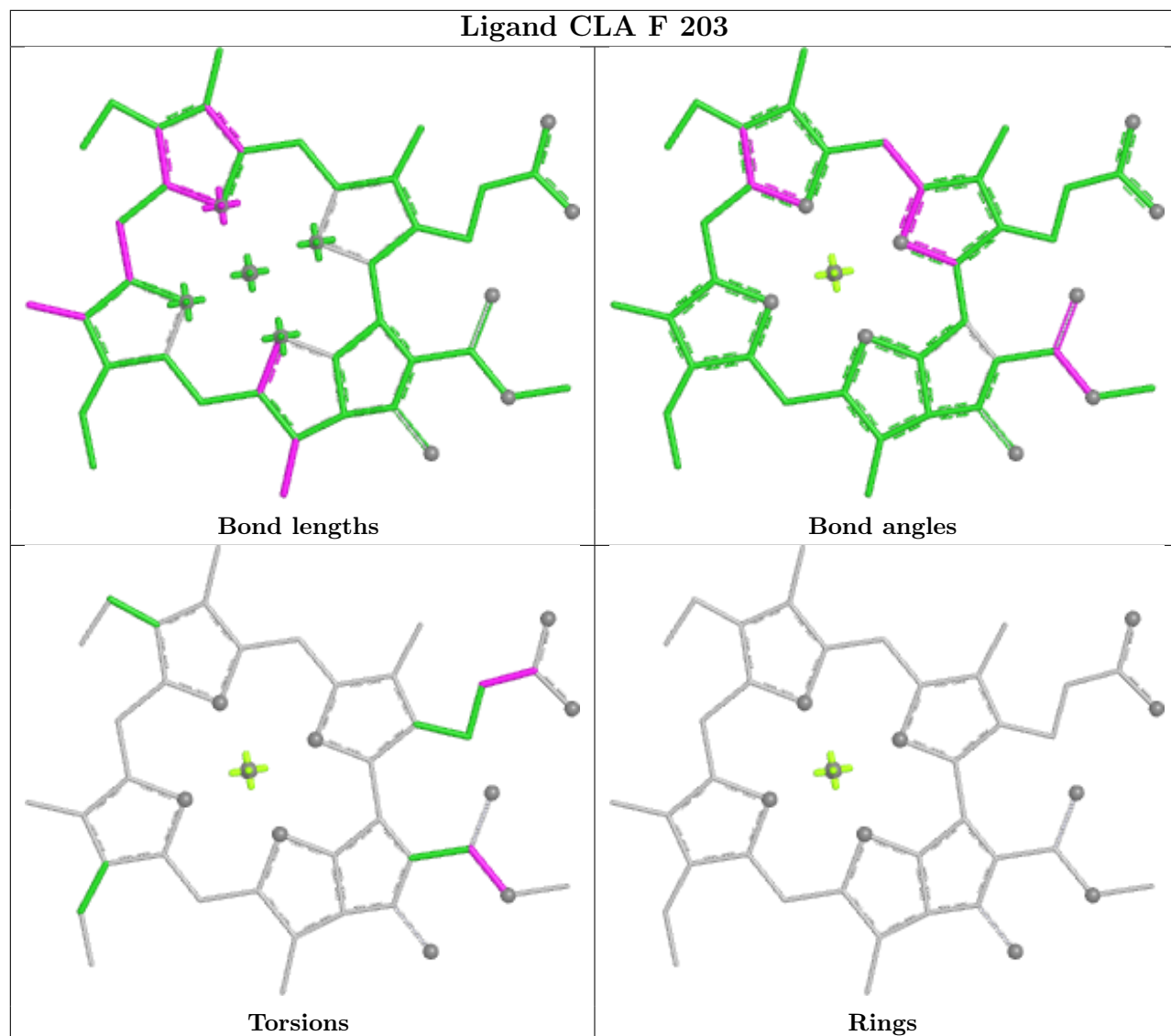
Torsions



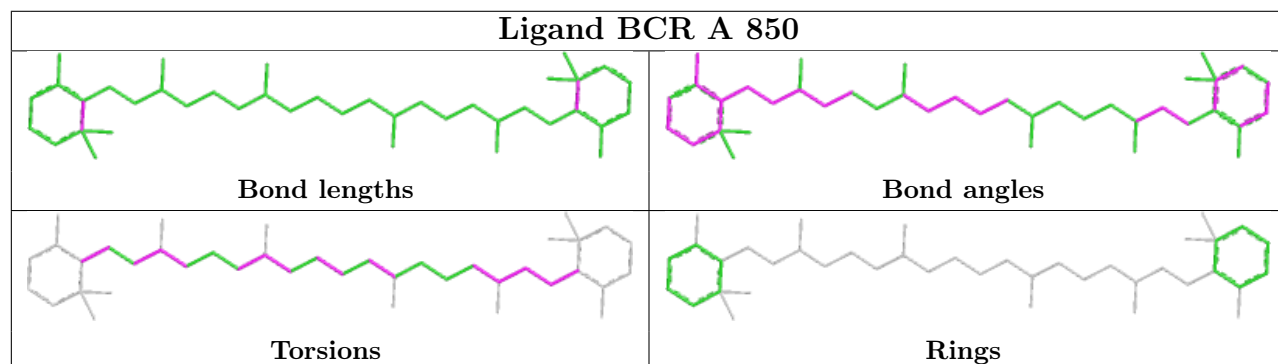
Rings

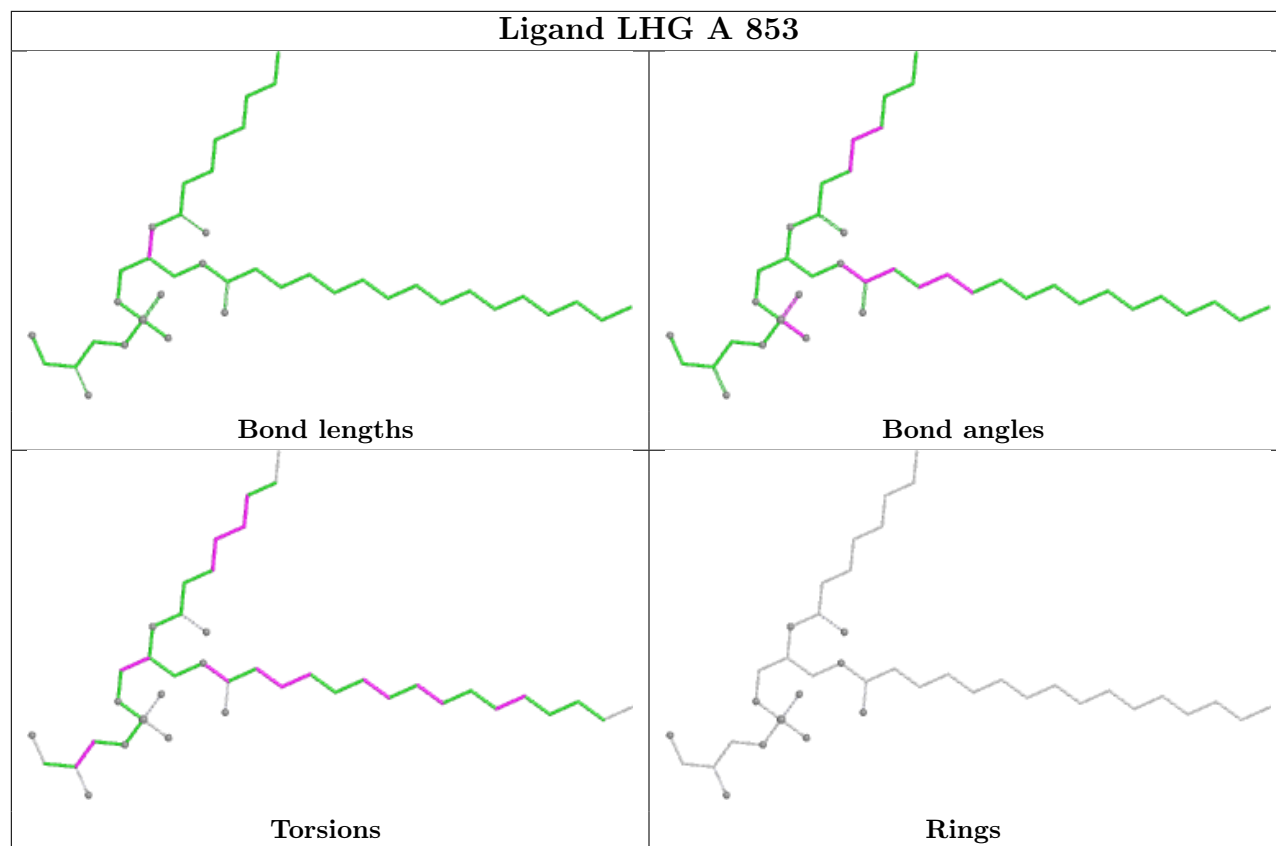


Ligand CLA F 203

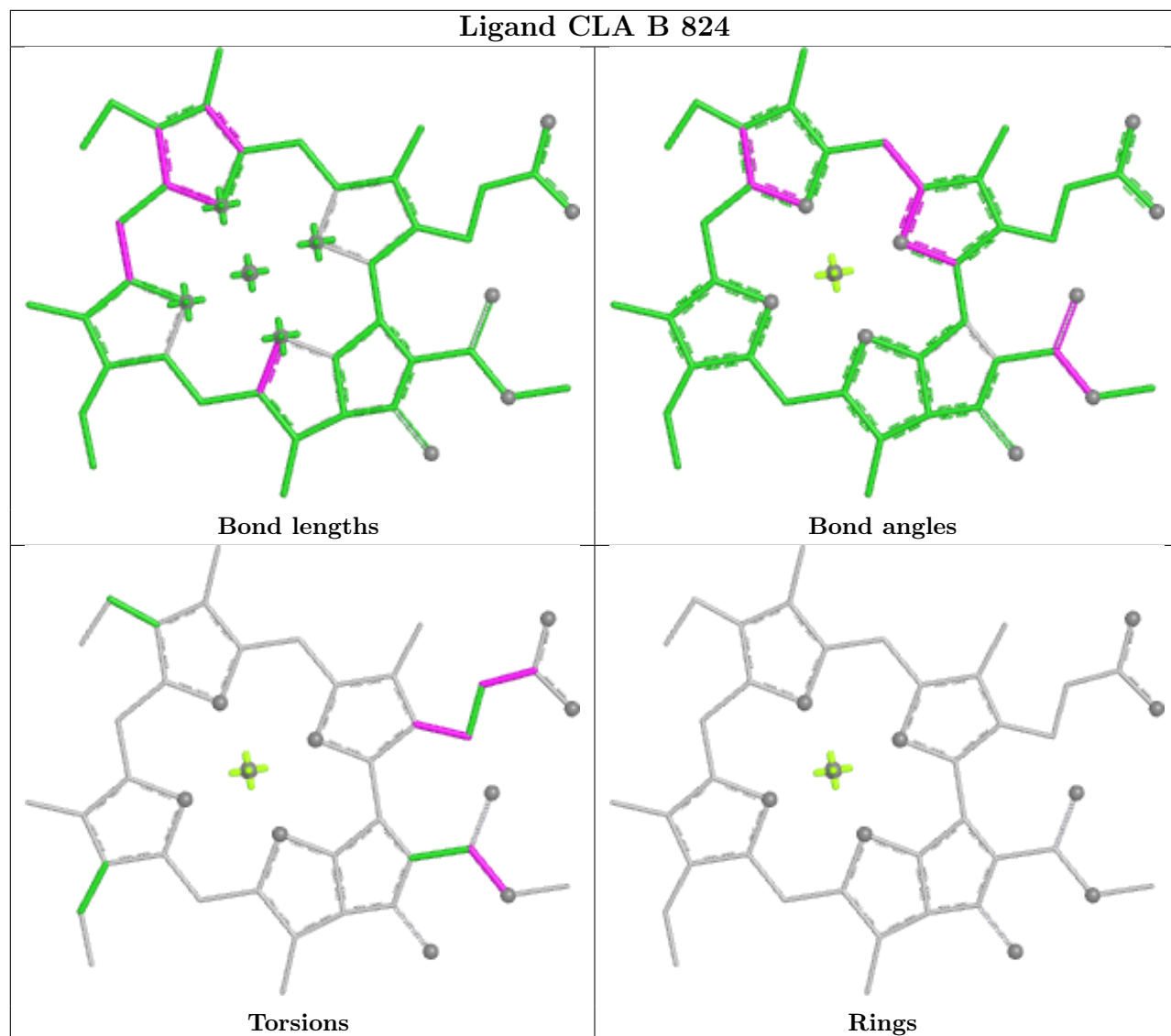


Ligand BCR A 850

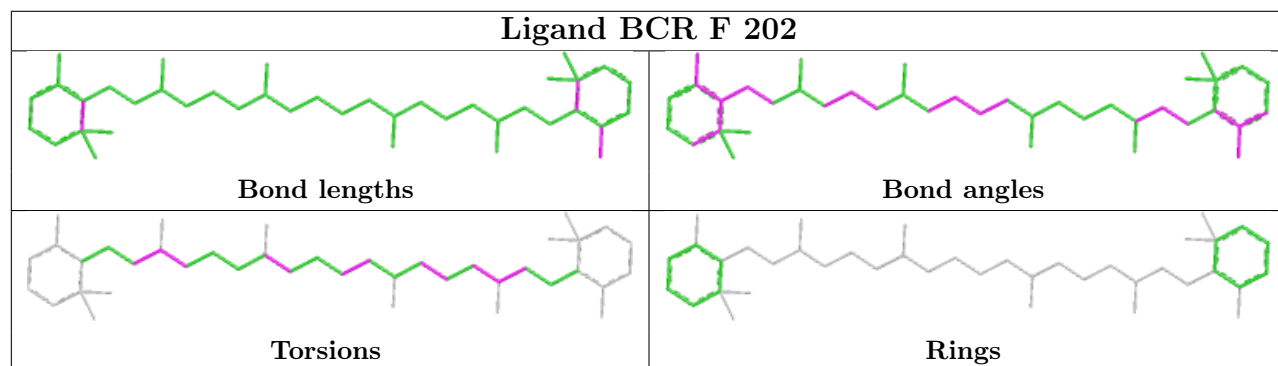


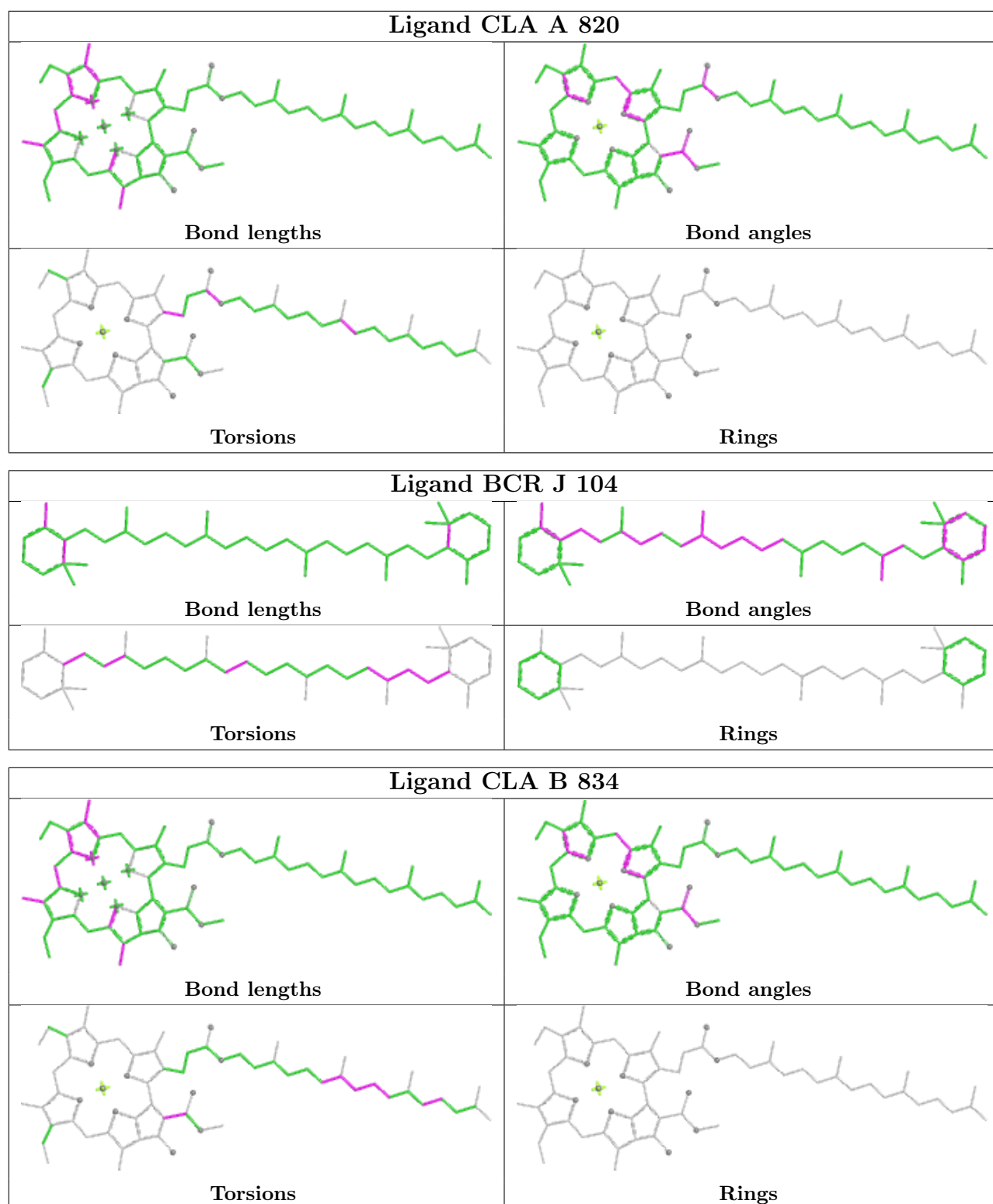


Ligand CLA B 824

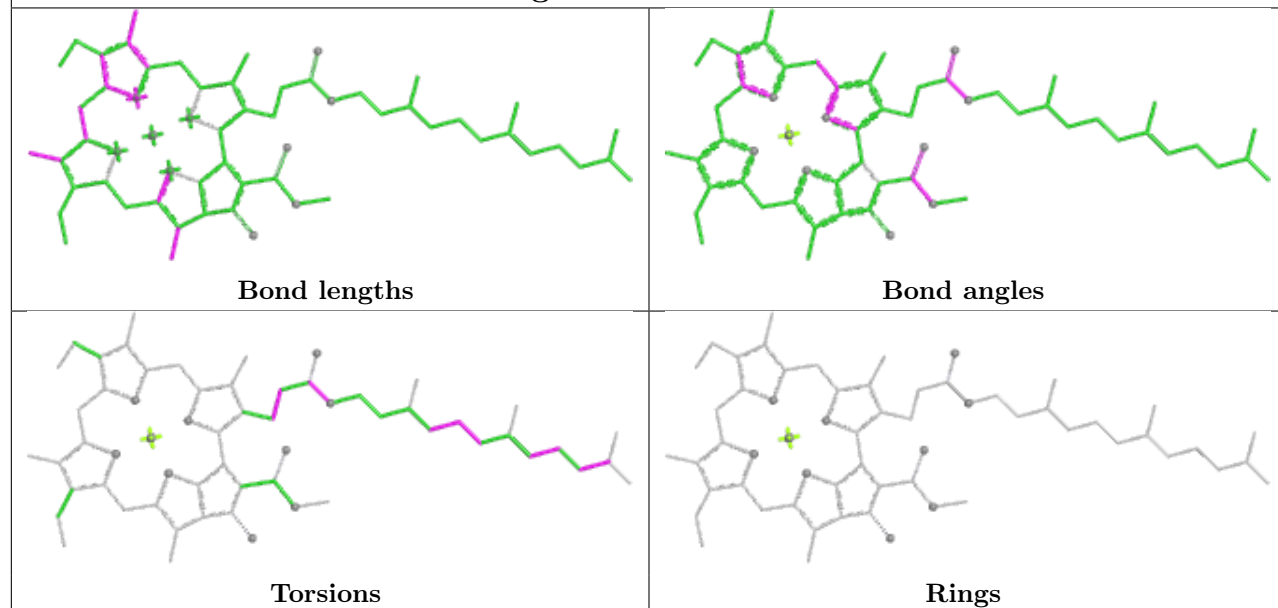


Ligand BCR F 202

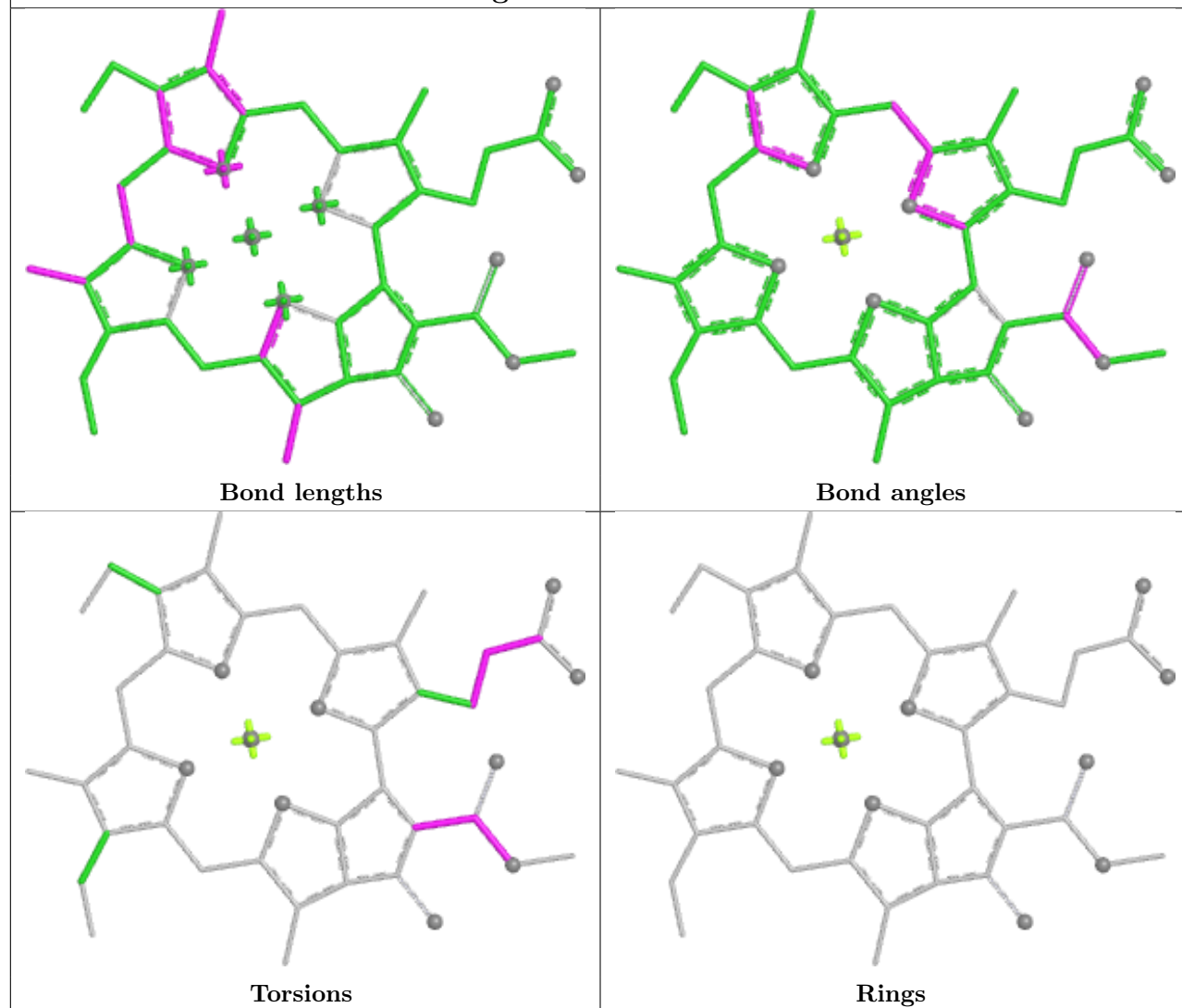


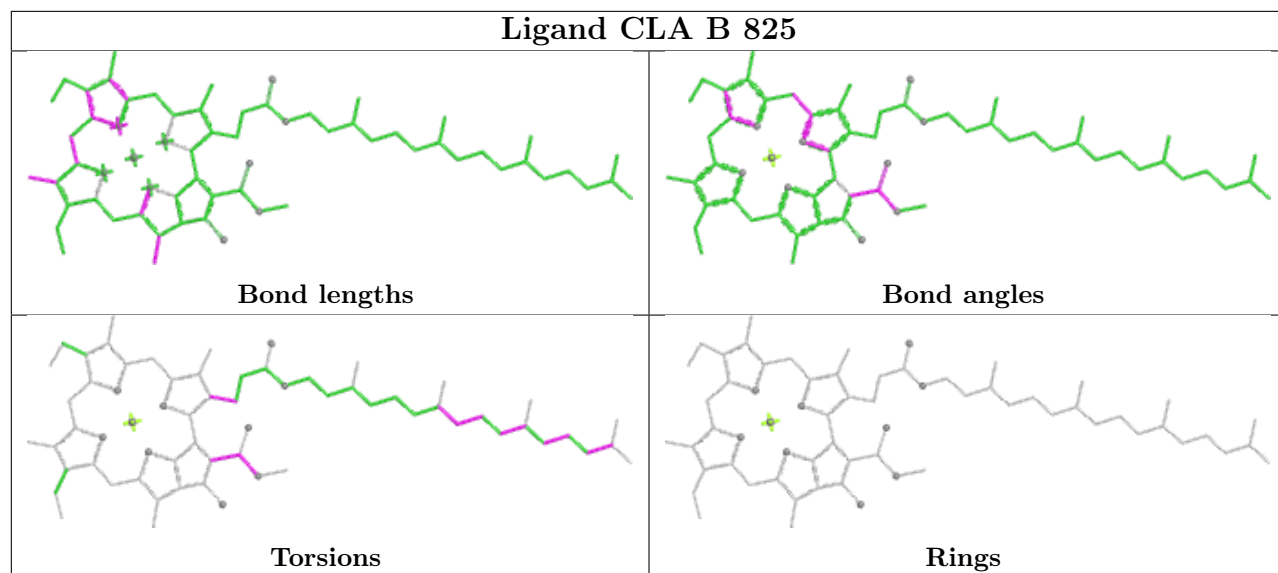
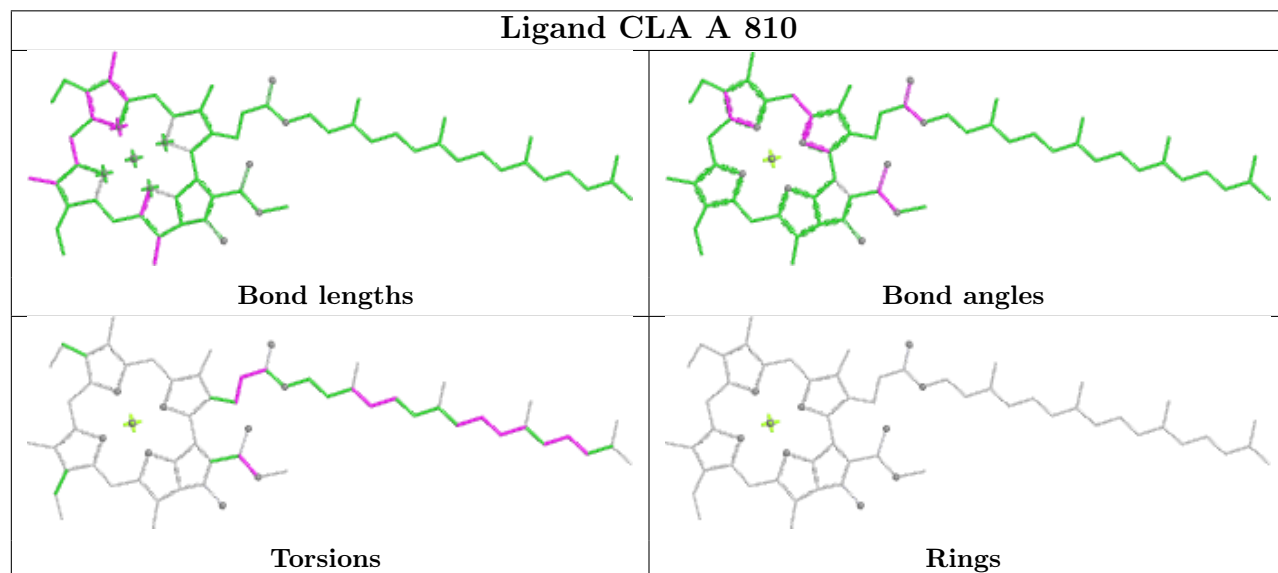
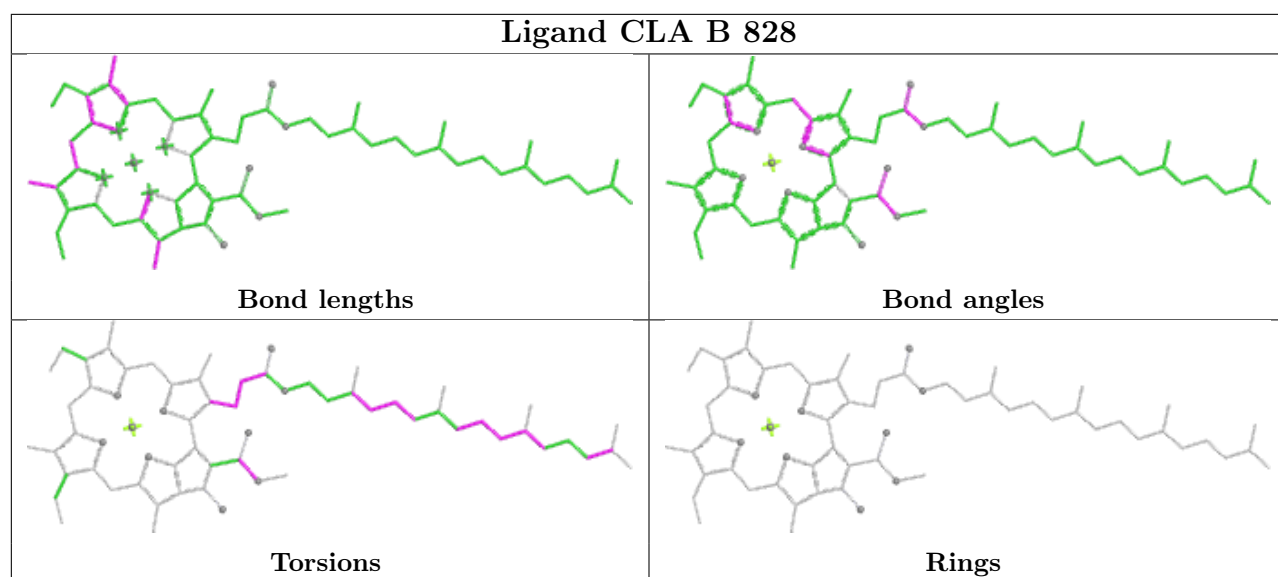


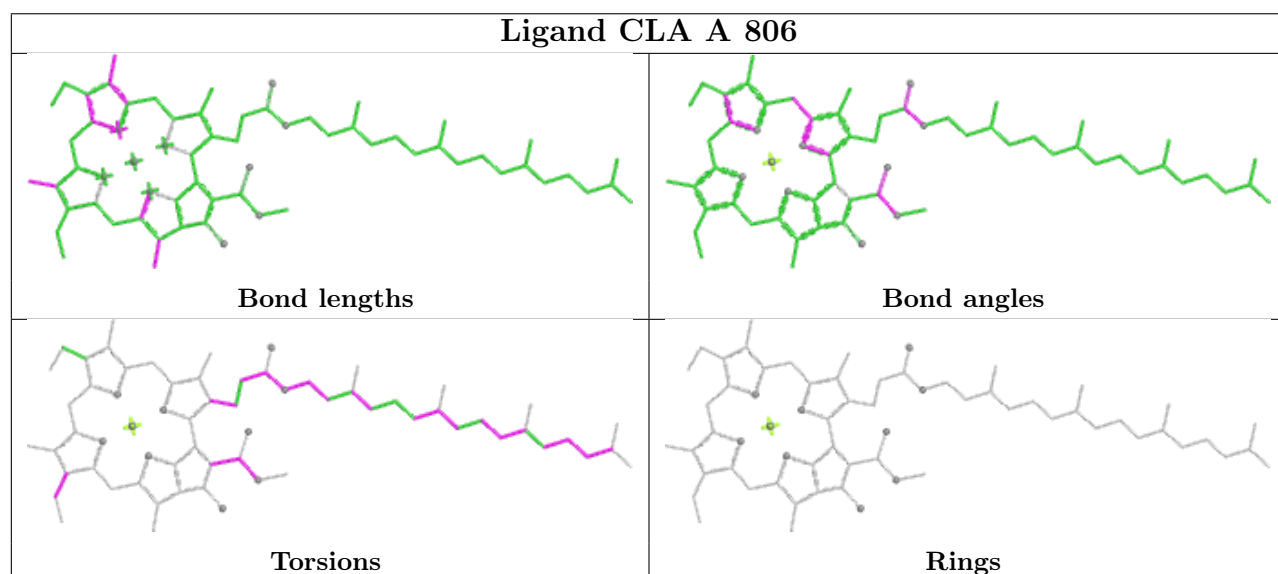
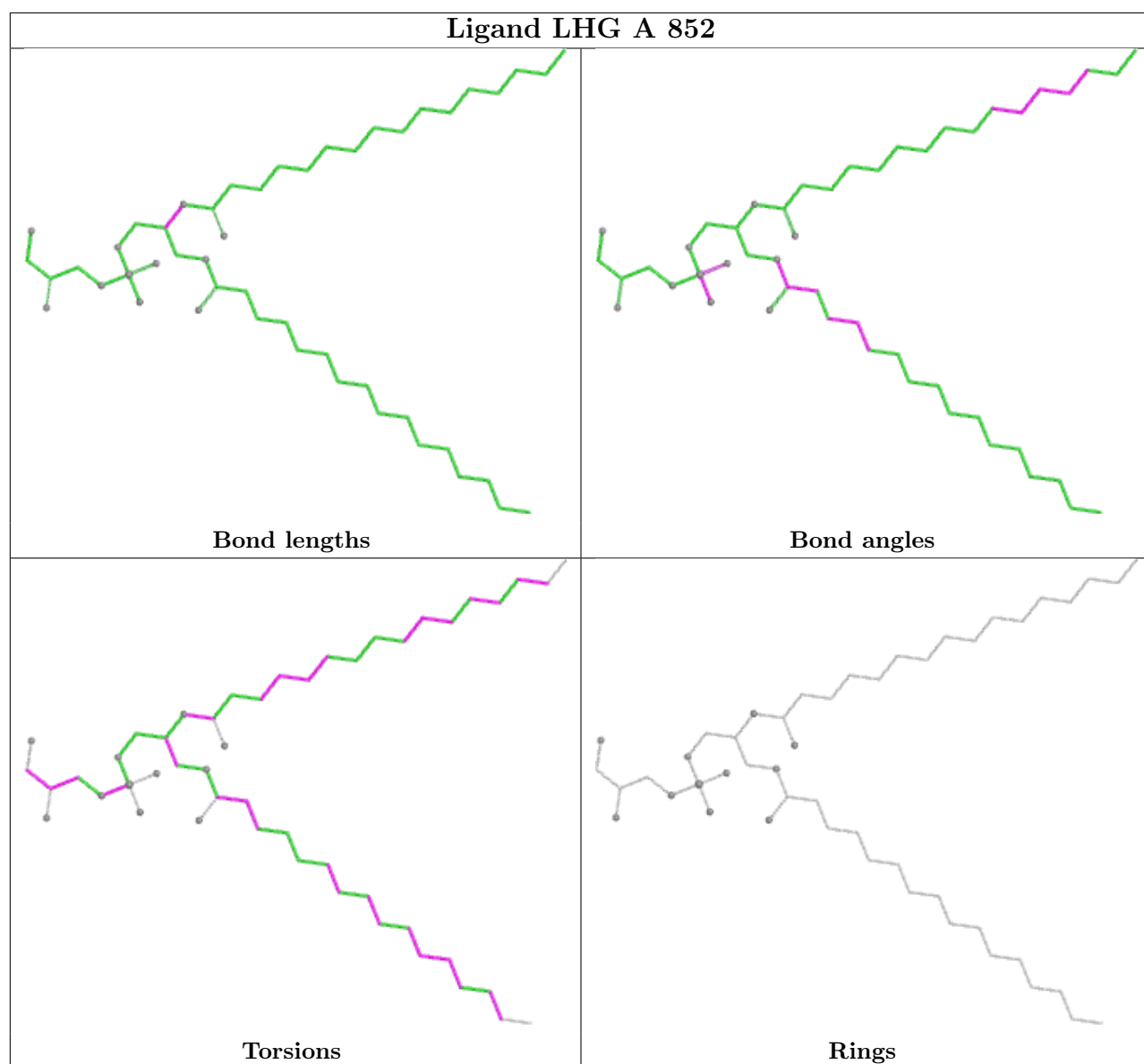
Ligand CLA A 832

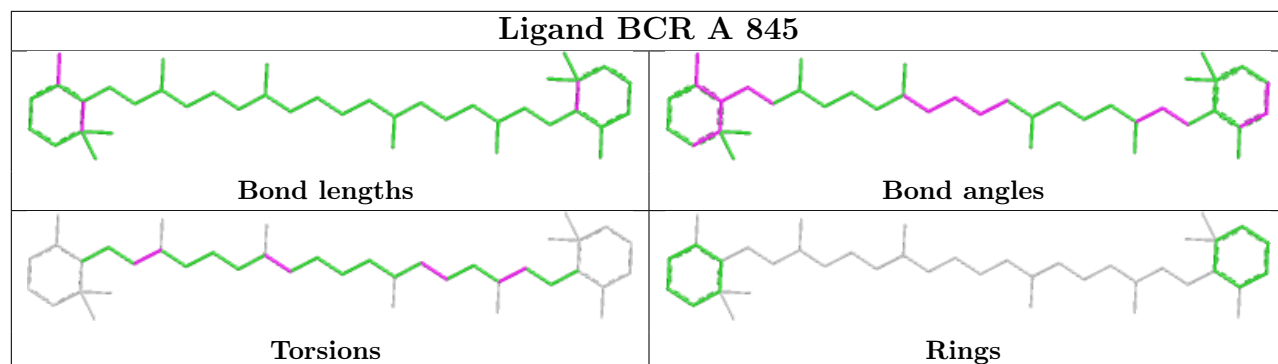
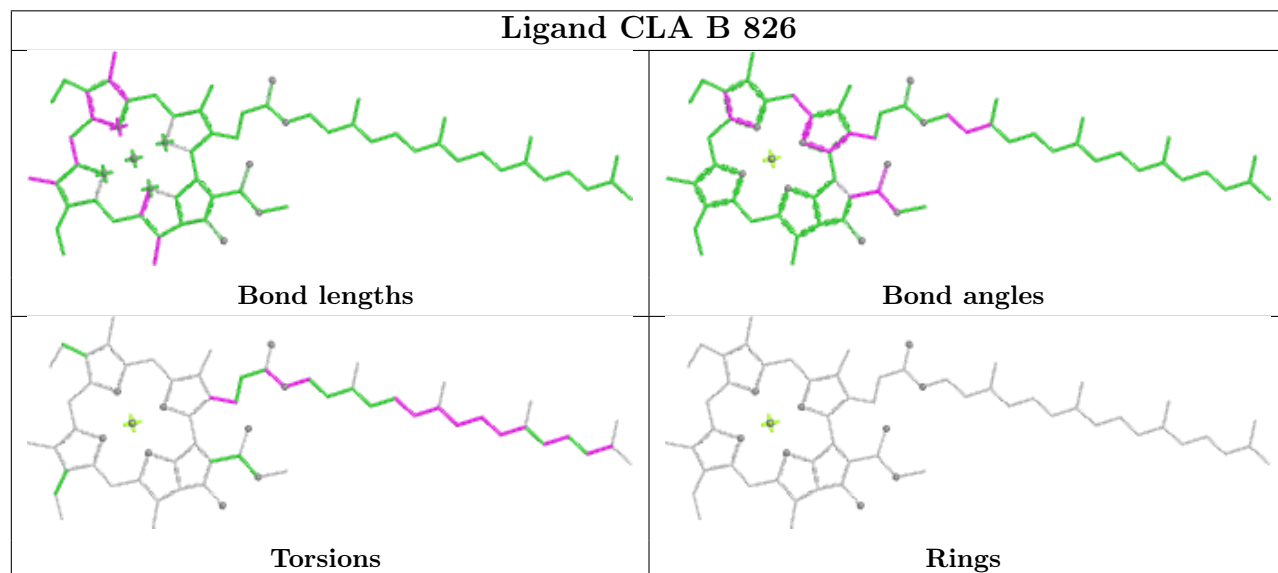
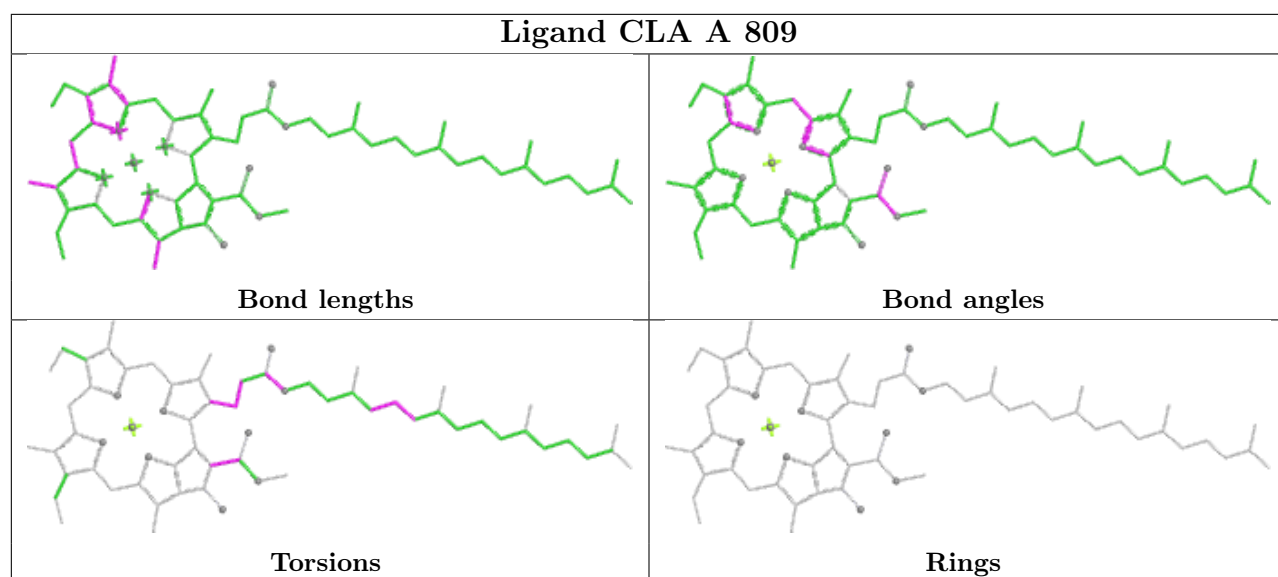


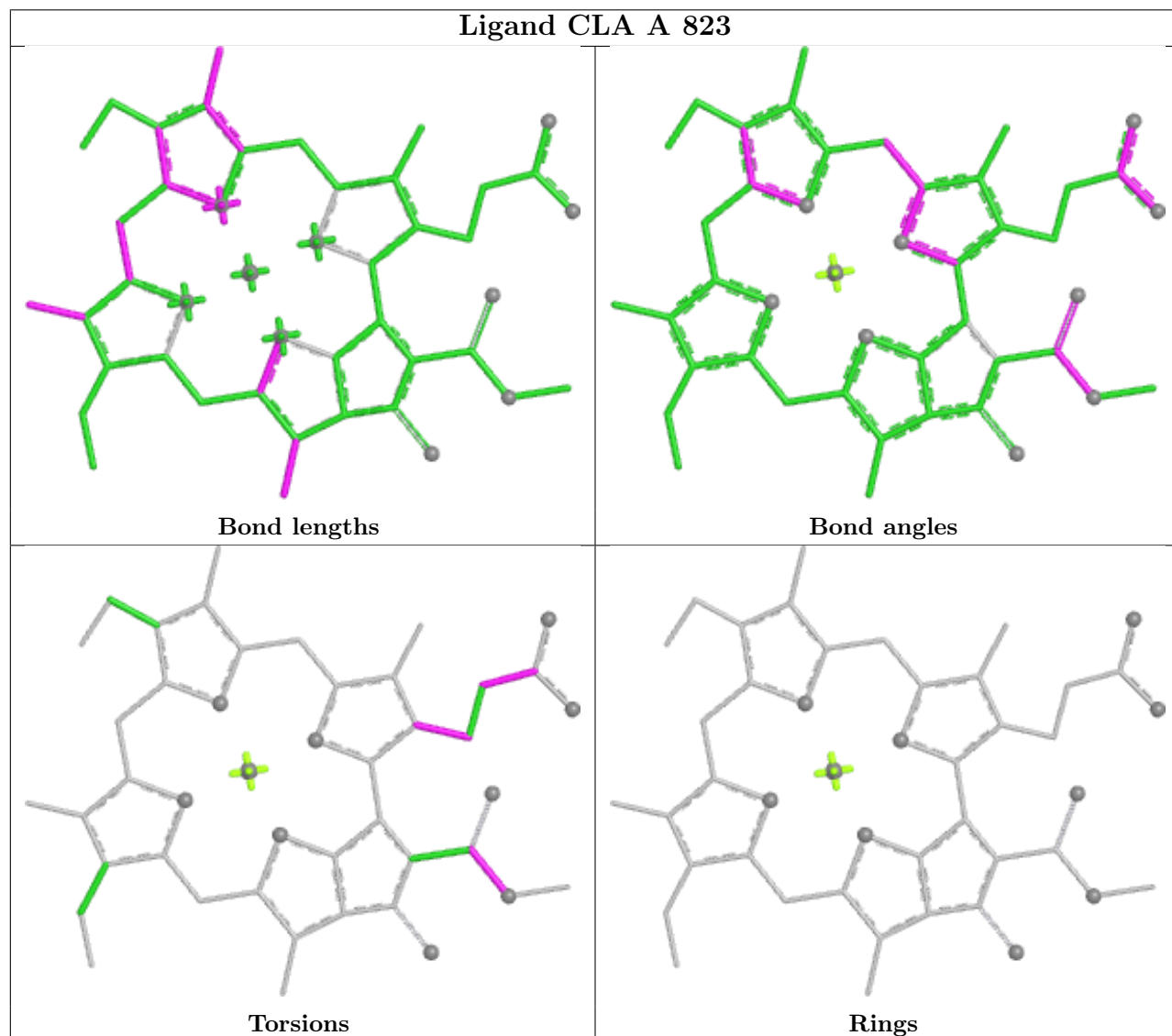
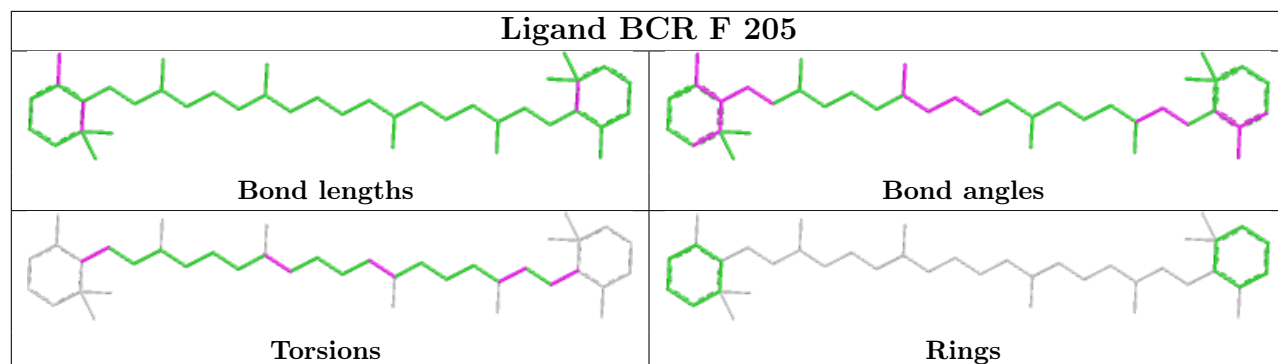
Ligand CLA B 822



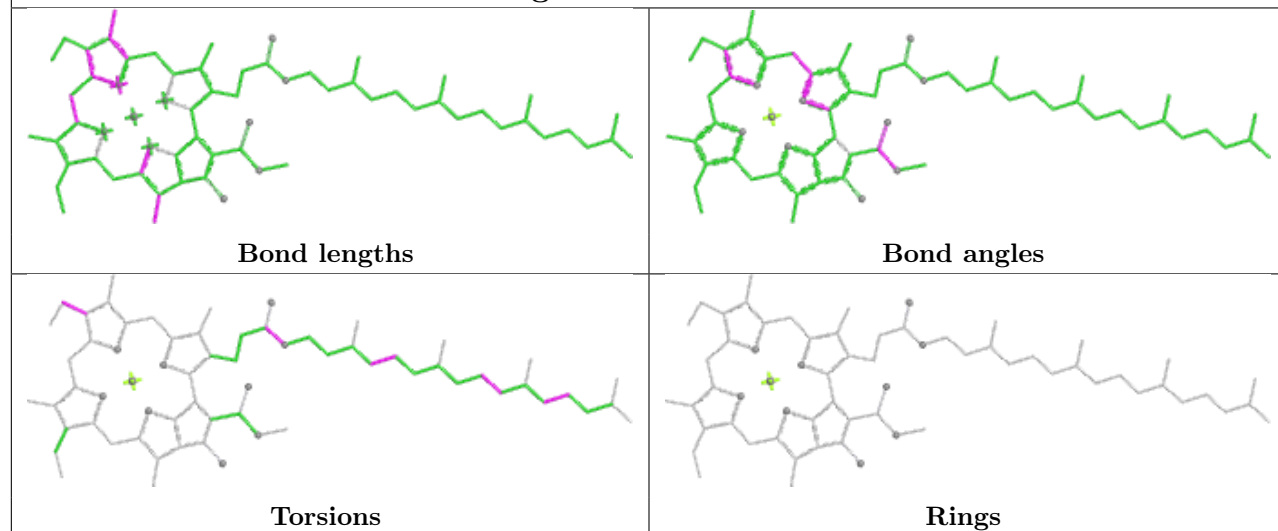




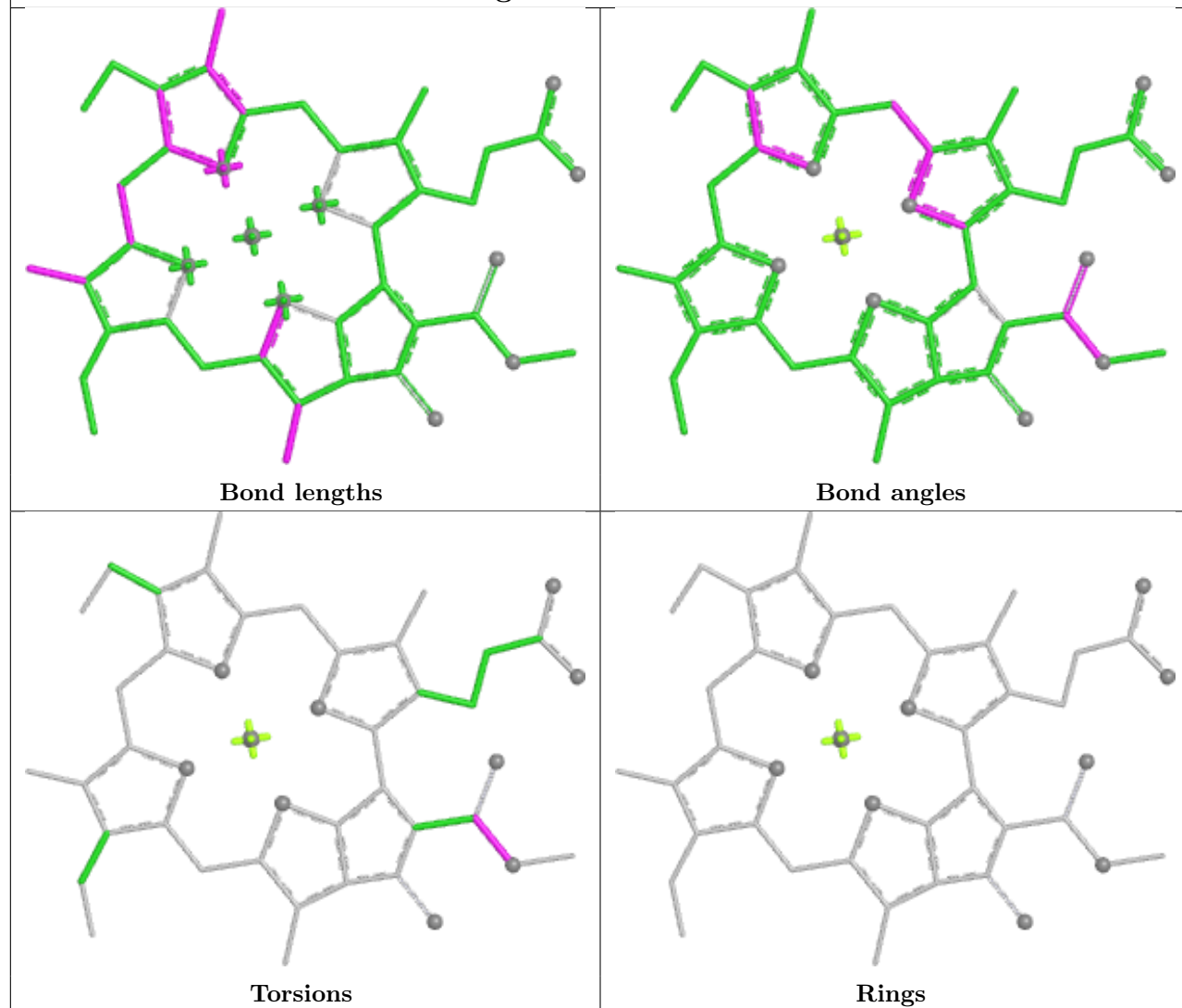


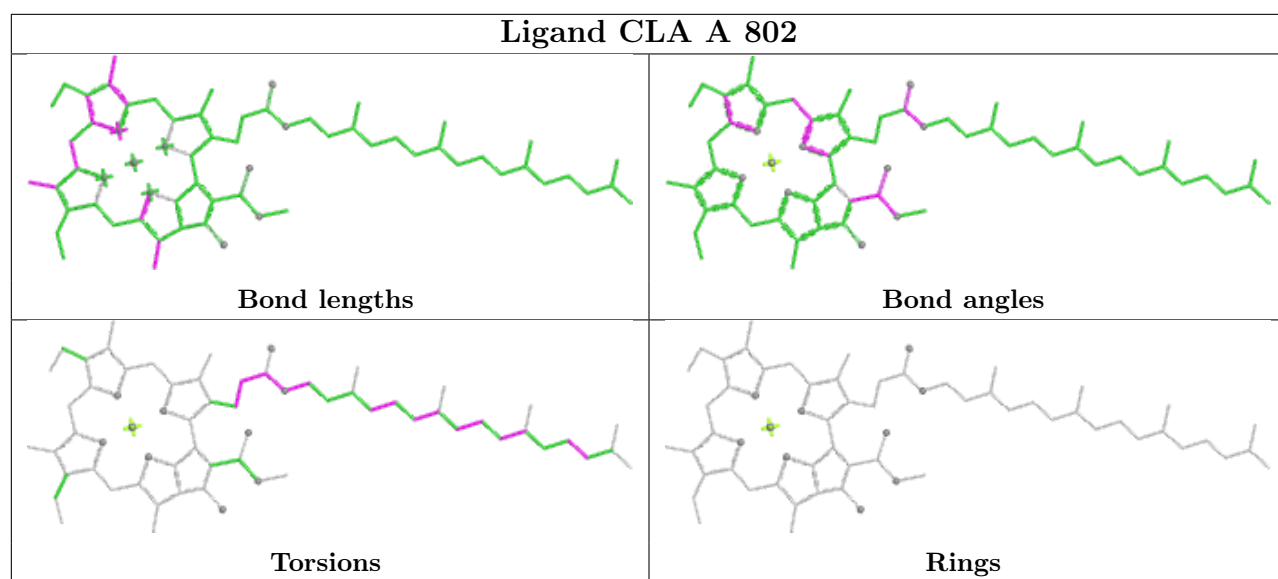


Ligand CLA A 840

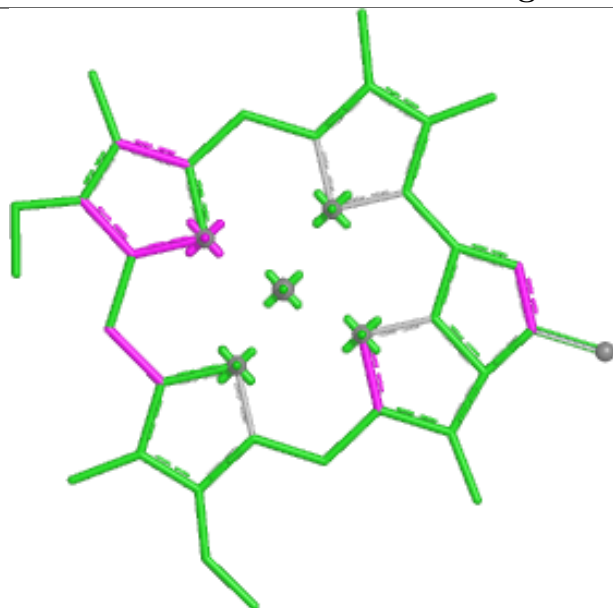


Ligand CLA J 101





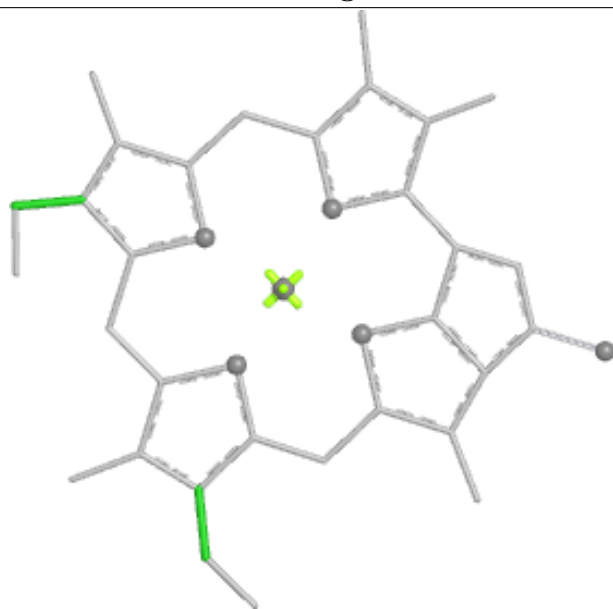
Ligand CLA J 102



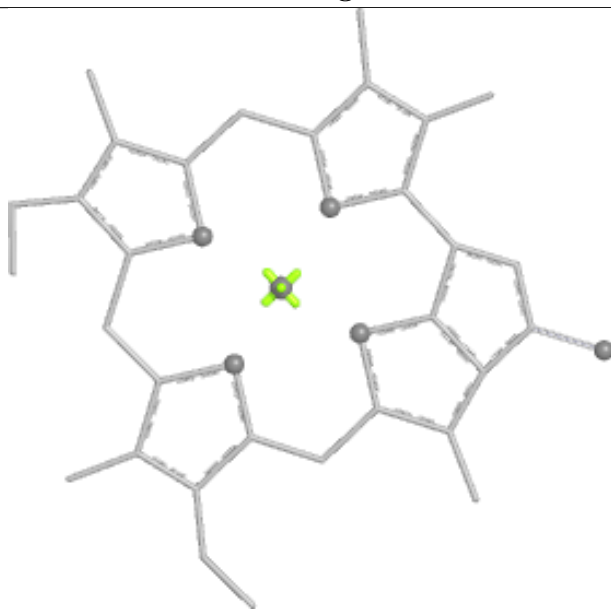
Bond lengths



Bond angles

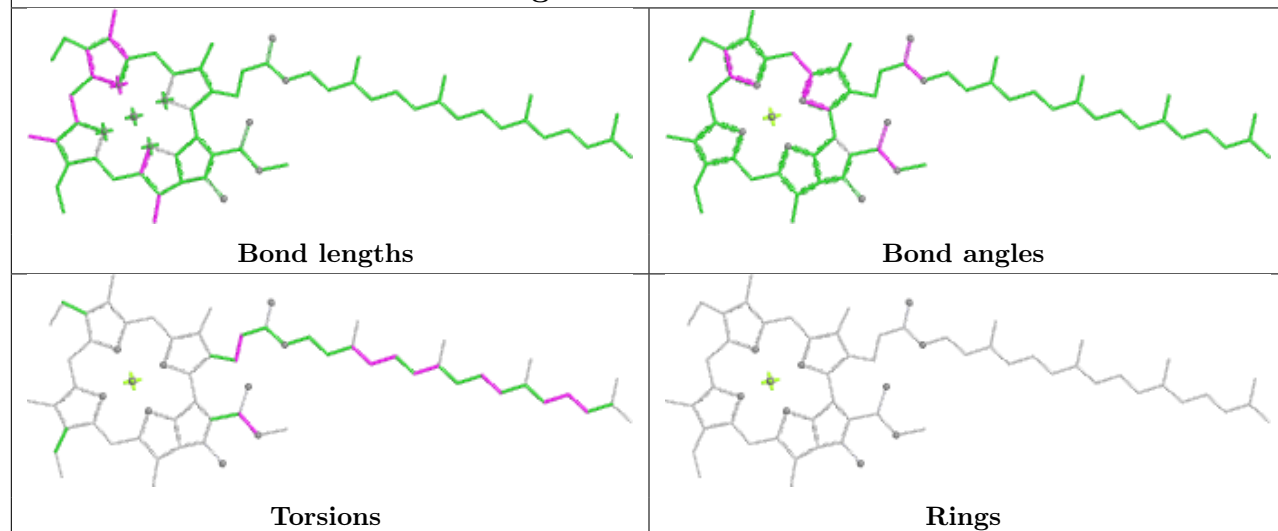


Torsions

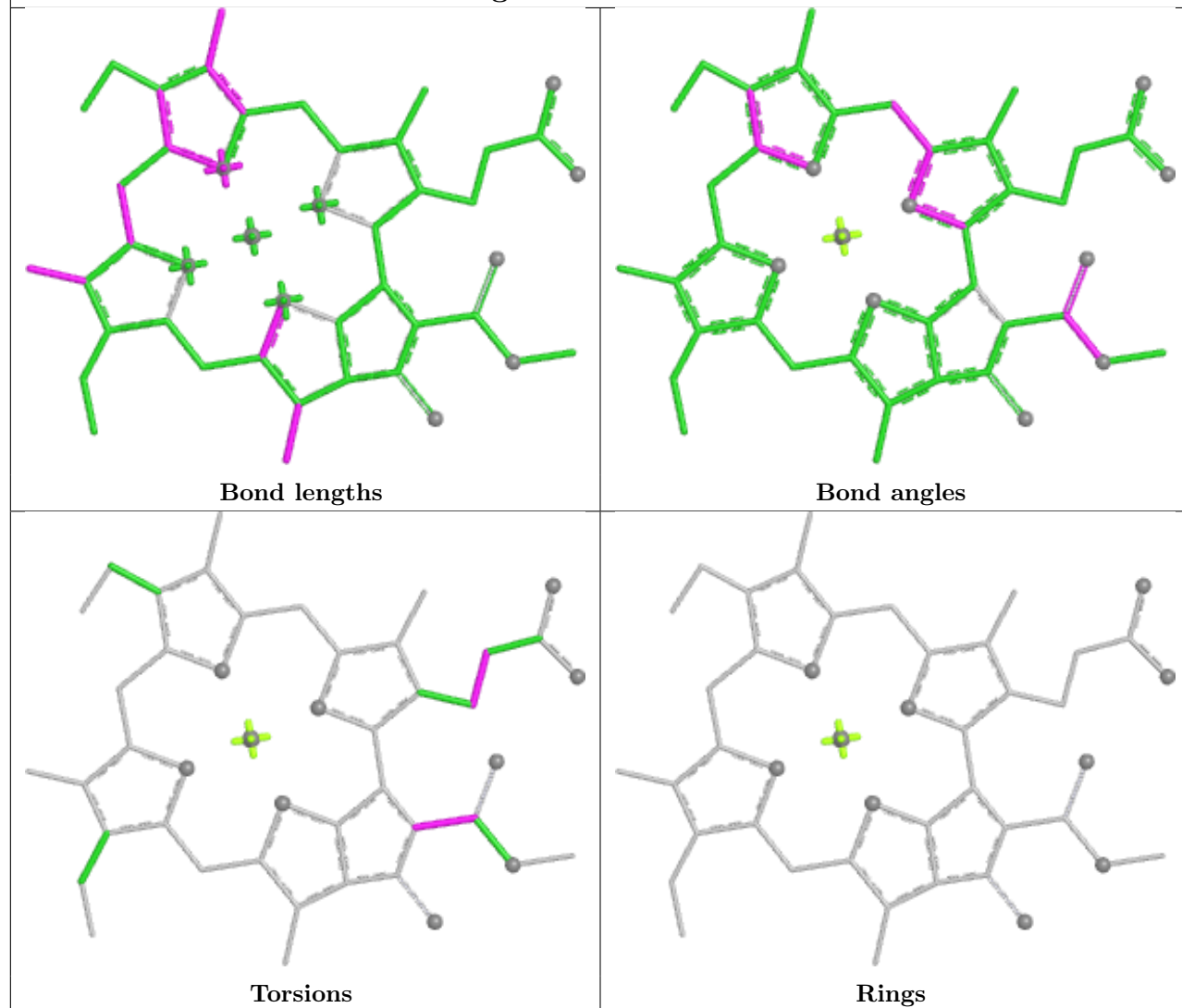


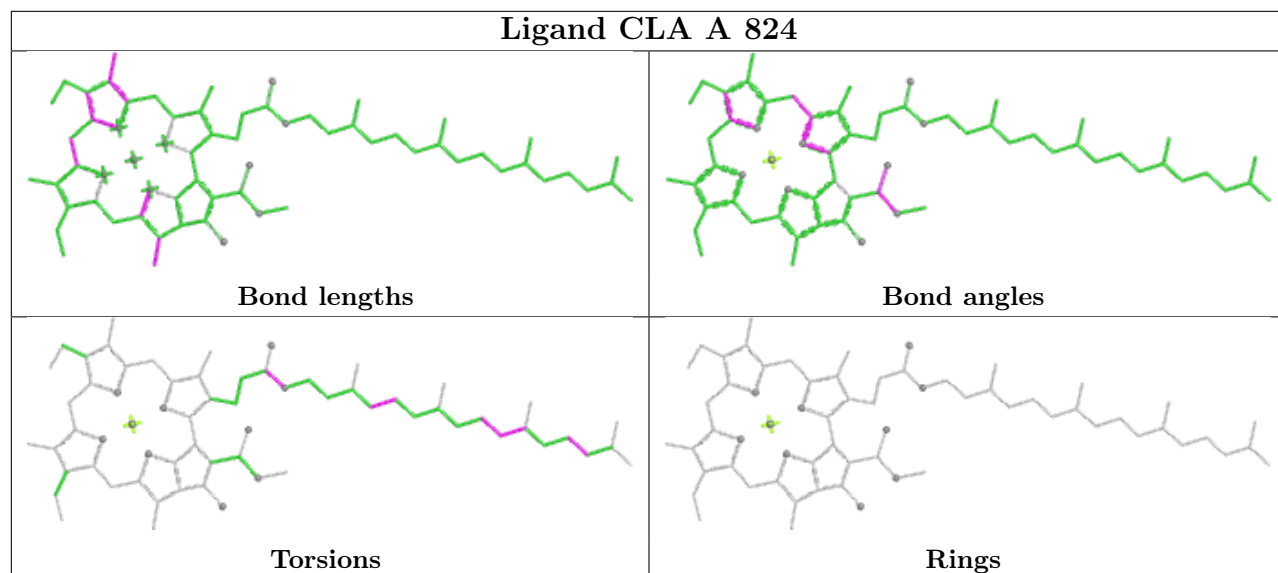
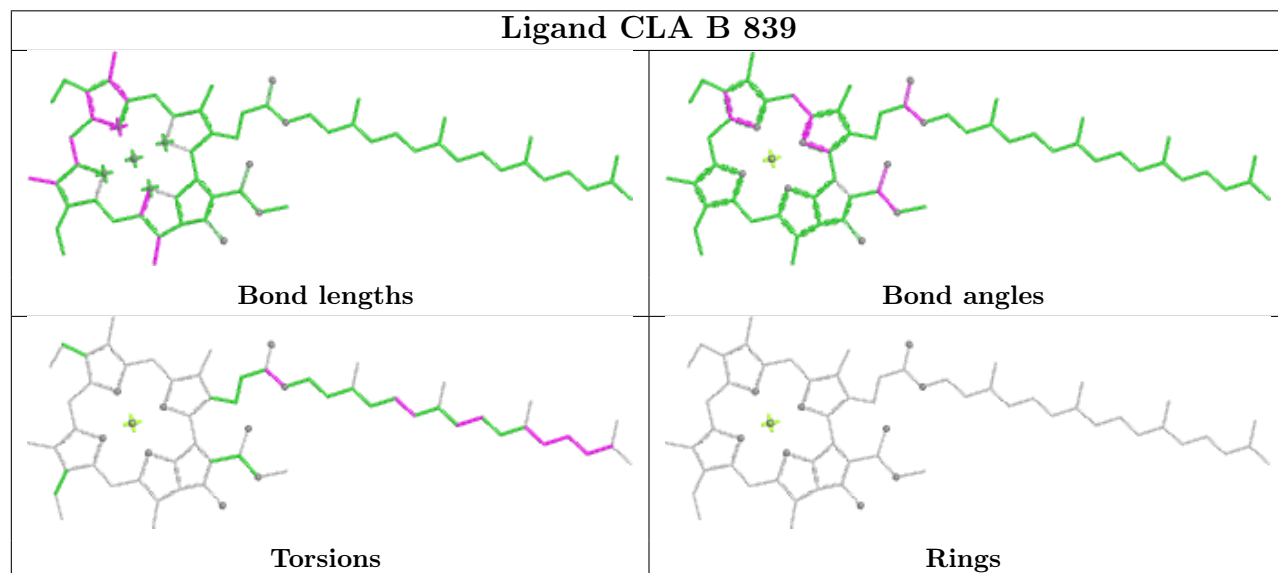
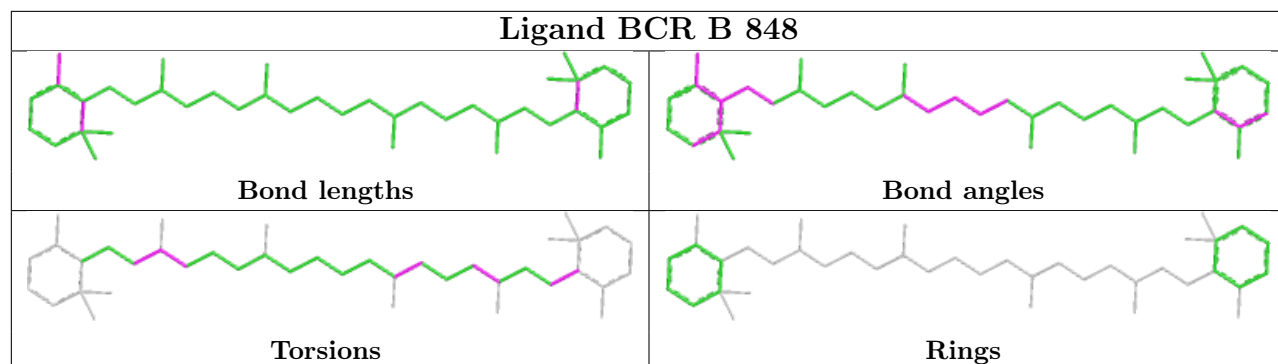
Rings

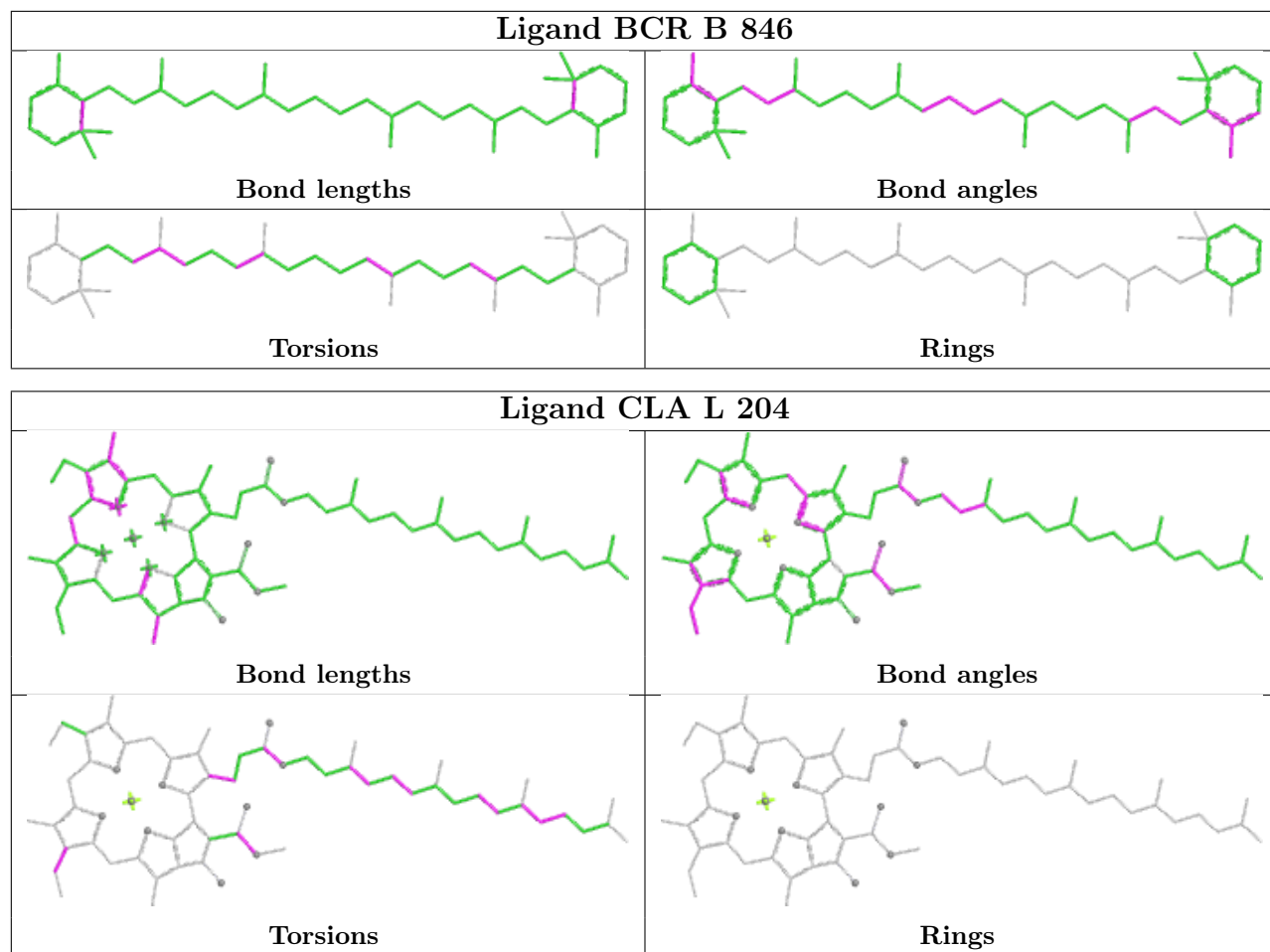
Ligand CLA A 803



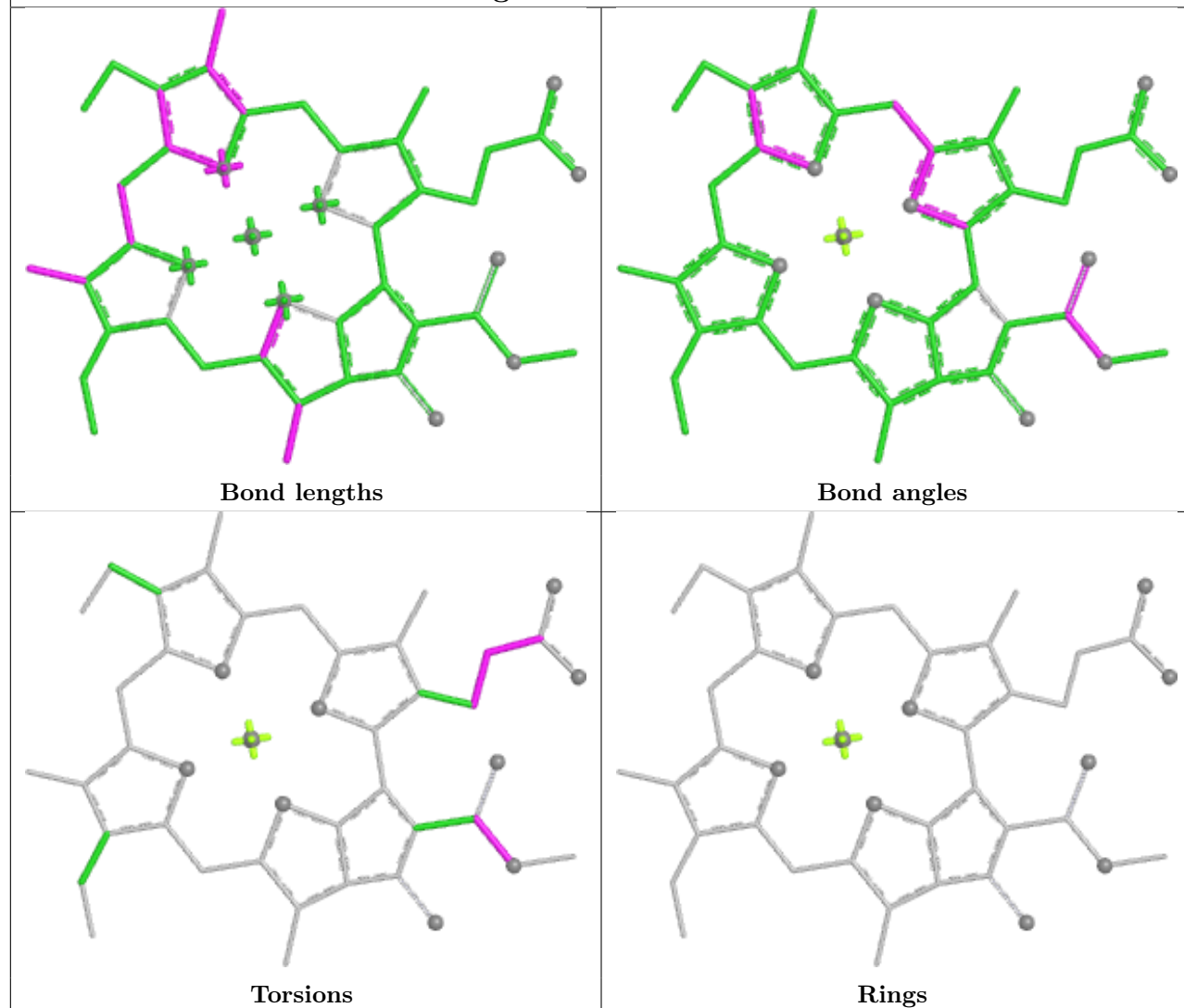
Ligand CLA A 843



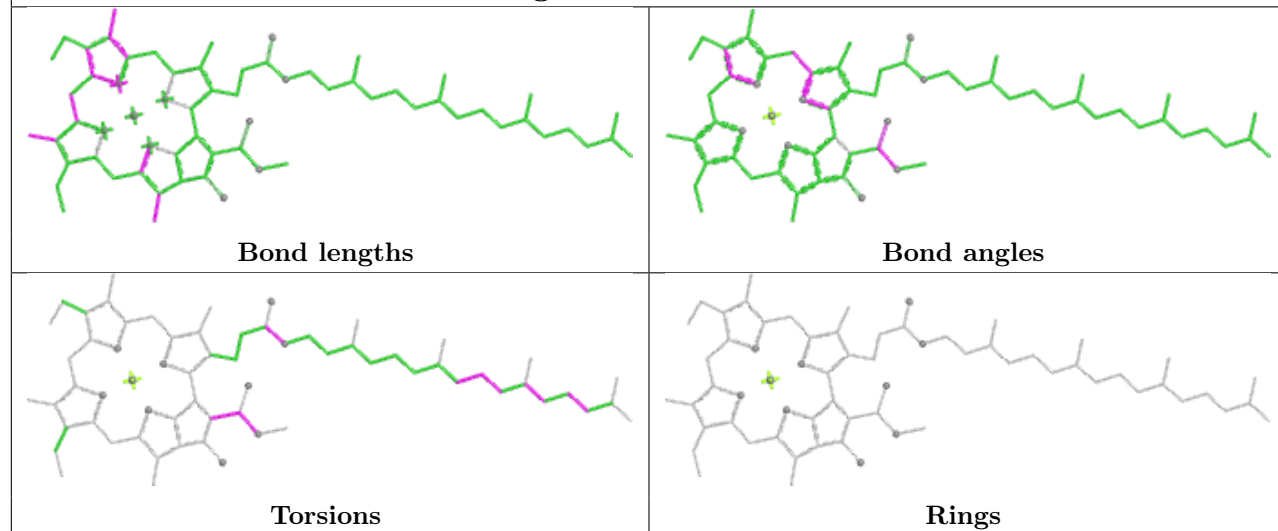




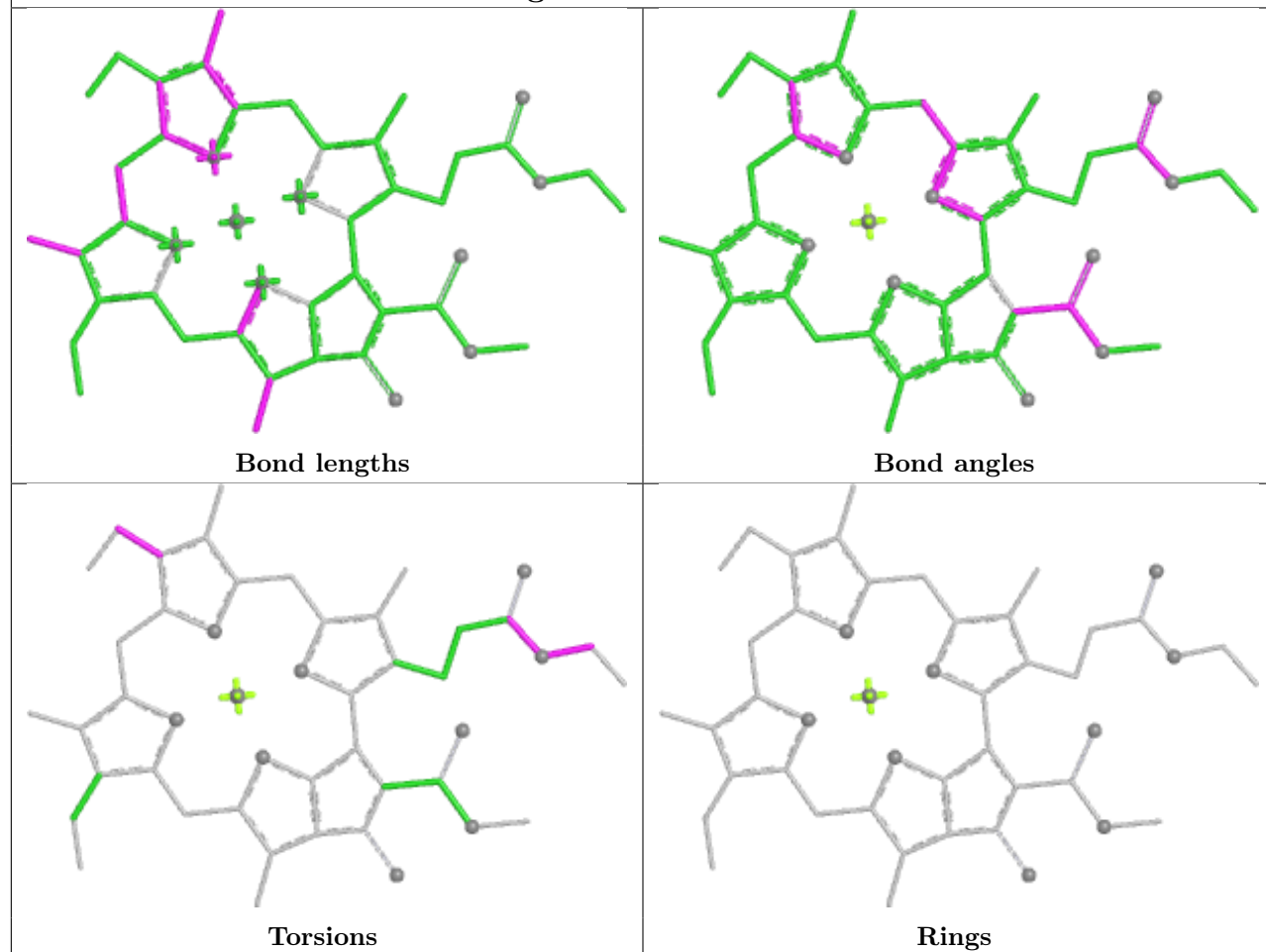
Ligand CLA B 813



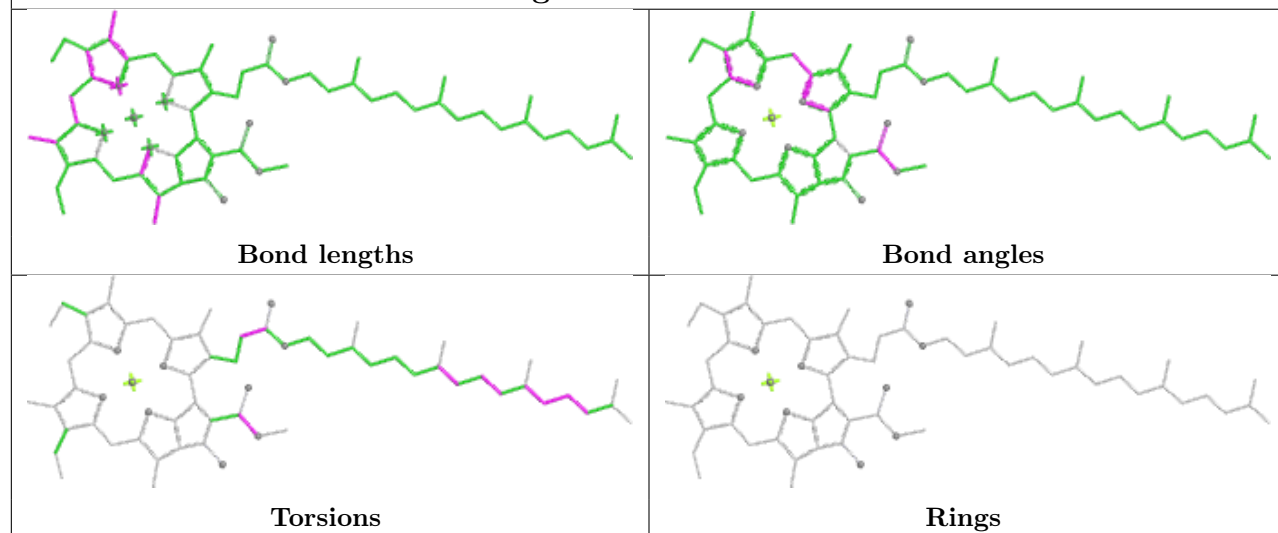
Ligand CLA B 835

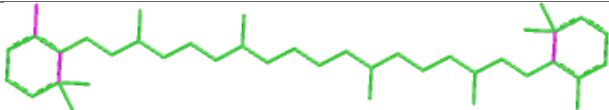
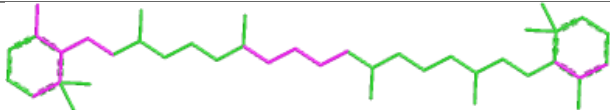
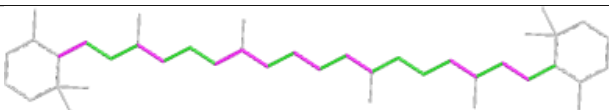
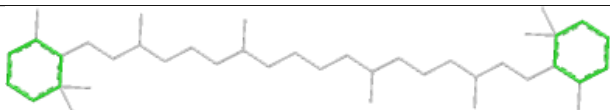


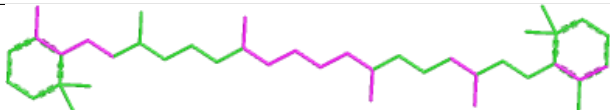
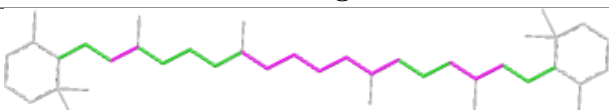
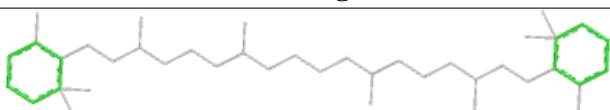
Ligand CLA B 840

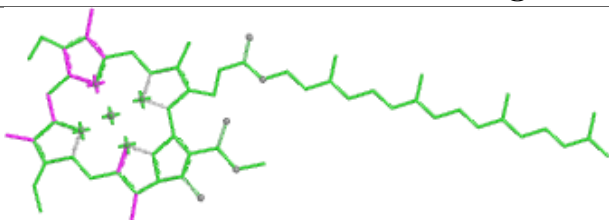
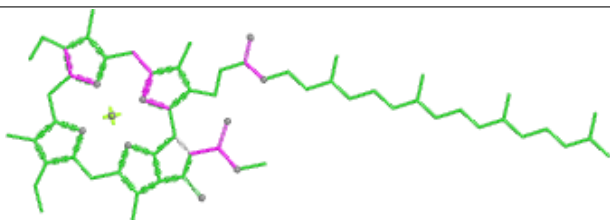
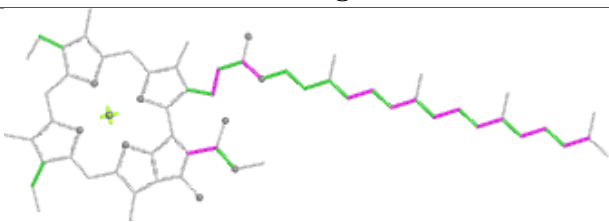
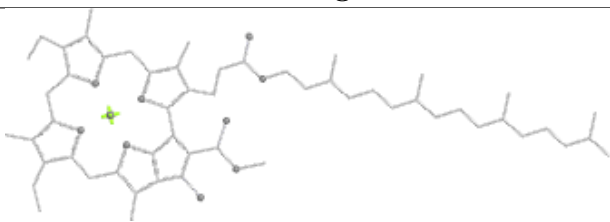


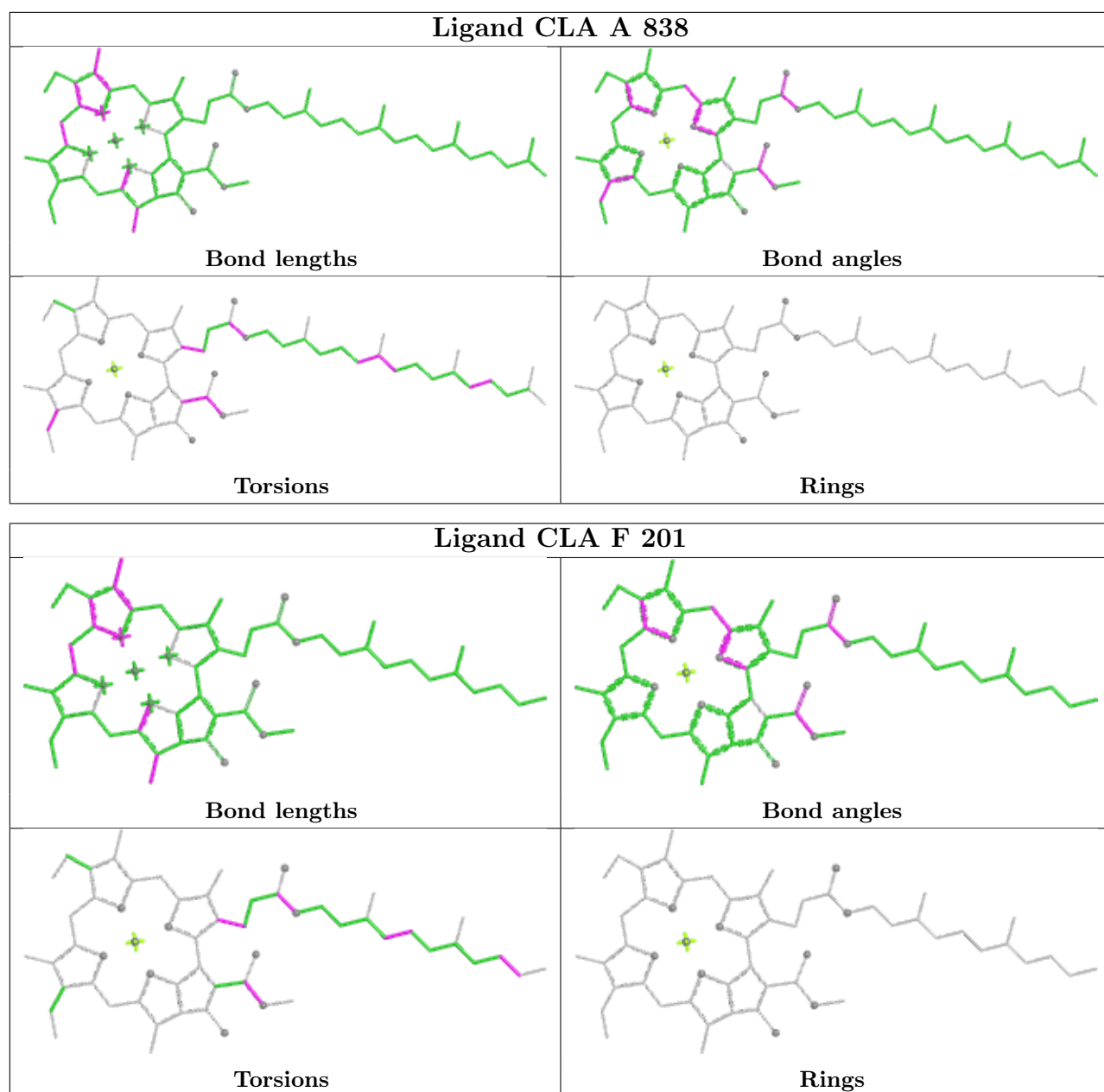
Ligand CLA B 804

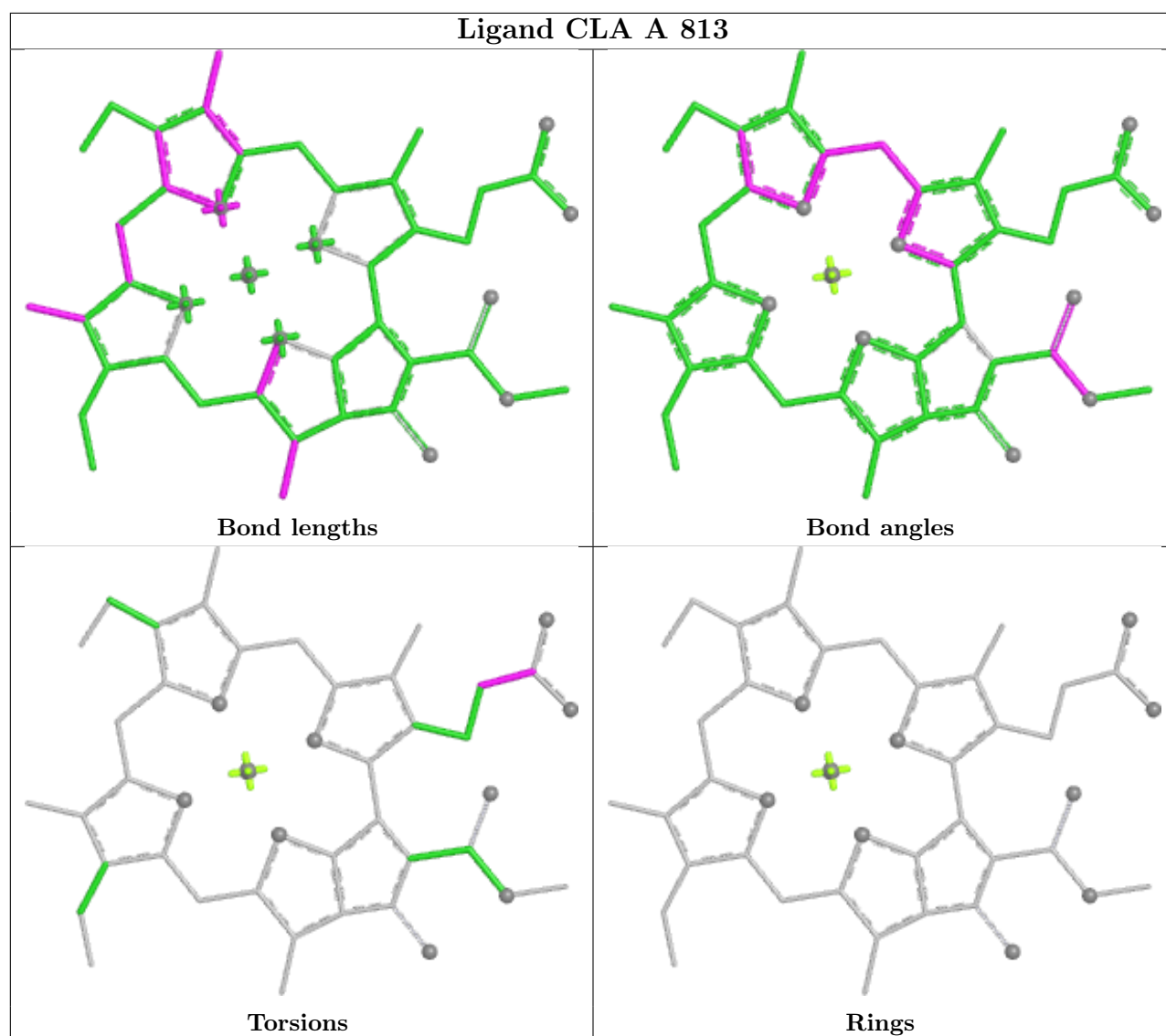


Ligand BCR I 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 847	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 839	
	
Bond lengths	Bond angles
	
Torsions	Rings





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.

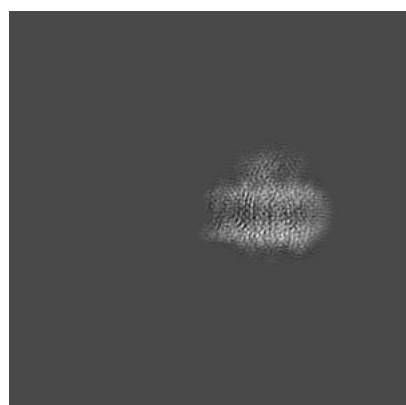
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10557. These allow visual inspection of the internal detail of the map and identification of artifacts.

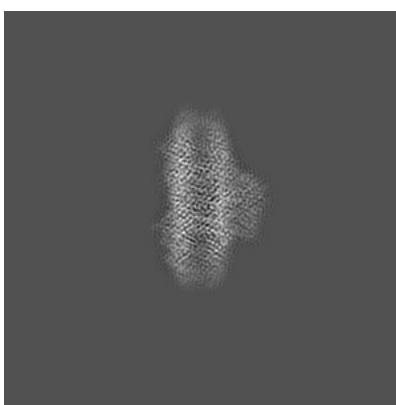
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

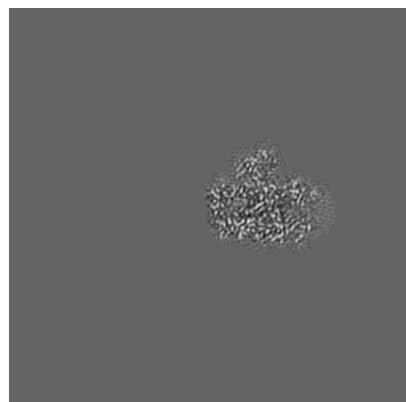


Z

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

6.2 Central slices [i](#)

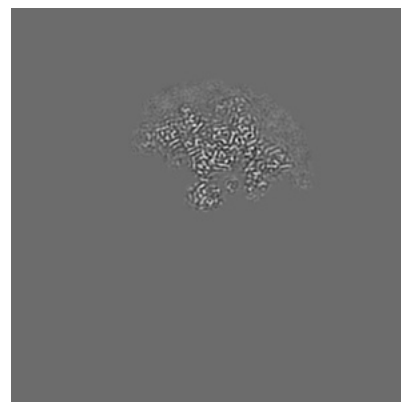
6.2.1 Primary map



X Index: 280



Y Index: 280

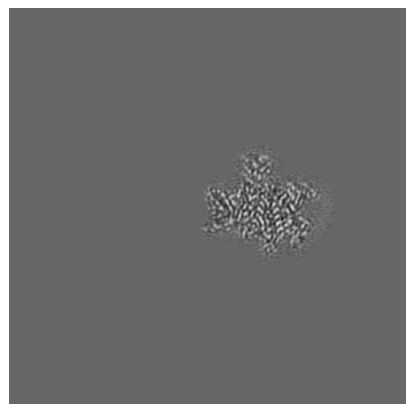


Z Index: 280

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

6.3 Largest variance slices [i](#)

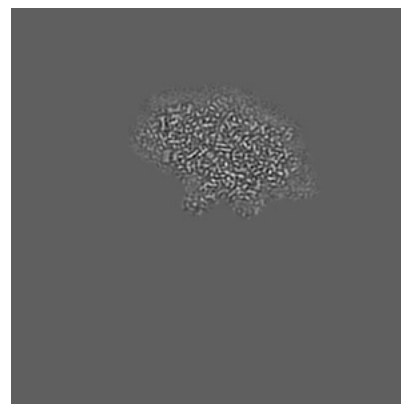
6.3.1 Primary map



X Index: 265



Y Index: 354

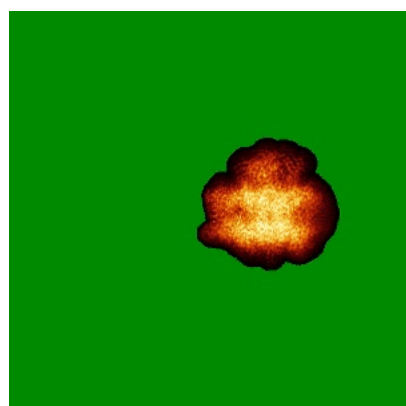


Z Index: 251

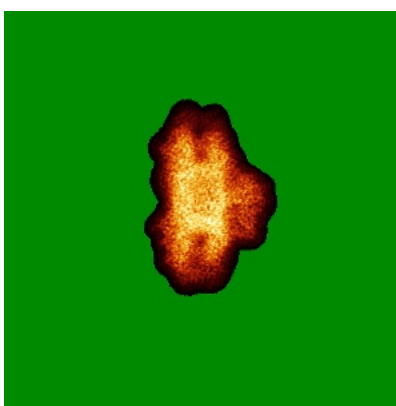
The images above show the largest variance slices of the map in three orthogonal directions.

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

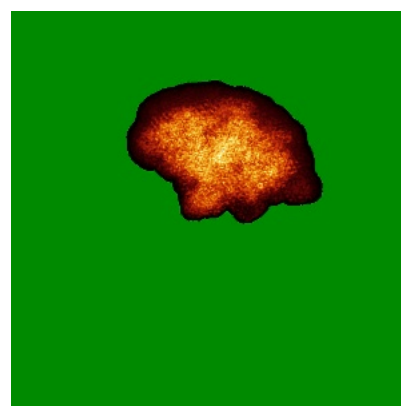
6.4.1 Primary map



X



Y

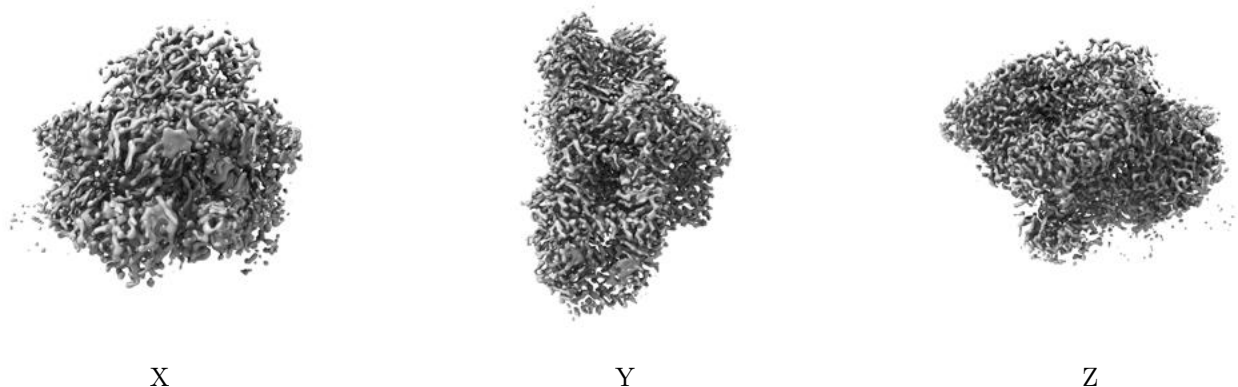


Z

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

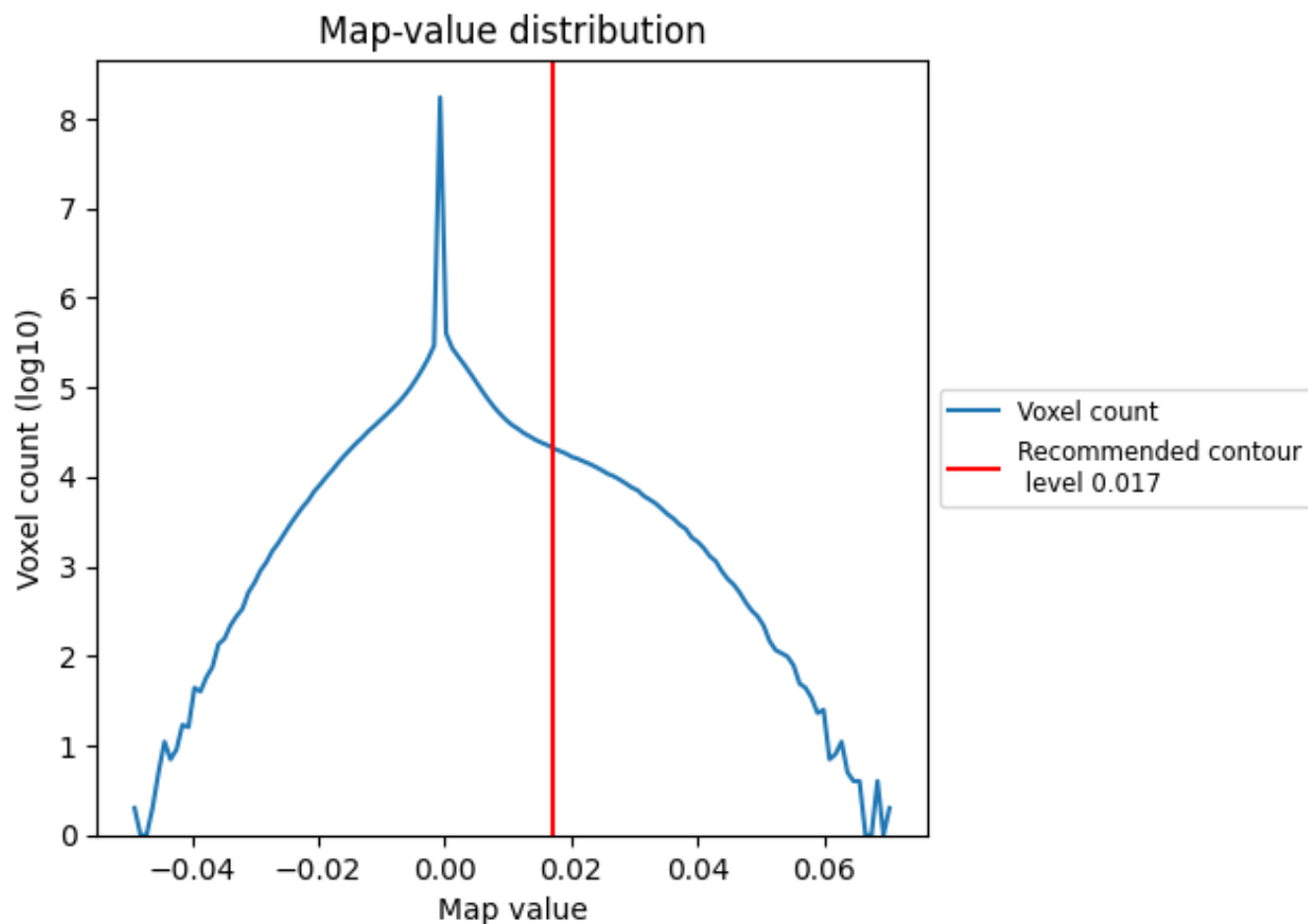
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

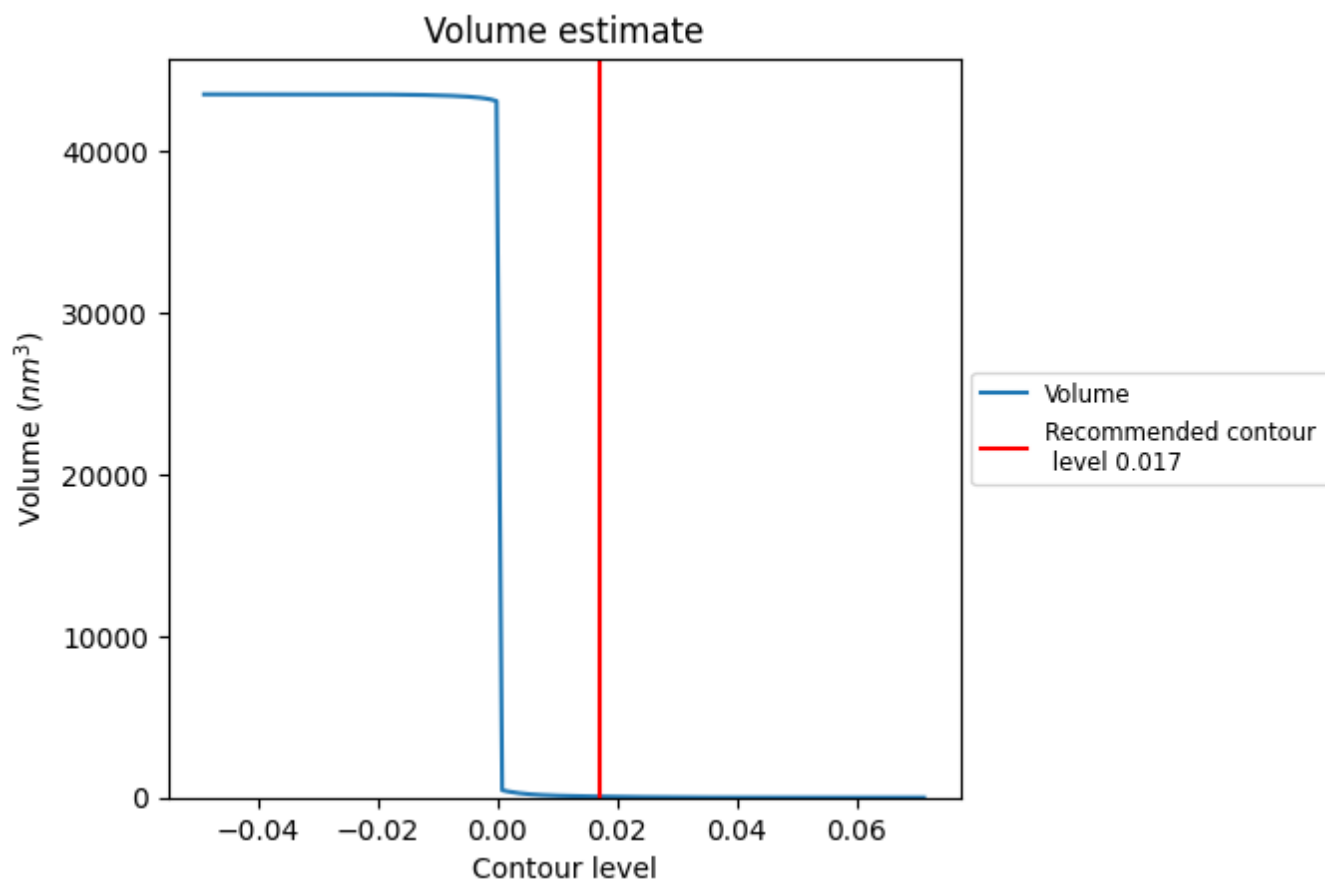
This section contains the results of statistical analysis of the map.

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.

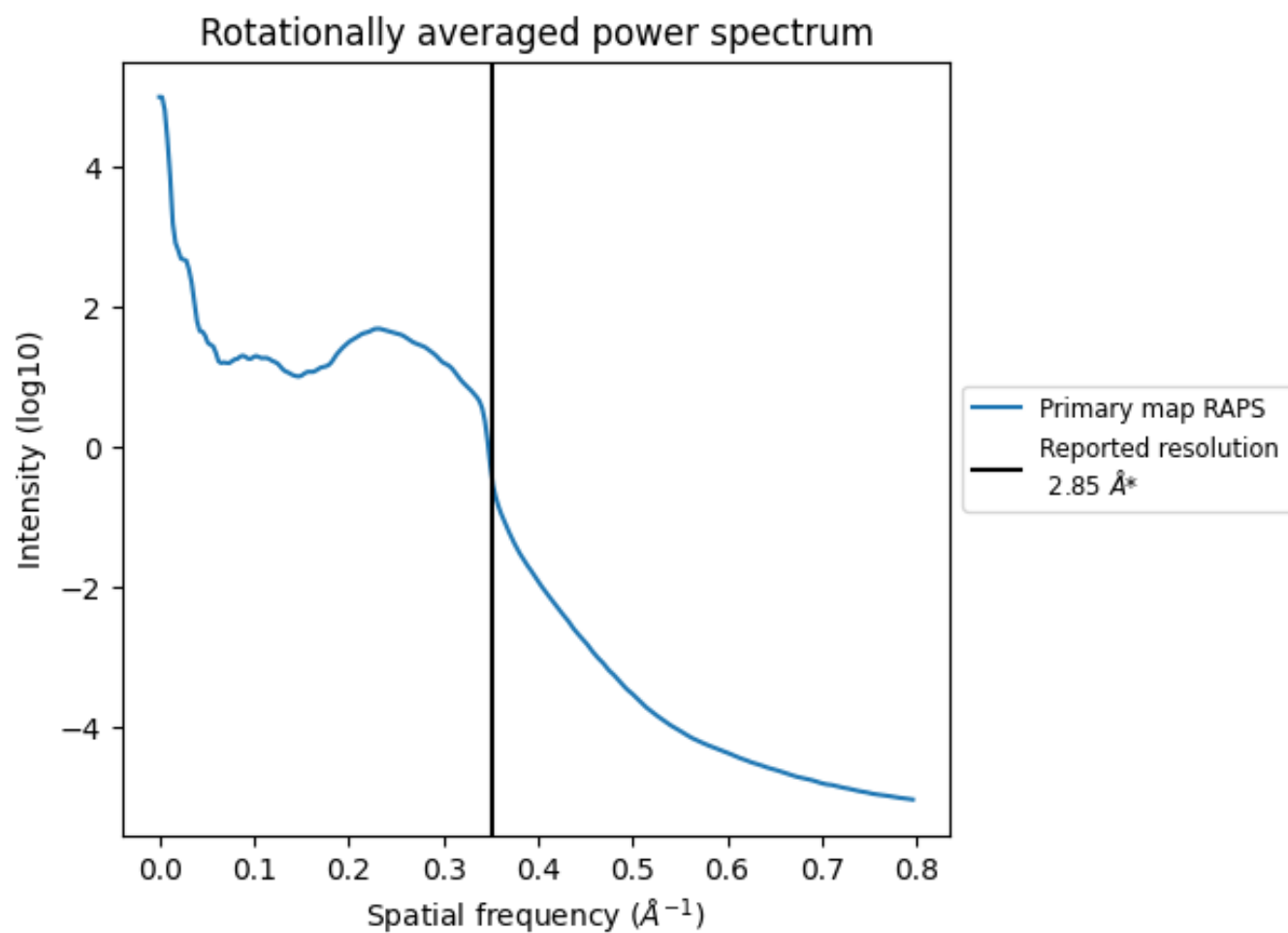
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 62 nm³; this corresponds to an approximate mass of 56 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 ⓘ

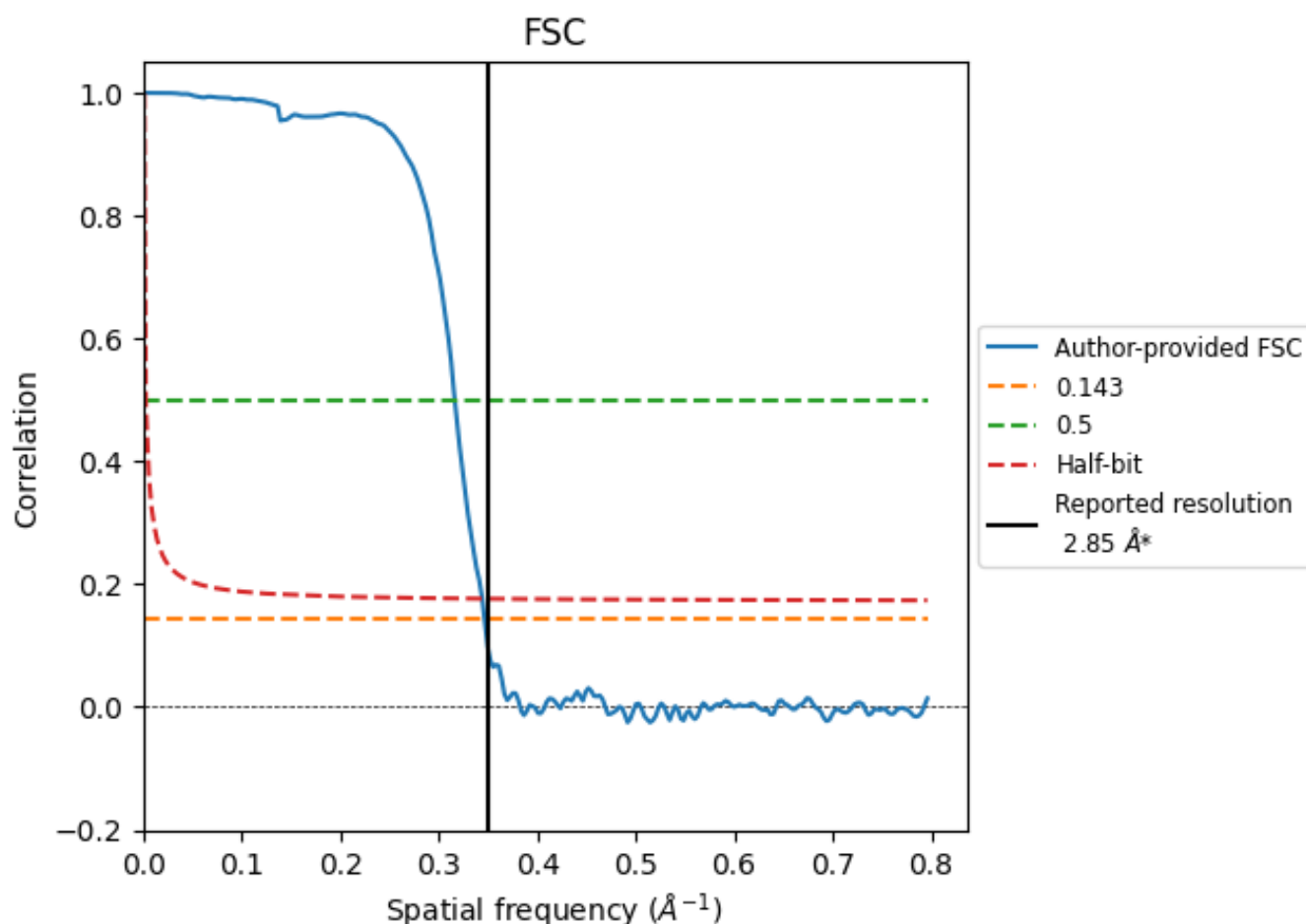


*Reported resolution corresponds to spatial frequency of 0.351 Å⁻¹

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 0.351 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

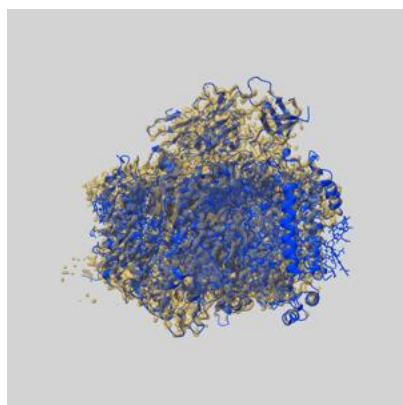
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.85	-	-
Author-provided FSC curve	2.89	3.16	2.91
Unmasked-calculated*	-	-	-

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

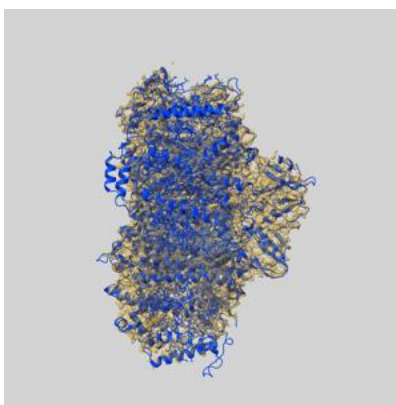
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10557 and PDB model 6TRA. Per-residue inclusion information can be found in section [3](#) on page [19](#).

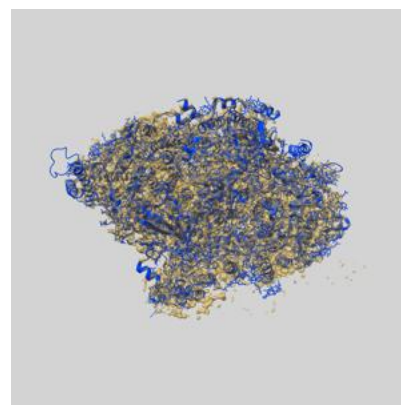
9.1 Map-model overlay [i](#)



X



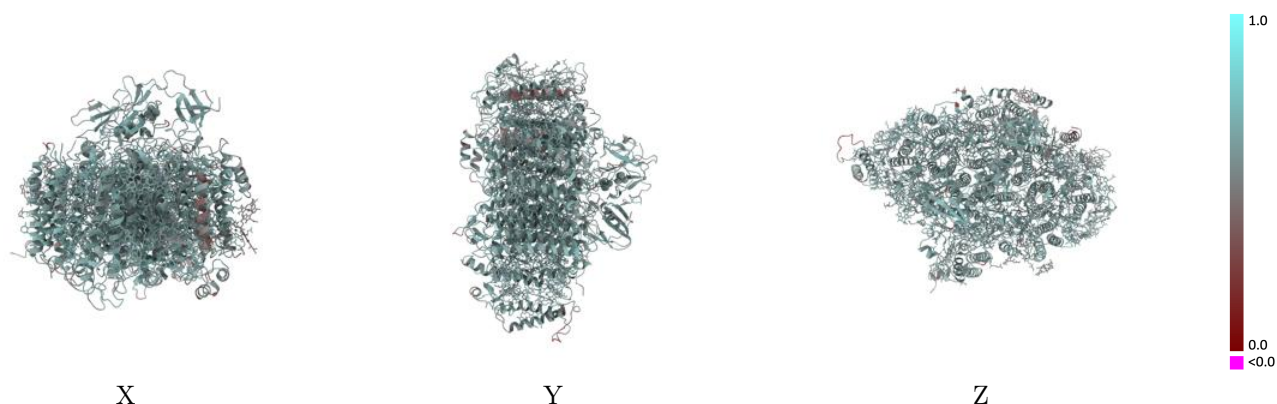
Y



Z

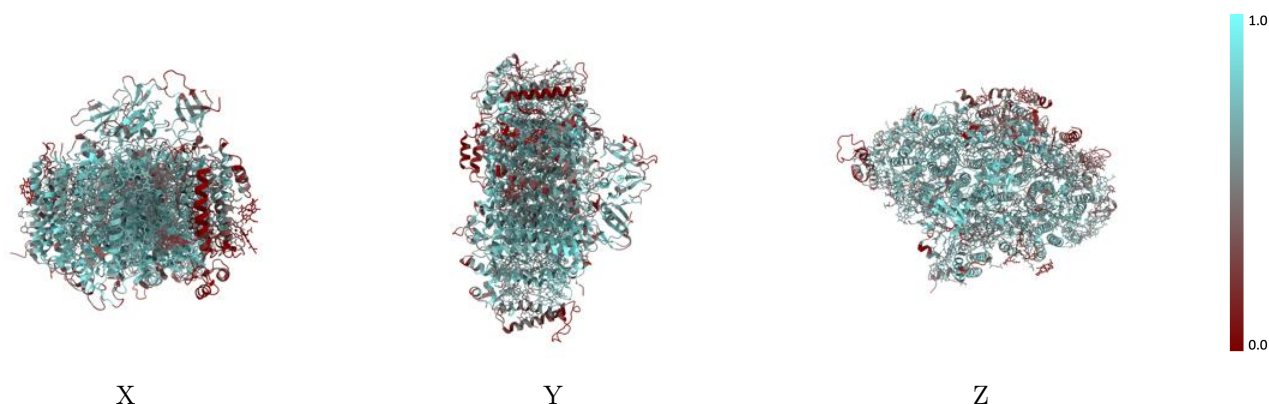
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



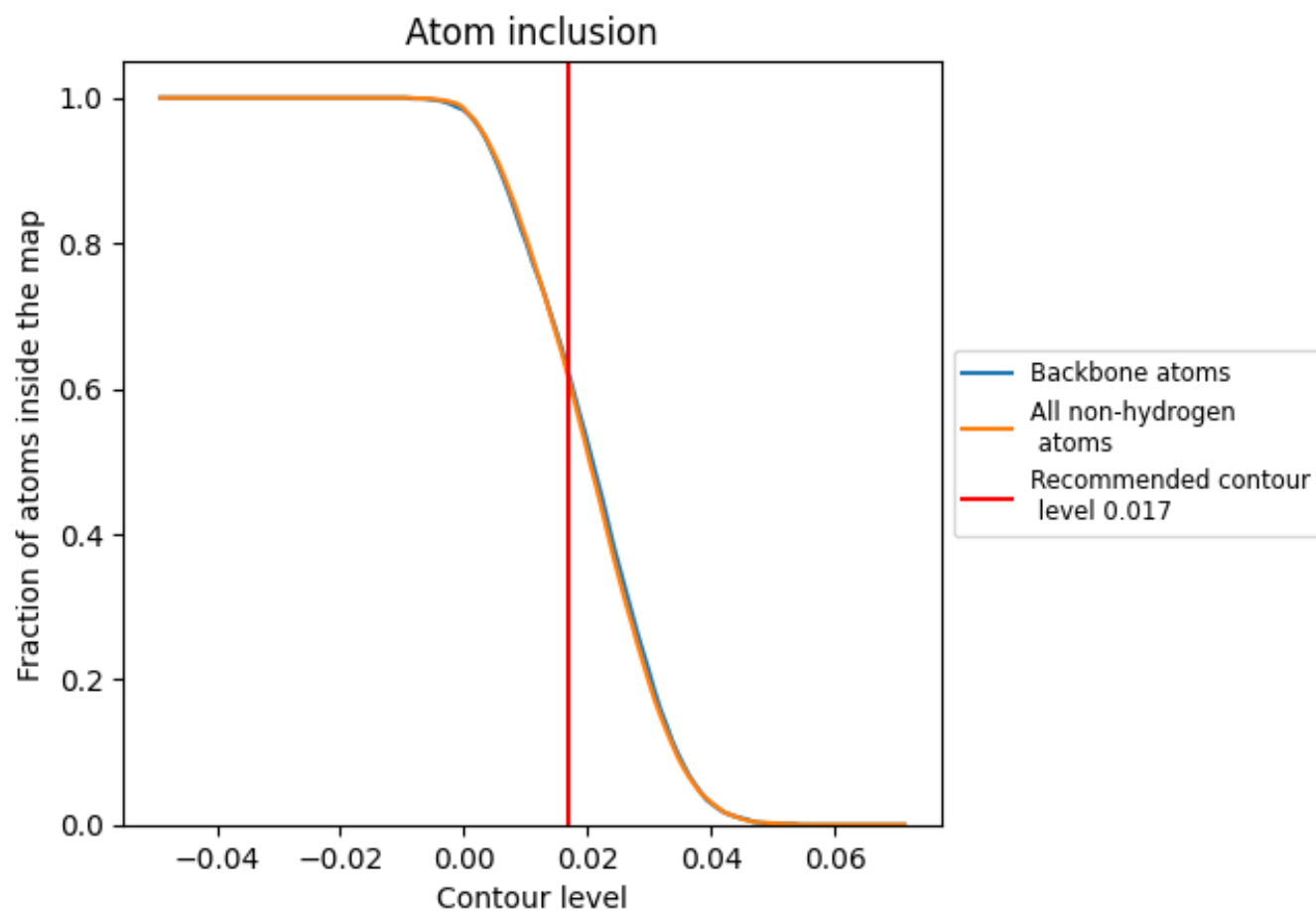
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.017).

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6120	0.5890
A	0.6900	0.6030
B	0.6630	0.5960
C	0.6800	0.5910
D	0.5620	0.5780
E	0.5090	0.5760
F	0.3120	0.5470
I	0.5890	0.5890
J	0.2920	0.5530
K	0.2630	0.5270
L	0.5880	0.5790
M	0.4870	0.5700
X	0.0150	0.4450

1.0

0.0

<0.0