



Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 12:36 AM UTC

PDB ID : 9SE7 / pdb_00009se7
EMDB ID : EMD-54804
Title : Structure of Cytochrome C6 bound Photosystem I from *Chlamydomonas reinhardtii* at 2.07 Å resolution
Authors : Mahapatra, G.P.; Schuller, J.M.
Deposited on : 2025-08-15
Resolution : 2.06 Å (reported)
Based on initial models : 7ZQC, 1CYI

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:

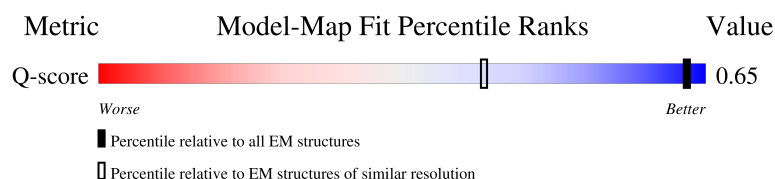
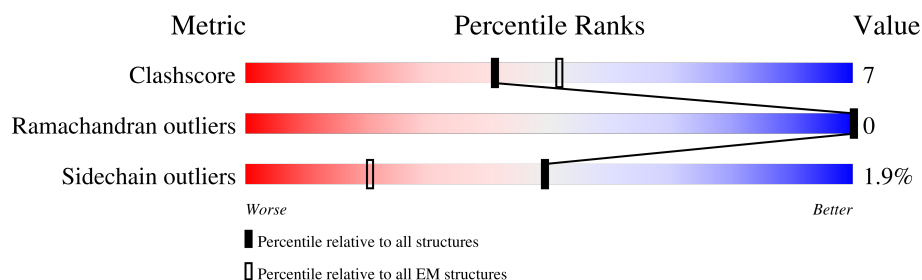
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.06 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	1895 (1.56 - 2.56)

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	742	 9% 88% 12%
2	B	733	 14% 87% 13%
3	C	80	 31% 88% 11%
4	D	144	 31% 83% 17%

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Mol	Chain	Length	Quality of chain
5	E	64	
6	I	37	
7	J	41	
8	T	89	
9	F	165	
10	L	138	

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
11	CLA	A	801	X	-	-	-
11	CLA	A	802	X	-	-	-
11	CLA	A	803	X	-	-	-
11	CLA	A	804	X	-	-	-
11	CLA	A	805	X	-	-	-
11	CLA	A	806	X	-	-	-
11	CLA	A	807	X	-	-	-
11	CLA	A	808	X	-	-	-
11	CLA	A	809	X	-	-	-
11	CLA	A	810	X	-	-	-
11	CLA	A	811	X	-	-	-
11	CLA	A	812	X	-	-	-
11	CLA	A	813	X	-	-	-
11	CLA	A	814	X	-	-	-
11	CLA	A	815	X	-	-	-
11	CLA	A	816	X	-	-	-
11	CLA	A	817	X	-	-	-
11	CLA	A	818	X	-	-	-
11	CLA	A	819	X	-	-	-
11	CLA	A	820	X	-	-	-
11	CLA	A	821	X	-	-	-
11	CLA	A	822	X	-	-	-
11	CLA	A	823	X	-	-	-
11	CLA	A	824	X	-	-	-
11	CLA	A	825	X	-	-	-
11	CLA	A	826	X	-	-	-
11	CLA	A	827	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	A	828	X	-	-	-
11	CLA	A	829	X	-	-	-
11	CLA	A	830	X	-	-	-
11	CLA	A	831	X	-	-	-
11	CLA	A	832	X	-	-	-
11	CLA	A	833	X	-	-	-
11	CLA	A	834	X	-	-	-
11	CLA	A	835	X	-	-	-
11	CLA	A	836	X	-	-	-
11	CLA	A	837	X	-	-	-
11	CLA	A	838	X	-	-	-
11	CLA	A	839	X	-	-	-
11	CLA	A	840	X	-	-	-
11	CLA	A	841	X	-	-	-
11	CLA	A	842	X	-	-	-
11	CLA	A	844	X	-	-	-
11	CLA	B	801	X	-	-	-
11	CLA	B	802	X	-	-	-
11	CLA	B	803	X	-	-	-
11	CLA	B	804	X	-	-	-
11	CLA	B	805	X	-	-	-
11	CLA	B	806	X	-	-	-
11	CLA	B	807	X	-	-	-
11	CLA	B	808	X	-	-	-
11	CLA	B	809	X	-	-	-
11	CLA	B	810	X	-	-	-
11	CLA	B	811	X	-	-	-
11	CLA	B	812	X	-	-	-
11	CLA	B	813	X	-	-	-
11	CLA	B	814	X	-	-	-
11	CLA	B	815	X	-	-	-
11	CLA	B	816	X	-	-	-
11	CLA	B	817	X	-	-	-
11	CLA	B	818	X	-	-	-
11	CLA	B	819	X	-	-	-
11	CLA	B	820	X	-	-	-
11	CLA	B	821	X	-	-	-
11	CLA	B	822	X	-	-	-
11	CLA	B	823	X	-	-	-
11	CLA	B	824	X	-	-	-
11	CLA	B	825	X	-	-	-
11	CLA	B	826	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	B	827	X	-	-	-
11	CLA	B	828	X	-	-	-
11	CLA	B	829	X	-	-	-
11	CLA	B	830	X	-	-	-
11	CLA	B	831	X	-	-	-
11	CLA	B	832	X	-	-	-
11	CLA	B	833	X	-	-	-
11	CLA	B	834	X	-	-	-
11	CLA	B	835	X	-	-	-
11	CLA	B	836	X	-	-	-
11	CLA	B	837	X	-	-	-
11	CLA	B	838	X	-	-	-
11	CLA	B	839	X	-	-	-
11	CLA	B	840	X	-	-	-
11	CLA	B	841	X	-	-	-
11	CLA	B	842	X	-	-	-
11	CLA	B	852	X	-	-	-
11	CLA	F	803	X	-	-	-
11	CLA	F	804	X	-	-	-
11	CLA	J	103	X	-	-	-
11	CLA	L	202	X	-	-	-
11	CLA	L	203	X	-	-	-

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 24300 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	742	Total	C	N	O	S	0	0
			5825	3808	994	1001	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5824	3824	977	1005	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			601	369	103	117	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	144	Total	C	N	O	S	0	0
			1133	725	200	201	7		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	64	Total	C	N	O	0	0
			506	322	89	95		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	37	Total	C	N	O	S	0	0
			281	195	39	46	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	41	Total	C	N	O	S	0	0
			329	224	46	58	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	0	ACE	-	acetylation	UNP P59777

- Molecule 8 is a protein called Cytochrome c6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	T	89	Total	C	N	O	S	0	0
			674	424	114	131	5		

- Molecule 9 is a protein called Photosystem I reaction center subunit III, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	165	Total	C	N	O	S	0	0
			1266	817	213	233	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	124	Total	C	N	O	S	0	0
			899	586	146	164	3		

- Molecule 11 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
11	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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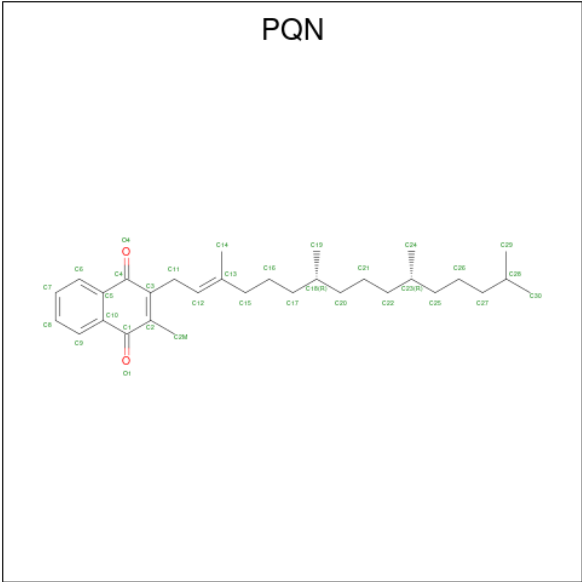
Mol	Chain	Residues	Atoms					AltConf
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
11	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	

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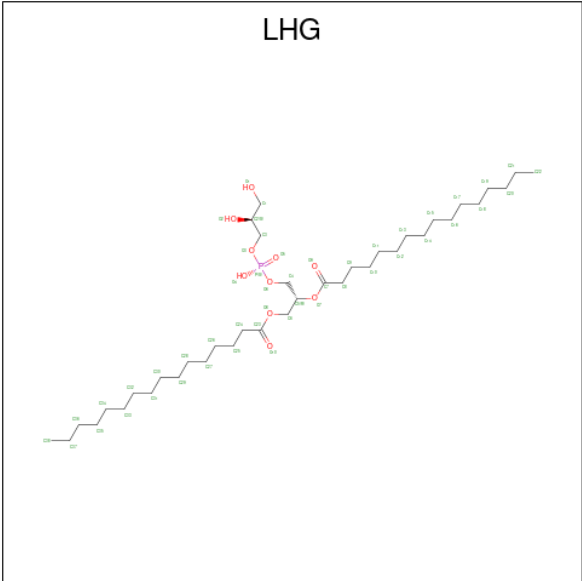
Mol	Chain	Residues	Atoms					AltConf
11	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0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

- Molecule 12 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 13 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



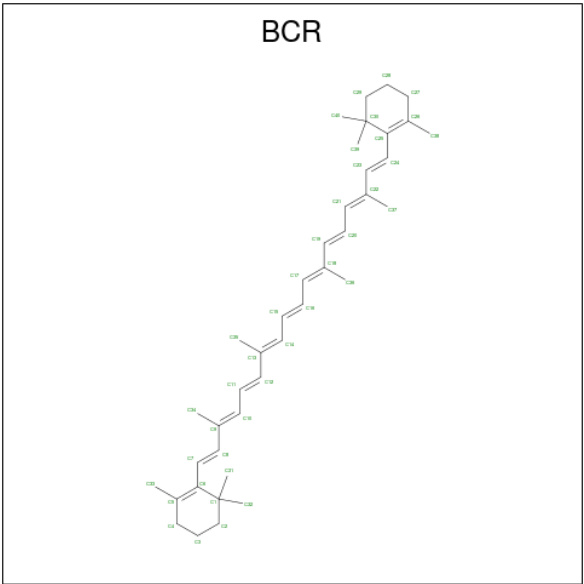
Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	O	P	0
			38	27	10	1	
13	B	1	Total	C	O	P	0
			45	34	10	1	

- Molecule 14 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



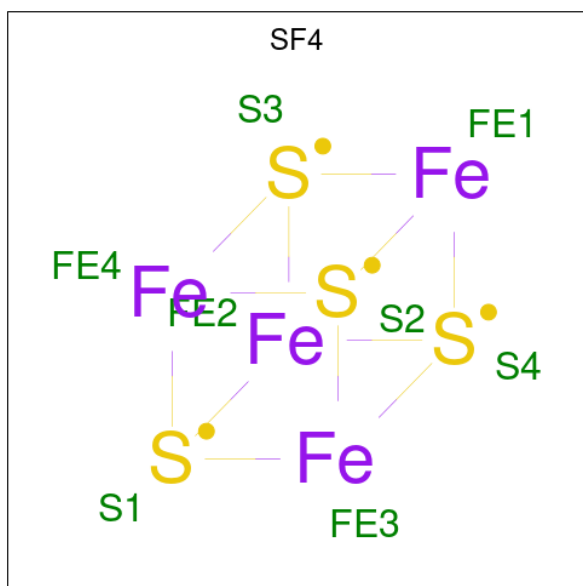
Mol	Chain	Residues	Atoms		AltConf
14	A	1	Total	C	0
			40	40	
14	A	1	Total	C	0
			40	40	
14	A	1	Total	C	0
			40	40	
14	A	1	Total	C	0
			40	40	
14	A	1	Total	C	0
			40	40	
14	B	1	Total	C	0
			40	40	
14	B	1	Total	C	0
			40	40	
14	B	1	Total	C	0
			40	40	
14	B	1	Total	C	0
			40	40	

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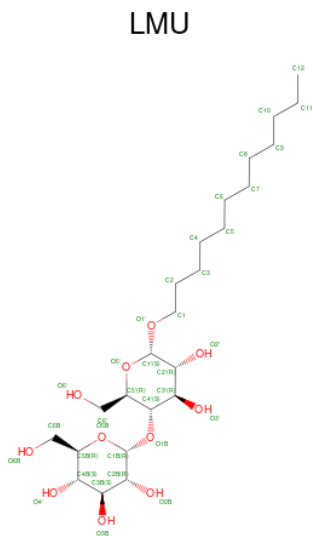
Mol	Chain	Residues	Atoms	AltConf
14	B	1	Total C 40 40	0
14	I	1	Total C 40 40	0
14	J	1	Total C 40 40	0
14	F	1	Total C 40 40	0
14	L	1	Total C 40 40	0
14	L	1	Total C 40 40	0

- Molecule 15 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



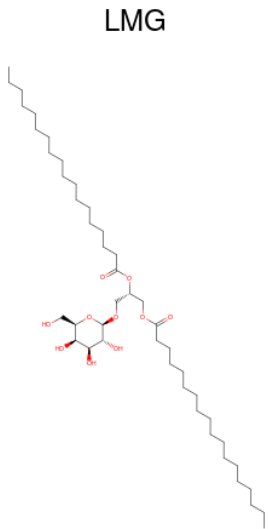
Mol	Chain	Residues	Atoms	AltConf
15	A	1	Total Fe S 8 4 4	0
15	C	1	Total Fe S 8 4 4	0
15	C	1	Total Fe S 8 4 4	0

- Molecule 16 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $\text{C}_{24}\text{H}_{46}\text{O}_{11}$).



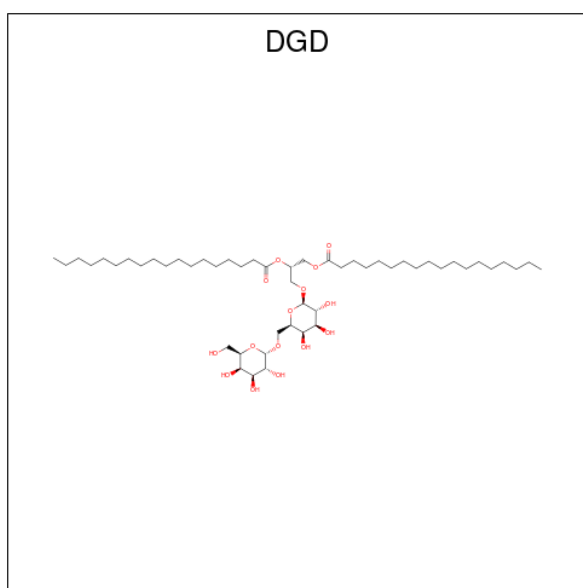
Mol	Chain	Residues	Atoms			AltConf
16	A	1	Total 34	C 23	O 11	0
16	A	1	Total 35	C 24	O 11	0
16	A	1	Total 24	C 18	O 6	0

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



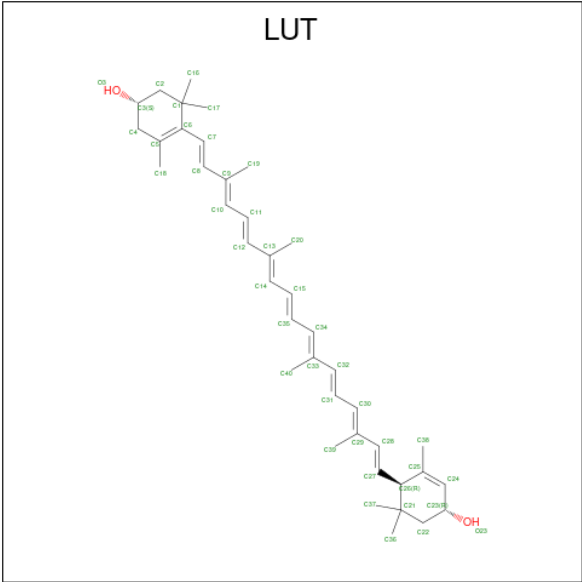
Mol	Chain	Residues	Atoms			AltConf
17	A	1	Total	C	O	0
			40	30	10	
17	B	1	Total	C	O	0
			43	33	10	
17	J	1	Total	C	O	0
			32	22	10	
17	J	1	Total	C	O	0
			42	32	10	
17	F	1	Total	C	O	0
			35	25	10	

- Molecule 18 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



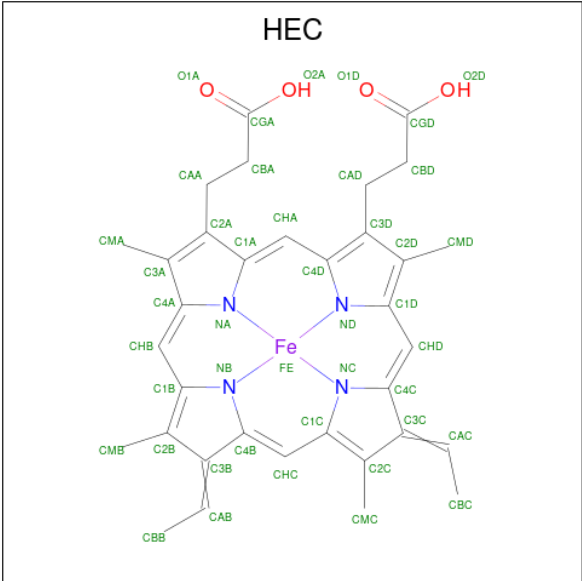
Mol	Chain	Residues	Atoms			AltConf
18	B	1	Total	C	O	0
			59	44	15	

- Molecule 19 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
19	J	1	Total	C	O	0
			42	40	2	
19	F	1	Total	C	O	0
			42	40	2	

- Molecule 20 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
20	T	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

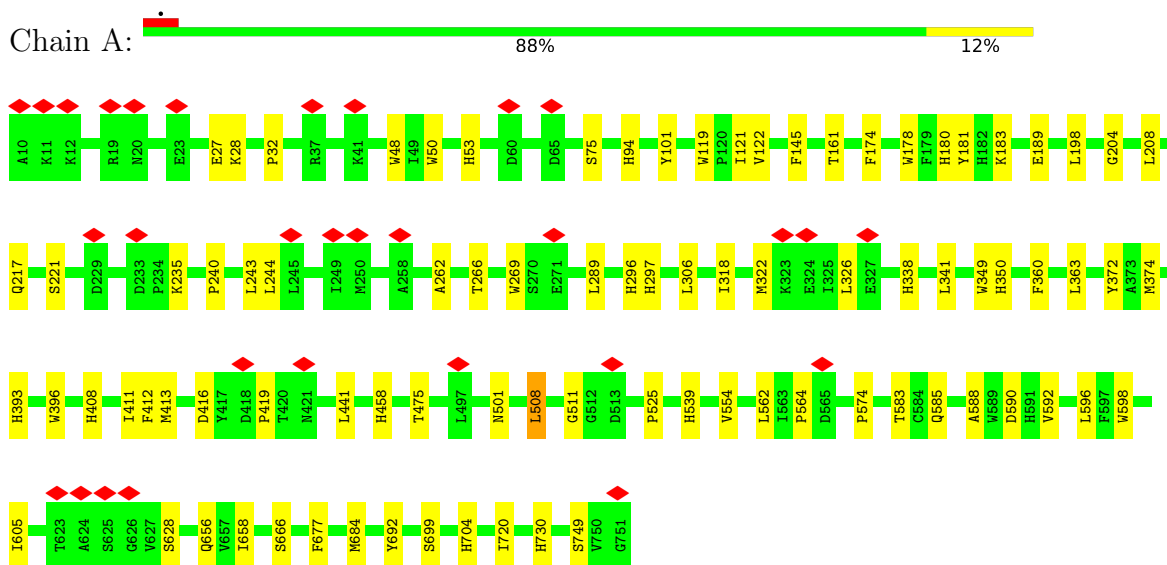
- Molecule 21 is water.

Mol	Chain	Residues	Atoms		AltConf
21	A	103	Total 103	O 103	0
21	B	107	Total 107	O 107	0
21	C	2	Total 2	O 2	0
21	D	3	Total 3	O 3	0
21	E	3	Total 3	O 3	0
21	J	6	Total 6	O 6	0
21	T	4	Total 4	O 4	0
21	F	24	Total 24	O 24	0

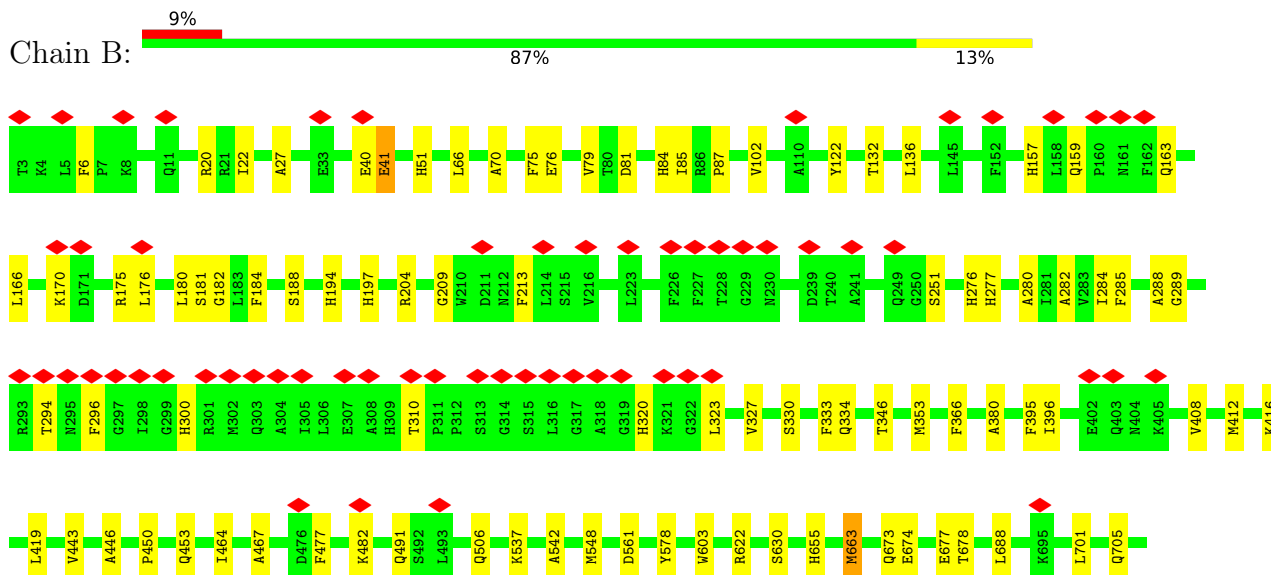
3 Residue-property plots

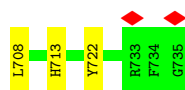
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

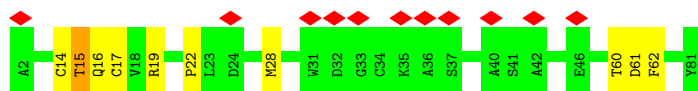
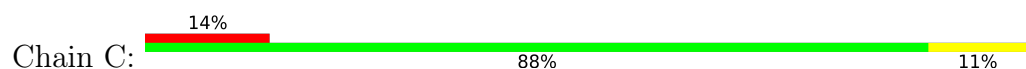


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

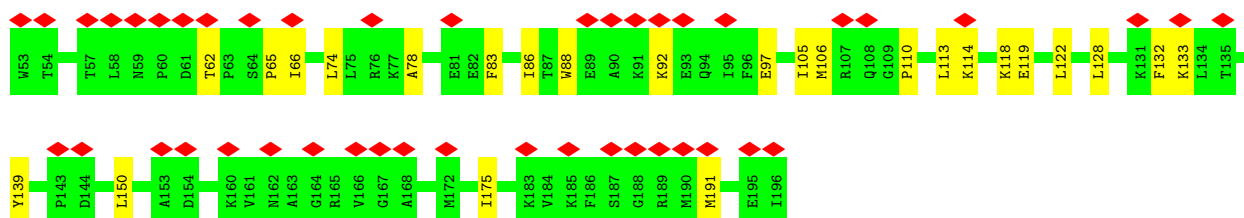
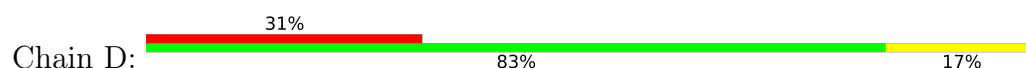




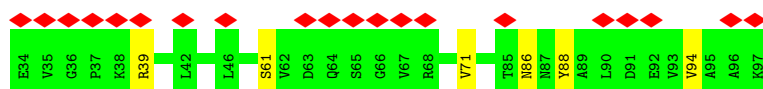
- Molecule 3: Photosystem I iron-sulfur center



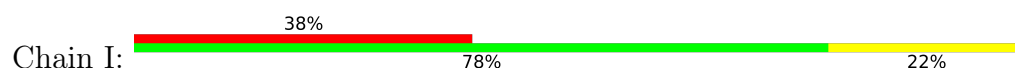
- Molecule 4: Photosystem I reaction center subunit II, chloroplastic



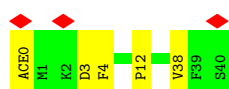
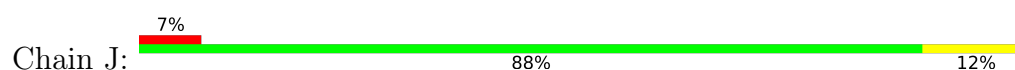
- Molecule 5: Photosystem I reaction center subunit IV, chloroplastic



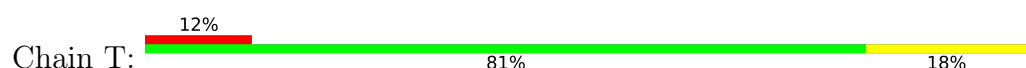
- Molecule 6: Photosystem I reaction center subunit VIII



- Molecule 7: Photosystem I reaction center subunit IX

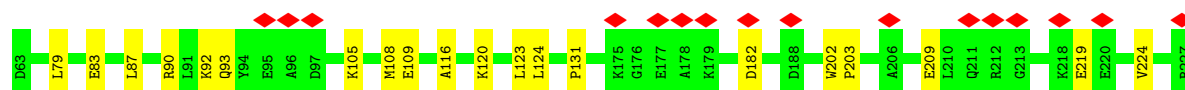
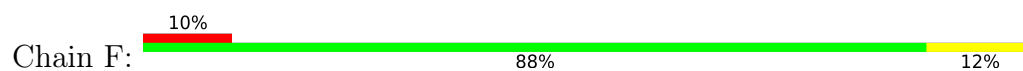


- Molecule 8: Cytochrome c6, chloroplastic

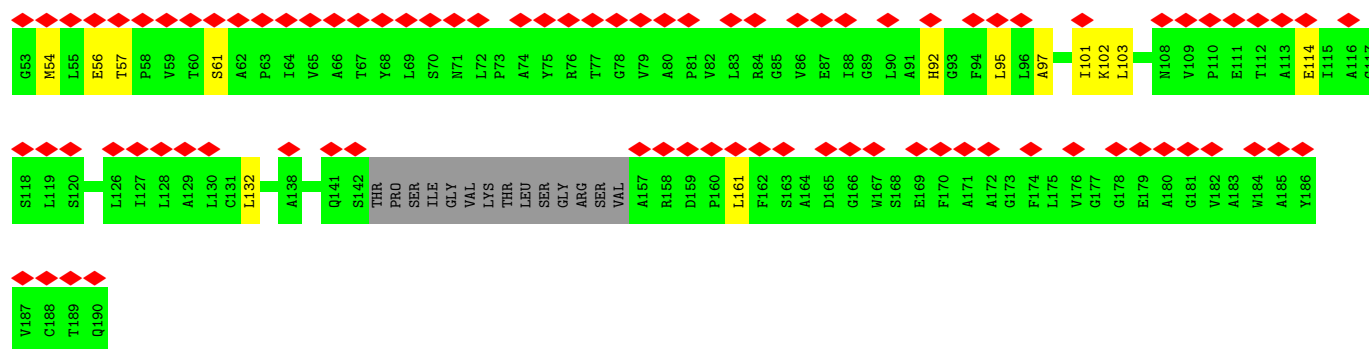
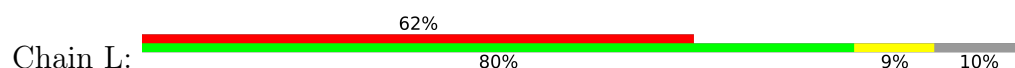




- Molecule 9: Photosystem I reaction center subunit III, chloroplastic



- Molecule 10: Photosystem I reaction center subunit XI, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53904	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.266	Depositor
Minimum map value	-0.106	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	373.76, 373.76, 373.76	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.73, 0.73, 0.73	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LUT, HEC, SF4, CLA, LMU, BCR, LHG, LMG, DGD, ACE, PQN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.15	0/6021	0.31	0/8208
2	B	0.15	0/6036	0.32	1/8240 (0.0%)
3	C	0.13	0/611	0.35	0/826
4	D	0.11	0/1161	0.31	0/1567
5	E	0.11	0/516	0.28	0/700
6	I	0.15	0/293	0.32	0/406
7	J	0.18	0/338	0.36	0/464
8	T	0.11	0/686	0.30	0/925
9	F	0.14	0/1292	0.30	0/1747
10	L	0.11	0/920	0.27	0/1257
All	All	0.14	0/17874	0.31	1/24340 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	663	MET	CA-CB-CG	5.65	125.41	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5825	0	5675	68	0
2	B	5824	0	5577	76	0
3	C	601	0	581	7	0
4	D	1133	0	1150	13	0
5	E	506	0	504	2	0
6	I	281	0	292	8	0
7	J	329	0	328	4	0
8	T	674	0	650	8	0
9	F	1266	0	1300	9	0
10	L	899	0	905	10	0
11	A	2554	0	2596	84	0
11	B	2588	0	2666	98	0
11	F	110	0	105	2	0
11	J	55	0	49	1	0
11	L	110	0	105	5	0
12	A	33	0	46	2	0
12	B	33	0	46	3	0
13	A	87	0	123	2	0
13	B	45	0	63	2	0
14	A	200	0	280	13	0
14	B	200	0	280	10	0
14	F	40	0	56	1	0
14	I	40	0	56	3	0
14	J	40	0	56	2	0
14	L	80	0	112	5	0
15	A	8	0	0	0	0
15	C	16	0	0	1	0
16	A	93	0	122	3	0
17	A	40	0	50	1	0
17	B	43	0	56	2	0
17	F	35	0	40	0	0
17	J	74	0	91	1	0
18	B	59	0	79	5	0
19	F	42	0	56	1	0
19	J	42	0	56	2	0
20	T	43	0	31	2	0
21	A	103	0	0	0	0
21	B	107	0	0	0	0
21	C	2	0	0	0	0
21	D	3	0	0	0	0
21	E	3	0	0	0	0
21	F	24	0	0	0	0
21	J	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	T	4	0	0	0	0
All	All	24300	0	24182	333	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 (333) 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:198:LEU:HD12	1:A:322:MET:HE1	1.58	0.85
1:A:684:MET:HB2	11:A:802:CLA:C1C	2.09	0.82
2:B:663:MET:HB3	11:B:804:CLA:C1C	2.12	0.79
2:B:300:HIS:NE2	11:B:822:CLA:ND	2.31	0.78
11:A:840:CLA:H112	11:A:840:CLA:HAB	1.71	0.72
11:B:814:CLA:H172	14:B:844:BCR:H271	1.73	0.70
11:A:827:CLA:HED1	11:A:835:CLA:HAB	1.76	0.68
1:A:374:MET:HE2	11:A:827:CLA:HMC2	1.78	0.65
8:T:10:PHE:HA	8:T:14:CYS:SG	2.37	0.65
2:B:40:GLU:HG2	2:B:166:LEU:HD11	1.78	0.64
1:A:161:THR:HG21	11:A:816:CLA:HAA2	1.78	0.64
1:A:217:GLN:HA	1:A:221:SER:HB2	1.80	0.64
1:A:240:PRO:HA	1:A:243:LEU:HD12	1.79	0.64
11:B:832:CLA:HBC2	11:B:839:CLA:HMC2	1.80	0.62
2:B:708:LEU:HD22	18:B:849:DGD:HB22	1.80	0.62
2:B:204:ARG:HG2	2:B:251:SER:HB2	1.80	0.62
2:B:673:GLN:O	2:B:677:GLU:HG3	2.01	0.61
14:A:851:BCR:H362	11:B:802:CLA:H2	1.83	0.61
4:D:88:TRP:HE1	4:D:106:MET:HE2	1.66	0.61
2:B:416:LYS:HA	2:B:419:LEU:HD12	1.83	0.60
7:J:38:VAL:HG11	9:F:123:LEU:HD21	1.83	0.60
2:B:663:MET:HB3	11:B:804:CLA:C2C	2.31	0.60
11:A:817:CLA:H171	11:A:818:CLA:H141	1.83	0.59
11:B:831:CLA:HAB	11:B:839:CLA:HAB	1.83	0.59
2:B:464:ILE:HD11	11:B:837:CLA:H12	1.83	0.59
2:B:157:HIS:CE1	11:B:812:CLA:NA	2.71	0.59
2:B:175:ARG:HB2	11:B:814:CLA:HBC2	1.85	0.58
1:A:396:TRP:CD1	11:A:828:CLA:HAB	2.38	0.58
2:B:27:ALA:HA	11:B:830:CLA:H42	1.86	0.58
11:A:821:CLA:H102	11:A:824:CLA:H93	1.85	0.58
2:B:705:GLN:HG3	18:B:849:DGD:HA22	1.85	0.58
11:B:804:CLA:H201	11:B:841:CLA:H51	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:839:CLA:H102	14:A:850:BCR:H373	1.86	0.57
2:B:280:ALA:O	2:B:284:ILE:HG13	2.05	0.57
7:J:0:ACE:H2	7:J:4:PHE:H	1.70	0.57
11:A:810:CLA:H51	11:A:813:CLA:H193	1.86	0.57
14:B:844:BCR:HC8	14:B:844:BCR:H311	1.87	0.56
11:B:818:CLA:H152	11:B:836:CLA:HBA1	1.86	0.56
1:A:75:SER:OG	1:A:181:TYR:HB2	2.06	0.56
14:B:846:BCR:H352	13:B:850:LHG:H162	1.88	0.56
3:C:60:THR:HG22	3:C:62:PHE:O	2.06	0.56
11:B:804:CLA:HBC2	11:B:804:CLA:HHD	1.86	0.55
1:A:32:PRO:HB2	1:A:48:TRP:HH2	1.71	0.55
2:B:300:HIS:CE1	11:B:822:CLA:NA	2.75	0.55
2:B:300:HIS:NE2	11:B:822:CLA:C4D	2.69	0.54
2:B:688:LEU:HB3	14:L:201:BCR:HC31	1.89	0.54
2:B:184:PHE:HE1	11:B:814:CLA:H52	1.71	0.54
2:B:408:VAL:O	2:B:412:MET:HG2	2.07	0.54
11:B:826:CLA:HAA2	11:B:827:CLA:OBD	2.08	0.54
6:I:86:VAL:O	6:I:90:ILE:HD12	2.07	0.54
11:A:819:CLA:HAB	11:A:819:CLA:H8	1.91	0.53
11:A:842:CLA:H72	11:B:840:CLA:H43	1.91	0.53
1:A:554:VAL:HG21	14:A:850:BCR:HC31	1.90	0.53
11:B:811:CLA:HBB2	6:I:84:GLY:HA3	1.89	0.53
1:A:393:HIS:CE1	11:A:828:CLA:ND	2.77	0.53
2:B:41:GLU:HG3	2:B:166:LEU:HB2	1.91	0.53
11:B:840:CLA:H172	14:I:201:BCR:H353	1.91	0.53
5:E:39:ARG:HD3	5:E:61:SER:HA	1.91	0.52
8:T:78:TYR:CE1	8:T:82:GLN:NE2	2.77	0.52
2:B:184:PHE:CE1	11:B:814:CLA:H52	2.45	0.52
11:A:840:CLA:HAA2	11:B:832:CLA:HMB2	1.92	0.52
11:B:840:CLA:HBB2	12:B:843:PQN:H141	1.91	0.52
11:B:829:CLA:H52	14:B:844:BCR:H23C	1.92	0.52
10:L:132:LEU:HD21	14:L:204:BCR:H24C	1.92	0.52
2:B:6:PHE:HE2	2:B:22:ILE:HA	1.75	0.52
1:A:684:MET:HB2	11:A:802:CLA:NC	2.25	0.52
11:B:802:CLA:HBB	11:B:803:CLA:H202	1.92	0.52
11:B:852:CLA:HMC2	19:F:805:LUT:H27	1.92	0.51
10:L:101:ILE:HG23	10:L:114:GLU:HA	1.91	0.51
1:A:297:HIS:HB2	11:A:818:CLA:C1B	2.41	0.51
4:D:128:LEU:HA	4:D:132:PHE:HD2	1.76	0.51
2:B:713:HIS:NE2	11:B:841:CLA:NA	2.60	0.50
8:T:28:GLU:HG2	8:T:29:LYS:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:HIS:HB3	2:B:323:LEU:HD12	1.93	0.50
3:C:28:MET:HA	3:C:28:MET:HE2	1.94	0.50
2:B:70:ALA:HB2	2:B:136:LEU:HB2	1.93	0.50
11:B:809:CLA:O1A	11:B:828:CLA:HBD	2.12	0.50
11:A:833:CLA:HBB2	10:L:103:LEU:HD13	1.94	0.49
11:A:809:CLA:H142	19:J:101:LUT:H192	1.93	0.49
8:T:63:TRP:CD1	20:T:200:HEC:HBB2	2.47	0.49
11:B:807:CLA:H172	11:B:829:CLA:HBB2	1.93	0.49
11:A:831:CLA:H62	13:A:846:LHG:H241	1.94	0.49
11:B:819:CLA:H8	11:B:819:CLA:HAB	1.93	0.49
2:B:87:PRO:HB3	2:B:122:TYR:CD2	2.47	0.48
3:C:14:CYS:O	3:C:15:THR:HG22	2.13	0.48
11:A:805:CLA:H201	14:A:847:BCR:H12C	1.95	0.48
1:A:596:LEU:HD21	11:A:830:CLA:HBC1	1.93	0.48
1:A:658:ILE:HD12	2:B:622:ARG:HG3	1.94	0.48
11:A:826:CLA:HMB3	11:A:826:CLA:HBB1	1.96	0.48
1:A:204:GLY:O	1:A:208:LEU:HB2	2.13	0.48
1:A:441:LEU:HD22	11:A:839:CLA:HBB1	1.96	0.48
11:A:809:CLA:H162	11:A:809:CLA:H141	1.72	0.48
1:A:180:HIS:CE1	11:A:810:CLA:NA	2.82	0.47
9:F:202:TRP:CD1	9:F:203:PRO:HD3	2.49	0.47
11:B:817:CLA:CHD	11:B:818:CLA:HBB2	2.44	0.47
11:A:838:CLA:C1C	17:A:855:LMG:H191	2.44	0.47
2:B:327:VAL:HG22	2:B:333:PHE:CE1	2.50	0.47
11:B:826:CLA:H202	11:B:835:CLA:HBC1	1.94	0.47
11:A:809:CLA:HBB1	14:J:104:BCR:H23C	1.95	0.47
1:A:350:HIS:CE1	1:A:411:ILE:HG21	2.49	0.47
2:B:294:THR:HG23	2:B:296:PHE:H	1.79	0.47
11:A:819:CLA:H92	11:A:829:CLA:H91	1.96	0.47
1:A:119:TRP:CD2	11:A:809:CLA:HED3	2.51	0.47
11:B:826:CLA:HMA1	14:B:847:BCR:H14C	1.96	0.47
11:B:828:CLA:H62	11:B:828:CLA:H102	1.73	0.46
9:F:105:LYS:O	9:F:109:GLU:HG2	2.15	0.46
2:B:674:GLU:O	2:B:678:THR:HG23	2.14	0.46
17:B:851:LMG:H142	17:B:851:LMG:H302	1.98	0.46
1:A:121:ILE:HG13	1:A:122:VAL:HG13	1.96	0.46
2:B:194:HIS:CE1	11:B:815:CLA:NA	2.84	0.46
2:B:285:PHE:CE1	11:B:820:CLA:HAB	2.51	0.46
11:A:831:CLA:HBA2	13:A:846:LHG:HC91	1.96	0.46
11:B:801:CLA:HBB1	11:B:801:CLA:HMB3	1.97	0.46
11:A:812:CLA:HMB1	11:A:812:CLA:HBB1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:701:LEU:HD21	12:B:843:PQN:H151	1.97	0.46
1:A:338:HIS:CD2	11:A:824:CLA:ND	2.84	0.46
2:B:209:GLY:O	2:B:213:PHE:HB3	2.15	0.46
6:I:96:PHE:HB2	14:L:204:BCR:H12C	1.97	0.46
11:L:202:CLA:H61	11:L:202:CLA:H41	1.71	0.46
11:A:833:CLA:HAB	11:A:834:CLA:HBB	1.98	0.46
20:T:200:HEC:HBB3	20:T:200:HEC:HMB3	1.96	0.46
1:A:412:PHE:CD1	1:A:416:ASP:HB2	2.51	0.46
11:A:840:CLA:H193	11:F:803:CLA:H52	1.97	0.46
2:B:22:ILE:H	2:B:22:ILE:HG13	1.62	0.46
11:B:814:CLA:H43	14:B:844:BCR:H19C	1.97	0.46
4:D:65:PRO:HG2	4:D:113:LEU:HD11	1.98	0.46
1:A:349:TRP:HB3	11:A:805:CLA:HAC1	1.98	0.46
2:B:277:HIS:HB2	11:B:818:CLA:CHB	2.46	0.46
1:A:564:PRO:HD2	4:D:119:GLU:OE1	2.16	0.46
2:B:157:HIS:HE1	11:B:812:CLA:C1A	2.28	0.46
2:B:176:LEU:O	2:B:180:LEU:HD12	2.16	0.46
11:B:818:CLA:H3A	11:B:818:CLA:HBA2	1.40	0.46
1:A:730:HIS:CE1	11:A:841:CLA:NA	2.84	0.45
14:A:847:BCR:H20C	14:A:847:BCR:H361	1.84	0.45
2:B:288:ALA:HB2	11:B:820:CLA:HBC2	1.98	0.45
11:B:809:CLA:H92	14:B:848:BCR:HC7	1.97	0.45
11:B:837:CLA:H143	11:B:837:CLA:H111	1.71	0.45
11:A:842:CLA:H122	11:A:842:CLA:H8	1.62	0.45
8:T:68:SER:OG	8:T:71:GLU:HG3	2.16	0.45
8:T:70:GLU:H	8:T:70:GLU:CD	2.23	0.45
10:L:95:LEU:HD11	11:L:202:CLA:HMA3	1.98	0.45
11:A:837:CLA:H11	11:A:838:CLA:O1A	2.15	0.45
16:A:856:LMU:H31	17:J:102:LMG:H302	1.97	0.45
2:B:181:SER:HB3	2:B:289:GLY:HA3	1.97	0.45
1:A:574:PRO:HB3	1:A:720:ILE:HB	1.99	0.45
11:A:840:CLA:H101	11:B:833:CLA:H43	1.99	0.45
2:B:346:THR:HB	2:B:380:ALA:HB2	1.98	0.45
2:B:722:TYR:HB2	11:B:803:CLA:HED2	1.99	0.45
1:A:174:PHE:HB3	16:A:856:LMU:H92	1.99	0.45
11:B:831:CLA:H3A	11:B:832:CLA:OBD	2.16	0.45
3:C:61:ASP:HA	3:C:62:PHE:HA	1.83	0.45
1:A:318:ILE:HG13	11:A:820:CLA:HED2	1.99	0.45
1:A:511:GLY:HA2	1:A:525:PRO:HB3	1.99	0.45
1:A:656:GLN:HG2	1:A:749:SER:HB2	1.99	0.45
1:A:666:SER:HB2	2:B:446:ALA:HB1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:TRP:HE1	11:B:804:CLA:C1D	2.30	0.45
11:B:811:CLA:H142	11:B:811:CLA:H112	1.81	0.45
11:B:819:CLA:H8	11:B:819:CLA:CAB	2.47	0.45
11:B:840:CLA:H111	11:B:841:CLA:H112	1.99	0.45
11:B:834:CLA:H101	11:B:834:CLA:H62	1.67	0.44
3:C:15:THR:O	3:C:19:ARG:HG3	2.17	0.44
2:B:330:SER:O	2:B:334:GLN:HG3	2.17	0.44
11:A:805:CLA:H72	14:A:848:BCR:H323	1.99	0.44
2:B:630:SER:HB3	8:T:25:VAL:HG22	1.99	0.44
11:B:807:CLA:H91	11:B:807:CLA:H112	1.79	0.44
10:L:92:HIS:NE2	11:L:202:CLA:NA	2.65	0.44
11:A:825:CLA:H61	11:A:825:CLA:H2	1.77	0.44
11:A:832:CLA:HMB1	11:A:842:CLA:HAA2	1.99	0.44
6:I:95:LEU:O	6:I:99:ILE:HG23	2.17	0.44
11:L:202:CLA:H152	11:L:202:CLA:H112	1.34	0.44
1:A:704:HIS:HE1	11:A:840:CLA:C4D	2.30	0.44
11:A:809:CLA:CBB	14:J:104:BCR:H23C	2.47	0.44
2:B:443:VAL:HG21	11:B:834:CLA:HAC2	2.00	0.44
11:B:834:CLA:H62	11:B:834:CLA:H41	1.59	0.44
18:B:849:DGD:HB52	18:B:849:DGD:HB21	1.74	0.44
11:J:103:CLA:H61	11:J:103:CLA:H41	1.43	0.44
10:L:132:LEU:CD2	14:L:204:BCR:H24C	2.48	0.44
1:A:27:GLU:HG3	1:A:28:LYS:N	2.32	0.44
1:A:262:ALA:O	1:A:266:THR:HG23	2.16	0.44
1:A:677:PHE:CG	14:A:851:BCR:H363	2.53	0.44
11:A:805:CLA:H112	11:A:805:CLA:H151	1.49	0.44
11:B:816:CLA:H2A	11:B:816:CLA:HED2	2.00	0.44
11:A:834:CLA:H2A	11:A:834:CLA:O2D	2.17	0.44
4:D:133:LYS:HD3	4:D:133:LYS:N	2.33	0.44
1:A:198:LEU:HD23	1:A:198:LEU:HA	1.79	0.43
11:A:806:CLA:H112	11:A:806:CLA:H152	1.80	0.43
4:D:66:ILE:HB	4:D:105:ILE:HB	2.00	0.43
1:A:338:HIS:HB3	1:A:341:LEU:HD12	2.01	0.43
2:B:688:LEU:HD23	2:B:688:LEU:HA	1.91	0.43
11:B:852:CLA:H161	11:B:852:CLA:H192	1.82	0.43
1:A:178:TRP:HB2	11:A:811:CLA:CMC	2.49	0.43
2:B:450:PRO:O	2:B:453:GLN:HG2	2.18	0.43
1:A:360:PHE:HE1	11:A:829:CLA:H171	1.83	0.43
1:A:539:HIS:HE1	1:A:605:ILE:HG22	1.84	0.43
11:A:811:CLA:H141	11:A:811:CLA:H161	1.67	0.43
2:B:277:HIS:HB2	11:B:818:CLA:C1B	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:824:CLA:HBA2	11:B:824:CLA:H3A	1.57	0.43
6:I:96:PHE:CD1	6:I:96:PHE:C	2.96	0.43
11:A:819:CLA:H111	11:A:819:CLA:H72	1.62	0.43
11:B:815:CLA:H61	11:B:815:CLA:H2	1.82	0.43
11:B:818:CLA:H151	11:B:818:CLA:H18	1.65	0.43
14:B:845:BCR:H371	14:B:845:BCR:H24C	1.78	0.43
11:A:809:CLA:HBB1	11:A:809:CLA:HMB3	2.00	0.43
2:B:467:ALA:HB2	2:B:477:PHE:CZ	2.53	0.43
3:C:17:CYS:HB3	15:C:102:SF4:S4	2.59	0.43
3:C:22:PRO:C	4:D:122:LEU:HD23	2.43	0.43
4:D:74:LEU:HD12	4:D:78:ALA:HB2	2.01	0.43
11:A:839:CLA:H93	11:A:839:CLA:H111	1.82	0.43
2:B:66:LEU:HD11	14:B:845:BCR:H271	2.01	0.43
2:B:188:SER:HB3	2:B:282:ALA:HB2	2.00	0.43
2:B:353:MET:HE2	2:B:353:MET:HB3	1.88	0.43
11:B:817:CLA:H41	11:B:817:CLA:H61	1.56	0.43
1:A:562:LEU:HD21	1:A:583:THR:HG22	2.01	0.43
11:B:806:CLA:HBA1	11:B:806:CLA:H3A	1.50	0.43
1:A:289:LEU:HD21	1:A:374:MET:HB3	2.01	0.42
2:B:75:PHE:O	2:B:79:VAL:HG13	2.19	0.42
2:B:482:LYS:HE2	2:B:482:LYS:HB2	1.71	0.42
9:F:124:LEU:O	9:F:131:PRO:HA	2.19	0.42
1:A:53:HIS:CE1	11:A:803:CLA:ND	2.87	0.42
1:A:183:LYS:HA	1:A:183:LYS:HD2	1.90	0.42
1:A:296:HIS:CE1	11:A:817:CLA:NA	2.87	0.42
9:F:90:ARG:O	9:F:93:GLN:HG2	2.18	0.42
2:B:655:HIS:NE2	11:B:803:CLA:NA	2.68	0.42
11:B:840:CLA:H191	6:I:89:ALA:HB2	2.01	0.42
12:B:843:PQN:H301	18:B:849:DGD:HA82	2.00	0.42
1:A:408:HIS:CE1	11:A:830:CLA:NA	2.88	0.42
1:A:692:TYR:CE2	2:B:537:LYS:HD3	2.55	0.42
11:A:831:CLA:HMA1	10:L:57:THR:HG21	2.02	0.42
2:B:81:ASP:HB3	2:B:85:ILE:HD12	2.00	0.42
11:B:812:CLA:H92	11:B:812:CLA:H62	1.72	0.42
14:A:849:BCR:H20C	14:A:849:BCR:H361	1.83	0.42
2:B:713:HIS:HE1	11:B:841:CLA:C4D	2.32	0.42
11:B:818:CLA:H102	11:B:818:CLA:H62	1.78	0.42
11:B:812:CLA:H202	11:B:812:CLA:H161	1.74	0.42
11:B:837:CLA:H92	11:B:837:CLA:H61	1.86	0.42
1:A:458:HIS:CE1	11:A:834:CLA:NA	2.88	0.42
11:B:805:CLA:HHC	11:B:807:CLA:OBD	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:845:BCR:H20C	14:B:845:BCR:H361	1.91	0.42
2:B:51:HIS:NE2	11:B:806:CLA:NA	2.68	0.42
2:B:76:GLU:OE1	2:B:132:THR:HA	2.20	0.42
2:B:276:HIS:HE1	11:B:817:CLA:C4D	2.33	0.42
2:B:285:PHE:CZ	11:B:820:CLA:HAB	2.55	0.42
11:B:840:CLA:H111	11:B:841:CLA:H13	2.02	0.42
10:L:97:ALA:O	10:L:101:ILE:HG13	2.18	0.42
1:A:269:TRP:HZ3	11:A:817:CLA:H51	1.84	0.42
11:A:802:CLA:CGA	11:A:802:CLA:H3A	2.50	0.42
2:B:20:ARG:HH22	18:B:849:DGD:HE1	1.84	0.42
11:B:824:CLA:HBB1	11:B:824:CLA:HMB3	2.02	0.42
5:E:86:ASN:HB3	5:E:88:TYR:CE2	2.55	0.42
9:F:116:ALA:O	9:F:120:LYS:HE2	2.20	0.42
11:B:836:CLA:H3A	11:B:836:CLA:HBA2	1.75	0.42
11:B:826:CLA:H3A	11:B:826:CLA:HBA2	1.69	0.41
1:A:204:GLY:HA2	11:A:820:CLA:HBC1	2.02	0.41
11:A:803:CLA:H203	11:A:803:CLA:H161	1.82	0.41
2:B:548:MET:HE3	2:B:561:ASP:OD1	2.20	0.41
11:B:820:CLA:H142	11:B:824:CLA:H51	2.02	0.41
11:A:806:CLA:HBA1	11:A:806:CLA:H3A	1.85	0.41
2:B:310:THR:N	11:B:842:CLA:HMD3	2.34	0.41
2:B:366:PHE:HB3	2:B:603:TRP:CZ3	2.55	0.41
2:B:396:ILE:HD11	2:B:542:ALA:HB1	2.01	0.41
14:I:201:BCR:H24C	14:I:201:BCR:H371	1.86	0.41
9:F:202:TRP:CG	9:F:203:PRO:HD3	2.55	0.41
14:L:204:BCR:H20C	14:L:204:BCR:H361	1.89	0.41
1:A:244:LEU:HD23	1:A:244:LEU:HA	1.82	0.41
1:A:326:LEU:O	1:A:338:HIS:HB2	2.21	0.41
1:A:363:LEU:HD11	11:A:819:CLA:H51	2.03	0.41
14:A:851:BCR:H362	11:B:802:CLA:C2	2.49	0.41
16:A:854:LMU:H22	16:A:854:LMU:H1'	1.78	0.41
2:B:197:HIS:CE1	11:B:816:CLA:NA	2.88	0.41
11:B:810:CLA:H91	11:B:810:CLA:H111	1.80	0.41
11:B:821:CLA:H62	11:B:821:CLA:H2	1.65	0.41
10:L:102:LYS:HD3	10:L:102:LYS:HA	1.86	0.41
1:A:501:ASN:HB2	11:A:836:CLA:O1D	2.20	0.41
11:A:826:CLA:HBA2	11:A:826:CLA:H3A	1.89	0.41
11:B:809:CLA:CGA	11:B:809:CLA:C1A	2.98	0.41
11:B:809:CLA:H2	11:B:809:CLA:H61	1.76	0.41
1:A:94:HIS:CE1	11:A:807:CLA:NA	2.88	0.41
1:A:235:LYS:HE3	1:A:235:LYS:HB3	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:PRO:HG3	4:D:97:GLU:HB2	2.01	0.41
11:A:808:CLA:HBA1	11:A:808:CLA:C4A	2.51	0.41
11:B:831:CLA:HMB3	11:B:831:CLA:HBB1	2.02	0.41
7:J:12:PRO:HB2	19:J:101:LUT:H163	2.02	0.41
10:L:56:GLU:HB3	10:L:61:SER:OG	2.21	0.41
11:A:825:CLA:H101	11:A:825:CLA:H62	1.76	0.41
11:A:840:CLA:HBC1	12:A:843:PQN:H211	2.02	0.41
2:B:159:GLN:O	2:B:163:GLN:HG3	2.20	0.41
11:B:838:CLA:H62	11:B:838:CLA:H102	1.82	0.41
8:T:57:LYS:O	8:T:60:MET:HB3	2.21	0.41
1:A:50:TRP:HZ2	11:F:803:CLA:HBB1	1.85	0.41
11:A:817:CLA:H143	11:A:817:CLA:H111	1.88	0.41
2:B:182:GLY:HA3	11:B:814:CLA:HBB1	2.03	0.41
11:B:841:CLA:H161	11:B:841:CLA:H193	1.83	0.41
13:B:850:LHG:H301	13:B:850:LHG:H332	1.88	0.41
6:I:91:ALA:O	6:I:95:LEU:HD12	2.21	0.41
12:A:843:PQN:H162	14:F:801:BCR:H382	2.03	0.41
11:B:811:CLA:CBB	6:I:84:GLY:HA3	2.51	0.41
11:B:841:CLA:H61	11:B:841:CLA:H41	1.89	0.41
4:D:62:THR:HG23	4:D:110:PRO:HB2	2.03	0.41
4:D:92:LYS:HE2	4:D:92:LYS:HB2	1.79	0.41
4:D:118:LYS:HE3	4:D:150:LEU:HD13	2.02	0.41
11:A:805:CLA:HBA1	11:A:805:CLA:H3A	1.72	0.41
11:A:808:CLA:H172	11:A:830:CLA:H191	2.02	0.41
2:B:81:ASP:OD2	2:B:84:HIS:HB2	2.21	0.41
2:B:102:VAL:HG22	17:B:851:LMG:HC3	2.03	0.41
2:B:310:THR:H	11:B:842:CLA:HMD3	1.86	0.41
4:D:83:PHE:CE2	4:D:114:LYS:HD3	2.56	0.41
1:A:393:HIS:HE1	11:A:828:CLA:ND	2.19	0.40
14:A:848:BCR:H24C	14:A:848:BCR:H371	1.84	0.40
11:B:803:CLA:H102	11:B:803:CLA:H62	1.89	0.40
9:F:79:LEU:O	9:F:83:GLU:HG3	2.20	0.40
9:F:87:LEU:HB3	9:F:108:MET:HE2	2.03	0.40
1:A:27:GLU:HA	7:J:3:ASP:CG	2.46	0.40
1:A:318:ILE:HD11	11:A:820:CLA:H2A	2.03	0.40
11:A:808:CLA:H91	11:A:808:CLA:H112	1.88	0.40
11:A:826:CLA:CHB	11:A:839:CLA:HAA2	2.51	0.40
11:A:839:CLA:H162	14:A:850:BCR:H371	2.04	0.40
2:B:87:PRO:HB3	2:B:122:TYR:CG	2.56	0.40
11:B:811:CLA:H171	11:B:811:CLA:H13	1.83	0.40
11:A:821:CLA:C4A	11:A:821:CLA:HBA2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:202:CLA:H192	11:L:202:CLA:H162	1.82	0.40
1:A:588:ALA:O	1:A:592:VAL:HG23	2.22	0.40
11:A:805:CLA:H61	11:A:805:CLA:H2	1.64	0.40
11:A:833:CLA:H71	11:A:833:CLA:H112	1.88	0.40
11:A:837:CLA:HMB3	11:A:837:CLA:HBB1	2.03	0.40
14:A:849:BCR:H24C	14:A:849:BCR:H371	1.86	0.40
2:B:277:HIS:CE1	11:B:818:CLA:ND	2.90	0.40
1:A:101:TYR:HA	1:A:145:PHE:CE2	2.57	0.40
1:A:508:LEU:HD13	1:A:508:LEU:HA	1.91	0.40
1:A:585:GLN:HA	1:A:590:ASP:OD2	2.22	0.40
1:A:677:PHE:CD2	14:A:851:BCR:H363	2.57	0.40
11:A:839:CLA:H111	11:A:839:CLA:H142	1.88	0.40
11:B:834:CLA:H112	11:B:834:CLA:H91	1.67	0.40
14:I:201:BCR:HC7	14:I:201:BCR:H311	1.71	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	740/742 (100%)	726 (98%)	14 (2%)	0	100	100
2	B	731/733 (100%)	712 (97%)	19 (3%)	0	100	100
3	C	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
4	D	142/144 (99%)	136 (96%)	6 (4%)	0	100	100
5	E	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
6	I	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
7	J	39/41 (95%)	39 (100%)	0	0	100	100
8	T	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
9	F	163/165 (99%)	160 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	L	120/138 (87%)	117 (98%)	3 (2%)	0	100	100
All	All	2197/2233 (98%)	2147 (98%)	50 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	601/601 (100%)	593 (99%)	8 (1%)	61	62
2	B	596/596 (100%)	590 (99%)	6 (1%)	68	71
3	C	69/69 (100%)	67 (97%)	2 (3%)	37	33
4	D	121/121 (100%)	117 (97%)	4 (3%)	33	28
5	E	55/55 (100%)	53 (96%)	2 (4%)	31	25
6	I	31/31 (100%)	31 (100%)	0	100	100
7	J	36/36 (100%)	36 (100%)	0	100	100
8	T	66/66 (100%)	61 (92%)	5 (8%)	12	6
9	F	127/127 (100%)	122 (96%)	5 (4%)	28	23
10	L	90/102 (88%)	88 (98%)	2 (2%)	45	43
All	All	1792/1804 (99%)	1758 (98%)	34 (2%)	49	49

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	GLU
1	A	306	LEU
1	A	372	TYR
1	A	413	MET
1	A	475	THR
1	A	508	LEU
1	A	628	SER
1	A	699	SER

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Mol	Chain	Res	Type
2	B	41	GLU
2	B	170	LYS
2	B	395	PHE
2	B	491	GLN
2	B	506	GLN
2	B	578	TYR
3	C	15	THR
3	C	16	GLN
4	D	86	ILE
4	D	139	TYR
4	D	175	ILE
4	D	191	MET
5	E	71	VAL
5	E	94	VAL
8	T	3	LEU
8	T	26	MET
8	T	73	GLN
8	T	82	GLN
8	T	89	LYS
9	F	92	LYS
9	F	182	ASP
9	F	209	GLU
9	F	219	GLU
9	F	224	VAL
10	L	54	MET
10	L	161	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	GLN
1	A	296	HIS
1	A	704	HIS
2	B	15	GLN
2	B	157	HIS
2	B	276	HIS
2	B	445	GLN
2	B	453	GLN
2	B	506	GLN
4	D	108	GLN
4	D	177	GLN
8	T	13	ASN

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Mol	Chain	Res	Type
9	F	117	ASN
10	L	139	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

126 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	A	819	1	69,73,73	1.16	8 (11%)	82,113,113	1.29	8 (9%)
16	LMU	A	854	-	36,36,36	0.43	0	47,47,47	1.20	4 (8%)
11	CLA	A	829	1	69,73,73	1.16	7 (10%)	82,113,113	1.24	7 (8%)
11	CLA	B	829	2	69,73,73	1.15	9 (13%)	82,113,113	1.21	7 (8%)
11	CLA	A	809	1	69,73,73	1.14	8 (11%)	82,113,113	1.34	8 (9%)
11	CLA	B	827	2	69,73,73	1.17	9 (13%)	82,113,113	1.26	7 (8%)
11	CLA	L	203	-	49,53,73	1.40	7 (14%)	58,89,113	1.36	4 (6%)
11	CLA	B	833	2	69,73,73	1.15	8 (11%)	82,113,113	1.27	5 (6%)
14	BCR	F	801	-	41,41,41	0.34	0	56,56,56	1.08	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	A	834	1	69,73,73	1.16	7 (10%)	82,113,113	1.30	7 (8%)
11	CLA	B	805	2	49,53,73	1.38	8 (16%)	58,89,113	1.41	5 (8%)
11	CLA	B	838	2	69,73,73	1.15	7 (10%)	82,113,113	1.25	6 (7%)
11	CLA	B	841	2	69,73,73	1.16	7 (10%)	82,113,113	1.29	5 (6%)
14	BCR	A	848	-	41,41,41	0.32	0	56,56,56	0.44	0
11	CLA	A	817	1	69,73,73	1.17	8 (11%)	82,113,113	1.27	7 (8%)
11	CLA	A	807	1	54,58,73	1.31	8 (14%)	64,95,113	1.41	6 (9%)
14	BCR	A	851	-	41,41,41	0.33	0	56,56,56	0.53	0
11	CLA	B	821	2	60,64,73	1.26	7 (11%)	71,102,113	1.33	5 (7%)
14	BCR	A	847	-	41,41,41	0.30	0	56,56,56	0.47	0
11	CLA	B	834	2	62,66,73	1.20	8 (12%)	73,104,113	1.37	8 (10%)
14	BCR	J	104	-	41,41,41	0.31	0	56,56,56	0.72	1 (1%)
14	BCR	A	849	-	41,41,41	0.31	0	56,56,56	0.59	0
11	CLA	F	803	21	69,73,73	1.16	7 (10%)	82,113,113	1.29	6 (7%)
11	CLA	J	103	7	59,63,73	1.26	7 (11%)	70,101,113	1.39	8 (11%)
16	LMU	A	853	-	35,35,36	0.47	0	46,46,47	0.77	1 (2%)
11	CLA	A	831	1	59,63,73	1.26	8 (13%)	70,101,113	1.33	6 (8%)
14	BCR	A	850	-	41,41,41	0.30	0	56,56,56	0.66	1 (1%)
11	CLA	B	835	2	64,68,73	1.21	6 (9%)	76,107,113	1.31	6 (7%)
12	PQN	B	843	-	34,34,34	0.36	0	43,45,45	0.63	1 (2%)
16	LMU	A	856	-	24,24,36	0.35	0	29,29,47	0.79	1 (3%)
11	CLA	B	837	2	64,68,73	1.21	7 (10%)	76,107,113	1.29	7 (9%)
11	CLA	B	803	2	69,73,73	1.13	7 (10%)	82,113,113	1.30	5 (6%)
11	CLA	A	830	1	69,73,73	1.16	8 (11%)	82,113,113	1.26	6 (7%)
11	CLA	A	802	-	69,73,73	1.14	7 (10%)	82,113,113	1.21	7 (8%)
11	CLA	A	838	1	69,73,73	1.16	8 (11%)	82,113,113	1.26	6 (7%)
11	CLA	A	827	1	69,73,73	1.16	8 (11%)	82,113,113	1.26	6 (7%)
11	CLA	B	802	21	69,73,73	1.16	6 (8%)	82,113,113	1.21	3 (3%)
11	CLA	B	831	2	49,53,73	1.38	8 (16%)	58,89,113	1.42	5 (8%)
11	CLA	A	821	21	69,73,73	1.16	8 (11%)	82,113,113	1.28	6 (7%)
11	CLA	A	826	21	69,73,73	1.15	8 (11%)	82,113,113	1.34	10 (12%)
11	CLA	A	810	1	66,70,73	1.18	7 (10%)	77,108,113	1.28	7 (9%)
14	BCR	L	204	-	41,41,41	0.32	0	56,56,56	0.58	0
11	CLA	B	818	2	69,73,73	1.16	9 (13%)	82,113,113	1.24	5 (6%)
11	CLA	B	810	2	69,73,73	1.16	8 (11%)	82,113,113	1.27	6 (7%)
11	CLA	B	825	21	69,73,73	1.18	7 (10%)	82,113,113	1.24	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	A	804	11,1	59,63,73	1.26	6 (10%)	70,101,113	1.34	7 (10%)
11	CLA	B	817	2	60,64,73	1.25	8 (13%)	71,102,113	1.32	4 (5%)
13	LHG	A	845	-	48,48,48	0.52	0	51,54,54	0.56	0
11	CLA	B	826	21	69,73,73	1.15	7 (10%)	82,113,113	1.30	6 (7%)
11	CLA	B	836	21	49,53,73	1.38	6 (12%)	58,89,113	1.43	5 (8%)
14	BCR	B	844	-	41,41,41	0.35	0	56,56,56	0.69	0
11	CLA	A	820	1	46,50,73	1.40	7 (15%)	53,85,113	1.46	5 (9%)
11	CLA	B	808	2	59,63,73	1.25	8 (13%)	70,101,113	1.33	7 (10%)
11	CLA	B	830	2	69,73,73	1.16	7 (10%)	82,113,113	1.21	5 (6%)
11	CLA	B	832	2	59,63,73	1.26	8 (13%)	70,101,113	1.32	8 (11%)
12	PQN	A	843	-	34,34,34	0.36	0	43,45,45	0.60	1 (2%)
11	CLA	B	815	2	64,68,73	1.22	8 (12%)	76,107,113	1.25	4 (5%)
11	CLA	B	820	-	64,68,73	1.21	8 (12%)	76,107,113	1.32	7 (9%)
19	LUT	F	805	-	42,43,43	0.30	0	51,60,60	0.77	2 (3%)
11	CLA	B	812	2	69,73,73	1.17	6 (8%)	82,113,113	1.22	5 (6%)
11	CLA	B	813	2	45,49,73	1.42	7 (15%)	54,84,113	1.49	6 (11%)
11	CLA	B	822	2	46,50,73	1.41	7 (15%)	53,85,113	1.43	4 (7%)
11	CLA	A	842	21	69,73,73	1.17	8 (11%)	82,113,113	1.27	6 (7%)
11	CLA	B	840	-	69,73,73	1.16	7 (10%)	82,113,113	1.27	6 (7%)
11	CLA	A	803	1	69,73,73	1.15	7 (10%)	82,113,113	1.32	8 (9%)
17	LMG	J	102	-	32,32,55	0.59	0	40,40,63	0.67	0
11	CLA	A	824	1	59,63,73	1.27	7 (11%)	70,101,113	1.34	6 (8%)
11	CLA	B	839	2	54,58,73	1.31	7 (12%)	64,95,113	1.39	7 (10%)
11	CLA	B	816	2	69,73,73	1.16	7 (10%)	82,113,113	1.28	6 (7%)
11	CLA	B	811	2	69,73,73	1.16	7 (10%)	82,113,113	1.29	5 (6%)
11	CLA	A	837	1	55,59,73	1.31	8 (14%)	64,96,113	1.42	7 (10%)
11	CLA	L	202	10	69,73,73	1.17	7 (10%)	82,113,113	1.28	6 (7%)
11	CLA	A	825	21	69,73,73	1.18	7 (10%)	82,113,113	1.28	5 (6%)
11	CLA	A	836	1	49,53,73	1.39	8 (16%)	58,89,113	1.42	5 (8%)
11	CLA	A	818	1	64,68,73	1.23	9 (14%)	76,107,113	1.29	6 (7%)
11	CLA	A	806	1	69,73,73	1.16	7 (10%)	82,113,113	1.27	4 (4%)
11	CLA	A	808	1	69,73,73	1.13	7 (10%)	82,113,113	1.31	5 (6%)
11	CLA	A	832	1	49,53,73	1.39	8 (16%)	58,89,113	1.46	6 (10%)
11	CLA	B	828	2	69,73,73	1.17	7 (10%)	82,113,113	1.26	6 (7%)
14	BCR	B	847	-	41,41,41	0.31	0	56,56,56	0.87	0
13	LHG	A	846	11	37,37,48	0.58	0	40,43,54	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	BCR	B	846	-	41,41,41	0.29	0	56,56,56	0.68	0
14	BCR	B	845	-	41,41,41	0.32	0	56,56,56	0.55	0
19	LUT	J	101	-	42,43,43	0.30	0	51,60,60	0.74	2 (3%)
14	BCR	B	848	-	41,41,41	0.31	0	56,56,56	0.73	0
11	CLA	B	806	2	69,73,73	1.16	7 (10%)	82,113,113	1.26	6 (7%)
11	CLA	A	841	1	69,73,73	1.16	9 (13%)	82,113,113	1.23	5 (6%)
11	CLA	A	815	1	46,50,73	1.40	8 (17%)	53,85,113	1.49	6 (11%)
11	CLA	A	835	1	69,73,73	1.17	7 (10%)	82,113,113	1.26	5 (6%)
20	HEC	T	200	8	46,50,50	1.84	6 (13%)	58,82,82	1.89	4 (6%)
11	CLA	A	814	1	59,63,73	1.26	8 (13%)	70,101,113	1.31	5 (7%)
11	CLA	A	840	1	69,73,73	1.15	8 (11%)	82,113,113	1.25	6 (7%)
15	SF4	A	852	2,1	0,12,12	-	-	-	-	-
11	CLA	B	814	2	69,73,73	1.18	9 (13%)	82,113,113	1.26	6 (7%)
11	CLA	A	812	1	59,63,73	1.25	8 (13%)	70,101,113	1.36	7 (10%)
11	CLA	A	805	1	69,73,73	1.15	7 (10%)	82,113,113	1.26	6 (7%)
11	CLA	B	823	2	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
11	CLA	B	801	21	69,73,73	1.15	6 (8%)	82,113,113	1.22	6 (7%)
17	LMG	F	802	-	35,35,55	0.57	0	43,43,63	0.75	0
11	CLA	B	842	13	69,73,73	1.18	8 (11%)	82,113,113	1.30	7 (8%)
11	CLA	A	839	1	69,73,73	1.17	8 (11%)	82,113,113	1.29	6 (7%)
11	CLA	B	804	-	69,73,73	1.15	6 (8%)	82,113,113	1.25	8 (9%)
11	CLA	A	816	21	59,63,73	1.26	9 (15%)	70,101,113	1.40	6 (8%)
11	CLA	B	819	2	69,73,73	1.16	9 (13%)	82,113,113	1.29	7 (8%)
11	CLA	A	811	11,1	69,73,73	1.15	6 (8%)	82,113,113	1.23	6 (7%)
11	CLA	A	822	1	49,53,73	1.39	8 (16%)	58,89,113	1.42	4 (6%)
14	BCR	I	201	-	41,41,41	0.32	0	56,56,56	0.84	1 (1%)
17	LMG	J	105	-	42,42,55	0.54	0	50,50,63	0.67	0
13	LHG	B	850	11	44,44,48	0.54	0	47,50,54	0.57	0
11	CLA	A	833	1	69,73,73	1.17	8 (11%)	82,113,113	1.28	6 (7%)
15	SF4	C	101	3	0,12,12	-	-	-	-	-
15	SF4	C	102	3	0,12,12	-	-	-	-	-
11	CLA	B	807	2	69,73,73	1.17	8 (11%)	82,113,113	1.27	6 (7%)
11	CLA	B	824	2	69,73,73	1.17	7 (10%)	82,113,113	1.25	5 (6%)
17	LMG	A	855	-	40,40,55	0.53	0	48,48,63	0.65	0
11	CLA	A	813	1	69,73,73	1.16	8 (11%)	82,113,113	1.28	5 (6%)
17	LMG	B	851	-	43,43,55	0.53	0	51,51,63	0.67	0
11	CLA	B	809	2	69,73,73	1.16	8 (11%)	82,113,113	1.30	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	A	801	1	69,73,73	0.75	4 (5%)	82,113,113	1.04	4 (4%)
11	CLA	A	828	1	69,73,73	1.15	6 (8%)	82,113,113	1.26	6 (7%)
11	CLA	A	844	13	49,53,73	1.39	9 (18%)	58,89,113	1.43	4 (6%)
11	CLA	A	823	1	49,53,73	1.38	6 (12%)	58,89,113	1.38	5 (8%)
14	BCR	L	201	-	41,41,41	0.32	0	56,56,56	0.54	0
18	DGD	B	849	-	60,60,67	0.55	0	74,74,81	0.79	1 (1%)
11	CLA	B	852	9	69,73,73	1.17	8 (11%)	82,113,113	1.20	4 (4%)
11	CLA	F	804	21	49,53,73	1.39	7 (14%)	58,89,113	1.43	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
11	CLA	A	819	1	1/1/15/20	4/39/115/115	-
16	LMU	A	854	-	-	11/21/61/61	0/2/2/2
11	CLA	A	829	1	1/1/15/20	4/39/115/115	-
11	CLA	B	829	2	1/1/15/20	10/39/115/115	-
11	CLA	A	809	1	1/1/15/20	10/39/115/115	-
11	CLA	B	827	2	1/1/15/20	6/39/115/115	-
11	CLA	L	203	-	1/1/11/20	6/15/91/115	-
11	CLA	B	833	2	1/1/15/20	8/39/115/115	-
14	BCR	F	801	-	-	4/29/63/63	0/2/2/2
11	CLA	A	834	1	1/1/15/20	9/39/115/115	-
11	CLA	B	805	2	1/1/11/20	3/15/91/115	-
11	CLA	B	838	2	1/1/15/20	8/39/115/115	-
11	CLA	B	841	2	1/1/15/20	12/39/115/115	-
14	BCR	A	848	-	-	0/29/63/63	0/2/2/2
11	CLA	A	817	1	1/1/15/20	8/39/115/115	-
11	CLA	A	807	1	1/1/12/20	2/21/97/115	-
14	BCR	A	851	-	-	8/29/63/63	0/2/2/2
11	CLA	B	821	2	1/1/13/20	12/29/105/115	-
14	BCR	A	847	-	-	4/29/63/63	0/2/2/2
11	CLA	B	834	2	1/1/13/20	9/31/107/115	-
14	BCR	J	104	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BCR	A	849	-	-	3/29/63/63	0/2/2/2
11	CLA	F	803	21	1/1/15/20	6/39/115/115	-
11	CLA	J	103	7	1/1/13/20	9/27/103/115	-
16	LMU	A	853	-	-	3/20/60/61	0/2/2/2
11	CLA	A	831	1	1/1/13/20	7/27/103/115	-
14	BCR	A	850	-	-	5/29/63/63	0/2/2/2
11	CLA	B	835	2	1/1/14/20	8/33/109/115	-
12	PQN	B	843	-	-	0/23/43/43	0/2/2/2
16	LMU	A	856	-	-	5/15/35/61	0/1/1/2
11	CLA	B	837	2	1/1/14/20	8/33/109/115	-
11	CLA	B	803	2	1/1/15/20	7/39/115/115	-
11	CLA	A	830	1	1/1/15/20	9/39/115/115	-
11	CLA	A	802	-	1/1/15/20	8/39/115/115	-
11	CLA	A	838	1	1/1/15/20	7/39/115/115	-
11	CLA	A	827	1	1/1/15/20	6/39/115/115	-
11	CLA	B	802	21	1/1/15/20	15/39/115/115	-
11	CLA	B	831	2	1/1/11/20	0/15/91/115	-
11	CLA	A	821	21	1/1/15/20	4/39/115/115	-
11	CLA	A	826	21	1/1/15/20	8/39/115/115	-
11	CLA	A	810	1	1/1/14/20	5/33/109/115	-
14	BCR	L	204	-	-	6/29/63/63	0/2/2/2
11	CLA	B	818	2	1/1/15/20	11/39/115/115	-
11	CLA	B	810	2	1/1/15/20	10/39/115/115	-
11	CLA	B	825	21	1/1/15/20	7/39/115/115	-
11	CLA	A	804	11,1	1/1/13/20	5/27/103/115	-
11	CLA	B	817	2	1/1/13/20	5/29/105/115	-
13	LHG	A	845	-	-	9/53/53/53	-
11	CLA	B	826	21	1/1/15/20	12/39/115/115	-
11	CLA	B	836	21	1/1/11/20	5/15/91/115	-
14	BCR	B	844	-	-	8/29/63/63	0/2/2/2
11	CLA	A	820	1	1/1/10/20	5/12/88/115	-
11	CLA	B	808	2	1/1/13/20	6/27/103/115	-
11	CLA	B	830	2	1/1/15/20	8/39/115/115	-
11	CLA	B	832	2	1/1/13/20	3/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PQN	A	843	-	-	2/23/43/43	0/2/2/2
11	CLA	B	815	2	1/1/14/20	4/33/109/115	-
11	CLA	B	820	-	1/1/14/20	11/33/109/115	-
19	LUT	F	805	-	-	7/29/67/67	0/2/2/2
11	CLA	B	812	2	1/1/15/20	10/39/115/115	-
11	CLA	B	813	2	1/1/10/20	0/10/86/115	-
11	CLA	B	822	2	1/1/10/20	5/12/88/115	-
11	CLA	A	842	21	1/1/15/20	14/39/115/115	-
11	CLA	B	840	-	1/1/15/20	12/39/115/115	-
11	CLA	A	803	1	1/1/15/20	1/39/115/115	-
17	LMG	J	102	-	-	11/27/47/70	0/1/1/1
11	CLA	A	824	1	1/1/13/20	9/27/103/115	-
11	CLA	B	839	2	1/1/12/20	2/21/97/115	-
11	CLA	B	816	2	1/1/15/20	15/39/115/115	-
11	CLA	B	811	2	1/1/15/20	7/39/115/115	-
11	CLA	A	837	1	1/1/12/20	4/23/99/115	-
11	CLA	L	202	10	1/1/15/20	16/39/115/115	-
11	CLA	A	825	21	1/1/15/20	8/39/115/115	-
11	CLA	A	836	1	1/1/11/20	3/15/91/115	-
11	CLA	A	818	1	1/1/14/20	13/33/109/115	-
11	CLA	A	806	1	1/1/15/20	8/39/115/115	-
11	CLA	A	808	1	1/1/15/20	11/39/115/115	-
11	CLA	A	832	1	1/1/11/20	1/15/91/115	-
11	CLA	B	828	2	1/1/15/20	12/39/115/115	-
14	BCR	B	847	-	-	2/29/63/63	0/2/2/2
13	LHG	A	846	11	-	11/42/42/53	-
14	BCR	B	846	-	-	3/29/63/63	0/2/2/2
14	BCR	B	845	-	-	5/29/63/63	0/2/2/2
19	LUT	J	101	-	-	7/29/67/67	0/2/2/2
14	BCR	B	848	-	-	3/29/63/63	0/2/2/2
11	CLA	B	806	2	1/1/15/20	11/39/115/115	-
11	CLA	A	841	1	1/1/15/20	7/39/115/115	-
11	CLA	A	815	1	1/1/10/20	4/12/88/115	-
11	CLA	A	835	1	1/1/15/20	7/39/115/115	-
20	HEC	T	200	8	-	6/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	A	814	1	1/1/13/20	4/27/103/115	-
11	CLA	A	840	1	1/1/15/20	10/39/115/115	-
15	SF4	A	852	2,1	-	-	0/6/5/5
11	CLA	B	814	2	1/1/15/20	12/39/115/115	-
11	CLA	A	812	1	1/1/13/20	3/27/103/115	-
11	CLA	A	805	1	1/1/15/20	13/39/115/115	-
11	CLA	B	823	2	1/1/11/20	3/15/91/115	-
11	CLA	B	801	21	1/1/15/20	8/39/115/115	-
17	LMG	F	802	-	-	11/30/50/70	0/1/1/1
11	CLA	B	842	13	1/1/15/20	13/39/115/115	-
11	CLA	A	839	1	1/1/15/20	9/39/115/115	-
11	CLA	B	804	-	1/1/15/20	7/39/115/115	-
11	CLA	A	816	21	1/1/13/20	5/27/103/115	-
11	CLA	B	819	2	1/1/15/20	9/39/115/115	-
11	CLA	A	811	11,1	1/1/15/20	9/39/115/115	-
11	CLA	A	822	1	1/1/11/20	10/15/91/115	-
14	BCR	I	201	-	-	5/29/63/63	0/2/2/2
17	LMG	J	105	-	-	7/37/57/70	0/1/1/1
13	LHG	B	850	11	-	16/49/49/53	-
11	CLA	A	833	1	1/1/15/20	4/39/115/115	-
15	SF4	C	101	3	-	-	0/6/5/5
15	SF4	C	102	3	-	-	0/6/5/5
11	CLA	B	807	2	1/1/15/20	7/39/115/115	-
11	CLA	B	824	2	1/1/15/20	13/39/115/115	-
17	LMG	A	855	-	-	11/35/55/70	0/1/1/1
11	CLA	A	813	1	1/1/15/20	10/39/115/115	-
17	LMG	B	851	-	-	10/38/58/70	0/1/1/1
11	CLA	B	809	2	1/1/15/20	10/39/115/115	-
11	CLA	A	801	1	1/1/15/20	2/39/115/115	-
11	CLA	A	828	1	1/1/15/20	11/39/115/115	-
11	CLA	A	844	13	1/1/11/20	7/15/91/115	-
11	CLA	A	823	1	1/1/11/20	5/15/91/115	-
14	BCR	L	201	-	-	4/29/63/63	0/2/2/2
18	DGD	B	849	-	-	16/48/88/95	0/2/2/2
11	CLA	B	852	9	1/1/15/20	24/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	F	804	21	1/1/11/20	2/15/91/115	-

All (685) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	T	200	HEC	CAC-C3C	6.18	1.55	1.35
20	T	200	HEC	CAB-C3B	6.17	1.55	1.35
20	T	200	HEC	C3D-C2D	5.66	1.53	1.38
11	A	820	CLA	C1D-ND	3.65	1.42	1.37
11	A	834	CLA	C1D-ND	3.63	1.42	1.37
11	A	832	CLA	C1D-ND	3.62	1.42	1.37
11	B	811	CLA	C1D-ND	3.61	1.42	1.37
11	B	821	CLA	C1D-ND	3.61	1.42	1.37
11	L	203	CLA	C1D-ND	3.60	1.42	1.37
11	A	836	CLA	C1D-ND	3.60	1.42	1.37
11	A	816	CLA	C1D-ND	3.58	1.42	1.37
11	B	825	CLA	C1D-ND	3.56	1.42	1.37
11	B	824	CLA	C1D-ND	3.56	1.42	1.37
11	A	844	CLA	C1D-ND	3.55	1.42	1.37
11	B	827	CLA	C1D-ND	3.55	1.42	1.37
11	A	812	CLA	C1D-ND	3.54	1.42	1.37
11	B	828	CLA	C1D-ND	3.54	1.42	1.37
11	B	839	CLA	C1D-ND	3.54	1.42	1.37
11	A	822	CLA	C1D-ND	3.54	1.42	1.37
11	A	819	CLA	C1D-ND	3.54	1.42	1.37
11	A	837	CLA	C1D-ND	3.54	1.42	1.37
11	F	803	CLA	C1D-ND	3.53	1.42	1.37
11	B	823	CLA	C1D-ND	3.53	1.42	1.37
11	A	824	CLA	C1D-ND	3.53	1.42	1.37
11	B	807	CLA	C1D-ND	3.52	1.42	1.37
11	B	815	CLA	C1D-ND	3.52	1.42	1.37
11	A	839	CLA	C1D-ND	3.51	1.42	1.37
11	F	804	CLA	C1D-ND	3.51	1.42	1.37
11	A	823	CLA	C1D-ND	3.51	1.42	1.37
11	B	812	CLA	C1D-ND	3.50	1.42	1.37
11	B	814	CLA	C1D-ND	3.50	1.42	1.37
11	B	822	CLA	C1D-ND	3.50	1.42	1.37
11	A	815	CLA	C1D-ND	3.49	1.42	1.37
11	A	827	CLA	C1D-ND	3.49	1.42	1.37
11	B	803	CLA	C1D-ND	3.49	1.42	1.37
11	A	825	CLA	C1D-ND	3.49	1.42	1.37
11	B	813	CLA	C1D-ND	3.49	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	810	CLA	C1D-ND	3.48	1.42	1.37
11	A	828	CLA	C1D-ND	3.48	1.42	1.37
11	B	831	CLA	C1D-ND	3.48	1.42	1.37
11	L	202	CLA	C1D-ND	3.48	1.42	1.37
11	B	836	CLA	C1D-ND	3.46	1.42	1.37
11	A	814	CLA	C1D-ND	3.46	1.42	1.37
11	A	817	CLA	C1D-ND	3.45	1.42	1.37
11	A	804	CLA	C1D-ND	3.45	1.42	1.37
11	A	829	CLA	C1D-ND	3.45	1.42	1.37
11	B	829	CLA	C1D-ND	3.45	1.42	1.37
11	B	832	CLA	C1D-ND	3.45	1.42	1.37
11	A	806	CLA	C1D-ND	3.44	1.42	1.37
11	B	840	CLA	C1D-ND	3.44	1.42	1.37
11	A	813	CLA	C1D-ND	3.44	1.42	1.37
11	A	818	CLA	C1D-ND	3.44	1.42	1.37
11	A	807	CLA	C1D-ND	3.44	1.42	1.37
11	J	103	CLA	C1D-ND	3.44	1.42	1.37
11	A	811	CLA	C1D-ND	3.43	1.42	1.37
11	B	810	CLA	C1D-ND	3.43	1.42	1.37
11	B	842	CLA	C1D-ND	3.43	1.42	1.37
11	A	805	CLA	C1D-ND	3.43	1.42	1.37
11	B	835	CLA	C1D-ND	3.43	1.42	1.37
11	A	838	CLA	C1D-ND	3.43	1.42	1.37
11	B	852	CLA	C1D-ND	3.43	1.42	1.37
11	A	821	CLA	C1D-ND	3.43	1.42	1.37
11	B	817	CLA	C1D-ND	3.43	1.42	1.37
11	B	802	CLA	C1D-ND	3.42	1.42	1.37
11	B	820	CLA	C1D-ND	3.42	1.42	1.37
11	A	831	CLA	C1D-ND	3.42	1.42	1.37
11	B	837	CLA	C1D-ND	3.42	1.42	1.37
11	B	819	CLA	C1D-ND	3.42	1.42	1.37
11	B	816	CLA	C1D-ND	3.41	1.42	1.37
11	B	806	CLA	C1D-ND	3.41	1.42	1.37
11	A	835	CLA	C1D-ND	3.41	1.42	1.37
11	A	803	CLA	C1D-ND	3.40	1.42	1.37
11	A	833	CLA	C1D-ND	3.40	1.42	1.37
11	B	805	CLA	C1D-ND	3.40	1.42	1.37
11	B	818	CLA	C1D-ND	3.39	1.42	1.37
11	B	808	CLA	C1D-ND	3.39	1.42	1.37
11	A	830	CLA	C1D-ND	3.39	1.42	1.37
11	B	830	CLA	C1D-ND	3.38	1.42	1.37
11	A	841	CLA	C1D-ND	3.38	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	801	CLA	C1D-ND	3.37	1.42	1.37
11	B	838	CLA	C1D-ND	3.36	1.42	1.37
11	B	834	CLA	C1D-ND	3.34	1.42	1.37
11	B	841	CLA	C1D-ND	3.34	1.42	1.37
11	B	833	CLA	C1D-ND	3.32	1.42	1.37
11	B	826	CLA	C1D-ND	3.30	1.42	1.37
11	A	826	CLA	C1D-ND	3.29	1.42	1.37
11	A	808	CLA	C1D-ND	3.28	1.42	1.37
11	A	809	CLA	C1D-ND	3.27	1.42	1.37
11	A	840	CLA	C1D-ND	3.26	1.42	1.37
11	A	842	CLA	C1D-ND	3.26	1.42	1.37
11	B	809	CLA	C1D-ND	3.25	1.42	1.37
11	B	852	CLA	C4B-NB	3.23	1.42	1.37
11	B	804	CLA	C1D-ND	3.19	1.42	1.37
11	A	802	CLA	C4B-NB	3.19	1.42	1.37
11	B	841	CLA	C4B-NB	3.16	1.42	1.37
11	B	809	CLA	C4B-NB	3.16	1.42	1.37
11	A	824	CLA	C4B-NB	3.14	1.42	1.37
11	B	821	CLA	C4B-NB	3.14	1.42	1.37
11	A	802	CLA	C1D-ND	3.11	1.42	1.37
11	A	818	CLA	C4B-NB	3.11	1.41	1.37
11	L	203	CLA	C4B-NB	3.10	1.41	1.37
11	B	825	CLA	C4B-NB	3.09	1.41	1.37
11	B	842	CLA	C4B-NB	3.09	1.41	1.37
11	B	801	CLA	C4B-NB	3.08	1.41	1.37
11	B	823	CLA	C4B-NB	3.08	1.41	1.37
11	A	841	CLA	C4B-NB	3.06	1.41	1.37
11	A	835	CLA	C4B-NB	3.06	1.41	1.37
11	A	844	CLA	C4B-NB	3.06	1.41	1.37
11	B	813	CLA	C4B-NB	3.05	1.41	1.37
11	B	822	CLA	C4B-NB	3.05	1.41	1.37
11	B	817	CLA	C4B-NB	3.04	1.41	1.37
11	B	819	CLA	C4B-NB	3.04	1.41	1.37
11	A	804	CLA	C4B-NB	3.04	1.41	1.37
11	A	836	CLA	C4B-NB	3.04	1.41	1.37
11	B	839	CLA	C4B-NB	3.04	1.41	1.37
11	A	807	CLA	C4B-NB	3.03	1.41	1.37
11	A	825	CLA	C4B-NB	3.03	1.41	1.37
11	A	823	CLA	C4B-NB	3.02	1.41	1.37
11	B	812	CLA	C4B-NB	3.02	1.41	1.37
11	A	811	CLA	C4B-NB	3.02	1.41	1.37
11	B	820	CLA	C4B-NB	3.01	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	L	202	CLA	C4B-NB	3.01	1.41	1.37
11	A	832	CLA	C4B-NB	3.01	1.41	1.37
11	A	822	CLA	C4B-NB	3.01	1.41	1.37
11	B	830	CLA	C4B-NB	3.01	1.41	1.37
11	A	831	CLA	C4B-NB	3.00	1.41	1.37
11	A	842	CLA	C4B-NB	3.00	1.41	1.37
11	A	830	CLA	C4B-NB	3.00	1.41	1.37
11	B	838	CLA	C4B-NB	3.00	1.41	1.37
11	B	818	CLA	C4B-NB	2.99	1.41	1.37
11	B	805	CLA	C4B-NB	2.99	1.41	1.37
11	A	806	CLA	C4B-NB	2.99	1.41	1.37
11	B	836	CLA	C4B-NB	2.98	1.41	1.37
11	B	816	CLA	C4B-NB	2.98	1.41	1.37
11	B	810	CLA	C4B-NB	2.98	1.41	1.37
11	B	804	CLA	C4B-NB	2.98	1.41	1.37
11	A	819	CLA	C4B-NB	2.98	1.41	1.37
11	A	817	CLA	C4B-NB	2.97	1.41	1.37
11	B	815	CLA	C4B-NB	2.97	1.41	1.37
11	B	802	CLA	C4B-NB	2.97	1.41	1.37
11	A	833	CLA	C4B-NB	2.96	1.41	1.37
11	A	840	CLA	C4B-NB	2.96	1.41	1.37
11	A	839	CLA	C4B-NB	2.95	1.41	1.37
11	A	814	CLA	C4B-NB	2.95	1.41	1.37
11	B	808	CLA	C4B-NB	2.95	1.41	1.37
11	A	821	CLA	C4B-NB	2.94	1.41	1.37
11	F	804	CLA	C4B-NB	2.94	1.41	1.37
11	A	820	CLA	C4B-NB	2.94	1.41	1.37
11	A	815	CLA	C4B-NB	2.92	1.41	1.37
11	B	806	CLA	C4B-NB	2.92	1.41	1.37
11	A	826	CLA	C4B-NB	2.92	1.41	1.37
11	B	840	CLA	C4B-NB	2.92	1.41	1.37
11	B	824	CLA	C4B-NB	2.91	1.41	1.37
11	B	828	CLA	C4B-NB	2.91	1.41	1.37
11	B	833	CLA	C4B-NB	2.90	1.41	1.37
11	B	835	CLA	C4B-NB	2.90	1.41	1.37
11	B	826	CLA	C4B-NB	2.90	1.41	1.37
11	B	831	CLA	C4B-NB	2.89	1.41	1.37
11	F	803	CLA	C4B-NB	2.89	1.41	1.37
11	A	834	CLA	C4B-NB	2.89	1.41	1.37
11	B	814	CLA	C4B-NB	2.87	1.41	1.37
11	A	816	CLA	C4B-NB	2.87	1.41	1.37
11	A	825	CLA	C1B-C2B	2.86	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	827	CLA	C4B-NB	2.86	1.41	1.37
11	L	203	CLA	C1B-C2B	2.84	1.49	1.43
11	A	813	CLA	C4B-NB	2.84	1.41	1.37
11	B	808	CLA	C1B-C2B	2.84	1.49	1.43
11	B	814	CLA	C1B-C2B	2.83	1.49	1.43
11	B	824	CLA	C1B-C2B	2.83	1.49	1.43
11	A	812	CLA	C4B-NB	2.83	1.41	1.37
11	B	839	CLA	C1B-C2B	2.83	1.49	1.43
11	A	810	CLA	C4B-NB	2.83	1.41	1.37
11	A	837	CLA	C4B-NB	2.83	1.41	1.37
11	B	823	CLA	C1B-C2B	2.82	1.49	1.43
11	B	825	CLA	C1B-C2B	2.82	1.49	1.43
11	B	807	CLA	C4B-NB	2.82	1.41	1.37
11	B	836	CLA	C1B-C2B	2.82	1.49	1.43
11	A	805	CLA	C4B-NB	2.82	1.41	1.37
11	J	103	CLA	C4B-NB	2.82	1.41	1.37
11	A	807	CLA	C1B-C2B	2.82	1.49	1.43
11	A	829	CLA	C4B-NB	2.81	1.41	1.37
11	B	803	CLA	C1B-C2B	2.81	1.49	1.43
11	B	832	CLA	C4B-NB	2.81	1.41	1.37
11	B	834	CLA	C4B-NB	2.81	1.41	1.37
11	A	803	CLA	C4B-NB	2.81	1.41	1.37
11	A	808	CLA	C4B-NB	2.81	1.41	1.37
11	B	802	CLA	C1B-C2B	2.81	1.49	1.43
11	L	202	CLA	C1B-C2B	2.80	1.49	1.43
11	A	801	CLA	C1D-C2D	-2.80	1.39	1.45
11	A	844	CLA	C1B-C2B	2.80	1.49	1.43
11	B	829	CLA	C4B-NB	2.79	1.41	1.37
11	A	820	CLA	C1B-C2B	2.79	1.49	1.43
11	A	838	CLA	C4B-NB	2.78	1.41	1.37
11	B	852	CLA	C1B-C2B	2.78	1.49	1.43
11	B	837	CLA	C4B-NB	2.78	1.41	1.37
11	A	827	CLA	C4B-NB	2.77	1.41	1.37
11	B	811	CLA	C4B-NB	2.76	1.41	1.37
11	A	801	CLA	MG-NC	2.76	2.12	2.06
11	A	836	CLA	C1B-C2B	2.76	1.49	1.43
11	A	817	CLA	C1B-C2B	2.76	1.49	1.43
11	A	839	CLA	C1B-C2B	2.76	1.49	1.43
11	A	815	CLA	C1B-C2B	2.75	1.49	1.43
11	B	807	CLA	C1B-C2B	2.75	1.49	1.43
11	A	833	CLA	C1B-C2B	2.74	1.49	1.43
11	F	804	CLA	C1B-C2B	2.74	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	817	CLA	C1B-C2B	2.74	1.49	1.43
11	B	835	CLA	C1B-C2B	2.74	1.49	1.43
11	A	838	CLA	C1B-C2B	2.74	1.49	1.43
11	B	828	CLA	C1B-C2B	2.73	1.49	1.43
11	A	834	CLA	C1B-C2B	2.73	1.49	1.43
11	A	814	CLA	C1B-C2B	2.73	1.49	1.43
11	A	842	CLA	C1B-C2B	2.72	1.49	1.43
11	B	810	CLA	C1B-C2B	2.72	1.49	1.43
11	A	816	CLA	C1B-C2B	2.72	1.49	1.43
11	B	811	CLA	C1B-C2B	2.72	1.49	1.43
11	B	833	CLA	C1B-C2B	2.72	1.49	1.43
11	A	808	CLA	C1B-C2B	2.71	1.49	1.43
11	B	821	CLA	C1B-C2B	2.71	1.49	1.43
11	B	822	CLA	C1B-C2B	2.71	1.49	1.43
11	B	838	CLA	C1B-C2B	2.71	1.49	1.43
11	F	803	CLA	C1B-C2B	2.71	1.49	1.43
11	B	830	CLA	C1B-C2B	2.70	1.49	1.43
11	B	840	CLA	C1B-C2B	2.70	1.49	1.43
11	B	827	CLA	C1B-C2B	2.70	1.49	1.43
11	A	811	CLA	C1B-C2B	2.70	1.49	1.43
11	B	812	CLA	C1B-C2B	2.69	1.49	1.43
11	B	813	CLA	C1B-C2B	2.69	1.49	1.43
11	A	828	CLA	C1B-C2B	2.68	1.49	1.43
11	A	840	CLA	C1B-C2B	2.68	1.49	1.43
11	A	823	CLA	C1B-C2B	2.68	1.49	1.43
11	A	804	CLA	C1B-C2B	2.68	1.49	1.43
11	A	803	CLA	C1B-C2B	2.68	1.49	1.43
11	B	820	CLA	C1B-C2B	2.68	1.49	1.43
11	A	821	CLA	C1B-C2B	2.68	1.49	1.43
11	B	831	CLA	C1B-C2B	2.68	1.49	1.43
11	B	842	CLA	C1B-C2B	2.67	1.49	1.43
11	A	812	CLA	C1B-C2B	2.67	1.49	1.43
11	A	829	CLA	C1B-C2B	2.67	1.49	1.43
11	A	813	CLA	C1B-C2B	2.67	1.49	1.43
11	B	841	CLA	C1B-C2B	2.67	1.49	1.43
11	A	831	CLA	C1B-C2B	2.67	1.49	1.43
11	A	824	CLA	C1B-C2B	2.67	1.49	1.43
11	A	830	CLA	C1B-C2B	2.66	1.49	1.43
11	A	832	CLA	C1B-C2B	2.66	1.49	1.43
11	A	828	CLA	C4B-NB	2.65	1.41	1.37
11	A	805	CLA	C1B-C2B	2.65	1.49	1.43
11	A	818	CLA	C1B-C2B	2.65	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	829	CLA	C1B-C2B	2.65	1.49	1.43
11	A	827	CLA	C1B-C2B	2.65	1.49	1.43
11	B	806	CLA	C1B-C2B	2.65	1.49	1.43
11	B	815	CLA	C1B-C2B	2.64	1.49	1.43
11	A	810	CLA	C1B-C2B	2.64	1.49	1.43
11	J	103	CLA	C1B-C2B	2.64	1.49	1.43
11	B	801	CLA	C1B-C2B	2.64	1.49	1.43
11	A	837	CLA	C1B-C2B	2.63	1.49	1.43
11	B	816	CLA	C1B-C2B	2.63	1.49	1.43
11	A	835	CLA	C1B-C2B	2.63	1.49	1.43
11	B	826	CLA	C1B-C2B	2.63	1.49	1.43
11	A	841	CLA	C1B-C2B	2.63	1.49	1.43
11	A	822	CLA	C1B-C2B	2.63	1.49	1.43
11	B	834	CLA	C1B-C2B	2.63	1.49	1.43
11	B	832	CLA	C1B-C2B	2.61	1.49	1.43
11	B	805	CLA	C1B-C2B	2.59	1.49	1.43
11	B	837	CLA	C1B-C2B	2.59	1.49	1.43
11	B	818	CLA	C1B-C2B	2.59	1.49	1.43
11	A	806	CLA	C1B-C2B	2.59	1.49	1.43
11	B	809	CLA	C1B-C2B	2.59	1.49	1.43
11	A	809	CLA	C4B-NB	2.58	1.41	1.37
11	A	826	CLA	C1B-C2B	2.55	1.49	1.43
11	A	802	CLA	C1B-C2B	2.55	1.49	1.43
11	B	819	CLA	C1B-C2B	2.54	1.49	1.43
11	B	803	CLA	C4B-NB	2.52	1.41	1.37
11	A	835	CLA	C3B-C4B	2.52	1.50	1.42
11	B	804	CLA	C1B-C2B	2.52	1.49	1.43
11	A	809	CLA	C1B-C2B	2.51	1.49	1.43
11	A	826	CLA	C3B-C4B	2.50	1.50	1.42
11	B	809	CLA	C3B-C4B	2.48	1.49	1.42
11	A	824	CLA	C3B-C4B	2.45	1.49	1.42
11	B	805	CLA	CHC-C1C	2.44	1.43	1.38
11	A	819	CLA	C1B-C2B	2.44	1.48	1.43
11	B	852	CLA	C3B-C4B	2.42	1.49	1.42
11	B	805	CLA	C3B-C4B	2.42	1.49	1.42
11	B	804	CLA	C3B-C4B	2.42	1.49	1.42
11	A	804	CLA	C3B-C4B	2.41	1.49	1.42
11	B	813	CLA	C3B-C4B	2.41	1.49	1.42
11	A	806	CLA	C3B-C4B	2.41	1.49	1.42
11	A	818	CLA	CHC-C1C	2.40	1.43	1.38
11	B	826	CLA	C3B-C4B	2.40	1.49	1.42
11	A	822	CLA	C3B-C4B	2.40	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	826	CLA	CHC-C1C	2.40	1.43	1.38
11	A	802	CLA	C3B-C4B	2.40	1.49	1.42
11	A	804	CLA	CHC-C1C	2.40	1.43	1.38
11	B	818	CLA	C3B-C4B	2.39	1.49	1.42
11	A	818	CLA	C3B-C4B	2.39	1.49	1.42
11	B	813	CLA	CHC-C1C	2.39	1.43	1.38
11	B	826	CLA	CHC-C1C	2.39	1.43	1.38
11	B	802	CLA	CHC-C1C	2.38	1.43	1.38
11	A	801	CLA	MG-NA	2.38	2.11	2.06
11	B	821	CLA	C3B-C4B	2.37	1.49	1.42
11	B	802	CLA	C3B-C4B	2.37	1.49	1.42
11	B	840	CLA	C3B-C4B	2.37	1.49	1.42
11	A	810	CLA	C3B-C4B	2.36	1.49	1.42
11	B	835	CLA	C3B-C4B	2.36	1.49	1.42
11	B	820	CLA	CHC-C1C	2.36	1.43	1.38
11	B	837	CLA	C3B-C4B	2.36	1.49	1.42
11	B	820	CLA	C3B-C4B	2.35	1.49	1.42
11	B	806	CLA	CHC-C1C	2.35	1.43	1.38
11	A	802	CLA	CHC-C1C	2.35	1.43	1.38
11	B	842	CLA	C3B-C4B	2.35	1.49	1.42
11	B	818	CLA	CHC-C1C	2.35	1.43	1.38
11	B	842	CLA	CHC-C1C	2.35	1.43	1.38
11	F	804	CLA	C3B-C4B	2.35	1.49	1.42
11	A	841	CLA	CHC-C1C	2.35	1.43	1.38
11	A	841	CLA	C3B-C4B	2.35	1.49	1.42
11	A	832	CLA	C3B-C4B	2.35	1.49	1.42
11	B	835	CLA	CHC-C1C	2.35	1.43	1.38
11	A	812	CLA	C3B-C4B	2.34	1.49	1.42
11	B	828	CLA	CHC-C1C	2.34	1.43	1.38
11	A	820	CLA	C3B-C4B	2.34	1.49	1.42
11	A	805	CLA	C3B-C4B	2.34	1.49	1.42
11	A	840	CLA	C3B-C4B	2.34	1.49	1.42
11	A	831	CLA	C3B-C4B	2.34	1.49	1.42
11	B	832	CLA	C3B-C4B	2.33	1.49	1.42
11	B	806	CLA	C3B-C4B	2.33	1.49	1.42
11	B	807	CLA	C3B-C4B	2.33	1.49	1.42
11	B	816	CLA	C3B-C4B	2.32	1.49	1.42
11	B	838	CLA	CHC-C1C	2.32	1.43	1.38
11	B	852	CLA	CHC-C1C	2.32	1.43	1.38
11	L	203	CLA	C3B-C4B	2.32	1.49	1.42
11	B	824	CLA	C3B-C4B	2.32	1.49	1.42
11	A	801	CLA	C1C-NC	2.32	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	816	CLA	CHC-C1C	2.32	1.43	1.38
11	A	805	CLA	CHC-C1C	2.32	1.43	1.38
11	B	801	CLA	C3B-C4B	2.31	1.49	1.42
11	A	815	CLA	C3B-C4B	2.31	1.49	1.42
11	B	815	CLA	CHC-C1C	2.31	1.43	1.38
11	A	813	CLA	C3B-C4B	2.31	1.49	1.42
11	A	819	CLA	CHC-C1C	2.31	1.43	1.38
11	A	829	CLA	C3B-C4B	2.31	1.49	1.42
11	B	817	CLA	C3B-C4B	2.30	1.49	1.42
11	B	819	CLA	C3B-C4B	2.30	1.49	1.42
11	B	809	CLA	CMD-C2D	-2.30	1.46	1.50
11	B	838	CLA	C3B-C4B	2.30	1.49	1.42
11	A	831	CLA	CHC-C1C	2.30	1.43	1.38
11	B	801	CLA	CHC-C1C	2.29	1.43	1.38
11	B	837	CLA	CHC-C1C	2.29	1.43	1.38
11	A	827	CLA	C3B-C4B	2.29	1.49	1.42
11	B	812	CLA	C3B-C4B	2.29	1.49	1.42
11	F	803	CLA	C3B-C4B	2.29	1.49	1.42
11	A	819	CLA	C3B-C4B	2.29	1.49	1.42
11	B	819	CLA	CHC-C1C	2.29	1.43	1.38
11	A	816	CLA	CHC-C1C	2.29	1.43	1.38
11	A	837	CLA	C3B-C4B	2.29	1.49	1.42
11	B	823	CLA	C3B-C4B	2.29	1.49	1.42
11	B	822	CLA	CHC-C1C	2.29	1.43	1.38
11	B	841	CLA	C3B-C4B	2.29	1.49	1.42
11	B	836	CLA	CHC-C1C	2.29	1.43	1.38
11	A	835	CLA	CHC-C1C	2.29	1.43	1.38
11	B	836	CLA	C3B-C4B	2.29	1.49	1.42
11	B	833	CLA	C3B-C4B	2.29	1.49	1.42
11	B	814	CLA	C3B-C4B	2.28	1.49	1.42
11	B	804	CLA	CHC-C1C	2.28	1.43	1.38
11	F	804	CLA	CHC-C1C	2.28	1.43	1.38
11	A	842	CLA	C3B-C4B	2.28	1.49	1.42
11	F	803	CLA	CHC-C1C	2.28	1.43	1.38
11	B	831	CLA	C3B-C4B	2.28	1.49	1.42
11	A	813	CLA	CHC-C1C	2.28	1.43	1.38
11	A	803	CLA	C3B-C4B	2.28	1.49	1.42
11	B	831	CLA	CHC-C1C	2.28	1.43	1.38
11	B	827	CLA	C3B-C4B	2.27	1.49	1.42
11	L	202	CLA	C3B-C4B	2.27	1.49	1.42
11	A	816	CLA	C3B-C4B	2.27	1.49	1.42
11	A	822	CLA	CHC-C1C	2.27	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	827	CLA	CHC-C1C	2.27	1.43	1.38
11	A	809	CLA	C3B-C4B	2.27	1.49	1.42
11	J	103	CLA	C3B-C4B	2.27	1.49	1.42
11	A	812	CLA	CHC-C1C	2.27	1.43	1.38
11	B	828	CLA	C3B-C4B	2.27	1.49	1.42
11	A	810	CLA	CHC-C1C	2.26	1.43	1.38
11	B	821	CLA	CHC-C1C	2.26	1.43	1.38
11	A	832	CLA	CHC-C1C	2.26	1.43	1.38
11	B	815	CLA	C3B-C4B	2.26	1.49	1.42
11	B	822	CLA	C3B-C4B	2.26	1.49	1.42
11	A	811	CLA	C3B-C4B	2.26	1.49	1.42
11	A	844	CLA	C3B-C4B	2.26	1.49	1.42
11	A	823	CLA	C3B-C4B	2.26	1.49	1.42
11	A	838	CLA	C3B-C4B	2.26	1.49	1.42
11	A	824	CLA	CHC-C1C	2.26	1.43	1.38
11	B	824	CLA	CHC-C1C	2.26	1.43	1.38
11	L	203	CLA	CHC-C1C	2.26	1.43	1.38
11	B	823	CLA	CMD-C2D	-2.25	1.46	1.50
11	A	817	CLA	C3B-C4B	2.25	1.49	1.42
11	A	828	CLA	CHC-C1C	2.25	1.43	1.38
11	B	812	CLA	CHC-C1C	2.25	1.43	1.38
11	A	807	CLA	CHC-C1C	2.25	1.43	1.38
11	A	809	CLA	CMD-C2D	-2.24	1.46	1.50
11	A	840	CLA	CHC-C1C	2.24	1.43	1.38
11	A	842	CLA	CHC-C1C	2.24	1.43	1.38
11	B	825	CLA	C3B-C4B	2.24	1.49	1.42
11	A	811	CLA	CHC-C1C	2.24	1.43	1.38
11	B	807	CLA	CHC-C1C	2.24	1.43	1.38
11	A	829	CLA	CHC-C1C	2.24	1.43	1.38
11	B	830	CLA	C3B-C4B	2.23	1.49	1.42
11	B	819	CLA	CMB-C2B	-2.23	1.46	1.50
11	A	844	CLA	CHC-C1C	2.23	1.43	1.38
11	B	810	CLA	C3B-C4B	2.23	1.49	1.42
11	B	832	CLA	CHC-C1C	2.23	1.43	1.38
11	J	103	CLA	CMD-C2D	-2.23	1.46	1.50
11	B	839	CLA	C3B-C4B	2.23	1.49	1.42
11	B	823	CLA	CHC-C1C	2.23	1.43	1.38
11	A	821	CLA	CHC-C1C	2.23	1.43	1.38
11	A	821	CLA	C3B-C4B	2.23	1.49	1.42
11	A	807	CLA	C3B-C4B	2.23	1.49	1.42
11	A	815	CLA	CHC-C1C	2.22	1.42	1.38
11	B	809	CLA	CHC-C1C	2.22	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	834	CLA	C3B-C4B	2.22	1.49	1.42
11	B	811	CLA	C3B-C4B	2.22	1.49	1.42
11	A	833	CLA	CMB-C2B	-2.22	1.46	1.50
11	A	838	CLA	CHC-C1C	2.22	1.42	1.38
11	L	202	CLA	CHC-C1C	2.22	1.42	1.38
11	A	817	CLA	CHC-C1C	2.21	1.42	1.38
11	B	808	CLA	C3B-C4B	2.21	1.49	1.42
11	B	817	CLA	CHC-C1C	2.21	1.42	1.38
11	B	829	CLA	C3B-C4B	2.21	1.49	1.42
11	A	806	CLA	CHC-C1C	2.21	1.42	1.38
11	B	829	CLA	CHC-C1C	2.21	1.42	1.38
11	A	819	CLA	CMB-C2B	-2.21	1.46	1.50
11	B	825	CLA	CMD-C2D	-2.21	1.46	1.50
11	A	839	CLA	C3B-C4B	2.21	1.49	1.42
11	A	830	CLA	CMB-C2B	-2.21	1.46	1.50
11	J	103	CLA	CHC-C1C	2.21	1.42	1.38
11	A	833	CLA	C3B-C4B	2.21	1.49	1.42
11	A	814	CLA	C3B-C4B	2.21	1.49	1.42
11	A	823	CLA	CHC-C1C	2.21	1.42	1.38
11	B	811	CLA	CHC-C1C	2.20	1.42	1.38
11	A	836	CLA	C3B-C4B	2.20	1.49	1.42
11	A	837	CLA	CHC-C1C	2.19	1.42	1.38
11	A	814	CLA	CHC-C1C	2.19	1.42	1.38
11	A	836	CLA	CHC-C1C	2.19	1.42	1.38
11	B	825	CLA	CHC-C1C	2.18	1.42	1.38
11	A	825	CLA	C3B-C4B	2.18	1.49	1.42
11	A	830	CLA	C3B-C4B	2.18	1.49	1.42
11	A	809	CLA	MG-NB	-2.18	2.01	2.05
11	B	839	CLA	CHC-C1C	2.18	1.42	1.38
11	B	814	CLA	CHC-C1C	2.18	1.42	1.38
11	B	830	CLA	CMB-C2B	-2.18	1.46	1.50
11	B	804	CLA	CMC-C2C	-2.18	1.46	1.50
11	A	803	CLA	CHC-C1C	2.18	1.42	1.38
11	B	802	CLA	CMD-C2D	-2.17	1.46	1.50
11	A	820	CLA	CHC-C1C	2.17	1.42	1.38
11	B	834	CLA	CHC-C1C	2.17	1.42	1.38
11	A	833	CLA	CHC-C1C	2.17	1.42	1.38
11	A	842	CLA	CMB-C2B	-2.17	1.46	1.50
11	B	840	CLA	CMD-C2D	-2.17	1.46	1.50
11	A	818	CLA	CMC-C2C	-2.16	1.46	1.50
11	A	830	CLA	CHC-C1C	2.16	1.42	1.38
11	A	842	CLA	CMD-C2D	-2.16	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	828	CLA	C3B-C4B	2.15	1.49	1.42
11	A	808	CLA	CHC-C1C	2.15	1.42	1.38
11	B	810	CLA	CMB-C2B	-2.15	1.46	1.50
11	A	808	CLA	CMD-C2D	-2.15	1.46	1.50
11	B	808	CLA	CHC-C1C	2.15	1.42	1.38
11	B	833	CLA	CHC-C1C	2.15	1.42	1.38
11	A	829	CLA	CMD-C2D	-2.15	1.46	1.50
11	B	837	CLA	CMD-C2D	-2.15	1.46	1.50
11	B	830	CLA	CMD-C2D	-2.15	1.46	1.50
11	B	837	CLA	MG-NB	-2.15	2.01	2.05
11	B	814	CLA	CMD-C2D	-2.15	1.46	1.50
11	A	809	CLA	CHC-C1C	2.14	1.42	1.38
11	B	815	CLA	CMD-C2D	-2.14	1.46	1.50
11	A	825	CLA	CHC-C1C	2.14	1.42	1.38
11	B	827	CLA	MG-NB	-2.14	2.01	2.05
11	A	839	CLA	CHC-C1C	2.14	1.42	1.38
11	F	803	CLA	CMD-C2D	-2.14	1.46	1.50
11	B	834	CLA	C3B-C4B	2.14	1.49	1.42
11	A	811	CLA	CMD-C2D	-2.14	1.46	1.50
11	B	809	CLA	CMC-C2C	-2.14	1.46	1.50
11	A	808	CLA	C3B-C4B	2.14	1.49	1.42
11	A	827	CLA	MG-NB	-2.14	2.01	2.05
11	A	818	CLA	CMD-C2D	-2.13	1.46	1.50
11	A	827	CLA	CMC-C2C	-2.13	1.46	1.50
11	B	832	CLA	MG-NB	-2.13	2.01	2.05
11	A	827	CLA	CMD-C2D	-2.13	1.46	1.50
11	A	826	CLA	CMD-C2D	-2.13	1.46	1.50
11	A	838	CLA	CMD-C2D	-2.13	1.46	1.50
11	B	822	CLA	CMB-C2B	-2.13	1.46	1.50
11	A	840	CLA	CMD-C2D	-2.13	1.46	1.50
11	A	813	CLA	CMD-C2D	-2.13	1.46	1.50
11	B	840	CLA	CHC-C1C	2.13	1.42	1.38
11	F	804	CLA	CMD-C2D	-2.13	1.46	1.50
11	B	818	CLA	CMD-C2D	-2.12	1.46	1.50
11	B	827	CLA	CMC-C2C	-2.12	1.46	1.50
11	B	829	CLA	CMD-C2D	-2.12	1.46	1.50
11	B	830	CLA	CHC-C1C	2.12	1.42	1.38
11	B	805	CLA	MG-NB	-2.12	2.01	2.05
11	A	840	CLA	CMB-C2B	-2.12	1.46	1.50
11	B	834	CLA	CMB-C2B	-2.12	1.46	1.50
11	B	842	CLA	CMD-C2D	-2.12	1.46	1.50
11	B	831	CLA	CMB-C2B	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	813	CLA	CMC-C2C	-2.11	1.46	1.50
11	B	827	CLA	CHC-C1C	2.11	1.42	1.38
11	B	838	CLA	CMD-C2D	-2.11	1.46	1.50
11	B	816	CLA	CMD-C2D	-2.11	1.46	1.50
11	A	821	CLA	CMB-C2B	-2.11	1.46	1.50
11	B	803	CLA	CMD-C2D	-2.11	1.46	1.50
11	J	103	CLA	MG-NB	-2.11	2.01	2.05
11	B	815	CLA	MG-NB	-2.11	2.01	2.05
11	A	822	CLA	CMD-C2D	-2.11	1.46	1.50
11	A	805	CLA	CMD-C2D	-2.11	1.46	1.50
11	A	813	CLA	MG-NB	-2.11	2.01	2.05
11	A	821	CLA	MG-NB	-2.11	2.01	2.05
11	A	834	CLA	CHC-C1C	2.11	1.42	1.38
11	B	814	CLA	MG-NB	-2.10	2.01	2.05
11	A	835	CLA	CMD-C2D	-2.10	1.46	1.50
11	A	832	CLA	CMB-C2B	-2.10	1.46	1.50
11	B	816	CLA	CMC-C2C	-2.10	1.46	1.50
11	B	841	CLA	CMB-C2B	-2.10	1.46	1.50
11	A	829	CLA	MG-NB	-2.10	2.01	2.05
11	B	828	CLA	CMB-C2B	-2.10	1.46	1.50
11	A	833	CLA	CMD-C2D	-2.10	1.46	1.50
11	B	824	CLA	CMC-C2C	-2.10	1.46	1.50
11	A	839	CLA	MG-NB	-2.10	2.01	2.05
11	A	839	CLA	CMD-C2D	-2.10	1.46	1.50
11	A	832	CLA	MG-NB	-2.10	2.01	2.05
11	B	806	CLA	CMD-C2D	-2.10	1.46	1.50
11	B	842	CLA	MG-NB	-2.10	2.01	2.05
11	B	805	CLA	CMD-C2D	-2.10	1.46	1.50
11	A	836	CLA	CMD-C2D	-2.09	1.46	1.50
11	B	827	CLA	CMD-C2D	-2.09	1.46	1.50
11	A	814	CLA	CMB-C2B	-2.09	1.46	1.50
11	A	823	CLA	CMD-C2D	-2.09	1.46	1.50
11	A	837	CLA	CMD-C2D	-2.09	1.46	1.50
11	A	806	CLA	CMB-C2B	-2.09	1.46	1.50
11	A	842	CLA	MG-NB	-2.09	2.01	2.05
11	B	852	CLA	CMC-C2C	-2.09	1.46	1.50
11	A	831	CLA	CMD-C2D	-2.09	1.46	1.50
11	B	818	CLA	MG-NB	-2.09	2.01	2.05
11	A	834	CLA	CMB-C2B	-2.09	1.46	1.50
11	A	836	CLA	MG-NB	-2.09	2.01	2.05
11	B	841	CLA	CMD-C2D	-2.09	1.46	1.50
11	A	832	CLA	CMD-C2D	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	841	CLA	CMB-C2B	-2.08	1.46	1.50
11	B	817	CLA	CMB-C2B	-2.08	1.46	1.50
11	B	841	CLA	CHC-C1C	2.08	1.42	1.38
11	A	814	CLA	MG-NB	-2.08	2.01	2.05
11	B	811	CLA	CMD-C2D	-2.08	1.46	1.50
11	B	827	CLA	CMB-C2B	-2.08	1.46	1.50
11	A	838	CLA	MG-NB	-2.08	2.01	2.05
11	A	820	CLA	CMD-C2D	-2.08	1.46	1.50
11	B	838	CLA	MG-NB	-2.08	2.01	2.05
11	B	833	CLA	MG-NB	-2.08	2.01	2.05
11	B	839	CLA	CMD-C2D	-2.08	1.46	1.50
11	A	818	CLA	MG-NB	-2.08	2.01	2.05
11	B	821	CLA	MG-NB	-2.08	2.01	2.05
11	A	835	CLA	CMB-C2B	-2.08	1.46	1.50
11	A	810	CLA	CMD-C2D	-2.07	1.46	1.50
11	B	833	CLA	CMD-C2D	-2.07	1.46	1.50
11	B	810	CLA	CHC-C1C	2.07	1.42	1.38
11	A	815	CLA	CMD-C2D	-2.07	1.46	1.50
11	B	807	CLA	CMD-C2D	-2.07	1.46	1.50
11	B	840	CLA	CMB-C2B	-2.07	1.46	1.50
11	A	804	CLA	CMD-C2D	-2.07	1.46	1.50
11	A	817	CLA	MG-NB	-2.07	2.01	2.05
11	B	807	CLA	MG-NB	-2.07	2.01	2.05
11	A	803	CLA	MG-NB	-2.07	2.01	2.05
11	B	808	CLA	CMD-C2D	-2.07	1.46	1.50
11	A	808	CLA	CMC-C2C	-2.07	1.46	1.50
11	A	831	CLA	MG-NB	-2.07	2.01	2.05
11	B	826	CLA	CMD-C2D	-2.07	1.46	1.50
11	A	844	CLA	CMD-C2D	-2.07	1.46	1.50
11	B	808	CLA	CMB-C2B	-2.07	1.46	1.50
11	A	830	CLA	CMD-C2D	-2.07	1.46	1.50
11	B	819	CLA	CMC-C2C	-2.07	1.46	1.50
11	A	825	CLA	CMD-C2D	-2.07	1.46	1.50
11	B	820	CLA	CMD-C2D	-2.07	1.46	1.50
11	A	807	CLA	CMB-C2B	-2.06	1.46	1.50
11	B	818	CLA	CMC-C2C	-2.06	1.46	1.50
11	A	819	CLA	MG-NB	-2.06	2.01	2.05
11	B	819	CLA	CMD-C2D	-2.06	1.46	1.50
11	A	839	CLA	CMB-C2B	-2.06	1.46	1.50
11	B	832	CLA	CMD-C2D	-2.06	1.46	1.50
11	A	824	CLA	CMD-C2D	-2.06	1.46	1.50
11	B	834	CLA	MG-NB	-2.06	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	833	CLA	MG-NB	-2.06	2.01	2.05
11	A	819	CLA	CMD-C2D	-2.06	1.46	1.50
11	A	836	CLA	CMB-C2B	-2.06	1.46	1.50
11	A	803	CLA	CMD-C2D	-2.06	1.46	1.50
11	B	829	CLA	CMB-C2B	-2.06	1.46	1.50
11	A	841	CLA	CMD-C2D	-2.06	1.46	1.50
11	B	817	CLA	MG-NB	-2.06	2.01	2.05
11	F	804	CLA	MG-NB	-2.06	2.01	2.05
11	L	203	CLA	CMD-C2D	-2.06	1.46	1.50
11	A	825	CLA	MG-NB	-2.06	2.01	2.05
11	L	203	CLA	CMB-C2B	-2.05	1.46	1.50
11	B	822	CLA	MG-NB	-2.05	2.01	2.05
11	B	810	CLA	MG-NB	-2.05	2.01	2.05
11	B	820	CLA	MG-NB	-2.05	2.01	2.05
11	B	815	CLA	CMB-C2B	-2.05	1.46	1.50
11	B	829	CLA	MG-NB	-2.05	2.01	2.05
11	A	831	CLA	CMB-C2B	-2.05	1.46	1.50
11	A	828	CLA	CMD-C2D	-2.05	1.46	1.50
11	B	801	CLA	CMD-C2D	-2.05	1.46	1.50
11	A	822	CLA	MG-NB	-2.05	2.01	2.05
11	B	831	CLA	CMD-C2D	-2.05	1.46	1.50
11	A	838	CLA	CMB-C2B	-2.05	1.46	1.50
11	A	844	CLA	CMB-C2B	-2.05	1.46	1.50
11	B	809	CLA	CMB-C2B	-2.05	1.46	1.50
11	B	852	CLA	CMD-C2D	-2.05	1.46	1.50
11	A	817	CLA	CMD-C2D	-2.05	1.46	1.50
11	A	824	CLA	CMB-C2B	-2.05	1.46	1.50
11	A	812	CLA	CMD-C2D	-2.05	1.46	1.50
11	B	806	CLA	MG-NB	-2.05	2.01	2.05
11	A	802	CLA	CMD-C2D	-2.04	1.46	1.50
11	A	805	CLA	CMC-C2C	-2.04	1.46	1.50
11	B	828	CLA	CMD-C2D	-2.04	1.46	1.50
11	A	841	CLA	MG-NB	-2.04	2.01	2.05
11	B	813	CLA	CMD-C2D	-2.04	1.46	1.50
11	B	803	CLA	MG-NB	-2.04	2.01	2.05
11	B	807	CLA	CMC-C2C	-2.04	1.46	1.50
11	B	832	CLA	CMB-C2B	-2.04	1.46	1.50
11	A	822	CLA	CMB-C2B	-2.04	1.46	1.50
11	L	202	CLA	CMD-C2D	-2.04	1.46	1.50
11	B	835	CLA	CMD-C2D	-2.04	1.46	1.50
11	B	808	CLA	MG-NB	-2.04	2.01	2.05
11	B	852	CLA	CMB-C2B	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	816	CLA	CMC-C2C	-2.03	1.46	1.50
11	B	813	CLA	CMB-C2B	-2.03	1.46	1.50
11	A	837	CLA	MG-NB	-2.03	2.01	2.05
20	T	200	HEC	CMB-C2B	2.03	1.54	1.50
11	A	807	CLA	CMD-C2D	-2.03	1.46	1.50
11	B	839	CLA	MG-NB	-2.03	2.01	2.05
11	A	818	CLA	CMB-C2B	-2.03	1.46	1.50
11	B	829	CLA	CMC-C2C	-2.03	1.46	1.50
11	A	830	CLA	MG-NB	-2.03	2.01	2.05
20	T	200	HEC	CMC-C2C	2.03	1.54	1.50
11	A	820	CLA	CMB-C2B	-2.03	1.46	1.50
11	A	815	CLA	MG-NB	-2.03	2.01	2.05
11	B	842	CLA	CMB-C2B	-2.03	1.46	1.50
11	B	826	CLA	CMC-C2C	-2.03	1.46	1.50
11	B	803	CLA	CMC-C2C	-2.03	1.46	1.50
11	B	819	CLA	MG-NB	-2.03	2.01	2.05
11	B	814	CLA	CMC-C2C	-2.03	1.46	1.50
11	A	806	CLA	CMD-C2D	-2.03	1.46	1.50
11	A	816	CLA	MG-NB	-2.03	2.01	2.05
11	A	837	CLA	CMB-C2B	-2.03	1.46	1.50
11	A	812	CLA	CMC-C2C	-2.02	1.46	1.50
11	B	834	CLA	CMC-C2C	-2.02	1.46	1.50
11	A	814	CLA	CMD-C2D	-2.02	1.46	1.50
11	B	817	CLA	CMD-C2D	-2.02	1.46	1.50
11	B	814	CLA	CMB-C2B	-2.02	1.46	1.50
11	A	807	CLA	CMC-C2C	-2.02	1.46	1.50
11	A	816	CLA	CMD-C2D	-2.02	1.46	1.50
11	A	840	CLA	CMC-C2C	-2.02	1.46	1.50
11	B	823	CLA	CMB-C2B	-2.02	1.46	1.50
11	B	805	CLA	CMC-C2C	-2.02	1.46	1.50
11	B	812	CLA	CMB-C2B	-2.02	1.46	1.50
11	A	810	CLA	CMC-C2C	-2.02	1.46	1.50
11	A	821	CLA	CMD-C2D	-2.02	1.46	1.50
11	B	831	CLA	MG-NB	-2.02	2.01	2.05
11	A	809	CLA	CMB-C2B	-2.02	1.46	1.50
11	L	202	CLA	CMB-C2B	-2.02	1.46	1.50
11	A	826	CLA	CMC-C2C	-2.01	1.46	1.50
11	A	844	CLA	CMC-C2C	-2.01	1.46	1.50
11	B	824	CLA	CMD-C2D	-2.01	1.46	1.50
20	T	200	HEC	C3C-C2C	-2.01	1.34	1.41
11	B	833	CLA	CMB-C2B	-2.01	1.46	1.50
11	F	803	CLA	MG-NB	-2.01	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	810	CLA	CMD-C2D	-2.01	1.46	1.50
11	B	836	CLA	CMD-C2D	-2.01	1.46	1.50
11	A	812	CLA	MG-NB	-2.01	2.01	2.05
11	A	802	CLA	CMB-C2B	-2.01	1.46	1.50
11	B	823	CLA	CMC-C2C	-2.01	1.46	1.50
11	B	811	CLA	MG-NB	-2.01	2.01	2.05
11	B	803	CLA	CMB-C2B	-2.01	1.46	1.50
11	A	817	CLA	CMB-C2B	-2.01	1.46	1.50
11	B	820	CLA	CMB-C2B	-2.01	1.46	1.50
11	A	816	CLA	CMB-C2B	-2.01	1.46	1.50
11	A	826	CLA	MG-NB	-2.01	2.01	2.05
11	B	818	CLA	CMB-C2B	-2.00	1.46	1.50
11	A	844	CLA	MG-NB	-2.00	2.01	2.05
11	B	825	CLA	CMB-C2B	-2.00	1.46	1.50
11	A	815	CLA	CMB-C2B	-2.00	1.46	1.50
11	A	834	CLA	MG-NB	-2.00	2.01	2.05
11	A	841	CLA	CMC-C2C	-2.00	1.46	1.50
11	B	821	CLA	CMB-C2B	-2.00	1.46	1.50

All (559) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	T	200	HEC	CBC-CAC-C3C	-8.58	110.28	127.43
11	B	803	CLA	C4A-NA-C1A	7.95	110.31	106.68
20	T	200	HEC	CBB-CAB-C3B	-7.53	112.38	127.43
11	A	808	CLA	C4A-NA-C1A	7.47	110.08	106.68
11	B	841	CLA	C4A-NA-C1A	7.26	109.99	106.68
11	A	816	CLA	C4A-NA-C1A	7.11	109.92	106.68
11	A	828	CLA	C4A-NA-C1A	7.05	109.90	106.68
11	A	839	CLA	C4A-NA-C1A	6.99	109.87	106.68
11	A	815	CLA	C4A-NA-C1A	6.95	109.85	106.68
11	B	810	CLA	C4A-NA-C1A	6.95	109.85	106.68
11	A	825	CLA	C4A-NA-C1A	6.91	109.83	106.68
11	A	820	CLA	C4A-NA-C1A	6.88	109.82	106.68
11	A	844	CLA	C4A-NA-C1A	6.86	109.81	106.68
11	B	820	CLA	C4A-NA-C1A	6.85	109.80	106.68
11	A	832	CLA	C4A-NA-C1A	6.84	109.80	106.68
11	A	807	CLA	C4A-NA-C1A	6.83	109.79	106.68
11	B	825	CLA	C4A-NA-C1A	6.81	109.79	106.68
11	B	835	CLA	C4A-NA-C1A	6.80	109.78	106.68
11	F	803	CLA	C4A-NA-C1A	6.76	109.77	106.68
11	J	103	CLA	C4A-NA-C1A	6.76	109.76	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	821	CLA	C4A-NA-C1A	6.74	109.76	106.68
11	B	809	CLA	C4A-NA-C1A	6.72	109.74	106.68
11	B	842	CLA	C4A-NA-C1A	6.71	109.74	106.68
11	B	828	CLA	C4A-NA-C1A	6.69	109.73	106.68
11	L	202	CLA	C4A-NA-C1A	6.69	109.73	106.68
11	B	836	CLA	C4A-NA-C1A	6.69	109.73	106.68
11	A	806	CLA	C4A-NA-C1A	6.68	109.73	106.68
11	B	823	CLA	C4A-NA-C1A	6.68	109.72	106.68
11	B	806	CLA	C4A-NA-C1A	6.66	109.72	106.68
11	B	808	CLA	C4A-NA-C1A	6.66	109.72	106.68
11	A	842	CLA	C4A-NA-C1A	6.65	109.71	106.68
11	B	814	CLA	C4A-NA-C1A	6.64	109.71	106.68
11	A	817	CLA	C4A-NA-C1A	6.61	109.69	106.68
11	B	821	CLA	C4A-NA-C1A	6.61	109.69	106.68
11	B	833	CLA	C4A-NA-C1A	6.61	109.69	106.68
11	A	830	CLA	C4A-NA-C1A	6.58	109.68	106.68
11	A	834	CLA	C4A-NA-C1A	6.58	109.68	106.68
11	B	817	CLA	C4A-NA-C1A	6.57	109.68	106.68
11	A	812	CLA	C4A-NA-C1A	6.57	109.67	106.68
11	A	835	CLA	C4A-NA-C1A	6.56	109.67	106.68
11	B	840	CLA	C4A-NA-C1A	6.56	109.67	106.68
11	B	819	CLA	C4A-NA-C1A	6.55	109.67	106.68
11	A	809	CLA	C4A-NA-C1A	6.54	109.66	106.68
11	B	826	CLA	C4A-NA-C1A	6.54	109.66	106.68
11	B	838	CLA	C4A-NA-C1A	6.54	109.66	106.68
11	B	839	CLA	C4A-NA-C1A	6.51	109.65	106.68
11	A	803	CLA	C4A-NA-C1A	6.51	109.65	106.68
11	A	804	CLA	C4A-NA-C1A	6.50	109.64	106.68
11	B	852	CLA	C4A-NA-C1A	6.49	109.64	106.68
11	A	824	CLA	C4A-NA-C1A	6.48	109.64	106.68
11	B	822	CLA	C4A-NA-C1A	6.47	109.63	106.68
11	A	827	CLA	C4A-NA-C1A	6.47	109.63	106.68
11	B	811	CLA	C4A-NA-C1A	6.47	109.63	106.68
11	A	810	CLA	C4A-NA-C1A	6.47	109.63	106.68
11	A	814	CLA	C4A-NA-C1A	6.47	109.63	106.68
11	A	840	CLA	C4A-NA-C1A	6.46	109.63	106.68
11	A	833	CLA	C4A-NA-C1A	6.45	109.62	106.68
11	F	804	CLA	C4A-NA-C1A	6.45	109.62	106.68
11	B	802	CLA	C4A-NA-C1A	6.44	109.62	106.68
11	A	813	CLA	C4A-NA-C1A	6.44	109.61	106.68
11	A	822	CLA	C4A-NA-C1A	6.41	109.61	106.68
11	A	841	CLA	C4A-NA-C1A	6.41	109.60	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	813	CLA	C4A-NA-C1A	6.41	109.60	106.68
11	A	805	CLA	C4A-NA-C1A	6.39	109.59	106.68
11	A	838	CLA	C4A-NA-C1A	6.37	109.58	106.68
11	B	807	CLA	C4A-NA-C1A	6.37	109.58	106.68
11	B	827	CLA	C4A-NA-C1A	6.36	109.58	106.68
11	B	815	CLA	C4A-NA-C1A	6.35	109.57	106.68
11	B	837	CLA	C4A-NA-C1A	6.33	109.57	106.68
11	A	836	CLA	C4A-NA-C1A	6.32	109.56	106.68
11	A	837	CLA	C4A-NA-C1A	6.31	109.56	106.68
11	B	816	CLA	C4A-NA-C1A	6.30	109.55	106.68
11	B	831	CLA	C4A-NA-C1A	6.29	109.55	106.68
11	B	824	CLA	C4A-NA-C1A	6.24	109.53	106.68
11	B	818	CLA	C4A-NA-C1A	6.23	109.52	106.68
11	A	826	CLA	C4A-NA-C1A	6.23	109.52	106.68
11	A	831	CLA	C4A-NA-C1A	6.22	109.52	106.68
11	A	823	CLA	C4A-NA-C1A	6.21	109.51	106.68
11	L	203	CLA	C4A-NA-C1A	6.21	109.51	106.68
11	B	832	CLA	C4A-NA-C1A	6.18	109.50	106.68
11	B	801	CLA	C4A-NA-C1A	6.16	109.49	106.68
11	A	818	CLA	C4A-NA-C1A	6.14	109.48	106.68
11	B	830	CLA	C4A-NA-C1A	6.11	109.47	106.68
11	B	805	CLA	C4A-NA-C1A	6.11	109.47	106.68
11	A	811	CLA	C4A-NA-C1A	6.02	109.42	106.68
11	B	812	CLA	C4A-NA-C1A	6.01	109.42	106.68
11	A	819	CLA	C4A-NA-C1A	5.90	109.37	106.68
11	B	829	CLA	C4A-NA-C1A	5.81	109.33	106.68
11	A	829	CLA	C4A-NA-C1A	5.80	109.33	106.68
11	B	834	CLA	C4A-NA-C1A	5.77	109.31	106.68
11	A	801	CLA	C4A-NA-C1A	5.73	109.29	106.68
11	A	802	CLA	C4A-NA-C1A	5.34	109.11	106.68
11	B	804	CLA	C4A-NA-C1A	4.46	108.72	106.68
20	T	200	HEC	C4D-ND-C1D	3.73	111.90	105.82
16	A	854	LMU	C1'-O5'-C5'	3.58	120.71	113.72
11	A	803	CLA	O2D-CGD-O1D	-3.48	117.08	123.85
11	A	834	CLA	O2D-CGD-O1D	-3.44	117.15	123.85
11	B	834	CLA	O2D-CGD-O1D	-3.39	117.25	123.85
14	I	201	BCR	C7-C8-C9	-3.35	121.28	126.23
11	B	839	CLA	O2D-CGD-O1D	-3.34	117.35	123.85
11	B	826	CLA	O2D-CGD-O1D	-3.29	117.45	123.85
11	A	818	CLA	C3B-C4B-NB	-3.28	107.61	110.53
11	A	811	CLA	O2D-CGD-O1D	-3.27	117.47	123.85
11	B	805	CLA	C3B-C4B-NB	-3.26	107.62	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	818	CLA	C3B-C4B-NB	-3.23	107.65	110.53
11	A	830	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
18	B	849	DGD	C2G-O2G-C1B	3.18	125.39	117.80
11	A	807	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
11	A	826	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
11	B	808	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
11	B	805	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
11	B	838	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
11	A	842	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
11	A	812	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
11	A	815	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
11	A	841	CLA	C3B-C4B-NB	-3.12	107.74	110.53
11	B	809	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
11	A	840	CLA	C3B-C4B-NB	-3.11	107.75	110.53
11	A	804	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
11	A	835	CLA	C3B-C4B-NB	-3.11	107.76	110.53
11	B	804	CLA	CAC-C3C-C4C	3.10	128.82	124.79
11	A	806	CLA	C3B-C4B-NB	-3.10	107.77	110.53
11	A	841	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
11	A	825	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
11	A	833	CLA	C1-C2-C3	-3.08	121.14	126.20
11	B	816	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
11	B	827	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
11	B	813	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
11	A	822	CLA	C3B-C4B-NB	-3.05	107.81	110.53
11	B	804	CLA	C3B-C4B-NB	-3.05	107.81	110.53
11	L	203	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
11	A	819	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
11	A	808	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
11	A	820	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
11	A	839	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
11	B	801	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
11	B	835	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
14	F	801	BCR	C16-C15-C14	-3.01	117.37	123.52
11	A	801	CLA	C3B-C4B-NB	-3.00	107.85	110.53
11	A	831	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
11	A	816	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
11	F	804	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
11	B	802	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
11	B	819	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
11	B	822	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
11	A	824	CLA	O2D-CGD-O1D	-2.96	118.08	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	830	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
11	A	827	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
11	B	821	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
11	A	826	CLA	C3B-C4B-NB	-2.95	107.89	110.53
11	B	842	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
11	B	840	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
11	A	822	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
11	B	828	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
11	A	809	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
11	A	813	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
11	B	803	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
11	B	833	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
11	A	840	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
11	A	804	CLA	C3B-C4B-NB	-2.92	107.92	110.53
11	B	820	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
11	A	818	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
11	B	811	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
11	L	202	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
11	A	836	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
11	A	831	CLA	C3B-C4B-NB	-2.91	107.93	110.53
11	A	833	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
11	B	812	CLA	O2D-CGD-O1D	-2.90	118.19	123.85
11	B	841	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
11	A	837	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
11	A	829	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
11	A	821	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
11	A	817	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
11	A	823	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
11	A	838	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
11	B	836	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
11	A	805	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
16	A	854	LMU	C3'-C4'-C5'	-2.87	104.56	110.93
11	B	809	CLA	C3B-C4B-NB	-2.87	107.96	110.53
11	B	815	CLA	C3B-C4B-NB	-2.87	107.96	110.53
11	B	818	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
11	B	835	CLA	C3B-C4B-NB	-2.87	107.97	110.53
11	B	817	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
11	A	802	CLA	CMB-C2B-C1B	-2.86	121.06	125.42
11	B	831	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
11	B	820	CLA	C3B-C4B-NB	-2.86	107.98	110.53
11	B	824	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
11	A	833	CLA	C3B-C4B-NB	-2.86	107.98	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	827	CLA	C3B-C4B-NB	-2.85	107.98	110.53
11	B	806	CLA	C3B-C4B-NB	-2.85	107.99	110.53
11	B	812	CLA	C3B-C4B-NB	-2.84	107.99	110.53
11	A	806	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
20	T	200	HEC	C2A-C1A-NA	-2.84	107.58	110.32
11	B	823	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
11	B	829	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
11	B	837	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
11	A	824	CLA	C3B-C4B-NB	-2.82	108.02	110.53
11	B	813	CLA	C3B-C4B-NB	-2.82	108.02	110.53
11	A	810	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
11	B	815	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
11	B	834	CLA	C3B-C4B-NB	-2.81	108.03	110.53
11	A	814	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
11	B	816	CLA	C3B-C4B-NB	-2.80	108.03	110.53
11	B	840	CLA	C3B-C4B-NB	-2.80	108.03	110.53
11	A	805	CLA	C3B-C4B-NB	-2.80	108.03	110.53
11	A	842	CLA	C3B-C4B-NB	-2.80	108.03	110.53
11	B	817	CLA	C3B-C4B-NB	-2.80	108.03	110.53
11	B	825	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
11	A	832	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
11	A	802	CLA	C3B-C4B-NB	-2.79	108.04	110.53
11	A	808	CLA	C3B-C4B-NB	-2.78	108.05	110.53
11	A	802	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
11	B	814	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
11	A	813	CLA	C3B-C4B-NB	-2.77	108.06	110.53
11	B	807	CLA	C3B-C4B-NB	-2.77	108.06	110.53
11	A	844	CLA	O2D-CGD-O1D	-2.77	118.47	123.85
11	B	822	CLA	C3B-C4B-NB	-2.76	108.06	110.53
11	B	842	CLA	C3B-C4B-NB	-2.75	108.07	110.53
11	B	826	CLA	C3B-C4B-NB	-2.75	108.08	110.53
11	B	807	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
11	B	806	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
11	A	809	CLA	C1-C2-C3	-2.74	121.70	126.20
11	B	809	CLA	O2A-CGA-O1A	-2.74	116.77	123.63
11	L	202	CLA	C3B-C4B-NB	-2.74	108.08	110.53
11	B	852	CLA	C3B-C4B-NB	-2.74	108.09	110.53
11	A	832	CLA	C3B-C4B-NB	-2.74	108.09	110.53
19	J	101	LUT	C26-C27-C28	2.73	128.83	124.58
11	A	811	CLA	C3B-C4B-NB	-2.73	108.10	110.53
11	F	803	CLA	C3B-C4B-NB	-2.72	108.10	110.53
11	A	809	CLA	C3B-C4B-NB	-2.72	108.10	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	811	CLA	C3B-C4B-NB	-2.72	108.10	110.53
11	J	103	CLA	C3B-C4B-NB	-2.71	108.11	110.53
11	B	832	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
11	B	852	CLA	O2D-CGD-O1D	-2.70	118.58	123.85
11	A	844	CLA	C3B-C4B-NB	-2.70	108.12	110.53
11	F	803	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
11	J	103	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
11	B	819	CLA	C1-C2-C3	-2.69	121.79	126.20
11	B	827	CLA	C3B-C4B-NB	-2.69	108.13	110.53
11	B	842	CLA	C1-C2-C3	-2.69	121.79	126.20
11	A	810	CLA	C3B-C4B-NB	-2.68	108.14	110.53
11	A	816	CLA	C1-C2-C3	-2.68	121.81	126.20
11	A	819	CLA	C1-C2-C3	-2.68	121.81	126.20
11	A	828	CLA	C3B-C4B-NB	-2.67	108.14	110.53
11	F	804	CLA	C3B-C4B-NB	-2.67	108.14	110.53
11	A	828	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
11	A	815	CLA	CHB-C4A-NA	2.67	128.26	124.40
11	B	810	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
11	A	837	CLA	C3B-C4B-NB	-2.66	108.15	110.53
11	A	819	CLA	C3B-C4B-NB	-2.66	108.16	110.53
11	B	814	CLA	C3B-C4B-NB	-2.66	108.16	110.53
11	A	835	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
11	A	814	CLA	C3B-C4B-NB	-2.65	108.16	110.53
11	B	814	CLA	C1-C2-C3	-2.65	121.86	126.20
11	A	826	CLA	CAA-C2A-C1A	-2.65	103.29	111.97
11	J	103	CLA	C1-C2-C3	-2.64	121.87	126.20
11	B	837	CLA	C3B-C4B-NB	-2.64	108.17	110.53
11	A	807	CLA	C1-C2-C3	-2.63	122.51	126.76
11	B	838	CLA	C3B-C4B-NB	-2.63	108.19	110.53
11	F	803	CLA	C1-C2-C3	-2.62	121.91	126.20
11	B	831	CLA	C3B-C4B-NB	-2.61	108.20	110.53
11	A	834	CLA	O2D-CGD-CBD	2.60	115.77	111.23
11	A	835	CLA	CHB-C4A-NA	2.60	128.15	124.40
11	B	835	CLA	CHB-C4A-NA	2.59	128.13	124.40
11	B	803	CLA	C3B-C4B-NB	-2.59	108.22	110.53
11	B	828	CLA	C1-C2-C3	-2.58	121.96	126.20
11	B	834	CLA	CAA-C2A-C1A	-2.58	103.52	111.97
11	A	838	CLA	C3B-C4B-NB	-2.58	108.23	110.53
11	B	819	CLA	C3B-C4B-NB	-2.58	108.23	110.53
11	A	803	CLA	C3B-C4B-NB	-2.57	108.23	110.53
11	A	816	CLA	CHB-C4A-NA	2.57	128.11	124.40
11	A	820	CLA	C3B-C4B-NB	-2.57	108.24	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	816	CLA	CHB-C4A-NA	2.56	128.10	124.40
11	A	820	CLA	CHB-C4A-NA	2.56	128.09	124.40
11	B	841	CLA	C3B-C4B-NB	-2.55	108.25	110.53
11	A	812	CLA	C3B-C4B-NB	-2.55	108.25	110.53
12	B	843	PQN	C11-C3-C4	-2.55	115.89	118.58
11	J	103	CLA	CHB-C4A-NA	2.55	128.08	124.40
11	A	829	CLA	C3B-C4B-NB	-2.55	108.26	110.53
11	A	817	CLA	C3B-C4B-NB	-2.54	108.26	110.53
11	A	803	CLA	CHB-C4A-NA	2.54	128.06	124.40
11	A	813	CLA	CHB-C4A-NA	2.53	128.06	124.40
11	B	832	CLA	C3B-C4B-NB	-2.53	108.27	110.53
11	A	840	CLA	CHB-C4A-NA	2.53	128.05	124.40
11	A	816	CLA	C3B-C4B-NB	-2.53	108.27	110.53
11	A	834	CLA	C3B-C4B-NB	-2.52	108.28	110.53
11	A	801	CLA	C1D-CHD-C4C	-2.52	120.66	126.02
11	A	812	CLA	CHB-C4A-NA	2.52	128.04	124.40
11	A	808	CLA	CHB-C4A-NA	2.51	128.03	124.40
11	B	820	CLA	CHB-C4A-NA	2.51	128.02	124.40
11	A	806	CLA	CHB-C4A-NA	2.51	128.02	124.40
11	B	813	CLA	CAA-C2A-C3A	-2.50	110.49	116.23
11	A	833	CLA	CHB-C4A-NA	2.50	128.01	124.40
11	A	821	CLA	C3B-C4B-NB	-2.50	108.30	110.53
11	B	841	CLA	CHB-C4A-NA	2.50	128.00	124.40
11	A	805	CLA	CHB-C4A-NA	2.49	127.99	124.40
11	B	840	CLA	CHB-C4A-NA	2.48	127.98	124.40
11	A	834	CLA	CHB-C4A-NA	2.48	127.98	124.40
19	J	101	LUT	C36-C21-C26	2.48	113.30	109.55
11	A	844	CLA	CHB-C4A-NA	2.48	127.97	124.40
11	A	810	CLA	CHB-C4A-NA	2.48	127.97	124.40
11	A	832	CLA	CHB-C4A-NA	2.47	127.97	124.40
11	B	813	CLA	CHB-C4A-NA	2.47	127.97	124.40
11	A	826	CLA	CHB-C4A-NA	2.47	127.96	124.40
11	B	818	CLA	CHB-C4A-NA	2.47	127.96	124.40
11	A	807	CLA	C3B-C4B-NB	-2.47	108.33	110.53
11	B	811	CLA	CHB-C4A-NA	2.47	127.96	124.40
11	A	831	CLA	CHB-C4A-NA	2.46	127.94	124.40
11	B	825	CLA	CHB-C4A-NA	2.45	127.94	124.40
11	B	807	CLA	CHB-C4A-NA	2.45	127.94	124.40
11	A	824	CLA	CHB-C4A-NA	2.45	127.93	124.40
16	A	853	LMU	C1B-O5B-C5B	2.45	118.50	113.72
11	B	824	CLA	C3B-C4B-NB	-2.44	108.35	110.53
11	B	830	CLA	C3B-C4B-NB	-2.44	108.35	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	826	CLA	CHB-C4A-NA	2.44	127.92	124.40
11	A	809	CLA	CMB-C2B-C1B	-2.43	121.72	125.42
11	B	817	CLA	CHB-C4A-NA	2.43	127.91	124.40
11	B	834	CLA	O2A-CGA-O1A	-2.42	117.57	123.63
11	B	819	CLA	CHB-C4A-NA	2.42	127.89	124.40
11	A	811	CLA	O2D-CGD-CBD	2.42	115.46	111.23
11	A	830	CLA	C3B-C4B-NB	-2.42	108.37	110.53
11	B	822	CLA	CHB-C4A-NA	2.42	127.89	124.40
11	A	804	CLA	CHB-C4A-NA	2.42	127.89	124.40
11	B	806	CLA	CHB-C4A-NA	2.41	127.89	124.40
11	B	808	CLA	C3B-C4B-NB	-2.41	108.38	110.53
11	A	827	CLA	CHB-C4A-NA	2.41	127.88	124.40
11	B	831	CLA	CHB-C4A-NA	2.41	127.88	124.40
11	A	830	CLA	CHB-C4A-NA	2.41	127.88	124.40
11	A	822	CLA	CHB-C4A-NA	2.41	127.87	124.40
11	B	836	CLA	CHB-C4A-NA	2.41	127.87	124.40
11	A	819	CLA	O2A-CGA-O1A	-2.40	117.62	123.63
11	A	838	CLA	C1-C2-C3	-2.40	122.27	126.20
11	A	809	CLA	CHB-C4A-NA	2.40	127.86	124.40
11	A	832	CLA	CMB-C2B-C1B	-2.40	121.77	125.42
11	A	831	CLA	C1-C2-C3	-2.40	122.27	126.20
11	B	837	CLA	CMB-C2B-C1B	-2.39	121.77	125.42
11	A	826	CLA	O2A-CGA-O1A	-2.39	117.64	123.63
11	B	815	CLA	CHB-C4A-NA	2.39	127.85	124.40
11	A	838	CLA	O2A-CGA-O1A	-2.39	117.64	123.63
11	A	817	CLA	CHB-C4A-NA	2.39	127.85	124.40
11	B	828	CLA	C3B-C4B-NB	-2.38	108.40	110.53
11	B	812	CLA	CHB-C4A-NA	2.38	127.84	124.40
11	A	807	CLA	CHB-C4A-NA	2.38	127.83	124.40
11	A	839	CLA	CHB-C4A-NA	2.37	127.83	124.40
11	A	825	CLA	CHB-C4A-NA	2.37	127.83	124.40
11	A	841	CLA	CHB-C4A-NA	2.37	127.83	124.40
11	B	808	CLA	CHB-C4A-NA	2.37	127.82	124.40
11	L	203	CLA	C3B-C4B-NB	-2.37	108.41	110.53
11	B	809	CLA	CHB-C4A-NA	2.37	127.82	124.40
11	B	832	CLA	CHB-C4A-NA	2.37	127.82	124.40
11	A	815	CLA	C3B-C4B-NB	-2.37	108.42	110.53
11	F	804	CLA	CHB-C4A-NA	2.37	127.82	124.40
11	B	837	CLA	CHB-C4A-NA	2.37	127.81	124.40
11	A	821	CLA	CHB-C4A-NA	2.36	127.81	124.40
11	A	803	CLA	O2D-CGD-CBD	2.36	115.36	111.23
11	A	837	CLA	CHB-C4A-NA	2.36	127.81	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	837	CLA	CMB-C2B-C1B	-2.36	121.83	125.42
11	F	803	CLA	CHB-C4A-NA	2.35	127.80	124.40
11	B	814	CLA	CHB-C4A-NA	2.35	127.80	124.40
11	A	829	CLA	C1-C2-C3	-2.35	122.34	126.20
11	A	838	CLA	CHB-C4A-NA	2.35	127.80	124.40
11	B	825	CLA	C3B-C4B-NB	-2.35	108.43	110.53
11	A	834	CLA	C1-C2-C3	-2.35	122.34	126.20
11	A	839	CLA	C1-C2-C3	-2.35	122.34	126.20
11	A	802	CLA	CHB-C4A-NA	2.35	127.79	124.40
11	A	818	CLA	CHB-C4A-NA	2.35	127.79	124.40
11	B	827	CLA	CHB-C4A-NA	2.35	127.78	124.40
11	A	842	CLA	CHB-C4A-NA	2.34	127.78	124.40
11	B	821	CLA	C3B-C4B-NB	-2.34	108.44	110.53
11	B	824	CLA	CHB-C4A-NA	2.34	127.78	124.40
11	A	837	CLA	C1-C2-C3	-2.34	122.36	126.20
11	B	829	CLA	C3B-C4B-NB	-2.34	108.44	110.53
11	A	817	CLA	CMB-C2B-C1B	-2.34	121.86	125.42
11	B	802	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
11	B	836	CLA	C3B-C4B-NB	-2.34	108.44	110.53
11	B	829	CLA	CMB-C2B-C1B	-2.33	121.86	125.42
11	B	838	CLA	CHB-C4A-NA	2.33	127.77	124.40
11	A	833	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
11	B	805	CLA	CHB-C4A-NA	2.32	127.75	124.40
11	B	840	CLA	C1-C2-C3	-2.32	122.39	126.20
11	L	202	CLA	CHB-C4A-NA	2.32	127.74	124.40
11	B	821	CLA	CHB-C4A-NA	2.32	127.74	124.40
11	A	826	CLA	C1-C2-C3	-2.32	122.40	126.20
11	B	842	CLA	CHB-C4A-NA	2.32	127.74	124.40
11	B	804	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
11	A	814	CLA	CHB-C4A-NA	2.31	127.73	124.40
11	B	823	CLA	CHB-C4A-NA	2.31	127.73	124.40
11	A	839	CLA	C3B-C4B-NB	-2.30	108.48	110.53
11	A	828	CLA	C1-C2-C3	-2.30	122.43	126.20
11	B	839	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
11	A	803	CLA	C1-C2-C3	-2.30	122.43	126.20
11	A	826	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
11	A	802	CLA	CMB-C2B-C3B	2.30	131.95	126.55
11	A	809	CLA	O2A-CGA-O1A	-2.30	117.89	123.63
11	B	810	CLA	C3B-C4B-NB	-2.30	108.48	110.53
11	L	202	CLA	C1-C2-C3	-2.29	122.44	126.20
11	B	833	CLA	CHB-C4A-NA	2.29	127.71	124.40
11	L	202	CLA	O2A-CGA-O1A	-2.29	117.89	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	829	CLA	CHB-C4A-NA	2.29	127.70	124.40
11	B	832	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
11	A	828	CLA	CHB-C4A-NA	2.29	127.70	124.40
11	B	840	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
11	A	819	CLA	O2D-CGD-CBD	2.28	115.21	111.23
11	A	836	CLA	CHB-C4A-NA	2.28	127.68	124.40
11	A	824	CLA	C1-C2-C3	-2.28	122.47	126.20
11	B	808	CLA	O2D-CGD-CBD	2.27	115.21	111.23
11	A	804	CLA	C1-C2-C3	-2.27	122.47	126.20
11	B	839	CLA	C1-C2-C3	-2.27	123.08	126.76
11	A	804	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
11	L	203	CLA	CHB-C4A-NA	2.27	127.67	124.40
11	B	828	CLA	CHB-C4A-NA	2.27	127.67	124.40
11	B	833	CLA	O2A-CGA-O1A	-2.27	117.96	123.63
11	A	825	CLA	C3B-C4B-NB	-2.27	108.51	110.53
11	B	828	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
11	A	804	CLA	O2D-CGD-CBD	2.26	115.18	111.23
11	A	805	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
11	B	826	CLA	O2D-CGD-CBD	2.26	115.18	111.23
11	A	811	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
11	B	830	CLA	CHB-C4A-NA	2.25	127.65	124.40
11	A	812	CLA	CMB-C2B-C1B	-2.25	121.99	125.42
11	A	829	CLA	CMB-C2B-C1B	-2.25	122.00	125.42
11	A	834	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
11	B	827	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
11	B	852	CLA	CHB-C4A-NA	2.24	127.64	124.40
11	B	810	CLA	CHB-C4A-NA	2.24	127.64	124.40
11	B	842	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
11	A	840	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
11	A	811	CLA	CHB-C4A-NA	2.23	127.62	124.40
11	A	819	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
11	B	834	CLA	O2D-CGD-CBD	2.23	115.12	111.23
11	B	833	CLA	C3B-C4B-NB	-2.23	108.54	110.53
11	B	806	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
11	A	819	CLA	CHB-C4A-NA	2.22	127.61	124.40
11	B	839	CLA	O2D-CGD-CBD	2.22	115.11	111.23
11	A	813	CLA	C1-C2-C3	-2.22	122.57	126.20
11	A	808	CLA	O2A-CGA-O1A	-2.22	118.09	123.63
11	B	807	CLA	CMB-C2B-C1B	-2.21	122.05	125.42
11	A	810	CLA	CMB-C2B-C1B	-2.21	122.05	125.42
11	B	809	CLA	C1-C2-C3	-2.21	122.58	126.20
16	A	854	LMU	O5'-C1'-C2'	2.20	114.90	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	823	CLA	CHB-C4A-NA	2.20	127.58	124.40
11	A	807	CLA	O2D-CGD-CBD	2.20	115.08	111.23
11	B	811	CLA	C1-C2-C3	-2.20	122.59	126.20
11	A	818	CLA	CAC-C3C-C4C	2.20	127.65	124.79
11	A	842	CLA	C1-C2-C3	-2.19	122.60	126.20
11	B	804	CLA	C1-C2-C3	-2.19	122.61	126.20
11	A	836	CLA	C3B-C4B-NB	-2.19	108.58	110.53
14	F	801	BCR	C15-C16-C17	2.19	128.00	123.52
11	B	809	CLA	O2D-CGD-CBD	2.19	115.05	111.23
11	J	103	CLA	CMB-C2B-C1B	-2.18	122.09	125.42
11	B	826	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
11	B	823	CLA	C3B-C4B-NB	-2.18	108.58	110.53
11	A	812	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
11	B	841	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
11	B	820	CLA	O2A-CGA-O1A	-2.16	118.21	123.63
11	B	834	CLA	CHB-C4A-NA	2.16	127.52	124.40
11	A	809	CLA	CMB-C2B-C3B	2.16	131.63	126.55
11	B	839	CLA	CHB-C4A-NA	2.16	127.52	124.40
11	A	827	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
11	A	815	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
11	A	821	CLA	CMB-C2B-C1B	-2.16	122.14	125.42
11	B	810	CLA	C1-C2-C3	-2.16	122.67	126.20
14	F	801	BCR	C19-C18-C17	-2.15	115.62	119.01
11	A	803	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
11	B	803	CLA	O1D-CGD-CBD	2.15	128.76	124.52
11	A	836	CLA	CMB-C2B-C1B	-2.15	122.15	125.42
11	A	830	CLA	O2D-CGD-CBD	2.15	114.98	111.23
11	B	804	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
11	B	834	CLA	CAA-CBA-CGA	-2.14	107.12	113.21
11	A	801	CLA	C3D-C4D-ND	-2.14	106.50	109.99
11	B	835	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
11	A	829	CLA	CHB-C4A-NA	2.14	127.49	124.40
11	B	819	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
14	A	850	BCR	C24-C23-C22	-2.14	123.07	126.23
11	B	842	CLA	CMB-C2B-C1B	-2.14	122.17	125.42
11	A	827	CLA	C1-C2-C3	-2.13	122.70	126.20
11	A	815	CLA	O2D-CGD-CBD	2.13	114.96	111.23
11	B	837	CLA	CMB-C2B-C3B	2.13	131.57	126.55
16	A	856	LMU	C1-O1'-C1'	2.13	117.32	113.68
11	A	802	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
16	A	854	LMU	C1B-O5B-C5B	2.13	117.88	113.72
11	A	818	CLA	O2A-CGA-O1A	-2.13	118.31	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	803	CLA	CHB-C4A-NA	2.13	127.47	124.40
11	A	831	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
11	B	816	CLA	C1-C2-C3	-2.12	122.72	126.20
11	B	827	CLA	C1-C2-C3	-2.12	122.72	126.20
11	B	829	CLA	CMB-C2B-C3B	2.12	131.53	126.55
11	B	830	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
11	B	824	CLA	CMB-C2B-C1B	-2.11	122.20	125.42
11	B	838	CLA	CMB-C2B-C1B	-2.11	122.20	125.42
11	B	838	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
11	B	820	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
19	F	805	LUT	C22-C23-C24	2.10	114.31	111.18
11	B	836	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
11	B	837	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
11	A	825	CLA	O2D-CGD-CBD	2.10	114.90	111.23
11	A	841	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
11	B	825	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
11	J	103	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
11	A	830	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
11	A	810	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
11	A	826	CLA	CMB-C2B-C3B	2.10	131.48	126.55
11	B	814	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
11	F	803	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
11	A	805	CLA	C1-C2-C3	-2.08	122.78	126.20
11	B	839	CLA	C3B-C4B-NB	-2.08	108.67	110.53
11	B	810	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
11	A	803	CLA	CMB-C2B-C1B	-2.08	122.26	125.42
11	A	828	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
11	A	817	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
11	A	820	CLA	O2D-CGD-CBD	2.07	114.85	111.23
11	A	823	CLA	C3B-C4B-NB	-2.07	108.69	110.53
11	B	832	CLA	CMB-C2B-C3B	2.07	131.41	126.55
11	A	826	CLA	CAA-CBA-CGA	-2.07	107.34	113.21
11	B	804	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
11	B	819	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
11	A	837	CLA	CMB-C2B-C3B	2.06	131.40	126.55
11	B	808	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
11	A	817	CLA	CMB-C2B-C3B	2.06	131.39	126.55
11	B	816	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
11	A	829	CLA	CMB-C2B-C3B	2.05	131.38	126.55
11	A	824	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
11	B	801	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
11	B	801	CLA	CHB-C4A-NA	2.05	127.36	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	804	CLA	CHB-C4A-NA	2.05	127.36	124.40
11	B	821	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
11	A	812	CLA	CMB-C2B-C3B	2.05	131.37	126.55
14	F	801	BCR	C16-C17-C18	2.05	130.15	127.28
11	B	812	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
11	B	818	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
11	B	827	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
11	A	814	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
11	A	835	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
11	B	806	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
11	B	831	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
11	F	804	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
14	J	104	BCR	C8-C9-C10	-2.04	115.80	119.01
11	A	840	CLA	C1-C2-C3	-2.04	122.86	126.20
11	A	823	CLA	CMB-C2B-C1B	-2.04	122.32	125.42
11	B	801	CLA	C3B-C4B-NB	-2.04	108.71	110.53
11	B	807	CLA	CMB-C2B-C3B	2.03	131.33	126.55
11	B	813	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
12	A	843	PQN	C11-C3-C4	-2.03	116.44	118.58
11	A	816	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
11	A	810	CLA	CMB-C2B-C3B	2.02	131.31	126.55
11	J	103	CLA	CMB-C2B-C3B	2.02	131.31	126.55
11	A	842	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
11	B	808	CLA	C1-C2-C3	-2.02	122.89	126.20
11	B	832	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
11	B	829	CLA	O2A-CGA-O1A	-2.02	118.59	123.63
11	B	805	CLA	O2D-CGD-CBD	2.02	114.75	111.23
19	F	805	LUT	C28-C29-C30	-2.01	115.84	119.01
11	B	820	CLA	C1-C2-C3	-2.01	122.91	126.20
11	A	839	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
11	A	821	CLA	C1-C2-C3	-2.01	122.91	126.20
11	A	832	CLA	CMB-C2B-C3B	2.01	131.27	126.55
11	B	832	CLA	C1-C2-C3	-2.00	122.91	126.20
11	B	801	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
11	B	835	CLA	C1-C2-C3	-2.00	122.92	126.20

All (91) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	A	801	CLA	CBD
11	A	802	CLA	ND
11	A	803	CLA	ND

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Mol	Chain	Res	Type	Atom
11	A	804	CLA	ND
11	A	805	CLA	ND
11	A	806	CLA	ND
11	A	807	CLA	ND
11	A	808	CLA	ND
11	A	809	CLA	ND
11	A	810	CLA	ND
11	A	811	CLA	ND
11	A	812	CLA	ND
11	A	813	CLA	ND
11	A	814	CLA	ND
11	A	815	CLA	ND
11	A	816	CLA	ND
11	A	817	CLA	ND
11	A	818	CLA	ND
11	A	819	CLA	ND
11	A	820	CLA	ND
11	A	821	CLA	ND
11	A	822	CLA	ND
11	A	823	CLA	ND
11	A	824	CLA	ND
11	A	825	CLA	ND
11	A	826	CLA	ND
11	A	827	CLA	ND
11	A	828	CLA	ND
11	A	829	CLA	ND
11	A	830	CLA	ND
11	A	831	CLA	ND
11	A	832	CLA	ND
11	A	833	CLA	ND
11	A	834	CLA	ND
11	A	835	CLA	ND
11	A	836	CLA	ND
11	A	837	CLA	ND
11	A	838	CLA	ND
11	A	839	CLA	ND
11	A	840	CLA	ND
11	A	841	CLA	ND
11	A	842	CLA	ND
11	A	844	CLA	ND
11	B	801	CLA	ND
11	B	802	CLA	ND

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Mol	Chain	Res	Type	Atom
11	B	803	CLA	ND
11	B	804	CLA	ND
11	B	805	CLA	ND
11	B	806	CLA	ND
11	B	807	CLA	ND
11	B	808	CLA	ND
11	B	809	CLA	ND
11	B	810	CLA	ND
11	B	811	CLA	ND
11	B	812	CLA	ND
11	B	813	CLA	ND
11	B	814	CLA	ND
11	B	815	CLA	ND
11	B	816	CLA	ND
11	B	817	CLA	ND
11	B	818	CLA	ND
11	B	819	CLA	ND
11	B	820	CLA	ND
11	B	821	CLA	ND
11	B	822	CLA	ND
11	B	823	CLA	ND
11	B	824	CLA	ND
11	B	825	CLA	ND
11	B	826	CLA	ND
11	B	827	CLA	ND
11	B	828	CLA	ND
11	B	829	CLA	ND
11	B	830	CLA	ND
11	B	831	CLA	ND
11	B	832	CLA	ND
11	B	833	CLA	ND
11	B	834	CLA	ND
11	B	835	CLA	ND
11	B	836	CLA	ND
11	B	837	CLA	ND
11	B	838	CLA	ND
11	B	839	CLA	ND
11	B	840	CLA	ND
11	B	841	CLA	ND
11	B	842	CLA	ND
11	B	852	CLA	ND
11	J	103	CLA	ND

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Mol	Chain	Res	Type	Atom
11	F	803	CLA	ND
11	F	804	CLA	ND
11	L	202	CLA	ND
11	L	203	CLA	ND

All (908) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	805	CLA	C3A-C2A-CAA-CBA
11	A	808	CLA	CHA-CBD-CGD-O1D
11	A	808	CLA	CHA-CBD-CGD-O2D
11	A	815	CLA	CHA-CBD-CGD-O1D
11	A	815	CLA	CHA-CBD-CGD-O2D
11	A	816	CLA	CHA-CBD-CGD-O1D
11	A	816	CLA	CHA-CBD-CGD-O2D
11	A	818	CLA	C1A-C2A-CAA-CBA
11	A	818	CLA	C3A-C2A-CAA-CBA
11	A	822	CLA	CHA-CBD-CGD-O1D
11	A	822	CLA	CHA-CBD-CGD-O2D
11	A	825	CLA	CHA-CBD-CGD-O1D
11	A	825	CLA	CHA-CBD-CGD-O2D
11	A	828	CLA	CBD-CGD-O2D-CED
11	A	830	CLA	CHA-CBD-CGD-O1D
11	A	830	CLA	CHA-CBD-CGD-O2D
11	A	833	CLA	C4B-C3B-CAB-CBB
11	A	834	CLA	CHA-CBD-CGD-O1D
11	A	834	CLA	CHA-CBD-CGD-O2D
11	A	837	CLA	C1A-C2A-CAA-CBA
11	A	840	CLA	C4B-C3B-CAB-CBB
11	B	806	CLA	C3A-C2A-CAA-CBA
11	B	809	CLA	CHA-CBD-CGD-O1D
11	B	809	CLA	CHA-CBD-CGD-O2D
11	B	814	CLA	C1A-C2A-CAA-CBA
11	B	814	CLA	C3A-C2A-CAA-CBA
11	B	816	CLA	CBD-CGD-O2D-CED
11	B	818	CLA	C3A-C2A-CAA-CBA
11	B	822	CLA	CHA-CBD-CGD-O1D
11	B	822	CLA	CHA-CBD-CGD-O2D
11	B	824	CLA	C3A-C2A-CAA-CBA
11	B	826	CLA	C1A-C2A-CAA-CBA
11	B	826	CLA	CHA-CBD-CGD-O1D
11	B	826	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
11	B	830	CLA	CHA-CBD-CGD-O1D
11	B	830	CLA	CHA-CBD-CGD-O2D
11	B	834	CLA	CHA-CBD-CGD-O1D
11	B	834	CLA	CHA-CBD-CGD-O2D
11	B	834	CLA	C4-C3-C5-C6
11	B	835	CLA	C1A-C2A-CAA-CBA
11	B	836	CLA	C1A-C2A-CAA-CBA
11	B	841	CLA	C1A-C2A-CAA-CBA
11	B	841	CLA	C3A-C2A-CAA-CBA
11	B	842	CLA	C3A-C2A-CAA-CBA
11	B	852	CLA	C1A-C2A-CAA-CBA
11	B	852	CLA	CAD-CBD-CGD-O2D
11	L	202	CLA	C1A-C2A-CAA-CBA
11	L	203	CLA	CHA-CBD-CGD-O1D
11	L	203	CLA	CHA-CBD-CGD-O2D
13	A	845	LHG	C3-O3-P-O5
13	A	846	LHG	C3-O3-P-O5
13	B	850	LHG	C3-O3-P-O4
13	B	850	LHG	C3-O3-P-O6
14	A	849	BCR	C11-C12-C13-C14
14	A	850	BCR	C23-C24-C25-C26
14	B	844	BCR	C7-C8-C9-C10
14	B	844	BCR	C7-C8-C9-C34
14	B	844	BCR	C11-C12-C13-C14
14	B	844	BCR	C21-C22-C23-C24
14	J	104	BCR	C17-C18-C19-C20
14	J	104	BCR	C36-C18-C19-C20
14	J	104	BCR	C21-C22-C23-C24
14	F	801	BCR	C11-C12-C13-C14
14	L	204	BCR	C7-C8-C9-C10
14	L	204	BCR	C37-C22-C23-C24
14	L	204	BCR	C23-C24-C25-C26
14	L	204	BCR	C23-C24-C25-C30
16	A	854	LMU	C2'-C1'-O1'-C1
16	A	854	LMU	C2-C1-O1'-C1'
16	A	856	LMU	C2-C1-O1'-C1'
17	A	855	LMG	O6-C1-O1-C7
17	B	851	LMG	C2-C1-O1-C7
17	B	851	LMG	O6-C1-O1-C7
18	B	849	DGD	C2D-C1D-O3G-C3G
18	B	849	DGD	O6D-C1D-O3G-C3G
19	J	101	LUT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	J	101	LUT	C6-C7-C8-C9
19	J	101	LUT	C25-C26-C27-C28
19	F	805	LUT	C6-C7-C8-C9
19	F	805	LUT	C27-C28-C29-C30
20	T	200	HEC	C2B-C3B-CAB-CBB
20	T	200	HEC	C4B-C3B-CAB-CBB
20	T	200	HEC	C2C-C3C-CAC-CBC
11	A	802	CLA	CBD-CGD-O2D-CED
11	A	831	CLA	CBD-CGD-O2D-CED
11	B	815	CLA	CBD-CGD-O2D-CED
11	B	820	CLA	CBD-CGD-O2D-CED
11	B	823	CLA	CBD-CGD-O2D-CED
11	F	803	CLA	CBD-CGD-O2D-CED
11	B	823	CLA	O1D-CGD-O2D-CED
11	B	816	CLA	O1D-CGD-O2D-CED
11	A	805	CLA	C3-C5-C6-C7
11	A	806	CLA	C3-C5-C6-C7
11	A	809	CLA	C3-C5-C6-C7
11	B	802	CLA	C3-C5-C6-C7
11	A	805	CLA	CBD-CGD-O2D-CED
11	A	815	CLA	CBD-CGD-O2D-CED
11	B	818	CLA	CBD-CGD-O2D-CED
11	B	828	CLA	CBD-CGD-O2D-CED
11	B	804	CLA	C2C-C3C-CAC-CBC
11	A	828	CLA	O1D-CGD-O2D-CED
11	B	817	CLA	C4-C3-C5-C6
11	B	817	CLA	C2-C3-C5-C6
11	B	834	CLA	C2-C3-C5-C6
11	A	813	CLA	CBD-CGD-O2D-CED
11	B	815	CLA	O1D-CGD-O2D-CED
11	A	842	CLA	C2A-CAA-CBA-CGA
11	B	825	CLA	C2A-CAA-CBA-CGA
11	A	842	CLA	C3-C5-C6-C7
14	F	801	BCR	C15-C16-C17-C18
11	A	831	CLA	C3-C5-C6-C7
11	J	103	CLA	C3-C5-C6-C7
11	A	844	CLA	CBD-CGD-O2D-CED
11	L	203	CLA	CBD-CGD-O2D-CED
11	F	803	CLA	O1D-CGD-O2D-CED
11	A	811	CLA	CBA-CGA-O2A-C1
17	B	851	LMG	O6-C5-C6-O5
11	A	831	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	A	802	CLA	O1D-CGD-O2D-CED
11	B	809	CLA	C3-C5-C6-C7
11	B	821	CLA	C3-C5-C6-C7
11	A	814	CLA	CBD-CGD-O2D-CED
11	A	820	CLA	CBD-CGD-O2D-CED
11	A	841	CLA	CBD-CGD-O2D-CED
11	B	824	CLA	CBD-CGD-O2D-CED
11	L	202	CLA	CBD-CGD-O2D-CED
11	B	820	CLA	O1D-CGD-O2D-CED
11	J	103	CLA	C2-C3-C5-C6
11	A	822	CLA	CBD-CGD-O2D-CED
17	B	851	LMG	C4-C5-C6-O5
11	A	811	CLA	O1A-CGA-O2A-C1
16	A	854	LMU	O5'-C1'-O1'-C1
11	A	804	CLA	CBD-CGD-O2D-CED
11	A	806	CLA	CBD-CGD-O2D-CED
11	A	810	CLA	CBD-CGD-O2D-CED
11	A	818	CLA	CBD-CGD-O2D-CED
11	A	823	CLA	CBD-CGD-O2D-CED
11	A	839	CLA	CBD-CGD-O2D-CED
11	B	802	CLA	CBD-CGD-O2D-CED
11	B	821	CLA	CBD-CGD-O2D-CED
11	B	805	CLA	CBD-CGD-O2D-CED
11	B	807	CLA	CBD-CGD-O2D-CED
11	B	836	CLA	CBD-CGD-O2D-CED
11	B	842	CLA	CBD-CGD-O2D-CED
11	A	816	CLA	CBA-CGA-O2A-C1
11	A	842	CLA	CBA-CGA-O2A-C1
11	B	838	CLA	CBA-CGA-O2A-C1
11	B	852	CLA	CBA-CGA-O2A-C1
11	A	824	CLA	CBD-CGD-O2D-CED
11	J	103	CLA	C4-C3-C5-C6
11	L	202	CLA	C4-C3-C5-C6
11	A	811	CLA	CBD-CGD-O2D-CED
11	A	817	CLA	CBD-CGD-O2D-CED
11	B	804	CLA	C14-C13-C15-C16
11	B	820	CLA	C6-C7-C8-C9
11	B	826	CLA	C6-C7-C8-C9
11	B	829	CLA	C11-C12-C13-C14
11	B	818	CLA	O1D-CGD-O2D-CED
17	A	855	LMG	C2-C1-O1-C7
11	A	815	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	A	842	CLA	O1A-CGA-O2A-C1
14	A	849	BCR	C11-C12-C13-C35
14	A	850	BCR	C37-C22-C23-C24
14	A	851	BCR	C7-C8-C9-C34
14	B	844	BCR	C11-C12-C13-C35
14	B	844	BCR	C37-C22-C23-C24
14	J	104	BCR	C37-C22-C23-C24
14	F	801	BCR	C11-C12-C13-C35
14	L	204	BCR	C7-C8-C9-C34
19	J	101	LUT	C7-C8-C9-C19
19	F	805	LUT	C27-C28-C29-C39
14	A	850	BCR	C21-C22-C23-C24
14	L	204	BCR	C21-C22-C23-C24
11	B	852	CLA	O1A-CGA-O2A-C1
11	B	810	CLA	C13-C15-C16-C17
11	A	807	CLA	CBD-CGD-O2D-CED
11	B	801	CLA	CBD-CGD-O2D-CED
11	B	806	CLA	C15-C16-C17-C18
11	A	821	CLA	C15-C16-C17-C18
11	A	805	CLA	O1D-CGD-O2D-CED
11	A	808	CLA	CBD-CGD-O2D-CED
11	B	804	CLA	C4C-C3C-CAC-CBC
11	A	802	CLA	C12-C13-C15-C16
11	A	805	CLA	C11-C12-C13-C15
11	B	828	CLA	C6-C7-C8-C10
11	L	202	CLA	C11-C12-C13-C15
13	B	850	LHG	C24-C23-O8-C6
11	B	804	CLA	C13-C15-C16-C17
11	B	852	CLA	C15-C16-C17-C18
11	B	811	CLA	CBD-CGD-O2D-CED
11	B	810	CLA	CBA-CGA-O2A-C1
11	A	824	CLA	C5-C6-C7-C8
11	B	818	CLA	C13-C15-C16-C17
11	B	838	CLA	C5-C6-C7-C8
11	B	842	CLA	C10-C11-C12-C13
11	B	852	CLA	C13-C15-C16-C17
11	A	808	CLA	C2A-CAA-CBA-CGA
11	A	829	CLA	C2A-CAA-CBA-CGA
11	B	823	CLA	C2A-CAA-CBA-CGA
11	B	840	CLA	C2A-CAA-CBA-CGA
11	B	852	CLA	C2A-CAA-CBA-CGA
11	A	804	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
11	B	811	CLA	C10-C11-C12-C13
11	B	826	CLA	C13-C15-C16-C17
11	B	828	CLA	C13-C15-C16-C17
11	B	837	CLA	C5-C6-C7-C8
11	B	837	CLA	C10-C11-C12-C13
11	B	842	CLA	C8-C10-C11-C12
11	F	803	CLA	C13-C15-C16-C17
16	A	854	LMU	O5B-C5B-C6B-O6B
13	A	846	LHG	C23-C24-C25-C26
13	B	850	LHG	C7-C8-C9-C10
11	A	805	CLA	C8-C10-C11-C12
11	A	818	CLA	C10-C11-C12-C13
11	A	819	CLA	C15-C16-C17-C18
11	A	827	CLA	C15-C16-C17-C18
11	A	834	CLA	C13-C15-C16-C17
11	A	838	CLA	C8-C10-C11-C12
11	B	812	CLA	C15-C16-C17-C18
11	B	814	CLA	C10-C11-C12-C13
11	B	819	CLA	C15-C16-C17-C18
11	B	841	CLA	C5-C6-C7-C8
11	B	841	CLA	C13-C15-C16-C17
11	B	842	CLA	C13-C15-C16-C17
11	B	852	CLA	C5-C6-C7-C8
11	B	829	CLA	CBA-CGA-O2A-C1
11	A	816	CLA	O1A-CGA-O2A-C1
11	B	838	CLA	O1A-CGA-O2A-C1
11	L	203	CLA	O1D-CGD-O2D-CED
11	A	813	CLA	O1D-CGD-O2D-CED
11	B	828	CLA	O1D-CGD-O2D-CED
11	A	828	CLA	C5-C6-C7-C8
11	A	831	CLA	C5-C6-C7-C8
11	A	838	CLA	C10-C11-C12-C13
11	B	824	CLA	C13-C15-C16-C17
11	B	828	CLA	CBA-CGA-O2A-C1
11	J	103	CLA	CBA-CGA-O2A-C1
17	J	102	LMG	C29-C28-O8-C9
17	J	102	LMG	C11-C10-O7-C8
17	F	802	LMG	C11-C10-O7-C8
17	J	102	LMG	O9-C10-O7-C8
17	F	802	LMG	O9-C10-O7-C8
11	B	832	CLA	C2A-CAA-CBA-CGA
11	A	804	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
11	A	834	CLA	CBA-CGA-O2A-C1
11	B	839	CLA	CBA-CGA-O2A-C1
11	A	805	CLA	C10-C11-C12-C13
11	A	813	CLA	C15-C16-C17-C18
11	A	844	CLA	O1D-CGD-O2D-CED
11	A	811	CLA	C13-C15-C16-C17
11	B	802	CLA	C5-C6-C7-C8
11	B	820	CLA	C8-C10-C11-C12
11	B	837	CLA	CBA-CGA-O2A-C1
11	B	817	CLA	C3-C5-C6-C7
11	A	820	CLA	O1D-CGD-O2D-CED
11	B	824	CLA	O1D-CGD-O2D-CED
11	B	810	CLA	O1A-CGA-O2A-C1
19	J	101	LUT	C20-C13-C14-C15
11	A	828	CLA	C8-C10-C11-C12
11	B	817	CLA	C5-C6-C7-C8
14	B	847	BCR	C37-C22-C23-C24
14	I	201	BCR	C7-C8-C9-C34
14	I	201	BCR	C11-C12-C13-C35
14	I	201	BCR	C7-C8-C9-C10
11	B	828	CLA	O1A-CGA-O2A-C1
13	B	850	LHG	O10-C23-O8-C6
11	A	824	CLA	C2A-CAA-CBA-CGA
11	B	836	CLA	C2A-CAA-CBA-CGA
11	L	202	CLA	C10-C11-C12-C13
11	L	202	CLA	O1D-CGD-O2D-CED
11	B	808	CLA	C6-C7-C8-C9
11	B	810	CLA	C16-C17-C18-C19
11	A	814	CLA	O1D-CGD-O2D-CED
11	A	841	CLA	O1D-CGD-O2D-CED
11	B	829	CLA	O1A-CGA-O2A-C1
11	B	852	CLA	C3-C5-C6-C7
19	F	805	LUT	C28-C29-C30-C31
11	L	202	CLA	C2-C3-C5-C6
11	B	821	CLA	CBA-CGA-O2A-C1
11	A	827	CLA	C10-C11-C12-C13
11	B	810	CLA	C16-C17-C18-C20
11	A	834	CLA	O1A-CGA-O2A-C1
11	A	817	CLA	C10-C11-C12-C13
11	A	806	CLA	O1D-CGD-O2D-CED
11	A	822	CLA	O1D-CGD-O2D-CED
11	J	103	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	J	102	LMG	O10-C28-O8-C9
11	B	830	CLA	CBA-CGA-O2A-C1
18	B	849	DGD	C6A-C7A-C8A-C9A
11	A	841	CLA	C4B-C3B-CAB-CBB
11	B	821	CLA	O1D-CGD-O2D-CED
11	A	814	CLA	C5-C6-C7-C8
11	B	826	CLA	C6-C7-C8-C10
17	J	102	LMG	C11-C12-C13-C14
11	A	837	CLA	C3A-C2A-CAA-CBA
11	B	826	CLA	C3A-C2A-CAA-CBA
11	A	810	CLA	O1D-CGD-O2D-CED
11	B	812	CLA	C10-C11-C12-C13
11	B	814	CLA	C8-C10-C11-C12
11	A	818	CLA	O1D-CGD-O2D-CED
11	A	804	CLA	O1A-CGA-O2A-C1
11	B	839	CLA	O1A-CGA-O2A-C1
11	A	842	CLA	C8-C10-C11-C12
17	J	105	LMG	C15-C16-C17-C18
18	B	849	DGD	C9B-CAB-CBB-CCB
11	B	837	CLA	O1A-CGA-O2A-C1
18	B	849	DGD	C2B-C3B-C4B-C5B
11	A	804	CLA	O1D-CGD-O2D-CED
11	A	823	CLA	O1D-CGD-O2D-CED
11	A	833	CLA	C2B-C3B-CAB-CBB
11	A	840	CLA	C2B-C3B-CAB-CBB
11	A	841	CLA	C2B-C3B-CAB-CBB
14	A	850	BCR	C23-C24-C25-C30
14	B	844	BCR	C1-C6-C7-C8
14	B	844	BCR	C5-C6-C7-C8
14	I	201	BCR	C1-C6-C7-C8
14	F	801	BCR	C23-C24-C25-C26
14	L	201	BCR	C1-C6-C7-C8
14	L	201	BCR	C5-C6-C7-C8
13	A	845	LHG	C29-C30-C31-C32
11	B	821	CLA	O1A-CGA-O2A-C1
13	B	850	LHG	C11-C10-C9-C8
11	A	813	CLA	CBA-CGA-O2A-C1
11	A	835	CLA	CBA-CGA-O2A-C1
11	B	812	CLA	CBA-CGA-O2A-C1
11	B	841	CLA	CBA-CGA-O2A-C1
11	B	830	CLA	C14-C13-C15-C16
11	A	839	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	A	846	LHG	C11-C10-C9-C8
11	A	835	CLA	C3-C5-C6-C7
11	B	808	CLA	C6-C7-C8-C10
13	A	846	LHG	C8-C7-O7-C5
13	A	846	LHG	O9-C7-O7-C5
14	A	851	BCR	C37-C22-C23-C24
11	A	809	CLA	C2A-CAA-CBA-CGA
11	A	821	CLA	C2A-CAA-CBA-CGA
11	B	821	CLA	C11-C10-C8-C9
11	A	824	CLA	C4-C3-C5-C6
11	B	837	CLA	C4-C3-C5-C6
11	B	802	CLA	O1D-CGD-O2D-CED
11	B	807	CLA	O1D-CGD-O2D-CED
11	A	810	CLA	C5-C6-C7-C8
11	B	841	CLA	C15-C16-C17-C18
11	B	830	CLA	O1A-CGA-O2A-C1
11	A	802	CLA	C15-C16-C17-C18
11	B	840	CLA	C15-C16-C17-C18
17	F	802	LMG	O6-C5-C6-O5
11	A	808	CLA	C10-C11-C12-C13
11	B	836	CLA	O1D-CGD-O2D-CED
11	B	814	CLA	CBD-CGD-O2D-CED
11	B	842	CLA	O1D-CGD-O2D-CED
11	B	805	CLA	O1D-CGD-O2D-CED
17	B	851	LMG	C35-C36-C37-C38
17	J	105	LMG	C4-C5-C6-O5
11	A	840	CLA	C2-C3-C5-C6
11	B	837	CLA	C2-C3-C5-C6
11	A	822	CLA	C2A-CAA-CBA-CGA
11	B	801	CLA	C2A-CAA-CBA-CGA
11	B	804	CLA	C2A-CAA-CBA-CGA
11	F	804	CLA	C2A-CAA-CBA-CGA
11	A	824	CLA	CBA-CGA-O2A-C1
17	F	802	LMG	C30-C31-C32-C33
11	A	817	CLA	O1D-CGD-O2D-CED
11	A	824	CLA	O1D-CGD-O2D-CED
11	B	826	CLA	C16-C17-C18-C20
11	A	813	CLA	O1A-CGA-O2A-C1
11	A	805	CLA	C1A-C2A-CAA-CBA
11	A	822	CLA	C1A-C2A-CAA-CBA
11	A	824	CLA	C1A-C2A-CAA-CBA
11	A	830	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
11	B	806	CLA	C1A-C2A-CAA-CBA
11	B	818	CLA	C1A-C2A-CAA-CBA
11	B	824	CLA	C1A-C2A-CAA-CBA
11	B	842	CLA	C1A-C2A-CAA-CBA
11	J	103	CLA	C1A-C2A-CAA-CBA
11	A	835	CLA	O1A-CGA-O2A-C1
11	B	812	CLA	O1A-CGA-O2A-C1
11	B	841	CLA	O1A-CGA-O2A-C1
11	A	810	CLA	C11-C10-C8-C7
11	A	828	CLA	C6-C7-C8-C10
11	A	839	CLA	C12-C13-C15-C16
11	B	819	CLA	C11-C12-C13-C15
11	B	821	CLA	C6-C7-C8-C10
11	B	826	CLA	C11-C10-C8-C7
11	B	829	CLA	C12-C13-C15-C16
11	B	833	CLA	C6-C7-C8-C10
11	B	833	CLA	C11-C10-C8-C7
11	B	840	CLA	C6-C7-C8-C10
11	L	202	CLA	C6-C7-C8-C10
17	J	105	LMG	C28-C29-C30-C31
11	B	852	CLA	C4-C3-C5-C6
11	A	819	CLA	C2-C3-C5-C6
11	A	827	CLA	C2-C3-C5-C6
11	B	852	CLA	C2-C3-C5-C6
11	A	812	CLA	C2A-CAA-CBA-CGA
11	A	802	CLA	C14-C13-C15-C16
11	A	838	CLA	C14-C13-C15-C16
11	A	839	CLA	C6-C7-C8-C9
11	A	839	CLA	C14-C13-C15-C16
11	B	821	CLA	C6-C7-C8-C9
11	B	828	CLA	C14-C13-C15-C16
11	B	833	CLA	C11-C10-C8-C9
11	B	840	CLA	C6-C7-C8-C9
11	L	202	CLA	C6-C7-C8-C9
13	A	845	LHG	C14-C15-C16-C17
11	A	808	CLA	O1D-CGD-O2D-CED
11	B	816	CLA	CBA-CGA-O2A-C1
17	A	855	LMG	O6-C5-C6-O5
11	A	811	CLA	O1D-CGD-O2D-CED
11	B	801	CLA	O1D-CGD-O2D-CED
11	A	826	CLA	CBD-CGD-O2D-CED
11	A	826	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	B	849	DGD	O6E-C5E-C6E-O5E
11	B	826	CLA	C16-C17-C18-C19
11	A	807	CLA	O1D-CGD-O2D-CED
11	B	811	CLA	O1D-CGD-O2D-CED
16	A	854	LMU	O5'-C5'-C6'-O6'
16	A	854	LMU	C2-C3-C4-C5
18	B	849	DGD	CEB-CFB-CGB-CHB
11	A	819	CLA	C4-C3-C5-C6
11	A	827	CLA	C4-C3-C5-C6
11	A	840	CLA	C4-C3-C5-C6
11	B	816	CLA	C5-C6-C7-C8
11	B	818	CLA	C15-C16-C17-C18
14	A	851	BCR	C7-C8-C9-C10
14	I	201	BCR	C11-C12-C13-C14
16	A	854	LMU	C7-C8-C9-C10
11	A	824	CLA	O1A-CGA-O2A-C1
17	F	802	LMG	C29-C28-O8-C9
11	B	816	CLA	C15-C16-C17-C18
17	J	105	LMG	C14-C15-C16-C17
11	A	834	CLA	C5-C6-C7-C8
11	B	802	CLA	C2-C3-C5-C6
17	J	105	LMG	O6-C5-C6-O5
17	J	105	LMG	C19-C20-C21-C22
18	B	849	DGD	C6B-C7B-C8B-C9B
16	A	854	LMU	C11-C10-C9-C8
11	B	833	CLA	C5-C6-C7-C8
11	B	852	CLA	C8-C10-C11-C12
11	B	806	CLA	CBA-CGA-O2A-C1
17	J	102	LMG	C13-C14-C15-C16
17	A	855	LMG	C14-C15-C16-C17
11	B	802	CLA	C4-C3-C5-C6
11	B	806	CLA	C4-C3-C5-C6
17	J	105	LMG	C18-C19-C20-C21
16	A	853	LMU	C2-C1-O1'-C1'
11	A	805	CLA	C11-C12-C13-C14
11	A	805	CLA	C14-C13-C15-C16
11	A	810	CLA	C11-C10-C8-C9
11	A	828	CLA	C6-C7-C8-C9
11	A	838	CLA	C6-C7-C8-C9
11	B	809	CLA	C6-C7-C8-C9
11	B	826	CLA	C11-C10-C8-C9
11	B	828	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
11	B	829	CLA	C14-C13-C15-C16
11	B	833	CLA	C6-C7-C8-C9
11	B	835	CLA	C11-C10-C8-C9
11	B	852	CLA	C6-C7-C8-C9
11	A	818	CLA	C8-C10-C11-C12
11	A	808	CLA	C4B-C3B-CAB-CBB
11	A	834	CLA	C4B-C3B-CAB-CBB
11	B	822	CLA	C4B-C3B-CAB-CBB
11	B	834	CLA	C8-C10-C11-C12
11	B	829	CLA	C3-C5-C6-C7
11	A	813	CLA	C6-C7-C8-C10
11	A	827	CLA	C11-C12-C13-C15
11	A	838	CLA	C6-C7-C8-C10
11	A	838	CLA	C12-C13-C15-C16
11	A	839	CLA	C6-C7-C8-C10
11	A	840	CLA	C11-C10-C8-C7
11	B	809	CLA	C6-C7-C8-C10
11	B	819	CLA	C6-C7-C8-C10
11	B	828	CLA	C12-C13-C15-C16
11	B	835	CLA	C11-C10-C8-C7
11	B	852	CLA	C6-C7-C8-C10
11	B	824	CLA	C4-C3-C5-C6
11	B	829	CLA	C4-C3-C5-C6
11	B	835	CLA	C3A-C2A-CAA-CBA
11	B	836	CLA	C3A-C2A-CAA-CBA
11	L	202	CLA	C3A-C2A-CAA-CBA
11	A	830	CLA	C10-C11-C12-C13
11	B	819	CLA	C2-C3-C5-C6
11	A	826	CLA	O1A-CGA-O2A-C1
11	B	816	CLA	O1A-CGA-O2A-C1
11	B	820	CLA	CBA-CGA-O2A-C1
11	A	809	CLA	C16-C17-C18-C19
11	A	828	CLA	C16-C17-C18-C19
11	A	809	CLA	C10-C11-C12-C13
11	A	823	CLA	C2A-CAA-CBA-CGA
11	B	810	CLA	C2A-CAA-CBA-CGA
17	J	102	LMG	O1-C7-C8-C9
17	F	802	LMG	O1-C7-C8-C9
11	B	819	CLA	C4-C3-C5-C6
11	B	806	CLA	C2-C3-C5-C6
11	B	824	CLA	C2-C3-C5-C6
11	B	829	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
17	F	802	LMG	O10-C28-O8-C9
11	A	840	CLA	C8-C10-C11-C12
19	J	101	LUT	C1-C6-C7-C8
17	A	855	LMG	C34-C35-C36-C37
11	B	842	CLA	C15-C16-C17-C18
11	A	830	CLA	CBD-CGD-O2D-CED
13	B	850	LHG	C10-C11-C12-C13
14	A	849	BCR	C9-C10-C11-C12
17	J	102	LMG	C30-C31-C32-C33
11	A	826	CLA	C14-C13-C15-C16
11	A	827	CLA	C11-C12-C13-C14
11	B	814	CLA	C11-C10-C8-C9
11	B	828	CLA	C11-C10-C8-C9
11	B	852	CLA	C11-C12-C13-C14
13	A	845	LHG	C23-C24-C25-C26
11	A	802	CLA	C8-C10-C11-C12
11	A	820	CLA	C1A-C2A-CAA-CBA
11	L	202	CLA	C2A-CAA-CBA-CGA
11	B	835	CLA	C8-C10-C11-C12
13	A	846	LHG	C7-C8-C9-C10
11	L	202	CLA	CBA-CGA-O2A-C1
13	B	850	LHG	O7-C7-C8-C9
11	A	830	CLA	C13-C15-C16-C17
11	A	811	CLA	C15-C16-C17-C18
17	B	851	LMG	C29-C30-C31-C32
16	A	856	LMU	C4'-C5'-C6'-O6'
11	A	817	CLA	C11-C10-C8-C7
11	A	826	CLA	C12-C13-C15-C16
11	B	802	CLA	C11-C10-C8-C7
11	B	802	CLA	C12-C13-C15-C16
11	B	804	CLA	C11-C10-C8-C7
11	B	814	CLA	C11-C10-C8-C7
11	B	824	CLA	C11-C12-C13-C15
11	B	827	CLA	C12-C13-C15-C16
11	B	828	CLA	C11-C10-C8-C7
11	B	830	CLA	C11-C12-C13-C15
11	B	842	CLA	C12-C13-C15-C16
11	B	852	CLA	C11-C10-C8-C7
11	F	803	CLA	C11-C12-C13-C15
18	B	849	DGD	C8B-C9B-CAB-CBB
11	B	827	CLA	C13-C15-C16-C17
14	B	847	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
11	B	814	CLA	O1D-CGD-O2D-CED
11	A	805	CLA	C5-C6-C7-C8
11	A	828	CLA	C16-C17-C18-C20
11	B	806	CLA	O1A-CGA-O2A-C1
11	B	820	CLA	C3-C5-C6-C7
11	B	842	CLA	CBA-CGA-O2A-C1
11	B	810	CLA	C5-C6-C7-C8
13	B	850	LHG	C29-C30-C31-C32
11	A	809	CLA	C16-C17-C18-C20
11	A	824	CLA	C2-C3-C5-C6
11	B	828	CLA	C15-C16-C17-C18
11	B	807	CLA	C3-C5-C6-C7
17	F	802	LMG	O1-C7-C8-O7
11	B	812	CLA	C5-C6-C7-C8
11	B	804	CLA	C11-C10-C8-C9
11	B	812	CLA	C6-C7-C8-C9
11	B	830	CLA	C11-C12-C13-C14
11	B	852	CLA	C11-C10-C8-C9
11	F	803	CLA	C11-C12-C13-C14
11	B	820	CLA	O1A-CGA-O2A-C1
11	L	202	CLA	O1A-CGA-O2A-C1
11	B	802	CLA	C15-C16-C17-C18
11	B	803	CLA	C15-C16-C17-C18
11	B	842	CLA	C3-C5-C6-C7
17	B	851	LMG	C11-C10-O7-C8
16	A	856	LMU	C5-C6-C7-C8
11	B	827	CLA	CBA-CGA-O2A-C1
17	J	102	LMG	C12-C13-C14-C15
16	A	854	LMU	C1-C2-C3-C4
11	A	806	CLA	C4B-C3B-CAB-CBB
11	A	818	CLA	C4B-C3B-CAB-CBB
11	A	822	CLA	C4B-C3B-CAB-CBB
11	A	844	CLA	C1A-C2A-CAA-CBA
11	B	802	CLA	C1A-C2A-CAA-CBA
11	B	818	CLA	C4B-C3B-CAB-CBB
11	B	840	CLA	C4B-C3B-CAB-CBB
11	B	841	CLA	C4B-C3B-CAB-CBB
11	A	829	CLA	C4-C3-C5-C6
11	B	811	CLA	C4-C3-C5-C6
11	B	821	CLA	C4-C3-C5-C6
12	A	843	PQN	C26-C27-C28-C29
13	B	850	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
17	A	855	LMG	C13-C14-C15-C16
11	B	806	CLA	CBD-CGD-O2D-CED
11	A	833	CLA	C8-C10-C11-C12
11	A	808	CLA	C12-C13-C15-C16
11	A	825	CLA	C11-C12-C13-C15
11	B	809	CLA	C11-C12-C13-C15
11	B	829	CLA	C11-C12-C13-C15
11	B	833	CLA	C11-C12-C13-C15
11	L	202	CLA	C12-C13-C15-C16
11	B	824	CLA	CBA-CGA-O2A-C1
13	B	850	LHG	C16-C17-C18-C19
11	B	842	CLA	O1A-CGA-O2A-C1
11	A	826	CLA	O1D-CGD-O2D-CED
20	T	200	HEC	C4C-C3C-CAC-CBC
17	B	851	LMG	O9-C10-O7-C8
11	A	840	CLA	C11-C10-C8-C9
11	B	819	CLA	C6-C7-C8-C9
11	B	824	CLA	C11-C12-C13-C14
11	B	842	CLA	C14-C13-C15-C16
11	B	827	CLA	O1A-CGA-O2A-C1
14	J	104	BCR	C19-C20-C21-C22
11	B	802	CLA	C16-C17-C18-C19
11	A	830	CLA	O1D-CGD-O2D-CED
11	A	834	CLA	C3-C5-C6-C7
17	A	855	LMG	O7-C8-C9-O8
17	J	102	LMG	O1-C7-C8-O7
11	B	801	CLA	C10-C11-C12-C13
11	B	841	CLA	CBD-CGD-O2D-CED
11	A	831	CLA	CAD-CBD-CGD-O2D
11	A	844	CLA	CAD-CBD-CGD-O2D
11	B	824	CLA	O1A-CGA-O2A-C1
11	A	811	CLA	CHA-CBD-CGD-O1D
11	A	811	CLA	CHA-CBD-CGD-O2D
11	A	820	CLA	CHA-CBD-CGD-O1D
11	A	820	CLA	CHA-CBD-CGD-O2D
11	A	831	CLA	CAD-CBD-CGD-O1D
11	A	844	CLA	CAD-CBD-CGD-O1D
11	B	825	CLA	CHA-CBD-CGD-O1D
11	B	825	CLA	CHA-CBD-CGD-O2D
11	B	852	CLA	CAD-CBD-CGD-O1D
14	A	850	BCR	C19-C20-C21-C22
16	A	856	LMU	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
11	B	810	CLA	C8-C10-C11-C12
11	A	818	CLA	C2B-C3B-CAB-CBB
11	B	818	CLA	C2B-C3B-CAB-CBB
11	B	840	CLA	C2B-C3B-CAB-CBB
11	A	835	CLA	C16-C17-C18-C20
14	A	851	BCR	C21-C22-C23-C24
18	B	849	DGD	C1G-C2G-O2G-C1B
18	B	849	DGD	CAB-CBB-CCB-CDB
11	B	821	CLA	C2-C3-C5-C6
14	B	845	BCR	C9-C10-C11-C12
11	B	819	CLA	C5-C6-C7-C8
11	A	802	CLA	C11-C10-C8-C9
11	A	813	CLA	C6-C7-C8-C9
11	A	828	CLA	C11-C12-C13-C14
11	B	802	CLA	C11-C10-C8-C9
11	B	802	CLA	C14-C13-C15-C16
11	B	827	CLA	C14-C13-C15-C16
11	L	202	CLA	C11-C12-C13-C14
11	B	807	CLA	C6-C7-C8-C10
11	B	807	CLA	C11-C12-C13-C15
11	B	815	CLA	C6-C7-C8-C10
11	B	840	CLA	C11-C12-C13-C15
11	A	818	CLA	C2A-CAA-CBA-CGA
11	A	818	CLA	CBA-CGA-O2A-C1
11	A	818	CLA	CAA-CBA-CGA-O2A
11	B	806	CLA	O1D-CGD-O2D-CED
11	A	818	CLA	C2C-C3C-CAC-CBC
11	B	825	CLA	C16-C17-C18-C19
11	B	825	CLA	CBA-CGA-O2A-C1
18	B	849	DGD	CCB-CDB-CEB-CFB
14	A	847	BCR	C37-C22-C23-C24
17	J	102	LMG	C8-C7-O1-C1
11	B	803	CLA	C5-C6-C7-C8
11	A	837	CLA	C2A-CAA-CBA-CGA
11	B	808	CLA	C2A-CAA-CBA-CGA
11	B	811	CLA	C2A-CAA-CBA-CGA
11	B	824	CLA	C3-C5-C6-C7
11	A	829	CLA	C2-C3-C5-C6
16	A	854	LMU	C4B-C5B-C6B-O6B
11	B	825	CLA	O1A-CGA-O2A-C1
11	B	808	CLA	C3-C5-C6-C7
11	A	813	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
11	J	103	CLA	C6-C7-C8-C10
11	A	825	CLA	C11-C12-C13-C14
11	B	809	CLA	C11-C12-C13-C14
11	B	826	CLA	C11-C12-C13-C14
11	L	202	CLA	C14-C13-C15-C16
11	B	803	CLA	C4B-C3B-CAB-CBB
11	B	812	CLA	C4B-C3B-CAB-CBB
11	A	818	CLA	O1A-CGA-O2A-C1
11	A	830	CLA	C8-C10-C11-C12
11	B	812	CLA	C4-C3-C5-C6
17	B	851	LMG	O7-C10-C11-C12
11	B	841	CLA	O1D-CGD-O2D-CED
11	A	840	CLA	C11-C12-C13-C15
11	A	809	CLA	C13-C15-C16-C17
16	A	856	LMU	C2-C3-C4-C5
11	B	820	CLA	C10-C11-C12-C13
11	A	835	CLA	C16-C17-C18-C19
11	B	816	CLA	C16-C17-C18-C19
12	A	843	PQN	C26-C27-C28-C30
11	B	802	CLA	C3A-C2A-CAA-CBA
11	B	852	CLA	C3A-C2A-CAA-CBA
14	A	851	BCR	C11-C10-C9-C34
14	A	851	BCR	C16-C17-C18-C36
14	B	845	BCR	C11-C10-C9-C34
14	B	845	BCR	C20-C21-C22-C37
14	L	201	BCR	C11-C10-C9-C34
19	F	805	LUT	C20-C13-C14-C15
11	A	841	CLA	C15-C16-C17-C18
11	B	820	CLA	C5-C6-C7-C8
11	A	842	CLA	C2-C1-O2A-CGA
11	B	816	CLA	C13-C15-C16-C17
13	A	846	LHG	C10-C11-C12-C13
11	B	816	CLA	C4-C3-C5-C6
11	B	840	CLA	C4-C3-C5-C6
11	B	809	CLA	C8-C10-C11-C12
11	A	829	CLA	C10-C11-C12-C13
11	A	830	CLA	C6-C7-C8-C9
11	A	833	CLA	C11-C12-C13-C14
11	A	842	CLA	C11-C12-C13-C14
11	B	802	CLA	C11-C12-C13-C14
11	B	809	CLA	C14-C13-C15-C16
11	B	816	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
11	A	839	CLA	C16-C17-C18-C20
11	B	837	CLA	C11-C12-C13-C14
11	B	810	CLA	O1D-CGD-O2D-CED
11	B	810	CLA	CBD-CGD-O2D-CED
11	B	816	CLA	C2-C3-C5-C6
11	A	816	CLA	C1A-C2A-CAA-CBA
11	A	831	CLA	C1A-C2A-CAA-CBA
11	B	816	CLA	C1A-C2A-CAA-CBA
11	B	821	CLA	C1A-C2A-CAA-CBA
11	B	830	CLA	C1A-C2A-CAA-CBA
14	A	851	BCR	C11-C10-C9-C8
14	A	851	BCR	C16-C17-C18-C19
14	B	845	BCR	C11-C10-C9-C8
14	B	845	BCR	C20-C21-C22-C23
14	L	201	BCR	C11-C10-C9-C8
19	F	805	LUT	C12-C13-C14-C15
11	F	803	CLA	C15-C16-C17-C18
11	A	808	CLA	C2B-C3B-CAB-CBB
11	A	822	CLA	C2B-C3B-CAB-CBB
11	A	834	CLA	C2B-C3B-CAB-CBB
11	B	812	CLA	C2B-C3B-CAB-CBB
11	B	822	CLA	C2B-C3B-CAB-CBB
11	B	841	CLA	C2B-C3B-CAB-CBB
14	A	847	BCR	C23-C24-C25-C26
14	A	847	BCR	C23-C24-C25-C30
14	B	846	BCR	C23-C24-C25-C26
14	B	846	BCR	C23-C24-C25-C30
14	B	848	BCR	C1-C6-C7-C8
14	B	848	BCR	C5-C6-C7-C8
11	A	822	CLA	CAA-CBA-CGA-O1A
11	A	822	CLA	CAA-CBA-CGA-O2A
20	T	200	HEC	CAD-CBD-CGD-O2D
11	A	828	CLA	C4-C3-C5-C6
11	B	812	CLA	C2-C3-C5-C6
14	B	848	BCR	C13-C14-C15-C16
11	A	809	CLA	C11-C12-C13-C15
11	A	821	CLA	C6-C7-C8-C10
11	A	826	CLA	C6-C7-C8-C10
11	B	814	CLA	C12-C13-C15-C16
11	B	816	CLA	C6-C7-C8-C10
11	B	838	CLA	C6-C7-C8-C10
11	B	838	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
18	B	849	DGD	C2A-C3A-C4A-C5A
18	B	849	DGD	C7B-C8B-C9B-CAB
11	A	803	CLA	C16-C17-C18-C20
13	A	846	LHG	C11-C12-C13-C14
13	A	845	LHG	C13-C14-C15-C16
11	B	821	CLA	C11-C10-C8-C7
11	A	828	CLA	C3-C5-C6-C7
11	B	840	CLA	C13-C15-C16-C17
11	A	825	CLA	C8-C10-C11-C12
11	B	840	CLA	CBA-CGA-O2A-C1
11	B	814	CLA	C3-C5-C6-C7
16	A	854	LMU	C9-C10-C11-C12
11	L	203	CLA	C2A-CAA-CBA-CGA
11	B	806	CLA	C6-C7-C8-C9
11	B	852	CLA	CBD-CGD-O2D-CED
13	A	845	LHG	C19-C20-C21-C22
20	T	200	HEC	CAD-CBD-CGD-O1D
11	A	842	CLA	C4-C3-C5-C6
11	B	811	CLA	C2-C3-C5-C6
11	B	834	CLA	C5-C6-C7-C8
11	B	834	CLA	CBA-CGA-O2A-C1
11	B	834	CLA	O1A-CGA-O2A-C1
17	A	855	LMG	C7-C8-C9-O8
11	B	809	CLA	C15-C16-C17-C18
11	B	822	CLA	C1A-C2A-CAA-CBA
13	A	845	LHG	C34-C35-C36-C37
11	A	814	CLA	C4-C3-C5-C6
11	A	801	CLA	C4B-C3B-CAB-CBB
11	B	816	CLA	C4B-C3B-CAB-CBB
11	B	835	CLA	C4B-C3B-CAB-CBB
11	A	839	CLA	C5-C6-C7-C8
11	B	840	CLA	O1A-CGA-O2A-C1
11	A	809	CLA	C8-C10-C11-C12
11	B	852	CLA	O1D-CGD-O2D-CED
11	B	824	CLA	C16-C17-C18-C19
11	B	838	CLA	C16-C17-C18-C20
11	A	823	CLA	CAA-CBA-CGA-O2A
17	F	802	LMG	O6-C1-O1-C7
11	B	837	CLA	C11-C12-C13-C15
11	A	842	CLA	C11-C10-C8-C9
11	B	801	CLA	C11-C10-C8-C9
11	B	811	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
11	B	820	CLA	C11-C10-C8-C9
11	A	813	CLA	C2A-CAA-CBA-CGA
11	A	806	CLA	C2-C1-O2A-CGA
11	B	803	CLA	C2-C1-O2A-CGA
11	B	815	CLA	C2-C1-O2A-CGA
11	B	816	CLA	C2-C1-O2A-CGA
11	B	852	CLA	C2-C1-O2A-CGA
11	A	832	CLA	C3A-C2A-CAA-CBA
11	B	832	CLA	C3A-C2A-CAA-CBA
11	A	842	CLA	C2-C3-C5-C6
11	B	840	CLA	C2-C3-C5-C6
11	A	844	CLA	CAA-CBA-CGA-O2A
11	B	825	CLA	O2A-C1-C2-C3
13	A	846	LHG	C16-C17-C18-C19
11	A	836	CLA	CAA-CBA-CGA-O2A
11	B	807	CLA	C10-C11-C12-C13
17	A	855	LMG	C31-C32-C33-C34
11	A	836	CLA	CAA-CBA-CGA-O1A
11	A	844	CLA	CAA-CBA-CGA-O1A
11	B	841	CLA	C8-C10-C11-C12
11	B	818	CLA	CBA-CGA-O2A-C1
13	A	845	LHG	C24-C25-C26-C27
11	A	817	CLA	C11-C10-C8-C9
11	B	833	CLA	C11-C12-C13-C14
11	A	839	CLA	C16-C17-C18-C19
11	A	806	CLA	CAA-CBA-CGA-O2A
13	B	850	LHG	O9-C7-C8-C9
11	B	833	CLA	C3-C5-C6-C7
11	A	842	CLA	CAA-CBA-CGA-O2A
17	A	855	LMG	O8-C28-C29-C30
11	A	823	CLA	CAA-CBA-CGA-O1A
11	A	841	CLA	C2A-CAA-CBA-CGA
11	B	819	CLA	C2A-CAA-CBA-CGA
11	A	842	CLA	C11-C10-C8-C7
11	B	801	CLA	C11-C10-C8-C7
11	B	806	CLA	C6-C7-C8-C10
11	B	820	CLA	C6-C7-C8-C10
11	A	801	CLA	C2B-C3B-CAB-CBB
11	A	837	CLA	C2B-C3B-CAB-CBB
11	B	803	CLA	C2B-C3B-CAB-CBB
11	B	835	CLA	C2B-C3B-CAB-CBB
19	F	805	LUT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
11	A	835	CLA	C2-C1-O2A-CGA
11	B	827	CLA	C2-C1-O2A-CGA
11	B	832	CLA	C2-C1-O2A-CGA
11	B	835	CLA	C2-C1-O2A-CGA
11	B	834	CLA	C10-C11-C12-C13
11	B	852	CLA	CAA-CBA-CGA-O2A
17	F	802	LMG	O8-C28-C29-C30
11	B	808	CLA	C2-C3-C5-C6
11	A	825	CLA	C15-C16-C17-C18
11	B	808	CLA	C4-C3-C5-C6
13	B	850	LHG	C18-C19-C20-C21
13	B	850	LHG	C25-C26-C27-C28
11	B	818	CLA	O1A-CGA-O2A-C1
11	A	805	CLA	C6-C7-C8-C9
11	A	808	CLA	C11-C10-C8-C9
11	A	841	CLA	C11-C12-C13-C14
11	B	814	CLA	C14-C13-C15-C16
11	A	825	CLA	CAA-CBA-CGA-O2A
11	A	836	CLA	C1A-C2A-CAA-CBA
11	B	801	CLA	C1A-C2A-CAA-CBA
11	L	203	CLA	C4B-C3B-CAB-CBB
11	A	842	CLA	C10-C11-C12-C13
18	B	849	DGD	O1G-C1G-C2G-O2G
14	A	847	BCR	C21-C22-C23-C24
14	B	846	BCR	C19-C20-C21-C22
13	A	845	LHG	C35-C36-C37-C38
11	A	812	CLA	CAA-CBA-CGA-O2A
11	A	817	CLA	C4-C3-C5-C6
11	J	103	CLA	C2-C1-O2A-CGA
11	A	805	CLA	C11-C10-C8-C7
11	A	811	CLA	C11-C12-C13-C15
11	A	817	CLA	C15-C16-C17-C18
13	A	846	LHG	C12-C13-C14-C15
11	B	817	CLA	C2A-CAA-CBA-CGA
11	B	838	CLA	C2A-CAA-CBA-CGA
11	A	813	CLA	C10-C11-C12-C13
11	B	805	CLA	CAA-CBA-CGA-O1A
11	B	829	CLA	C5-C6-C7-C8
13	A	846	LHG	C13-C14-C15-C16
17	B	851	LMG	C37-C38-C39-C40
11	B	801	CLA	C3A-C2A-CAA-CBA
11	J	103	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
11	A	806	CLA	CAA-CBA-CGA-O1A
13	B	850	LHG	C30-C31-C32-C33
11	A	808	CLA	C14-C13-C15-C16
11	A	809	CLA	C11-C12-C13-C14
11	A	821	CLA	C6-C7-C8-C9
11	A	826	CLA	C6-C7-C8-C9
11	A	835	CLA	C11-C10-C8-C9
11	B	819	CLA	C11-C12-C13-C14
11	B	838	CLA	C11-C12-C13-C14
16	A	853	LMU	C5'-C4'-O1B-C1B
13	B	850	LHG	C9-C10-C11-C12
11	A	825	CLA	CAA-CBA-CGA-O1A
17	A	855	LMG	O10-C28-C29-C30
19	J	101	LUT	C21-C26-C27-C28
11	B	807	CLA	C15-C16-C17-C18
11	F	804	CLA	CAA-CBA-CGA-O2A
11	A	812	CLA	CAA-CBA-CGA-O1A
11	A	817	CLA	C5-C6-C7-C8
17	F	802	LMG	O10-C28-C29-C30
11	A	819	CLA	C2A-CAA-CBA-CGA
11	A	840	CLA	C2A-CAA-CBA-CGA
11	B	814	CLA	C2A-CAA-CBA-CGA
11	A	842	CLA	CAA-CBA-CGA-O1A
11	A	802	CLA	C13-C15-C16-C17
11	B	803	CLA	C8-C10-C11-C12
11	B	818	CLA	C10-C11-C12-C13
16	A	853	LMU	C3'-C4'-O1B-C1B
11	A	806	CLA	CAD-CBD-CGD-O2D
11	B	803	CLA	CAD-CBD-CGD-O2D
11	A	838	CLA	C15-C16-C17-C18
18	B	849	DGD	C3B-C4B-C5B-C6B
11	B	852	CLA	CAA-CBA-CGA-O1A
11	A	809	CLA	CAA-CBA-CGA-O2A
11	A	840	CLA	C10-C11-C12-C13

There are no ring outliers.

107 monomers are involved in 222 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	819	CLA	4	0
16	A	854	LMU	1	0
11	A	829	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	829	CLA	2	0
11	A	809	CLA	6	0
11	B	827	CLA	1	0
11	B	833	CLA	1	0
14	F	801	BCR	1	0
11	A	834	CLA	3	0
11	B	805	CLA	1	0
11	B	838	CLA	1	0
11	B	841	CLA	7	0
14	A	848	BCR	2	0
11	A	817	CLA	4	0
11	A	807	CLA	1	0
14	A	851	BCR	4	0
11	B	821	CLA	1	0
14	A	847	BCR	2	0
11	B	834	CLA	4	0
14	J	104	BCR	2	0
14	A	849	BCR	2	0
11	F	803	CLA	2	0
11	J	103	CLA	1	0
11	A	831	CLA	3	0
14	A	850	BCR	3	0
11	B	835	CLA	1	0
12	B	843	PQN	3	0
16	A	856	LMU	2	0
11	B	837	CLA	3	0
11	B	803	CLA	4	0
11	A	830	CLA	3	0
11	A	802	CLA	3	0
11	A	838	CLA	2	0
11	A	827	CLA	2	0
11	B	802	CLA	3	0
11	B	831	CLA	3	0
11	A	821	CLA	2	0
11	A	826	CLA	3	0
11	A	810	CLA	2	0
14	L	204	BCR	4	0
11	B	818	CLA	8	0
11	B	810	CLA	1	0
11	B	817	CLA	3	0
11	B	826	CLA	4	0
11	B	836	CLA	2	0

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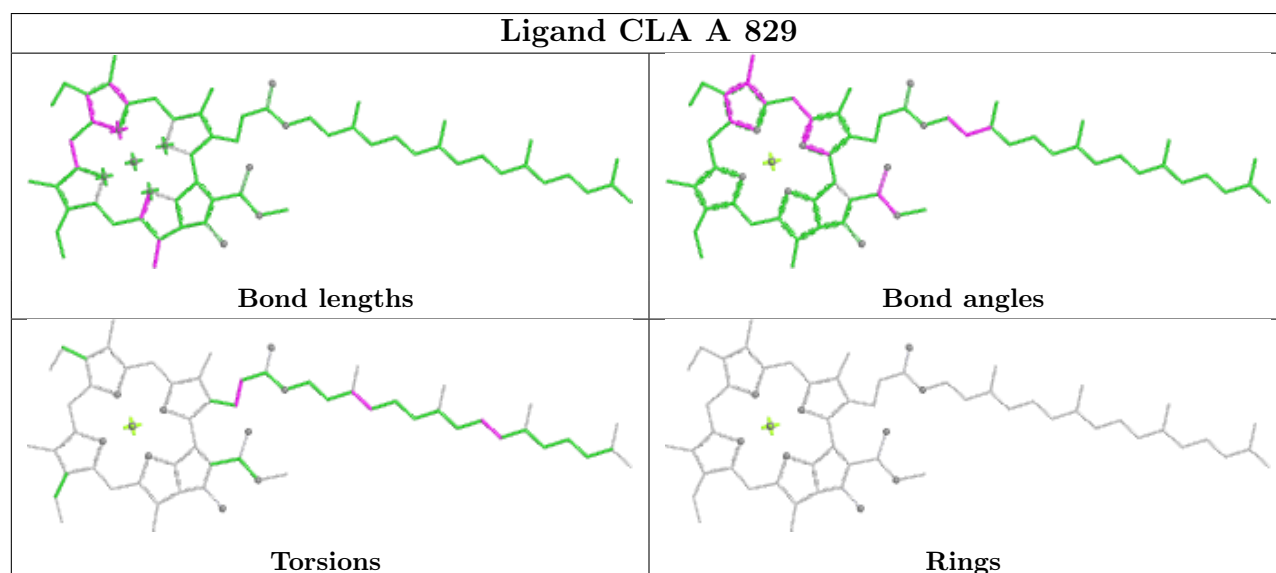
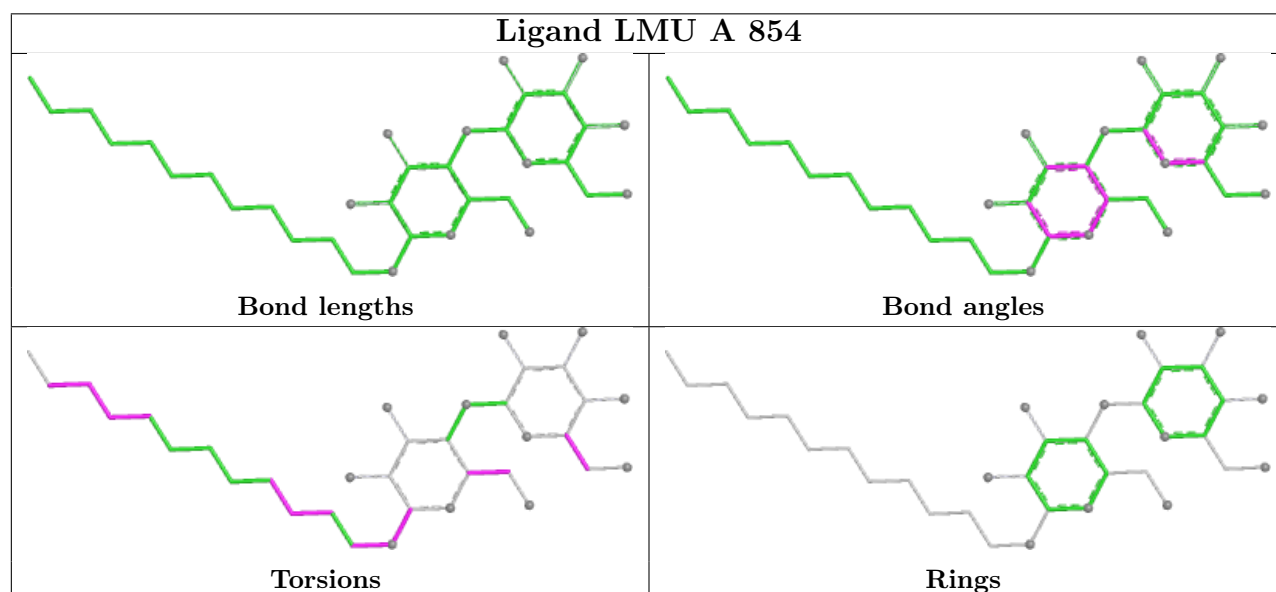
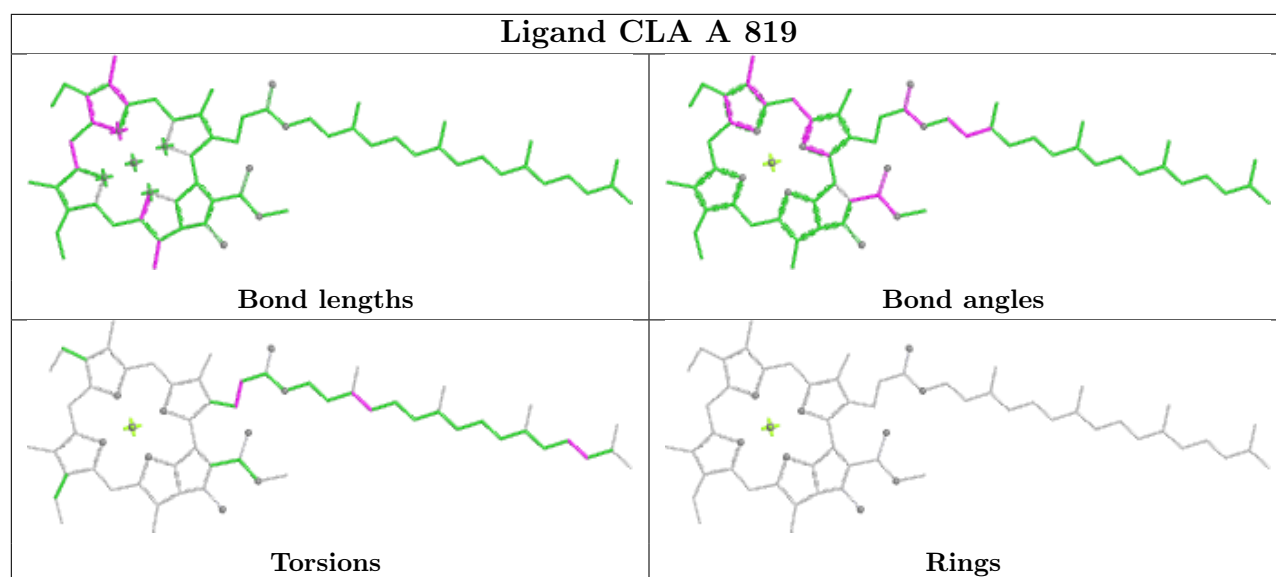
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	844	BCR	4	0
11	A	820	CLA	3	0
11	B	830	CLA	1	0
11	B	832	CLA	3	0
12	A	843	PQN	2	0
11	B	815	CLA	2	0
11	B	820	CLA	4	0
19	F	805	LUT	1	0
11	B	812	CLA	4	0
11	B	822	CLA	3	0
11	A	842	CLA	3	0
11	B	840	CLA	6	0
11	A	803	CLA	2	0
17	J	102	LMG	1	0
11	A	824	CLA	2	0
11	B	839	CLA	2	0
11	B	816	CLA	2	0
11	B	811	CLA	4	0
11	A	837	CLA	2	0
11	L	202	CLA	5	0
11	A	825	CLA	2	0
11	A	836	CLA	1	0
11	A	818	CLA	2	0
11	A	806	CLA	2	0
11	A	808	CLA	3	0
11	A	832	CLA	1	0
11	B	828	CLA	2	0
14	B	847	BCR	1	0
13	A	846	LHG	2	0
14	B	846	BCR	1	0
14	B	845	BCR	3	0
19	J	101	LUT	2	0
14	B	848	BCR	1	0
11	B	806	CLA	2	0
11	A	841	CLA	1	0
11	A	835	CLA	1	0
20	T	200	HEC	2	0
11	A	840	CLA	6	0
11	B	814	CLA	6	0
11	A	812	CLA	1	0
11	A	805	CLA	6	0
11	B	801	CLA	1	0

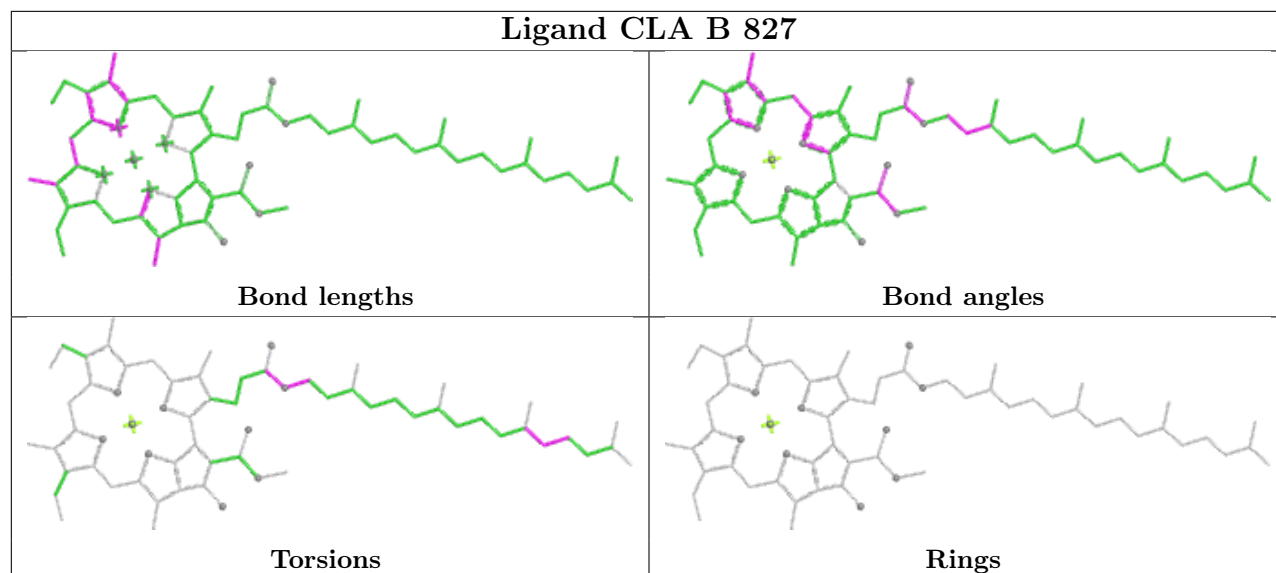
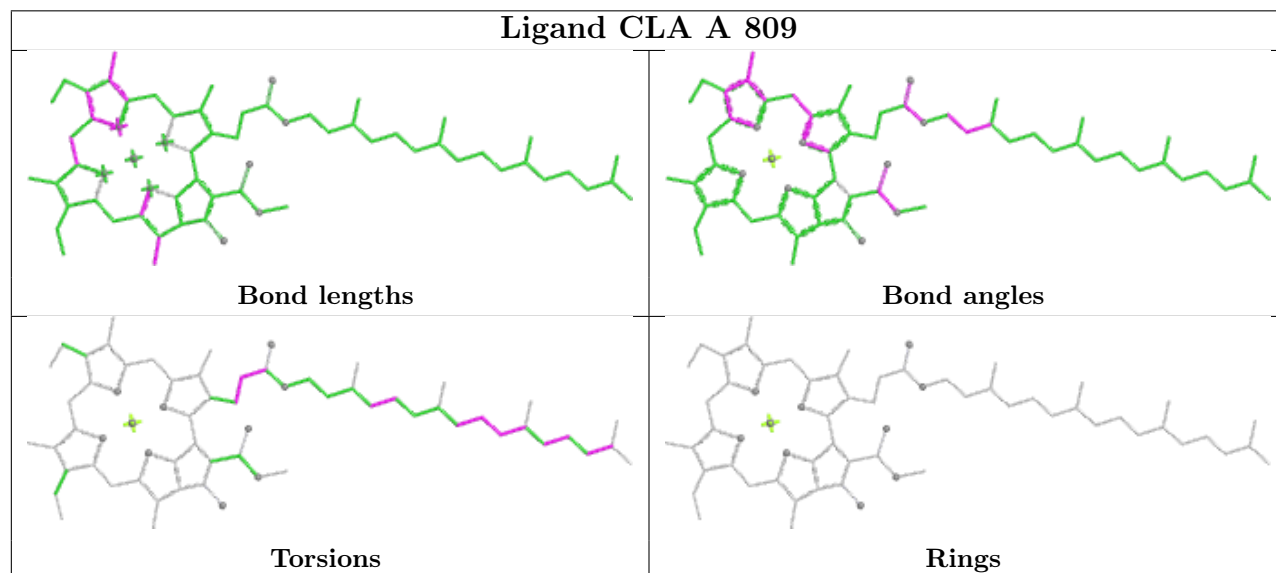
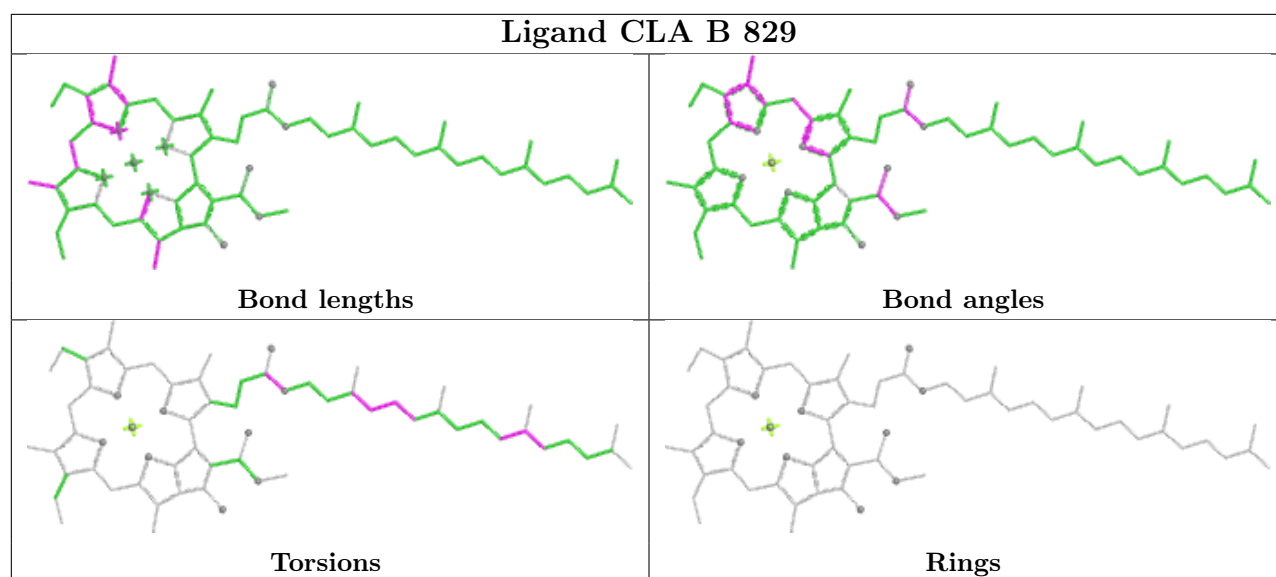
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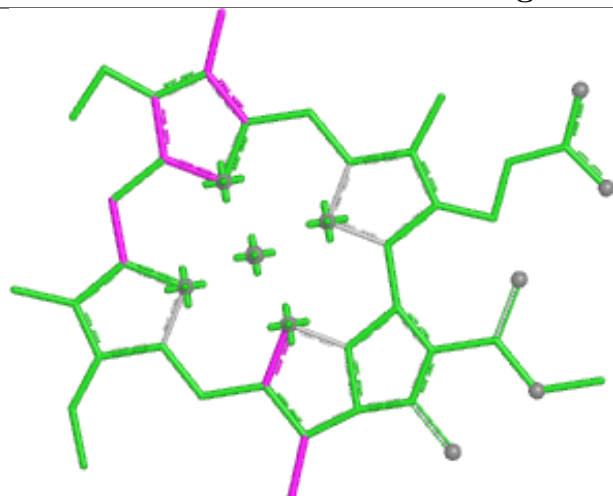
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	842	CLA	2	0
11	A	839	CLA	6	0
11	B	804	CLA	5	0
11	A	816	CLA	1	0
11	B	819	CLA	2	0
11	A	811	CLA	2	0
14	I	201	BCR	3	0
13	B	850	LHG	2	0
11	A	833	CLA	3	0
15	C	102	SF4	1	0
11	B	807	CLA	3	0
11	B	824	CLA	3	0
17	A	855	LMG	1	0
11	A	813	CLA	1	0
17	B	851	LMG	2	0
11	B	809	CLA	4	0
11	A	828	CLA	3	0
14	L	201	BCR	1	0
18	B	849	DGD	5	0
11	B	852	CLA	2	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.

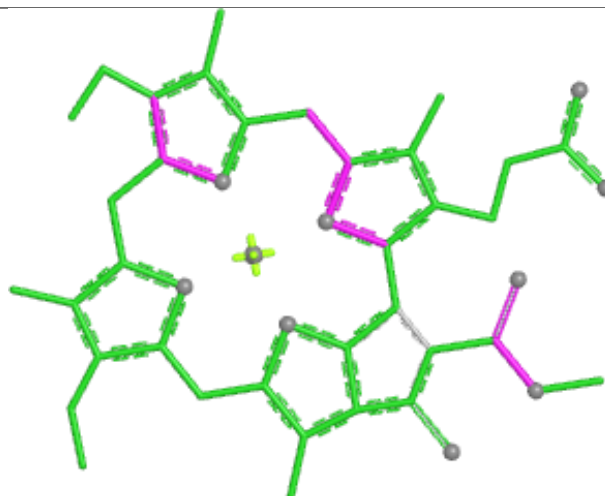




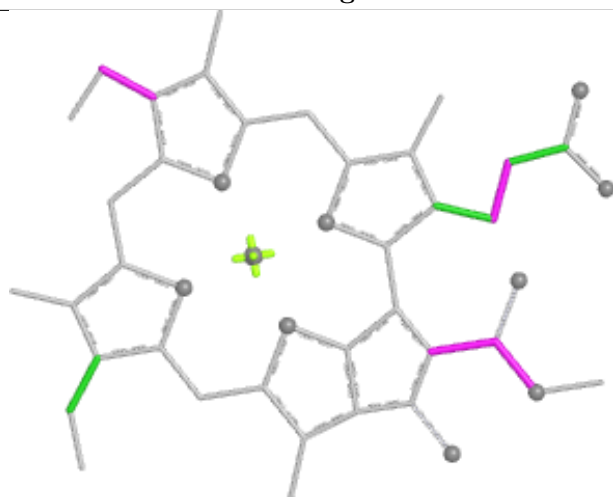
Ligand CLA L 203



Bond lengths



Bond angles

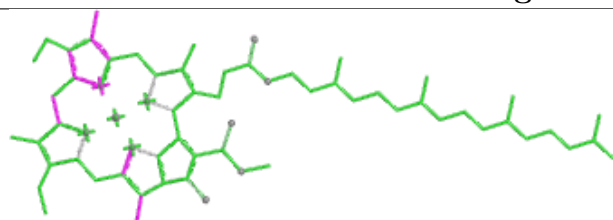


Torsions

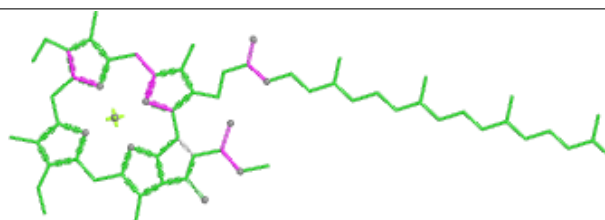


Rings

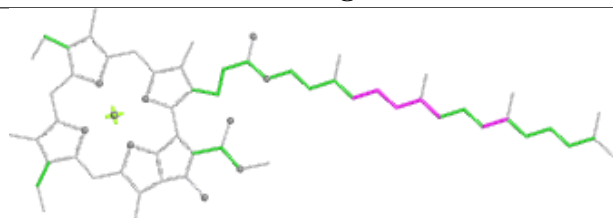
Ligand CLA B 833



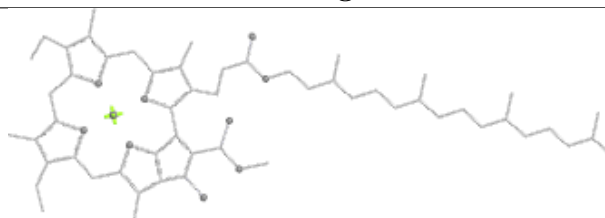
Bond lengths



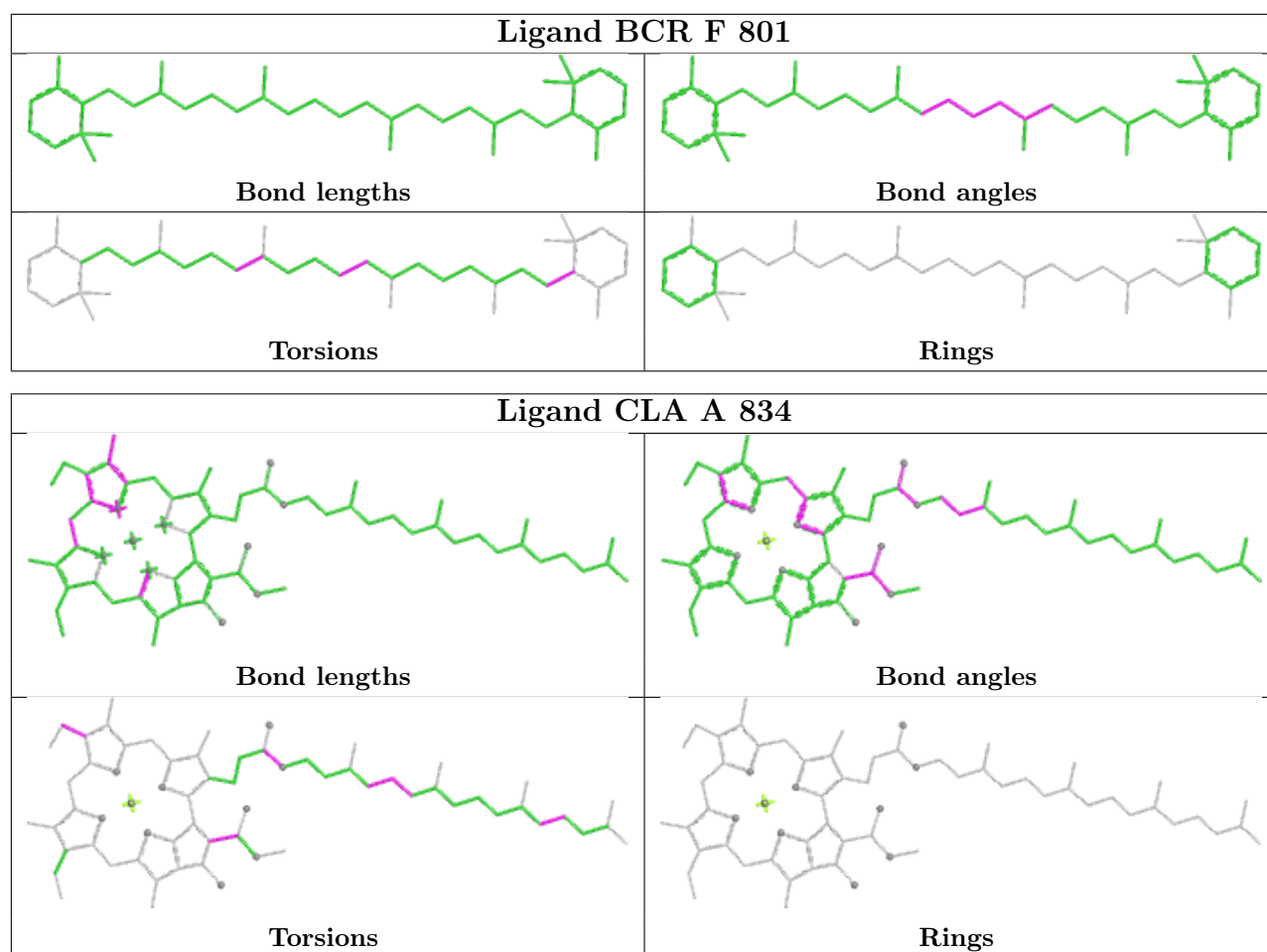
Bond angles



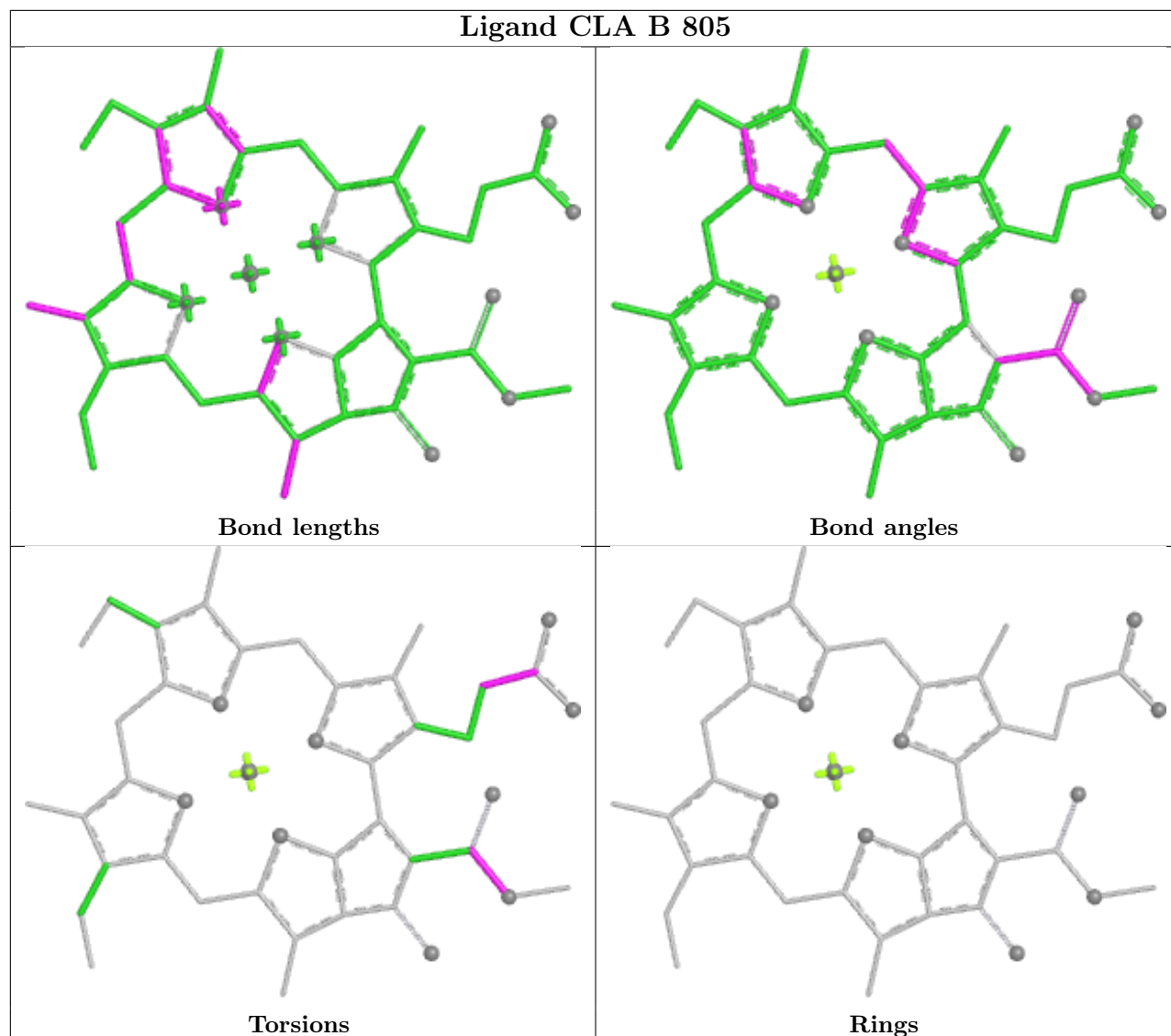
Torsions



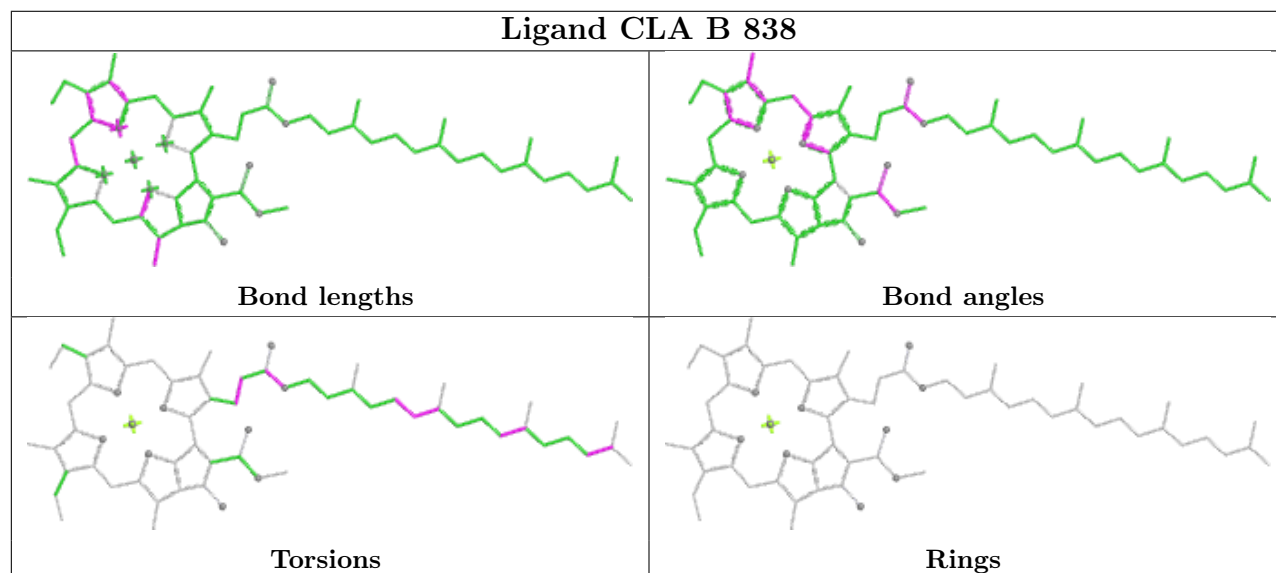
Rings

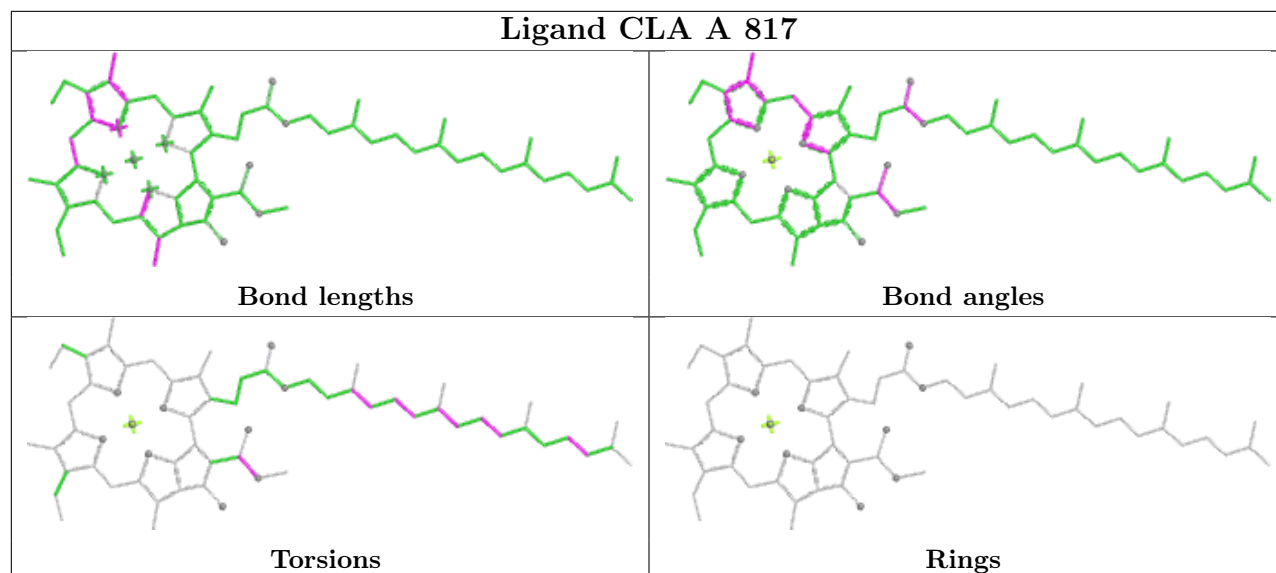
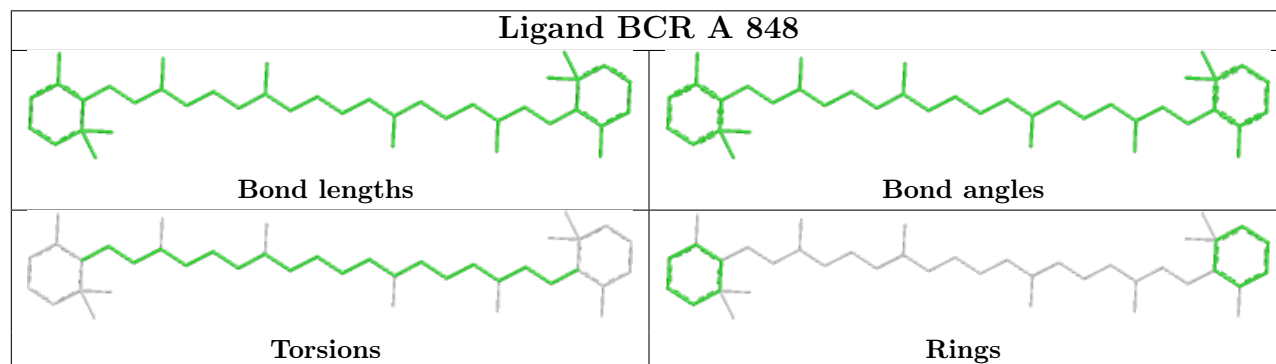
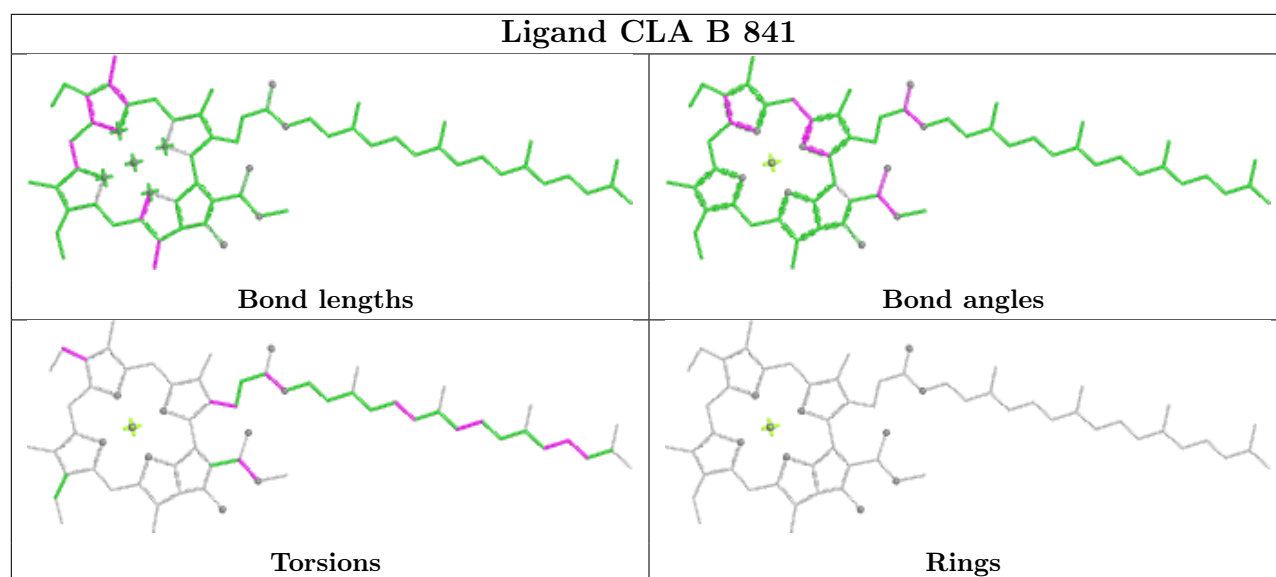


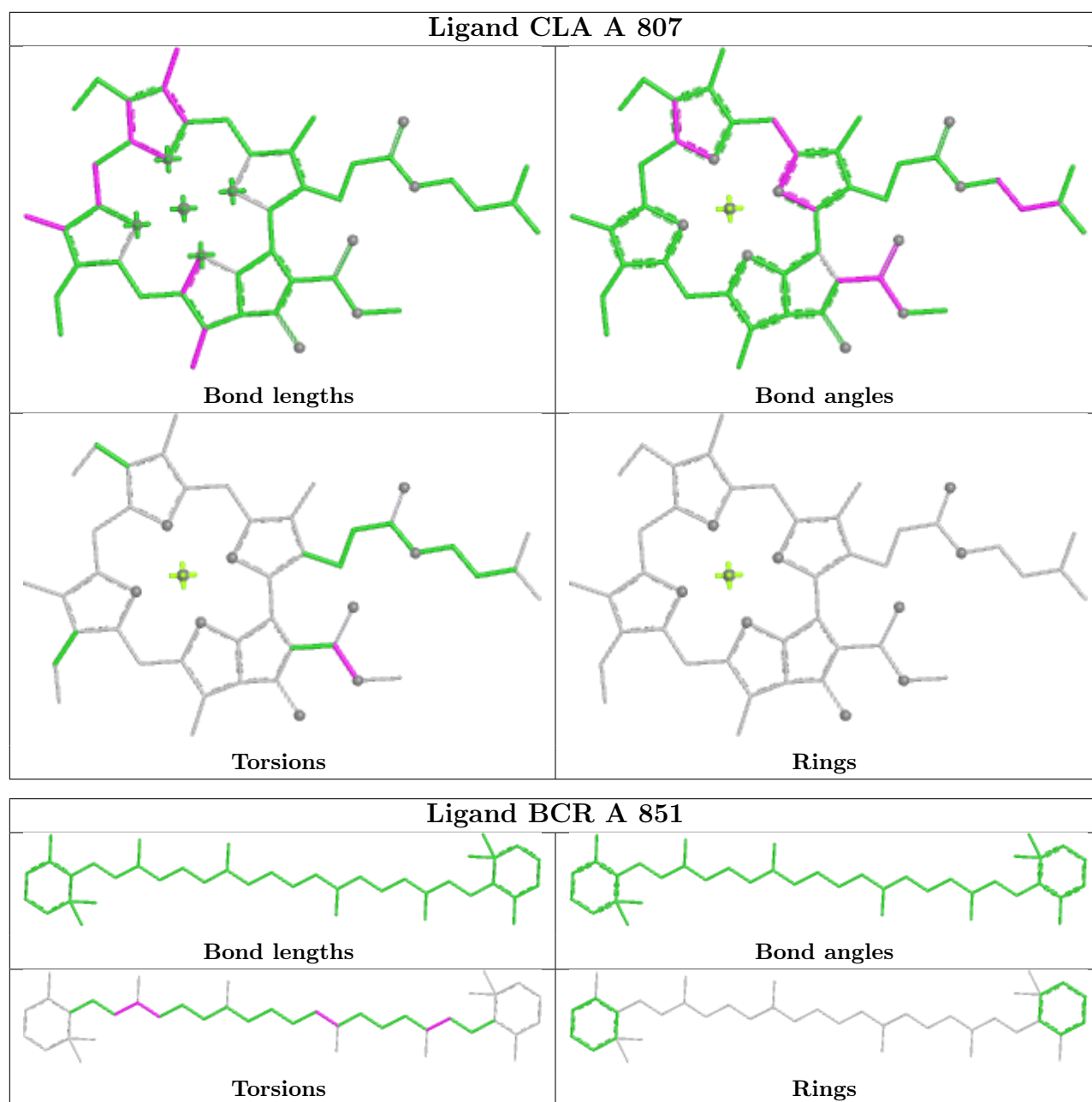
Ligand CLA B 805

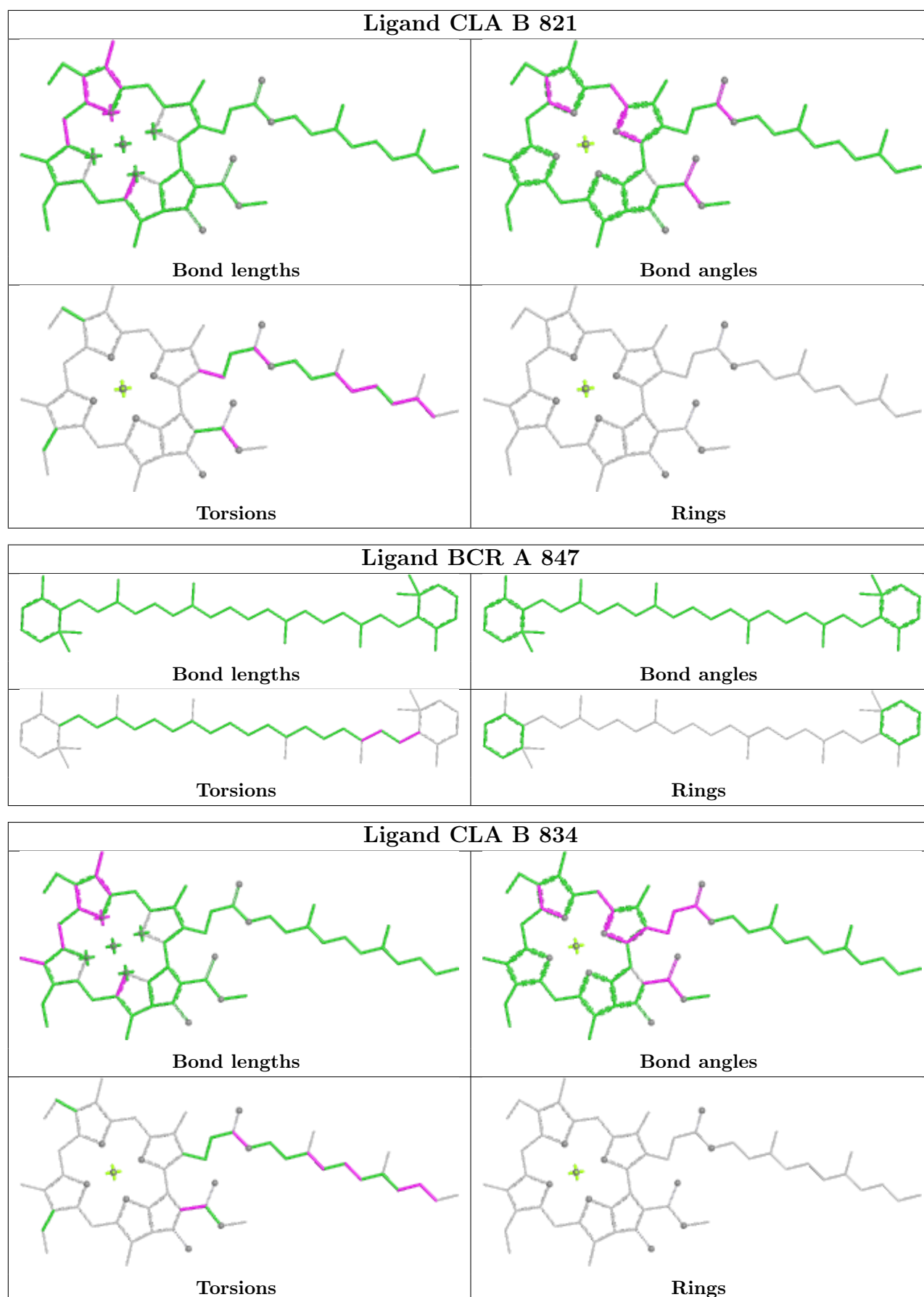


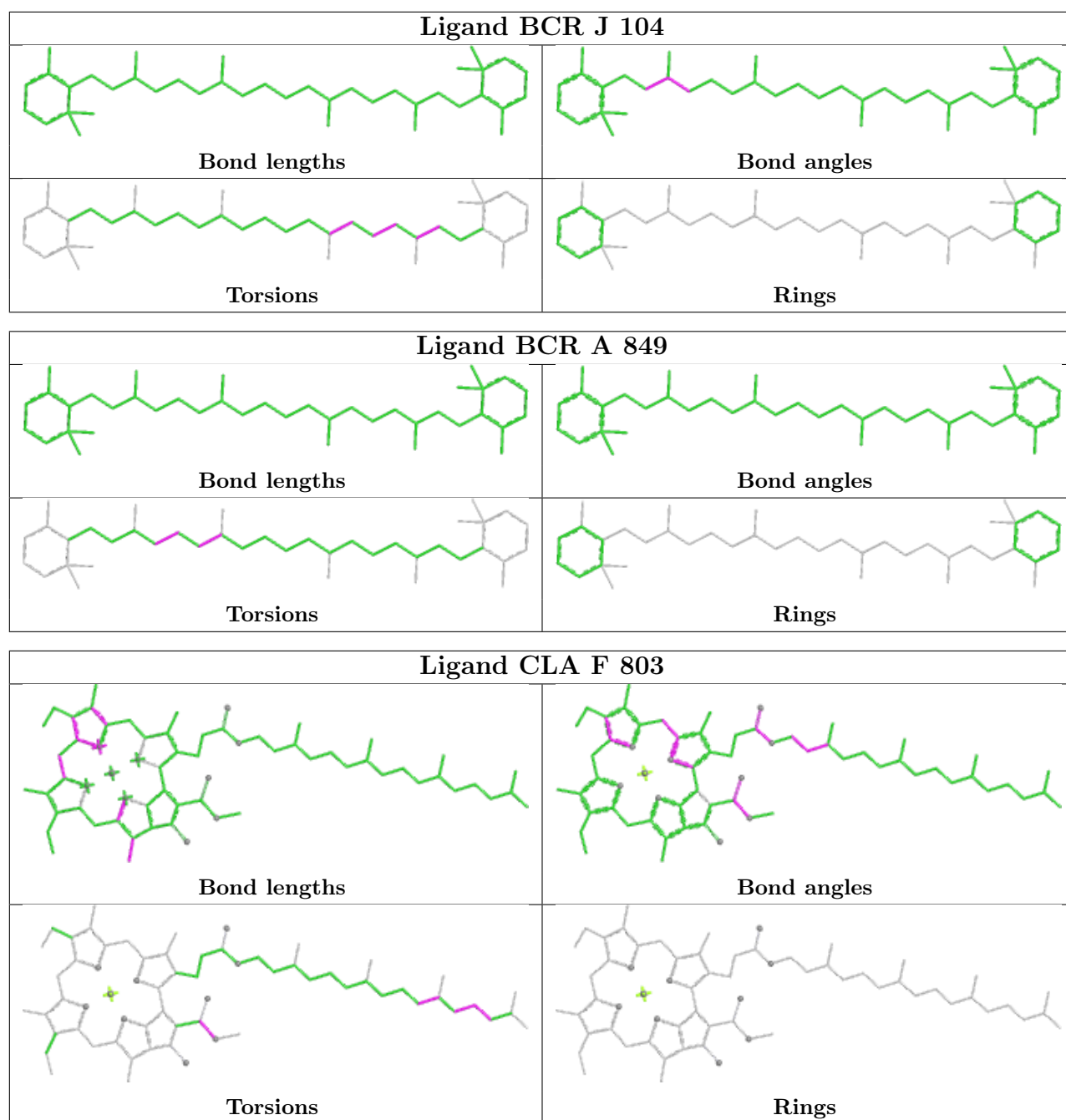
Ligand CLA B 838



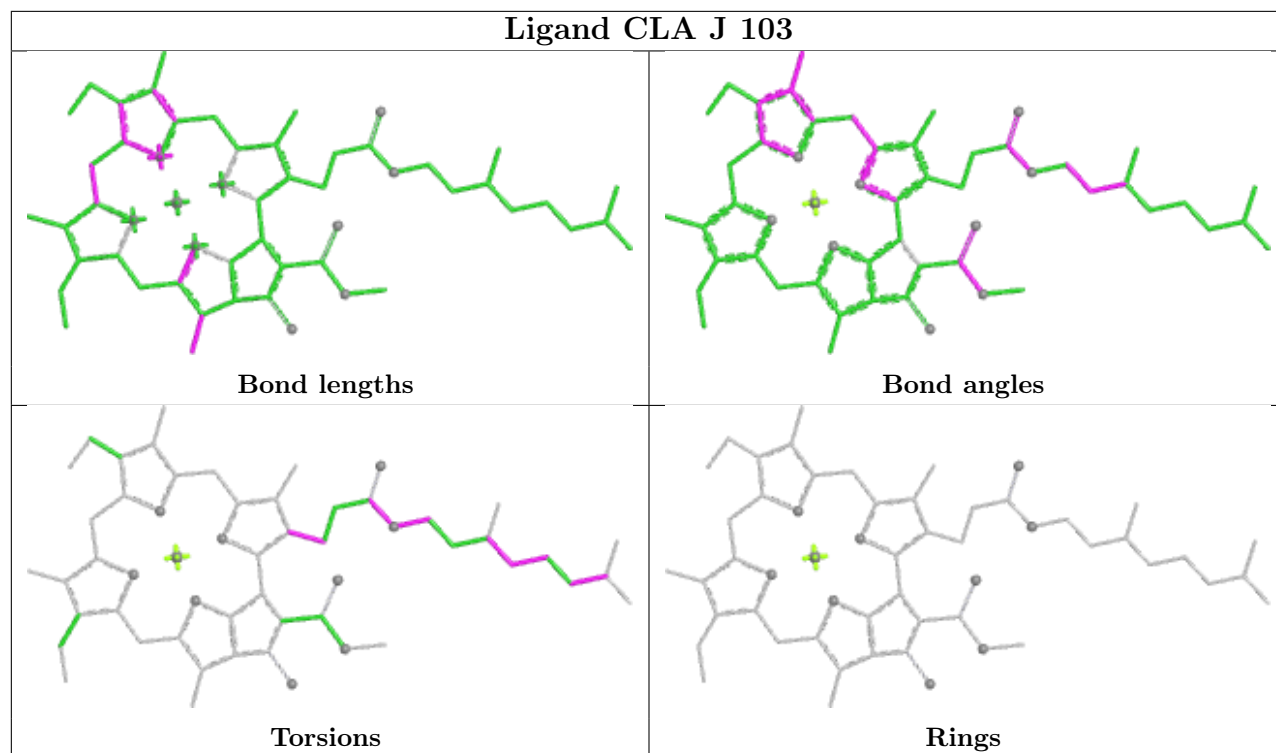




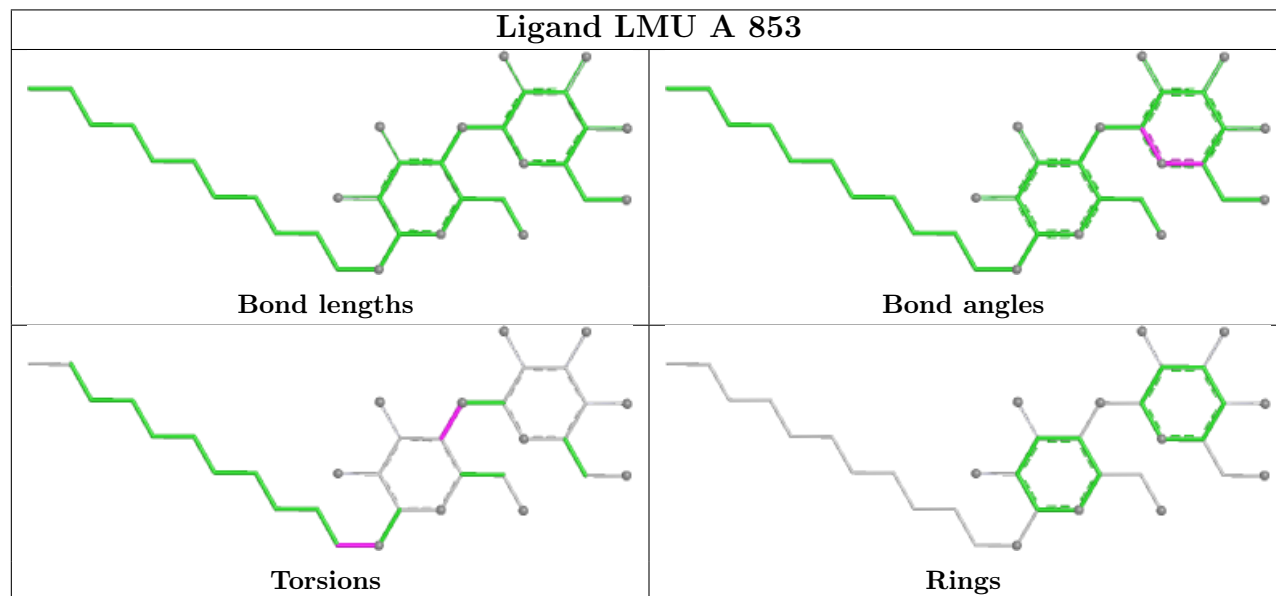




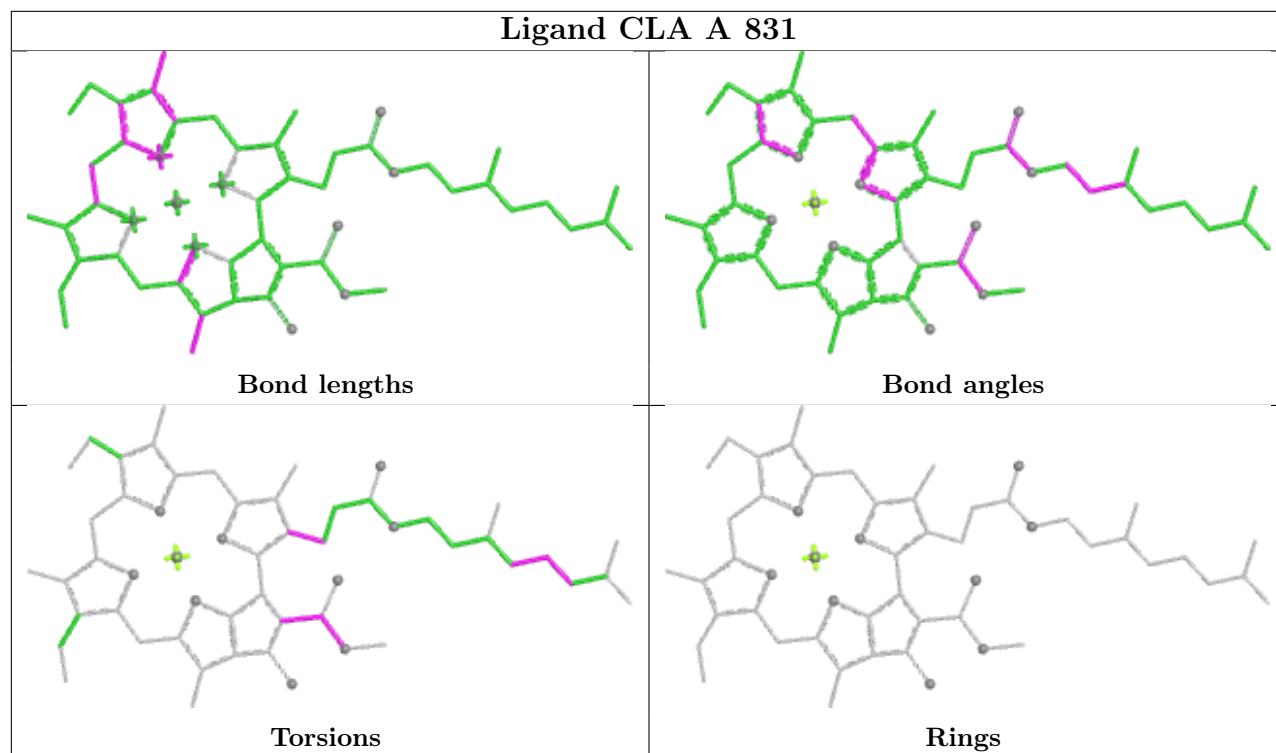
Ligand CLA J 103



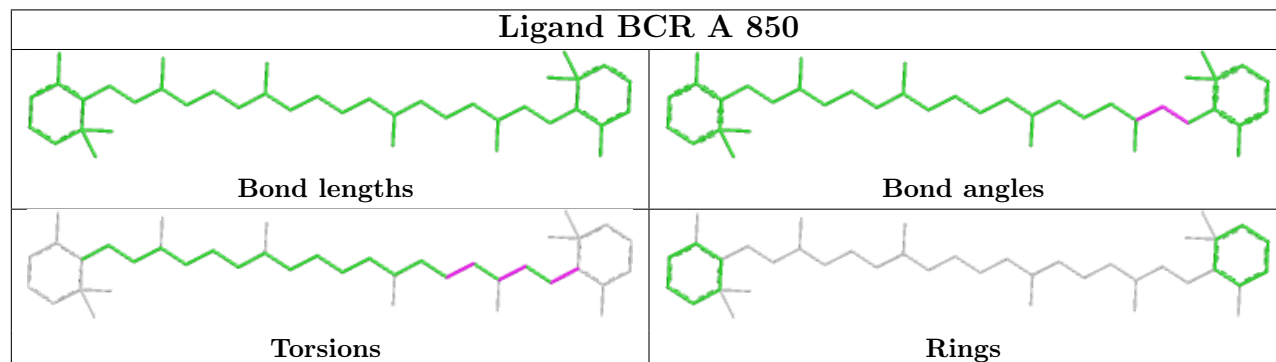
Ligand LMU A 853



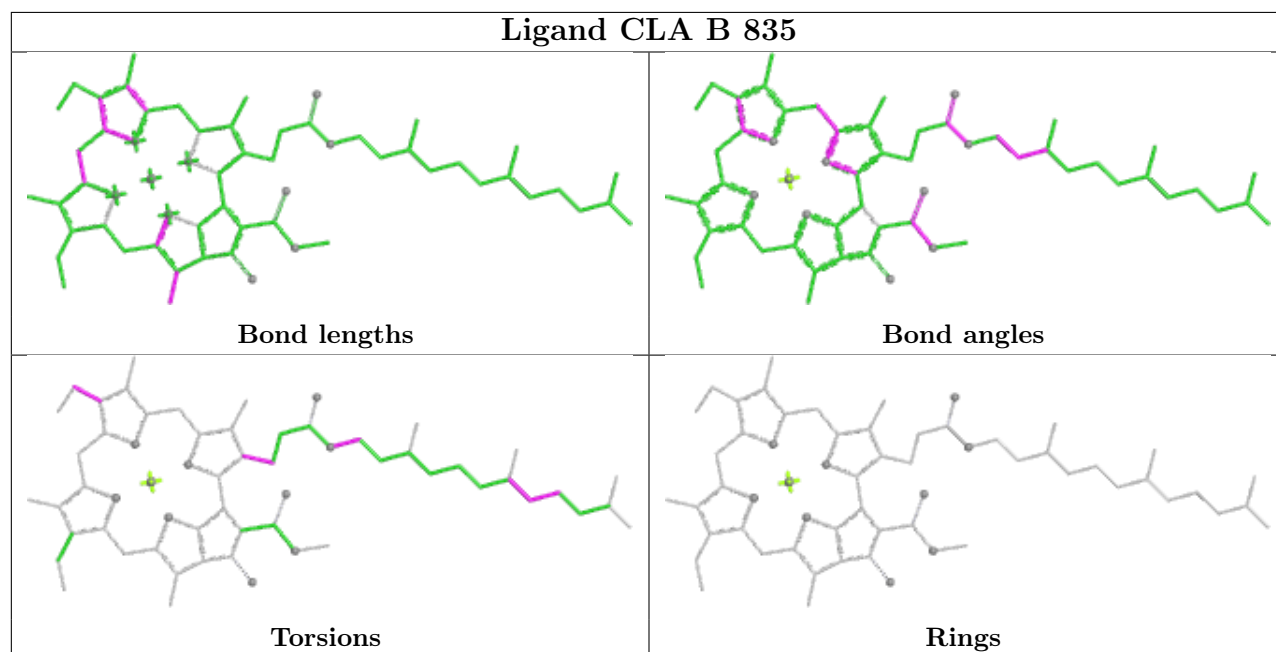
Ligand CLA A 831

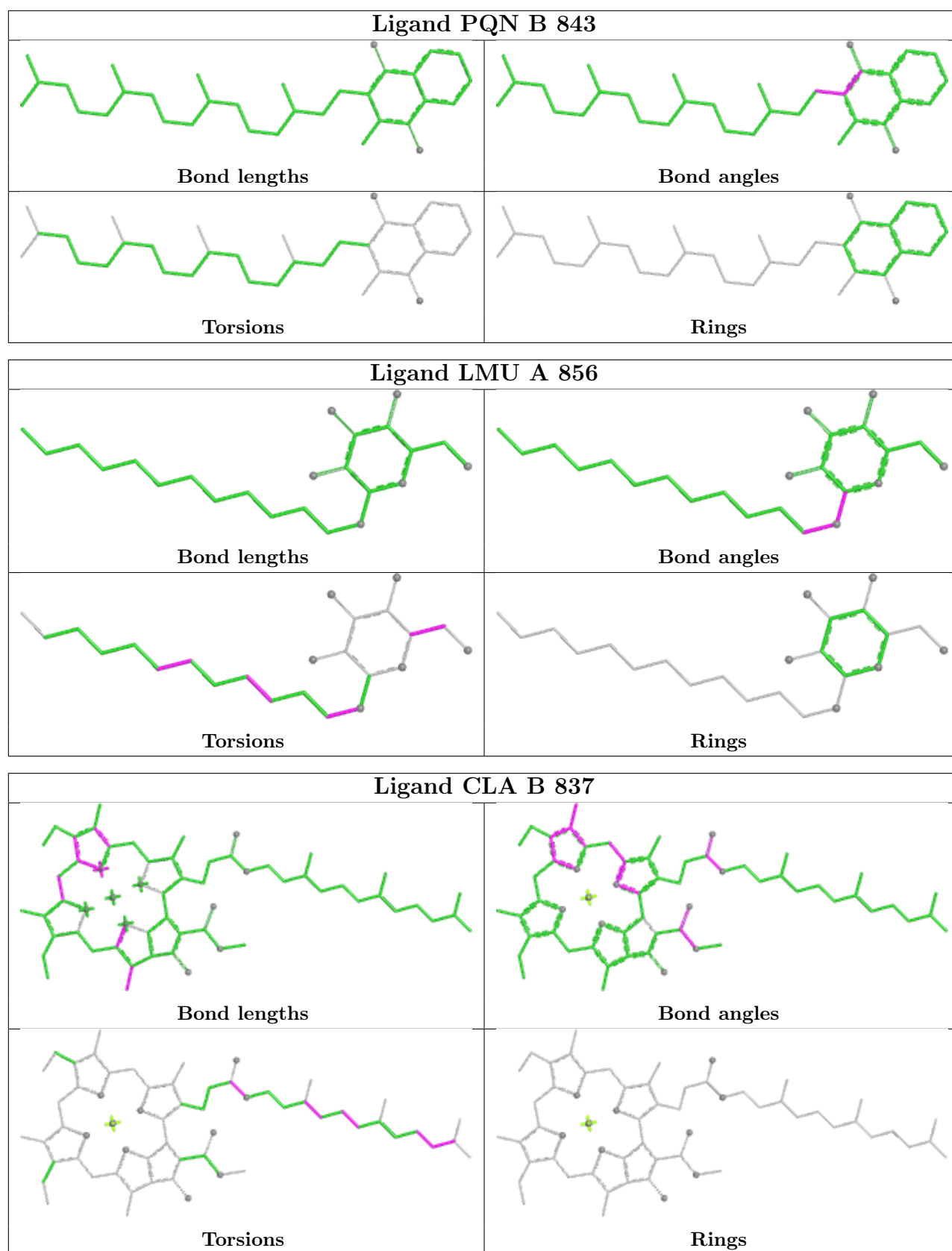


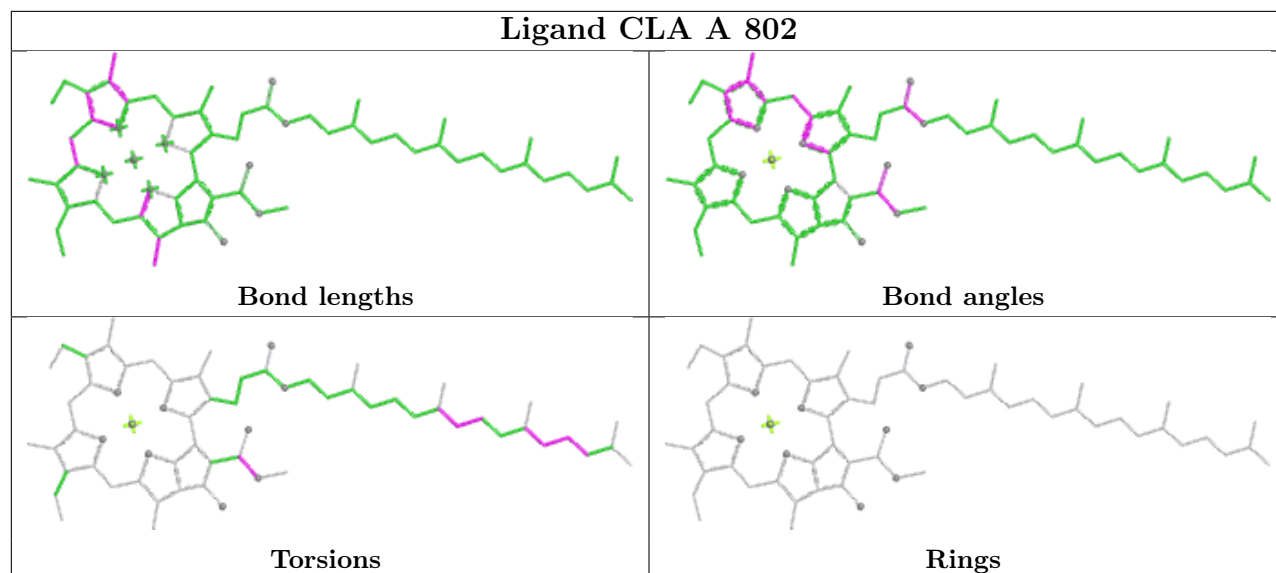
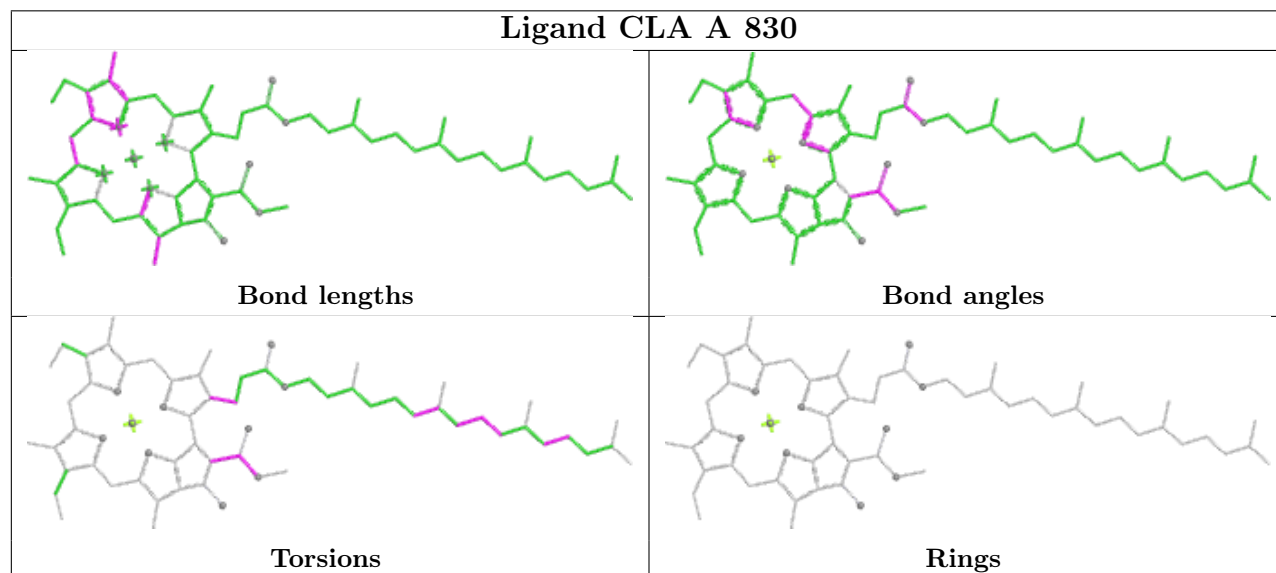
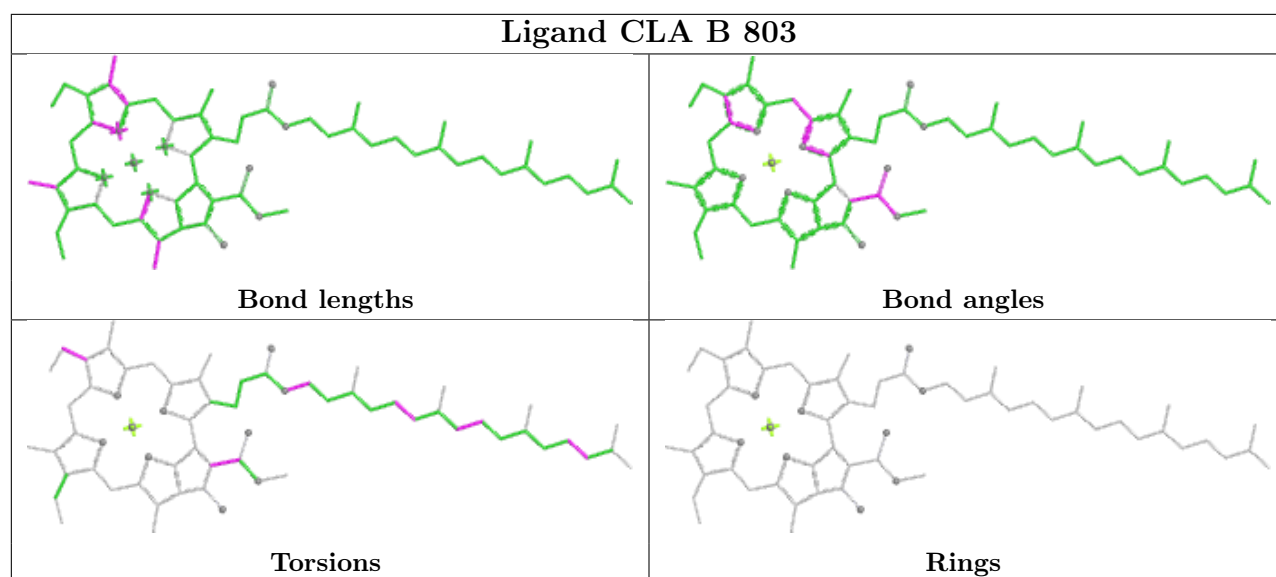
Ligand BCR A 850

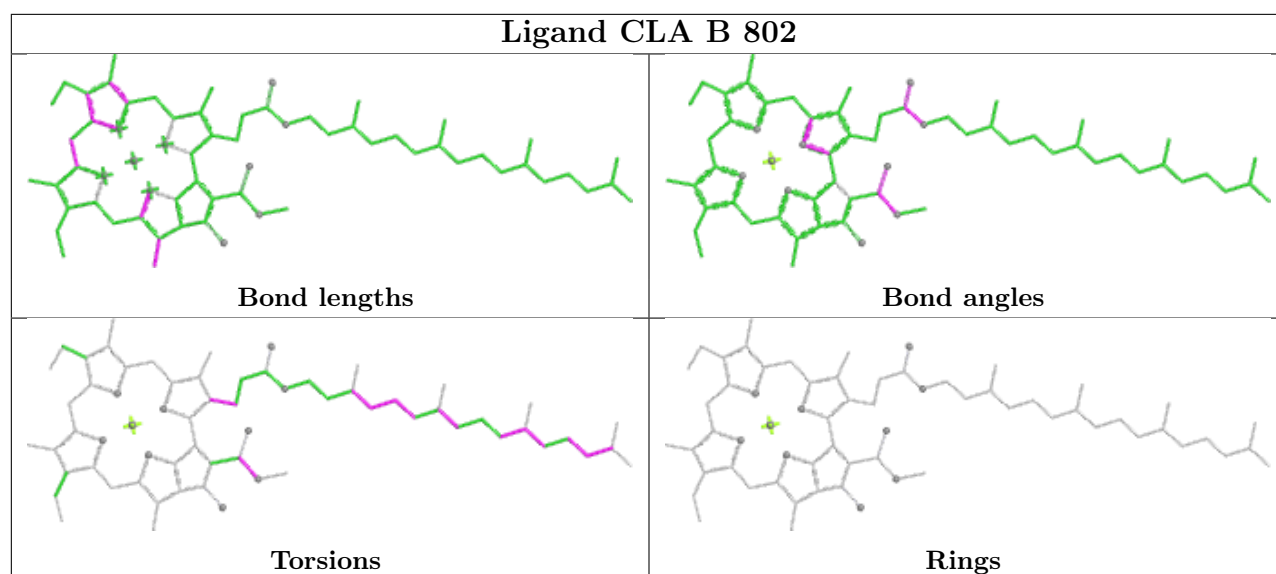
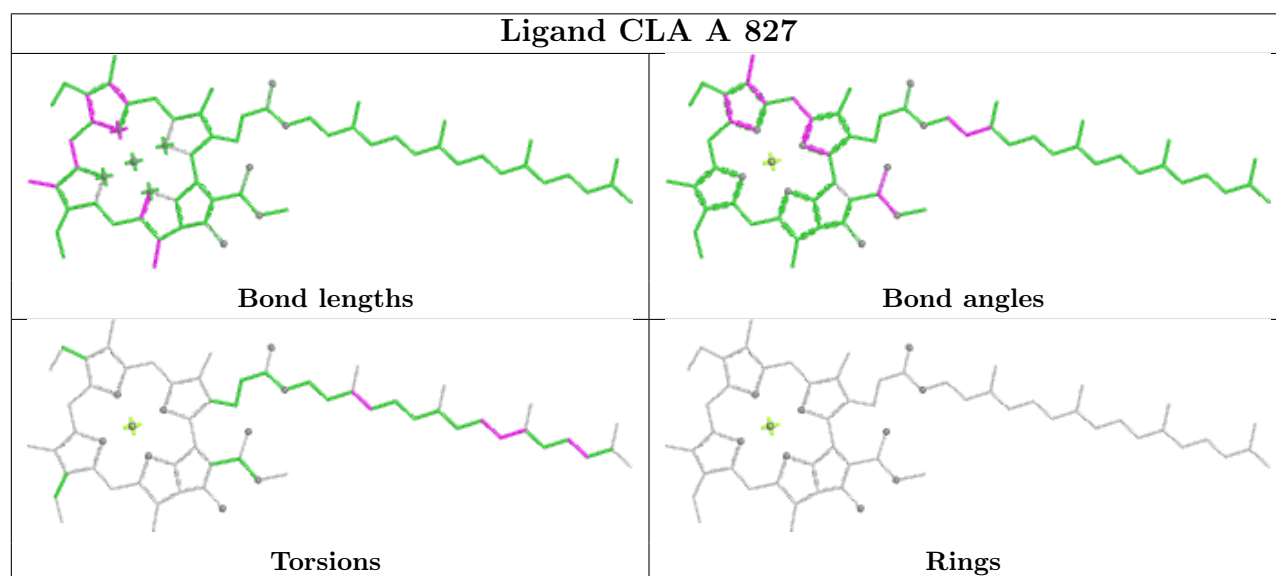
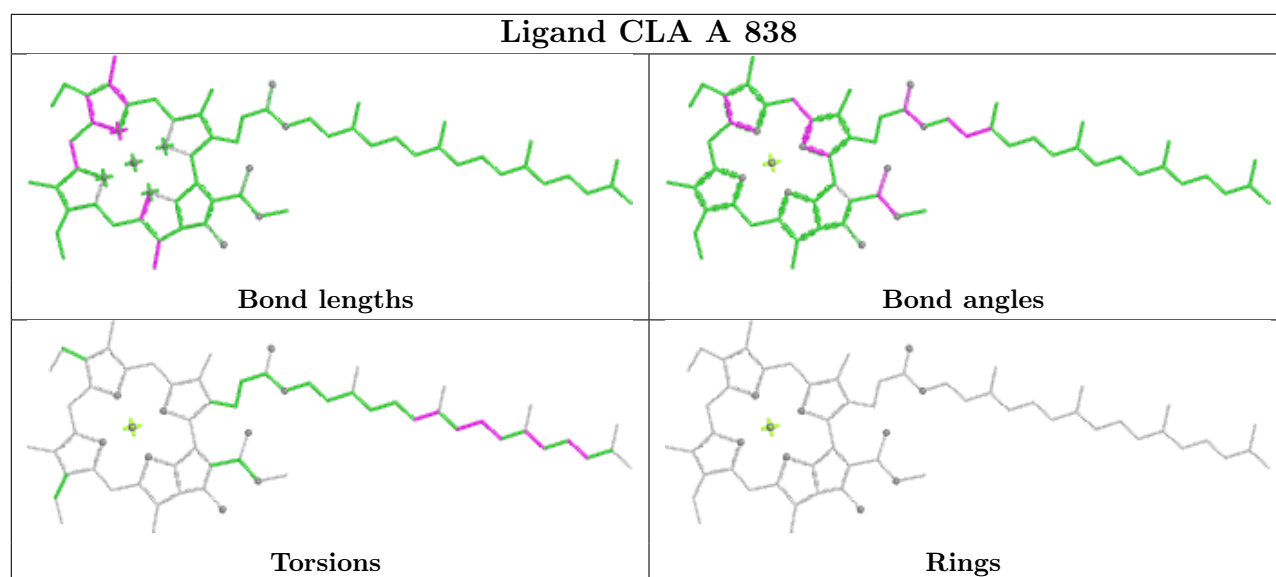


Ligand CLA B 835

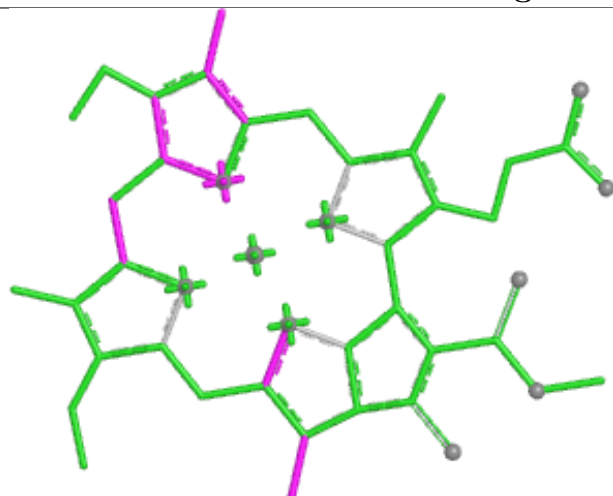




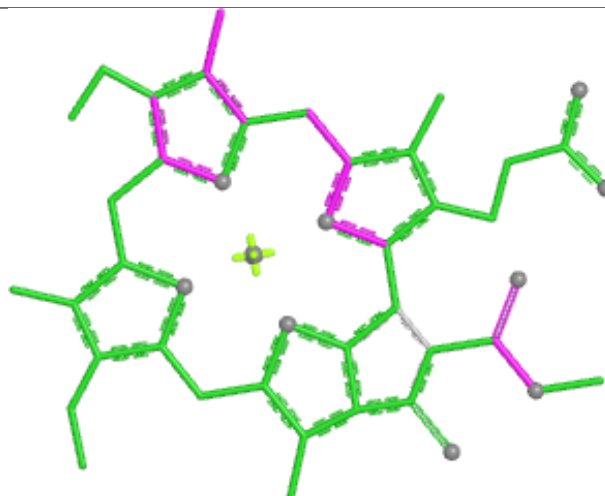




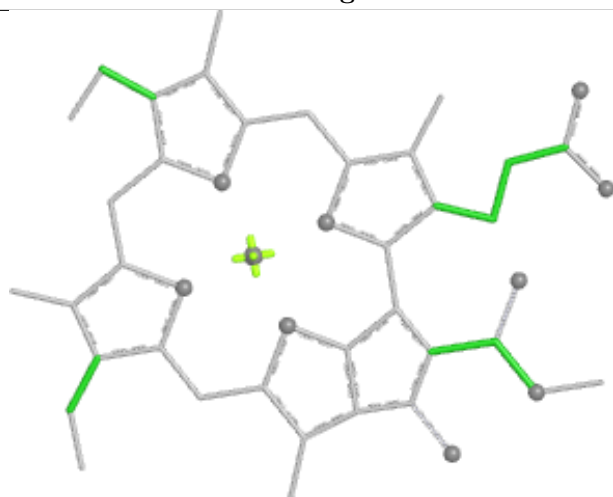
Ligand CLA B 831



Bond lengths



Bond angles

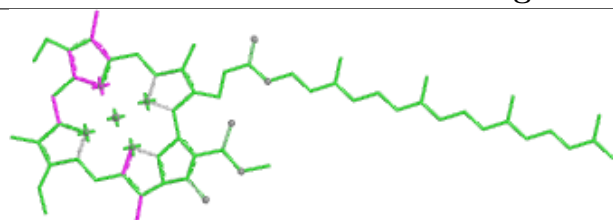


Torsions

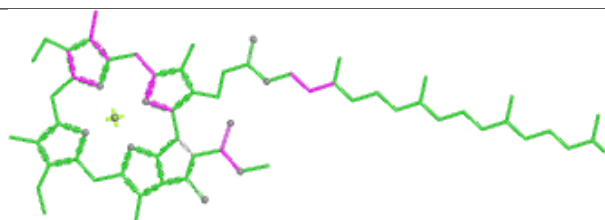


Rings

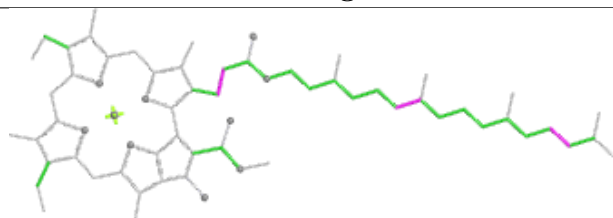
Ligand CLA A 821



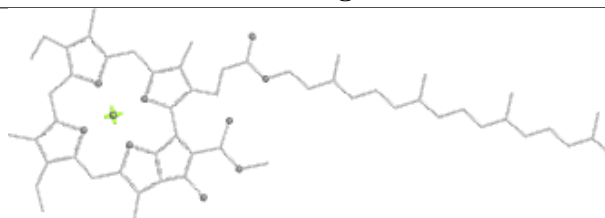
Bond lengths



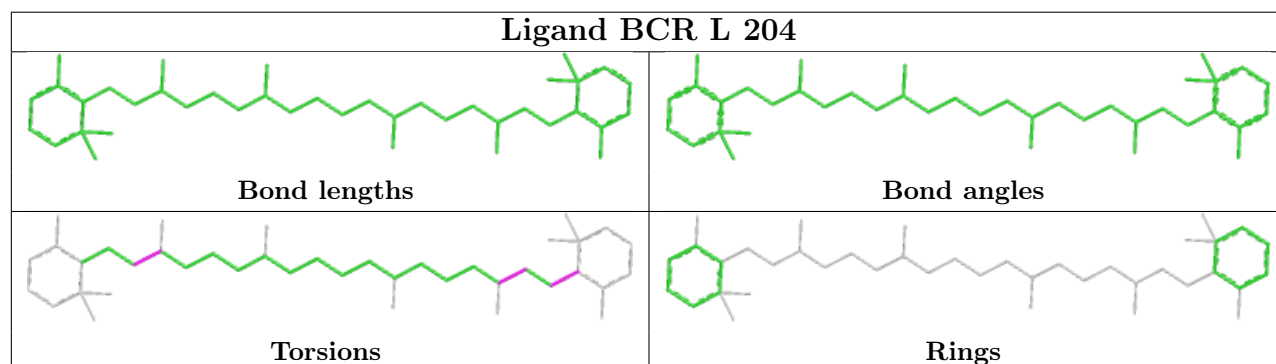
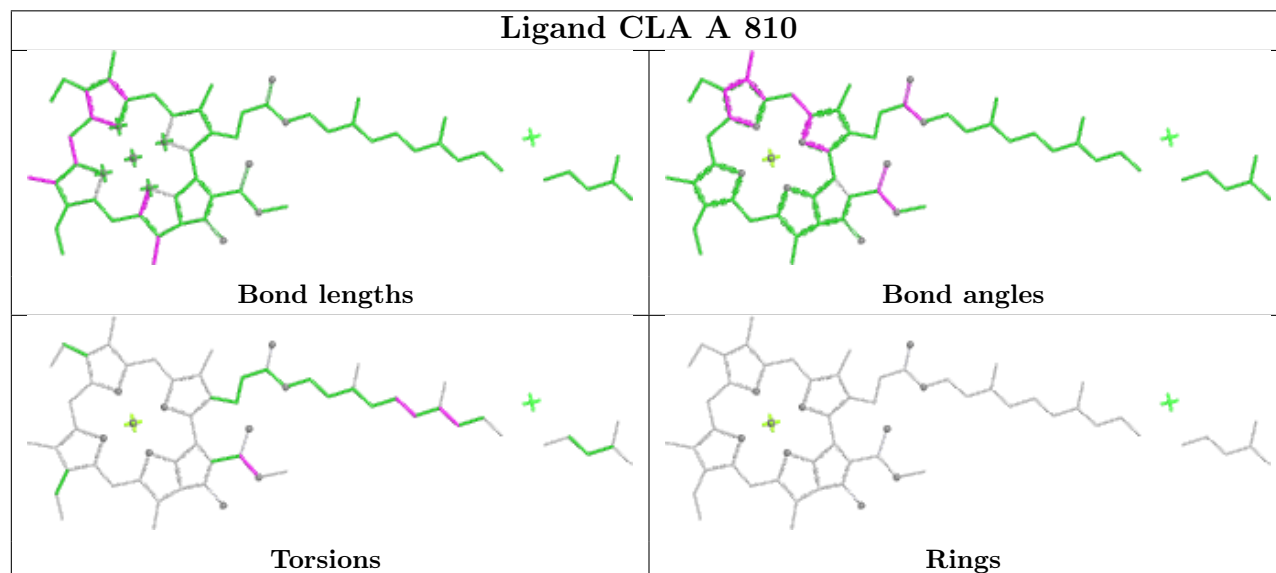
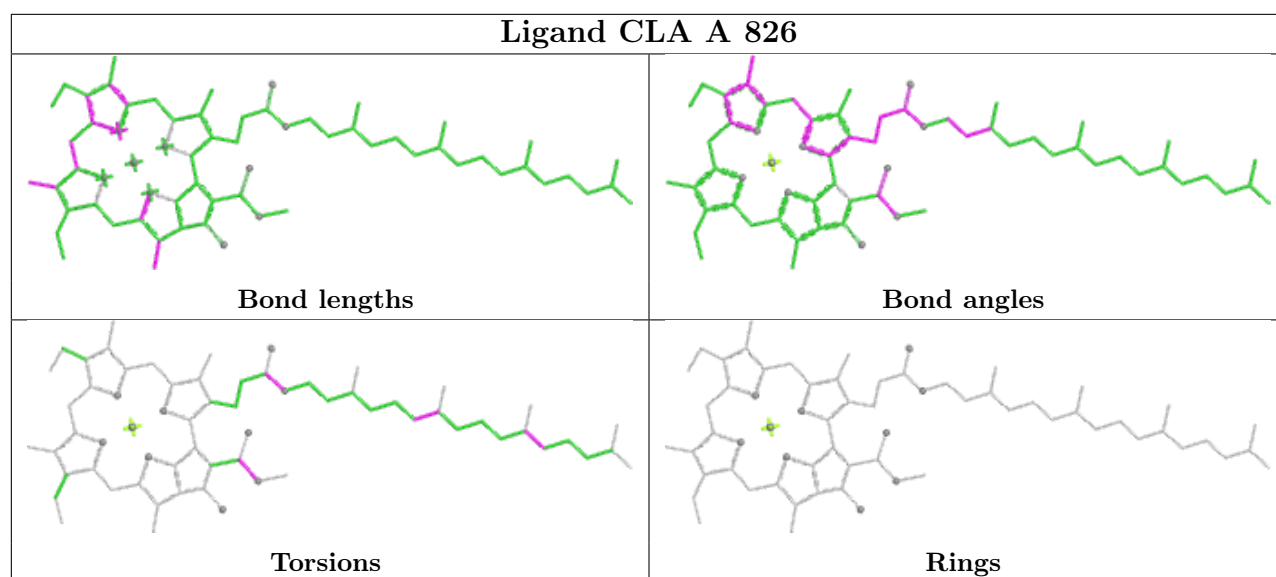
Bond angles

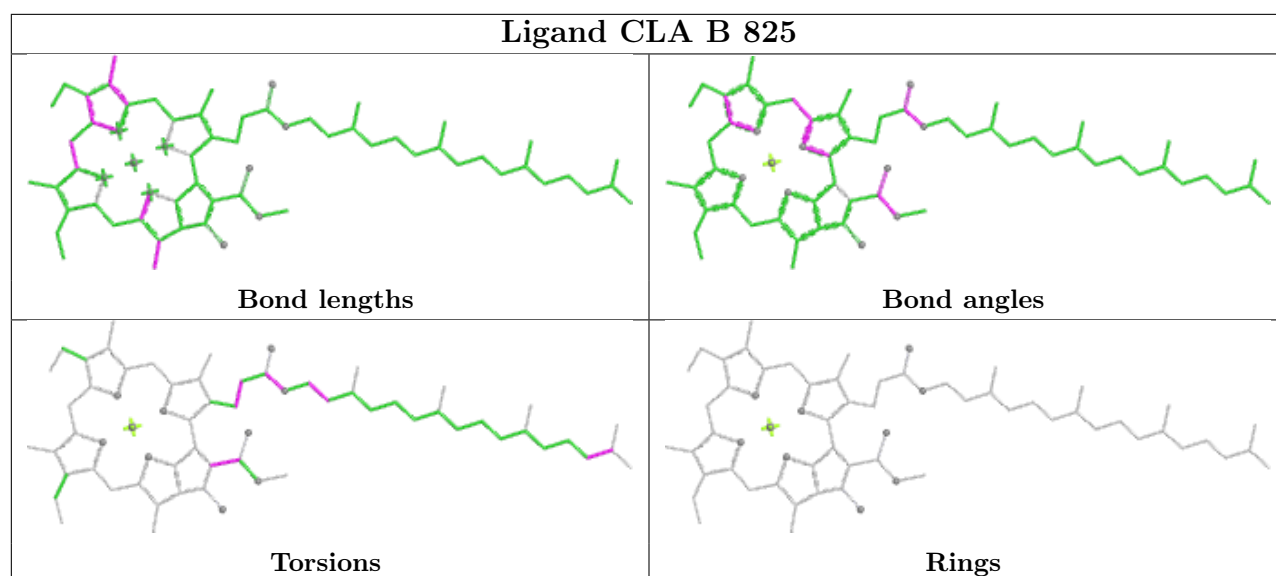
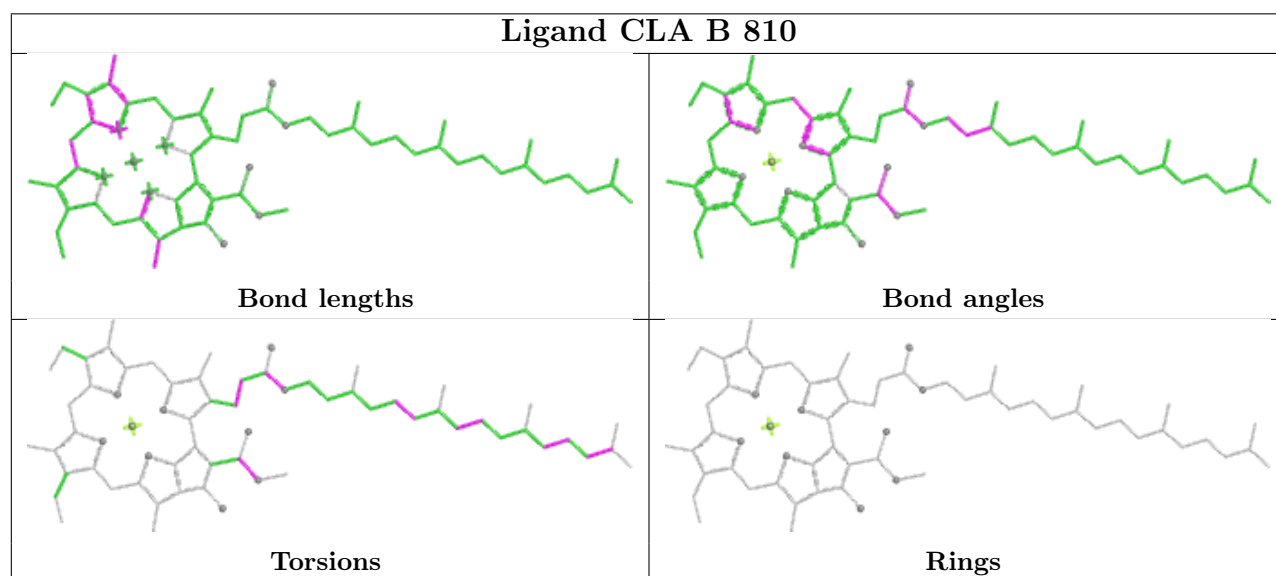
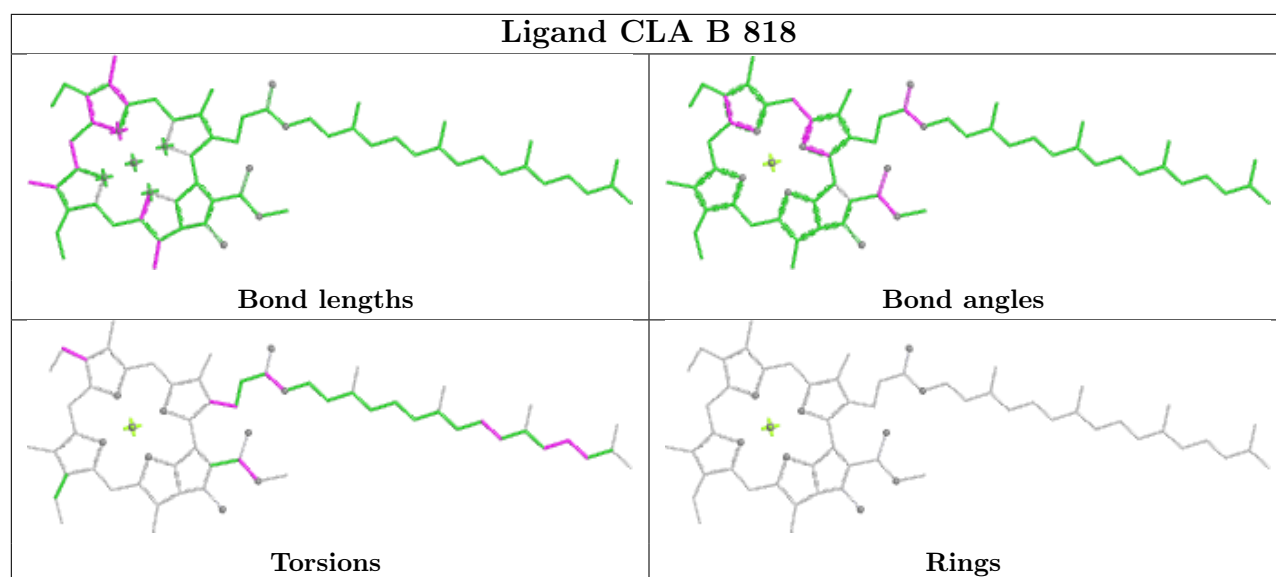


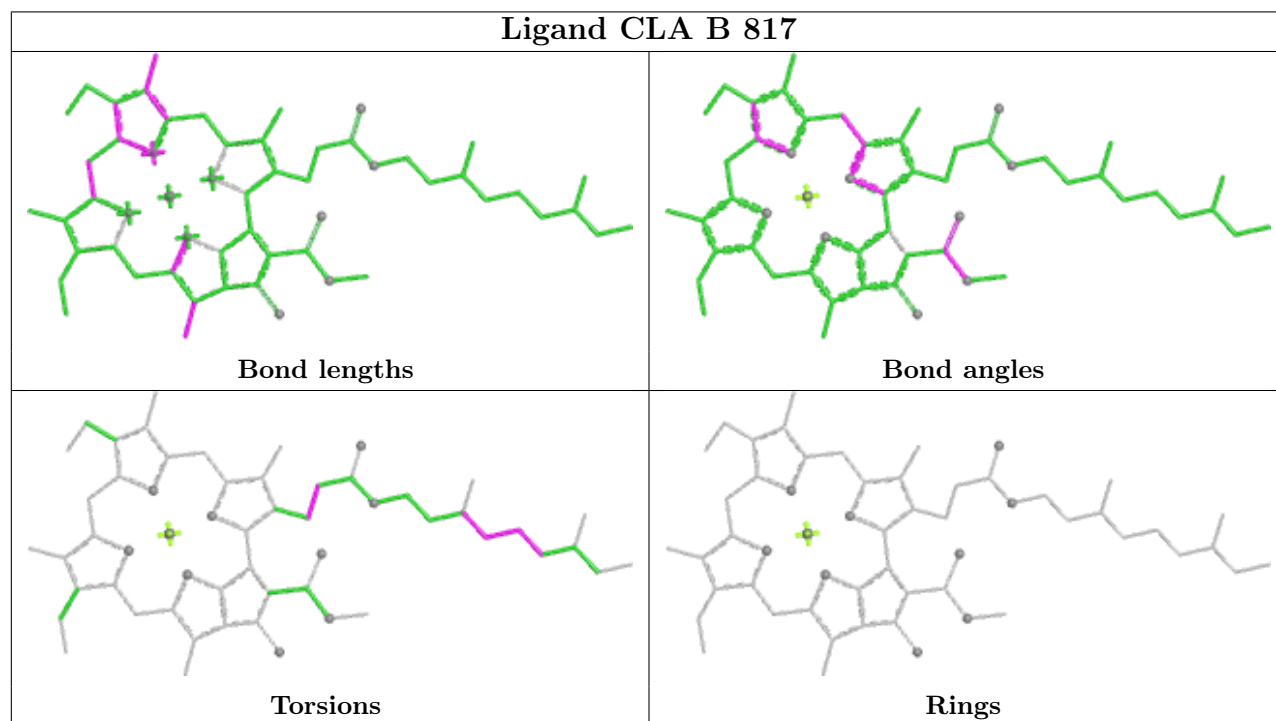
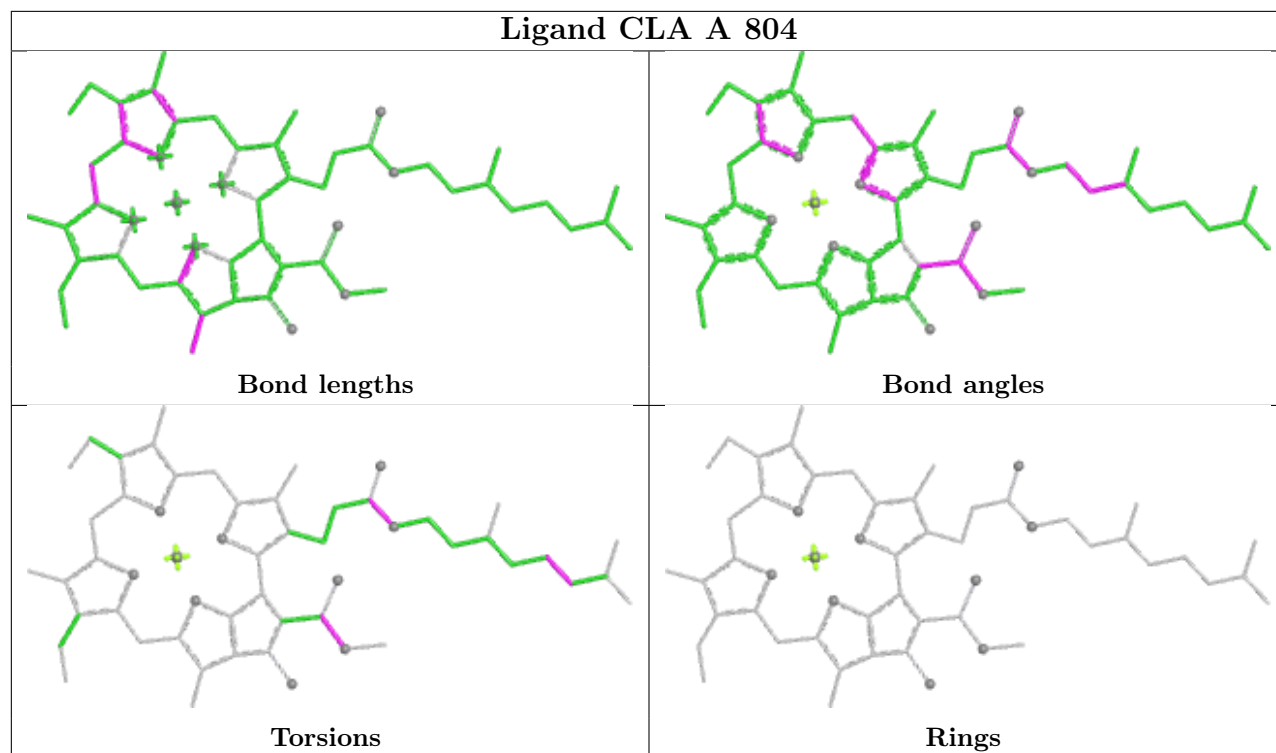
Torsions

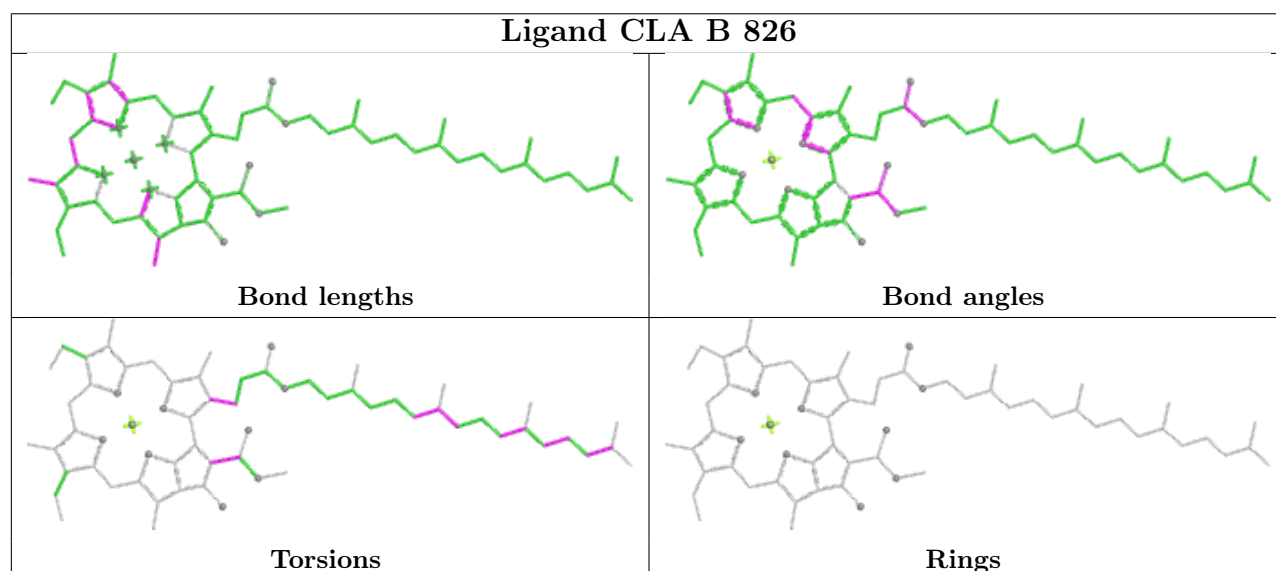
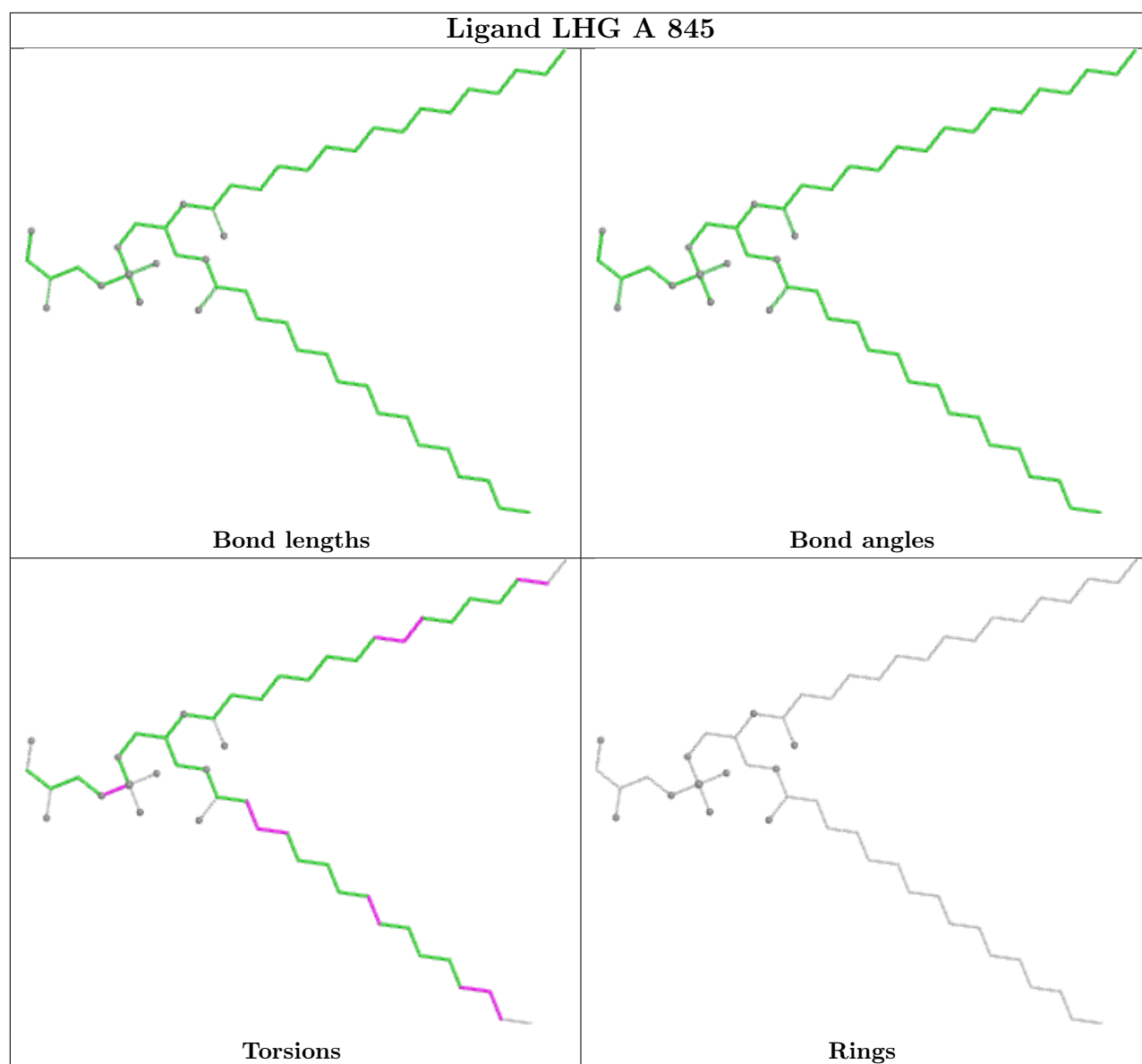


Rings

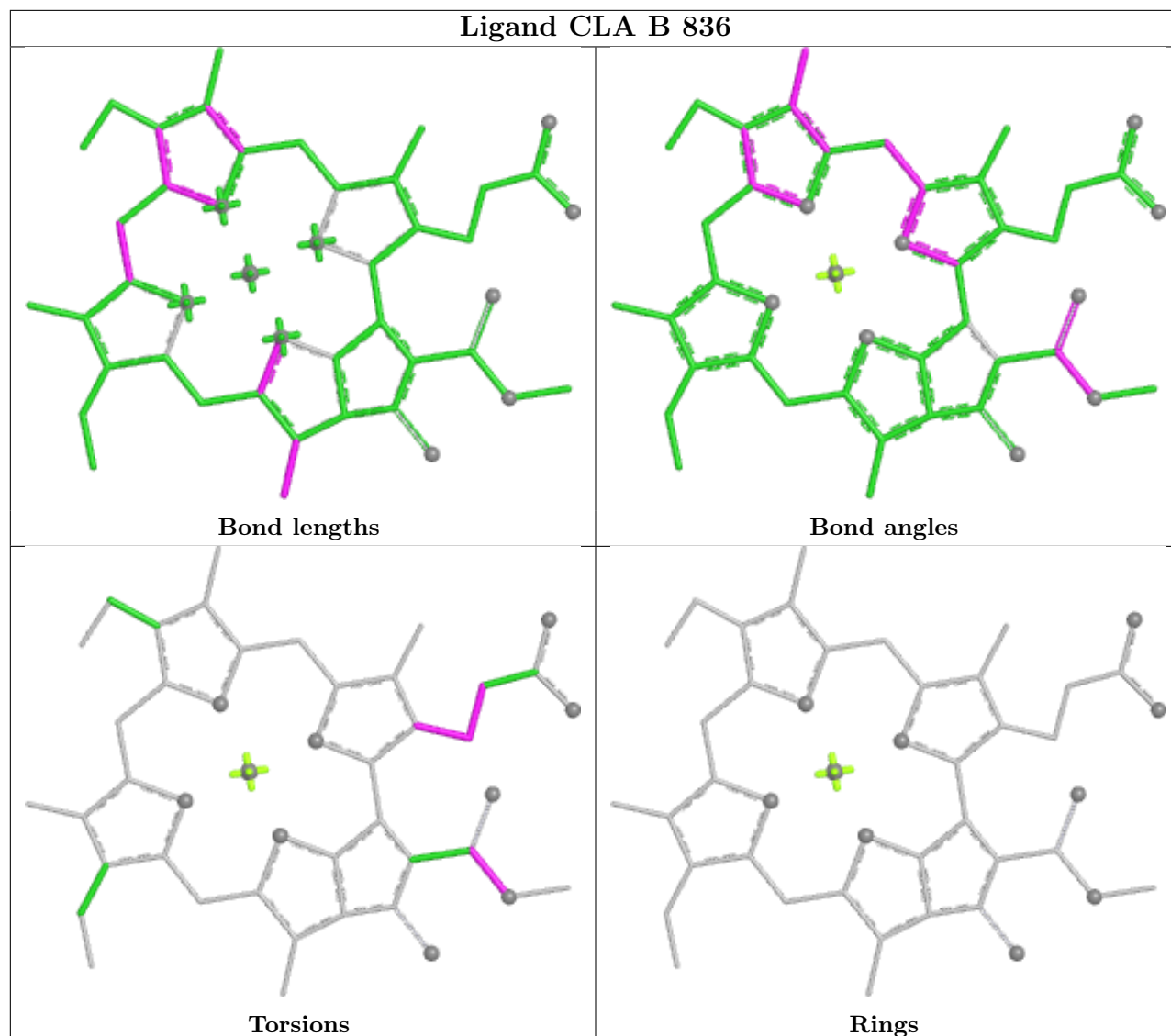




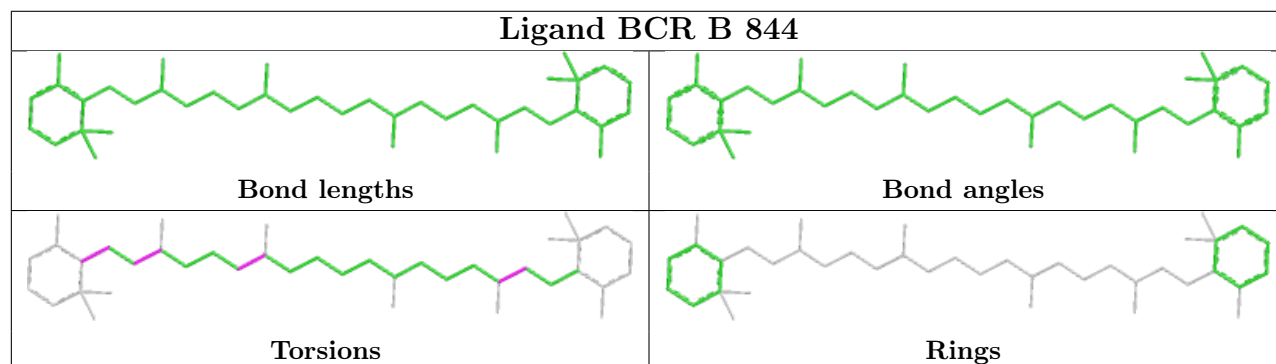




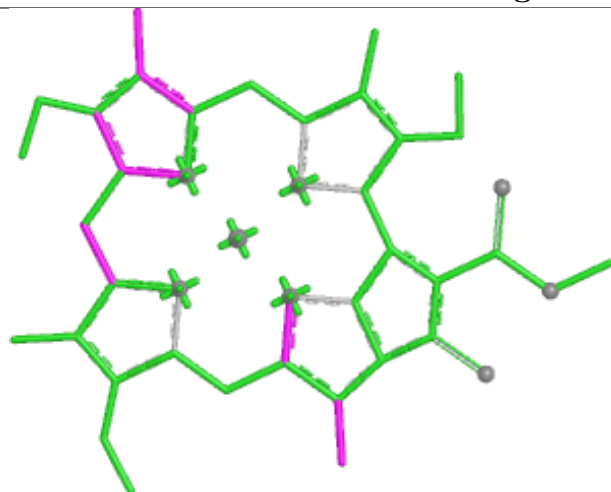
Ligand CLA B 836



Ligand BCR B 844



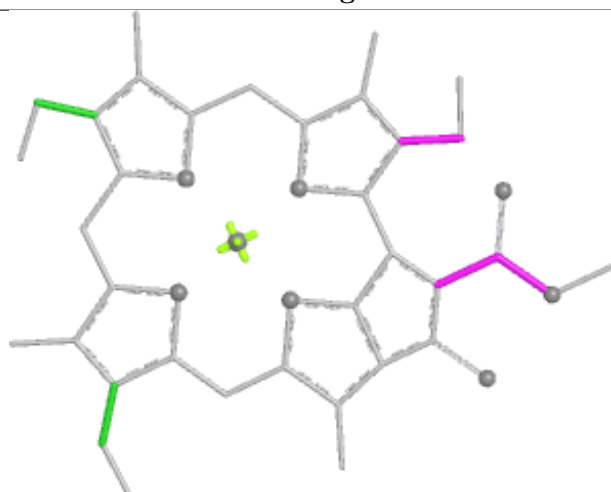
Ligand CLA A 820



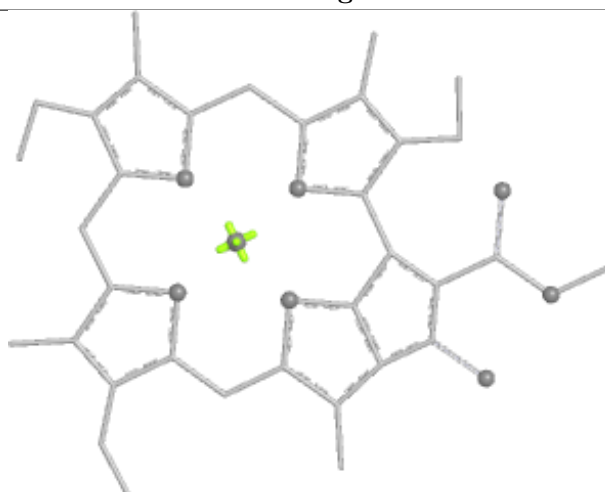
Bond lengths



Bond angles

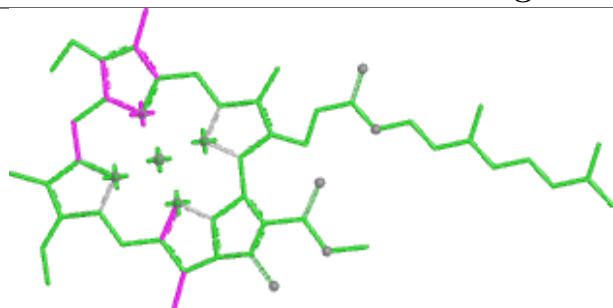


Torsions

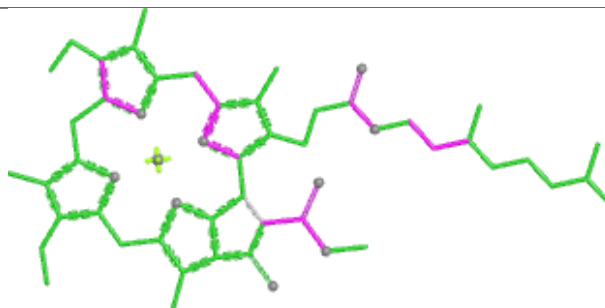


Rings

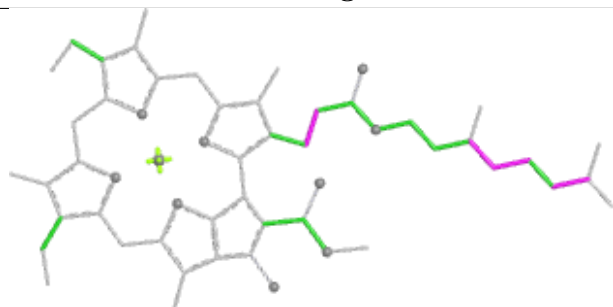
Ligand CLA B 808



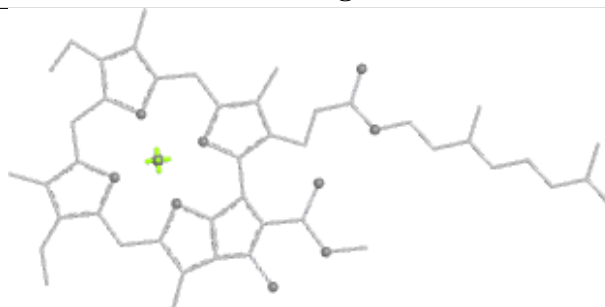
Bond lengths



Bond angles

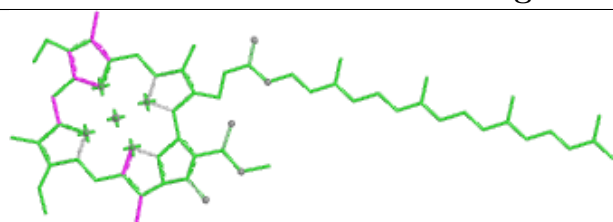


Torsions

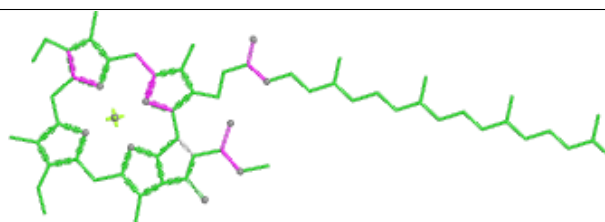


Rings

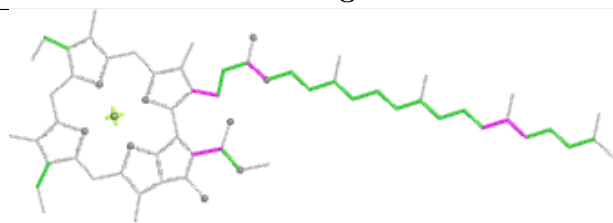
Ligand CLA B 830



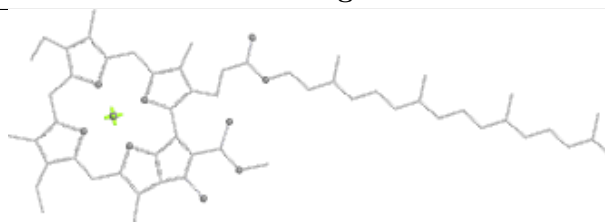
Bond lengths



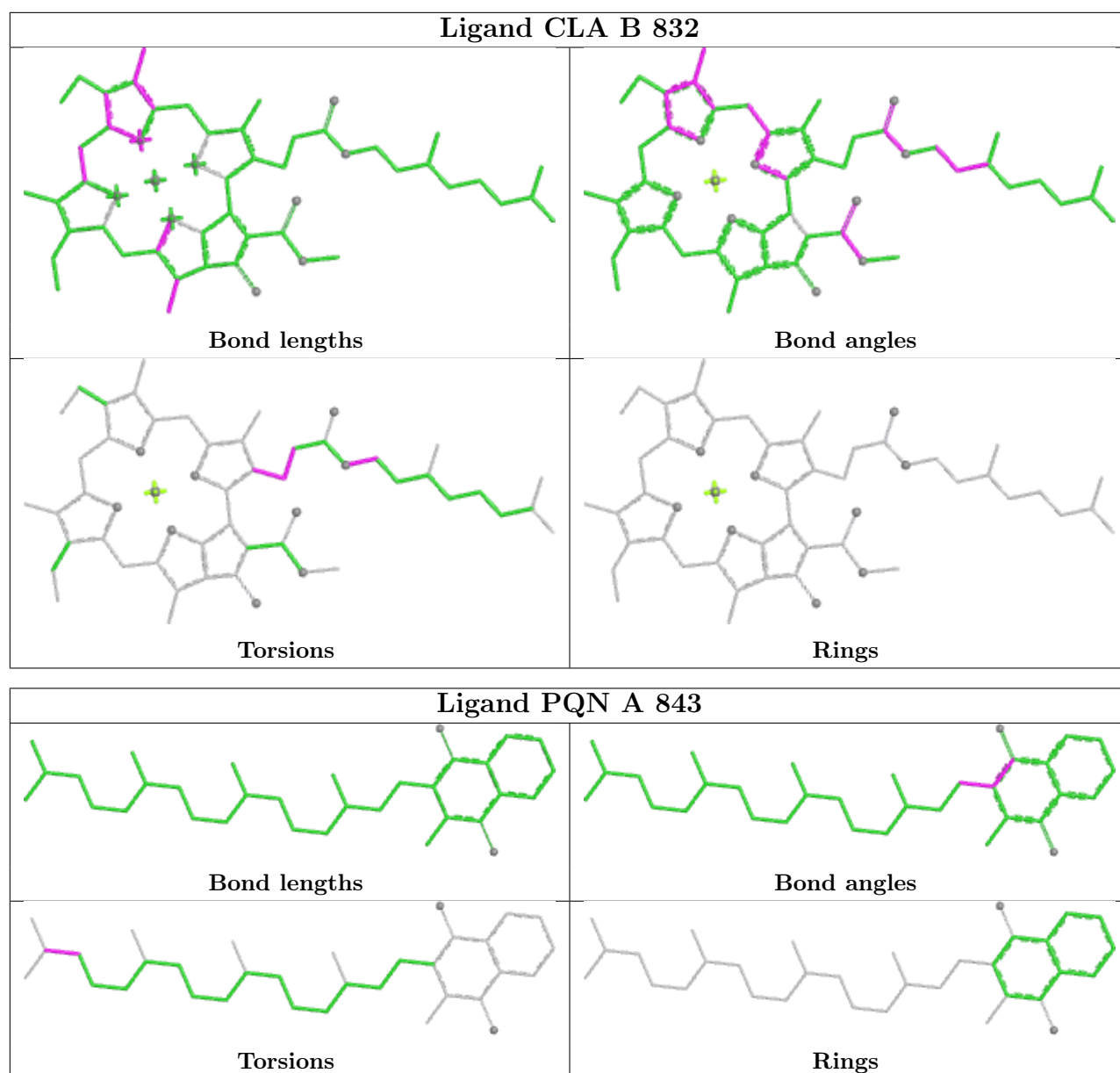
Bond angles

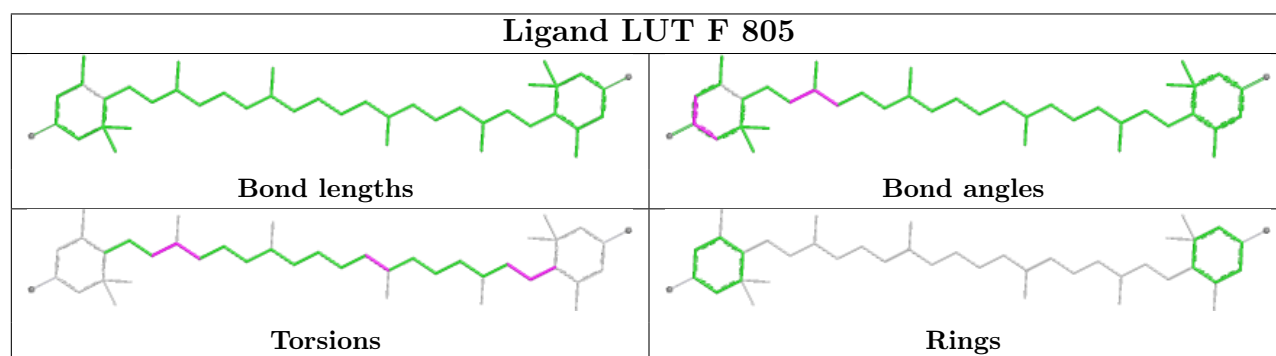
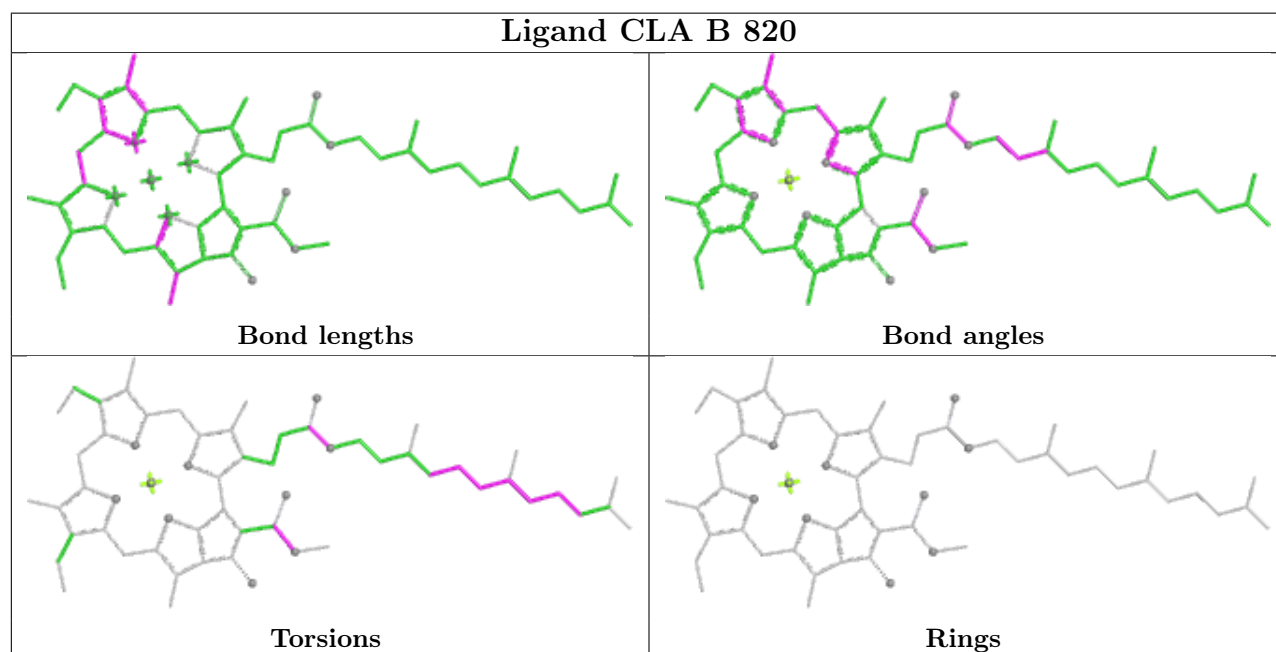
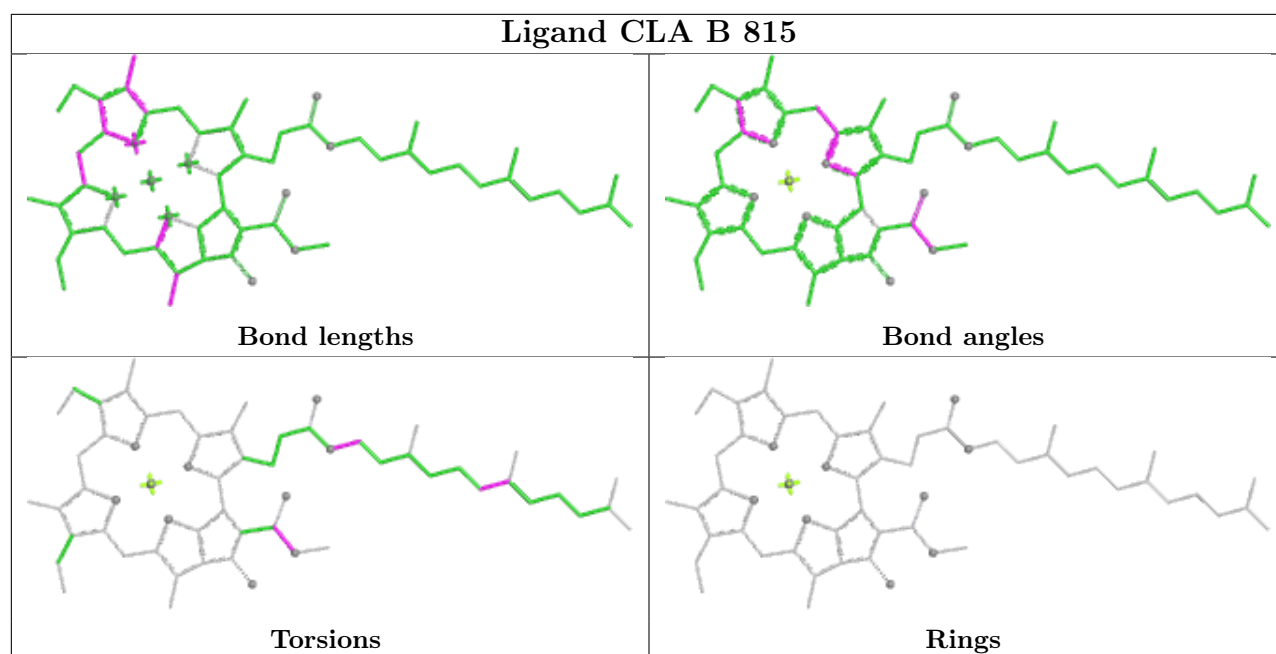


Torsions

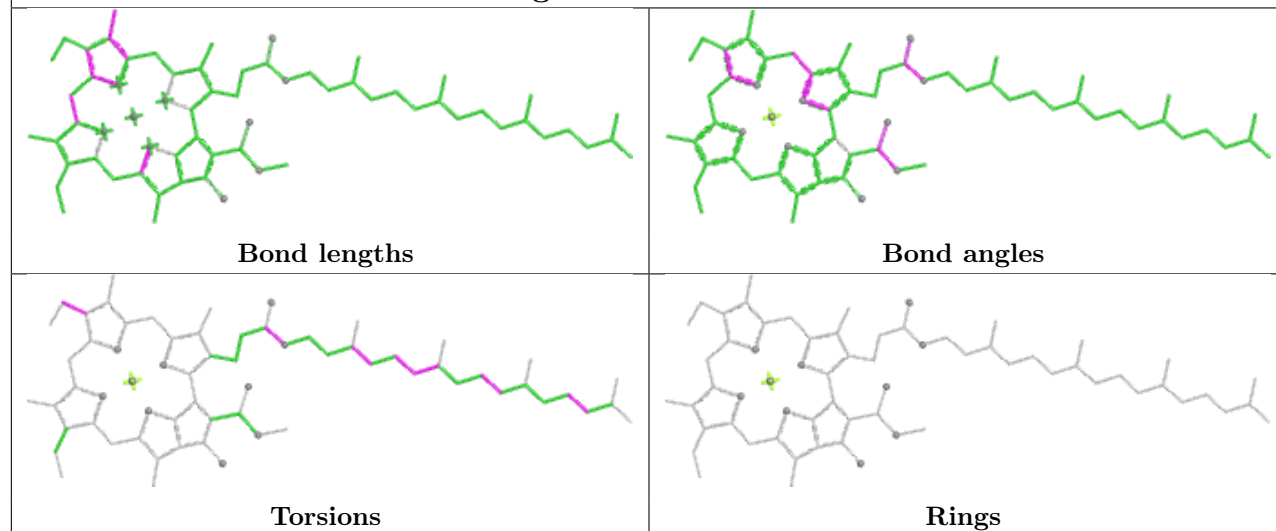


Rings

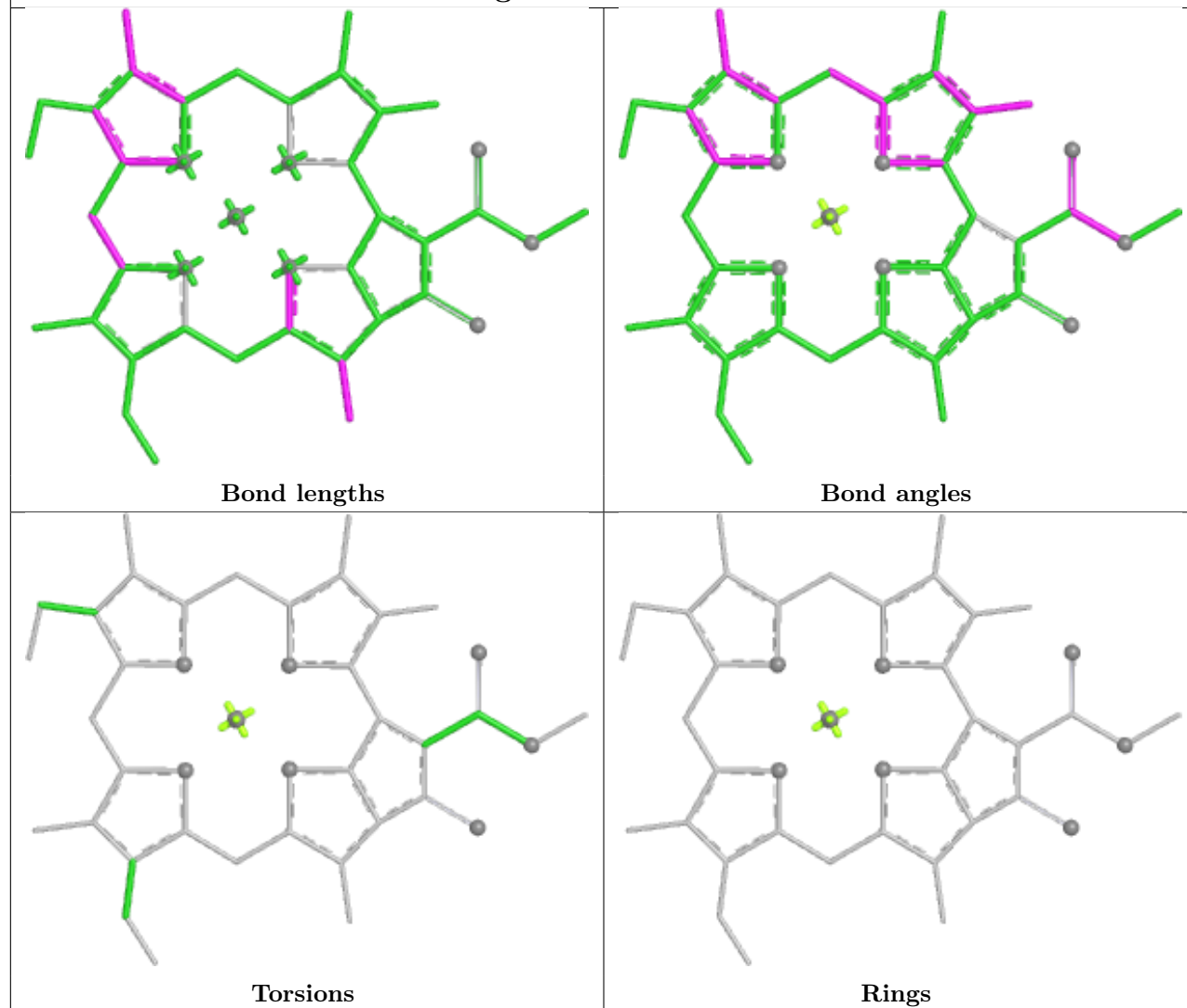




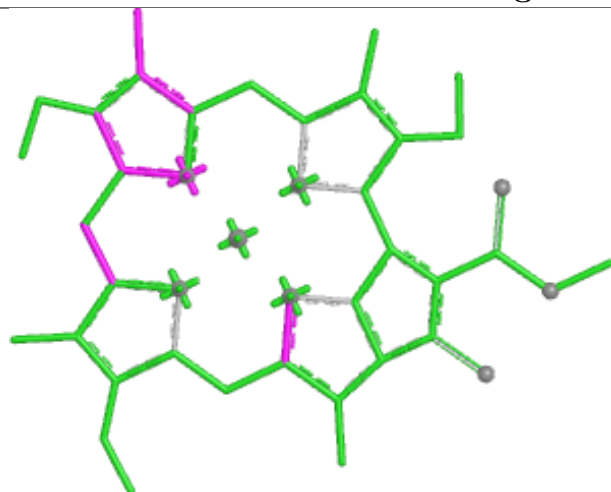
Ligand CLA B 812



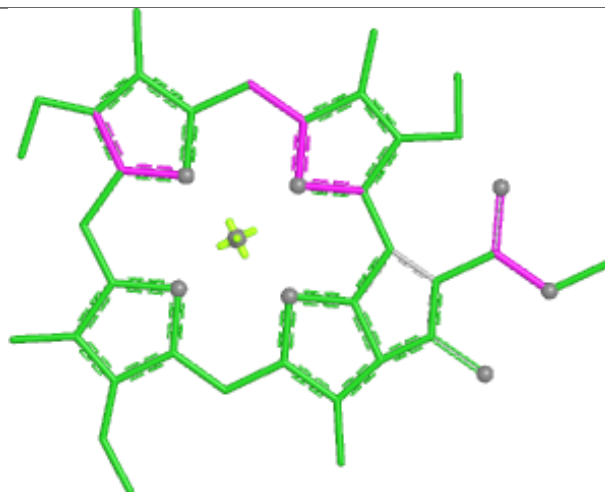
Ligand CLA B 813



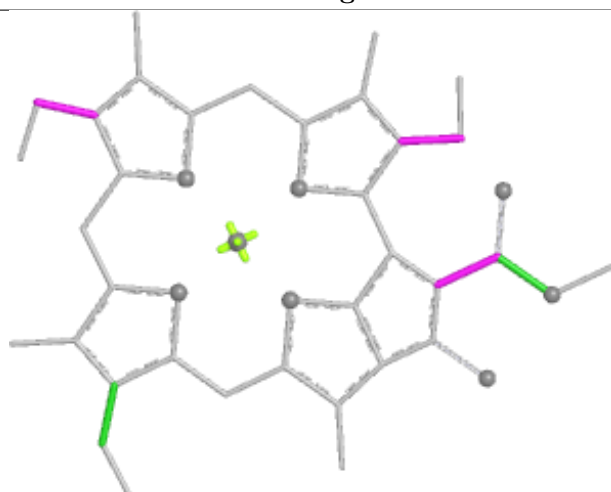
Ligand CLA B 822



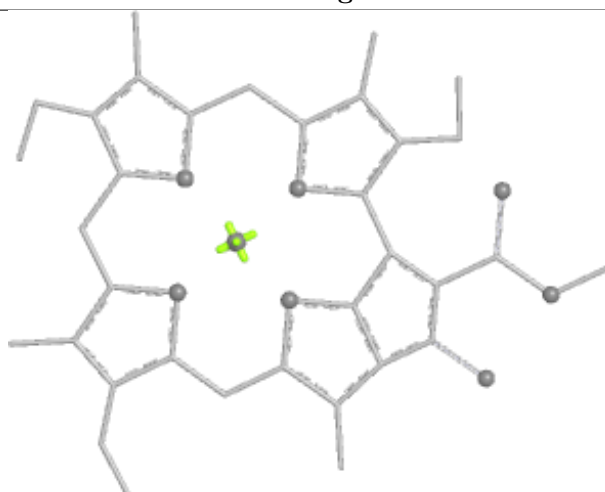
Bond lengths



Bond angles

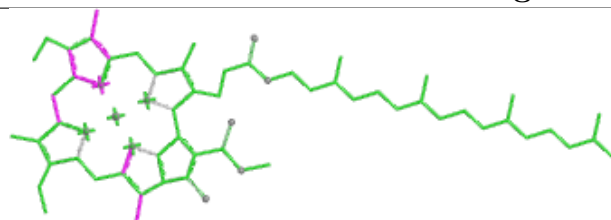


Torsions

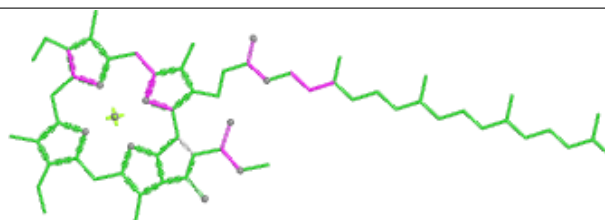


Rings

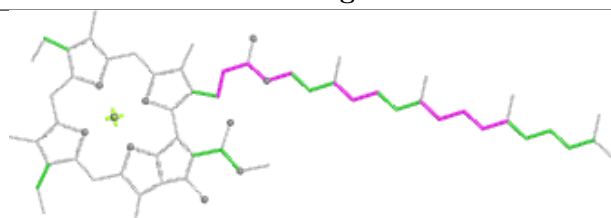
Ligand CLA A 842



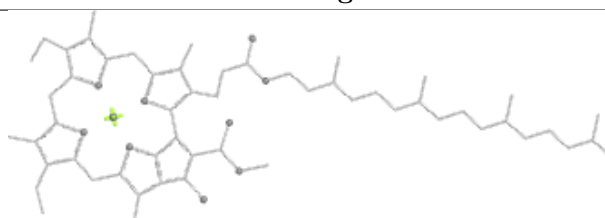
Bond lengths



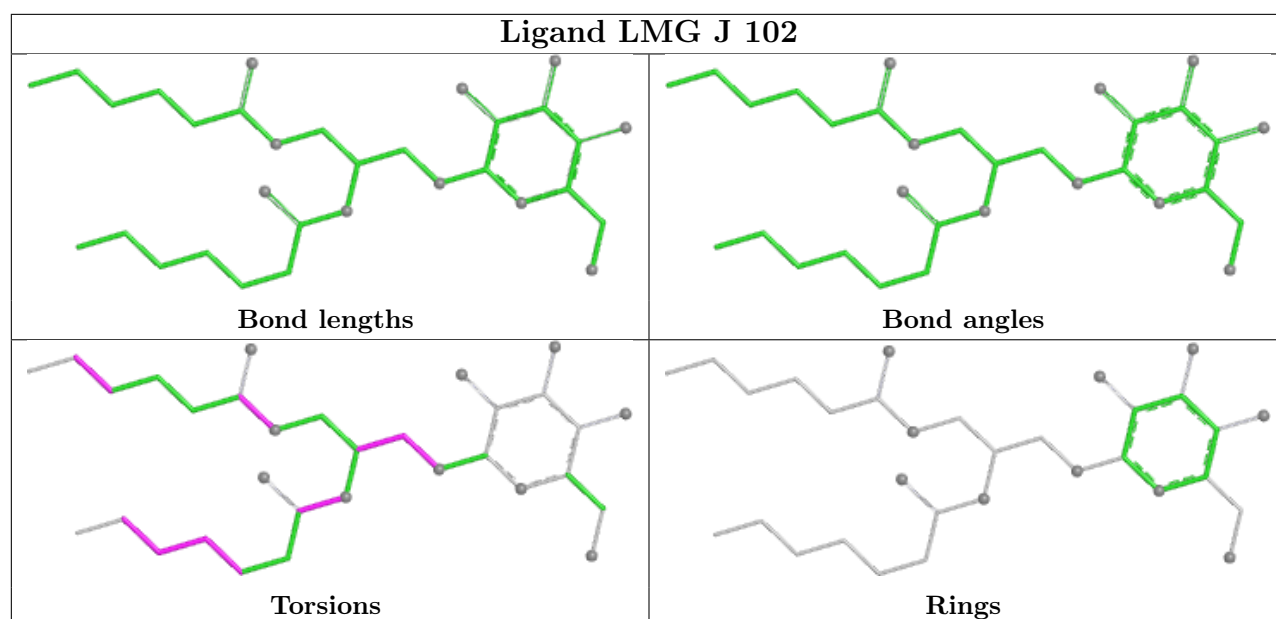
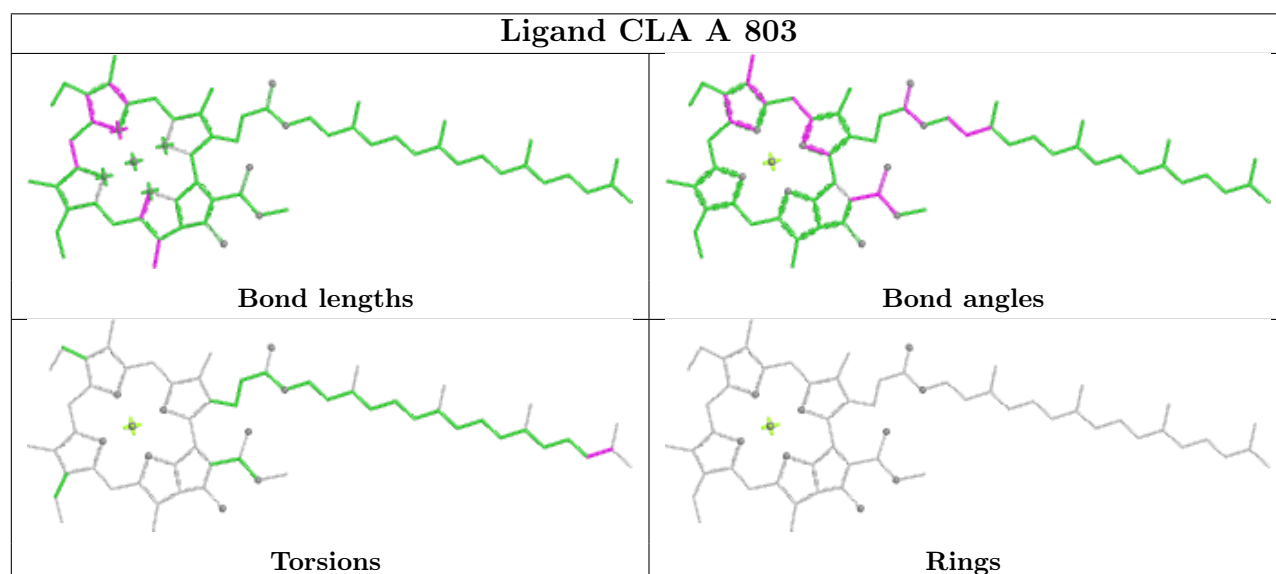
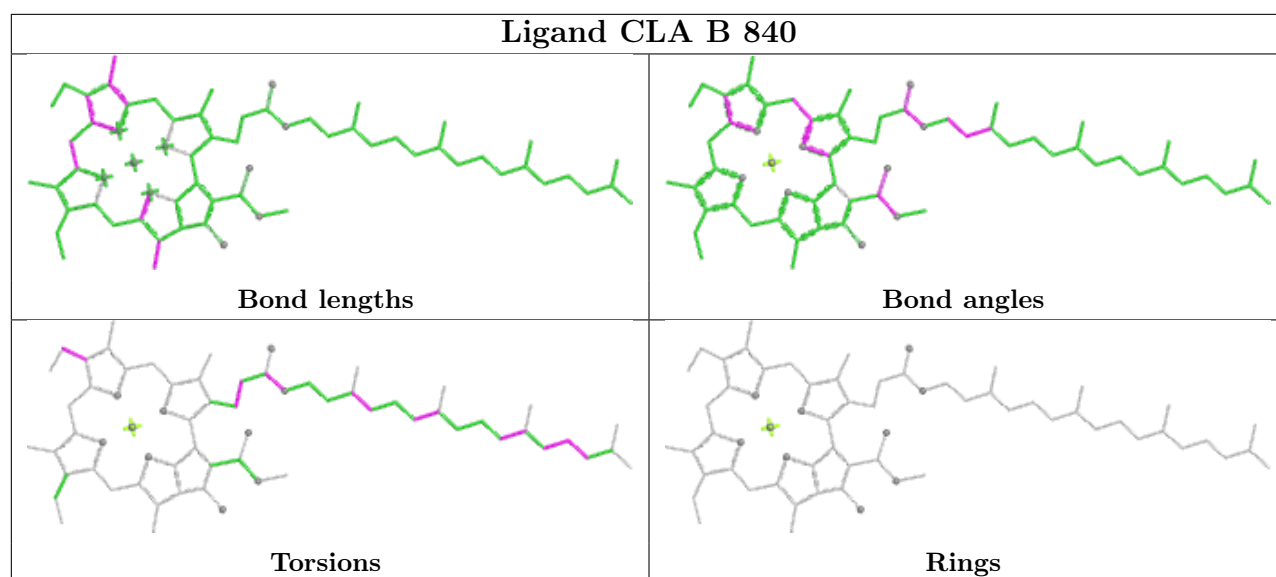
Bond angles



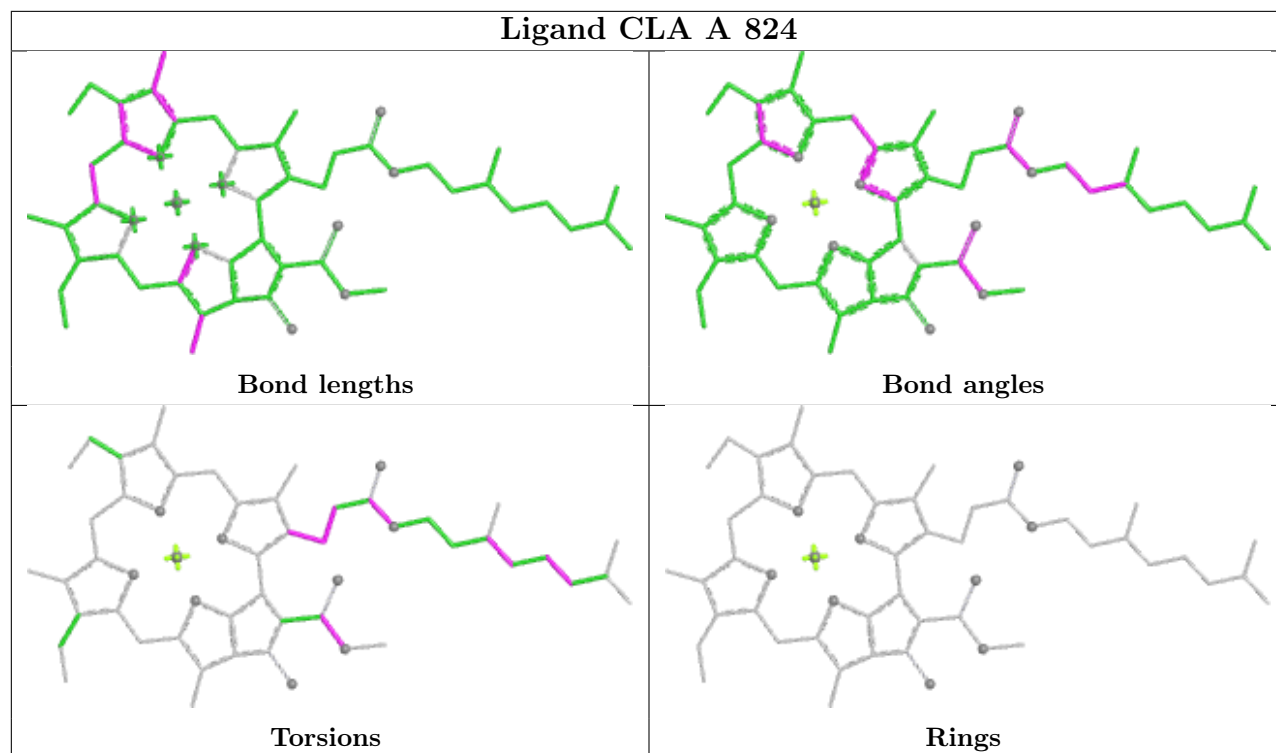
Torsions



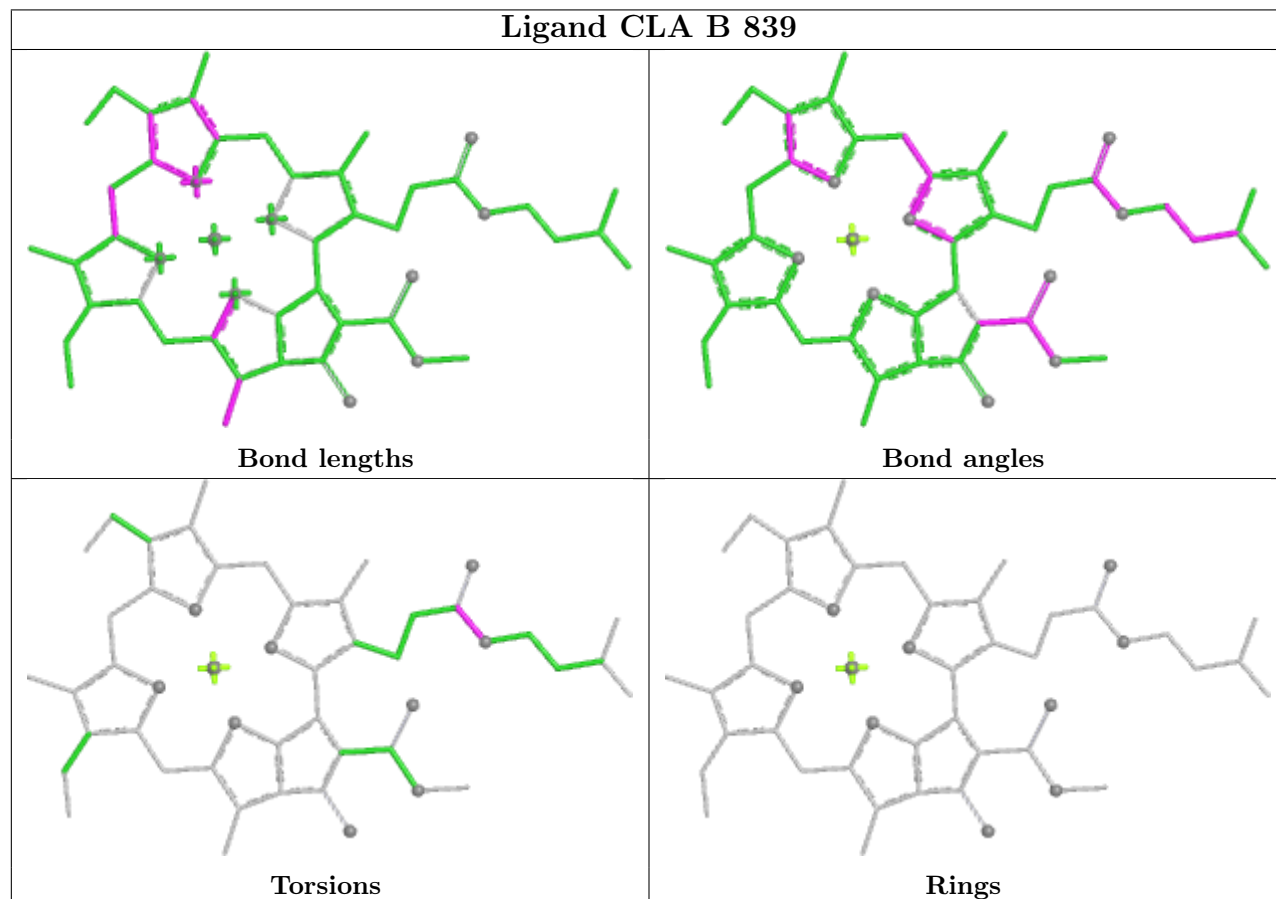
Rings

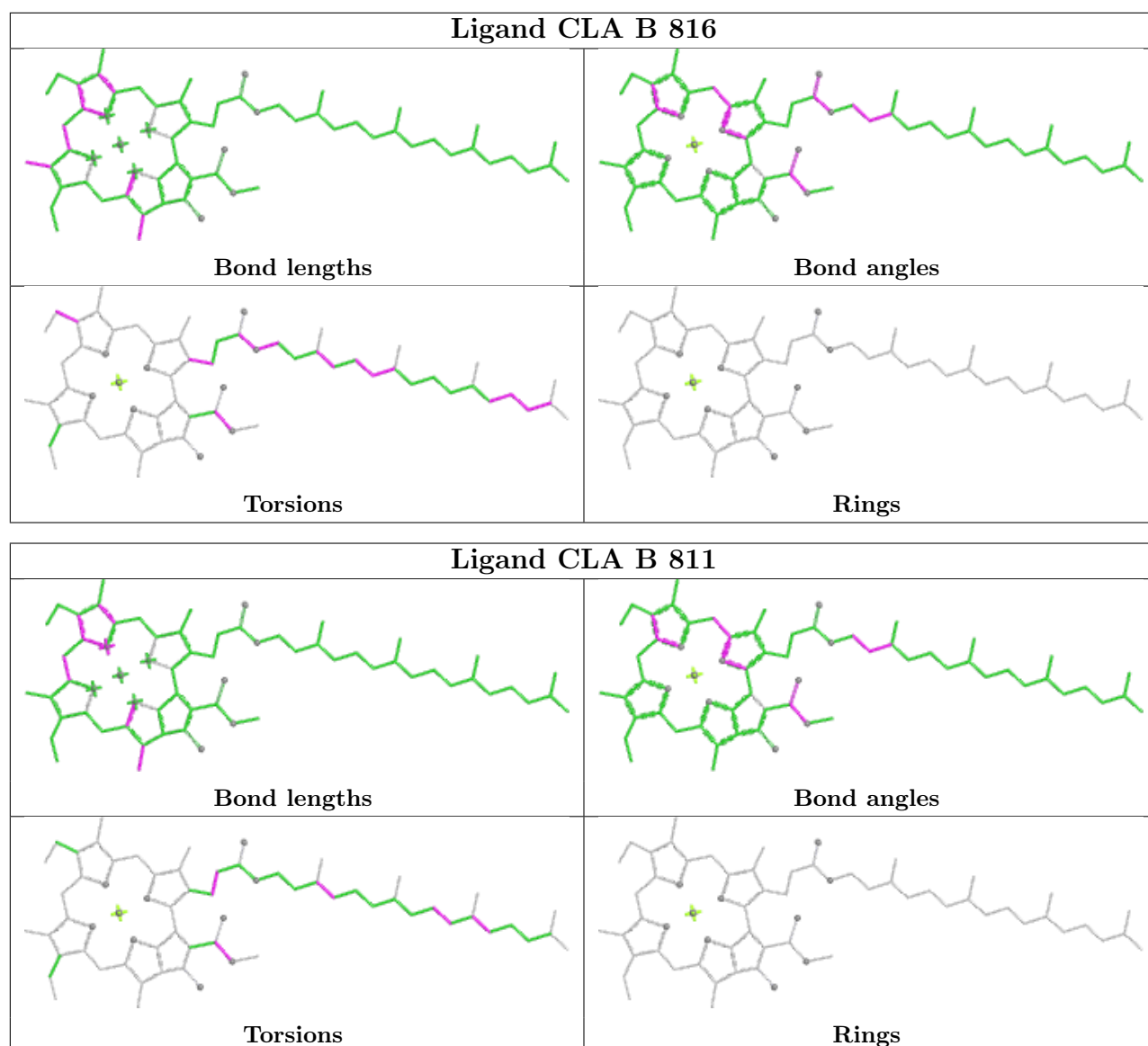


Ligand CLA A 824

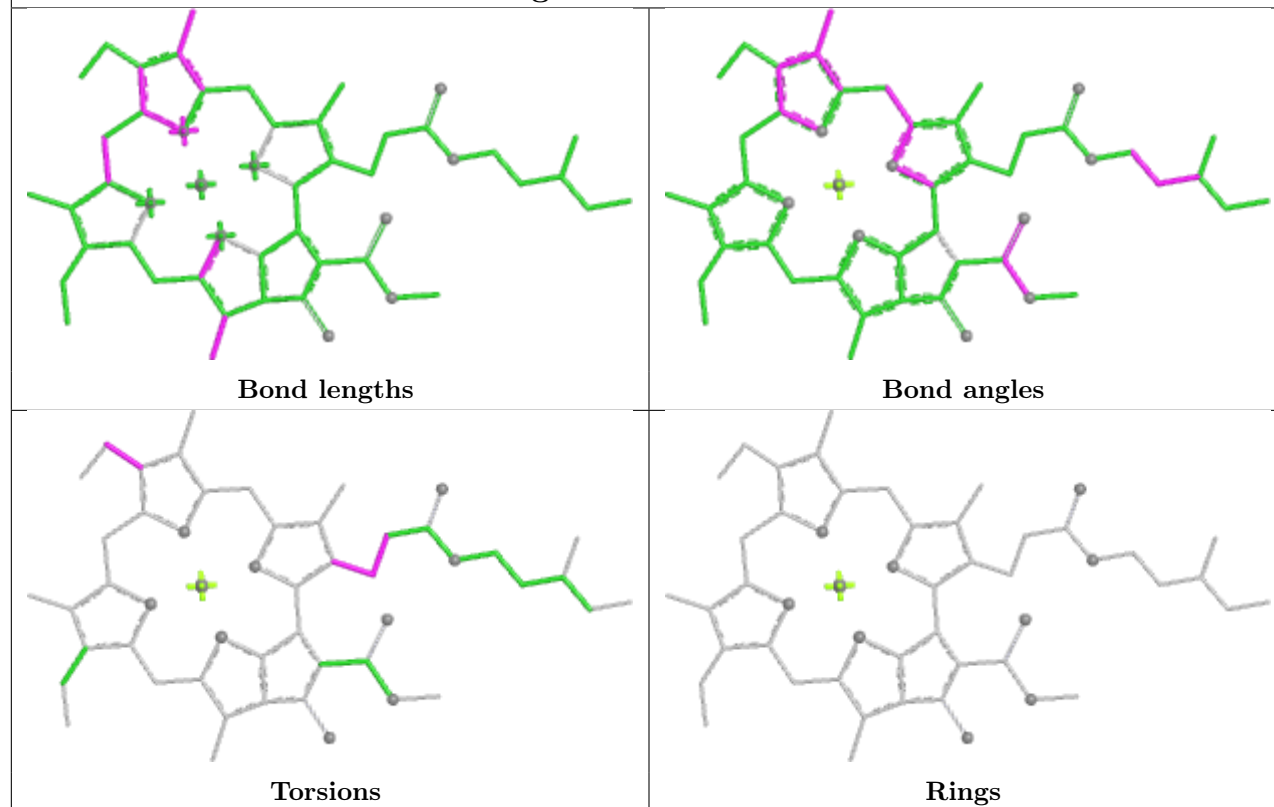


Ligand CLA B 839

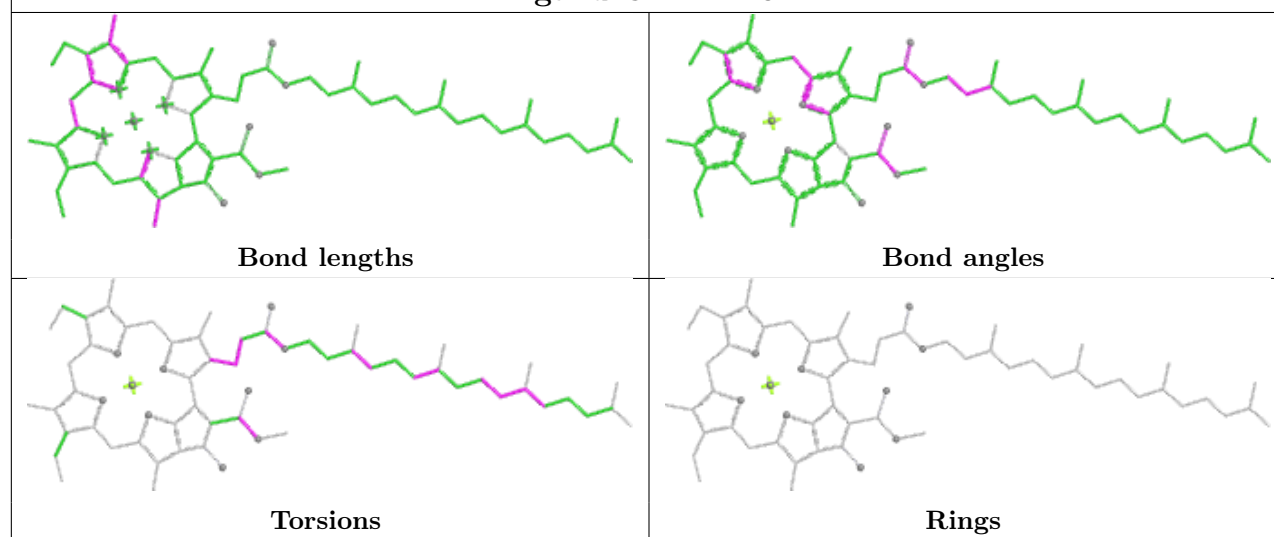


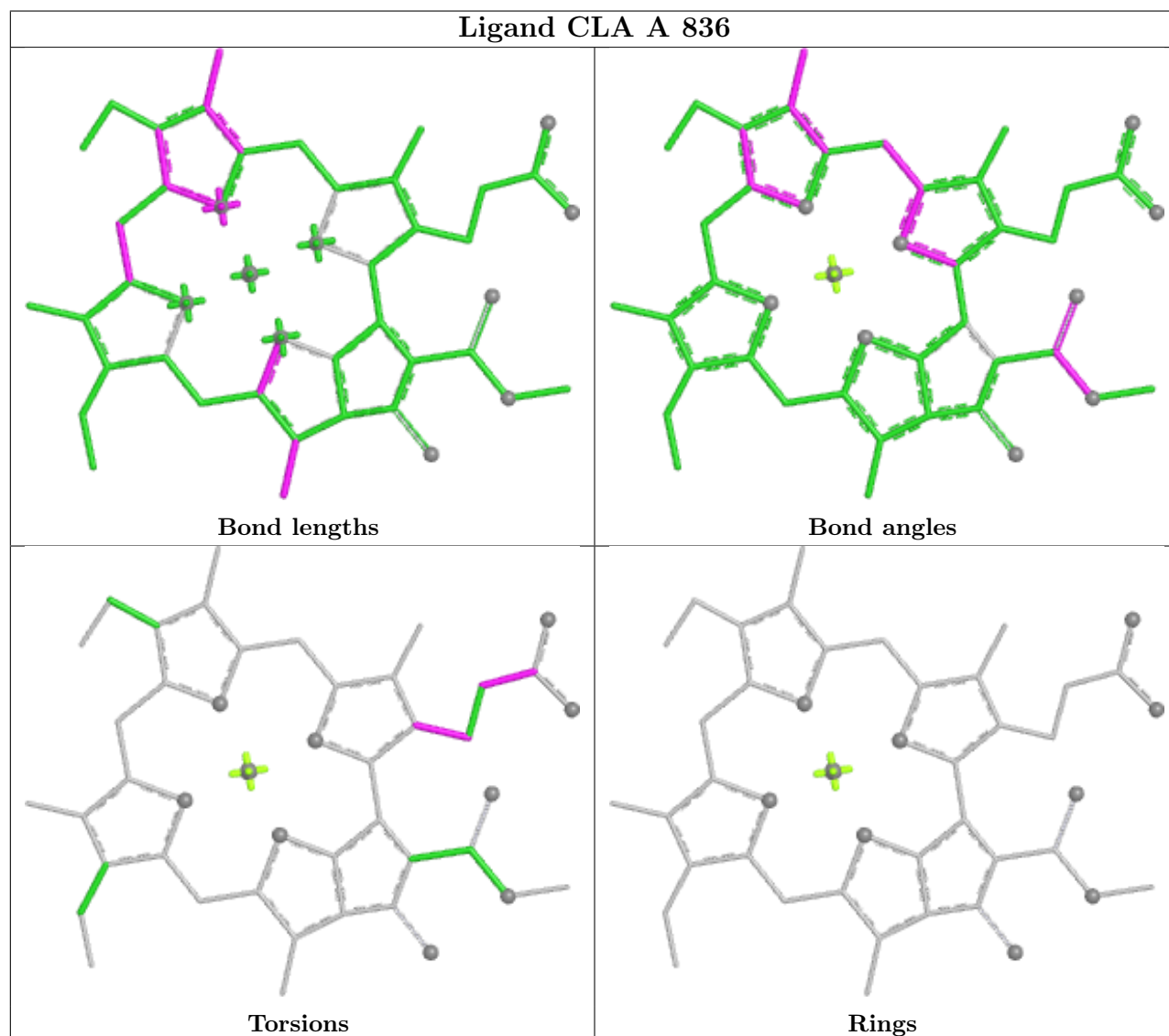
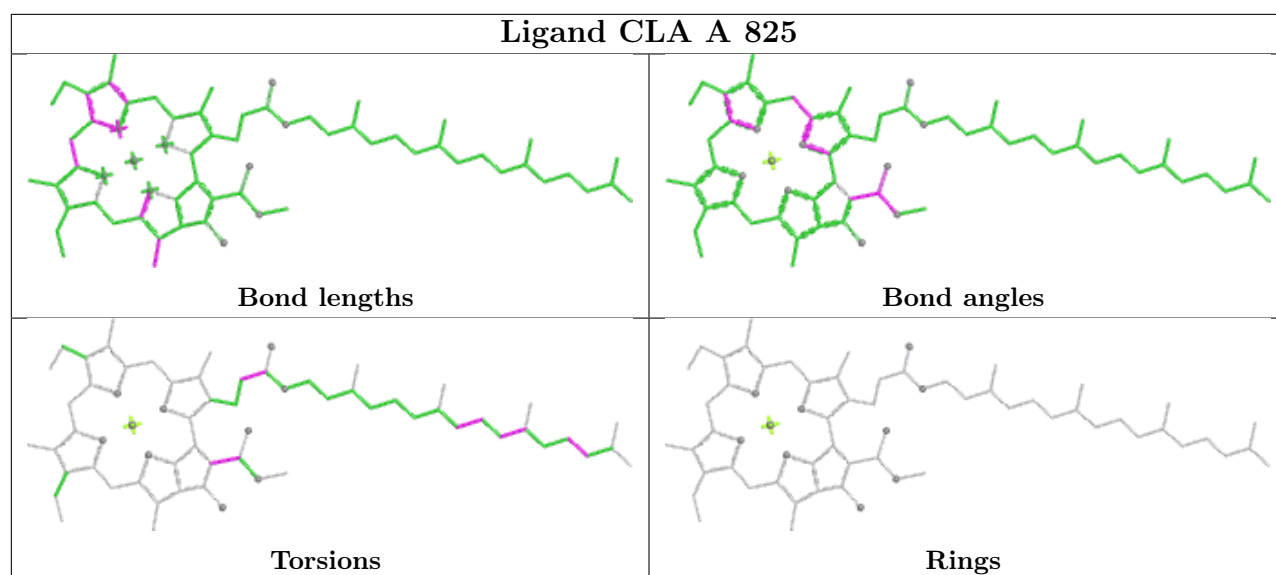


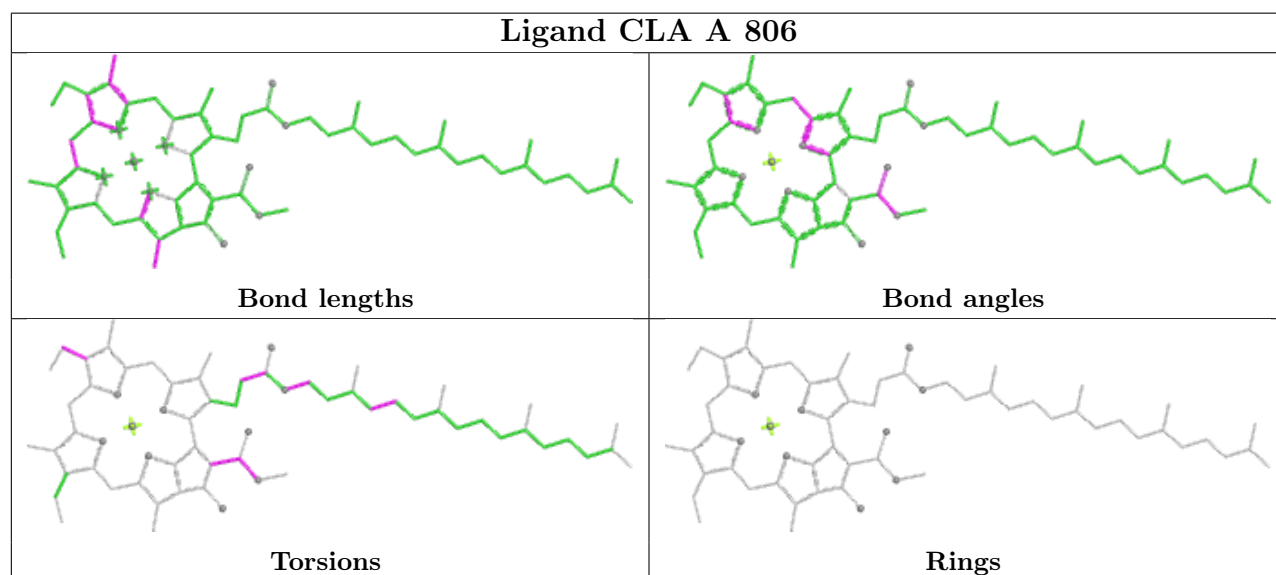
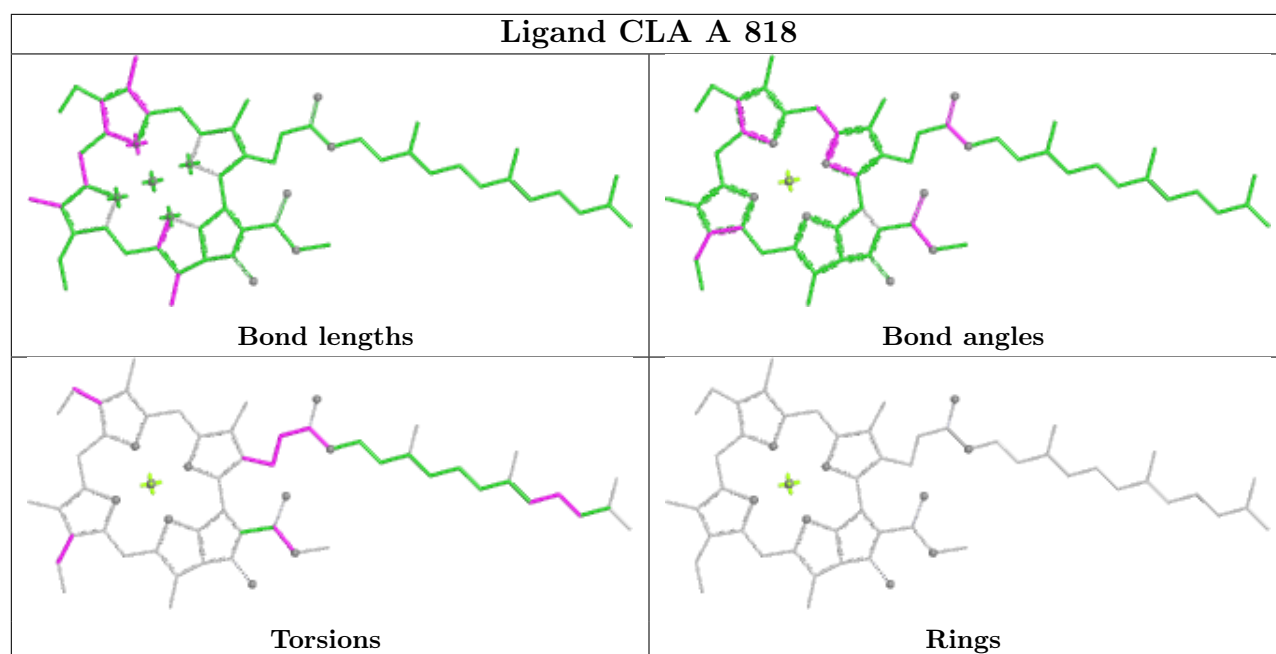
Ligand CLA A 837

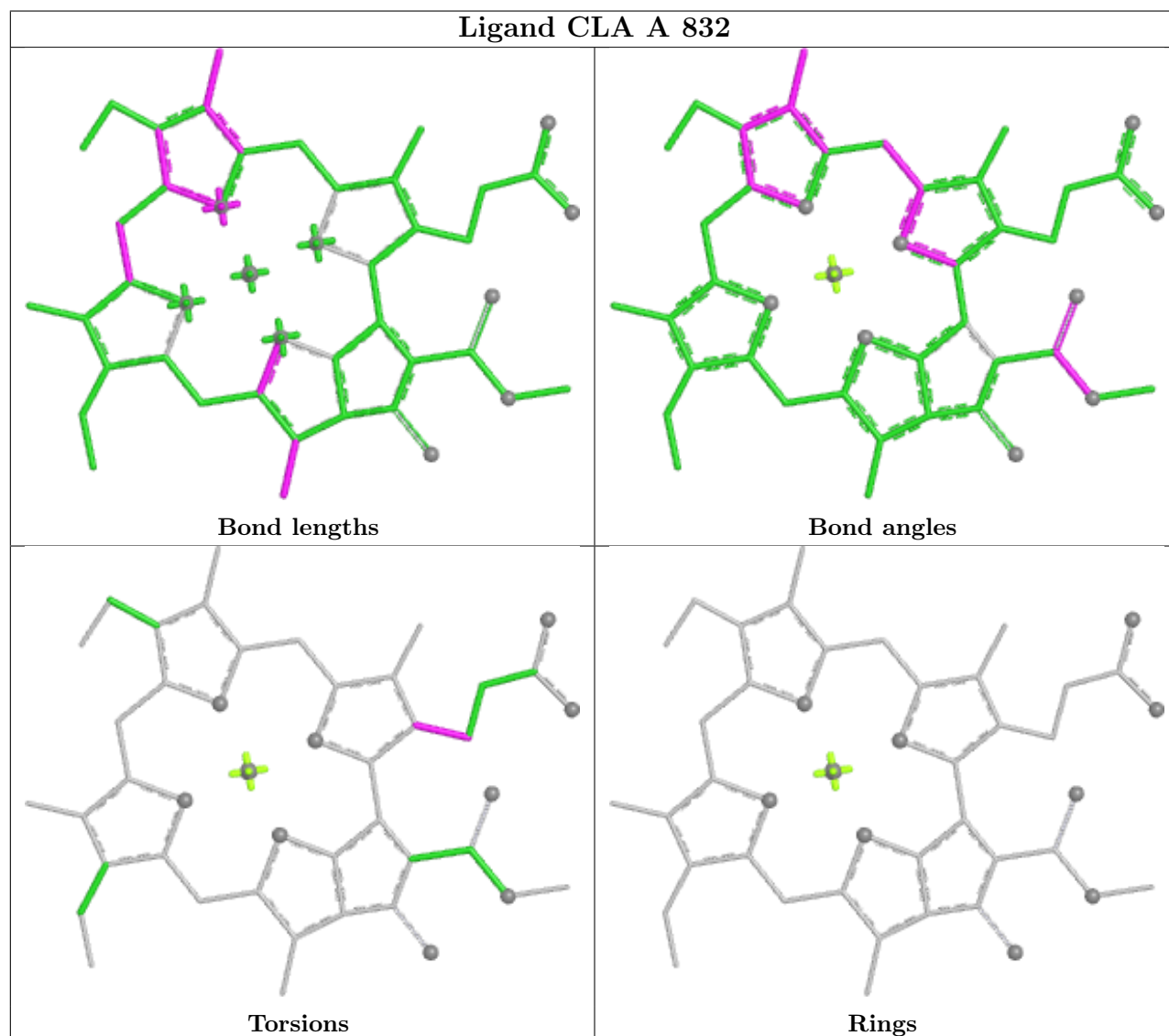
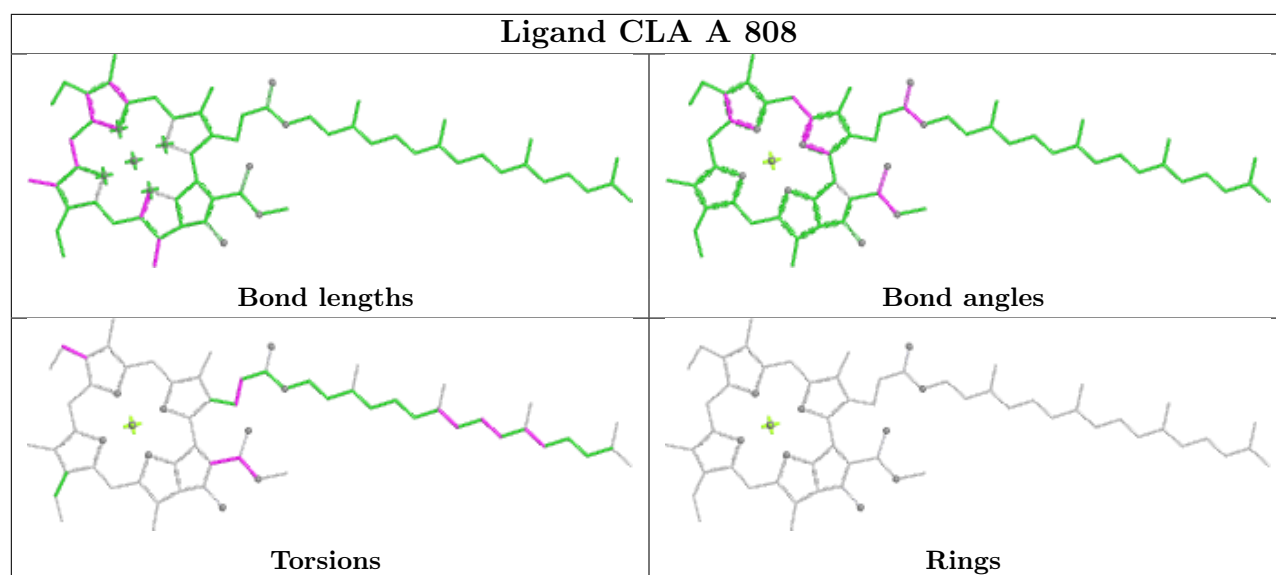


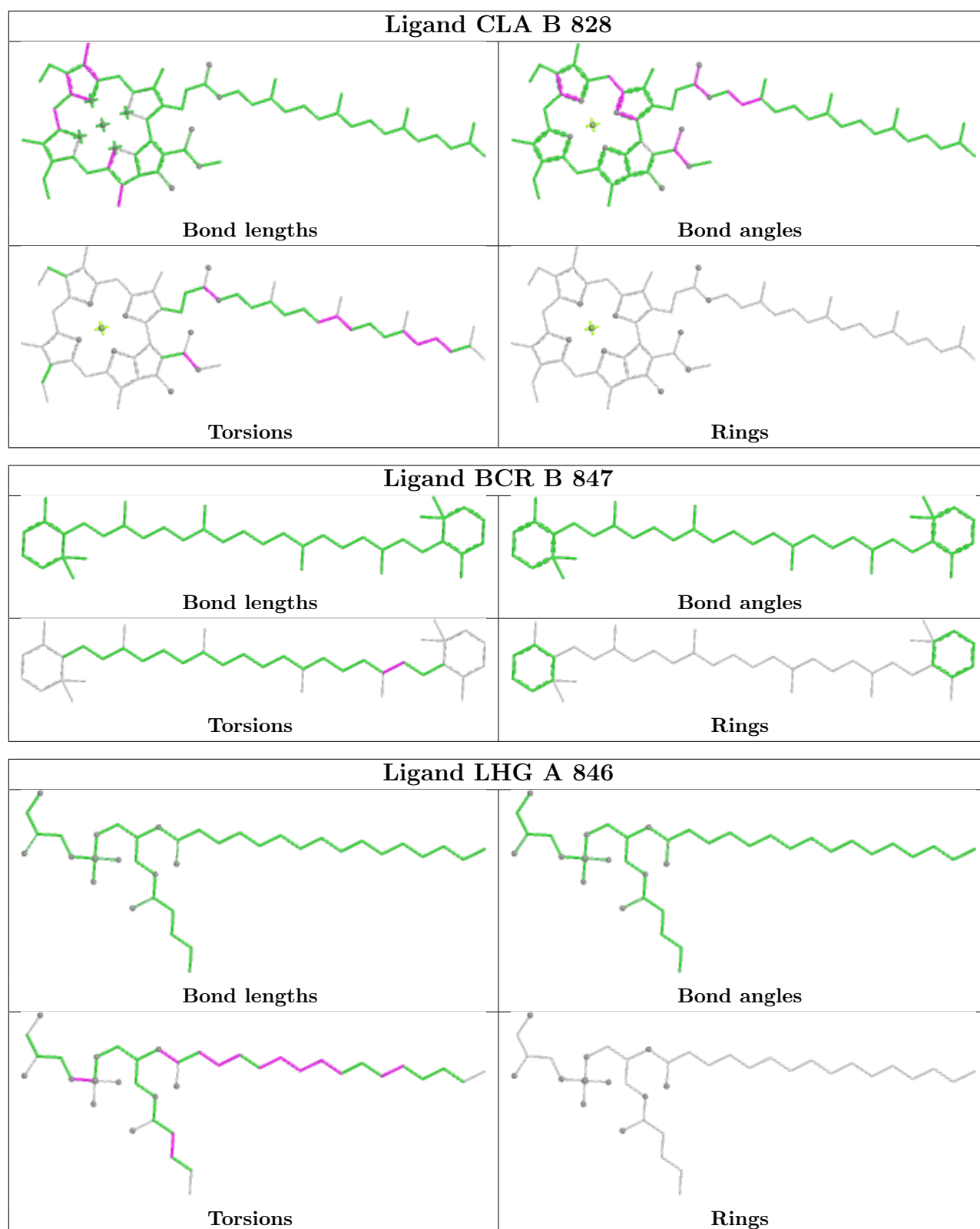
Ligand CLA L 202

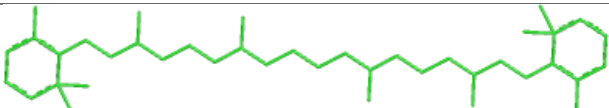
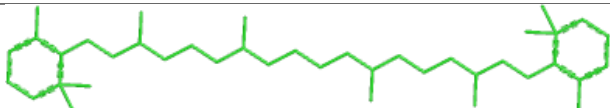
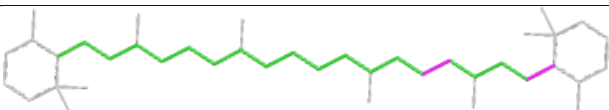
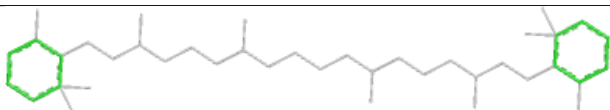




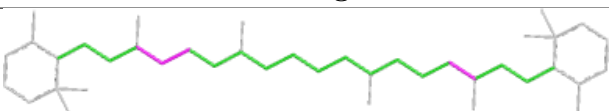
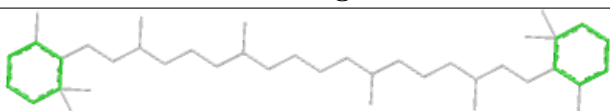


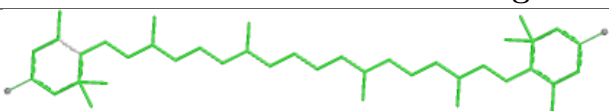
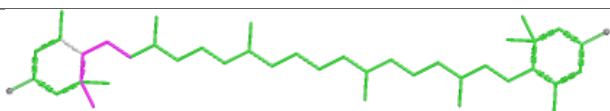
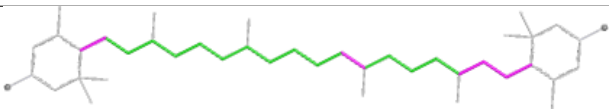
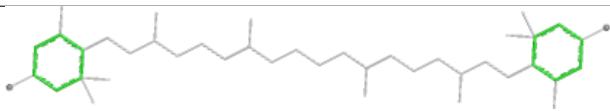


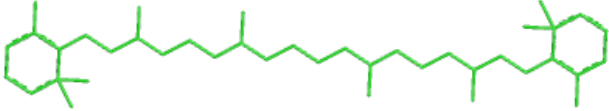
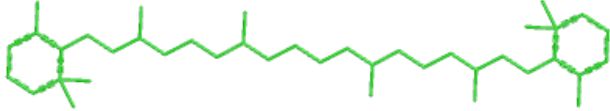
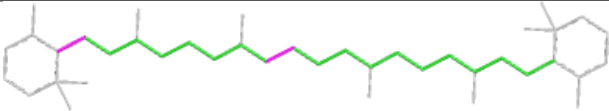
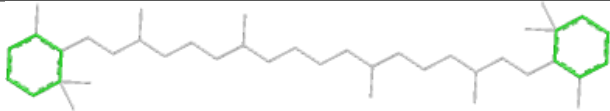


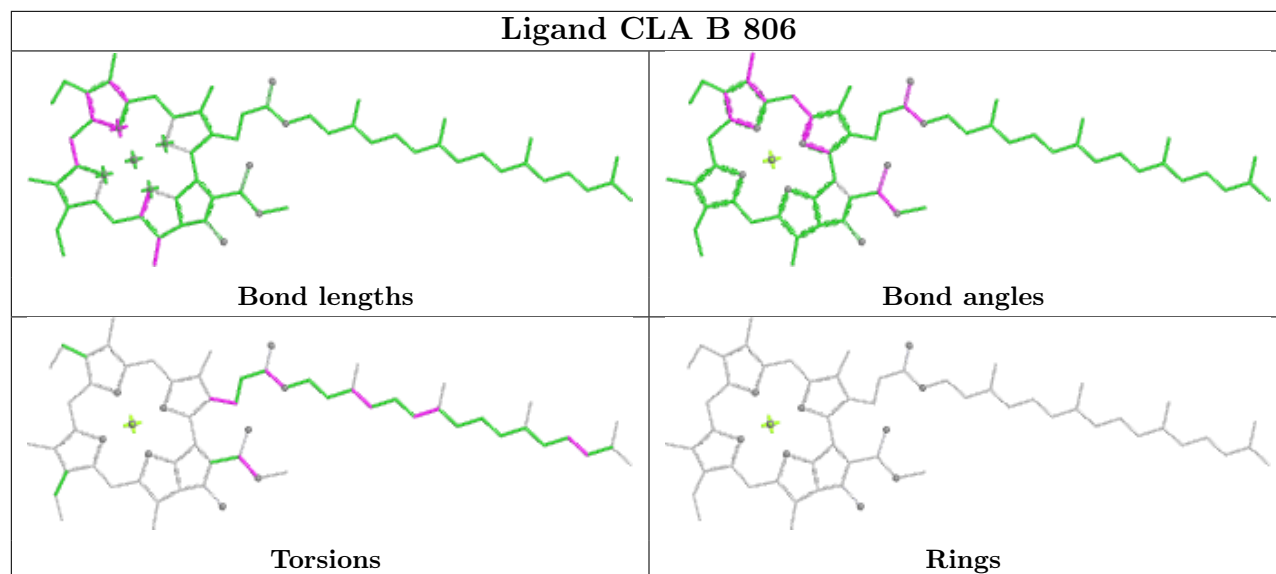
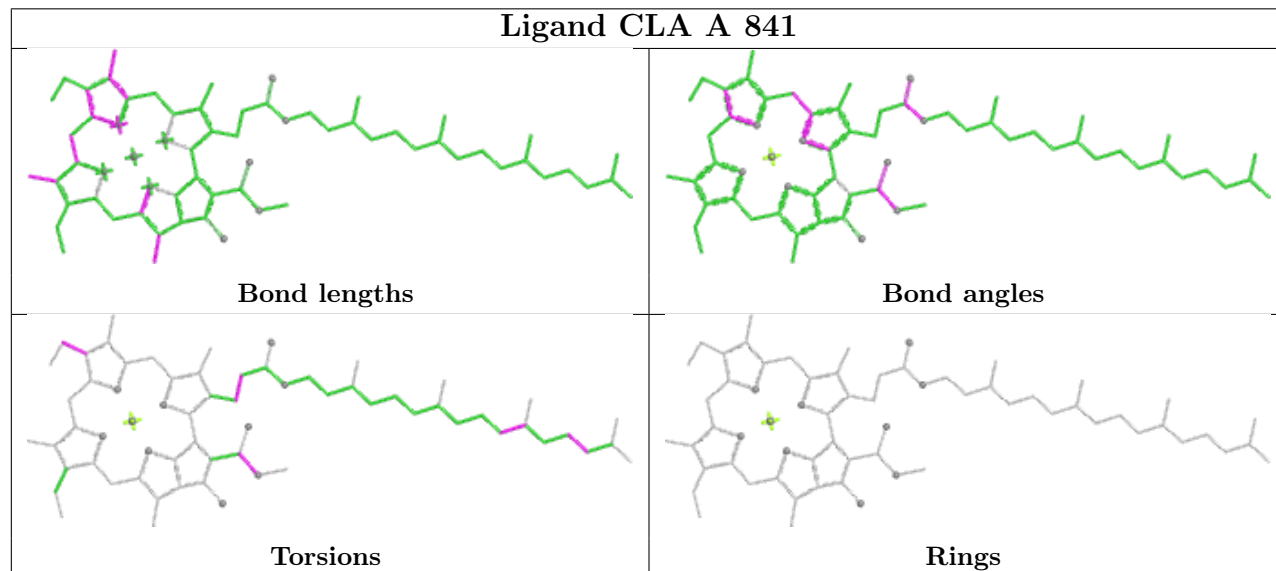


Ligand BCR B 846	
	
Bond lengths	Bond angles
	
Torsions	Rings

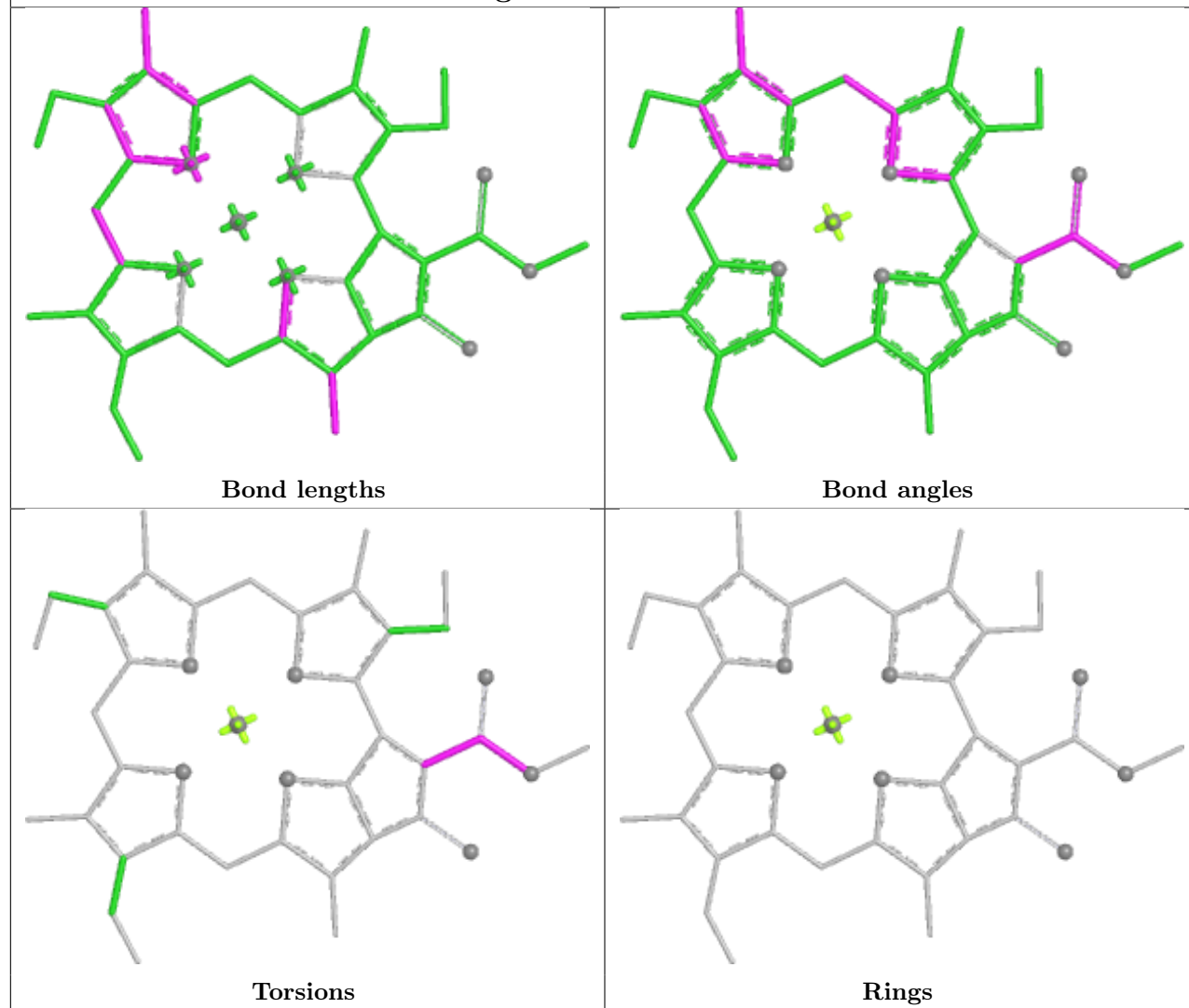
Ligand BCR B 845	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT J 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

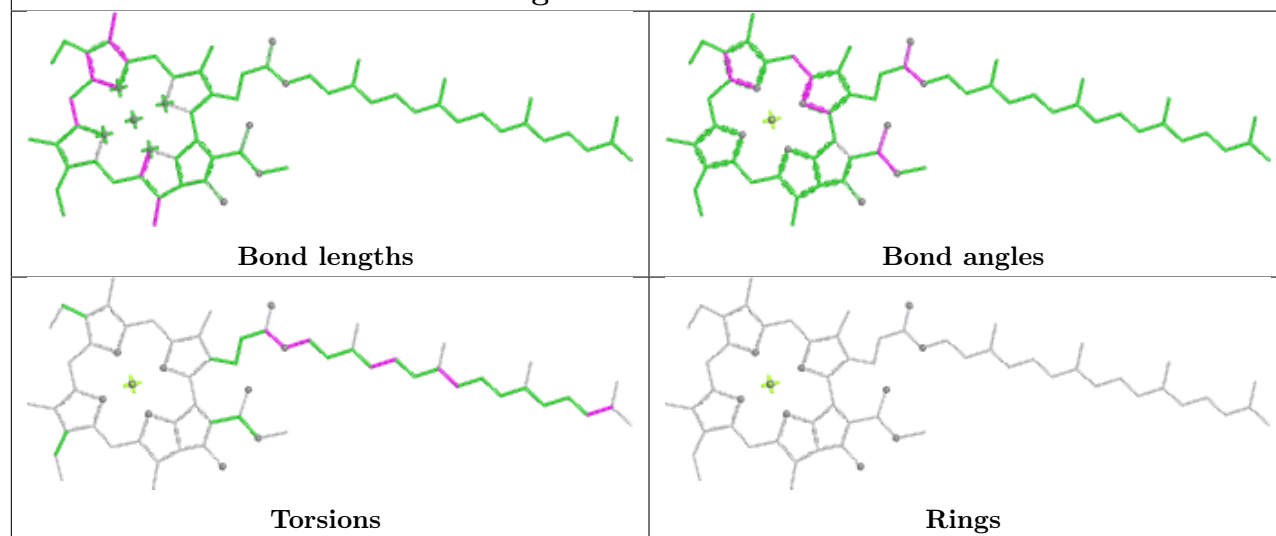
Ligand BCR B 848	
	
Bond lengths	Bond angles
	
Torsions	Rings

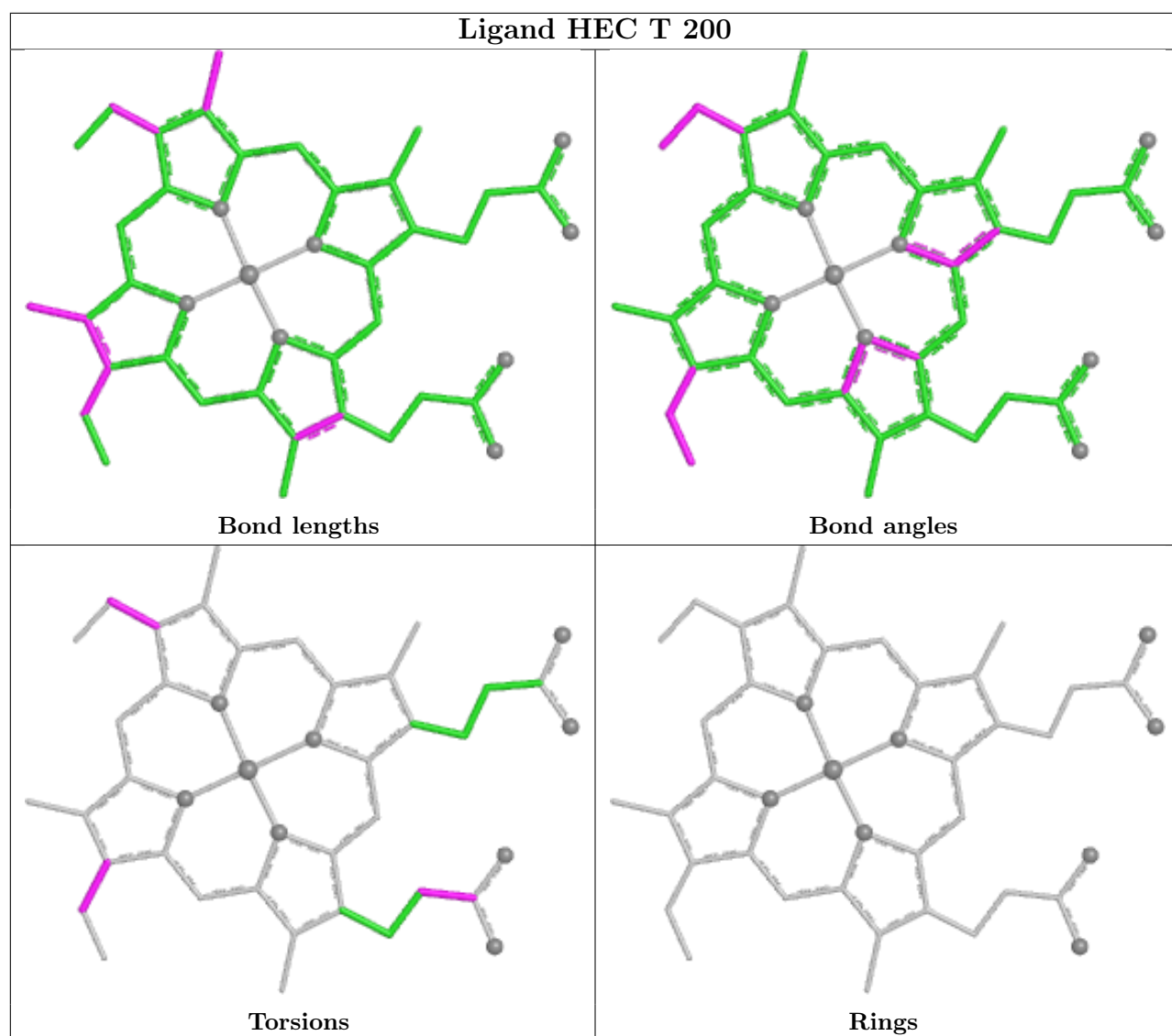
Ligand CLA B 806**Ligand CLA A 841**

Ligand CLA A 815

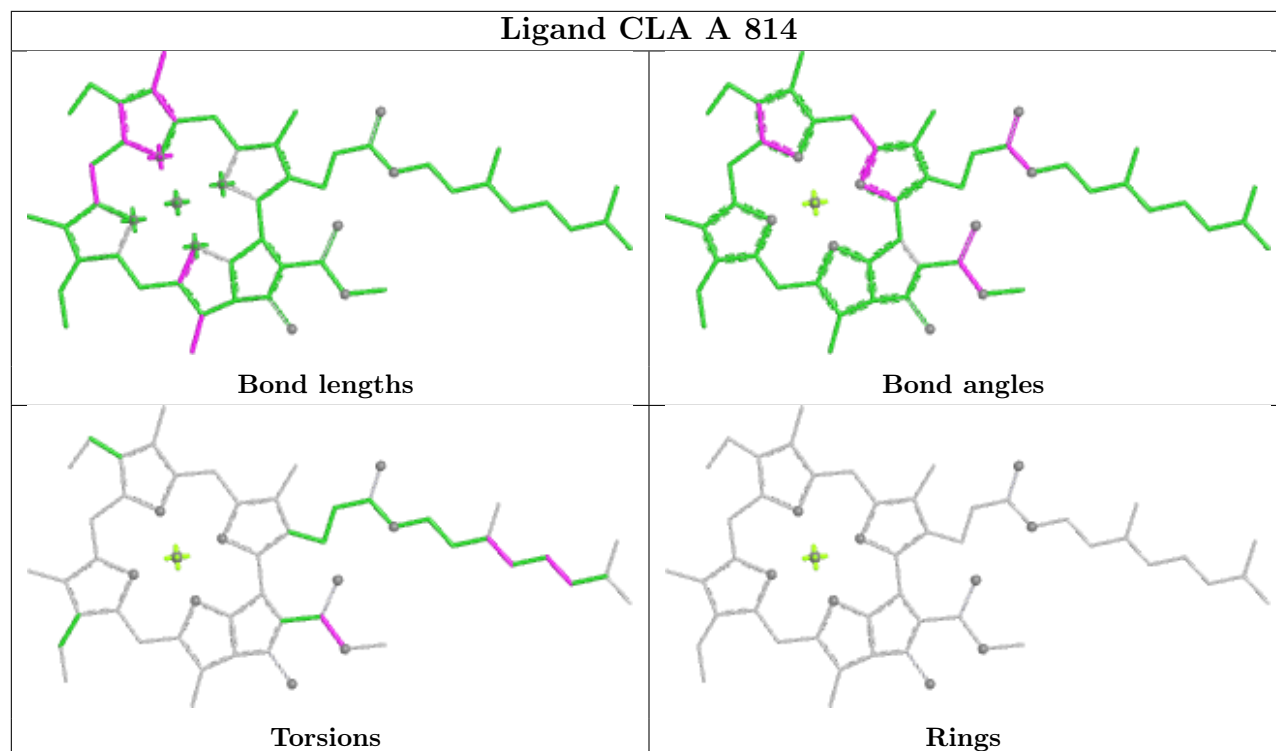


Ligand CLA A 835

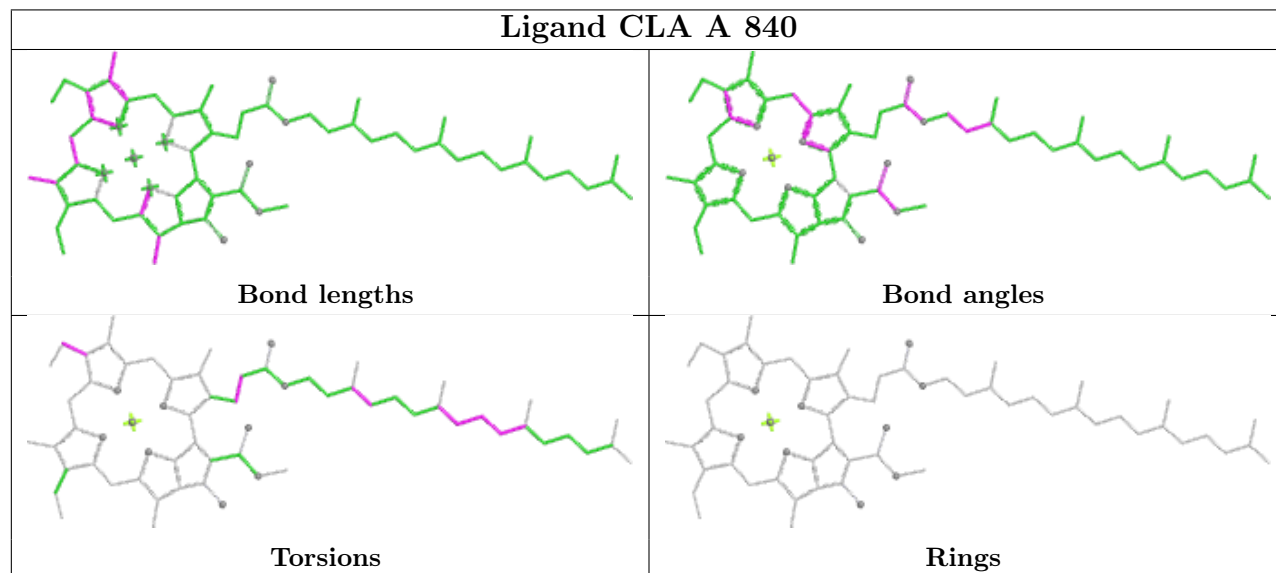


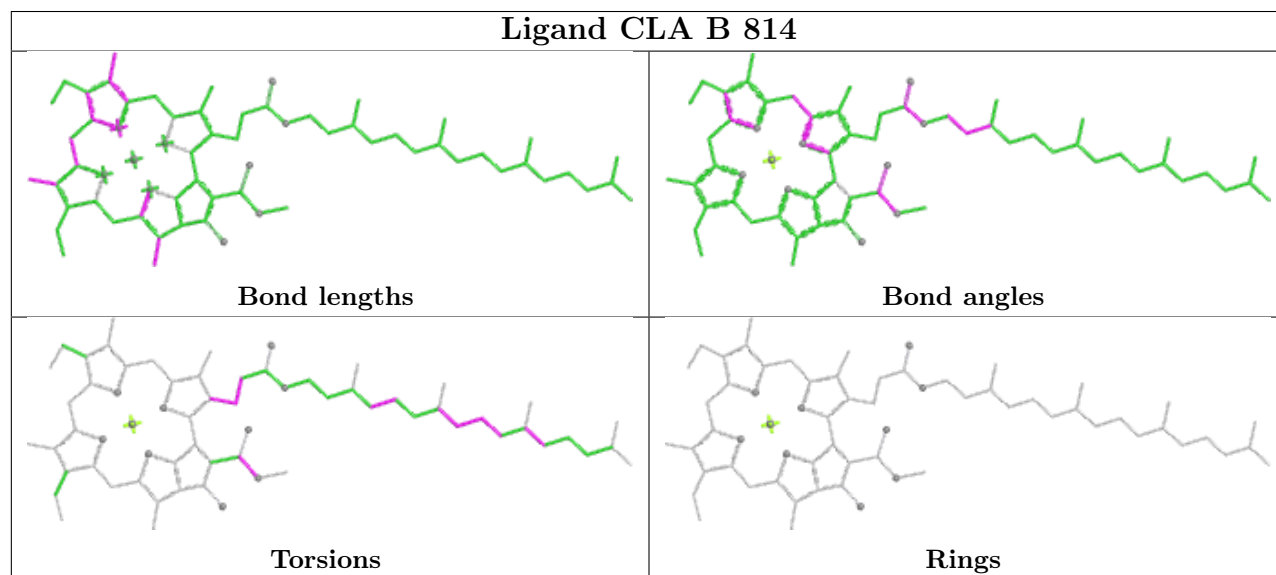
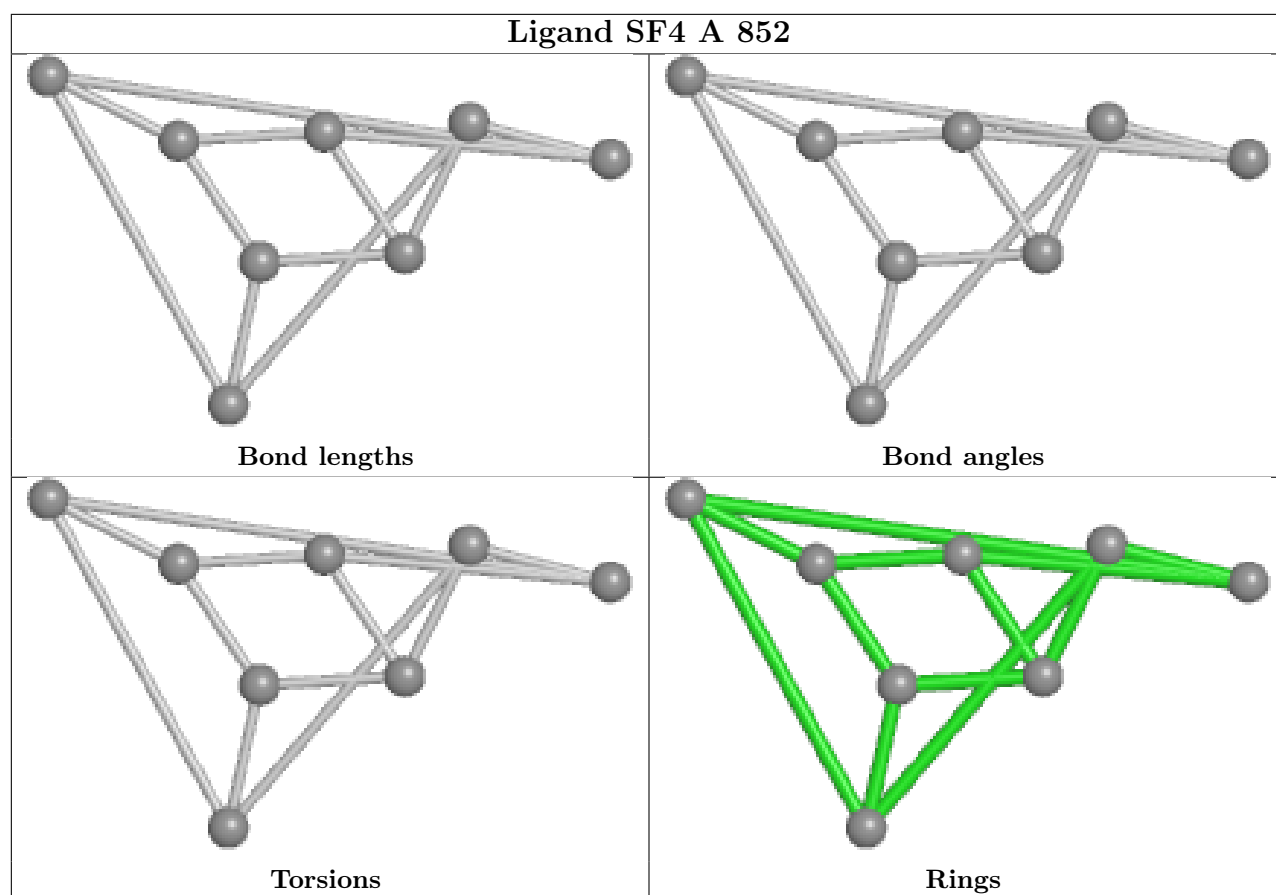


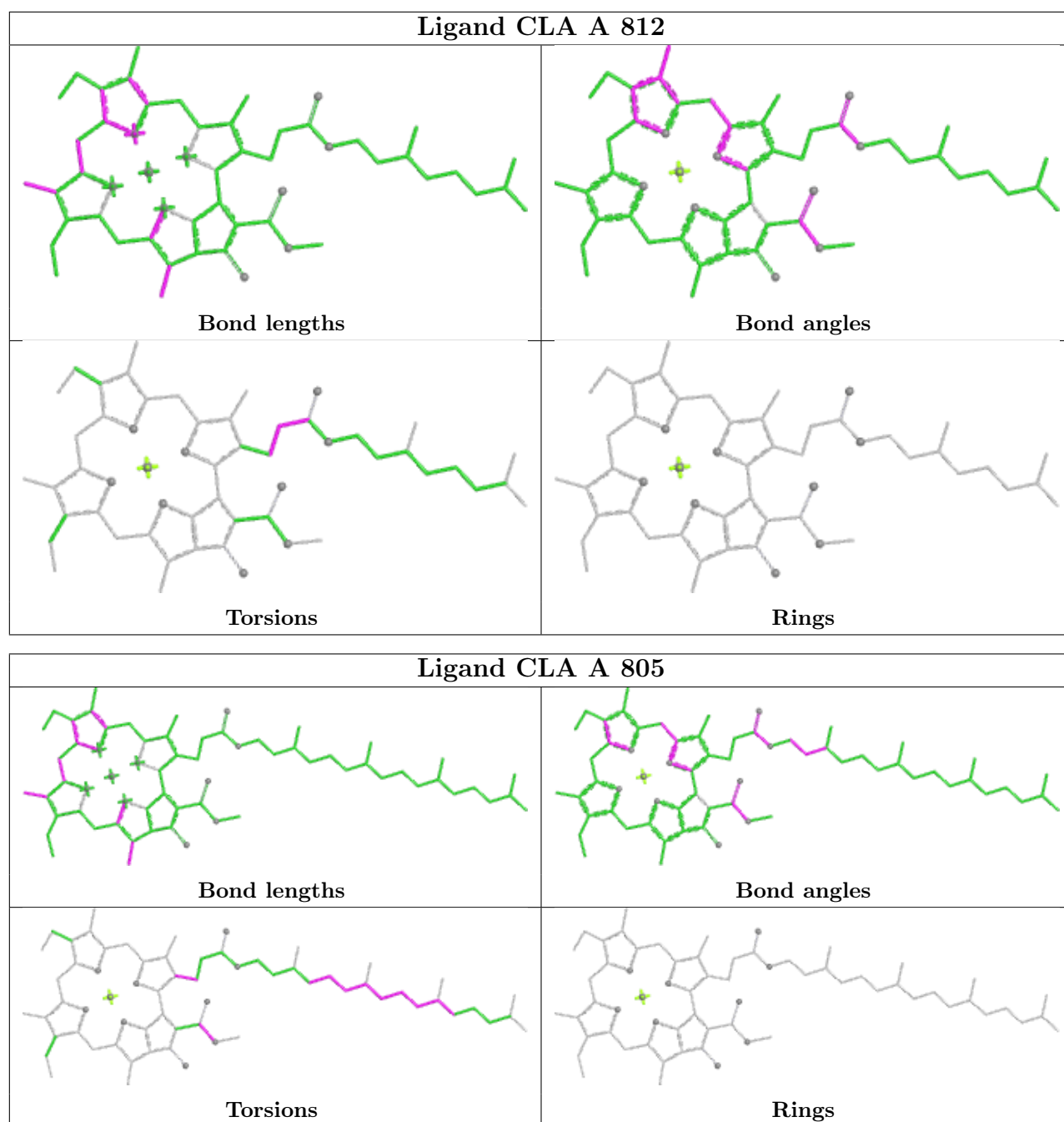
Ligand CLA A 814



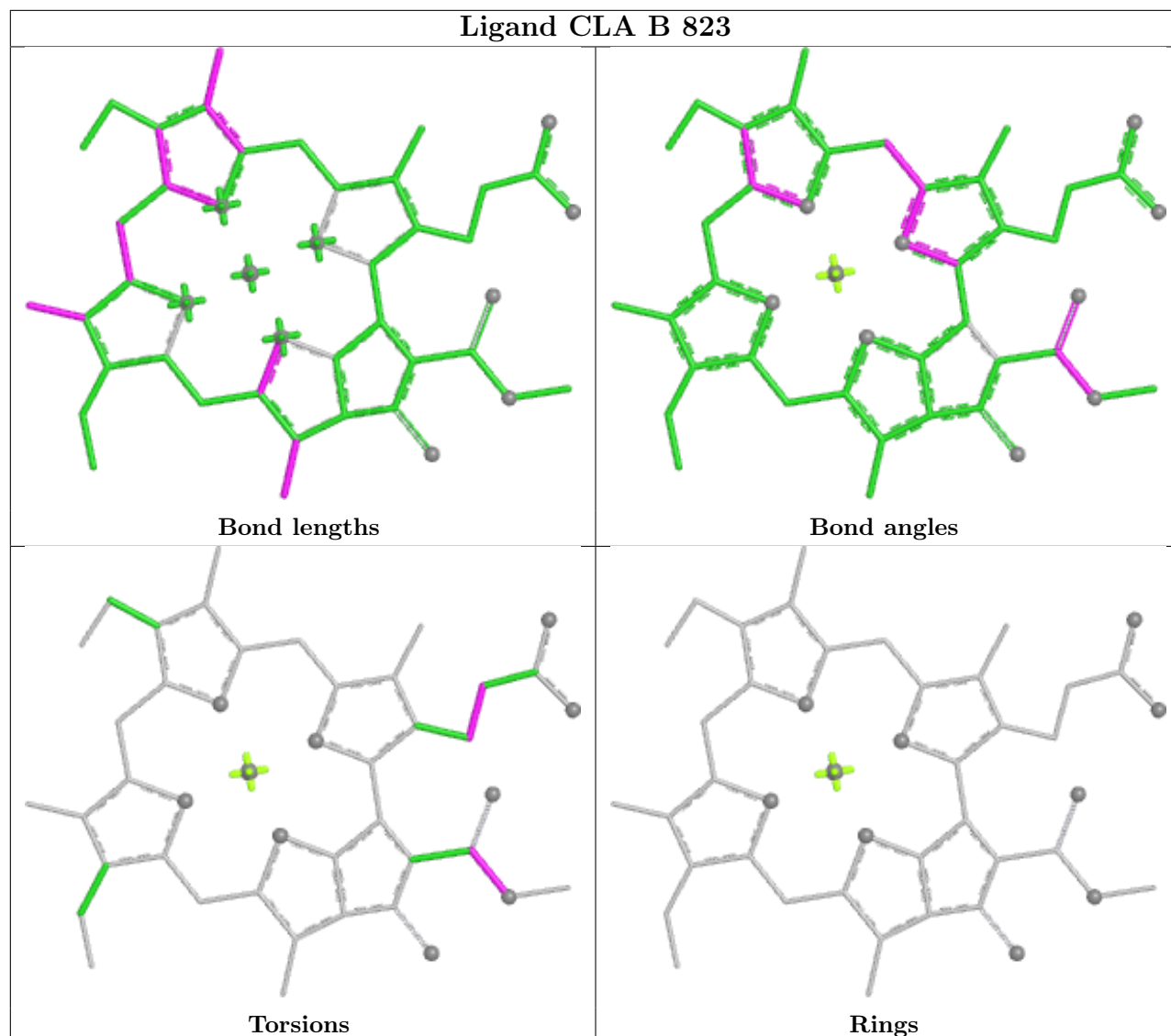
Ligand CLA A 840



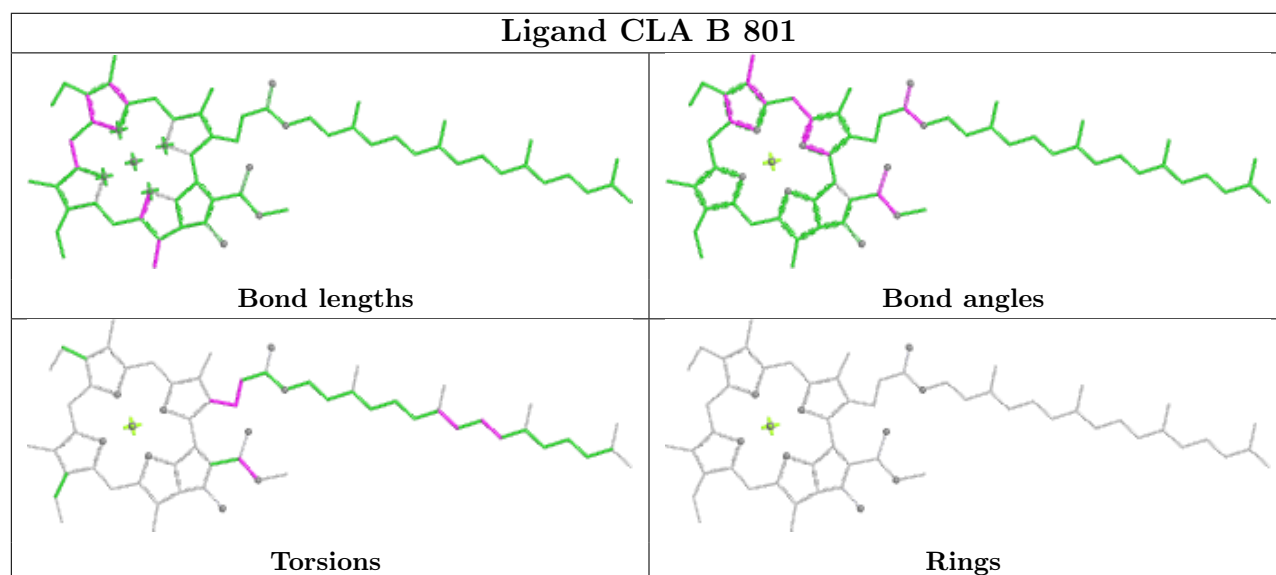


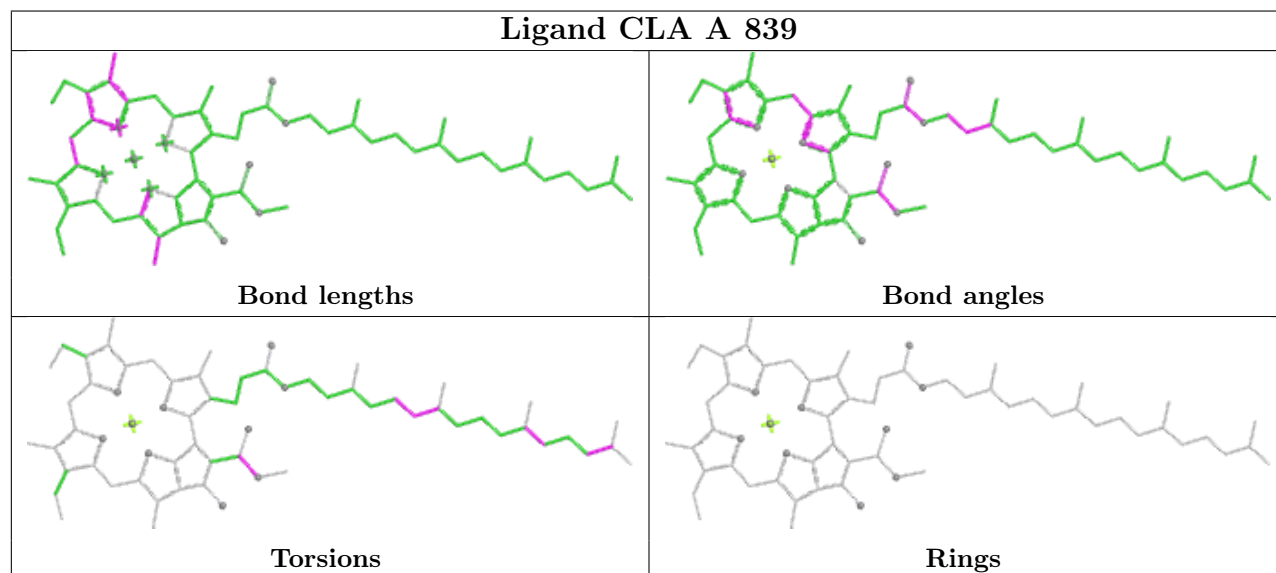
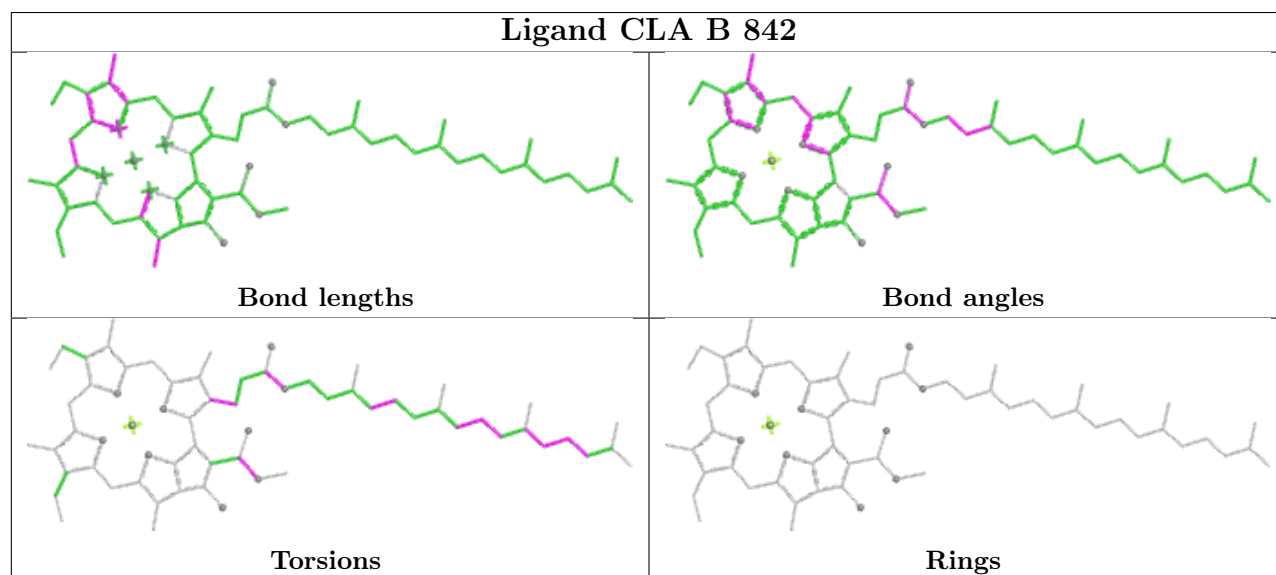
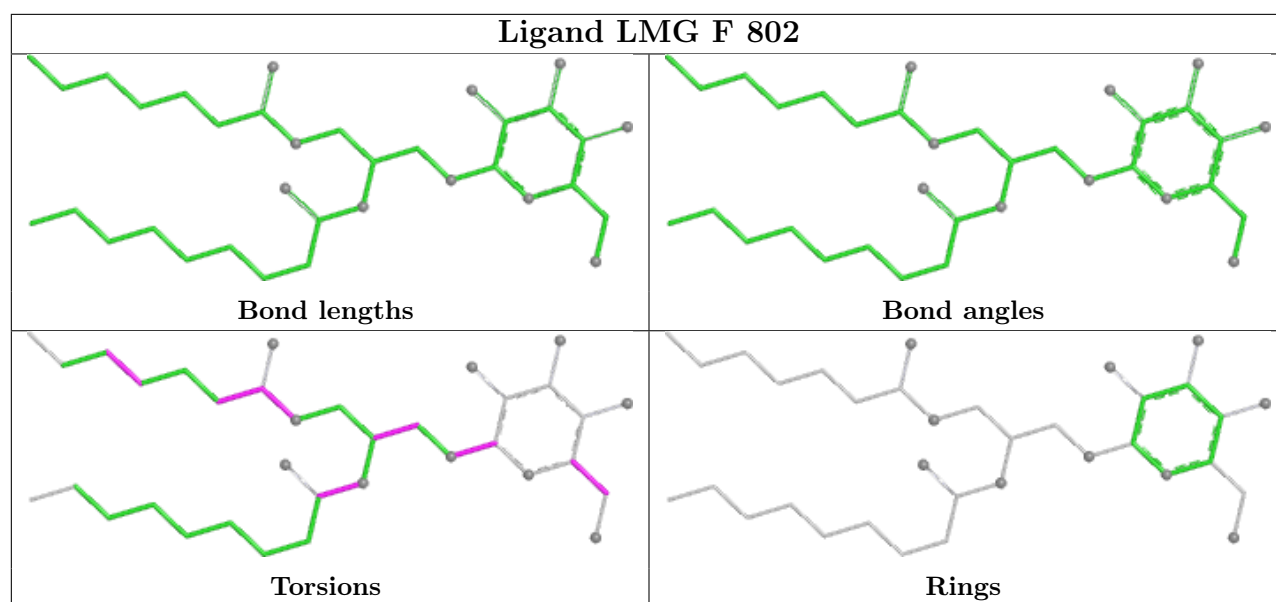


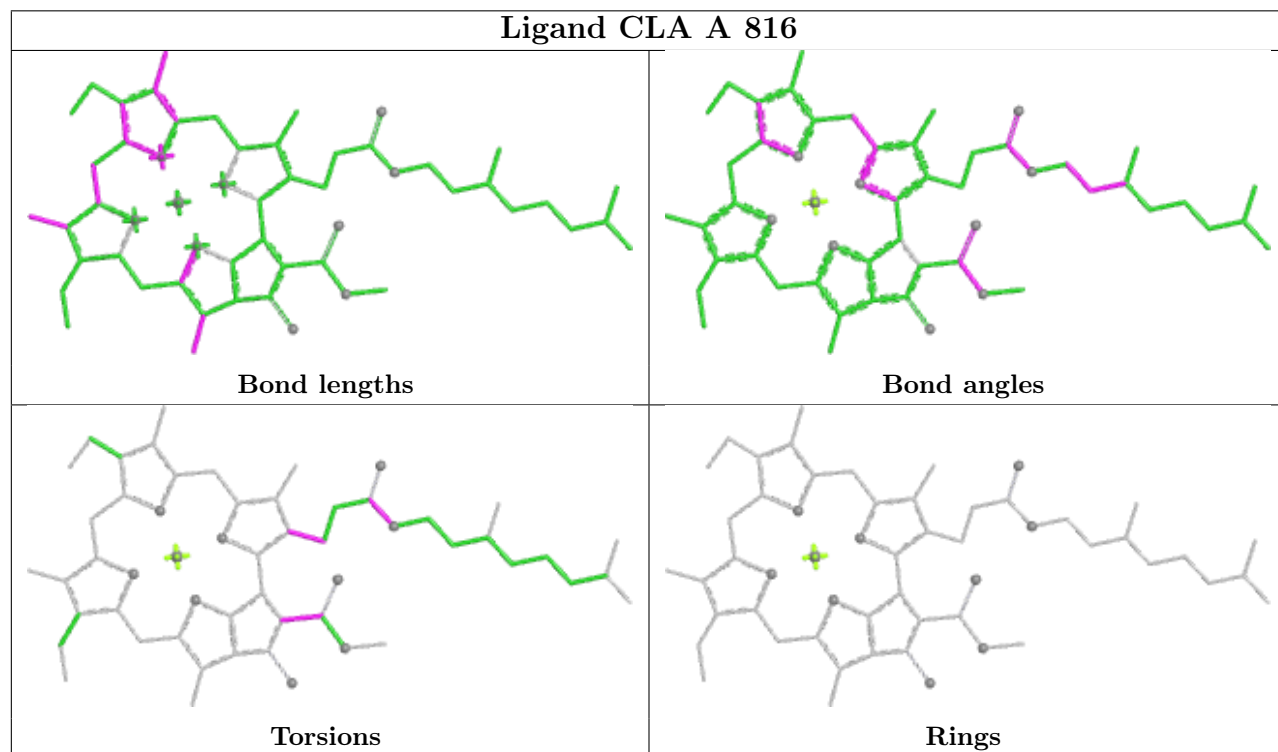
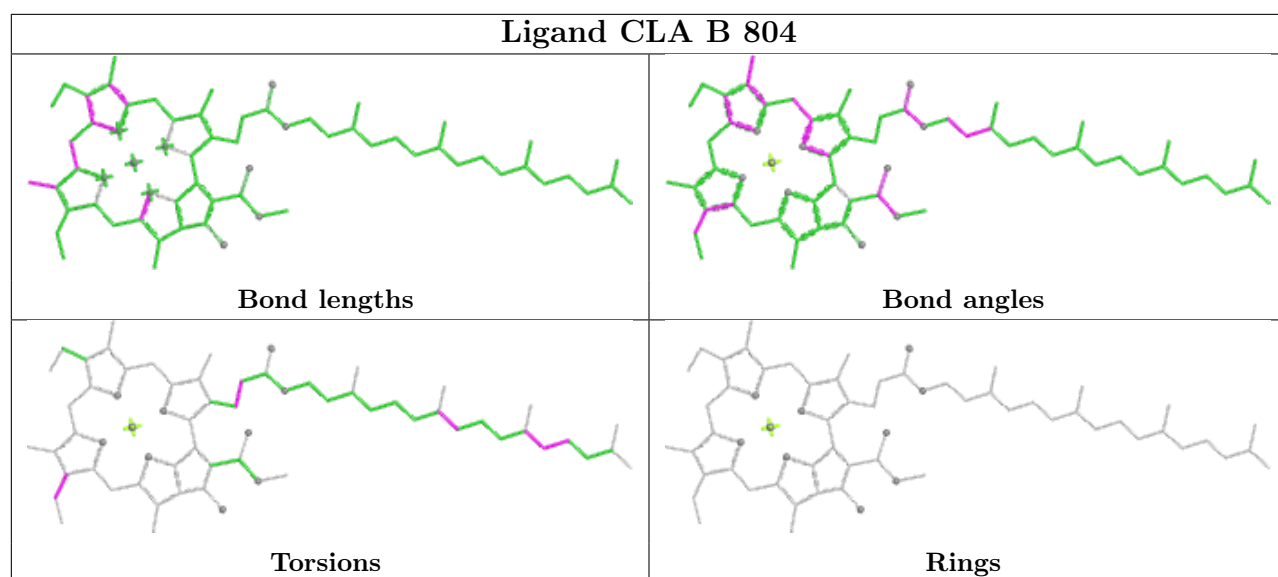
Ligand CLA B 823

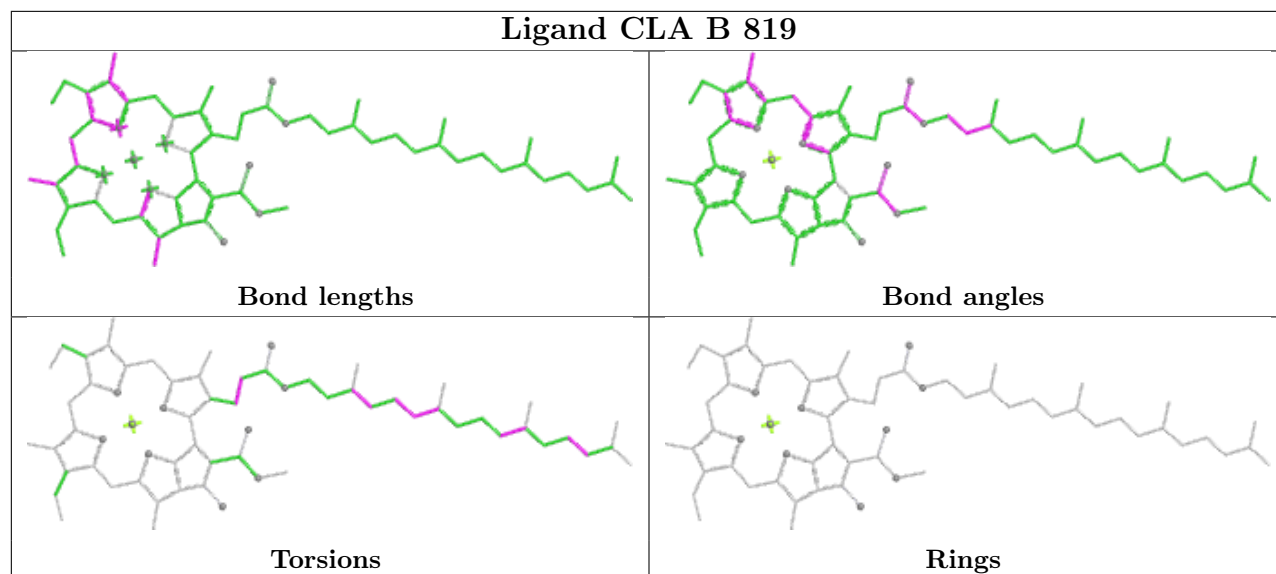
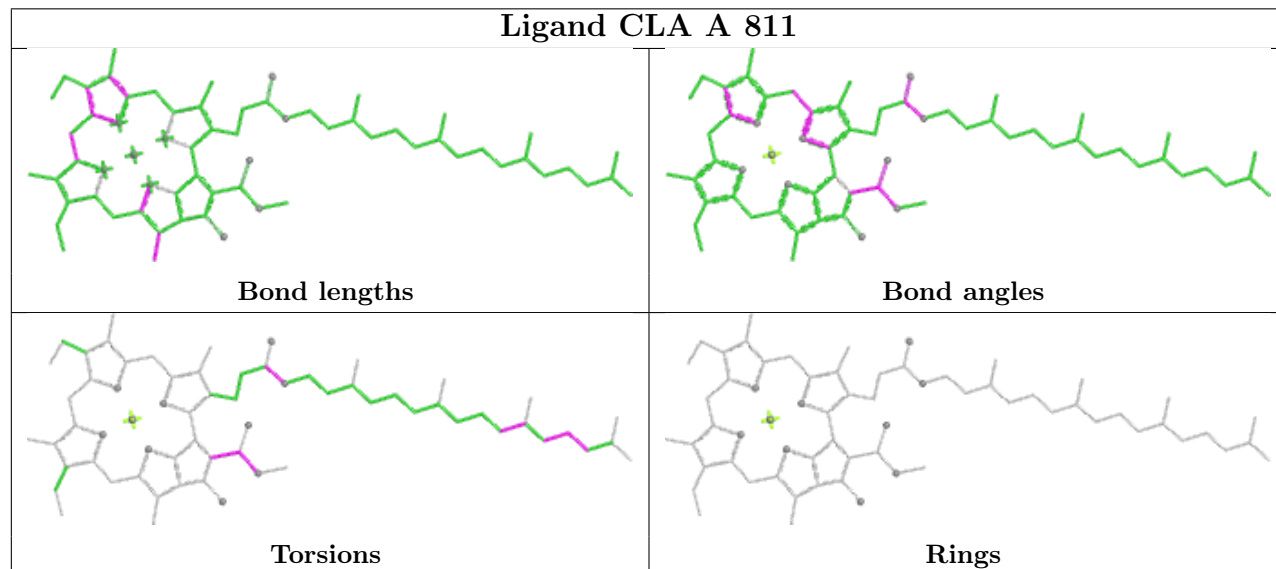


Ligand CLA B 801

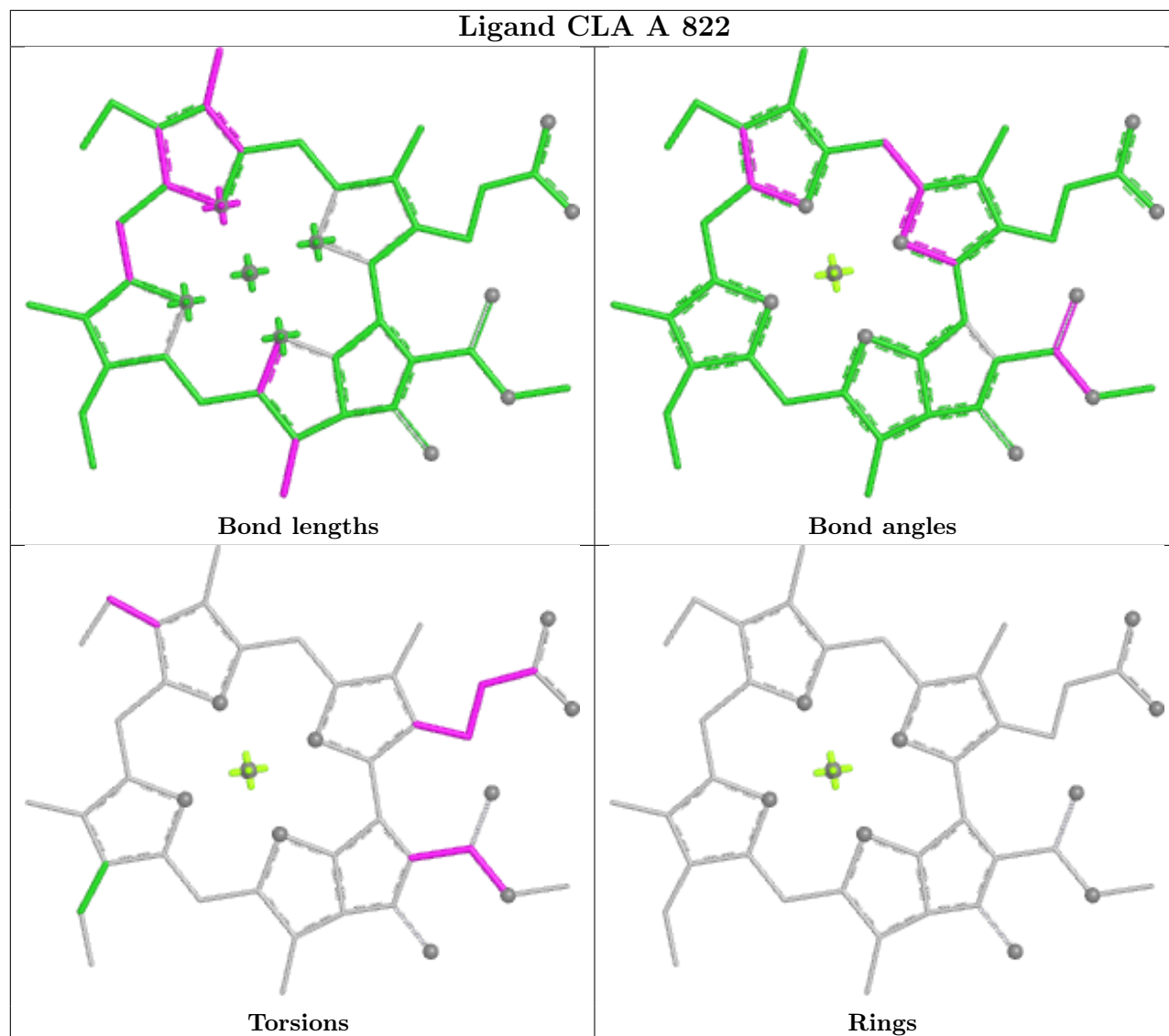




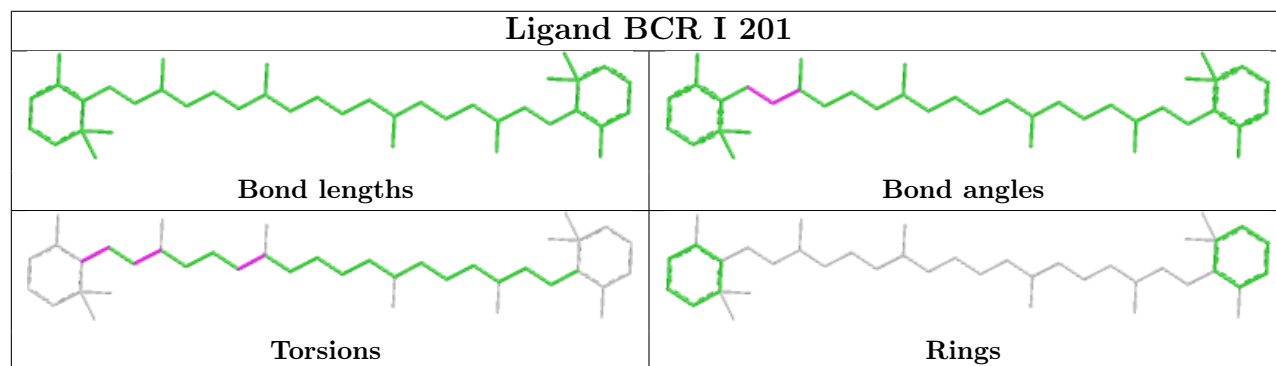


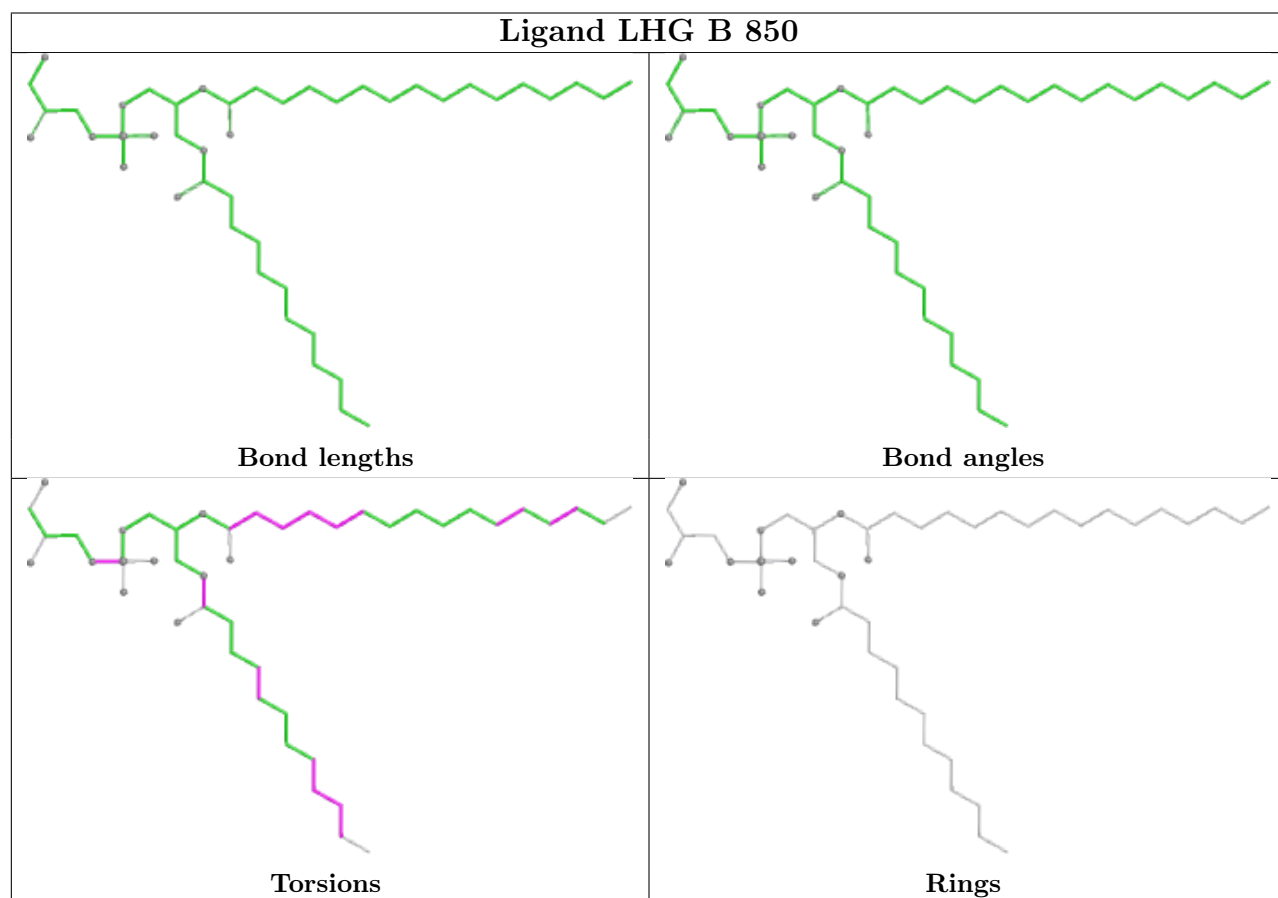
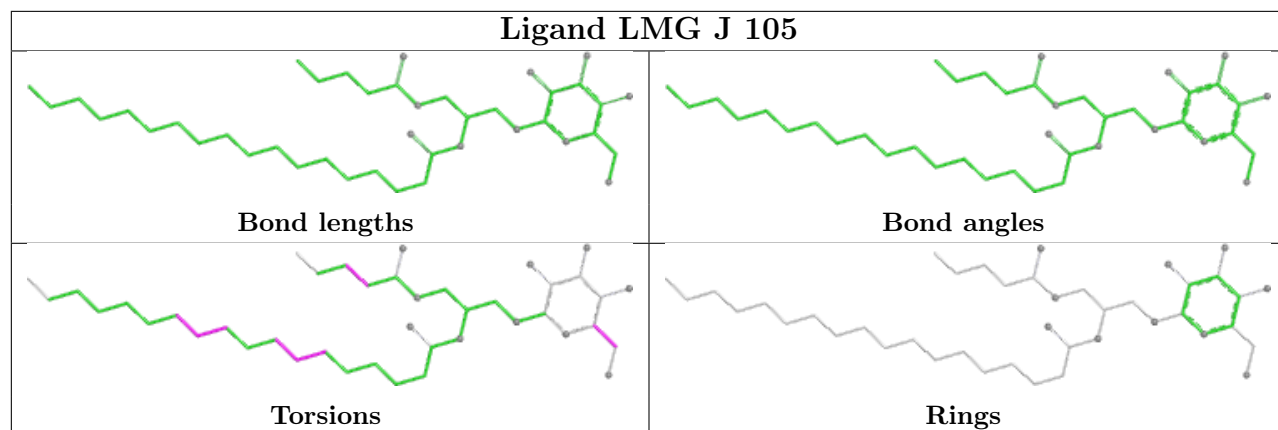
Ligand CLA B 819**Ligand CLA A 811**

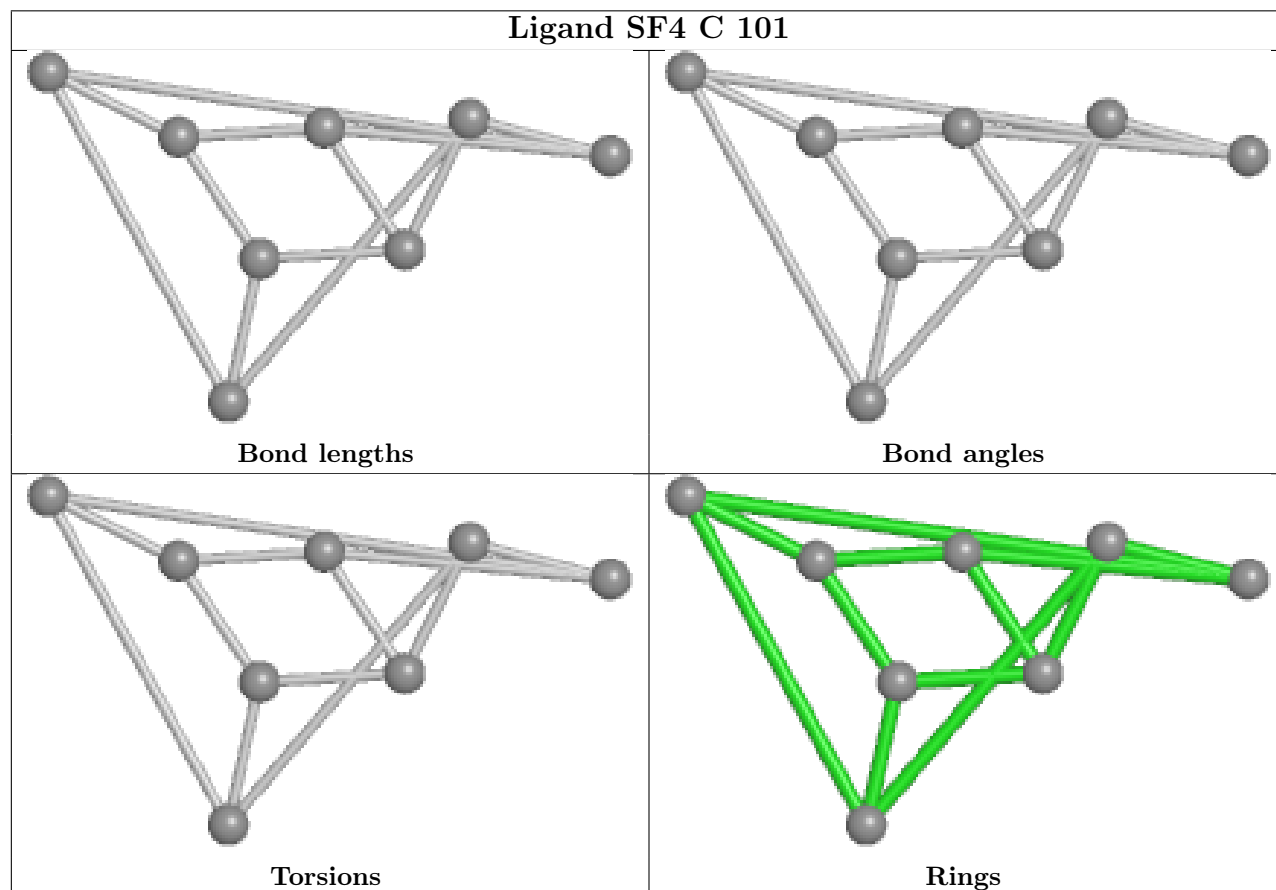
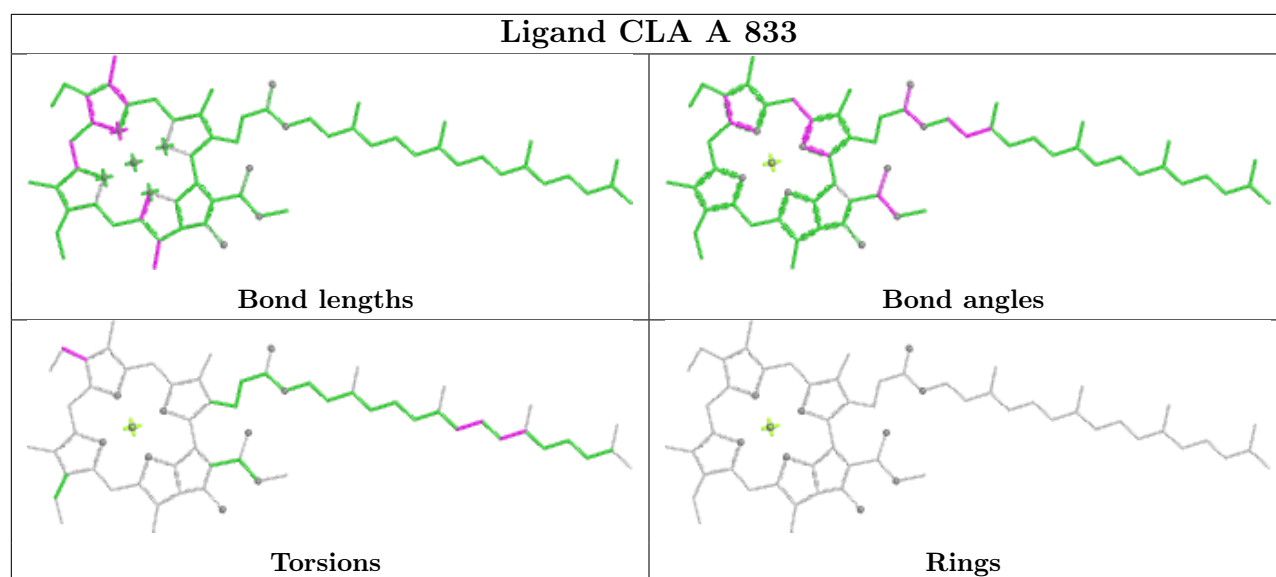
Ligand CLA A 822

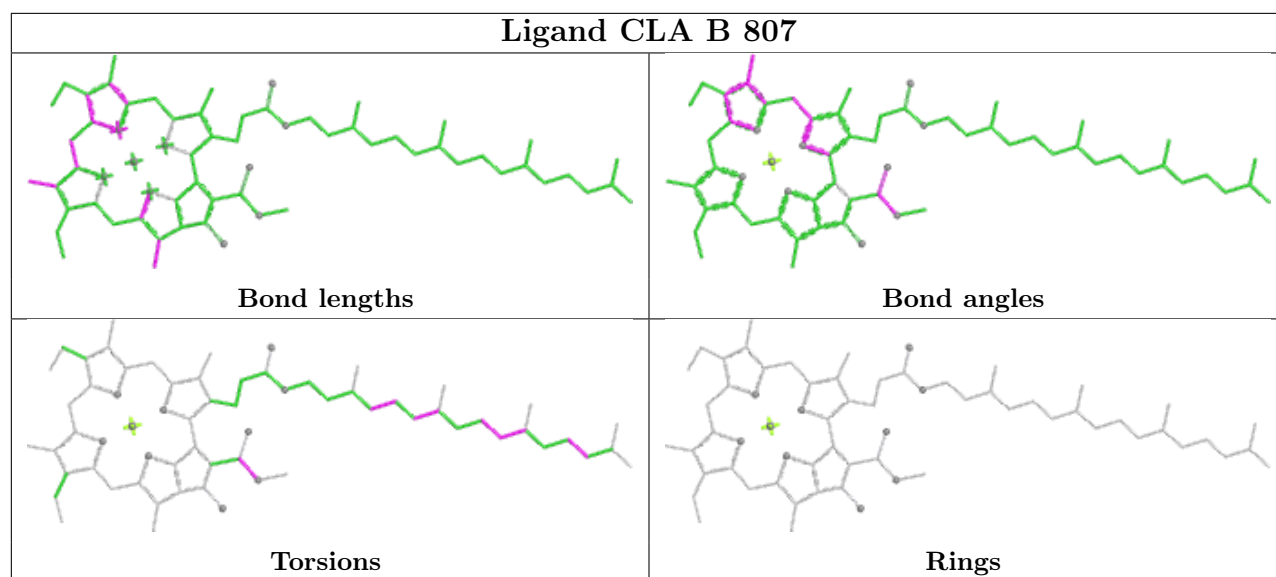
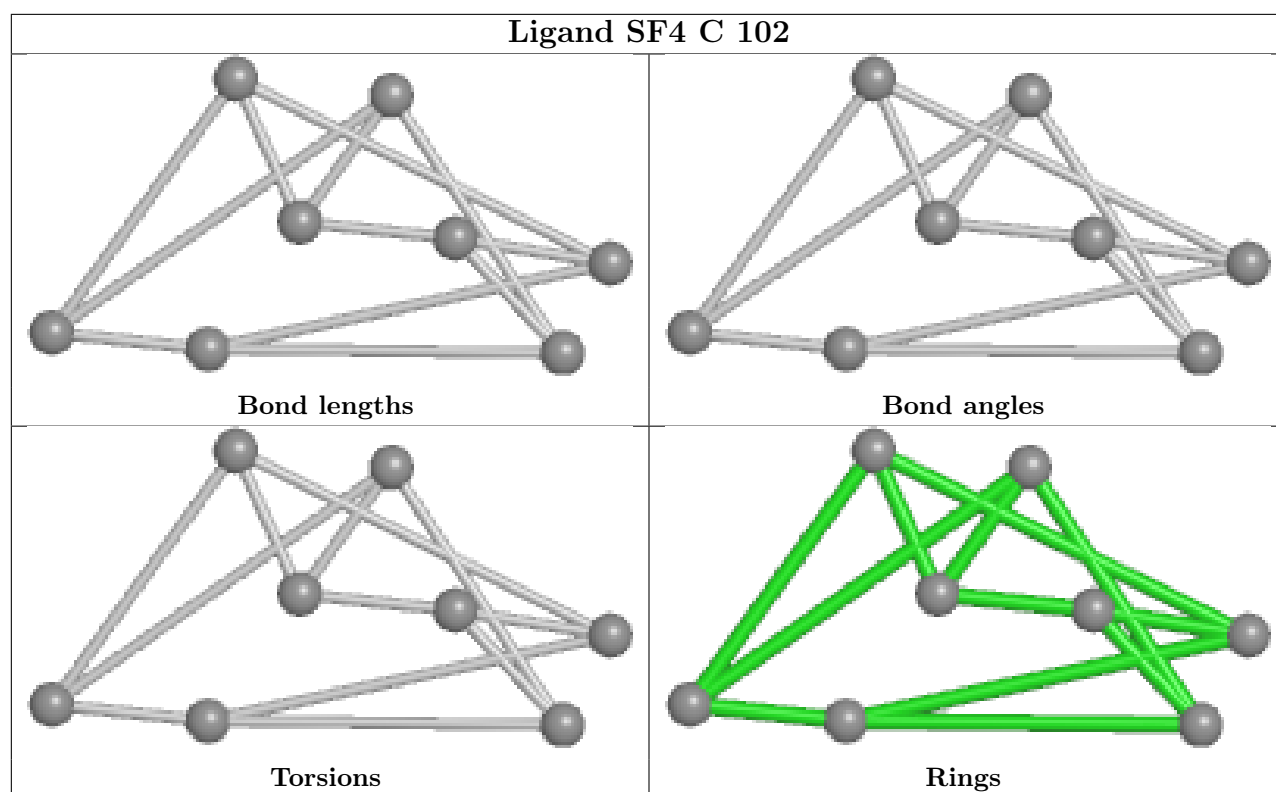


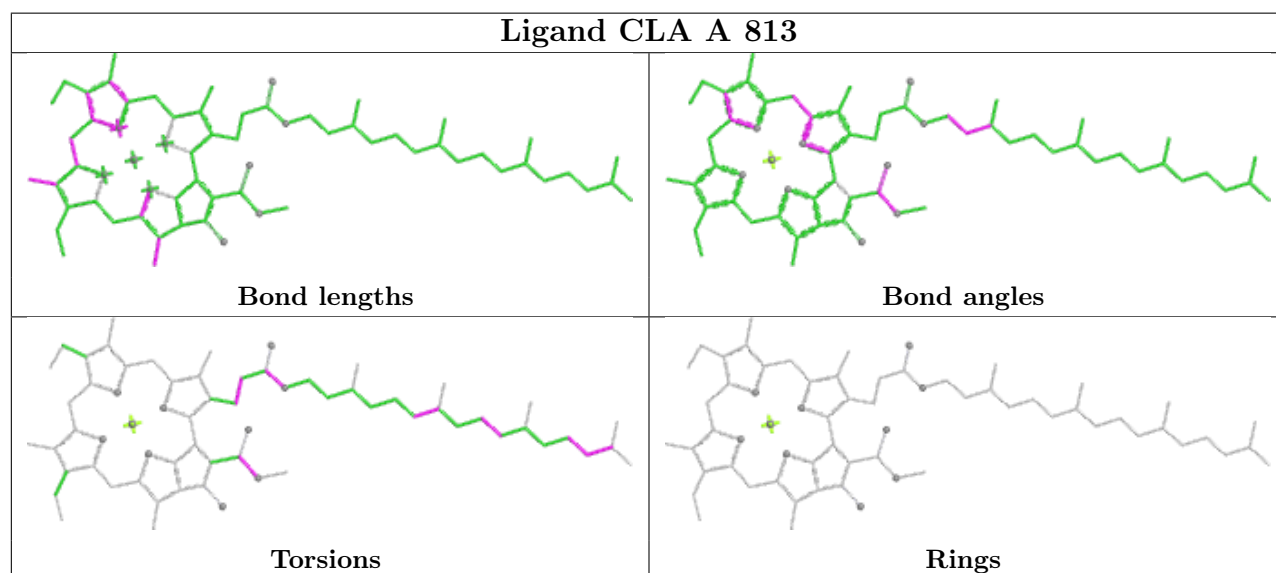
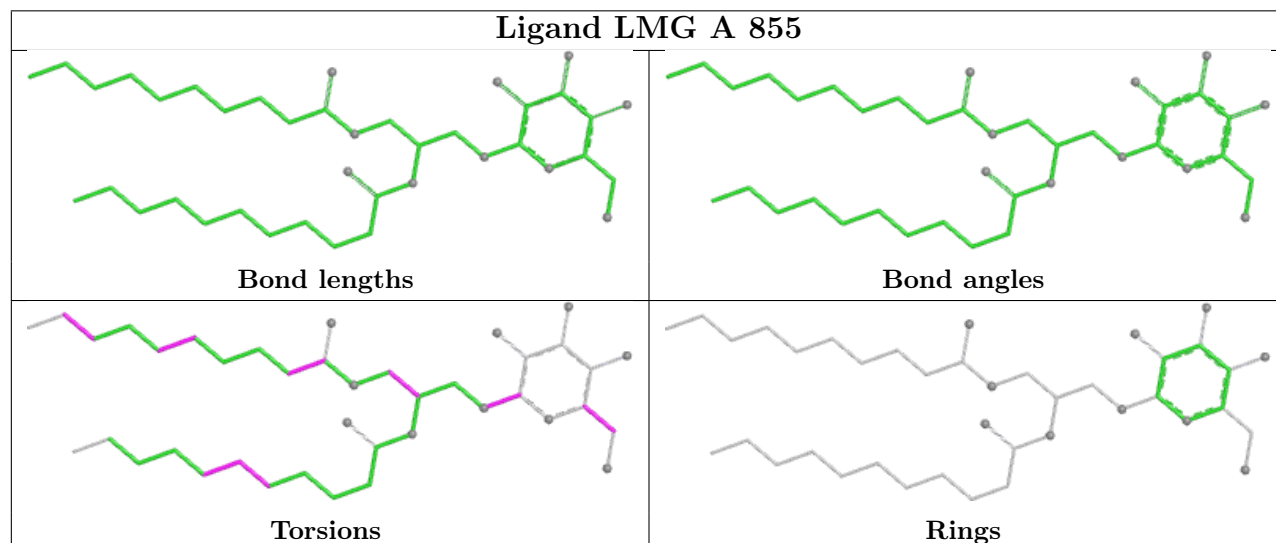
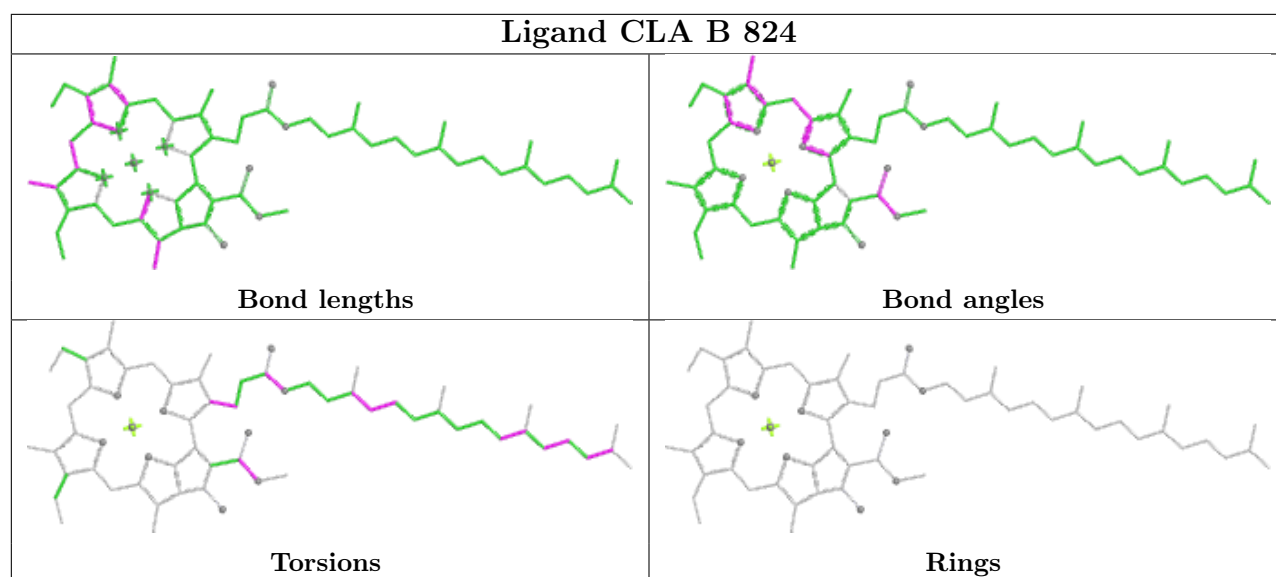
Ligand BCR I 201

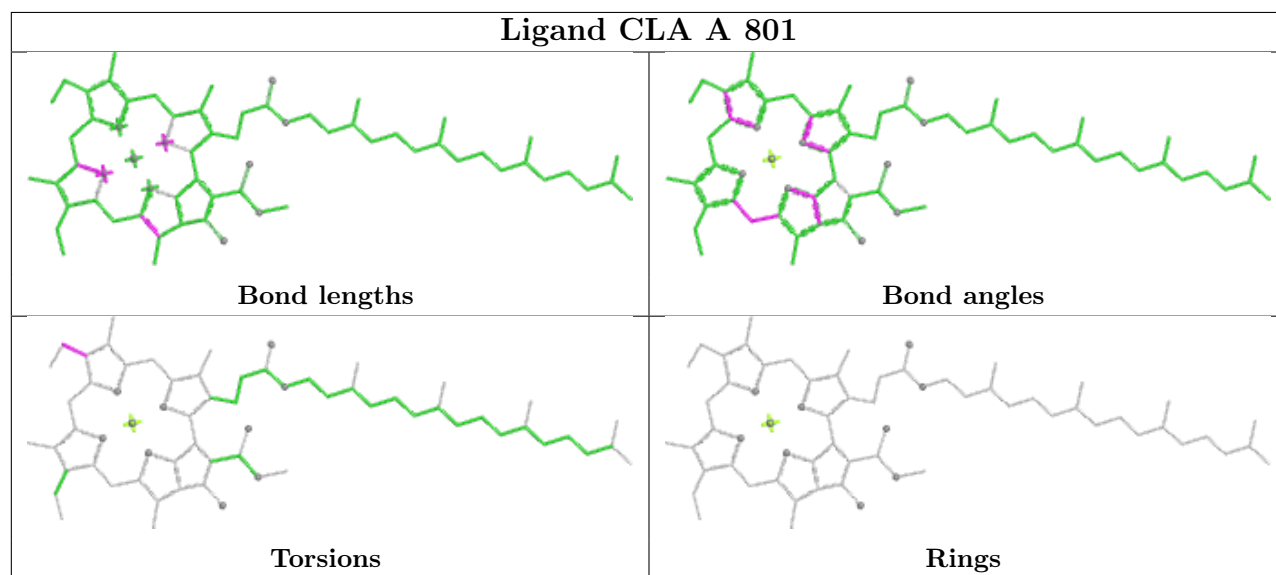
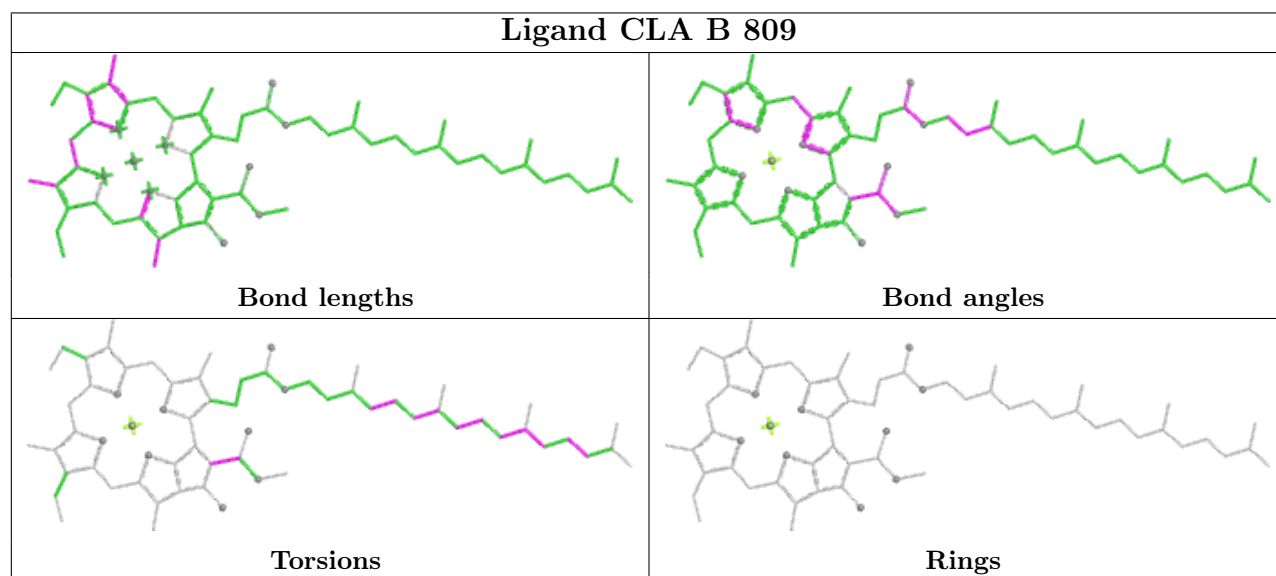
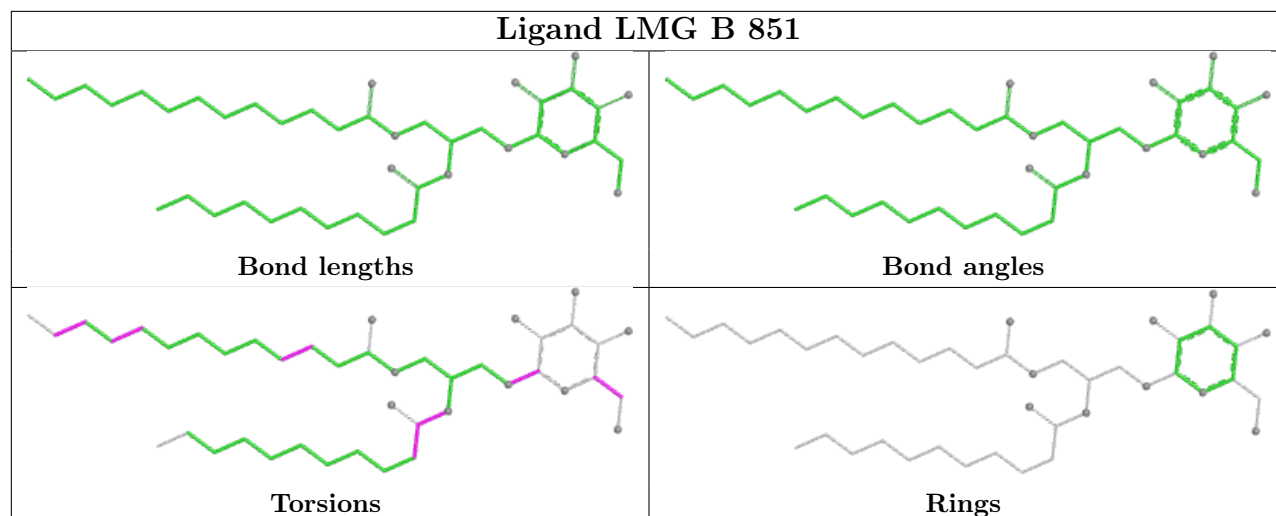


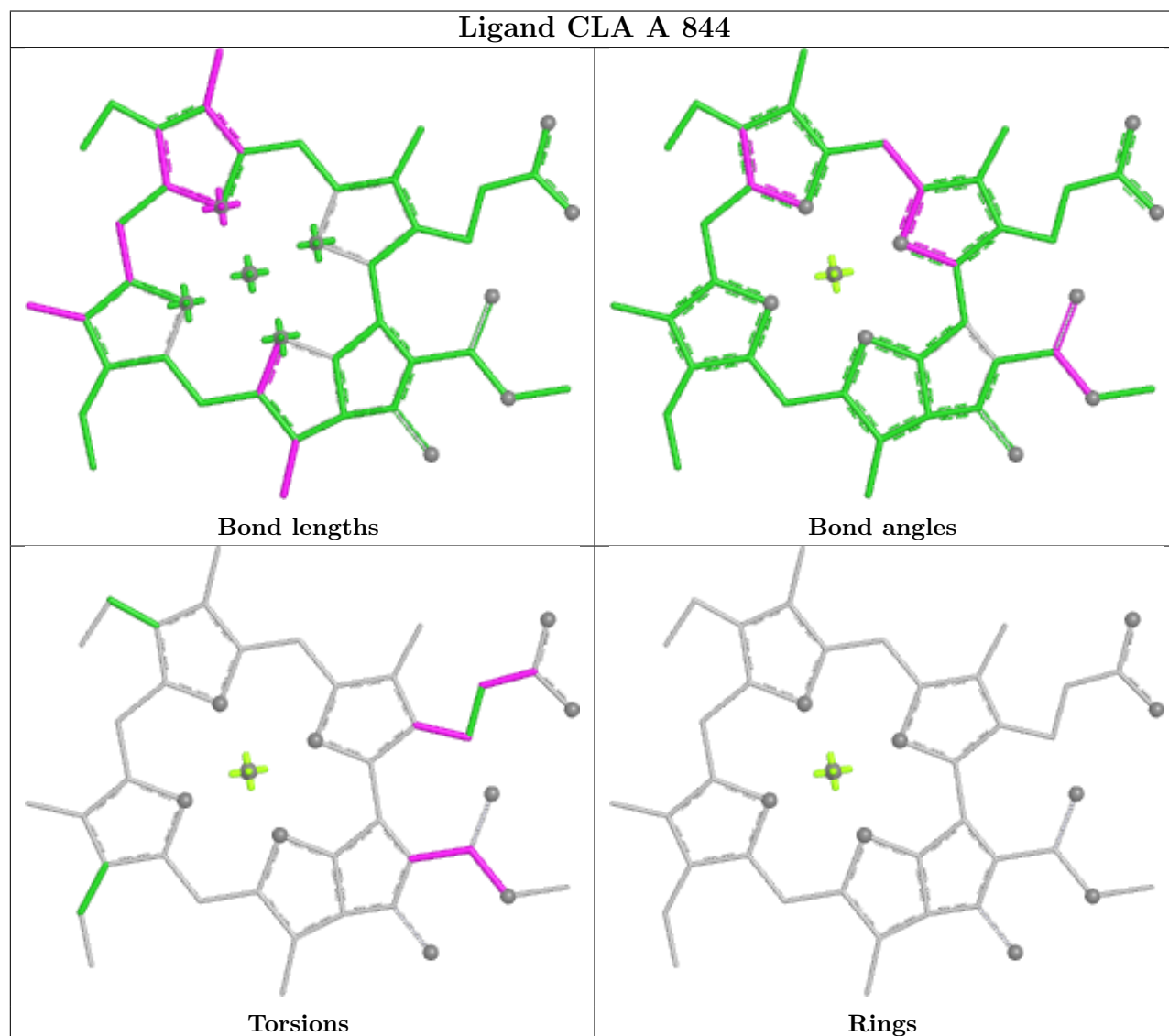
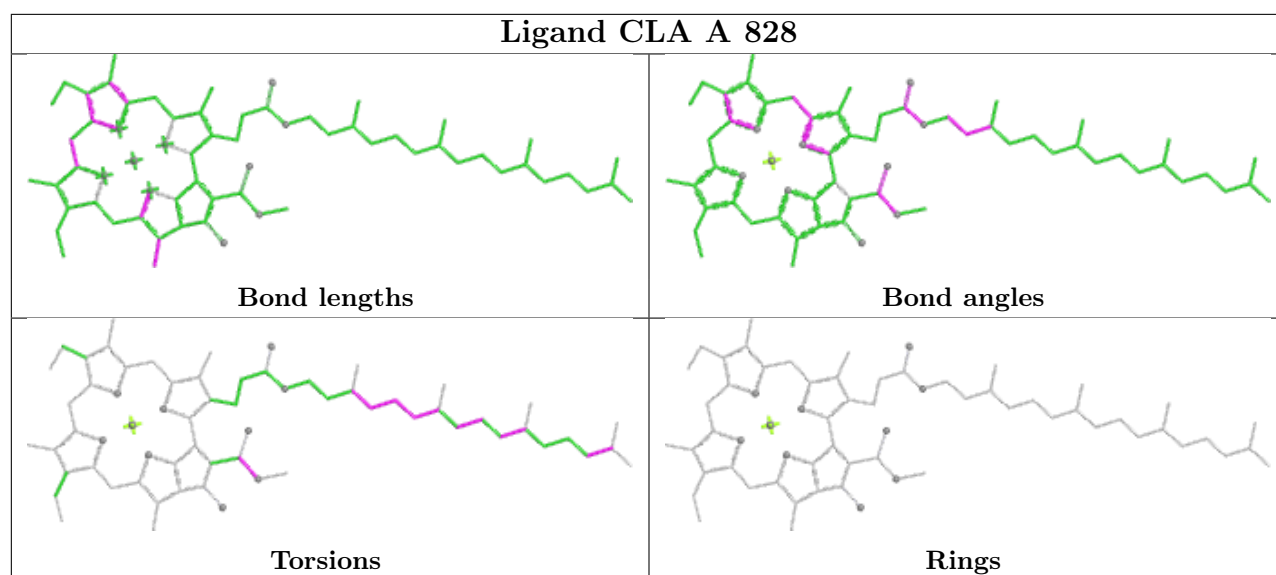


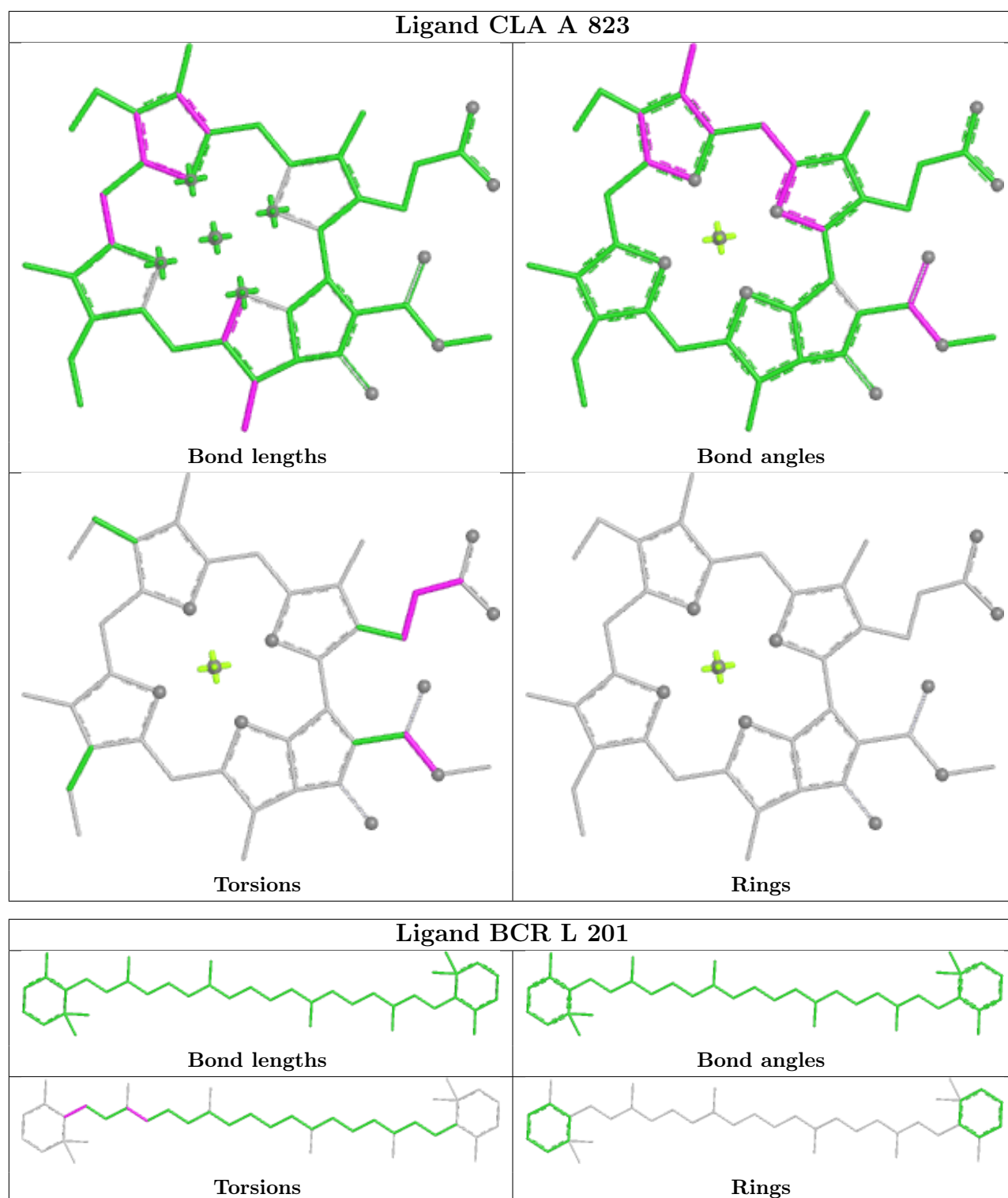


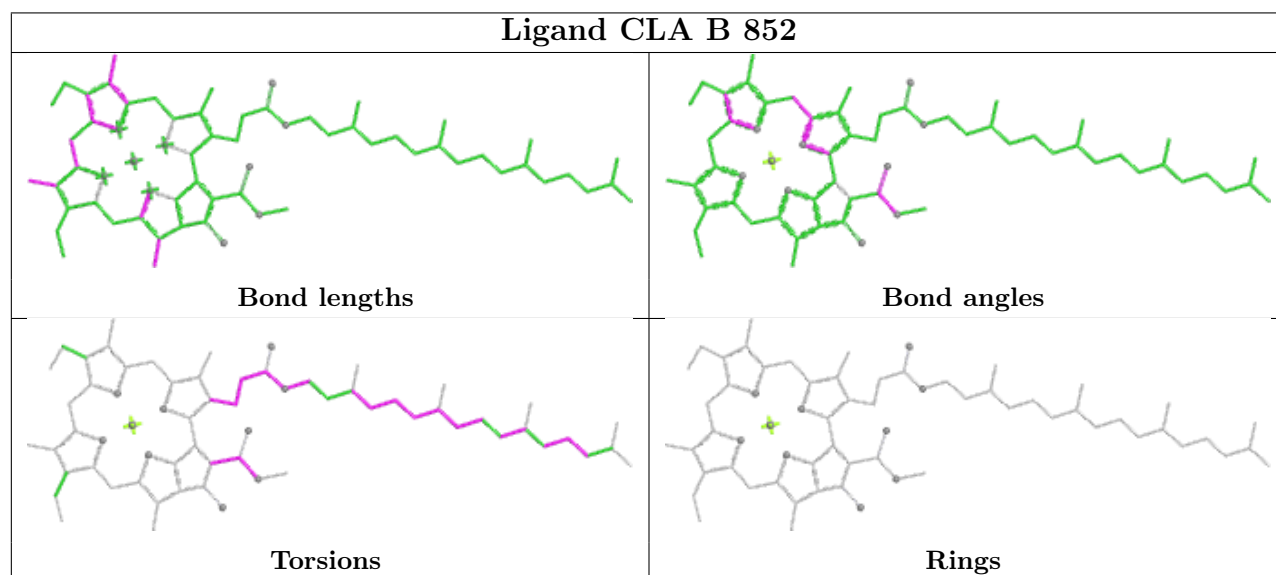
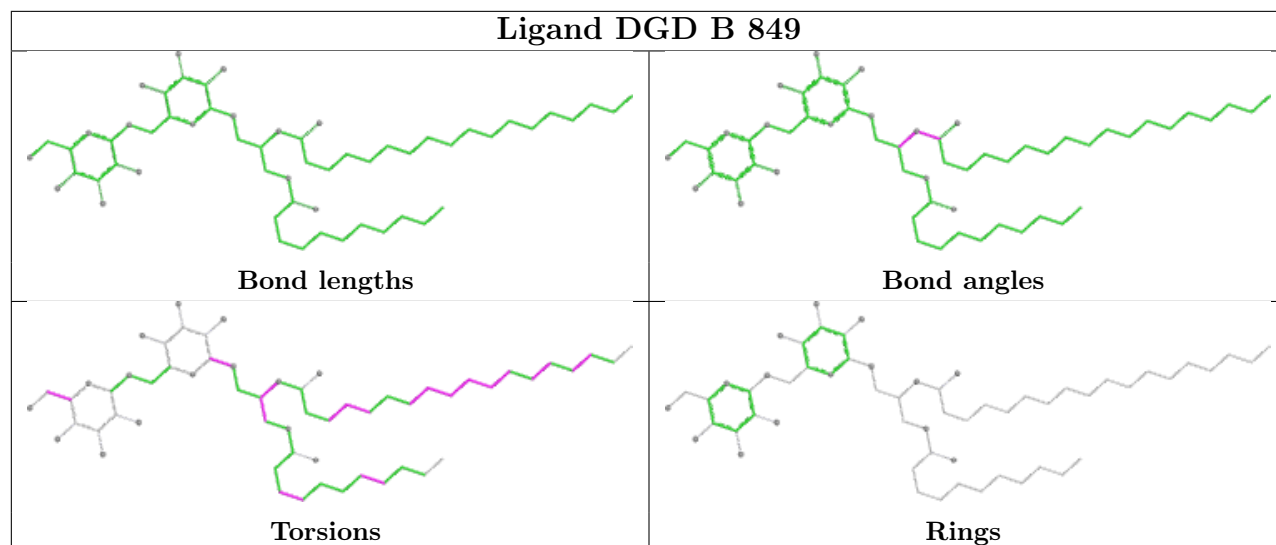


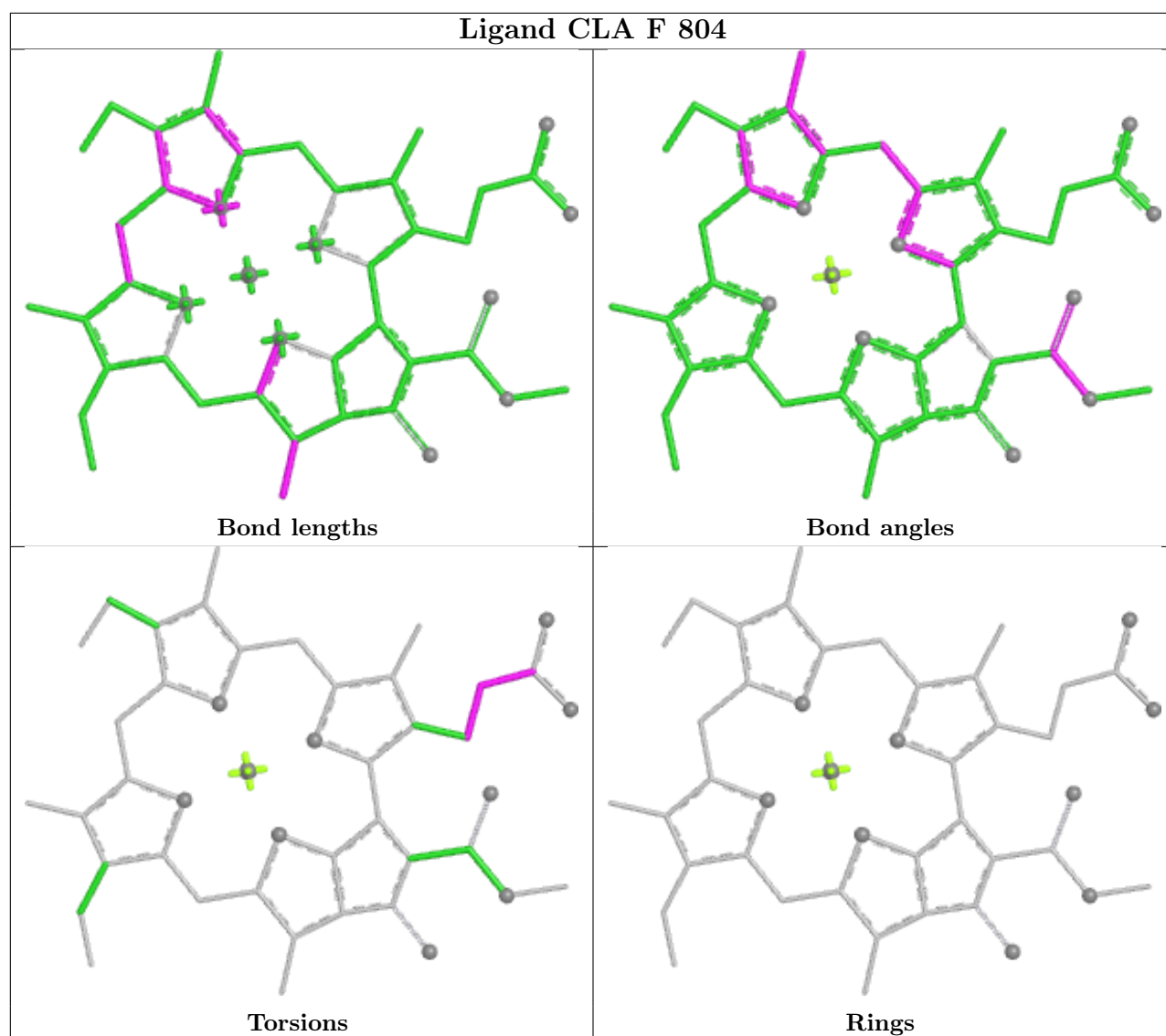












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

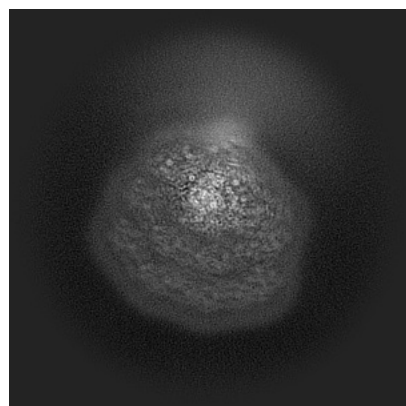
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54804. These allow visual inspection of the internal detail of the map and identification of artifacts.

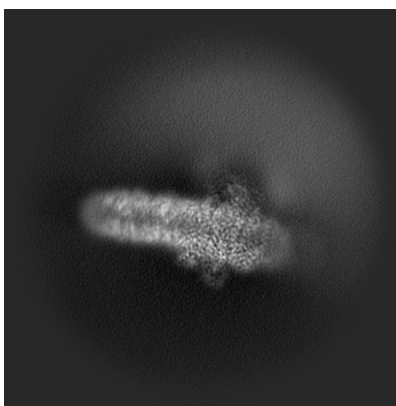
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

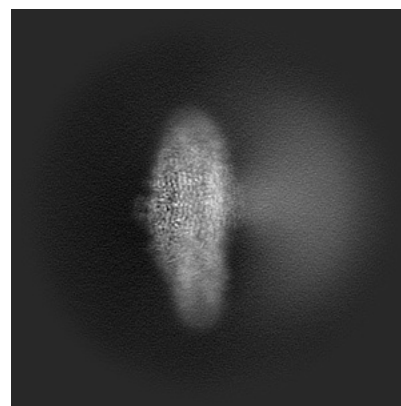
6.1.1 Primary map



X

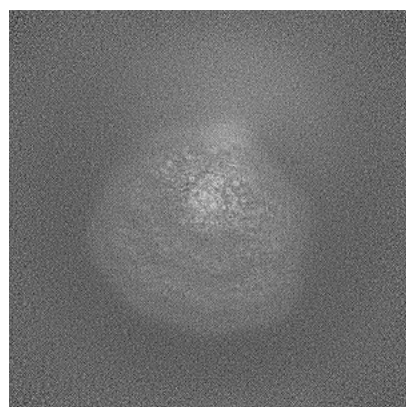


Y

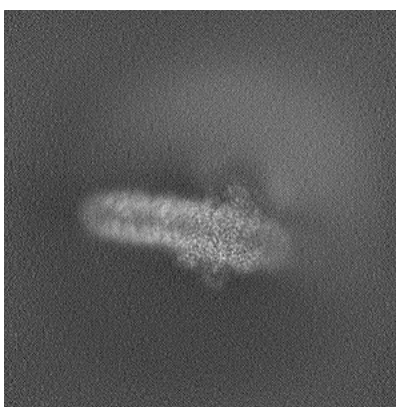


Z

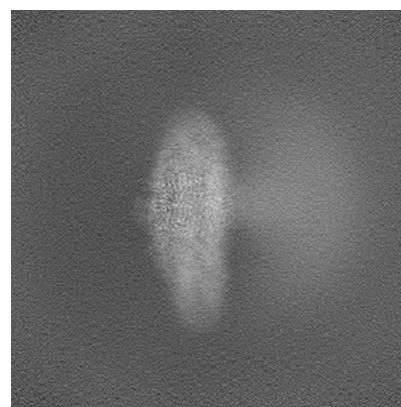
6.1.2 Raw map



X



Y

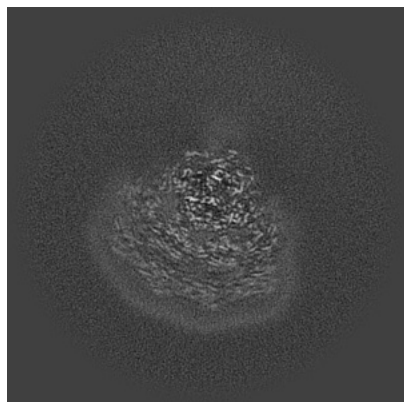


Z

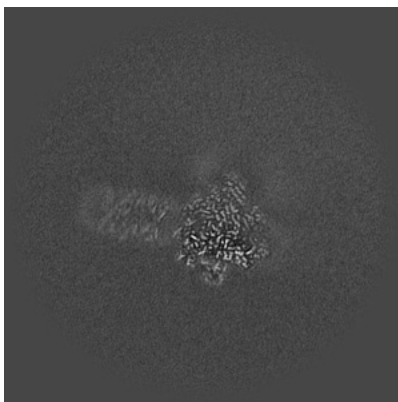
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

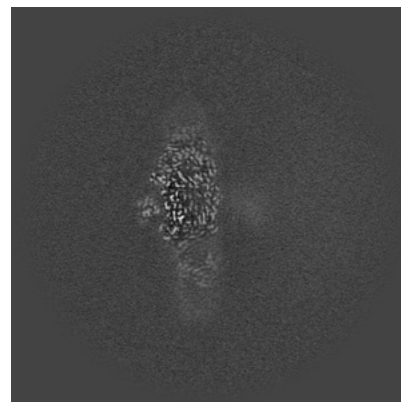
6.2.1 Primary map



X Index: 256

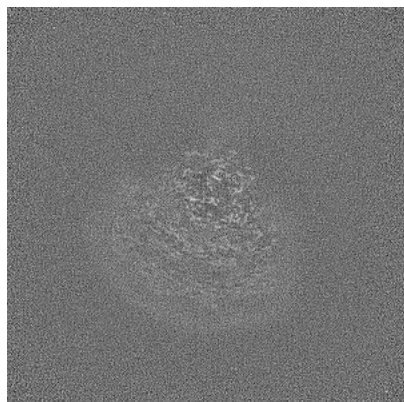


Y Index: 256

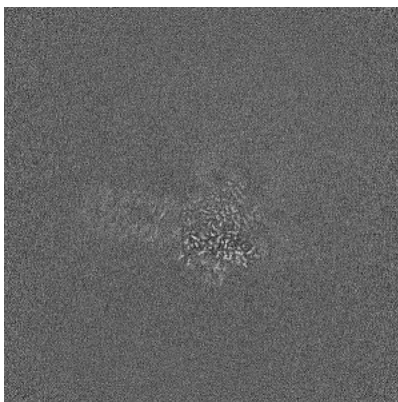


Z Index: 256

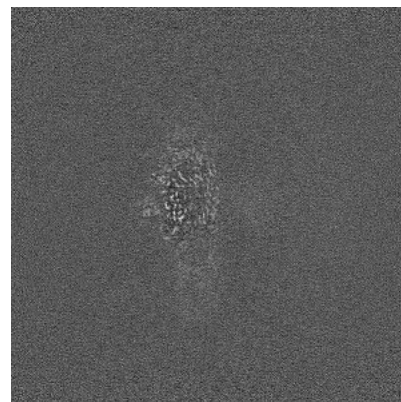
6.2.2 Raw map



X Index: 256



Y Index: 256

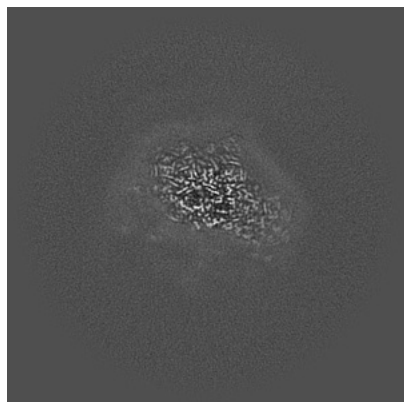


Z Index: 256

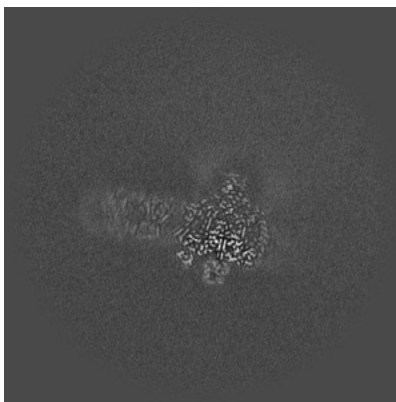
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

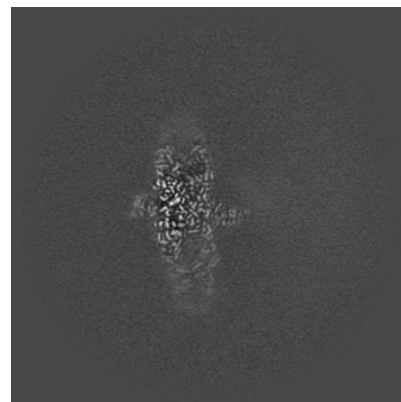
6.3.1 Primary map



X Index: 209

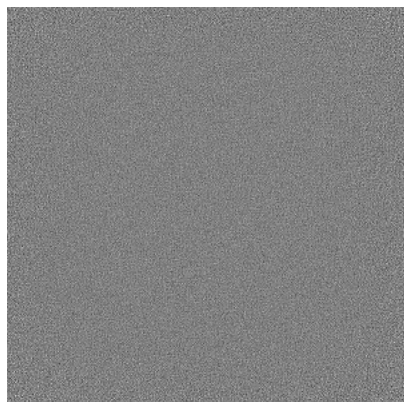


Y Index: 261

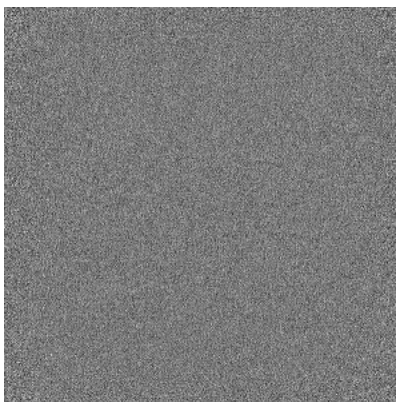


Z Index: 276

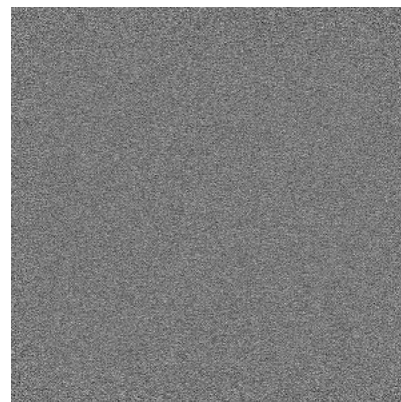
6.3.2 Raw map



X Index: 0



Y Index: 0

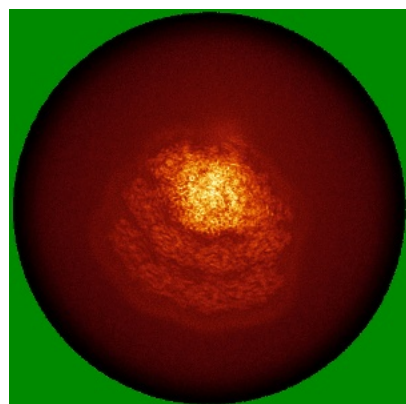


Z Index: 0

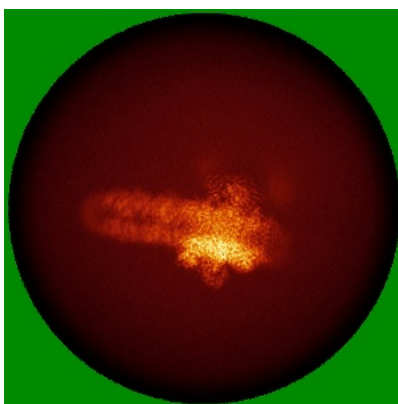
The images above show the largest variance slices of the map in three orthogonal directions.

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

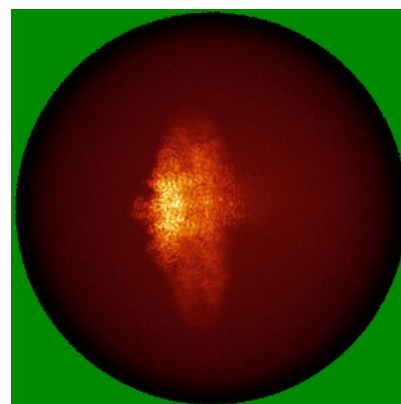
6.4.1 Primary map



X

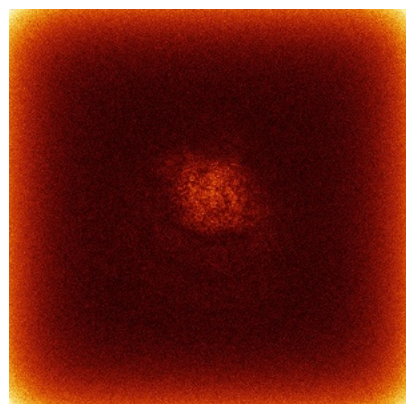


Y

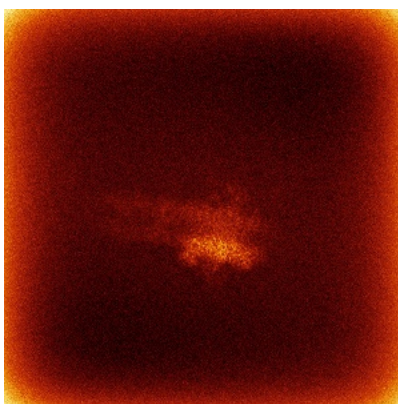


Z

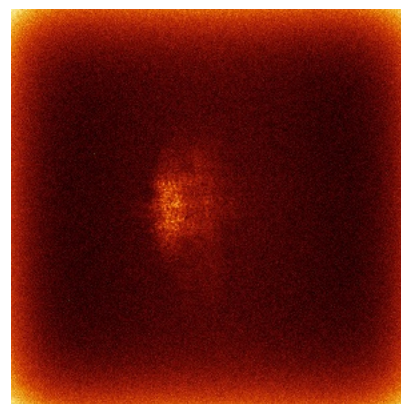
6.4.2 Raw map



X



Y

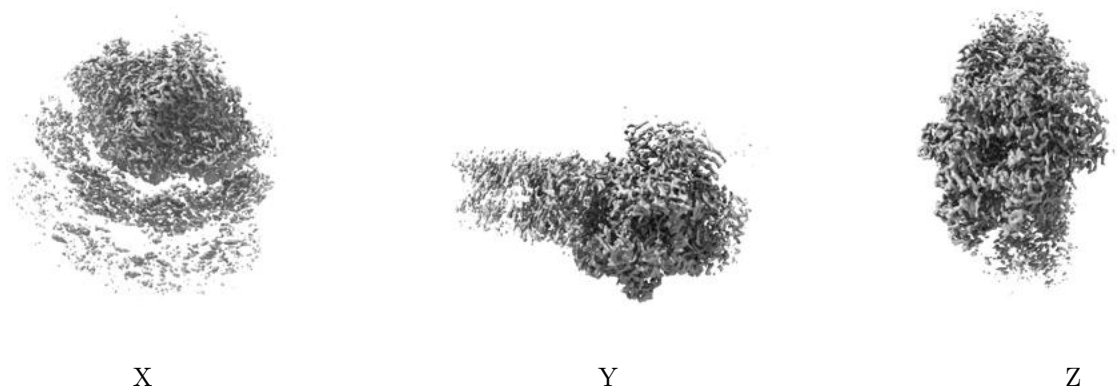


Z

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

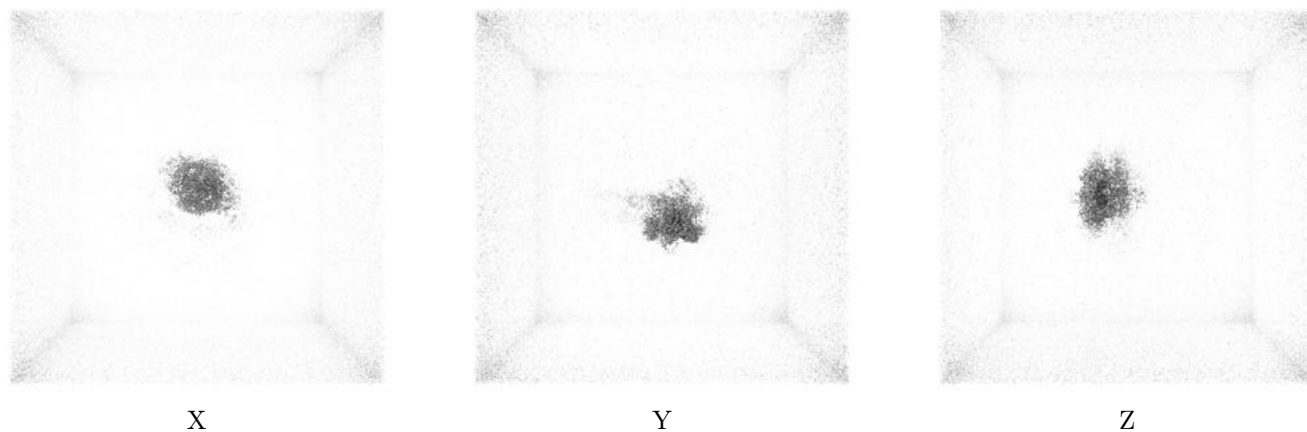
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

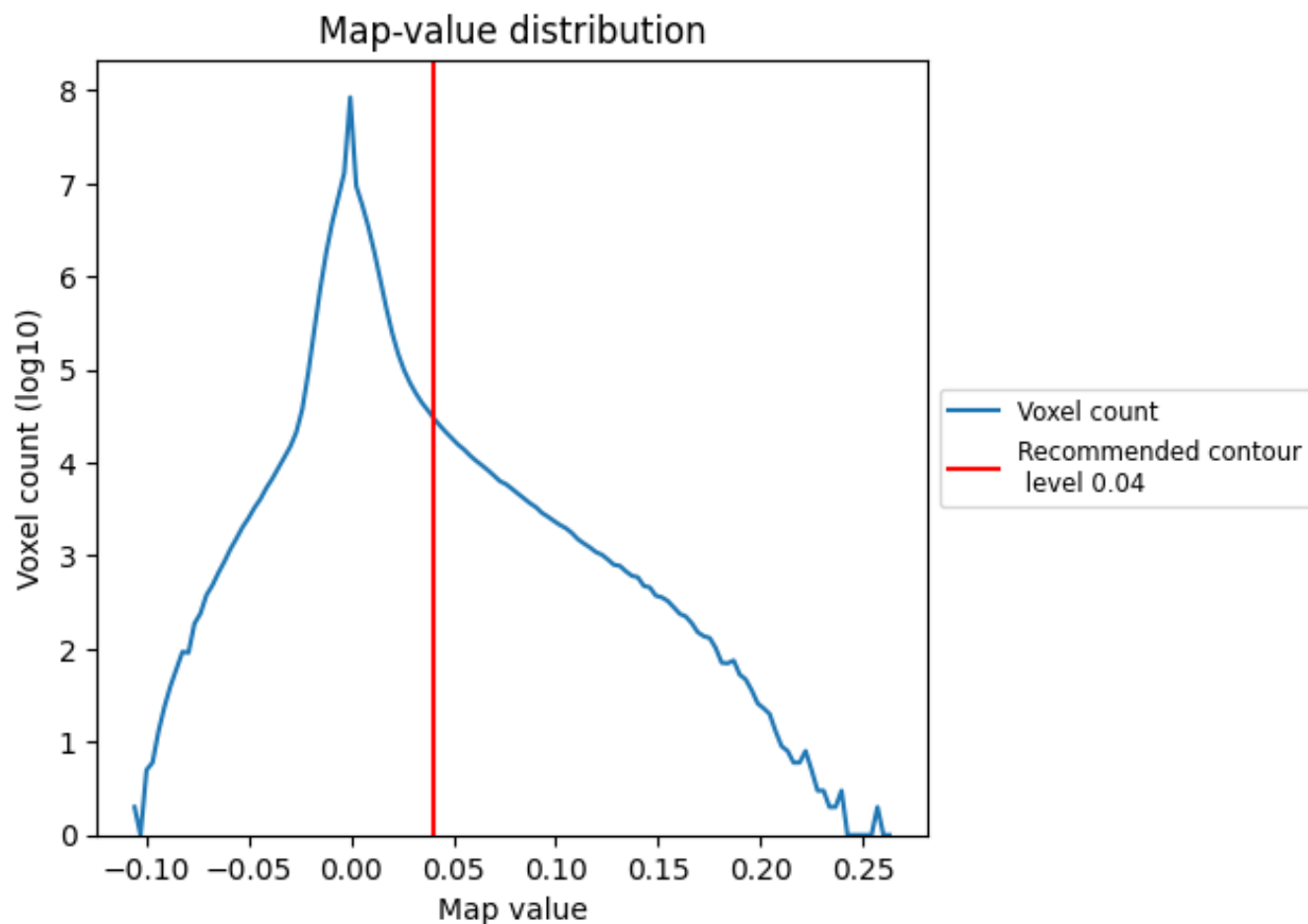
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

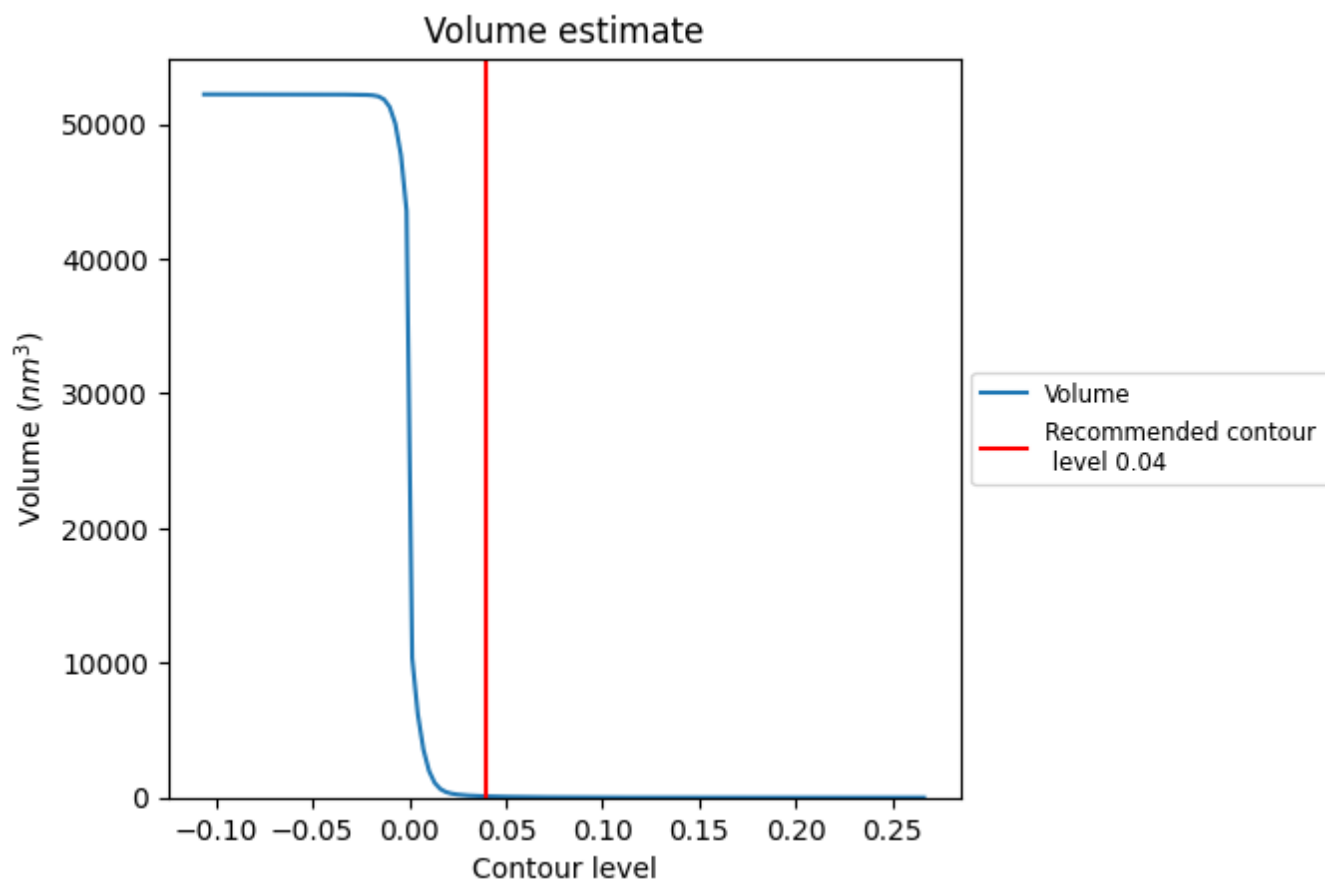
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

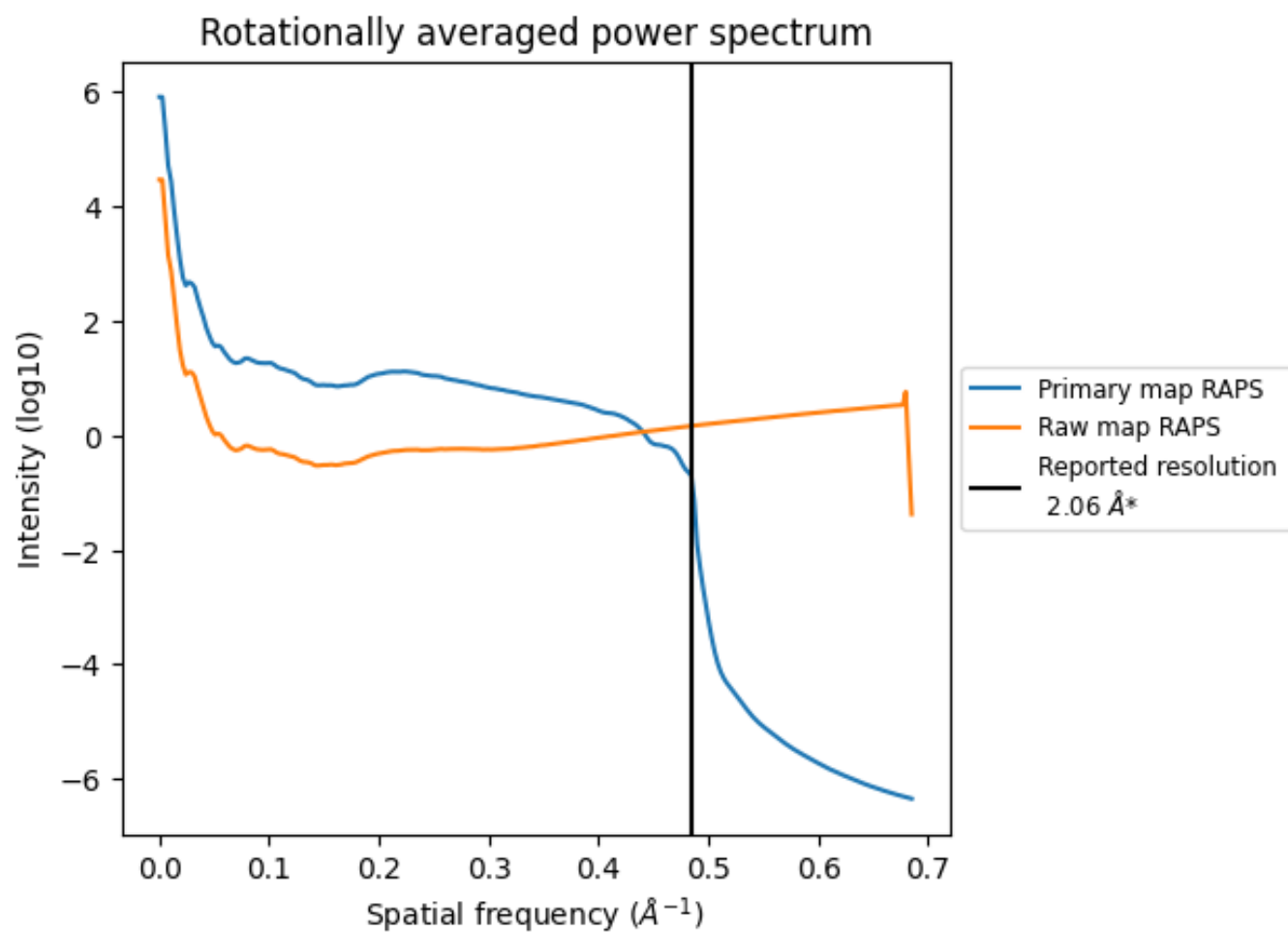
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 93 nm^3 ; this corresponds to an approximate mass of 84 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 ⓘ

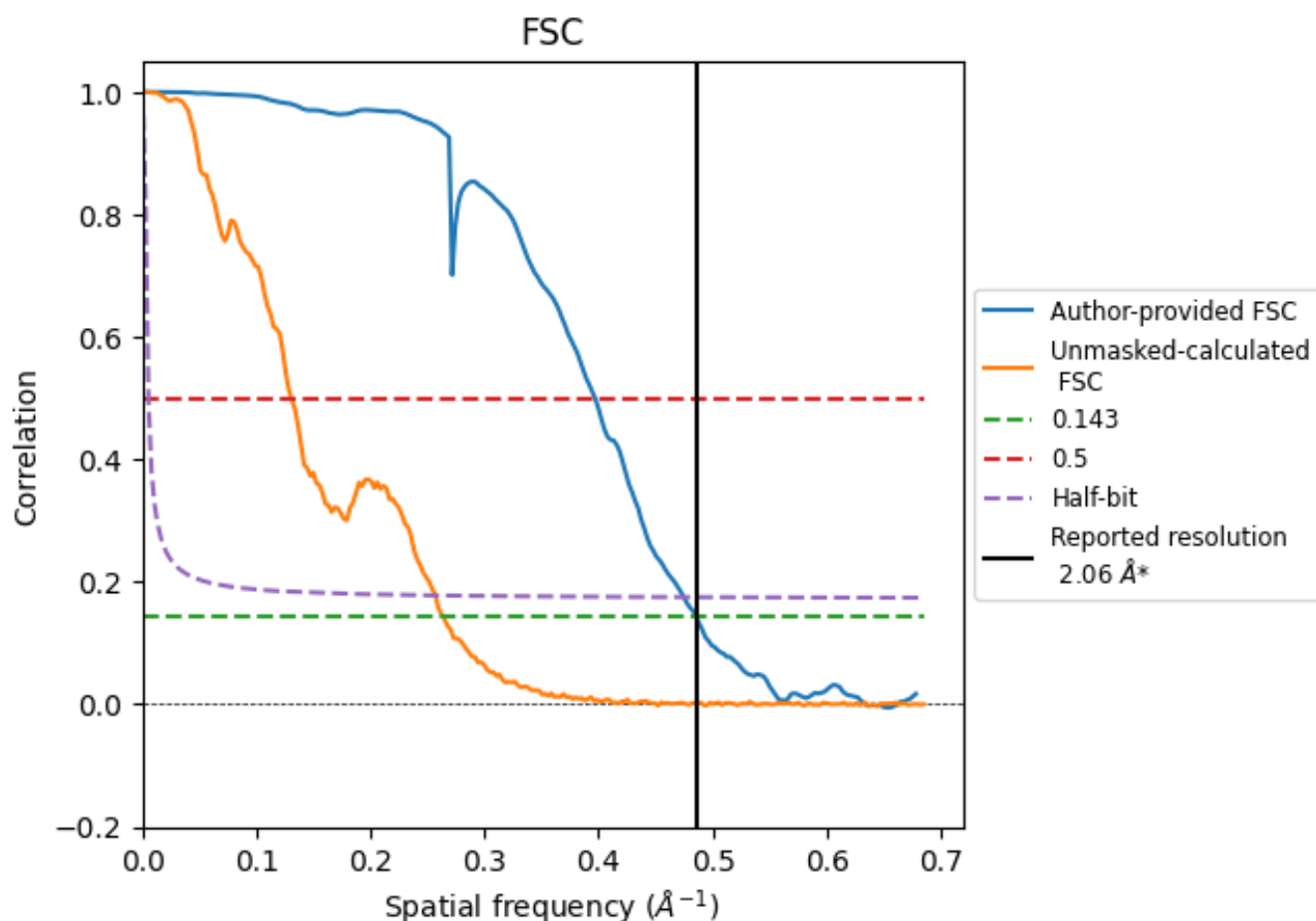


*Reported resolution corresponds to spatial frequency of 0.485 \AA^{-1}

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 0.485 Å⁻¹

8.2 Resolution estimates [i](#)

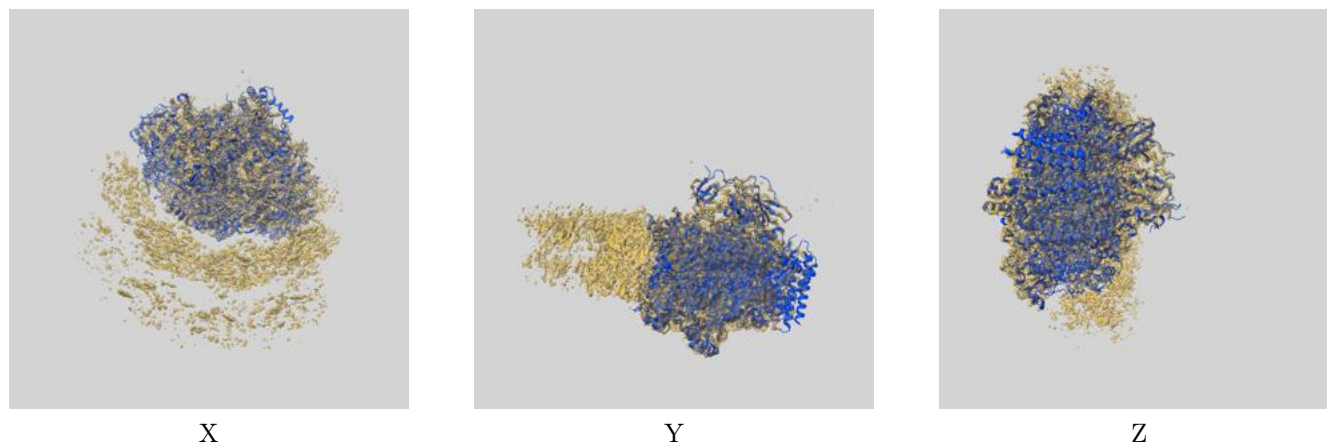
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.06	-	-
Author-provided FSC curve	2.06	2.52	2.11
Unmasked-calculated*	3.79	7.66	3.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.79 differs from the reported value 2.06 by more than 10 %

9 Map-model fit [i](#)

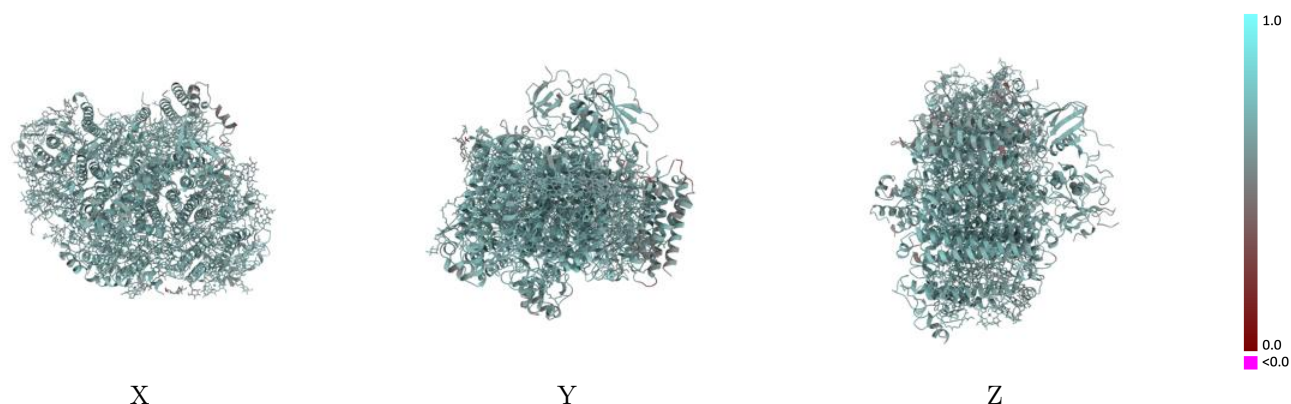
This section contains information regarding the fit between EMDB map EMD-54804 and PDB model 9SE7. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



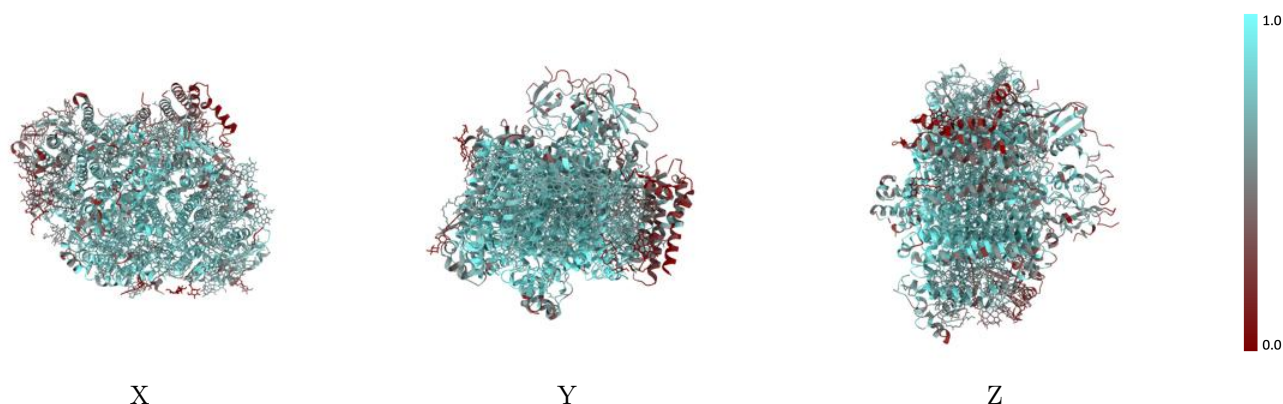
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



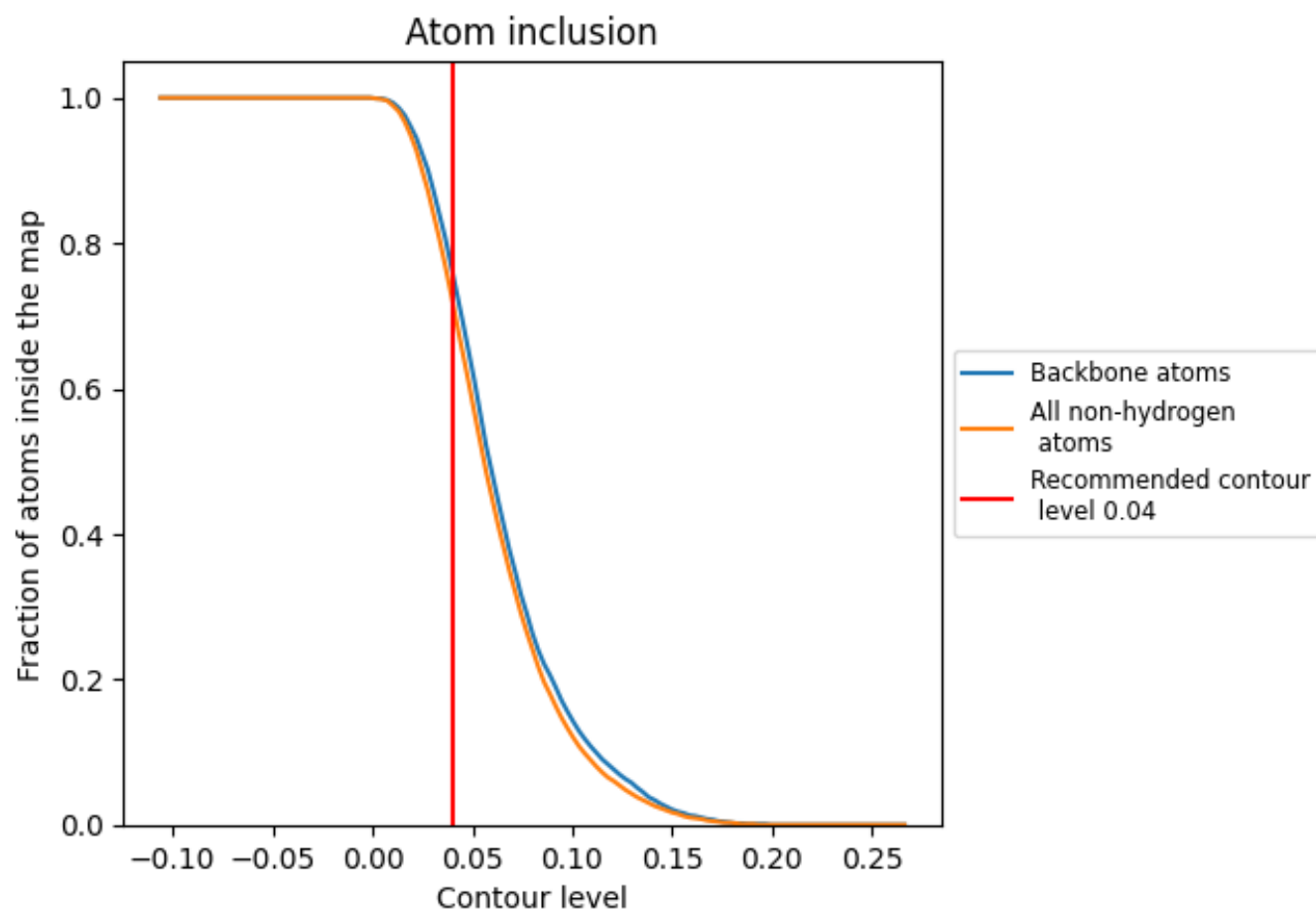
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion ⓘ



At the recommended contour level, 76% of all backbone atoms, 72% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7210	<div></div> 0.6500
A	<div></div> 0.8010	<div></div> 0.6660
B	<div></div> 0.7490	<div></div> 0.6590
C	<div></div> 0.6900	<div></div> 0.6350
D	<div></div> 0.5190	<div></div> 0.6200
E	<div></div> 0.5210	<div></div> 0.6040
F	<div></div> 0.7400	<div></div> 0.6460
I	<div></div> 0.4670	<div></div> 0.6210
J	<div></div> 0.6830	<div></div> 0.6380
L	<div></div> 0.2720	<div></div> 0.5550
T	<div></div> 0.6650	<div></div> 0.6120

1.0

0.0

<0.0