



Full wwPDB EM Validation Report ⓘ

Oct 12, 2026 – 02:29 PM JST

PDB ID : 9X4R / pdb_00009x4r
EMDB ID : EMD-66564
Title : photosystem I core from a green alga as lichen phycobiont
Authors : Su, X.D.; Wei, X.L.; Li, M.
Deposited on : 2025-10-11
Resolution : 3.46 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

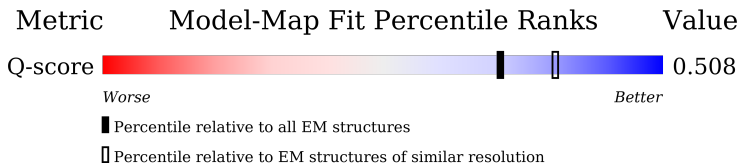
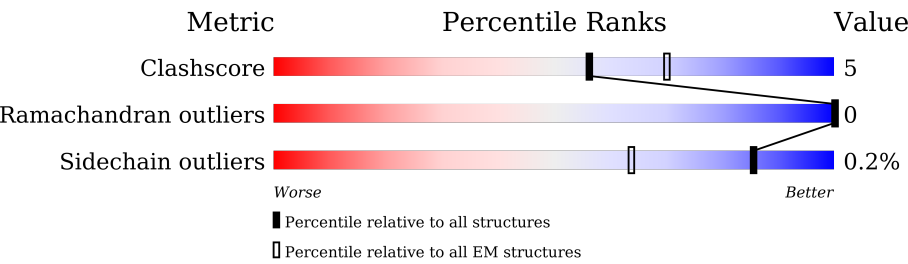
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.2
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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) : 2.51

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.46 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	13788 (2.96 - 3.96)

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

Mol	Chain	Length	Quality of chain
1	A	751	91% 8%
2	B	734	89% 7%
3	C	81	88% 11%
4	D	239	7% 54% 5% 40%

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Mol	Chain	Length	Quality of chain
5	E	111	
6	F	251	
7	I	106	
8	J	41	
9	K	126	
10	L	176	
11	M	32	

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
16	SF4	C	102	-	-	X	-

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 21846 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 PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	741	Total	C	N	O	S	0	0
			5834	3819	995	1002	18		

- Molecule 2 is a protein called PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	703	Total	C	N	O	S	0	0
			5601	3687	942	961	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			600	369	103	116	12		

- Molecule 4 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	143	Total	C	N	O	S	0	0
			1120	717	198	200	5		

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	62	Total	C	N	O	0	0
			484	309	86	89		

- Molecule 6 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	68	Total	C	N	O	S	0	0
			521	352	84	84	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	34	Total	C	N	O	S	0	0
			256	176	36	43	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	40	Total	C	N	O	S	0	0
			326	222	46	57	1		

- Molecule 9 is a protein called PsaK.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	K	81	Total	C	N	O	0	0
			571	363	97	111		

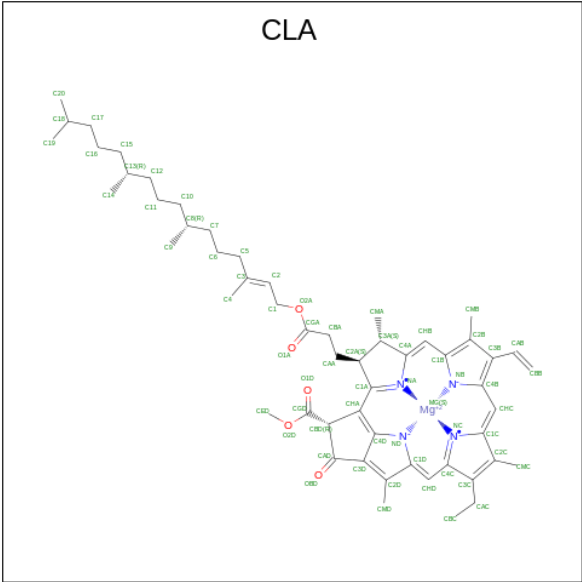
- Molecule 10 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	122	Total	C	N	O	S	0	0
			889	582	146	159	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	32	Total	C	N	O	S	0	0
			246	163	38	44	1		

- Molecule 12 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
12	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
12	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
12	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
12	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
12	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
12	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
12	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			57	48	1	4	4	
12	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
12	B	1	Total	C	Mg	N	O	0
			44	35	1	4	4	

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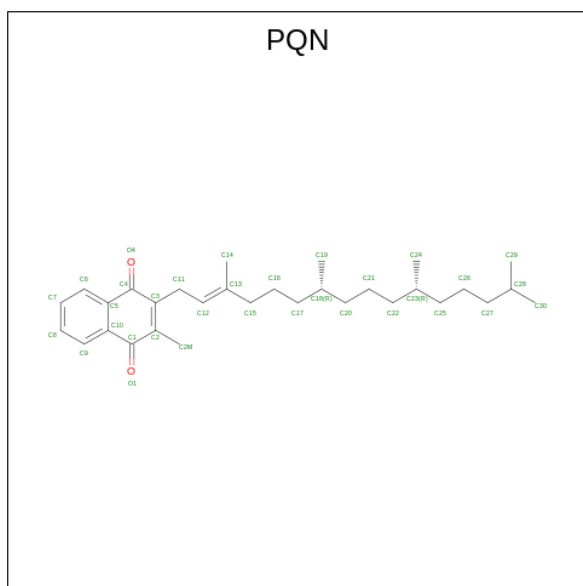
Mol	Chain	Residues	Atoms					AltConf
12	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			54	45	1	4	4	
12	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
12	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
12	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
12	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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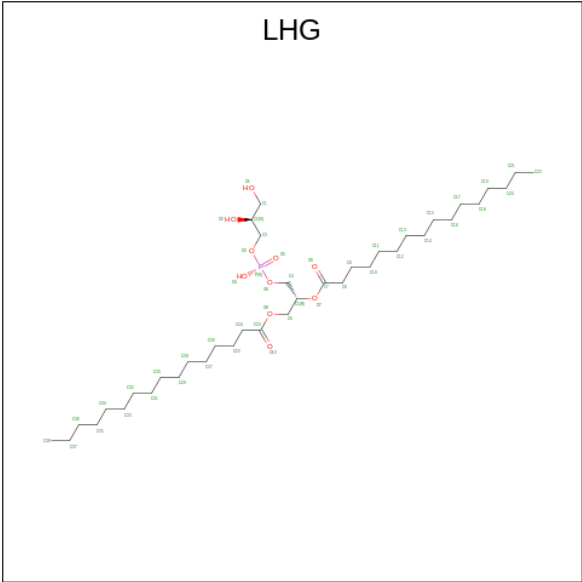
Mol	Chain	Residues	Atoms					AltConf
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
12	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
12	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
12	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	K	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
12	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	L	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

- Molecule 13 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



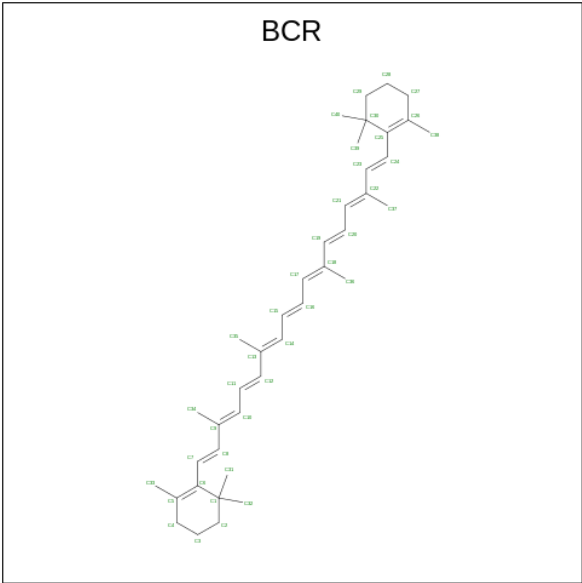
Mol	Chain	Residues	Atoms			AltConf
13	A	1	Total	C	O	0
			33	31	2	
13	B	1	Total	C	O	0
			33	31	2	

- Molecule 14 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
14	A	1	Total	C	O	P	0
			49	38	10	1	
14	A	1	Total	C	O	P	0
			45	34	10	1	

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



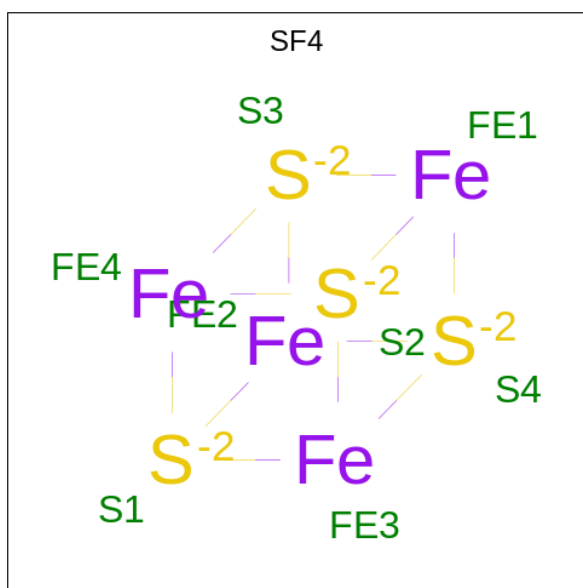
Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total	C	0
			40	40	
15	A	1	Total	C	0
			40	40	

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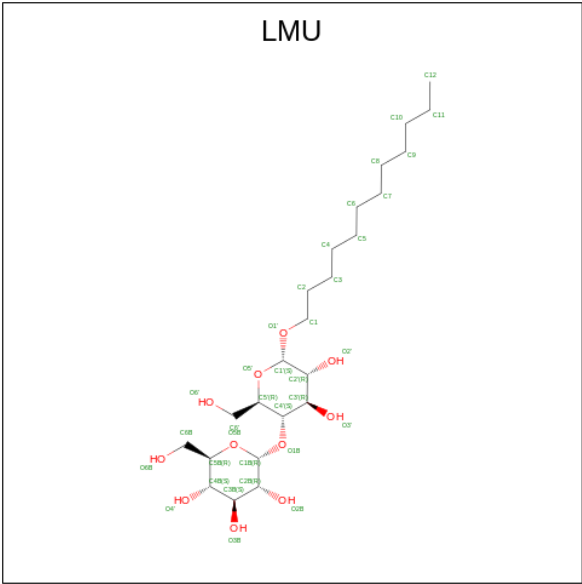
Mol	Chain	Residues	Atoms	AltConf
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	I	1	Total C 40 40	0
15	J	1	Total C 40 40	0
15	K	1	Total C 40 40	0
15	L	1	Total C 40 40	0
15	L	1	Total C 40 40	0
15	M	1	Total C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

- Molecule 16 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



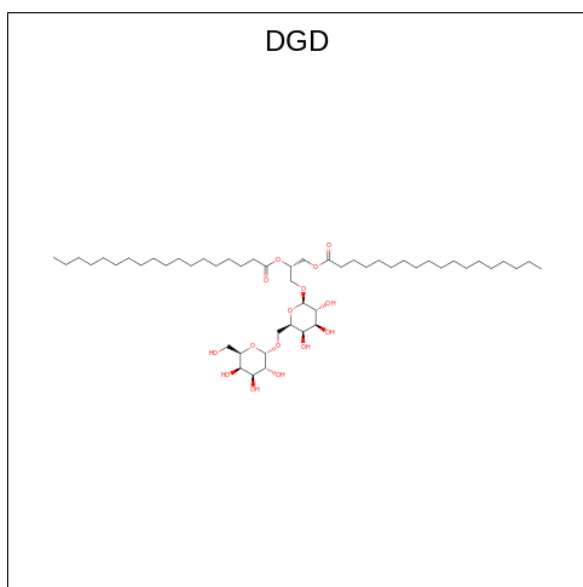
Mol	Chain	Residues	Atoms			AltConf
16	A	1	Total	Fe	S	0
			8	4	4	
16	C	1	Total	Fe	S	0
			8	4	4	
16	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 17 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			AltConf
17	A	1	Total	C	O	0
			34	24	10	

- Molecule 18 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).

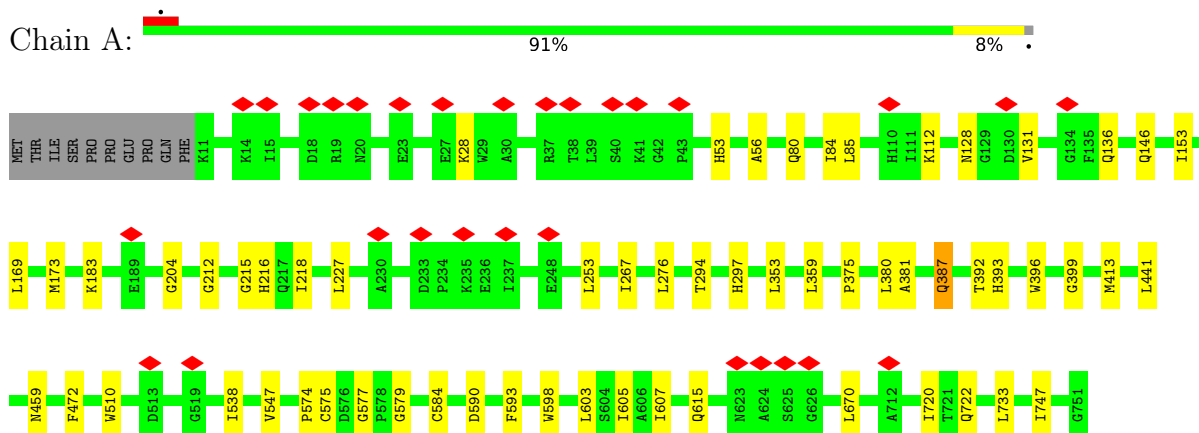


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
18	B	1	58	43	15	0

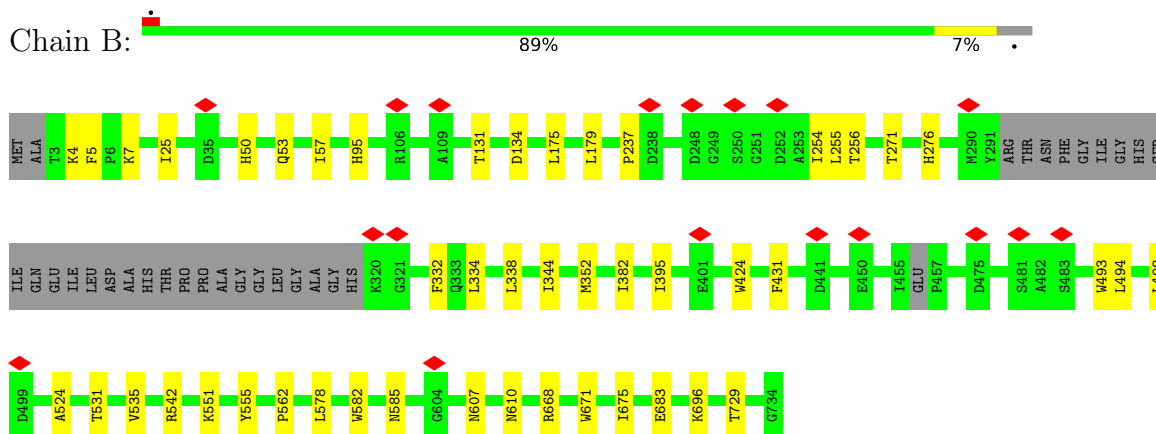
3 Residue-property plots

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.

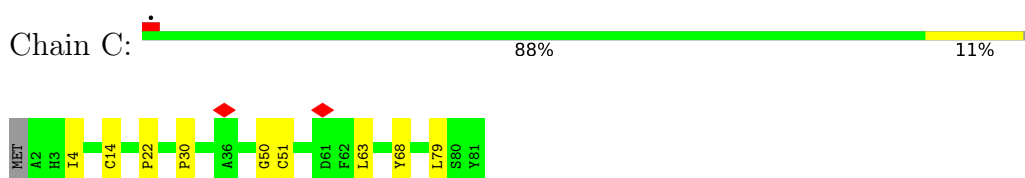
• Molecule 1: PsaA



• Molecule 2: PsaB

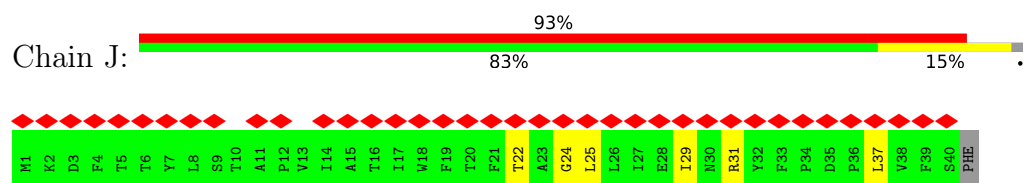


• Molecule 3: Photosystem I iron-sulfur center

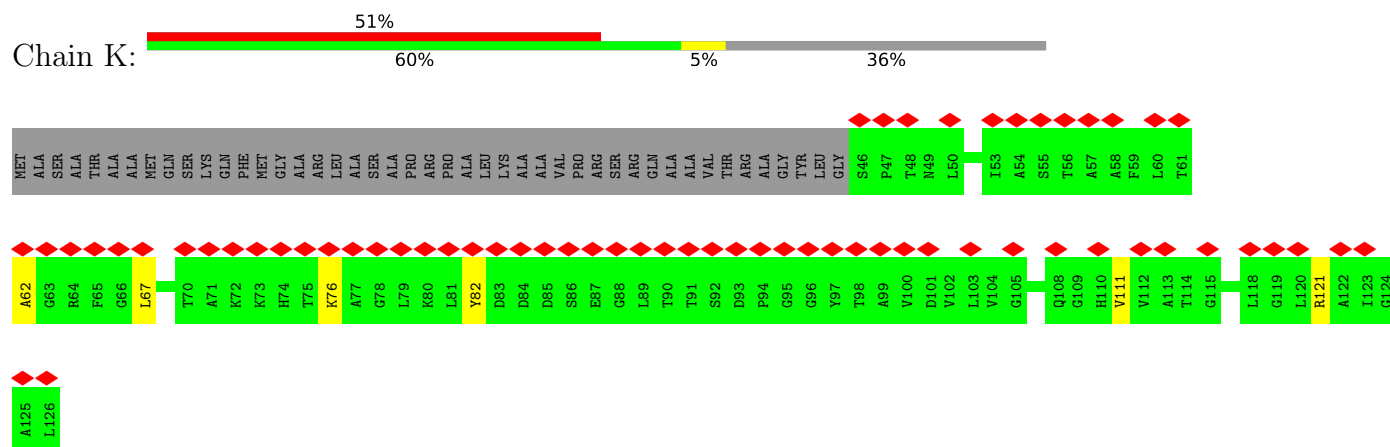


• Molecule 4: PsaD

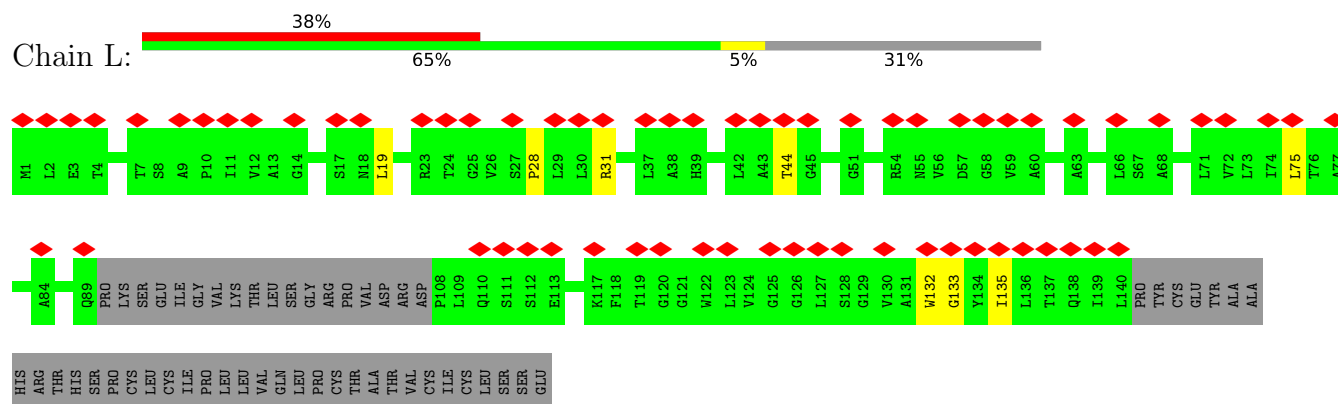
- Molecule 8: Photosystem I reaction center subunit IX



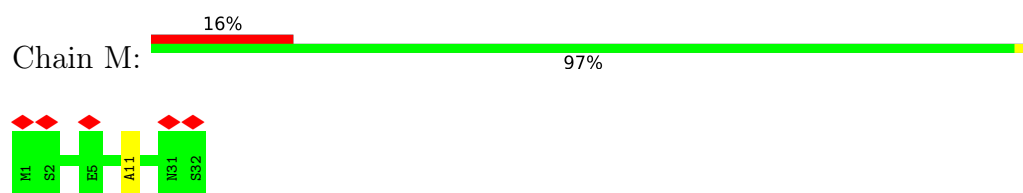
- Molecule 9: PsaK



- Molecule 10: PsaL



- Molecule 11: Photosystem I reaction center subunit XII



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	44940	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.257	Depositor
Minimum map value	-0.102	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	261.12, 261.12, 261.12	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.02, 1.02, 1.02	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.20	0/6030	0.44	2/8224 (0.0%)
2	B	0.20	0/5808	0.44	0/7937
3	C	0.18	0/610	0.51	0/826
4	D	0.16	0/1146	0.45	0/1545
5	E	0.13	0/495	0.34	0/674
6	F	0.23	0/536	0.48	0/727
7	I	0.39	0/265	0.75	0/367
8	J	0.26	0/337	0.65	0/462
9	K	0.21	0/580	0.47	0/789
10	L	0.20	0/908	0.45	0/1238
11	M	0.18	0/249	0.39	0/335
All	All	0.20	0/16964	0.46	2/23124 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	153	ILE	CA-C-N	5.12	129.68	122.46
1	A	153	ILE	C-N-CA	5.12	129.68	122.46

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5834	0	5700	45	0
2	B	5601	0	5365	38	0
3	C	600	0	581	9	0
4	D	1120	0	1137	8	0
5	E	484	0	481	2	0
6	F	521	0	530	3	0
7	I	256	0	268	3	0
8	J	326	0	327	4	0
9	K	571	0	582	4	0
10	L	889	0	927	5	0
11	M	246	0	260	1	0
12	A	2153	0	1981	57	0
12	B	2087	0	1950	43	0
12	F	41	0	29	0	0
12	J	42	0	31	1	0
12	K	138	0	109	0	0
12	L	101	0	85	4	0
13	A	33	0	46	1	0
13	B	33	0	46	5	0
14	A	94	0	137	5	0
15	A	160	0	224	15	0
15	B	160	0	224	12	0
15	I	40	0	56	4	0
15	J	40	0	56	5	0
15	K	40	0	56	2	0
15	L	80	0	111	13	0
15	M	40	0	56	3	0
16	A	8	0	0	0	0
16	C	16	0	0	3	0
17	A	34	0	44	1	0
18	B	58	0	74	0	0
All	All	21846	0	21473	212	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 5.

All (212) 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)
3:C:14:CYS:HB3	16:C:102:SF4:S1	2.11	0.91
12:B:802:CLA:C4B	12:B:807:CLA:HBB1	1.98	0.87
3:C:51:CYS:HB3	16:C:101:SF4:S3	2.20	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:820:CLA:H101	15:A:847:BCR:H21C	1.72	0.71
12:A:828:CLA:H2	15:A:845:BCR:H24C	1.76	0.68
1:A:353:LEU:HD11	12:A:829:CLA:HBB1	1.79	0.65
1:A:216:HIS:CE1	12:A:813:CLA:ND	2.65	0.64
12:B:801:CLA:HBB1	12:B:805:CLA:C4B	2.29	0.63
12:A:805:CLA:H151	12:A:828:CLA:HBB2	1.80	0.62
12:A:818:CLA:HAB	12:A:818:CLA:H8	1.82	0.61
12:B:821:CLA:HBA2	12:B:825:CLA:HBB2	1.82	0.61
12:L:203:CLA:HAC2	15:L:204:BCR:HC42	1.84	0.59
1:A:399:GLY:HA3	1:A:603:LEU:HD11	1.83	0.59
12:A:810:CLA:H72	15:J:101:BCR:H312	1.86	0.57
12:B:838:CLA:H8	12:B:839:CLA:H121	1.85	0.57
8:J:24:GLY:HA3	12:J:102:CLA:HAB	1.87	0.57
1:A:359:LEU:HD21	12:A:820:CLA:H71	1.87	0.56
1:A:441:LEU:HD22	12:A:837:CLA:HBB1	1.86	0.56
2:B:585:ASN:HB2	12:B:805:CLA:HBC2	1.86	0.56
1:A:80:GLN:HE21	1:A:84:ILE:HG13	1.71	0.56
1:A:112:LYS:HB2	1:A:131:VAL:HB	1.88	0.56
12:A:804:CLA:H41	15:A:845:BCR:H23C	1.87	0.56
1:A:579:GLY:HA3	3:C:50:GLY:HA3	1.88	0.55
1:A:733:LEU:HD22	12:A:839:CLA:HMA1	1.88	0.55
12:A:802:CLA:HAB	15:J:101:BCR:H313	1.88	0.55
12:B:838:CLA:HAB	13:B:840:PQN:H162	1.88	0.55
12:B:810:CLA:H151	12:B:827:CLA:HBB2	1.89	0.55
1:A:396:TRP:CD1	12:A:827:CLA:HAB	2.42	0.54
12:A:807:CLA:H2	15:B:804:BCR:H391	1.89	0.54
4:D:216:SER:HB3	4:D:218:ARG:HD3	1.89	0.54
2:B:334:LEU:HD11	12:B:828:CLA:HBB1	1.90	0.53
2:B:493:TRP:HH2	12:B:834:CLA:H2A	1.74	0.52
12:A:811:CLA:HED2	12:A:812:CLA:HAC1	1.92	0.52
1:A:227:LEU:HG	1:A:253:LEU:HD21	1.91	0.51
12:B:811:CLA:HBC1	11:M:11:ALA:HB1	1.93	0.51
1:A:204:GLY:HA3	12:A:812:CLA:HBB1	1.92	0.51
2:B:95:HIS:NE2	12:B:814:CLA:NA	2.58	0.51
6:F:194:TYR:HB2	6:F:219:VAL:HG21	1.92	0.51
2:B:237:PRO:HB3	2:B:256:THR:HG21	1.92	0.51
12:B:839:CLA:HAC1	13:B:840:PQN:H172	1.93	0.51
2:B:4:LYS:HE3	7:I:103:ALA:HA	1.92	0.51
12:A:820:CLA:H61	15:A:846:BCR:H352	1.93	0.51
12:A:831:CLA:HBB1	12:B:803:CLA:HBA2	1.93	0.51
12:B:811:CLA:HMB3	12:B:812:CLA:HHB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:831:CLA:HBB2	15:L:202:BCR:H373	1.93	0.50
1:A:267:ILE:HG22	9:K:121:ARG:HH22	1.76	0.50
12:B:839:CLA:H42	13:B:840:PQN:H292	1.94	0.50
4:D:98:LEU:HD22	4:D:102:ALA:HB2	1.93	0.50
7:I:95:LEU:HD22	15:L:204:BCR:H271	1.94	0.49
12:A:826:CLA:H152	12:A:833:CLA:H112	1.95	0.49
2:B:582:TRP:NE1	12:B:801:CLA:ND	2.60	0.49
12:B:802:CLA:H191	12:B:813:CLA:H2	1.93	0.49
3:C:4:ILE:HG23	3:C:68:TYR:HB2	1.94	0.49
12:B:821:CLA:H143	12:B:834:CLA:HAA2	1.93	0.49
8:J:31:ARG:HD3	15:J:101:BCR:H291	1.93	0.49
1:A:218:ILE:HD11	1:A:276:LEU:HD21	1.95	0.49
12:A:826:CLA:HBA1	15:A:847:BCR:H12C	1.95	0.49
8:J:22:THR:HA	8:J:25:LEU:HD12	1.95	0.49
1:A:387:GLN:HA	1:A:387:GLN:HE21	1.78	0.49
2:B:494:LEU:O	2:B:498:LEU:HB2	2.13	0.48
10:L:132:TRP:HA	10:L:135:ILE:HG22	1.94	0.48
2:B:5:PHE:HB2	7:I:99:ILE:HA	1.94	0.48
2:B:332:PHE:HE1	15:B:842:BCR:H312	1.77	0.48
12:B:838:CLA:H93	15:I:201:BCR:H382	1.95	0.48
1:A:670:LEU:HB3	12:B:805:CLA:H92	1.96	0.48
2:B:25:ILE:HD11	15:L:204:BCR:H383	1.94	0.48
2:B:395:ILE:HD13	2:B:555:TYR:HA	1.95	0.48
1:A:56:ALA:HB3	12:A:829:CLA:H12	1.96	0.48
12:B:810:CLA:HHB	12:B:828:CLA:HAB	1.96	0.48
3:C:22:PRO:HB2	4:D:143:GLU:HG3	1.94	0.48
1:A:28:LYS:HB2	12:A:810:CLA:HAA2	1.96	0.47
10:L:19:LEU:HD22	12:L:203:CLA:HBD	1.96	0.47
1:A:146:GLN:HE21	1:A:380:LEU:HA	1.79	0.47
8:J:29:ILE:HD13	8:J:37:LEU:HD11	1.96	0.47
1:A:459:ASN:HD21	1:A:472:PHE:HB2	1.79	0.47
1:A:590:ASP:HA	1:A:593:PHE:HB3	1.97	0.47
12:A:838:CLA:H121	12:A:838:CLA:HAB	1.96	0.47
2:B:131:THR:HG23	2:B:134:ASP:H	1.80	0.47
2:B:542:ARG:HH21	2:B:551:LYS:HD3	1.79	0.47
5:E:53:LYS:HA	5:E:53:LYS:HD2	1.75	0.46
12:A:820:CLA:H72	15:A:847:BCR:H19C	1.97	0.46
2:B:95:HIS:CE1	12:B:814:CLA:NB	2.84	0.46
12:B:819:CLA:H2	12:B:819:CLA:H62	1.71	0.46
15:B:843:BCR:H15C	15:B:843:BCR:H351	1.71	0.46
5:E:84:TYR:HA	5:E:104:GLY:HA2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:338:LEU:HD22	2:B:382:ILE:HG23	1.97	0.46
12:B:832:CLA:H8	12:B:832:CLA:H52	1.81	0.46
14:A:843:LHG:H201	14:A:843:LHG:H301	1.98	0.46
2:B:53:GLN:HE21	2:B:57:ILE:HG13	1.81	0.46
15:A:846:BCR:H15C	15:A:846:BCR:H351	1.77	0.46
12:B:811:CLA:H93	15:M:101:BCR:H353	1.98	0.46
12:B:824:CLA:HMA1	15:B:842:BCR:H17C	1.98	0.46
15:A:844:BCR:H15C	15:A:844:BCR:H351	1.75	0.46
2:B:431:PHE:HD1	15:B:804:BCR:H332	1.81	0.46
15:L:202:BCR:H15C	15:L:202:BCR:H351	1.79	0.46
12:A:822:CLA:H191	9:K:111:VAL:HG11	1.97	0.45
12:B:812:CLA:HAB	12:B:813:CLA:HBA1	1.98	0.45
12:B:834:CLA:HBA2	12:B:834:CLA:H3A	1.53	0.45
3:C:14:CYS:CB	16:C:102:SF4:S1	2.95	0.45
1:A:547:VAL:HG21	12:A:837:CLA:HMA1	1.99	0.45
2:B:175:LEU:O	2:B:179:LEU:HB2	2.16	0.45
1:A:212:GLY:HA2	12:A:814:CLA:HBB2	1.98	0.45
1:A:574:PRO:HB3	1:A:720:ILE:HB	1.99	0.45
15:B:841:BCR:H15C	15:B:841:BCR:H351	1.84	0.45
12:B:811:CLA:H2	12:B:811:CLA:H61	1.76	0.45
1:A:85:LEU:HD13	1:A:169:LEU:HB3	1.99	0.45
6:F:190:VAL:HG22	6:F:220:CYS:HA	1.99	0.45
12:A:820:CLA:H102	12:A:823:CLA:H91	1.98	0.45
12:A:838:CLA:H3A	12:A:838:CLA:HBA2	1.70	0.45
12:A:812:CLA:H61	12:A:812:CLA:H102	1.83	0.44
12:A:832:CLA:H143	12:A:832:CLA:H111	1.84	0.44
4:D:123:PRO:HD3	4:D:148:LEU:HD13	1.99	0.44
9:K:76:LYS:HE3	9:K:82:TYR:HB3	2.00	0.44
12:A:839:CLA:HAA1	13:A:840:PQN:H301	2.00	0.44
12:B:812:CLA:H72	15:B:843:BCR:H382	1.99	0.44
2:B:50:HIS:NE2	12:B:809:CLA:NA	2.66	0.44
2:B:683:GLU:HG2	4:D:100:ARG:HH21	1.82	0.44
1:A:294:THR:HG21	12:A:818:CLA:HED3	2.00	0.44
15:A:845:BCR:H11C	15:A:845:BCR:H341	1.85	0.44
2:B:254:ILE:HG13	2:B:255:LEU:HG	2.00	0.44
12:A:805:CLA:H202	12:A:805:CLA:H161	1.88	0.44
15:A:847:BCR:H351	15:A:847:BCR:H15C	1.84	0.44
15:L:202:BCR:H281	12:L:203:CLA:ND	2.32	0.44
3:C:63:LEU:H	3:C:63:LEU:HG	1.64	0.44
15:J:101:BCR:H15C	15:J:101:BCR:H351	1.76	0.43
12:A:837:CLA:H41	14:A:843:LHG:H331	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:44:THR:HG21	10:L:133:GLY:HA3	1.99	0.43
15:A:846:BCR:H361	15:A:846:BCR:H20C	1.81	0.43
15:I:201:BCR:H11C	15:I:201:BCR:H341	1.84	0.43
1:A:392:THR:HG23	1:A:607:ILE:HG21	1.99	0.43
1:A:598:TRP:CH2	12:B:802:CLA:HAB	2.54	0.43
1:A:393:HIS:CE1	12:A:827:CLA:ND	2.86	0.43
1:A:510:TRP:HH2	12:A:835:CLA:HED3	1.83	0.43
14:A:842:LHG:H262	14:A:842:LHG:H291	1.86	0.43
6:F:187:ILE:H	6:F:187:ILE:HG13	1.68	0.43
1:A:173:MET:HE1	12:A:812:CLA:H92	2.01	0.43
1:A:375:PRO:HG3	1:A:381:ALA:HB2	1.99	0.43
1:A:605:ILE:HD12	12:A:801:CLA:H122	2.00	0.43
17:A:849:LMU:H92	17:A:849:LMU:H61	1.82	0.43
1:A:441:LEU:HD21	1:A:547:VAL:HG12	2.01	0.42
12:A:837:CLA:H51	14:A:843:LHG:H331	2.01	0.42
10:L:75:LEU:HD13	15:L:204:BCR:H323	2.01	0.42
12:A:826:CLA:H2	12:A:826:CLA:H61	1.76	0.42
4:D:115:LYS:HG2	4:D:158:LEU:HD21	2.01	0.42
15:M:101:BCR:H15C	15:M:101:BCR:H351	1.86	0.42
1:A:538:ILE:HD12	12:A:801:CLA:H172	2.01	0.42
12:A:812:CLA:H122	12:A:812:CLA:H8	1.87	0.42
12:L:201:CLA:H2	12:L:201:CLA:H62	1.87	0.42
15:L:204:BCR:H11C	15:L:204:BCR:H341	1.77	0.42
12:A:823:CLA:H62	12:A:837:CLA:H42	2.00	0.42
15:B:804:BCR:H20C	15:B:804:BCR:H361	1.78	0.42
15:B:843:BCR:H11C	15:B:843:BCR:H341	1.77	0.42
1:A:722:GLN:HE21	14:A:842:LHG:HC81	1.83	0.42
15:A:846:BCR:H11C	15:A:846:BCR:H341	1.83	0.42
2:B:256:THR:H	2:B:271:THR:HB	1.84	0.42
2:B:276:HIS:HE1	12:B:821:CLA:ND	2.17	0.42
12:A:823:CLA:H142	12:A:823:CLA:H112	1.86	0.42
15:L:204:BCR:H15C	15:L:204:BCR:H351	1.80	0.42
2:B:671:TRP:O	2:B:675:ILE:HG12	2.19	0.42
13:B:840:PQN:H2M1	13:B:840:PQN:H111	1.83	0.42
15:K:202:BCR:H20C	15:K:202:BCR:H361	1.78	0.42
10:L:28:PRO:HA	10:L:31:ARG:HD3	2.00	0.42
4:D:138:LYS:HE2	4:D:138:LYS:HB3	1.90	0.42
15:J:101:BCR:H11C	15:J:101:BCR:H341	1.75	0.42
1:A:128:ASN:HB3	1:A:136:GLN:HB3	2.01	0.42
12:A:815:CLA:HBA1	12:A:815:CLA:H3A	1.55	0.42
12:A:824:CLA:HBA1	12:A:828:CLA:H193	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:494:LEU:HD12	2:B:494:LEU:HA	1.90	0.42
15:L:204:BCR:H20C	15:L:204:BCR:H361	1.86	0.42
1:A:575:CYS:HB3	1:A:584:CYS:HA	2.01	0.41
1:A:577:GLY:HA2	2:B:562:PRO:HD3	2.02	0.41
2:B:7:LYS:HE2	2:B:7:LYS:HB3	1.96	0.41
2:B:578:LEU:HB3	12:B:801:CLA:HMD1	2.01	0.41
15:B:843:BCR:H24C	15:B:843:BCR:H371	1.89	0.41
15:L:202:BCR:H24C	15:L:202:BCR:H371	1.81	0.41
12:A:822:CLA:H111	15:K:202:BCR:HC41	2.01	0.41
15:I:201:BCR:H392	15:L:202:BCR:H353	2.02	0.41
12:A:818:CLA:HBA2	12:A:818:CLA:H3A	1.65	0.41
12:A:829:CLA:H142	12:A:829:CLA:H111	1.91	0.41
15:L:202:BCR:H11C	15:L:202:BCR:H341	1.82	0.41
12:A:804:CLA:H93	12:A:804:CLA:H61	1.92	0.41
12:B:810:CLA:H101	12:B:810:CLA:H13	1.91	0.41
3:C:30:PRO:HG3	4:D:187:ALA:HA	2.03	0.41
1:A:53:HIS:HE1	12:A:802:CLA:ND	2.17	0.41
1:A:413:MET:HB3	1:A:413:MET:HE3	1.82	0.41
15:A:844:BCR:H371	15:A:844:BCR:H24C	1.76	0.41
15:A:844:BCR:H11C	15:A:844:BCR:H341	1.86	0.41
15:A:847:BCR:H20C	15:A:847:BCR:H361	1.96	0.41
12:B:824:CLA:CAD	12:B:835:CLA:HBB1	2.51	0.41
1:A:297:HIS:HE2	12:A:818:CLA:C2B	2.34	0.41
2:B:524:ALA:HB2	12:B:836:CLA:HMA1	2.03	0.41
12:B:811:CLA:H3A	12:B:812:CLA:HMB2	2.02	0.41
15:B:842:BCR:H15C	15:B:842:BCR:H351	1.88	0.41
1:A:615:GLN:HE21	1:A:747:ILE:HD13	1.86	0.41
12:A:803:CLA:HBA1	12:A:803:CLA:H3A	1.78	0.41
2:B:424:TRP:CE2	12:B:830:CLA:HAB	2.56	0.41
15:I:201:BCR:H15C	15:I:201:BCR:H351	1.78	0.41
2:B:668:ARG:HB2	13:B:840:PQN:H7	2.03	0.41
12:B:826:CLA:H3A	12:B:826:CLA:HBA2	1.56	0.41
1:A:183:LYS:HD3	1:A:183:LYS:HA	1.86	0.40
2:B:531:THR:O	2:B:535:VAL:HB	2.22	0.40
12:A:824:CLA:H202	12:A:824:CLA:H161	1.85	0.40
2:B:352:MET:HE3	2:B:352:MET:HB2	1.92	0.40
1:A:215:GLY:HA3	12:A:814:CLA:HAB	2.03	0.40
2:B:607:ASN:HA	2:B:610:ASN:HB2	2.03	0.40
2:B:696:LYS:HD2	3:C:79:LEU:HD23	2.03	0.40
15:B:804:BCR:H15C	15:B:804:BCR:H351	1.87	0.40
12:B:823:CLA:HBC3	12:B:823:CLA:H102	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:344:ILE:HG23	12:B:822:CLA:H72	2.04	0.40
2:B:582:TRP:CH2	12:B:805:CLA:HAB	2.56	0.40
9:K:62:ALA:HA	9:K:67:LEU:HD13	2.03	0.40
15:M:101:BCR:H24C	15:M:101:BCR:H371	1.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/751 (98%)	709 (96%)	30 (4%)	0	100	100
2	B	697/734 (95%)	673 (97%)	24 (3%)	0	100	100
3	C	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
4	D	141/239 (59%)	133 (94%)	8 (6%)	0	100	100
5	E	60/111 (54%)	56 (93%)	4 (7%)	0	100	100
6	F	64/251 (26%)	60 (94%)	4 (6%)	0	100	100
7	I	32/106 (30%)	30 (94%)	2 (6%)	0	100	100
8	J	38/41 (93%)	35 (92%)	3 (8%)	0	100	100
9	K	79/126 (63%)	76 (96%)	3 (4%)	0	100	100
10	L	118/176 (67%)	115 (98%)	3 (2%)	0	100	100
11	M	30/32 (94%)	30 (100%)	0	0	100	100
All	All	2076/2648 (78%)	1990 (96%)	86 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	604/614 (98%)	603 (100%)	1 (0%)	87	84
2	B	574/595 (96%)	573 (100%)	1 (0%)	87	84
3	C	69/70 (99%)	69 (100%)	0	100	100
4	D	119/194 (61%)	118 (99%)	1 (1%)	73	77
5	E	53/89 (60%)	53 (100%)	0	100	100
6	F	49/190 (26%)	49 (100%)	0	100	100
7	I	28/76 (37%)	28 (100%)	0	100	100
8	J	36/37 (97%)	36 (100%)	0	100	100
9	K	58/87 (67%)	58 (100%)	0	100	100
10	L	91/140 (65%)	91 (100%)	0	100	100
11	M	27/27 (100%)	27 (100%)	0	100	100
All	All	1708/2119 (81%)	1705 (100%)	3 (0%)	85	84

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	387	GLN
2	B	729	THR
4	D	215	VAL

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

Mol	Chain	Res	Type
1	A	136	GLN
1	A	216	HIS
1	A	252	GLN
1	A	459	ASN
1	A	488	GLN
1	A	504	ASN
1	A	539	HIS

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Mol	Chain	Res	Type
1	A	568	ASN
1	A	609	HIS
1	A	615	GLN
1	A	653	GLN
1	A	656	GLN
1	A	705	ASN
2	B	114	ASN
2	B	205	HIS
2	B	242	HIS
2	B	350	GLN
2	B	375	HIS
2	B	403	ASN
2	B	444	GLN
2	B	452	GLN
2	B	464	GLN
2	B	684	HIS
4	D	132	GLN
4	D	186	ASN
4	D	204	ASN
9	K	49	ASN
11	M	31	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

108 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
12	CLA	A	830	1	49,53,73	1.49	8 (16%)	59,89,113	1.33	6 (10%)
15	BCR	M	101	-	41,41,41	0.66	0	56,56,56	1.82	15 (26%)
12	CLA	B	807	-	69,73,73	1.24	8 (11%)	83,113,113	1.20	7 (8%)
12	CLA	B	820	2	58,62,73	1.36	6 (10%)	69,99,113	1.21	4 (5%)
12	CLA	A	806	1	49,53,73	1.47	5 (10%)	59,89,113	1.31	4 (6%)
12	CLA	B	821	2	63,67,73	1.32	8 (12%)	75,105,113	1.20	7 (9%)
12	CLA	A	825	-	54,58,73	1.41	7 (12%)	65,95,113	1.23	6 (9%)
12	CLA	A	832	1	69,73,73	1.25	7 (10%)	83,113,113	1.17	8 (9%)
12	CLA	A	819	1	50,54,73	1.45	7 (14%)	60,90,113	1.37	4 (6%)
12	CLA	B	819	2	56,60,73	1.39	6 (10%)	67,97,113	1.20	5 (7%)
12	CLA	A	811	1	45,49,73	1.55	8 (17%)	54,84,113	1.35	9 (16%)
12	CLA	A	834	1	45,49,73	1.52	7 (15%)	54,84,113	1.35	7 (12%)
12	CLA	B	805	-	60,64,73	1.34	8 (13%)	72,102,113	1.26	8 (11%)
14	LHG	A	842	-	48,48,48	0.94	2 (4%)	51,54,54	0.96	2 (3%)
12	CLA	A	836	1	59,63,73	1.35	7 (11%)	71,101,113	1.24	7 (9%)
12	CLA	B	809	2	69,73,73	1.24	8 (11%)	83,113,113	1.29	8 (9%)
12	CLA	B	802	-	69,73,73	1.25	7 (10%)	83,113,113	1.22	8 (9%)
12	CLA	A	841	14	43,48,73	1.55	6 (13%)	51,83,113	1.30	4 (7%)
12	CLA	A	820	-	64,68,73	1.30	8 (12%)	77,107,113	1.15	7 (9%)
12	CLA	A	815	-	49,53,73	1.49	6 (12%)	59,89,113	1.25	5 (8%)
12	CLA	A	807	1	55,59,73	1.38	7 (12%)	66,96,113	1.24	7 (10%)
12	CLA	A	812	1	68,72,73	1.25	7 (10%)	81,111,113	1.25	5 (6%)
12	CLA	B	812	2	69,73,73	1.24	8 (11%)	83,113,113	1.15	8 (9%)
12	CLA	B	831	2	49,53,73	1.49	7 (14%)	59,89,113	1.41	5 (8%)
15	BCR	A	846	-	41,41,41	0.68	0	56,56,56	2.03	17 (30%)
15	BCR	K	202	-	41,41,41	0.70	0	56,56,56	2.10	15 (26%)
15	BCR	A	845	-	41,41,41	0.70	0	56,56,56	1.89	17 (30%)
12	CLA	B	803	-	68,72,73	1.26	9 (13%)	81,111,113	1.20	8 (9%)
12	CLA	B	839	2	69,73,73	1.26	7 (10%)	83,113,113	1.19	6 (7%)
12	CLA	K	201	9	45,49,73	1.52	6 (13%)	54,84,113	1.29	5 (9%)
16	SF4	A	848	2,1	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	B	813	2	67,71,73	1.28	8 (11%)	80,110,113	1.25	6 (7%)
12	CLA	B	808	2	45,49,73	1.51	7 (15%)	54,84,113	1.33	9 (16%)
12	CLA	B	832	2	59,63,73	1.36	7 (11%)	71,101,113	1.18	5 (7%)
12	CLA	B	835	2	46,50,73	1.50	7 (15%)	55,85,113	1.43	4 (7%)
13	PQN	A	840	-	34,34,34	0.38	0	42,45,45	1.00	2 (4%)
12	CLA	A	802	1	57,61,73	1.37	7 (12%)	68,98,113	1.28	5 (7%)
12	CLA	F	301	-	45,49,73	1.51	6 (13%)	54,84,113	1.32	8 (14%)
15	BCR	B	804	-	41,41,41	0.70	0	56,56,56	2.33	17 (30%)
12	CLA	B	825	2	69,73,73	1.26	7 (10%)	83,113,113	1.19	4 (4%)
12	CLA	B	817	2	48,52,73	1.46	5 (10%)	56,87,113	1.38	4 (7%)
15	BCR	B	843	-	41,41,41	0.70	0	56,56,56	1.97	14 (25%)
15	BCR	B	842	-	41,41,41	0.72	0	56,56,56	2.08	21 (37%)
12	CLA	A	823	1	69,73,73	1.25	6 (8%)	83,113,113	1.15	4 (4%)
12	CLA	A	835	1	54,58,73	1.39	5 (9%)	65,95,113	1.38	7 (10%)
12	CLA	B	823	-	60,64,73	1.34	6 (10%)	72,102,113	1.23	8 (11%)
16	SF4	C	101	3	0,12,12	-	-	-	-	-
12	CLA	B	828	2	59,63,73	1.34	6 (10%)	71,101,113	1.18	5 (7%)
12	CLA	A	810	1,12	63,67,73	1.30	6 (9%)	75,105,113	1.17	5 (6%)
12	CLA	A	833	1	61,65,73	1.34	7 (11%)	73,103,113	1.25	7 (9%)
12	CLA	A	816	1	64,68,73	1.29	7 (10%)	77,107,113	1.19	3 (3%)
12	CLA	B	826	2	64,68,73	1.27	7 (10%)	77,107,113	1.18	8 (10%)
12	CLA	B	827	2	69,73,73	1.27	7 (10%)	83,113,113	1.13	7 (8%)
12	CLA	A	813	1	47,51,73	1.48	7 (14%)	56,86,113	1.28	6 (10%)
12	CLA	B	814	2	61,65,73	1.33	7 (11%)	72,102,113	1.28	5 (6%)
12	CLA	A	805	1	68,72,73	1.26	6 (8%)	81,111,113	1.23	5 (6%)
12	CLA	B	816	2	46,50,73	1.51	7 (15%)	55,85,113	1.43	4 (7%)
12	CLA	A	803	1,12	56,60,73	1.38	7 (12%)	67,97,113	1.26	9 (13%)
12	CLA	K	203	-	59,63,73	1.37	6 (10%)	71,101,113	1.20	4 (5%)
12	CLA	B	833	2	50,54,73	1.45	7 (14%)	60,90,113	1.29	6 (10%)
12	CLA	J	102	8	46,50,73	1.51	5 (10%)	55,85,113	1.26	4 (7%)
12	CLA	A	818	1	69,73,73	1.25	8 (11%)	83,113,113	1.24	8 (9%)
12	CLA	A	831	1	49,53,73	1.48	6 (12%)	59,89,113	1.44	6 (10%)
12	CLA	B	829	-	47,51,73	1.50	6 (12%)	56,86,113	1.25	4 (7%)
15	BCR	I	201	-	41,41,41	0.72	0	56,56,56	2.06	16 (28%)
12	CLA	B	822	2	57,61,73	1.38	6 (10%)	68,98,113	1.34	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	LHG	A	843	12	44,44,48	0.96	2 (4%)	47,50,54	1.00	2 (4%)
12	CLA	A	808	1	54,58,73	1.41	6 (11%)	65,95,113	1.25	6 (9%)
12	CLA	B	838	-	59,63,73	1.35	8 (13%)	71,101,113	1.18	6 (8%)
18	DGD	B	844	-	59,59,67	0.92	2 (3%)	73,73,81	1.01	4 (5%)
12	CLA	A	801	1	69,73,73	1.25	7 (10%)	83,113,113	1.12	7 (8%)
12	CLA	A	817	1	60,64,73	1.34	6 (10%)	72,102,113	1.27	9 (12%)
15	BCR	J	101	-	41,41,41	0.67	0	56,56,56	2.04	13 (23%)
12	CLA	A	837	1	61,65,73	1.32	5 (8%)	73,103,113	1.18	7 (9%)
15	BCR	L	202	-	41,41,41	0.69	0	56,56,56	2.15	16 (28%)
17	LMU	A	849	-	34,35,36	1.26	3 (8%)	42,45,47	1.24	5 (11%)
12	CLA	L	201	1	64,68,73	1.29	6 (9%)	77,107,113	1.22	8 (10%)
12	CLA	A	839	1	46,50,73	1.50	8 (17%)	55,85,113	1.30	6 (10%)
15	BCR	A	844	-	41,41,41	0.67	0	56,56,56	1.99	18 (32%)
12	CLA	A	824	-	68,72,73	1.27	7 (10%)	81,111,113	1.31	5 (6%)
12	CLA	A	814	1	45,49,73	1.51	5 (11%)	54,84,113	1.38	7 (12%)
12	CLA	A	828	1	69,73,73	1.25	8 (11%)	83,113,113	1.15	8 (9%)
15	BCR	B	841	-	41,41,41	0.69	0	56,56,56	2.09	15 (26%)
12	CLA	B	815	2	56,61,73	1.45	7 (12%)	70,99,113	1.22	8 (11%)
12	CLA	L	203	10	45,49,73	1.52	6 (13%)	54,84,113	1.45	5 (9%)
12	CLA	B	811	2	63,67,73	1.31	6 (9%)	75,105,113	1.24	5 (6%)
15	BCR	A	847	-	41,41,41	0.77	0	56,56,56	1.96	14 (25%)
12	CLA	A	826	1	66,70,73	1.28	9 (13%)	79,109,113	1.25	5 (6%)
12	CLA	A	827	1	54,58,73	1.40	8 (14%)	65,95,113	1.27	9 (13%)
16	SF4	C	102	3	0,12,12	-	-	-		
12	CLA	A	804	1	65,69,73	1.28	8 (12%)	78,108,113	1.31	6 (7%)
12	CLA	B	818	2	49,53,73	1.47	7 (14%)	59,89,113	1.36	7 (11%)
13	PQN	B	840	-	34,34,34	0.61	0	42,45,45	0.97	1 (2%)
12	CLA	B	810	2	69,73,73	1.25	6 (8%)	83,113,113	1.22	9 (10%)
12	CLA	B	824	-	54,58,73	1.42	7 (12%)	65,95,113	1.24	10 (15%)
12	CLA	B	801	2	64,68,73	1.30	8 (12%)	77,107,113	1.36	5 (6%)
12	CLA	A	821	1	46,50,73	1.51	5 (10%)	55,85,113	1.25	4 (7%)
12	CLA	B	830	2	47,51,73	1.48	6 (12%)	56,86,113	1.28	7 (12%)
15	BCR	L	204	-	41,41,41	0.66	0	56,56,56	2.17	16 (28%)
12	CLA	B	806	2	69,73,73	1.24	7 (10%)	83,113,113	1.11	6 (7%)
12	CLA	B	837	2	51,55,73	1.45	6 (11%)	61,91,113	1.28	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	A	822	1	69,73,73	1.26	7 (10%)	83,113,113	1.17	7 (8%)
12	CLA	A	829	1	69,73,73	1.24	7 (10%)	83,113,113	1.14	3 (3%)
12	CLA	A	809	1	46,50,73	1.50	6 (13%)	55,85,113	1.25	3 (5%)
12	CLA	K	204	9	46,50,73	1.52	7 (15%)	55,85,113	1.38	4 (7%)
12	CLA	B	836	2	62,66,73	1.33	8 (12%)	74,104,113	1.20	6 (8%)
12	CLA	B	834	-	49,53,73	1.49	7 (14%)	59,89,113	1.40	5 (8%)
12	CLA	A	838	1	69,73,73	1.25	7 (10%)	83,113,113	1.19	8 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	A	830	1	-	4/15/91/115	-
15	BCR	M	101	-	-	4/29/63/63	0/2/2/2
12	CLA	B	807	-	-	13/39/115/115	-
12	CLA	B	820	2	-	12/25/101/115	-
12	CLA	A	806	1	-	6/15/91/115	-
12	CLA	B	821	2	-	8/32/108/115	-
12	CLA	A	825	-	-	8/21/97/115	-
12	CLA	A	832	1	-	19/39/115/115	-
12	CLA	A	819	1	-	12/17/93/115	-
12	CLA	B	819	2	-	10/24/100/115	-
12	CLA	A	811	1	-	5/10/86/115	-
12	CLA	A	834	1	-	6/10/86/115	-
12	CLA	B	805	-	-	8/29/105/115	-
14	LHG	A	842	-	-	12/53/53/53	-
12	CLA	A	836	1	-	8/27/103/115	-
12	CLA	B	809	2	-	12/39/115/115	-
12	CLA	B	802	-	-	11/39/115/115	-
12	CLA	A	841	14	-	4/8/84/115	-
12	CLA	A	820	-	-	16/33/109/115	-
12	CLA	A	815	-	-	9/15/91/115	-
12	CLA	A	807	1	-	8/23/99/115	-
12	CLA	A	812	1	-	9/37/113/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	B	812	2	-	16/39/115/115	-
12	CLA	B	831	2	-	7/15/91/115	-
15	BCR	A	846	-	-	2/29/63/63	0/2/2/2
15	BCR	K	202	-	-	4/29/63/63	0/2/2/2
15	BCR	A	845	-	-	0/29/63/63	0/2/2/2
12	CLA	B	803	-	-	16/37/113/115	-
12	CLA	B	839	2	-	11/39/115/115	-
12	CLA	K	201	9	-	6/10/86/115	-
16	SF4	A	848	2,1	-	-	0/6/5/5
12	CLA	B	813	2	-	14/37/113/115	-
12	CLA	B	808	2	-	0/10/86/115	-
12	CLA	B	832	2	-	9/27/103/115	-
12	CLA	B	835	2	-	4/12/88/115	-
13	PQN	A	840	-	-	7/23/43/43	0/2/2/2
12	CLA	A	802	1	-	7/25/101/115	-
12	CLA	F	301	-	-	4/10/86/115	-
15	BCR	B	804	-	-	11/29/63/63	0/2/2/2
12	CLA	B	825	2	-	12/39/115/115	-
12	CLA	B	817	2	-	2/13/90/115	-
15	BCR	B	843	-	-	2/29/63/63	0/2/2/2
15	BCR	B	842	-	-	2/29/63/63	0/2/2/2
12	CLA	A	823	1	-	18/39/115/115	-
12	CLA	A	835	1	-	6/21/97/115	-
12	CLA	B	823	-	-	15/29/105/115	-
16	SF4	C	101	3	-	-	0/6/5/5
12	CLA	B	828	2	-	9/27/103/115	-
12	CLA	A	810	1,12	-	10/32/108/115	-
12	CLA	A	833	1	-	10/30/106/115	-
12	CLA	A	816	1	-	9/33/109/115	-
12	CLA	B	826	2	-	15/33/109/115	-
12	CLA	B	827	2	-	14/39/115/115	-
12	CLA	A	813	1	-	5/13/89/115	-
12	CLA	B	814	2	-	9/29/105/115	-
12	CLA	A	805	1	-	13/37/113/115	-
12	CLA	B	816	2	-	7/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	A	803	1,12	-	9/24/100/115	-
12	CLA	K	203	-	-	12/27/103/115	-
12	CLA	B	833	2	-	7/17/93/115	-
12	CLA	J	102	8	-	7/12/88/115	-
12	CLA	A	818	1	-	16/39/115/115	-
12	CLA	A	831	1	-	4/15/91/115	-
12	CLA	B	829	-	-	6/13/89/115	-
15	BCR	I	201	-	-	3/29/63/63	0/2/2/2
12	CLA	B	822	2	-	7/25/101/115	-
14	LHG	A	843	12	-	10/49/49/53	-
12	CLA	A	808	1	-	8/21/97/115	-
12	CLA	B	838	-	-	9/27/103/115	-
18	DGD	B	844	-	-	6/47/87/95	0/2/2/2
12	CLA	A	801	1	-	13/39/115/115	-
12	CLA	A	817	1	-	11/29/105/115	-
15	BCR	J	101	-	-	6/29/63/63	0/2/2/2
12	CLA	A	837	1	-	11/30/106/115	-
15	BCR	L	202	-	-	3/29/63/63	0/2/2/2
17	LMU	A	849	-	-	8/21/57/61	0/2/2/2
12	CLA	L	201	1	-	15/33/109/115	-
12	CLA	A	839	1	-	6/12/88/115	-
15	BCR	A	844	-	-	2/29/63/63	0/2/2/2
12	CLA	A	824	-	-	11/37/113/115	-
12	CLA	A	814	1	-	5/10/86/115	-
12	CLA	A	828	1	-	11/39/115/115	-
15	BCR	B	841	-	-	4/29/63/63	0/2/2/2
12	CLA	B	815	2	-	8/23/99/115	-
12	CLA	L	203	10	-	4/10/86/115	-
12	CLA	B	811	2	-	12/32/108/115	-
15	BCR	A	847	-	-	2/29/63/63	0/2/2/2
12	CLA	A	826	1	-	7/36/112/115	-
12	CLA	A	827	1	-	6/21/97/115	-
16	SF4	C	102	3	-	-	0/6/5/5
12	CLA	A	804	1	-	13/35/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	B	818	2	-	4/15/91/115	-
13	PQN	B	840	-	-	1/23/43/43	0/2/2/2
12	CLA	B	810	2	-	11/39/115/115	-
12	CLA	B	824	-	-	5/21/97/115	-
12	CLA	B	801	2	-	12/33/109/115	-
12	CLA	A	821	1	-	5/12/88/115	-
12	CLA	B	830	2	-	4/13/89/115	-
15	BCR	L	204	-	-	4/29/63/63	0/2/2/2
12	CLA	B	806	2	-	22/39/115/115	-
12	CLA	B	837	2	-	6/18/94/115	-
12	CLA	A	822	1	-	21/39/115/115	-
12	CLA	A	829	1	-	14/39/115/115	-
12	CLA	A	809	1	-	6/12/88/115	-
12	CLA	K	204	9	-	8/12/88/115	-
12	CLA	B	836	2	-	8/31/107/115	-
12	CLA	B	834	-	-	7/15/91/115	-
12	CLA	A	838	1	-	13/39/115/115	-

All (587) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	844	DGD	O1G-C1A	4.27	1.45	1.33
14	A	842	LHG	O8-C23	4.21	1.45	1.33
14	A	843	LHG	O8-C23	4.20	1.45	1.33
18	B	844	DGD	O2G-C1B	4.17	1.46	1.34
14	A	842	LHG	O7-C7	4.13	1.45	1.34
12	K	204	CLA	C1D-ND	4.02	1.42	1.37
12	A	824	CLA	C1D-ND	4.02	1.42	1.37
12	A	811	CLA	C4B-NB	4.00	1.42	1.37
12	A	822	CLA	C1D-ND	4.00	1.42	1.37
12	A	801	CLA	C1D-ND	3.99	1.42	1.37
12	A	831	CLA	C1D-ND	3.98	1.42	1.37
14	A	843	LHG	O7-C7	3.98	1.45	1.34
12	J	102	CLA	C1D-ND	3.95	1.42	1.37
12	A	805	CLA	C1D-ND	3.95	1.42	1.37
12	A	823	CLA	C1D-ND	3.95	1.42	1.37
12	A	827	CLA	C1D-ND	3.95	1.42	1.37
12	B	827	CLA	C1D-ND	3.95	1.42	1.37
12	B	817	CLA	C1D-ND	3.94	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	816	CLA	C1D-ND	3.93	1.42	1.37
12	K	203	CLA	C1D-ND	3.93	1.42	1.37
12	B	828	CLA	C1D-ND	3.92	1.42	1.37
12	B	834	CLA	C1D-ND	3.91	1.42	1.37
12	A	809	CLA	C1D-ND	3.90	1.42	1.37
12	B	832	CLA	C1D-ND	3.90	1.42	1.37
12	B	837	CLA	C1D-ND	3.90	1.42	1.37
12	A	838	CLA	C1D-ND	3.90	1.42	1.37
12	A	833	CLA	C1D-ND	3.90	1.42	1.37
12	B	815	CLA	C1D-ND	3.89	1.42	1.37
12	A	832	CLA	C1D-ND	3.89	1.42	1.37
12	A	815	CLA	C1D-ND	3.89	1.42	1.37
12	B	829	CLA	C1D-ND	3.89	1.42	1.37
12	A	829	CLA	C1D-ND	3.89	1.42	1.37
12	A	841	CLA	C1D-ND	3.88	1.42	1.37
12	B	831	CLA	C1D-ND	3.88	1.42	1.37
12	B	822	CLA	C1D-ND	3.87	1.42	1.37
12	A	836	CLA	C1D-ND	3.87	1.42	1.37
12	B	833	CLA	C1D-ND	3.87	1.42	1.37
12	A	826	CLA	C1D-ND	3.86	1.42	1.37
12	A	810	CLA	C1D-ND	3.86	1.42	1.37
12	B	810	CLA	C1D-ND	3.86	1.42	1.37
12	K	201	CLA	C1D-ND	3.86	1.42	1.37
12	L	203	CLA	C1D-ND	3.86	1.42	1.37
12	A	834	CLA	C1D-ND	3.86	1.42	1.37
12	B	823	CLA	C1D-ND	3.86	1.42	1.37
12	A	817	CLA	C1D-ND	3.86	1.42	1.37
12	A	814	CLA	C1D-ND	3.86	1.42	1.37
12	B	802	CLA	C1D-ND	3.86	1.42	1.37
12	B	819	CLA	C1D-ND	3.85	1.42	1.37
12	A	812	CLA	C1D-ND	3.85	1.42	1.37
12	A	804	CLA	C1D-ND	3.84	1.42	1.37
12	B	820	CLA	C1D-ND	3.84	1.42	1.37
12	A	830	CLA	C1D-ND	3.84	1.42	1.37
12	B	835	CLA	C1D-ND	3.84	1.42	1.37
12	A	837	CLA	C1D-ND	3.83	1.42	1.37
12	B	818	CLA	C1D-ND	3.83	1.42	1.37
12	L	201	CLA	C1D-ND	3.83	1.42	1.37
12	A	818	CLA	C1D-ND	3.82	1.42	1.37
12	B	809	CLA	C1D-ND	3.82	1.42	1.37
12	A	808	CLA	C1D-ND	3.82	1.42	1.37
12	B	825	CLA	C1D-ND	3.82	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	806	CLA	C1D-ND	3.81	1.42	1.37
12	A	821	CLA	C1D-ND	3.81	1.42	1.37
12	B	836	CLA	C1D-ND	3.81	1.42	1.37
12	B	806	CLA	C1D-ND	3.81	1.42	1.37
12	B	830	CLA	C1D-ND	3.81	1.42	1.37
12	B	839	CLA	C1D-ND	3.80	1.42	1.37
12	A	813	CLA	C1D-ND	3.79	1.42	1.37
12	A	839	CLA	C1D-ND	3.79	1.42	1.37
12	A	811	CLA	C1D-ND	3.79	1.42	1.37
12	A	816	CLA	C1D-ND	3.79	1.42	1.37
12	B	811	CLA	C1D-ND	3.79	1.42	1.37
12	B	824	CLA	C1D-ND	3.78	1.42	1.37
12	F	301	CLA	C1D-ND	3.78	1.42	1.37
12	A	807	CLA	C1D-ND	3.78	1.42	1.37
12	A	835	CLA	C1D-ND	3.77	1.42	1.37
12	B	808	CLA	C1D-ND	3.77	1.42	1.37
12	B	814	CLA	C1D-ND	3.77	1.42	1.37
12	A	820	CLA	C1D-ND	3.77	1.42	1.37
12	A	802	CLA	C1D-ND	3.76	1.42	1.37
12	B	821	CLA	C1D-ND	3.75	1.42	1.37
12	B	812	CLA	C1D-ND	3.75	1.42	1.37
12	A	821	CLA	C4B-NB	3.73	1.42	1.37
12	B	838	CLA	C1D-ND	3.71	1.42	1.37
12	B	813	CLA	C1D-ND	3.71	1.42	1.37
12	B	826	CLA	C1D-ND	3.71	1.42	1.37
12	B	829	CLA	C4B-NB	3.70	1.42	1.37
12	A	803	CLA	C1D-ND	3.70	1.42	1.37
12	K	201	CLA	C4B-NB	3.69	1.42	1.37
17	A	849	LMU	O5'-C1'	3.67	1.51	1.41
12	J	102	CLA	C4B-NB	3.67	1.42	1.37
12	B	834	CLA	C4B-NB	3.67	1.42	1.37
12	A	825	CLA	C1D-ND	3.67	1.42	1.37
12	B	831	CLA	C4B-NB	3.67	1.42	1.37
12	K	204	CLA	C4B-NB	3.66	1.42	1.37
12	A	819	CLA	C1D-ND	3.65	1.42	1.37
12	B	832	CLA	C4B-NB	3.64	1.42	1.37
12	A	813	CLA	C4B-NB	3.63	1.42	1.37
12	B	803	CLA	C1D-ND	3.63	1.42	1.37
12	A	828	CLA	C1D-ND	3.60	1.42	1.37
12	K	203	CLA	C4B-NB	3.59	1.42	1.37
12	B	819	CLA	C4B-NB	3.58	1.42	1.37
12	L	203	CLA	C4B-NB	3.58	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	841	CLA	C4B-NB	3.58	1.42	1.37
12	A	834	CLA	C4B-NB	3.58	1.42	1.37
12	A	803	CLA	C4B-NB	3.57	1.42	1.37
12	B	822	CLA	C4B-NB	3.57	1.42	1.37
12	B	805	CLA	C1D-ND	3.57	1.42	1.37
12	B	816	CLA	C4B-NB	3.57	1.42	1.37
12	B	815	CLA	C4B-NB	3.57	1.42	1.37
12	B	837	CLA	C4B-NB	3.56	1.42	1.37
12	B	801	CLA	C4B-NB	3.56	1.42	1.37
12	B	823	CLA	C4B-NB	3.56	1.42	1.37
12	B	838	CLA	C4B-NB	3.55	1.42	1.37
12	A	823	CLA	C4B-NB	3.55	1.42	1.37
12	A	816	CLA	C4B-NB	3.54	1.42	1.37
12	B	805	CLA	C4B-NB	3.54	1.42	1.37
12	B	820	CLA	C4B-NB	3.54	1.42	1.37
12	B	808	CLA	C4B-NB	3.53	1.42	1.37
12	B	821	CLA	C4B-NB	3.53	1.42	1.37
12	B	836	CLA	C4B-NB	3.53	1.42	1.37
12	A	809	CLA	C4B-NB	3.53	1.42	1.37
12	A	808	CLA	C4B-NB	3.52	1.42	1.37
12	A	839	CLA	C4B-NB	3.52	1.42	1.37
12	A	810	CLA	C4B-NB	3.51	1.42	1.37
12	A	815	CLA	C4B-NB	3.50	1.42	1.37
12	B	839	CLA	C4B-NB	3.50	1.42	1.37
12	A	805	CLA	C4B-NB	3.50	1.42	1.37
12	F	301	CLA	C4B-NB	3.50	1.42	1.37
12	A	828	CLA	C4B-NB	3.49	1.42	1.37
12	A	829	CLA	C4B-NB	3.49	1.42	1.37
12	A	814	CLA	C4B-NB	3.49	1.42	1.37
12	A	838	CLA	C4B-NB	3.48	1.42	1.37
12	A	804	CLA	C4B-NB	3.48	1.42	1.37
12	A	820	CLA	C4B-NB	3.47	1.42	1.37
12	A	822	CLA	C4B-NB	3.47	1.42	1.37
12	B	809	CLA	C4B-NB	3.46	1.42	1.37
12	B	827	CLA	C4B-NB	3.46	1.42	1.37
12	A	806	CLA	C4B-NB	3.46	1.42	1.37
12	A	819	CLA	C4B-NB	3.45	1.42	1.37
12	B	830	CLA	C4B-NB	3.45	1.42	1.37
12	B	833	CLA	C4B-NB	3.45	1.42	1.37
12	A	818	CLA	C4B-NB	3.45	1.42	1.37
12	B	807	CLA	C1D-ND	3.45	1.42	1.37
12	B	803	CLA	C4B-NB	3.44	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	806	CLA	C4B-NB	3.44	1.42	1.37
12	B	814	CLA	C4B-NB	3.44	1.42	1.37
12	B	818	CLA	C4B-NB	3.43	1.42	1.37
12	B	825	CLA	C4B-NB	3.43	1.42	1.37
12	A	825	CLA	C4B-NB	3.43	1.42	1.37
12	A	802	CLA	C4B-NB	3.43	1.42	1.37
12	A	836	CLA	C4B-NB	3.43	1.42	1.37
12	A	826	CLA	C4B-NB	3.43	1.42	1.37
12	B	810	CLA	C4B-NB	3.42	1.42	1.37
12	A	807	CLA	C4B-NB	3.42	1.42	1.37
17	A	849	LMU	O5B-C1B	3.41	1.50	1.41
12	B	811	CLA	C4B-NB	3.41	1.42	1.37
12	B	812	CLA	C4B-NB	3.41	1.42	1.37
12	A	831	CLA	C4B-NB	3.41	1.42	1.37
12	B	824	CLA	C4B-NB	3.41	1.42	1.37
12	A	833	CLA	C4B-NB	3.40	1.42	1.37
12	A	824	CLA	C4B-NB	3.40	1.42	1.37
12	A	832	CLA	C4B-NB	3.39	1.42	1.37
12	L	201	CLA	C4B-NB	3.39	1.42	1.37
12	A	812	CLA	C4B-NB	3.38	1.41	1.37
12	B	807	CLA	C4B-NB	3.38	1.41	1.37
12	A	837	CLA	C4B-NB	3.37	1.41	1.37
12	A	830	CLA	C4B-NB	3.36	1.41	1.37
12	B	813	CLA	C4B-NB	3.35	1.41	1.37
12	A	811	CLA	C3B-C4B	3.35	1.50	1.42
12	B	828	CLA	C4B-NB	3.33	1.41	1.37
12	A	817	CLA	C4B-NB	3.33	1.41	1.37
12	B	802	CLA	C4B-NB	3.31	1.41	1.37
12	A	827	CLA	C4B-NB	3.29	1.41	1.37
12	A	801	CLA	C4B-NB	3.29	1.41	1.37
12	B	835	CLA	C4B-NB	3.29	1.41	1.37
12	B	801	CLA	C3B-C4B	3.28	1.50	1.42
12	A	829	CLA	C1B-C2B	3.24	1.50	1.43
12	B	828	CLA	C1B-C2B	3.20	1.50	1.43
12	B	827	CLA	C4D-ND	-3.17	1.33	1.37
12	B	826	CLA	C4B-NB	3.16	1.41	1.37
12	A	835	CLA	C4B-NB	3.16	1.41	1.37
12	B	817	CLA	C4B-NB	3.15	1.41	1.37
12	A	827	CLA	C4D-ND	-3.13	1.33	1.37
12	B	801	CLA	C1D-ND	3.12	1.41	1.37
12	B	810	CLA	C4D-ND	-3.10	1.33	1.37
12	A	828	CLA	C4D-ND	-3.10	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	807	CLA	C4D-ND	-3.08	1.33	1.37
12	B	802	CLA	C4D-ND	-3.07	1.33	1.37
12	A	803	CLA	C3B-C4B	3.06	1.49	1.42
12	B	824	CLA	C4D-ND	-3.06	1.33	1.37
12	B	815	CLA	CAB-C3B	-3.06	1.44	1.50
12	B	808	CLA	C3B-C4B	3.05	1.49	1.42
12	B	805	CLA	C3B-C4B	3.04	1.49	1.42
12	A	837	CLA	C4D-ND	-3.03	1.33	1.37
12	B	811	CLA	C4D-ND	-3.01	1.33	1.37
12	A	835	CLA	C4D-ND	-3.01	1.33	1.37
12	B	821	CLA	C4D-ND	-3.01	1.33	1.37
12	B	839	CLA	C4D-ND	-3.01	1.33	1.37
12	A	817	CLA	C4D-ND	-3.00	1.33	1.37
12	A	808	CLA	C4D-ND	-2.99	1.33	1.37
12	B	814	CLA	C4D-ND	-2.99	1.33	1.37
12	B	801	CLA	C4D-ND	-2.98	1.33	1.37
12	A	825	CLA	C4D-ND	-2.98	1.33	1.37
12	B	832	CLA	C3B-C4B	2.98	1.49	1.42
12	A	820	CLA	C4D-ND	-2.98	1.33	1.37
12	B	833	CLA	C4D-ND	-2.97	1.33	1.37
12	B	824	CLA	C3B-C4B	2.96	1.49	1.42
12	B	815	CLA	C4D-ND	-2.96	1.33	1.37
12	B	837	CLA	C4D-ND	-2.96	1.33	1.37
12	A	803	CLA	C4D-ND	-2.95	1.33	1.37
12	L	201	CLA	C4D-ND	-2.95	1.33	1.37
12	B	819	CLA	C4D-ND	-2.95	1.33	1.37
12	B	803	CLA	C4D-ND	-2.95	1.33	1.37
12	B	838	CLA	C4D-ND	-2.95	1.33	1.37
12	A	838	CLA	C3B-C4B	2.94	1.49	1.42
12	B	825	CLA	C4D-ND	-2.94	1.33	1.37
12	B	830	CLA	C4D-ND	-2.94	1.33	1.37
12	A	836	CLA	C4D-ND	-2.94	1.33	1.37
12	A	819	CLA	C3B-C4B	2.94	1.49	1.42
12	A	814	CLA	C4D-ND	-2.94	1.33	1.37
12	B	837	CLA	C3B-C4B	2.93	1.49	1.42
12	A	805	CLA	C4D-ND	-2.93	1.33	1.37
12	A	829	CLA	C4D-ND	-2.93	1.33	1.37
12	A	841	CLA	C4D-ND	-2.93	1.33	1.37
12	A	810	CLA	C4D-ND	-2.93	1.33	1.37
12	A	806	CLA	C4D-ND	-2.93	1.33	1.37
12	A	809	CLA	C4D-ND	-2.92	1.33	1.37
12	A	821	CLA	C3B-C4B	2.92	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	826	CLA	C4D-ND	-2.92	1.33	1.37
12	K	201	CLA	C4D-ND	-2.92	1.33	1.37
12	F	301	CLA	C4D-ND	-2.92	1.33	1.37
12	A	814	CLA	C3B-C4B	2.92	1.49	1.42
12	B	836	CLA	C4D-ND	-2.92	1.33	1.37
12	A	802	CLA	C3B-C4B	2.92	1.49	1.42
12	B	805	CLA	C4D-ND	-2.92	1.33	1.37
12	A	834	CLA	C4D-ND	-2.91	1.33	1.37
12	A	830	CLA	C4D-ND	-2.91	1.33	1.37
12	B	813	CLA	C4D-ND	-2.91	1.33	1.37
12	B	822	CLA	C4D-ND	-2.91	1.33	1.37
12	A	839	CLA	C4D-ND	-2.91	1.33	1.37
12	A	816	CLA	C4D-ND	-2.91	1.33	1.37
12	A	821	CLA	C4D-ND	-2.91	1.33	1.37
12	A	807	CLA	C4D-ND	-2.91	1.33	1.37
12	B	834	CLA	C3B-C4B	2.91	1.49	1.42
12	K	203	CLA	C4D-ND	-2.90	1.33	1.37
12	A	832	CLA	C4D-ND	-2.90	1.33	1.37
12	A	826	CLA	C4D-ND	-2.90	1.33	1.37
12	B	808	CLA	C4D-ND	-2.90	1.33	1.37
12	A	834	CLA	C3B-C4B	2.89	1.49	1.42
12	A	815	CLA	C4D-ND	-2.89	1.33	1.37
12	B	818	CLA	C4D-ND	-2.89	1.33	1.37
12	B	820	CLA	C4D-ND	-2.89	1.33	1.37
12	B	809	CLA	C3B-C4B	2.89	1.49	1.42
12	B	835	CLA	C4D-ND	-2.88	1.33	1.37
12	A	822	CLA	C4D-ND	-2.88	1.33	1.37
12	A	820	CLA	C3B-C4B	2.88	1.49	1.42
12	B	818	CLA	C3B-C4B	2.88	1.49	1.42
12	B	832	CLA	C4D-ND	-2.87	1.33	1.37
12	K	203	CLA	C3B-C4B	2.87	1.49	1.42
12	B	806	CLA	C1B-C2B	2.87	1.50	1.43
12	A	825	CLA	C3B-C4B	2.86	1.49	1.42
12	K	204	CLA	C3B-C4B	2.86	1.49	1.42
12	B	820	CLA	C3B-C4B	2.86	1.49	1.42
12	A	813	CLA	C4D-ND	-2.86	1.33	1.37
12	A	822	CLA	C3B-C4B	2.86	1.49	1.42
12	A	818	CLA	C4D-ND	-2.86	1.33	1.37
12	A	838	CLA	C4D-ND	-2.85	1.33	1.37
12	B	823	CLA	C3B-C4B	2.85	1.49	1.42
12	B	828	CLA	C4D-ND	-2.85	1.33	1.37
12	A	827	CLA	C3B-C4B	2.85	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	819	CLA	C4D-ND	-2.85	1.33	1.37
12	L	201	CLA	C3B-C4B	2.85	1.49	1.42
12	A	813	CLA	C3B-C4B	2.85	1.49	1.42
12	A	831	CLA	C3B-C4B	2.84	1.49	1.42
12	B	838	CLA	C3B-C4B	2.84	1.49	1.42
12	A	841	CLA	C3B-C4B	2.84	1.49	1.42
12	A	828	CLA	C3B-C4B	2.84	1.49	1.42
12	J	102	CLA	C3B-C4B	2.84	1.49	1.42
12	A	833	CLA	C4D-ND	-2.84	1.33	1.37
12	B	817	CLA	C4D-ND	-2.84	1.33	1.37
12	B	836	CLA	C3B-C4B	2.84	1.49	1.42
12	B	825	CLA	C3B-C4B	2.84	1.49	1.42
12	B	816	CLA	C3B-C4B	2.84	1.49	1.42
12	A	817	CLA	C3B-C4B	2.84	1.49	1.42
12	A	823	CLA	C4D-ND	-2.84	1.33	1.37
12	B	823	CLA	C4D-ND	-2.83	1.33	1.37
12	A	812	CLA	C3B-C4B	2.83	1.49	1.42
12	B	830	CLA	C3B-C4B	2.83	1.49	1.42
12	K	201	CLA	C3B-C4B	2.83	1.49	1.42
12	B	829	CLA	C4D-ND	-2.83	1.33	1.37
12	A	836	CLA	C3B-C4B	2.83	1.49	1.42
12	B	812	CLA	C4D-ND	-2.83	1.33	1.37
12	B	821	CLA	C3B-C4B	2.83	1.49	1.42
12	B	831	CLA	C3B-C4B	2.83	1.49	1.42
12	J	102	CLA	C4D-ND	-2.82	1.33	1.37
12	B	833	CLA	C3B-C4B	2.82	1.49	1.42
12	F	301	CLA	C3B-C4B	2.82	1.49	1.42
12	B	819	CLA	C3B-C4B	2.82	1.49	1.42
12	B	827	CLA	C3B-C4B	2.82	1.49	1.42
12	A	831	CLA	C4D-ND	-2.81	1.33	1.37
12	A	839	CLA	C3B-C4B	2.81	1.49	1.42
12	A	811	CLA	C4D-ND	-2.81	1.33	1.37
12	A	809	CLA	C3B-C4B	2.81	1.49	1.42
12	A	833	CLA	C3B-C4B	2.80	1.49	1.42
12	B	811	CLA	C3B-C4B	2.80	1.49	1.42
12	A	832	CLA	C3B-C4B	2.80	1.49	1.42
12	A	812	CLA	C4D-ND	-2.80	1.33	1.37
12	B	831	CLA	C4D-ND	-2.80	1.33	1.37
12	A	801	CLA	C4D-ND	-2.80	1.33	1.37
12	A	816	CLA	C3B-C4B	2.80	1.49	1.42
12	B	814	CLA	C3B-C4B	2.80	1.49	1.42
12	A	818	CLA	C3B-C4B	2.79	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	802	CLA	C3B-C4B	2.79	1.49	1.42
12	A	829	CLA	C3B-C4B	2.79	1.49	1.42
12	B	810	CLA	C3B-C4B	2.78	1.49	1.42
12	A	810	CLA	C3B-C4B	2.78	1.49	1.42
12	A	815	CLA	C3B-C4B	2.78	1.49	1.42
12	B	803	CLA	C3B-C4B	2.78	1.49	1.42
12	A	830	CLA	C3B-C4B	2.78	1.49	1.42
12	A	806	CLA	C3B-C4B	2.78	1.49	1.42
12	B	826	CLA	C3B-C4B	2.78	1.49	1.42
12	A	837	CLA	C3B-C4B	2.77	1.49	1.42
12	B	807	CLA	C3B-C4B	2.77	1.49	1.42
12	K	204	CLA	C4D-ND	-2.77	1.33	1.37
12	A	807	CLA	C3B-C4B	2.77	1.49	1.42
12	B	829	CLA	C3B-C4B	2.77	1.49	1.42
12	L	203	CLA	C4D-ND	-2.77	1.33	1.37
12	A	824	CLA	C3B-C4B	2.77	1.49	1.42
12	A	802	CLA	C4D-ND	-2.76	1.33	1.37
12	A	826	CLA	C3B-C4B	2.76	1.49	1.42
12	A	808	CLA	C3B-C4B	2.76	1.49	1.42
12	B	839	CLA	C1B-C2B	2.75	1.49	1.43
12	A	804	CLA	C3B-C4B	2.74	1.49	1.42
12	B	809	CLA	C4D-ND	-2.74	1.33	1.37
12	A	805	CLA	C3B-C4B	2.73	1.49	1.42
12	B	828	CLA	C3B-C4B	2.73	1.49	1.42
12	B	834	CLA	C4D-ND	-2.72	1.33	1.37
12	L	203	CLA	C3B-C4B	2.72	1.49	1.42
12	B	816	CLA	C4D-ND	-2.72	1.34	1.37
12	B	806	CLA	C4D-ND	-2.72	1.34	1.37
12	B	822	CLA	C3B-C4B	2.71	1.49	1.42
12	B	835	CLA	C3B-C4B	2.71	1.49	1.42
12	B	812	CLA	C3B-C4B	2.71	1.49	1.42
12	A	804	CLA	C4D-ND	-2.71	1.34	1.37
12	B	829	CLA	C1B-C2B	2.70	1.49	1.43
12	B	817	CLA	C3B-C4B	2.70	1.49	1.42
12	A	823	CLA	C3B-C4B	2.70	1.49	1.42
12	A	801	CLA	C3B-C4B	2.69	1.49	1.42
12	K	203	CLA	C1B-C2B	2.69	1.49	1.43
12	B	806	CLA	C3B-C4B	2.68	1.49	1.42
12	K	201	CLA	C1B-C2B	2.68	1.49	1.43
12	B	815	CLA	C1B-C2B	2.68	1.49	1.43
12	A	824	CLA	C4D-ND	-2.68	1.34	1.37
12	A	801	CLA	C1B-C2B	2.66	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	811	CLA	C1B-C2B	2.66	1.49	1.43
12	A	809	CLA	C1B-C2B	2.65	1.49	1.43
12	A	804	CLA	C1B-C2B	2.65	1.49	1.43
12	A	805	CLA	C1B-C2B	2.65	1.49	1.43
12	A	815	CLA	C1B-C2B	2.65	1.49	1.43
12	A	841	CLA	C1B-C2B	2.65	1.49	1.43
12	J	102	CLA	C1B-C2B	2.65	1.49	1.43
12	B	817	CLA	C1B-C2B	2.63	1.49	1.43
12	B	819	CLA	C1B-C2B	2.63	1.49	1.43
12	K	204	CLA	C1B-C2B	2.62	1.49	1.43
12	L	203	CLA	C1B-C2B	2.62	1.49	1.43
12	B	816	CLA	C1B-C2B	2.62	1.49	1.43
12	F	301	CLA	C1B-C2B	2.62	1.49	1.43
12	B	831	CLA	C1B-C2B	2.62	1.49	1.43
12	A	822	CLA	C1B-C2B	2.62	1.49	1.43
12	B	813	CLA	C3B-C4B	2.62	1.48	1.42
12	A	824	CLA	C1B-C2B	2.62	1.49	1.43
12	A	835	CLA	C1B-C2B	2.62	1.49	1.43
12	A	808	CLA	C1B-C2B	2.62	1.49	1.43
12	B	810	CLA	C1B-C2B	2.61	1.49	1.43
12	B	820	CLA	C1B-C2B	2.61	1.49	1.43
12	A	823	CLA	C1B-C2B	2.61	1.49	1.43
12	B	818	CLA	C1B-C2B	2.61	1.49	1.43
12	A	834	CLA	C1B-C2B	2.60	1.49	1.43
12	A	806	CLA	C1B-C2B	2.60	1.49	1.43
12	A	812	CLA	C1B-C2B	2.60	1.49	1.43
12	B	835	CLA	C1B-C2B	2.60	1.49	1.43
12	A	810	CLA	C1B-C2B	2.59	1.49	1.43
12	A	816	CLA	C1B-C2B	2.59	1.49	1.43
12	A	832	CLA	C1B-C2B	2.59	1.49	1.43
12	B	812	CLA	C1B-C2B	2.59	1.49	1.43
12	A	814	CLA	C1B-C2B	2.59	1.49	1.43
12	B	815	CLA	C4B-C3B	2.58	1.49	1.43
12	B	838	CLA	C1B-C2B	2.58	1.49	1.43
12	A	839	CLA	C1B-C2B	2.58	1.49	1.43
12	B	837	CLA	C1B-C2B	2.58	1.49	1.43
12	A	821	CLA	C1B-C2B	2.57	1.49	1.43
12	A	826	CLA	C1B-C2B	2.57	1.49	1.43
12	B	825	CLA	C1B-C2B	2.57	1.49	1.43
12	B	833	CLA	C1B-C2B	2.57	1.49	1.43
12	A	819	CLA	C1B-C2B	2.57	1.49	1.43
12	B	814	CLA	C1B-C2B	2.56	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	807	CLA	C1B-C2B	2.56	1.49	1.43
12	B	830	CLA	C1B-C2B	2.56	1.49	1.43
12	A	837	CLA	C1B-C2B	2.55	1.49	1.43
12	B	836	CLA	C1B-C2B	2.55	1.49	1.43
12	B	803	CLA	C1B-C2B	2.55	1.49	1.43
12	A	802	CLA	C1B-C2B	2.54	1.49	1.43
12	B	809	CLA	C1B-C2B	2.54	1.49	1.43
12	B	823	CLA	C1B-C2B	2.54	1.49	1.43
12	A	827	CLA	C1B-C2B	2.54	1.49	1.43
12	A	838	CLA	C1B-C2B	2.54	1.49	1.43
12	B	827	CLA	C1B-C2B	2.54	1.49	1.43
12	A	830	CLA	C1B-C2B	2.54	1.49	1.43
12	A	825	CLA	C1B-C2B	2.54	1.49	1.43
12	A	835	CLA	C3B-C4B	2.53	1.48	1.42
12	B	822	CLA	C1B-C2B	2.51	1.49	1.43
12	B	834	CLA	C1B-C2B	2.51	1.49	1.43
12	A	833	CLA	C1B-C2B	2.51	1.49	1.43
12	A	813	CLA	C1B-C2B	2.51	1.49	1.43
12	A	807	CLA	C1B-C2B	2.51	1.49	1.43
12	A	817	CLA	C1B-C2B	2.51	1.49	1.43
12	B	826	CLA	C1B-C2B	2.50	1.49	1.43
12	B	805	CLA	CHC-C1C	2.49	1.43	1.38
12	B	832	CLA	C1B-C2B	2.49	1.49	1.43
12	A	820	CLA	C1B-C2B	2.49	1.49	1.43
12	A	831	CLA	C1B-C2B	2.48	1.49	1.43
12	B	808	CLA	C1B-C2B	2.48	1.49	1.43
12	B	813	CLA	CMB-C2B	-2.47	1.45	1.50
12	B	839	CLA	CMB-C2B	-2.47	1.45	1.50
12	A	836	CLA	C1B-C2B	2.47	1.49	1.43
12	B	801	CLA	CMD-C2D	-2.47	1.45	1.50
12	B	801	CLA	CHC-C1C	2.45	1.43	1.38
12	A	828	CLA	C1B-C2B	2.45	1.49	1.43
12	B	824	CLA	C1B-C2B	2.45	1.49	1.43
12	L	201	CLA	C1B-C2B	2.43	1.49	1.43
12	A	803	CLA	C1B-C2B	2.42	1.48	1.43
12	B	839	CLA	C3B-C4B	2.39	1.48	1.42
12	A	811	CLA	C1B-C2B	2.38	1.48	1.43
12	B	805	CLA	CMC-C2C	-2.37	1.45	1.50
12	B	813	CLA	C1B-C2B	2.37	1.48	1.43
12	B	802	CLA	C1B-C2B	2.36	1.48	1.43
12	A	818	CLA	C1B-C2B	2.33	1.48	1.43
12	B	807	CLA	CMC-C2C	-2.32	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	825	CLA	CMD-C2D	-2.30	1.45	1.50
12	B	838	CLA	CMD-C2D	-2.27	1.46	1.50
12	B	821	CLA	C1B-C2B	2.27	1.48	1.43
12	A	818	CLA	CMB-C2B	-2.27	1.46	1.50
12	A	811	CLA	CHC-C1C	2.26	1.43	1.38
12	B	805	CLA	C1B-C2B	2.26	1.48	1.43
12	A	803	CLA	CHC-C1C	2.26	1.43	1.38
12	B	801	CLA	C1B-C2B	2.25	1.48	1.43
12	A	828	CLA	CMD-C2D	-2.24	1.46	1.50
12	B	808	CLA	CHC-C1C	2.24	1.43	1.38
12	B	806	CLA	CMD-C2D	-2.23	1.46	1.50
12	B	821	CLA	CMB-C2B	-2.23	1.46	1.50
12	B	828	CLA	CMD-C2D	-2.22	1.46	1.50
12	B	827	CLA	CMD-C2D	-2.21	1.46	1.50
12	A	830	CLA	CMD-C2D	-2.21	1.46	1.50
12	B	809	CLA	CHC-C1C	2.20	1.43	1.38
12	B	812	CLA	CMD-C2D	-2.18	1.46	1.50
12	A	819	CLA	CHC-C1C	2.18	1.43	1.38
12	A	826	CLA	CMC-C2C	-2.18	1.46	1.50
12	B	824	CLA	CMD-C2D	-2.18	1.46	1.50
12	B	803	CLA	CMD-C2D	-2.17	1.46	1.50
12	A	802	CLA	CHC-C1C	2.17	1.42	1.38
12	B	812	CLA	CMC-C2C	-2.16	1.46	1.50
12	A	819	CLA	CMD-C2D	-2.15	1.46	1.50
12	A	833	CLA	CHC-C1C	2.14	1.42	1.38
12	A	802	CLA	CMD-C2D	-2.14	1.46	1.50
17	A	849	LMU	C3B-C2B	-2.14	1.49	1.52
12	B	832	CLA	CMD-C2D	-2.14	1.46	1.50
12	B	824	CLA	CHC-C1C	2.14	1.42	1.38
12	B	832	CLA	CHC-C1C	2.14	1.42	1.38
12	A	833	CLA	CMB-C2B	-2.14	1.46	1.50
12	A	804	CLA	CMC-C2C	-2.14	1.46	1.50
12	A	801	CLA	CMD-C2D	-2.13	1.46	1.50
12	B	801	CLA	MG-ND	-2.13	2.01	2.05
12	A	827	CLA	CHC-C1C	2.13	1.42	1.38
12	A	820	CLA	CMD-C2D	-2.13	1.46	1.50
12	A	801	CLA	CMB-C2B	-2.12	1.46	1.50
12	B	807	CLA	CMD-C2D	-2.12	1.46	1.50
12	B	835	CLA	CMD-C2D	-2.12	1.46	1.50
12	B	822	CLA	CMB-C2B	-2.12	1.46	1.50
12	B	827	CLA	CMC-C2C	-2.11	1.46	1.50
12	A	811	CLA	CMB-C2B	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	804	CLA	CMD-C2D	-2.10	1.46	1.50
12	A	822	CLA	CMD-C2D	-2.09	1.46	1.50
12	A	823	CLA	CMB-C2B	-2.09	1.46	1.50
12	B	814	CLA	CHC-C1C	2.08	1.42	1.38
12	A	839	CLA	CHC-C1C	2.08	1.42	1.38
12	B	826	CLA	CHC-C1C	2.08	1.42	1.38
12	B	810	CLA	CMD-C2D	-2.08	1.46	1.50
12	B	825	CLA	CMD-C2D	-2.08	1.46	1.50
12	A	808	CLA	CMD-C2D	-2.07	1.46	1.50
12	A	803	CLA	CMC-C2C	-2.07	1.46	1.50
12	B	813	CLA	CMD-C2D	-2.07	1.46	1.50
12	K	201	CLA	CMD-C2D	-2.07	1.46	1.50
12	A	838	CLA	CHC-C1C	2.07	1.42	1.38
12	B	831	CLA	CMD-C2D	-2.06	1.46	1.50
12	A	820	CLA	CHC-C1C	2.06	1.42	1.38
12	B	836	CLA	CHC-C1C	2.06	1.42	1.38
12	A	810	CLA	CMD-C2D	-2.06	1.46	1.50
12	A	830	CLA	CHC-C1C	2.06	1.42	1.38
12	A	807	CLA	CMD-C2D	-2.06	1.46	1.50
12	A	828	CLA	CHC-C1C	2.06	1.42	1.38
12	B	821	CLA	CHC-C1C	2.06	1.42	1.38
12	B	834	CLA	CHC-C1C	2.06	1.42	1.38
12	B	802	CLA	CHC-C1C	2.05	1.42	1.38
12	A	839	CLA	CMD-C2D	-2.05	1.46	1.50
12	B	805	CLA	CMD-C2D	-2.05	1.46	1.50
12	B	809	CLA	CMD-C2D	-2.05	1.46	1.50
12	A	831	CLA	CHC-C1C	2.05	1.42	1.38
12	B	823	CLA	CHC-C1C	2.05	1.42	1.38
12	A	818	CLA	CMC-C2C	-2.05	1.46	1.50
12	B	826	CLA	CMD-C2D	-2.05	1.46	1.50
12	K	203	CLA	CHC-C1C	2.05	1.42	1.38
12	A	826	CLA	CMD-C2D	-2.05	1.46	1.50
12	A	817	CLA	CHC-C1C	2.05	1.42	1.38
12	B	816	CLA	CHC-C1C	2.05	1.42	1.38
12	L	201	CLA	CMD-C2D	-2.05	1.46	1.50
12	A	828	CLA	CMB-C2B	-2.05	1.46	1.50
12	B	814	CLA	CMB-C2B	-2.05	1.46	1.50
12	B	812	CLA	CMB-C2B	-2.04	1.46	1.50
12	A	813	CLA	CHC-C1C	2.04	1.42	1.38
12	A	815	CLA	CMB-C2B	-2.04	1.46	1.50
12	A	816	CLA	CMC-C2C	-2.04	1.46	1.50
12	A	820	CLA	CMB-C2B	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	818	CLA	CHC-C1C	2.04	1.42	1.38
12	B	825	CLA	CHC-C1C	2.04	1.42	1.38
12	B	813	CLA	MG-NB	-2.04	2.01	2.05
12	A	813	CLA	CMD-C2D	-2.03	1.46	1.50
12	A	826	CLA	CHC-C1C	2.03	1.42	1.38
12	B	829	CLA	CMD-C2D	-2.03	1.46	1.50
12	B	816	CLA	CMD-C2D	-2.03	1.46	1.50
12	B	839	CLA	CMD-C2D	-2.03	1.46	1.50
12	B	820	CLA	CHC-C1C	2.03	1.42	1.38
12	B	837	CLA	CHC-C1C	2.03	1.42	1.38
12	B	811	CLA	CMD-C2D	-2.03	1.46	1.50
12	B	833	CLA	CMD-C2D	-2.03	1.46	1.50
12	B	835	CLA	CMB-C2B	-2.03	1.46	1.50
12	A	836	CLA	CMB-C2B	-2.03	1.46	1.50
12	B	803	CLA	CHC-C1C	2.03	1.42	1.38
12	A	816	CLA	CMD-C2D	-2.03	1.46	1.50
12	A	826	CLA	CMB-C2B	-2.03	1.46	1.50
12	B	803	CLA	CMC-C2C	-2.03	1.46	1.50
12	A	812	CLA	CHC-C1C	2.03	1.42	1.38
12	B	833	CLA	CHC-C1C	2.03	1.42	1.38
12	A	830	CLA	CMB-C2B	-2.03	1.46	1.50
12	B	830	CLA	CHC-C1C	2.03	1.42	1.38
12	A	824	CLA	CMD-C2D	-2.03	1.46	1.50
12	A	832	CLA	CMB-C2B	-2.03	1.46	1.50
12	A	827	CLA	CMD-C2D	-2.02	1.46	1.50
12	B	836	CLA	CMD-C2D	-2.02	1.46	1.50
12	A	829	CLA	CHC-C1C	2.02	1.42	1.38
12	A	834	CLA	CHC-C1C	2.02	1.42	1.38
12	A	827	CLA	CMC-C2C	-2.02	1.46	1.50
12	B	836	CLA	CMB-C2B	-2.02	1.46	1.50
12	B	838	CLA	CMC-C2C	-2.02	1.46	1.50
12	A	825	CLA	CMB-C2B	-2.02	1.46	1.50
12	B	808	CLA	CMD-C2D	-2.02	1.46	1.50
12	F	301	CLA	CHC-C1C	2.02	1.42	1.38
12	A	807	CLA	CMB-C2B	-2.02	1.46	1.50
12	A	841	CLA	CMC-C2C	-2.02	1.46	1.50
12	B	803	CLA	CMB-C2B	-2.02	1.46	1.50
12	A	818	CLA	CMD-C2D	-2.02	1.46	1.50
12	A	811	CLA	CMD-C2D	-2.02	1.46	1.50
12	B	819	CLA	CHC-C1C	2.02	1.42	1.38
12	A	812	CLA	CMC-C2C	-2.02	1.46	1.50
12	B	818	CLA	CMD-C2D	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	831	CLA	CHC-C1C	2.02	1.42	1.38
12	B	815	CLA	CMB-C2B	-2.01	1.46	1.50
12	B	834	CLA	CMB-C2B	-2.01	1.46	1.50
12	A	824	CLA	CMB-C2B	-2.01	1.46	1.50
12	B	806	CLA	CMC-C2C	-2.01	1.46	1.50
12	B	807	CLA	CMB-C2B	-2.01	1.46	1.50
12	A	839	CLA	CMB-C2B	-2.01	1.46	1.50
12	A	805	CLA	CMD-C2D	-2.01	1.46	1.50
12	K	204	CLA	CMD-C2D	-2.01	1.46	1.50
12	A	832	CLA	CMD-C2D	-2.01	1.46	1.50
12	A	836	CLA	CMD-C2D	-2.01	1.46	1.50
12	A	838	CLA	CMD-C2D	-2.01	1.46	1.50
12	K	204	CLA	CHC-C1C	2.01	1.42	1.38
12	B	802	CLA	CMD-C2D	-2.01	1.46	1.50
12	A	829	CLA	CMD-C2D	-2.01	1.46	1.50
12	B	838	CLA	CMB-C2B	-2.01	1.46	1.50
12	A	834	CLA	CMB-C2B	-2.01	1.46	1.50
12	L	203	CLA	CHC-C1C	2.01	1.42	1.38
12	A	809	CLA	CMD-C2D	-2.01	1.46	1.50
12	B	821	CLA	CMD-C2D	-2.00	1.46	1.50
12	A	822	CLA	CHC-C1C	2.00	1.42	1.38
12	A	804	CLA	CMB-C2B	-2.00	1.46	1.50
12	B	809	CLA	CMC-C2C	-2.00	1.46	1.50

All (760) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	804	BCR	C20-C21-C22	-7.06	117.23	127.31
15	B	804	BCR	C24-C23-C22	-6.96	115.72	126.23
15	I	201	BCR	C24-C23-C22	-6.55	116.33	126.23
15	L	202	BCR	C28-C27-C26	-6.46	102.55	114.08
12	B	809	CLA	C4A-NA-C1A	6.33	109.55	106.71
12	B	822	CLA	C4A-NA-C1A	6.31	109.54	106.71
15	L	204	BCR	C7-C8-C9	-6.30	116.72	126.23
12	B	816	CLA	C4A-NA-C1A	6.16	109.47	106.71
12	B	831	CLA	C4A-NA-C1A	6.15	109.47	106.71
12	A	804	CLA	C4A-NA-C1A	5.96	109.39	106.71
12	B	834	CLA	C4A-NA-C1A	5.96	109.39	106.71
12	B	814	CLA	C4A-NA-C1A	5.96	109.38	106.71
12	A	824	CLA	C4A-NA-C1A	5.92	109.37	106.71
12	A	826	CLA	C4A-NA-C1A	5.83	109.33	106.71
12	A	812	CLA	C4A-NA-C1A	5.80	109.31	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	835	CLA	C4A-NA-C1A	5.76	109.30	106.71
15	B	804	BCR	C16-C17-C18	-5.72	119.14	127.31
12	B	817	CLA	C4A-NA-C1A	5.70	109.27	106.71
12	A	831	CLA	C4A-NA-C1A	5.66	109.25	106.71
15	B	843	BCR	C7-C8-C9	-5.66	117.68	126.23
12	A	819	CLA	C4A-NA-C1A	5.64	109.24	106.71
12	A	829	CLA	C4A-NA-C1A	5.58	109.22	106.71
12	A	833	CLA	C4A-NA-C1A	5.58	109.21	106.71
12	B	825	CLA	C4A-NA-C1A	5.57	109.21	106.71
12	B	801	CLA	C4A-NA-C1A	5.49	109.17	106.71
15	B	841	BCR	C28-C27-C26	-5.47	104.32	114.08
12	K	204	CLA	C4A-NA-C1A	5.46	109.16	106.71
15	J	101	BCR	C15-C14-C13	-5.46	119.52	127.31
12	A	802	CLA	C4A-NA-C1A	5.44	109.15	106.71
12	B	807	CLA	C4A-NA-C1A	5.43	109.15	106.71
12	B	835	CLA	C4A-NA-C1A	5.39	109.13	106.71
15	I	201	BCR	C20-C21-C22	-5.39	119.62	127.31
15	B	841	BCR	C7-C8-C9	-5.36	118.14	126.23
12	L	203	CLA	C4A-NA-C1A	5.33	109.10	106.71
15	J	101	BCR	C11-C10-C9	-5.33	119.70	127.31
12	A	816	CLA	C4A-NA-C1A	5.33	109.10	106.71
15	B	843	BCR	C15-C14-C13	-5.32	119.72	127.31
15	J	101	BCR	C7-C8-C9	-5.30	118.23	126.23
12	B	810	CLA	C4A-NA-C1A	5.26	109.07	106.71
12	A	805	CLA	C4A-NA-C1A	5.25	109.07	106.71
12	B	828	CLA	C4A-NA-C1A	5.24	109.06	106.71
12	A	830	CLA	C4A-NA-C1A	5.12	109.01	106.71
12	B	811	CLA	C4A-NA-C1A	5.07	108.99	106.71
15	L	204	BCR	C28-C27-C26	-5.07	105.02	114.08
12	B	818	CLA	C4A-NA-C1A	5.07	108.99	106.71
15	K	202	BCR	C16-C17-C18	-5.05	120.10	127.31
12	A	836	CLA	C4A-NA-C1A	5.02	108.96	106.71
12	A	832	CLA	C4A-NA-C1A	5.01	108.96	106.71
12	B	823	CLA	C4A-NA-C1A	4.97	108.94	106.71
12	A	823	CLA	C4A-NA-C1A	4.94	108.93	106.71
15	B	841	BCR	C24-C23-C22	-4.92	118.81	126.23
12	K	203	CLA	C4A-NA-C1A	4.91	108.92	106.71
12	B	837	CLA	C4A-NA-C1A	4.91	108.91	106.71
15	B	842	BCR	C16-C17-C18	-4.90	120.32	127.31
12	A	814	CLA	C4A-NA-C1A	4.87	108.90	106.71
15	J	101	BCR	C28-C27-C26	-4.87	105.38	114.08
12	B	820	CLA	C4A-NA-C1A	4.86	108.89	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	843	BCR	C11-C10-C9	-4.85	120.39	127.31
12	B	829	CLA	C4A-NA-C1A	4.85	108.89	106.71
15	M	101	BCR	C16-C17-C18	-4.84	120.40	127.31
12	A	834	CLA	C4A-NA-C1A	4.84	108.88	106.71
12	B	838	CLA	C4A-NA-C1A	4.84	108.88	106.71
15	L	204	BCR	C11-C10-C9	-4.83	120.42	127.31
12	A	806	CLA	C4A-NA-C1A	4.78	108.85	106.71
12	B	836	CLA	C4A-NA-C1A	4.76	108.84	106.71
15	K	202	BCR	C3-C4-C5	-4.76	105.59	114.08
15	K	202	BCR	C4-C5-C6	-4.74	115.85	122.73
12	A	839	CLA	C4A-NA-C1A	4.73	108.83	106.71
15	A	844	BCR	C15-C14-C13	-4.72	120.57	127.31
15	L	204	BCR	C15-C14-C13	-4.72	120.57	127.31
12	B	819	CLA	C4A-NA-C1A	4.70	108.82	106.71
12	A	821	CLA	C4A-NA-C1A	4.69	108.82	106.71
15	A	847	BCR	C1-C6-C5	-4.68	116.02	122.61
12	A	838	CLA	C4A-NA-C1A	4.66	108.80	106.71
15	L	204	BCR	C16-C17-C18	-4.66	120.66	127.31
12	A	808	CLA	C4A-NA-C1A	4.65	108.80	106.71
12	B	813	CLA	C4A-NA-C1A	4.65	108.80	106.71
12	A	817	CLA	C4A-NA-C1A	4.65	108.80	106.71
12	A	818	CLA	C4A-NA-C1A	4.63	108.79	106.71
12	B	839	CLA	C4A-NA-C1A	4.63	108.79	106.71
12	A	813	CLA	C4A-NA-C1A	4.60	108.77	106.71
12	A	809	CLA	C4A-NA-C1A	4.58	108.77	106.71
12	B	833	CLA	C4A-NA-C1A	4.58	108.77	106.71
15	K	202	BCR	C1-C6-C5	-4.57	116.17	122.61
15	A	847	BCR	C4-C5-C6	-4.57	116.09	122.73
12	B	802	CLA	C4A-NA-C1A	4.57	108.76	106.71
12	B	821	CLA	C4A-NA-C1A	4.56	108.76	106.71
12	B	830	CLA	C4A-NA-C1A	4.52	108.74	106.71
15	L	202	BCR	C20-C21-C22	-4.51	120.87	127.31
15	L	202	BCR	C24-C23-C22	-4.51	119.42	126.23
12	A	841	CLA	C4A-NA-C1A	4.49	108.72	106.71
12	K	201	CLA	C4A-NA-C1A	4.49	108.72	106.71
12	A	815	CLA	C4A-NA-C1A	4.47	108.72	106.71
15	A	846	BCR	C15-C14-C13	-4.47	120.93	127.31
12	B	812	CLA	C4A-NA-C1A	4.47	108.72	106.71
12	B	826	CLA	C4A-NA-C1A	4.44	108.70	106.71
12	J	102	CLA	C4A-NA-C1A	4.43	108.70	106.71
12	A	807	CLA	C4A-NA-C1A	4.43	108.70	106.71
12	F	301	CLA	C4A-NA-C1A	4.41	108.69	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	820	CLA	C4A-NA-C1A	4.39	108.68	106.71
15	I	201	BCR	C15-C14-C13	-4.38	121.05	127.31
18	B	844	DGD	O2G-C1B-C2B	4.38	120.94	111.50
15	A	846	BCR	C24-C23-C22	-4.37	119.63	126.23
15	A	845	BCR	C16-C17-C18	-4.34	121.12	127.31
15	A	846	BCR	C20-C21-C22	-4.34	121.12	127.31
15	B	804	BCR	C15-C14-C13	-4.32	121.14	127.31
15	A	844	BCR	C24-C23-C22	-4.32	119.71	126.23
15	A	846	BCR	C3-C4-C5	-4.27	106.45	114.08
12	B	832	CLA	C4A-NA-C1A	4.26	108.62	106.71
12	A	825	CLA	C4A-NA-C1A	4.25	108.62	106.71
15	L	202	BCR	C16-C17-C18	-4.22	121.28	127.31
12	A	810	CLA	C4A-NA-C1A	4.17	108.58	106.71
12	A	827	CLA	C4A-NA-C1A	4.16	108.58	106.71
12	B	805	CLA	C4A-NA-C1A	4.14	108.57	106.71
15	B	804	BCR	C7-C8-C9	-4.13	120.00	126.23
12	B	827	CLA	C4A-NA-C1A	4.12	108.56	106.71
15	A	844	BCR	C20-C21-C22	-4.11	121.45	127.31
12	A	803	CLA	C4A-NA-C1A	4.11	108.55	106.71
15	L	202	BCR	C15-C14-C13	-4.06	121.52	127.31
12	L	201	CLA	C4A-NA-C1A	4.06	108.53	106.71
15	B	804	BCR	C20-C19-C18	-4.05	115.03	126.42
12	B	803	CLA	C4A-NA-C1A	4.05	108.53	106.71
12	B	815	CLA	C4A-NA-C1A	4.04	108.52	106.71
15	A	847	BCR	C16-C17-C18	-4.00	121.61	127.31
12	B	808	CLA	C4A-NA-C1A	3.99	108.50	106.71
15	A	847	BCR	C24-C23-C22	-3.98	120.22	126.23
15	A	846	BCR	C16-C17-C18	-3.92	121.71	127.31
12	A	822	CLA	C4A-NA-C1A	3.91	108.47	106.71
15	B	842	BCR	C20-C21-C22	-3.90	121.74	127.31
12	A	811	CLA	C4A-NA-C1A	3.86	108.44	106.71
15	B	841	BCR	C27-C26-C25	-3.84	117.15	122.73
15	K	202	BCR	C20-C21-C22	-3.83	121.84	127.31
15	K	202	BCR	C11-C10-C9	-3.83	121.84	127.31
15	L	202	BCR	C33-C5-C6	-3.82	120.23	124.53
12	L	203	CLA	CAA-C2A-C3A	-3.82	107.20	116.10
15	A	846	BCR	C11-C10-C9	-3.81	121.87	127.31
15	K	202	BCR	C15-C14-C13	-3.79	121.90	127.31
15	K	202	BCR	C7-C8-C9	-3.78	120.52	126.23
15	M	101	BCR	C20-C21-C22	-3.78	121.92	127.31
15	A	844	BCR	C7-C8-C9	-3.78	120.53	126.23
15	A	845	BCR	C15-C14-C13	-3.77	121.93	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	841	BCR	C16-C17-C18	-3.76	121.94	127.31
15	A	846	BCR	C38-C26-C25	-3.74	120.33	124.53
15	A	847	BCR	C33-C5-C4	3.73	120.77	113.62
15	A	844	BCR	C11-C10-C9	-3.71	122.01	127.31
15	B	842	BCR	C33-C5-C6	-3.71	120.37	124.53
15	A	844	BCR	C16-C17-C18	-3.69	122.04	127.31
15	B	842	BCR	C7-C8-C9	-3.69	120.67	126.23
15	M	101	BCR	C3-C4-C5	-3.67	107.52	114.08
15	L	204	BCR	C24-C23-C22	-3.67	120.70	126.23
15	L	204	BCR	C3-C4-C5	-3.64	107.58	114.08
15	L	202	BCR	C11-C10-C9	-3.63	122.13	127.31
15	I	201	BCR	C16-C17-C18	-3.60	122.17	127.31
15	L	204	BCR	C20-C21-C22	-3.60	122.17	127.31
15	A	845	BCR	C20-C21-C22	-3.60	122.17	127.31
14	A	842	LHG	O7-C7-C8	3.59	119.25	111.50
14	A	843	LHG	O7-C7-C8	3.59	119.25	111.50
15	I	201	BCR	C7-C8-C9	-3.59	120.81	126.23
15	B	843	BCR	C24-C23-C22	-3.56	120.85	126.23
15	I	201	BCR	C11-C10-C9	-3.55	122.24	127.31
15	M	101	BCR	C24-C23-C22	-3.55	120.86	126.23
15	A	847	BCR	C15-C14-C13	-3.55	122.25	127.31
15	L	202	BCR	C7-C8-C9	-3.55	120.88	126.23
12	A	837	CLA	C4A-NA-C1A	3.54	108.30	106.71
12	B	824	CLA	C4A-NA-C1A	3.54	108.30	106.71
15	K	202	BCR	C33-C5-C4	3.52	120.37	113.62
15	A	845	BCR	C38-C26-C25	-3.49	120.60	124.53
15	A	845	BCR	C11-C10-C9	-3.49	122.33	127.31
15	A	844	BCR	C3-C4-C5	-3.49	107.85	114.08
15	B	842	BCR	C28-C27-C26	-3.47	107.88	114.08
12	B	806	CLA	O2D-CGD-O1D	-3.46	117.08	123.84
12	B	835	CLA	CAA-C2A-C3A	-3.46	105.62	114.26
15	B	842	BCR	C24-C23-C22	-3.45	121.03	126.23
15	J	101	BCR	C16-C17-C18	-3.44	122.39	127.31
15	A	844	BCR	C28-C27-C26	-3.42	107.98	114.08
15	B	842	BCR	C33-C5-C4	3.41	120.17	113.62
15	B	804	BCR	C38-C26-C25	-3.41	120.70	124.53
15	B	843	BCR	C38-C26-C25	-3.41	120.70	124.53
15	B	841	BCR	C34-C9-C10	-3.41	118.15	122.92
15	A	846	BCR	C7-C8-C9	-3.39	121.11	126.23
15	B	842	BCR	C3-C4-C5	-3.37	108.06	114.08
12	B	806	CLA	C4A-NA-C1A	3.35	108.21	106.71
15	J	101	BCR	C20-C21-C22	-3.35	122.53	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	841	BCR	C15-C14-C13	-3.34	122.54	127.31
12	B	803	CLA	CAA-C2A-C3A	-3.33	103.65	112.78
12	A	824	CLA	CAA-C2A-C3A	-3.33	103.67	112.78
15	B	841	BCR	C38-C26-C27	3.32	119.99	113.62
15	M	101	BCR	C15-C14-C13	-3.32	122.58	127.31
17	A	849	LMU	C2'-C3'-C4'	3.31	117.24	109.68
15	A	847	BCR	C7-C8-C9	-3.30	121.24	126.23
15	A	845	BCR	C7-C8-C9	-3.30	121.25	126.23
15	A	847	BCR	C20-C21-C22	-3.28	122.62	127.31
15	A	846	BCR	C4-C5-C6	-3.27	117.98	122.73
15	A	844	BCR	C33-C5-C6	-3.26	120.87	124.53
15	B	843	BCR	C15-C16-C17	-3.26	116.81	123.47
15	A	847	BCR	C11-C10-C9	-3.24	122.68	127.31
12	A	801	CLA	C4A-NA-C1A	3.23	108.16	106.71
15	A	845	BCR	C24-C23-C22	-3.23	121.35	126.23
15	K	202	BCR	C38-C26-C25	-3.23	120.90	124.53
15	B	843	BCR	C3-C4-C5	-3.22	108.34	114.08
12	A	810	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
15	B	842	BCR	C38-C26-C25	-3.20	120.93	124.53
12	B	839	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
12	A	817	CLA	CMB-C2B-C1B	-3.18	120.53	125.37
15	B	842	BCR	C15-C14-C13	-3.17	122.78	127.31
12	L	201	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
15	B	843	BCR	C16-C17-C18	-3.12	122.85	127.31
12	A	839	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
12	A	814	CLA	CAA-C2A-C3A	-3.07	108.92	116.10
12	A	818	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
12	A	822	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
17	A	849	LMU	C1B-O1B-C4'	-3.06	110.39	117.96
12	B	814	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
12	A	828	CLA	C4A-NA-C1A	3.05	108.08	106.71
12	K	204	CLA	CAA-C2A-C3A	-3.05	106.64	114.26
15	B	842	BCR	C16-C15-C14	-3.05	117.23	123.47
12	A	811	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
12	B	816	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
12	B	823	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
15	J	101	BCR	C15-C16-C17	-3.02	117.28	123.47
17	A	849	LMU	C6B-C5B-C4B	-3.02	109.32	113.54
15	L	202	BCR	C38-C26-C27	3.02	119.42	113.62
15	B	842	BCR	C8-C7-C6	-3.01	118.74	127.20
12	B	837	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
12	B	812	CLA	O2D-CGD-O1D	-3.01	117.96	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	L	204	BCR	C27-C26-C25	-3.01	118.36	122.73
12	A	829	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
15	B	842	BCR	C38-C26-C27	3.00	119.39	113.62
12	B	801	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
12	B	828	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
15	I	201	BCR	C33-C5-C4	2.99	119.37	113.62
15	B	804	BCR	C11-C10-C9	-2.99	123.05	127.31
15	K	202	BCR	C24-C23-C22	-2.99	121.72	126.23
15	B	841	BCR	C20-C21-C22	-2.98	123.05	127.31
15	M	101	BCR	C7-C8-C9	-2.98	121.73	126.23
12	B	822	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
15	A	844	BCR	C33-C5-C4	2.96	119.30	113.62
12	A	819	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
15	A	846	BCR	C38-C26-C27	2.96	119.29	113.62
12	A	834	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
15	B	841	BCR	C37-C22-C21	-2.94	118.80	122.92
12	A	806	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
12	J	102	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
15	J	101	BCR	C11-C12-C13	-2.94	118.15	126.42
12	A	837	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
12	A	823	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
12	L	203	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
12	B	805	CLA	CMB-C2B-C1B	-2.92	120.92	125.37
12	B	818	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
12	B	831	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
12	A	824	CLA	CHB-C4A-NA	2.91	128.53	124.51
12	A	816	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
12	B	829	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
12	K	203	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
15	J	101	BCR	C29-C30-C25	2.89	114.93	110.48
12	A	811	CLA	CMB-C2B-C1B	-2.89	120.97	125.37
12	B	832	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
12	A	831	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
15	B	842	BCR	C10-C11-C12	-2.89	114.21	123.22
12	A	807	CLA	CHB-C4A-NA	2.89	128.50	124.51
12	B	805	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
12	A	826	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
12	B	801	CLA	CHB-C4A-NA	2.88	128.49	124.51
12	B	826	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
12	B	809	CLA	CHB-C4A-NA	2.87	128.48	124.51
12	B	819	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
15	A	845	BCR	C33-C5-C4	2.86	119.11	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	834	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
12	B	811	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
15	M	101	BCR	C33-C5-C6	-2.85	121.33	124.53
12	A	802	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
15	A	845	BCR	C33-C5-C6	-2.85	121.33	124.53
12	A	807	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
12	A	820	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
12	A	818	CLA	CMB-C2B-C1B	-2.84	121.04	125.37
12	A	825	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
12	B	802	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
12	A	805	CLA	CHB-C4A-NA	2.84	128.44	124.51
12	A	801	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
12	A	817	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
15	J	101	BCR	C40-C30-C25	-2.84	105.70	110.30
12	A	836	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
12	B	801	CLA	C3B-C4B-NB	-2.83	107.89	110.52
12	B	834	CLA	CHB-C4A-NA	2.83	128.42	124.51
12	A	827	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
12	B	803	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
15	I	201	BCR	C1-C6-C5	-2.83	118.63	122.61
12	B	835	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
15	B	804	BCR	C38-C26-C27	2.82	119.04	113.62
12	B	808	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
12	K	204	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
12	B	833	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
12	A	831	CLA	CMB-C2B-C1B	-2.82	121.08	125.37
12	B	820	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
12	A	803	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
15	B	804	BCR	C16-C15-C14	-2.81	117.72	123.47
12	B	813	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
12	A	832	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
12	A	814	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
12	A	813	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
12	B	839	CLA	CHC-C4B-NB	2.78	127.20	124.26
12	A	812	CLA	CHB-C4A-NA	2.78	128.36	124.51
12	B	830	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
12	A	804	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
12	B	816	CLA	CAA-C2A-C3A	-2.78	107.32	114.26
12	B	810	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
12	A	828	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
18	B	844	DGD	C2G-O2G-C1B	-2.76	110.99	117.79
12	B	835	CLA	CHB-C4A-NA	2.76	128.33	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	803	CLA	CHB-C4A-NA	2.76	128.33	124.51
12	A	809	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
12	A	835	CLA	CHB-C4A-NA	2.76	128.32	124.51
12	A	816	CLA	CHB-C4A-NA	2.76	128.32	124.51
12	B	825	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
12	B	838	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
12	A	838	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
12	B	836	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
15	M	101	BCR	C28-C27-C26	-2.74	109.18	114.08
15	L	204	BCR	C38-C26-C27	2.74	118.87	113.62
12	A	835	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
12	A	838	CLA	CHB-C4A-NA	2.72	128.28	124.51
12	A	833	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
12	B	821	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
15	L	202	BCR	C33-C5-C4	2.71	118.83	113.62
12	B	827	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
12	A	829	CLA	CHB-C4A-NA	2.71	128.26	124.51
12	B	807	CLA	CHB-C4A-NA	2.71	128.26	124.51
12	B	806	CLA	CHC-C4B-NB	2.71	127.12	124.26
12	B	812	CLA	CHB-C4A-NA	2.71	128.26	124.51
12	B	817	CLA	CHB-C4A-NA	2.71	128.26	124.51
12	F	301	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
15	M	101	BCR	C11-C10-C9	-2.70	123.45	127.31
12	A	819	CLA	CHB-C4A-NA	2.69	128.23	124.51
15	A	844	BCR	C38-C26-C25	-2.69	121.51	124.53
12	B	817	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
15	L	202	BCR	C38-C26-C25	-2.69	121.51	124.53
12	A	805	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
12	A	830	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
12	A	821	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
15	B	841	BCR	C29-C30-C25	2.68	114.61	110.48
12	B	803	CLA	CHB-C4A-NA	2.68	128.22	124.51
15	A	846	BCR	C30-C25-C26	-2.68	118.84	122.61
12	B	828	CLA	CHB-C4A-NA	2.67	128.20	124.51
12	A	808	CLA	O2D-CGD-O1D	-2.67	118.63	123.84
12	K	204	CLA	CHB-C4A-NA	2.66	128.20	124.51
12	B	820	CLA	CHB-C4A-NA	2.66	128.19	124.51
12	B	818	CLA	CMB-C2B-C1B	-2.66	121.32	125.37
12	B	805	CLA	CMB-C2B-C3B	2.65	133.01	126.59
12	B	818	CLA	CHB-C4A-NA	2.65	128.17	124.51
12	B	807	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
12	A	804	CLA	CMB-C2B-C1B	-2.65	121.34	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	I	201	BCR	C15-C16-C17	-2.65	118.06	123.47
12	A	809	CLA	CHB-C4A-NA	2.64	128.17	124.51
15	B	842	BCR	C23-C24-C25	-2.64	119.78	127.20
12	B	832	CLA	CHB-C4A-NA	2.64	128.16	124.51
15	M	101	BCR	C16-C15-C14	-2.64	118.07	123.47
12	B	815	CLA	O2D-CGD-O1D	-2.63	118.11	124.09
12	A	841	CLA	CAA-C2A-C3A	-2.63	109.96	116.10
12	A	804	CLA	CHB-C4A-NA	2.63	128.15	124.51
12	B	824	CLA	CMB-C2B-C1B	-2.63	121.37	125.37
13	B	840	PQN	C11-C12-C13	-2.63	122.42	126.79
15	B	843	BCR	C11-C12-C13	-2.63	119.04	126.42
12	A	826	CLA	CHB-C4A-NA	2.62	128.14	124.51
12	A	818	CLA	CHB-C1B-NB	2.62	127.03	124.26
12	K	201	CLA	CAA-C2A-C3A	-2.62	109.98	116.10
15	I	201	BCR	C33-C5-C6	-2.62	121.59	124.53
12	B	833	CLA	CHB-C4A-NA	2.62	128.13	124.51
12	A	824	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
12	B	810	CLA	CHB-C4A-NA	2.62	128.13	124.51
12	B	809	CLA	CMB-C2B-C1B	-2.61	121.39	125.37
12	K	201	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
12	B	833	CLA	CHD-C1D-ND	-2.61	122.05	124.45
15	A	845	BCR	C1-C6-C5	-2.61	118.94	122.61
12	A	823	CLA	CHB-C4A-NA	2.61	128.12	124.51
12	B	809	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
12	A	817	CLA	CMB-C2B-C3B	2.60	132.88	126.59
12	B	813	CLA	CHB-C1B-NB	2.60	127.01	124.26
15	I	201	BCR	C27-C26-C25	-2.59	118.97	122.73
12	A	841	CLA	O2D-CGD-O1D	-2.59	118.22	124.09
12	A	805	CLA	CAA-C2A-C3A	-2.59	105.70	112.78
12	L	201	CLA	CHB-C4A-NA	2.58	128.08	124.51
12	B	815	CLA	CHB-C4A-NA	2.58	128.08	124.51
15	B	843	BCR	C21-C20-C19	-2.58	115.16	123.22
12	B	811	CLA	CHB-C4A-NA	2.58	128.08	124.51
15	I	201	BCR	C30-C25-C26	-2.58	118.98	122.61
12	A	818	CLA	CHB-C4A-NA	2.58	128.07	124.51
12	A	812	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
12	A	839	CLA	CHB-C4A-NA	2.58	128.07	124.51
14	A	842	LHG	O8-C23-C24	2.57	119.99	111.91
12	A	815	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
12	A	834	CLA	CAA-C2A-C3A	-2.57	110.10	116.10
15	I	201	BCR	C4-C5-C6	-2.57	119.00	122.73
12	B	839	CLA	CHB-C4A-NA	2.57	128.06	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	L	202	BCR	C27-C26-C25	-2.56	119.01	122.73
12	A	837	CLA	CHB-C4A-NA	2.56	128.05	124.51
12	B	813	CLA	CMB-C2B-C1B	-2.56	121.47	125.37
15	B	804	BCR	C1-C6-C5	-2.56	119.01	122.61
12	A	806	CLA	CHB-C4A-NA	2.55	128.04	124.51
12	A	831	CLA	CAA-C2A-C3A	-2.55	105.80	112.78
12	B	827	CLA	CMB-C2B-C1B	-2.55	121.49	125.37
12	B	827	CLA	CHB-C4A-NA	2.55	128.04	124.51
13	A	840	PQN	C11-C12-C13	-2.55	122.55	126.79
12	B	806	CLA	O1D-CGD-CBD	2.55	129.69	124.48
15	M	101	BCR	C33-C5-C4	2.54	118.50	113.62
15	K	202	BCR	C20-C19-C18	-2.54	119.28	126.42
18	B	844	DGD	O1G-C1A-C2A	2.54	119.88	111.91
12	A	810	CLA	CHB-C4A-NA	2.54	128.02	124.51
12	B	823	CLA	CHB-C4A-NA	2.54	128.02	124.51
12	A	831	CLA	CHB-C4A-NA	2.53	128.01	124.51
12	B	838	CLA	CHB-C4A-NA	2.53	128.01	124.51
12	B	802	CLA	CMB-C2B-C1B	-2.53	121.52	125.37
12	B	808	CLA	CHB-C4A-NA	2.53	128.00	124.51
15	B	843	BCR	C2-C1-C6	2.52	114.37	110.48
12	B	829	CLA	CHB-C4A-NA	2.52	127.99	124.51
12	A	831	CLA	CMB-C2B-C3B	2.52	132.68	126.59
12	A	812	CLA	CAA-C2A-C3A	-2.52	105.89	112.78
14	A	843	LHG	O8-C23-C24	2.52	119.80	111.91
12	B	816	CLA	CHB-C4A-NA	2.51	127.99	124.51
12	A	811	CLA	CAA-C2A-C3A	-2.51	110.24	116.10
12	B	831	CLA	CHB-C4A-NA	2.51	127.98	124.51
12	B	815	CLA	CAB-C3B-C2B	2.51	130.10	123.59
12	B	814	CLA	C3B-C4B-NB	-2.51	108.19	110.52
12	A	830	CLA	CHB-C4A-NA	2.51	127.98	124.51
12	B	836	CLA	CHB-C4A-NA	2.51	127.98	124.51
12	A	813	CLA	CHB-C4A-NA	2.50	127.97	124.51
12	A	836	CLA	CHB-C4A-NA	2.50	127.97	124.51
12	A	815	CLA	CHB-C4A-NA	2.50	127.96	124.51
12	B	824	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
12	B	825	CLA	CHB-C4A-NA	2.49	127.96	124.51
15	B	841	BCR	C3-C4-C5	-2.49	109.63	114.08
15	B	843	BCR	C20-C21-C22	-2.49	123.75	127.31
12	A	803	CLA	C3B-C4B-NB	-2.49	108.21	110.52
15	A	845	BCR	C38-C26-C27	2.48	118.39	113.62
12	A	817	CLA	CHB-C4A-NA	2.48	127.94	124.51
12	B	819	CLA	CHB-C4A-NA	2.48	127.94	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	805	CLA	C2B-C1B-NB	2.48	111.89	110.23
12	B	808	CLA	CAA-C2A-C3A	-2.47	110.32	116.10
12	B	830	CLA	CHB-C4A-NA	2.47	127.93	124.51
12	A	821	CLA	CHB-C4A-NA	2.47	127.93	124.51
15	K	202	BCR	C16-C15-C14	-2.47	118.42	123.47
15	A	845	BCR	C8-C7-C6	-2.46	120.28	127.20
12	A	834	CLA	CHB-C4A-NA	2.46	127.91	124.51
12	B	814	CLA	CHB-C4A-NA	2.45	127.91	124.51
12	A	828	CLA	CHB-C4A-NA	2.45	127.90	124.51
12	B	821	CLA	CHB-C4A-NA	2.45	127.90	124.51
12	B	801	CLA	CHB-C1B-NB	2.45	126.85	124.26
12	J	102	CLA	CHB-C4A-NA	2.45	127.90	124.51
12	B	812	CLA	O2D-CGD-CBD	2.45	115.62	111.27
12	B	830	CLA	CHD-C1D-ND	-2.44	122.21	124.45
12	A	811	CLA	CHB-C1B-NB	2.44	126.84	124.26
12	A	841	CLA	CHB-C4A-NA	2.44	127.88	124.51
12	B	825	CLA	CAA-C2A-C3A	-2.44	106.11	112.78
12	L	201	CLA	CHB-C1B-NB	2.44	126.83	124.26
12	F	301	CLA	CHB-C4A-NA	2.43	127.88	124.51
12	B	817	CLA	CAA-C2A-C3A	-2.43	106.12	112.78
18	B	844	DGD	O6D-C5D-C6D	2.43	111.57	106.67
12	B	826	CLA	CHB-C4A-NA	2.42	127.86	124.51
12	B	808	CLA	CMB-C2B-C1B	-2.42	121.68	125.37
15	L	204	BCR	C11-C12-C13	-2.42	119.62	126.42
12	A	827	CLA	CHB-C4A-NA	2.42	127.86	124.51
15	L	202	BCR	C37-C22-C21	-2.42	119.54	122.92
12	A	820	CLA	CHB-C4A-NA	2.42	127.85	124.51
12	B	802	CLA	CAA-C2A-C3A	-2.41	106.17	112.78
12	A	832	CLA	CHB-C4A-NA	2.41	127.85	124.51
12	K	201	CLA	CHB-C4A-NA	2.41	127.84	124.51
12	A	801	CLA	CHC-C4B-NB	2.40	126.80	124.26
15	B	841	BCR	C8-C9-C10	2.40	122.62	118.94
12	A	805	CLA	C7-C6-C5	-2.40	109.28	114.49
12	A	822	CLA	CHB-C4A-NA	2.39	127.82	124.51
12	A	802	CLA	CHB-C4A-NA	2.39	127.82	124.51
12	B	837	CLA	CHB-C1B-NB	2.39	126.79	124.26
12	A	804	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
12	A	813	CLA	CHD-C1D-ND	-2.39	122.26	124.45
12	B	802	CLA	CMB-C2B-C3B	2.39	132.38	126.59
15	B	804	BCR	C3-C4-C5	-2.39	109.81	114.08
12	A	822	CLA	CHD-C1D-ND	-2.38	122.26	124.45
12	K	203	CLA	CHB-C4A-NA	2.38	127.81	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	811	CLA	CHD-C1D-ND	-2.38	122.27	124.45
15	B	804	BCR	C33-C5-C6	-2.38	121.86	124.53
12	A	828	CLA	CHB-C1B-NB	2.37	126.77	124.26
15	A	846	BCR	C1-C6-C5	-2.37	119.28	122.61
15	A	846	BCR	C33-C5-C4	2.37	118.17	113.62
12	A	808	CLA	CHB-C4A-NA	2.37	127.78	124.51
15	A	847	BCR	C16-C15-C14	-2.36	118.63	123.47
15	A	845	BCR	C16-C15-C14	-2.36	118.63	123.47
12	A	814	CLA	CHB-C4A-NA	2.36	127.78	124.51
12	B	826	CLA	CMB-C2B-C1B	-2.36	121.78	125.37
15	J	101	BCR	C24-C23-C22	-2.36	122.67	126.23
12	B	824	CLA	CHD-C1D-ND	-2.36	122.29	124.45
12	A	825	CLA	CHB-C4A-NA	2.36	127.77	124.51
12	B	822	CLA	CHB-C4A-NA	2.35	127.77	124.51
12	L	201	CLA	CHD-C1D-ND	-2.35	122.29	124.45
15	B	804	BCR	C33-C5-C4	2.35	118.13	113.62
12	A	814	CLA	CMB-C2B-C1B	-2.35	121.79	125.37
15	A	844	BCR	C15-C16-C17	-2.35	118.67	123.47
12	B	815	CLA	CMB-C2B-C3B	2.35	129.67	123.59
12	B	836	CLA	CHD-C1D-ND	-2.35	122.30	124.45
12	A	830	CLA	C3B-C4B-NB	-2.35	108.34	110.52
12	B	824	CLA	CHB-C4A-NA	2.34	127.75	124.51
12	B	821	CLA	CHB-C1B-NB	2.34	126.74	124.26
15	A	847	BCR	C38-C26-C25	-2.33	121.91	124.53
12	A	806	CLA	CHD-C1D-ND	-2.33	122.31	124.45
12	A	827	CLA	C3B-C4B-NB	-2.33	108.35	110.52
12	B	818	CLA	CMB-C2B-C3B	2.33	132.23	126.59
12	B	809	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
12	B	837	CLA	CHB-C4A-NA	2.33	127.73	124.51
12	F	301	CLA	CAA-C2A-C3A	-2.33	110.67	116.10
12	A	836	CLA	CHD-C1D-ND	-2.33	122.32	124.45
15	L	204	BCR	C2-C1-C6	2.32	114.06	110.48
15	L	202	BCR	C29-C30-C25	2.32	114.06	110.48
15	A	844	BCR	C38-C26-C27	2.32	118.07	113.62
12	B	824	CLA	CHB-C1B-NB	2.32	126.71	124.26
12	A	826	CLA	CAA-C2A-C3A	-2.32	106.44	112.78
12	A	835	CLA	CAA-C2A-C3A	-2.31	106.46	112.78
15	M	101	BCR	C10-C11-C12	-2.30	116.03	123.22
15	B	842	BCR	C1-C6-C5	-2.30	119.37	122.61
15	B	804	BCR	C34-C9-C8	2.30	121.70	118.08
12	B	826	CLA	CHC-C4B-NB	2.30	126.69	124.26
12	B	823	CLA	CHB-C1B-NB	2.30	126.69	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	803	CLA	CHD-C1D-ND	-2.30	122.34	124.45
12	A	824	CLA	C2A-C1A-CHA	2.30	127.87	123.86
12	B	813	CLA	CHB-C4A-NA	2.30	127.69	124.51
12	A	811	CLA	CHB-C4A-NA	2.29	127.68	124.51
15	A	847	BCR	C38-C26-C27	2.29	118.02	113.62
12	A	839	CLA	C3B-C4B-NB	-2.29	108.39	110.52
12	A	811	CLA	CHD-C1D-ND	-2.29	122.35	124.45
12	A	803	CLA	CHB-C1B-NB	2.29	126.68	124.26
12	A	838	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
15	M	101	BCR	C8-C7-C6	-2.29	120.78	127.20
12	A	803	CLA	CMB-C2B-C1B	-2.28	121.89	125.37
15	A	844	BCR	C1-C6-C5	-2.28	119.40	122.61
12	A	834	CLA	CHD-C1D-ND	-2.27	122.37	124.45
12	B	802	CLA	CHB-C4A-NA	2.26	127.64	124.51
15	K	202	BCR	C38-C26-C27	2.26	117.97	113.62
12	A	833	CLA	CHB-C4A-NA	2.26	127.64	124.51
15	B	842	BCR	C4-C5-C6	-2.26	119.45	122.73
12	B	806	CLA	CHB-C4A-NA	2.26	127.63	124.51
12	A	818	CLA	CHC-C4B-NB	2.25	126.64	124.26
12	B	824	CLA	CMB-C2B-C3B	2.25	132.04	126.59
12	B	808	CLA	CHB-C1B-NB	2.25	126.64	124.26
12	B	813	CLA	CHC-C4B-NB	2.25	126.64	124.26
15	M	101	BCR	C38-C26-C25	-2.25	122.00	124.53
12	A	827	CLA	CHB-C1B-NB	2.24	126.63	124.26
12	B	805	CLA	CHB-C4A-NA	2.24	127.61	124.51
12	B	802	CLA	C2B-C1B-NB	2.24	111.73	110.23
12	A	836	CLA	CHB-C1B-NB	2.24	126.63	124.26
12	K	203	CLA	CHD-C1D-ND	-2.24	122.40	124.45
12	A	833	CLA	C3B-C4B-NB	-2.24	108.44	110.52
12	A	820	CLA	CHB-C1B-NB	2.23	126.62	124.26
12	A	813	CLA	CMB-C2B-C1B	-2.23	121.97	125.37
12	A	837	CLA	CHC-C4B-NB	2.23	126.62	124.26
15	J	101	BCR	C38-C26-C27	2.23	117.90	113.62
12	A	838	CLA	CMB-C2B-C1B	-2.23	121.97	125.37
12	B	823	CLA	C3B-C4B-NB	-2.23	108.45	110.52
12	L	203	CLA	CHB-C4A-NA	2.23	127.60	124.51
12	B	812	CLA	CHC-C4B-NB	2.23	126.61	124.26
15	A	844	BCR	C8-C7-C6	-2.22	120.95	127.20
12	B	832	CLA	CHD-C1D-ND	-2.22	122.41	124.45
15	M	101	BCR	C20-C19-C18	-2.22	120.18	126.42
12	B	836	CLA	C3B-C4B-NB	-2.22	108.45	110.52
12	A	833	CLA	CHB-C1B-NB	2.22	126.61	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	828	CLA	CMB-C2B-C1B	-2.22	121.99	125.37
12	A	801	CLA	C3B-C4B-NB	-2.22	108.46	110.52
12	B	822	CLA	O2D-CGD-CBD	2.22	115.21	111.27
12	A	818	CLA	CMB-C2B-C3B	2.22	131.96	126.59
12	B	826	CLA	C3B-C4B-NB	-2.22	108.46	110.52
12	B	838	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
12	B	809	CLA	CMB-C2B-C3B	2.21	131.95	126.59
12	A	817	CLA	C1-C2-C3	-2.21	122.22	126.04
12	B	812	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
15	A	845	BCR	C30-C25-C26	-2.21	119.50	122.61
12	A	822	CLA	CHC-C4B-NB	2.21	126.59	124.26
12	A	804	CLA	CMB-C2B-C3B	2.21	131.93	126.59
12	A	825	CLA	CHD-C1D-ND	-2.21	122.43	124.45
15	A	845	BCR	C4-C5-C6	-2.20	119.53	122.73
17	A	849	LMU	C1'-C2'-C3'	2.20	114.58	110.00
12	B	836	CLA	CHB-C1B-NB	2.20	126.59	124.26
12	F	301	CLA	CHD-C1D-ND	-2.20	122.44	124.45
12	A	820	CLA	C3B-C4B-NB	-2.19	108.48	110.52
12	A	838	CLA	CHB-C1B-NB	2.19	126.58	124.26
12	A	836	CLA	C3B-C4B-NB	-2.19	108.48	110.52
12	B	830	CLA	C3B-C4B-NB	-2.19	108.48	110.52
12	B	810	CLA	CMB-C2B-C1B	-2.19	122.03	125.37
12	B	827	CLA	CHB-C1B-NB	2.19	126.57	124.26
12	B	815	CLA	CHD-C1D-ND	-2.19	122.45	124.45
12	B	826	CLA	CMB-C2B-C3B	2.18	131.87	126.59
12	L	201	CLA	O2D-CGD-CBD	2.18	115.14	111.27
12	B	828	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
12	A	832	CLA	C3B-C4B-NB	-2.18	108.50	110.52
15	B	804	BCR	C11-C12-C13	-2.17	120.31	126.42
12	A	802	CLA	CMB-C2B-C1B	-2.17	122.06	125.37
12	B	827	CLA	CMB-C2B-C3B	2.17	131.85	126.59
12	A	837	CLA	CHB-C1B-NB	2.17	126.56	124.26
15	A	846	BCR	C15-C16-C17	-2.17	119.03	123.47
12	B	803	CLA	C3B-C4B-NB	-2.17	108.50	110.52
12	B	819	CLA	CHD-C1D-ND	-2.17	122.46	124.45
12	A	828	CLA	C3B-C4B-NB	-2.17	108.51	110.52
12	A	808	CLA	CHD-C1D-ND	-2.16	122.47	124.45
15	B	843	BCR	C38-C26-C27	2.16	117.77	113.62
12	B	809	CLA	CHD-C1D-ND	-2.16	122.47	124.45
12	A	827	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
12	A	810	CLA	CHD-C1D-ND	-2.16	122.47	124.45
12	K	201	CLA	CHD-C1D-ND	-2.16	122.47	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	I	201	BCR	C8-C7-C6	-2.15	121.15	127.20
12	A	834	CLA	C3B-C4B-NB	-2.15	108.52	110.52
12	B	814	CLA	CHD-C1D-ND	-2.15	122.48	124.45
12	A	828	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
15	A	847	BCR	C21-C20-C19	-2.15	116.51	123.22
12	A	819	CLA	CAC-C3C-C4C	2.15	127.60	124.81
12	B	837	CLA	CHD-C1D-ND	-2.15	122.48	124.45
12	A	808	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
15	L	204	BCR	C23-C24-C25	-2.15	121.17	127.20
15	A	847	BCR	C10-C11-C12	-2.14	116.53	123.22
15	J	101	BCR	C38-C26-C25	-2.14	122.12	124.53
12	B	832	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
12	A	822	CLA	CHB-C1B-NB	2.13	126.52	124.26
12	A	832	CLA	CHB-C1B-NB	2.13	126.52	124.26
15	B	804	BCR	C10-C11-C12	-2.13	116.56	123.22
12	A	827	CLA	C1-C2-C3	-2.13	123.30	126.75
12	B	808	CLA	C3B-C4B-NB	-2.13	108.54	110.52
12	B	815	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
12	A	833	CLA	CHD-C1D-ND	-2.13	122.50	124.45
12	A	836	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
12	A	801	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
12	A	828	CLA	CHC-C4B-NB	2.13	126.51	124.26
12	A	838	CLA	CHD-C1D-ND	-2.13	122.50	124.45
12	L	201	CLA	CMB-C2B-C1B	-2.12	122.13	125.37
12	B	823	CLA	CHC-C4B-NB	2.12	126.50	124.26
12	B	809	CLA	C3B-C4B-NB	-2.12	108.55	110.52
12	B	830	CLA	CHB-C1B-NB	2.12	126.50	124.26
12	B	802	CLA	CHD-C1D-ND	-2.12	122.51	124.45
12	L	203	CLA	CHD-C1D-ND	-2.12	122.51	124.45
12	B	838	CLA	C3B-C4B-NB	-2.12	108.55	110.52
12	B	837	CLA	C3B-C4B-NB	-2.12	108.55	110.52
12	A	817	CLA	CHB-C1B-NB	2.12	126.50	124.26
12	A	810	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
12	A	807	CLA	CHD-C1D-ND	-2.12	122.51	124.45
12	A	803	CLA	CMB-C2B-C3B	2.12	131.71	126.59
15	B	842	BCR	C27-C26-C25	-2.11	119.66	122.73
12	B	808	CLA	CMB-C2B-C3B	2.11	131.70	126.59
12	B	823	CLA	CHD-C1D-ND	-2.11	122.51	124.45
12	A	814	CLA	CHD-C1D-ND	-2.11	122.52	124.45
12	A	835	CLA	CMB-C2B-C1B	-2.11	122.16	125.37
12	B	807	CLA	CHB-C1B-NB	2.11	126.49	124.26
12	A	815	CLA	O2A-CGA-O1A	-2.11	118.05	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	834	CLA	C2A-C1A-CHA	2.11	127.54	123.86
12	B	806	CLA	C3B-C4B-NB	-2.11	108.56	110.52
15	A	845	BCR	C3-C4-C5	-2.10	110.32	114.08
12	A	835	CLA	CMB-C2B-C3B	2.10	131.68	126.59
12	A	814	CLA	CMB-C2B-C3B	2.10	131.68	126.59
15	B	842	BCR	C20-C19-C18	-2.10	120.52	126.42
12	B	831	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
12	A	832	CLA	CHC-C4B-NB	2.10	126.48	124.26
12	B	812	CLA	C3B-C4B-NB	-2.10	108.57	110.52
12	A	821	CLA	CHD-C1D-ND	-2.10	122.53	124.45
12	B	808	CLA	CHD-C1D-ND	-2.10	122.53	124.45
12	A	835	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
12	A	820	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
13	A	840	PQN	C21-C20-C18	-2.09	109.15	115.92
15	I	201	BCR	C20-C19-C18	-2.09	120.54	126.42
12	A	826	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
12	A	834	CLA	CHB-C1B-NB	2.09	126.47	124.26
12	B	807	CLA	CHD-C1D-ND	-2.09	122.53	124.45
12	B	820	CLA	CHD-C1D-ND	-2.09	122.53	124.45
15	A	845	BCR	C23-C24-C25	-2.09	121.34	127.20
12	A	830	CLA	CHB-C1B-NB	2.09	126.47	124.26
12	A	839	CLA	CHD-C1D-ND	-2.09	122.54	124.45
12	A	811	CLA	CMA-C3A-C2A	-2.09	111.23	116.10
12	B	839	CLA	CHD-C1D-ND	-2.08	122.54	124.45
12	A	833	CLA	CMB-C2B-C1B	-2.08	122.19	125.37
15	L	202	BCR	C20-C19-C18	-2.08	120.56	126.42
15	B	841	BCR	C30-C25-C26	-2.08	119.68	122.61
12	B	824	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
15	B	843	BCR	C32-C1-C6	-2.08	106.92	110.30
12	A	837	CLA	CHD-C1D-ND	-2.08	122.54	124.45
12	B	815	CLA	C3B-C4B-NB	-2.08	108.84	110.23
12	B	818	CLA	CHD-C1D-ND	-2.08	122.54	124.45
12	B	833	CLA	O2D-CGD-CBD	2.08	114.96	111.27
12	B	821	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
12	A	807	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
12	L	201	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
15	K	202	BCR	C23-C24-C25	-2.07	121.38	127.20
12	A	801	CLA	CHB-C4A-NA	2.07	127.37	124.51
15	A	846	BCR	C20-C19-C18	-2.07	120.61	126.42
12	B	805	CLA	CAA-C2A-C3A	-2.07	107.12	112.78
12	A	822	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
12	B	822	CLA	CHD-C1D-ND	-2.07	122.56	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	830	CLA	O2D-CGD-CBD	2.06	114.94	111.27
15	B	842	BCR	C30-C25-C26	-2.06	119.71	122.61
17	A	849	LMU	O5B-C5B-C4B	2.06	112.91	110.06
12	A	832	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
12	F	301	CLA	CHB-C1B-NB	2.06	126.44	124.26
12	B	829	CLA	CHD-C1D-ND	-2.06	122.56	124.45
12	B	833	CLA	CHB-C1B-NB	2.06	126.44	124.26
12	A	817	CLA	CHD-C1D-ND	-2.06	122.56	124.45
12	B	810	CLA	CMB-C2B-C3B	2.06	131.57	126.59
12	B	810	CLA	C1-C2-C3	-2.05	122.49	126.04
12	B	831	CLA	C2A-C1A-CHA	2.05	127.45	123.86
12	B	803	CLA	C2A-C1A-CHA	2.05	127.45	123.86
15	A	844	BCR	C20-C19-C18	-2.05	120.65	126.42
12	B	810	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
12	A	802	CLA	CMB-C2B-C3B	2.05	131.56	126.59
12	B	810	CLA	CHD-C1D-ND	-2.05	122.57	124.45
12	B	805	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
12	B	821	CLA	CHD-C1D-ND	-2.05	122.57	124.45
12	B	834	CLA	O2A-CGA-O1A	-2.05	118.19	123.30
12	A	812	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
12	A	813	CLA	CMB-C2B-C3B	2.05	131.55	126.59
12	B	810	CLA	CAA-C2A-C3A	-2.05	107.17	112.78
12	B	807	CLA	CHC-C4B-NB	2.05	126.42	124.26
12	B	807	CLA	C3B-C4B-NB	-2.04	108.62	110.52
15	B	841	BCR	C10-C11-C12	-2.04	116.84	123.22
15	A	846	BCR	C11-C12-C13	-2.04	120.69	126.42
12	B	811	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
12	B	826	CLA	CHB-C1B-NB	2.04	126.41	124.26
12	B	823	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
12	A	807	CLA	CHB-C1B-NB	2.03	126.41	124.26
12	A	837	CLA	C3B-C4B-NB	-2.03	108.63	110.52
12	A	815	CLA	CHD-C1D-ND	-2.03	122.59	124.45
12	A	808	CLA	C1-C2-C3	-2.03	123.47	126.75
12	B	828	CLA	CHD-C1D-ND	-2.03	122.59	124.45
12	A	838	CLA	CMB-C2B-C3B	2.03	131.50	126.59
12	A	818	CLA	CHD-C1D-ND	-2.03	122.59	124.45
12	A	803	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
12	B	824	CLA	C3B-C4B-NB	-2.03	108.64	110.52
12	A	811	CLA	CMB-C2B-C3B	2.03	131.50	126.59
15	L	202	BCR	C8-C7-C6	-2.03	121.51	127.20
12	B	803	CLA	CHB-C1B-NB	2.03	126.40	124.26
12	A	823	CLA	CHD-C1D-ND	-2.03	122.59	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	827	CLA	CMB-C2B-C1B	-2.02	122.28	125.37
12	A	807	CLA	C3B-C4B-NB	-2.02	108.64	110.52
12	F	301	CLA	C3B-C4B-NB	-2.02	108.64	110.52
12	B	812	CLA	CHB-C1B-NB	2.02	126.40	124.26
12	A	817	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
12	B	818	CLA	O2A-CGA-O1A	-2.02	118.26	123.30
15	I	201	BCR	C3-C4-C5	-2.02	110.47	114.08
12	B	827	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
15	A	846	BCR	C28-C27-C26	-2.02	110.47	114.08
12	B	819	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
15	B	842	BCR	C30-C25-C24	2.02	121.49	115.78
12	A	825	CLA	C3B-C4B-NB	-2.02	108.64	110.52
12	J	102	CLA	CAA-C2A-C3A	-2.01	109.22	114.26
12	B	803	CLA	CAA-CBA-CGA	-2.01	107.37	113.25
12	A	825	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
12	A	830	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
15	L	204	BCR	C15-C16-C17	-2.01	119.35	123.47
12	A	820	CLA	CHD-C1D-ND	-2.01	122.61	124.45
15	A	844	BCR	C4-C5-C6	-2.01	119.81	122.73
12	B	821	CLA	CMB-C2B-C1B	-2.01	122.31	125.37
12	B	824	CLA	C1-C2-C3	-2.01	123.50	126.75
12	A	832	CLA	CHD-C1D-ND	-2.01	122.61	124.45
15	A	844	BCR	C11-C12-C13	-2.01	120.77	126.42
12	B	838	CLA	CHD-C1D-ND	-2.01	122.61	124.45
12	A	801	CLA	O1D-CGD-CBD	2.01	128.59	124.48
12	A	827	CLA	CHC-C4B-NB	2.01	126.38	124.26
15	L	204	BCR	C33-C5-C6	-2.01	122.28	124.53
12	A	839	CLA	CHB-C1B-NB	2.01	126.38	124.26
12	B	839	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
12	F	301	CLA	CHC-C4B-NB	2.00	126.38	124.26
15	L	204	BCR	C16-C15-C14	-2.00	119.38	123.47

There are no chirality outliers.

All (893) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	801	CLA	C2B-C3B-CAB-CBB
12	A	801	CLA	C4B-C3B-CAB-CBB
12	A	801	CLA	CBD-CGD-O2D-CED
12	A	801	CLA	O1D-CGD-O2D-CED
12	A	803	CLA	C3A-C2A-CAA-CBA
12	A	803	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
12	A	805	CLA	C2B-C3B-CAB-CBB
12	A	805	CLA	C4B-C3B-CAB-CBB
12	A	807	CLA	C3A-C2A-CAA-CBA
12	A	809	CLA	C1A-C2A-CAA-CBA
12	A	809	CLA	C3A-C2A-CAA-CBA
12	A	810	CLA	CBD-CGD-O2D-CED
12	A	810	CLA	O1D-CGD-O2D-CED
12	A	814	CLA	CHA-CBD-CGD-O1D
12	A	814	CLA	CHA-CBD-CGD-O2D
12	A	814	CLA	CBD-CGD-O2D-CED
12	A	815	CLA	C3A-C2A-CAA-CBA
12	A	817	CLA	C3A-C2A-CAA-CBA
12	A	818	CLA	C1A-C2A-CAA-CBA
12	A	818	CLA	C3A-C2A-CAA-CBA
12	A	819	CLA	CBA-CGA-O2A-C1
12	A	819	CLA	CHA-CBD-CGD-O1D
12	A	819	CLA	CHA-CBD-CGD-O2D
12	A	821	CLA	C1A-C2A-CAA-CBA
12	A	821	CLA	C3A-C2A-CAA-CBA
12	A	821	CLA	C4B-C3B-CAB-CBB
12	A	822	CLA	C1A-C2A-CAA-CBA
12	A	822	CLA	CHA-CBD-CGD-O1D
12	A	822	CLA	CHA-CBD-CGD-O2D
12	A	822	CLA	CAD-CBD-CGD-O1D
12	A	822	CLA	CAD-CBD-CGD-O2D
12	A	822	CLA	CBD-CGD-O2D-CED
12	A	823	CLA	C1A-C2A-CAA-CBA
12	A	823	CLA	C3A-C2A-CAA-CBA
12	A	828	CLA	C1A-C2A-CAA-CBA
12	A	829	CLA	C2B-C3B-CAB-CBB
12	A	829	CLA	C4B-C3B-CAB-CBB
12	A	830	CLA	C1A-C2A-CAA-CBA
12	A	830	CLA	C3A-C2A-CAA-CBA
12	A	832	CLA	C2B-C3B-CAB-CBB
12	A	832	CLA	C4B-C3B-CAB-CBB
12	A	832	CLA	CBD-CGD-O2D-CED
12	A	833	CLA	C1A-C2A-CAA-CBA
12	A	833	CLA	C3A-C2A-CAA-CBA
12	A	834	CLA	C2B-C3B-CAB-CBB
12	A	834	CLA	C4B-C3B-CAB-CBB
12	A	834	CLA	CHA-CBD-CGD-O1D
12	A	834	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
12	A	835	CLA	C1A-C2A-CAA-CBA
12	A	835	CLA	C3A-C2A-CAA-CBA
12	A	836	CLA	C2B-C3B-CAB-CBB
12	A	836	CLA	C4B-C3B-CAB-CBB
12	A	837	CLA	C1A-C2A-CAA-CBA
12	A	837	CLA	CHA-CBD-CGD-O1D
12	A	837	CLA	CHA-CBD-CGD-O2D
12	A	838	CLA	C1A-C2A-CAA-CBA
12	A	838	CLA	C3A-C2A-CAA-CBA
12	A	839	CLA	C1A-C2A-CAA-CBA
12	A	839	CLA	C3A-C2A-CAA-CBA
12	A	839	CLA	C2B-C3B-CAB-CBB
12	A	839	CLA	C4B-C3B-CAB-CBB
12	B	803	CLA	C2A-CAA-CBA-CGA
12	B	803	CLA	CHA-CBD-CGD-O1D
12	B	803	CLA	CHA-CBD-CGD-O2D
12	B	805	CLA	CHA-CBD-CGD-O1D
12	B	805	CLA	CHA-CBD-CGD-O2D
12	B	806	CLA	C2B-C3B-CAB-CBB
12	B	806	CLA	C4B-C3B-CAB-CBB
12	B	807	CLA	C2B-C3B-CAB-CBB
12	B	807	CLA	C4B-C3B-CAB-CBB
12	B	807	CLA	CBD-CGD-O2D-CED
12	B	809	CLA	C1A-C2A-CAA-CBA
12	B	809	CLA	C3A-C2A-CAA-CBA
12	B	809	CLA	CHA-CBD-CGD-O1D
12	B	809	CLA	CHA-CBD-CGD-O2D
12	B	809	CLA	CAD-CBD-CGD-O1D
12	B	811	CLA	C1A-C2A-CAA-CBA
12	B	811	CLA	C3A-C2A-CAA-CBA
12	B	812	CLA	C1A-C2A-CAA-CBA
12	B	812	CLA	C3A-C2A-CAA-CBA
12	B	812	CLA	C2B-C3B-CAB-CBB
12	B	812	CLA	C4B-C3B-CAB-CBB
12	B	813	CLA	C1A-C2A-CAA-CBA
12	B	813	CLA	C2A-CAA-CBA-CGA
12	B	814	CLA	C2A-CAA-CBA-CGA
12	B	814	CLA	C2B-C3B-CAB-CBB
12	B	814	CLA	C4B-C3B-CAB-CBB
12	B	814	CLA	CBD-CGD-O2D-CED
12	B	815	CLA	C1A-C2A-CAA-CBA
12	B	820	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
12	B	821	CLA	C2B-C3B-CAB-CBB
12	B	821	CLA	C4B-C3B-CAB-CBB
12	B	823	CLA	C2B-C3B-CAB-CBB
12	B	823	CLA	C4B-C3B-CAB-CBB
12	B	825	CLA	C1A-C2A-CAA-CBA
12	B	825	CLA	C3A-C2A-CAA-CBA
12	B	826	CLA	C1A-C2A-CAA-CBA
12	B	826	CLA	C3A-C2A-CAA-CBA
12	B	827	CLA	CHA-CBD-CGD-O1D
12	B	827	CLA	CHA-CBD-CGD-O2D
12	B	829	CLA	C1A-C2A-CAA-CBA
12	B	829	CLA	C3A-C2A-CAA-CBA
12	B	832	CLA	CBD-CGD-O2D-CED
12	B	833	CLA	C1A-C2A-CAA-CBA
12	B	833	CLA	C3A-C2A-CAA-CBA
12	B	834	CLA	C1A-C2A-CAA-CBA
12	B	834	CLA	CBD-CGD-O2D-CED
12	B	838	CLA	C2A-CAA-CBA-CGA
12	B	838	CLA	C4B-C3B-CAB-CBB
12	B	839	CLA	C2B-C3B-CAB-CBB
12	B	839	CLA	C4B-C3B-CAB-CBB
12	B	839	CLA	CBD-CGD-O2D-CED
12	J	102	CLA	CHA-CBD-CGD-O1D
12	J	102	CLA	CHA-CBD-CGD-O2D
12	J	102	CLA	CBD-CGD-O2D-CED
12	K	201	CLA	C2B-C3B-CAB-CBB
12	K	201	CLA	C4B-C3B-CAB-CBB
12	K	201	CLA	CHA-CBD-CGD-O1D
12	K	201	CLA	CHA-CBD-CGD-O2D
12	K	201	CLA	CBD-CGD-O2D-CED
12	K	201	CLA	O1D-CGD-O2D-CED
12	K	203	CLA	CHA-CBD-CGD-O1D
12	K	203	CLA	CHA-CBD-CGD-O2D
12	K	203	CLA	CAD-CBD-CGD-O1D
12	K	204	CLA	C2B-C3B-CAB-CBB
12	K	204	CLA	C4B-C3B-CAB-CBB
12	K	204	CLA	CHA-CBD-CGD-O1D
12	K	204	CLA	CHA-CBD-CGD-O2D
12	K	204	CLA	CAD-CBD-CGD-O1D
12	L	201	CLA	C1A-C2A-CAA-CBA
12	L	201	CLA	C3A-C2A-CAA-CBA
12	L	203	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
12	L	203	CLA	C4B-C3B-CAB-CBB
14	A	842	LHG	C4-O6-P-O5
14	A	843	LHG	C4-O6-P-O4
15	A	844	BCR	C7-C8-C9-C10
15	A	844	BCR	C7-C8-C9-C34
15	B	804	BCR	C7-C8-C9-C10
15	B	804	BCR	C7-C8-C9-C34
15	B	804	BCR	C21-C22-C23-C24
15	B	804	BCR	C37-C22-C23-C24
15	B	842	BCR	C7-C8-C9-C10
15	B	842	BCR	C7-C8-C9-C34
15	B	843	BCR	C7-C8-C9-C10
15	B	843	BCR	C7-C8-C9-C34
15	I	201	BCR	C21-C22-C23-C24
15	M	101	BCR	C7-C8-C9-C10
15	M	101	BCR	C7-C8-C9-C34
12	B	806	CLA	O1D-CGD-O2D-CED
12	B	810	CLA	O1D-CGD-O2D-CED
12	K	204	CLA	O1D-CGD-O2D-CED
12	A	813	CLA	O1D-CGD-O2D-CED
12	B	807	CLA	O1D-CGD-O2D-CED
12	B	834	CLA	O1D-CGD-O2D-CED
12	F	301	CLA	O1D-CGD-O2D-CED
12	A	802	CLA	CBD-CGD-O2D-CED
12	A	803	CLA	CBD-CGD-O2D-CED
12	A	813	CLA	CBD-CGD-O2D-CED
12	A	817	CLA	CBD-CGD-O2D-CED
12	A	827	CLA	CBD-CGD-O2D-CED
12	A	829	CLA	CBD-CGD-O2D-CED
12	B	801	CLA	CBD-CGD-O2D-CED
12	B	802	CLA	CBD-CGD-O2D-CED
12	B	805	CLA	CBD-CGD-O2D-CED
12	B	806	CLA	CBD-CGD-O2D-CED
12	B	810	CLA	CBD-CGD-O2D-CED
12	B	813	CLA	CBD-CGD-O2D-CED
12	B	818	CLA	CBD-CGD-O2D-CED
12	B	819	CLA	CBD-CGD-O2D-CED
12	B	820	CLA	CBD-CGD-O2D-CED
12	B	823	CLA	CBD-CGD-O2D-CED
12	B	828	CLA	CBD-CGD-O2D-CED
12	F	301	CLA	CBD-CGD-O2D-CED
12	K	204	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	A	820	CLA	O1A-CGA-O2A-C1
12	B	801	CLA	O1A-CGA-O2A-C1
12	B	809	CLA	O1A-CGA-O2A-C1
12	B	819	CLA	O1A-CGA-O2A-C1
12	B	838	CLA	O1A-CGA-O2A-C1
12	A	819	CLA	O1A-CGA-O2A-C1
12	A	822	CLA	O1D-CGD-O2D-CED
12	B	805	CLA	O1D-CGD-O2D-CED
12	B	819	CLA	O1D-CGD-O2D-CED
12	A	814	CLA	O1D-CGD-O2D-CED
12	A	832	CLA	O1D-CGD-O2D-CED
12	B	801	CLA	CBA-CGA-O2A-C1
12	B	819	CLA	CBA-CGA-O2A-C1
12	B	838	CLA	CBA-CGA-O2A-C1
12	A	806	CLA	CBD-CGD-O2D-CED
12	A	811	CLA	CBD-CGD-O2D-CED
12	A	823	CLA	CBD-CGD-O2D-CED
12	A	831	CLA	CBD-CGD-O2D-CED
12	A	834	CLA	CBD-CGD-O2D-CED
12	A	839	CLA	CBD-CGD-O2D-CED
12	B	829	CLA	CBD-CGD-O2D-CED
12	B	831	CLA	CBD-CGD-O2D-CED
12	L	201	CLA	CBD-CGD-O2D-CED
12	A	803	CLA	O1A-CGA-O2A-C1
12	A	805	CLA	O1A-CGA-O2A-C1
12	B	810	CLA	O1A-CGA-O2A-C1
12	B	811	CLA	O1A-CGA-O2A-C1
12	B	823	CLA	O1A-CGA-O2A-C1
12	B	832	CLA	O1A-CGA-O2A-C1
12	B	814	CLA	O1D-CGD-O2D-CED
12	B	832	CLA	O1D-CGD-O2D-CED
12	B	839	CLA	O1D-CGD-O2D-CED
12	J	102	CLA	O1D-CGD-O2D-CED
12	A	820	CLA	CBD-CGD-O2D-CED
12	A	825	CLA	CBD-CGD-O2D-CED
12	A	802	CLA	O1D-CGD-O2D-CED
12	A	828	CLA	O1A-CGA-O2A-C1
12	A	802	CLA	C3-C5-C6-C7
12	A	817	CLA	C3-C5-C6-C7
12	A	822	CLA	C3-C5-C6-C7
12	B	801	CLA	C3-C5-C6-C7
12	B	803	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
12	B	813	CLA	C3-C5-C6-C7
12	B	826	CLA	C3-C5-C6-C7
12	L	201	CLA	C3-C5-C6-C7
13	B	840	PQN	C13-C15-C16-C17
12	A	805	CLA	CBA-CGA-O2A-C1
12	A	820	CLA	CBA-CGA-O2A-C1
12	B	809	CLA	CBA-CGA-O2A-C1
12	B	810	CLA	CBA-CGA-O2A-C1
12	B	811	CLA	CBA-CGA-O2A-C1
12	B	823	CLA	CBA-CGA-O2A-C1
12	B	832	CLA	CBA-CGA-O2A-C1
12	A	826	CLA	CBD-CGD-O2D-CED
12	B	802	CLA	C2A-CAA-CBA-CGA
12	B	810	CLA	C2A-CAA-CBA-CGA
12	B	815	CLA	C2A-CAA-CBA-CGA
12	B	826	CLA	C2A-CAA-CBA-CGA
12	B	827	CLA	C2A-CAA-CBA-CGA
12	A	827	CLA	O1A-CGA-O2A-C1
12	A	803	CLA	CBA-CGA-O2A-C1
12	A	810	CLA	CBA-CGA-O2A-C1
12	A	827	CLA	CBA-CGA-O2A-C1
12	A	828	CLA	CBA-CGA-O2A-C1
12	A	836	CLA	CBA-CGA-O2A-C1
12	B	801	CLA	O1D-CGD-O2D-CED
12	A	809	CLA	CBD-CGD-O2D-CED
12	A	819	CLA	CBD-CGD-O2D-CED
12	A	817	CLA	O1D-CGD-O2D-CED
12	A	827	CLA	O1D-CGD-O2D-CED
12	B	818	CLA	O1D-CGD-O2D-CED
12	A	832	CLA	O1A-CGA-O2A-C1
12	B	806	CLA	O1A-CGA-O2A-C1
12	B	820	CLA	O1D-CGD-O2D-CED
12	A	833	CLA	C3-C5-C6-C7
12	A	832	CLA	CBA-CGA-O2A-C1
12	B	836	CLA	CBA-CGA-O2A-C1
12	L	201	CLA	CBA-CGA-O2A-C1
12	A	822	CLA	O1A-CGA-O2A-C1
12	B	836	CLA	O1A-CGA-O2A-C1
12	B	828	CLA	O1D-CGD-O2D-CED
12	L	203	CLA	CBD-CGD-O2D-CED
12	A	818	CLA	CBD-CGD-O2D-CED
12	A	822	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	B	806	CLA	CBA-CGA-O2A-C1
12	A	803	CLA	O1D-CGD-O2D-CED
12	B	823	CLA	O1D-CGD-O2D-CED
12	A	810	CLA	O1A-CGA-O2A-C1
12	A	836	CLA	O1A-CGA-O2A-C1
12	L	201	CLA	O1A-CGA-O2A-C1
12	B	819	CLA	C3-C5-C6-C7
12	A	812	CLA	C2A-CAA-CBA-CGA
12	A	827	CLA	C2A-CAA-CBA-CGA
12	B	805	CLA	C2A-CAA-CBA-CGA
12	B	802	CLA	O1D-CGD-O2D-CED
12	B	813	CLA	O1D-CGD-O2D-CED
12	A	818	CLA	CBA-CGA-O2A-C1
12	A	835	CLA	CBA-CGA-O2A-C1
12	B	821	CLA	CBA-CGA-O2A-C1
12	A	829	CLA	O1D-CGD-O2D-CED
12	A	818	CLA	O1A-CGA-O2A-C1
12	B	821	CLA	O1A-CGA-O2A-C1
12	A	828	CLA	C3-C5-C6-C7
12	A	811	CLA	O1D-CGD-O2D-CED
12	B	824	CLA	CBA-CGA-O2A-C1
12	B	827	CLA	CBA-CGA-O2A-C1
12	B	828	CLA	CBA-CGA-O2A-C1
12	A	806	CLA	O1D-CGD-O2D-CED
12	L	201	CLA	O1D-CGD-O2D-CED
12	A	812	CLA	C13-C15-C16-C17
12	B	824	CLA	O1A-CGA-O2A-C1
12	B	826	CLA	C11-C10-C8-C9
12	B	831	CLA	O1D-CGD-O2D-CED
12	A	820	CLA	C2A-CAA-CBA-CGA
15	B	804	BCR	C11-C12-C13-C35
15	B	804	BCR	C36-C18-C19-C20
15	I	201	BCR	C37-C22-C23-C24
15	J	101	BCR	C7-C8-C9-C34
15	K	202	BCR	C7-C8-C9-C34
15	L	204	BCR	C7-C8-C9-C34
15	B	804	BCR	C11-C12-C13-C14
15	J	101	BCR	C7-C8-C9-C10
15	K	202	BCR	C7-C8-C9-C10
15	L	204	BCR	C7-C8-C9-C10
14	A	842	LHG	C23-C24-C25-C26
12	B	827	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	A	816	CLA	C3-C5-C6-C7
12	A	820	CLA	C3-C5-C6-C7
12	A	823	CLA	C3-C5-C6-C7
12	B	832	CLA	C3-C5-C6-C7
12	A	824	CLA	C15-C16-C17-C18
12	B	826	CLA	C10-C11-C12-C13
12	B	827	CLA	C8-C10-C11-C12
12	A	839	CLA	O1D-CGD-O2D-CED
12	A	823	CLA	O1D-CGD-O2D-CED
12	B	829	CLA	O1D-CGD-O2D-CED
12	B	828	CLA	C5-C6-C7-C8
12	A	831	CLA	O1D-CGD-O2D-CED
12	A	822	CLA	C5-C6-C7-C8
12	B	807	CLA	C13-C15-C16-C17
12	B	802	CLA	C13-C15-C16-C17
12	A	823	CLA	C12-C13-C15-C16
12	B	826	CLA	C11-C10-C8-C7
12	B	812	CLA	C3-C5-C6-C7
12	A	820	CLA	O1D-CGD-O2D-CED
12	A	825	CLA	O1D-CGD-O2D-CED
12	A	834	CLA	O1D-CGD-O2D-CED
12	B	806	CLA	C8-C10-C11-C12
13	A	840	PQN	C23-C25-C26-C27
12	B	836	CLA	C3-C5-C6-C7
12	A	837	CLA	C8-C10-C11-C12
12	A	835	CLA	O1A-CGA-O2A-C1
12	B	828	CLA	O1A-CGA-O2A-C1
12	A	805	CLA	C15-C16-C17-C18
12	A	826	CLA	O1D-CGD-O2D-CED
12	A	832	CLA	C13-C15-C16-C17
12	A	822	CLA	C4-C3-C5-C6
12	L	201	CLA	C4-C3-C5-C6
13	A	840	PQN	C25-C26-C27-C28
12	B	812	CLA	C2A-CAA-CBA-CGA
12	B	821	CLA	C2A-CAA-CBA-CGA
12	B	806	CLA	C3-C5-C6-C7
12	A	838	CLA	CBA-CGA-O2A-C1
12	A	836	CLA	C5-C6-C7-C8
12	A	836	CLA	C6-C7-C8-C10
17	A	849	LMU	C3-C4-C5-C6
12	A	819	CLA	O1D-CGD-O2D-CED
12	A	809	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	A	843	LHG	C25-C26-C27-C28
17	A	849	LMU	C2'-C1'-O1'-C1
12	B	803	CLA	C11-C10-C8-C7
12	B	812	CLA	C16-C17-C18-C19
12	A	802	CLA	C4-C3-C5-C6
12	A	802	CLA	C2-C3-C5-C6
12	A	822	CLA	C2-C3-C5-C6
12	L	201	CLA	C2-C3-C5-C6
12	A	818	CLA	C6-C7-C8-C9
17	A	849	LMU	C4-C5-C6-C7
12	A	807	CLA	C4B-C3B-CAB-CBB
12	A	808	CLA	C4B-C3B-CAB-CBB
12	A	810	CLA	C4B-C3B-CAB-CBB
12	A	815	CLA	C4B-C3B-CAB-CBB
12	A	816	CLA	C4B-C3B-CAB-CBB
12	A	823	CLA	C4B-C3B-CAB-CBB
12	A	826	CLA	C4B-C3B-CAB-CBB
12	A	830	CLA	C4B-C3B-CAB-CBB
12	B	801	CLA	C4B-C3B-CAB-CBB
12	B	811	CLA	C4B-C3B-CAB-CBB
12	B	816	CLA	C4B-C3B-CAB-CBB
12	B	819	CLA	C4B-C3B-CAB-CBB
12	B	822	CLA	C4B-C3B-CAB-CBB
12	B	825	CLA	C4B-C3B-CAB-CBB
12	B	829	CLA	C4B-C3B-CAB-CBB
12	B	830	CLA	C4B-C3B-CAB-CBB
12	B	832	CLA	C4B-C3B-CAB-CBB
12	B	836	CLA	C4B-C3B-CAB-CBB
12	B	837	CLA	C4B-C3B-CAB-CBB
12	J	102	CLA	C4B-C3B-CAB-CBB
12	K	203	CLA	C4B-C3B-CAB-CBB
12	A	832	CLA	C16-C17-C18-C20
12	A	836	CLA	C6-C7-C8-C9
12	B	826	CLA	C11-C12-C13-C15
12	B	823	CLA	C5-C6-C7-C8
12	A	805	CLA	C3A-C2A-CAA-CBA
12	A	808	CLA	C3A-C2A-CAA-CBA
12	A	822	CLA	C3A-C2A-CAA-CBA
12	A	824	CLA	C3A-C2A-CAA-CBA
12	A	831	CLA	C3A-C2A-CAA-CBA
12	A	832	CLA	C3A-C2A-CAA-CBA
12	A	837	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	B	806	CLA	C3A-C2A-CAA-CBA
12	B	807	CLA	C3A-C2A-CAA-CBA
12	B	813	CLA	C3A-C2A-CAA-CBA
12	B	814	CLA	C3A-C2A-CAA-CBA
12	B	839	CLA	C3A-C2A-CAA-CBA
12	K	203	CLA	C3A-C2A-CAA-CBA
12	B	811	CLA	C3-C5-C6-C7
12	A	801	CLA	C4-C3-C5-C6
12	B	809	CLA	C4-C3-C5-C6
12	B	811	CLA	C4-C3-C5-C6
12	B	826	CLA	C4-C3-C5-C6
12	A	820	CLA	C2-C3-C5-C6
12	A	832	CLA	C2-C3-C5-C6
12	A	838	CLA	C2-C3-C5-C6
12	B	809	CLA	C2-C3-C5-C6
12	B	826	CLA	C2-C3-C5-C6
12	B	823	CLA	C2A-CAA-CBA-CGA
12	A	838	CLA	O1A-CGA-O2A-C1
12	B	812	CLA	C16-C17-C18-C20
12	B	826	CLA	C11-C12-C13-C14
12	A	807	CLA	C2B-C3B-CAB-CBB
12	A	808	CLA	C2B-C3B-CAB-CBB
12	A	810	CLA	C2B-C3B-CAB-CBB
12	A	815	CLA	C2B-C3B-CAB-CBB
12	A	821	CLA	C2B-C3B-CAB-CBB
12	A	823	CLA	C2B-C3B-CAB-CBB
12	A	826	CLA	C2B-C3B-CAB-CBB
12	A	830	CLA	C2B-C3B-CAB-CBB
12	B	801	CLA	C2B-C3B-CAB-CBB
12	B	811	CLA	C2B-C3B-CAB-CBB
12	B	816	CLA	C2B-C3B-CAB-CBB
12	B	819	CLA	C2B-C3B-CAB-CBB
12	B	829	CLA	C2B-C3B-CAB-CBB
12	B	832	CLA	C2B-C3B-CAB-CBB
12	B	836	CLA	C2B-C3B-CAB-CBB
12	B	837	CLA	C2B-C3B-CAB-CBB
12	B	838	CLA	C2B-C3B-CAB-CBB
12	J	102	CLA	C2B-C3B-CAB-CBB
12	K	203	CLA	C2B-C3B-CAB-CBB
12	A	823	CLA	C8-C10-C11-C12
18	B	844	DGD	C4E-C5E-C6E-O5E
12	B	812	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
12	A	829	CLA	C16-C17-C18-C19
15	A	846	BCR	C1-C6-C7-C8
15	A	846	BCR	C5-C6-C7-C8
15	A	847	BCR	C1-C6-C7-C8
15	A	847	BCR	C5-C6-C7-C8
15	B	804	BCR	C1-C6-C7-C8
15	B	804	BCR	C5-C6-C7-C8
15	J	101	BCR	C5-C6-C7-C8
15	K	202	BCR	C5-C6-C7-C8
15	M	101	BCR	C23-C24-C25-C26
15	M	101	BCR	C23-C24-C25-C30
12	A	823	CLA	C5-C6-C7-C8
12	A	832	CLA	C4-C3-C5-C6
12	A	801	CLA	C2-C3-C5-C6
12	A	810	CLA	C11-C10-C8-C7
12	A	818	CLA	C6-C7-C8-C10
12	B	811	CLA	C2-C3-C5-C6
12	B	812	CLA	C11-C10-C8-C7
12	B	820	CLA	C6-C7-C8-C10
12	A	805	CLA	C2A-CAA-CBA-CGA
12	A	838	CLA	C2A-CAA-CBA-CGA
12	B	822	CLA	C2A-CAA-CBA-CGA
12	B	836	CLA	C2A-CAA-CBA-CGA
12	A	818	CLA	O1D-CGD-O2D-CED
17	A	849	LMU	C1-C2-C3-C4
12	A	816	CLA	CBA-CGA-O2A-C1
12	B	803	CLA	CBD-CGD-O2D-CED
12	B	837	CLA	CBD-CGD-O2D-CED
12	L	203	CLA	O1D-CGD-O2D-CED
12	A	838	CLA	CBD-CGD-O2D-CED
12	B	807	CLA	C10-C11-C12-C13
12	B	812	CLA	C15-C16-C17-C18
12	A	820	CLA	C4-C3-C5-C6
12	A	829	CLA	C4-C3-C5-C6
12	A	838	CLA	C4-C3-C5-C6
12	A	810	CLA	C11-C10-C8-C9
12	B	812	CLA	C11-C10-C8-C9
12	A	817	CLA	C2A-CAA-CBA-CGA
12	A	804	CLA	C8-C10-C11-C12
12	A	803	CLA	C1A-C2A-CAA-CBA
12	A	805	CLA	C1A-C2A-CAA-CBA
12	A	806	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	A	807	CLA	C1A-C2A-CAA-CBA
12	A	808	CLA	C1A-C2A-CAA-CBA
12	A	810	CLA	C1A-C2A-CAA-CBA
12	A	815	CLA	C1A-C2A-CAA-CBA
12	A	817	CLA	C1A-C2A-CAA-CBA
12	A	827	CLA	C1A-C2A-CAA-CBA
12	A	829	CLA	C1A-C2A-CAA-CBA
12	A	831	CLA	C1A-C2A-CAA-CBA
12	A	832	CLA	C1A-C2A-CAA-CBA
12	B	806	CLA	C1A-C2A-CAA-CBA
12	B	814	CLA	C1A-C2A-CAA-CBA
12	B	818	CLA	C1A-C2A-CAA-CBA
12	B	819	CLA	C1A-C2A-CAA-CBA
12	B	820	CLA	C1A-C2A-CAA-CBA
12	B	827	CLA	C1A-C2A-CAA-CBA
12	B	828	CLA	C1A-C2A-CAA-CBA
12	B	830	CLA	C1A-C2A-CAA-CBA
12	B	832	CLA	C1A-C2A-CAA-CBA
12	B	837	CLA	C1A-C2A-CAA-CBA
12	B	839	CLA	C1A-C2A-CAA-CBA
12	K	203	CLA	C1A-C2A-CAA-CBA
12	A	829	CLA	C16-C17-C18-C20
12	A	832	CLA	C16-C17-C18-C19
12	B	820	CLA	C6-C7-C8-C9
12	B	816	CLA	CBD-CGD-O2D-CED
12	A	838	CLA	C3-C5-C6-C7
12	B	833	CLA	CBA-CGA-O2A-C1
14	A	843	LHG	C8-C7-O7-C5
12	A	823	CLA	C13-C15-C16-C17
12	A	838	CLA	C13-C15-C16-C17
18	B	844	DGD	C2B-C1B-O2G-C2G
12	A	823	CLA	C4-C3-C5-C6
12	A	837	CLA	C4-C3-C5-C6
12	A	823	CLA	C2-C3-C5-C6
12	A	833	CLA	CBA-CGA-O2A-C1
18	B	844	DGD	O6E-C5E-C6E-O5E
12	A	808	CLA	C2A-CAA-CBA-CGA
12	A	815	CLA	C2A-CAA-CBA-CGA
12	A	816	CLA	O1A-CGA-O2A-C1
12	B	802	CLA	C15-C16-C17-C18
12	A	808	CLA	CBA-CGA-O2A-C1
12	B	830	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
12	A	832	CLA	C10-C11-C12-C13
12	A	824	CLA	C4-C3-C5-C6
12	A	804	CLA	C11-C10-C8-C7
12	A	805	CLA	C12-C13-C15-C16
12	A	818	CLA	C11-C10-C8-C7
12	A	824	CLA	C2-C3-C5-C6
12	A	832	CLA	C11-C10-C8-C7
12	B	806	CLA	C6-C7-C8-C10
12	B	806	CLA	C11-C10-C8-C7
12	B	810	CLA	C12-C13-C15-C16
12	B	825	CLA	C12-C13-C15-C16
12	B	827	CLA	C11-C12-C13-C15
12	A	805	CLA	C14-C13-C15-C16
12	A	818	CLA	C11-C10-C8-C9
12	A	820	CLA	C6-C7-C8-C9
12	A	822	CLA	C11-C10-C8-C9
12	A	838	CLA	C14-C13-C15-C16
12	B	801	CLA	C6-C7-C8-C9
12	B	806	CLA	C11-C10-C8-C9
12	B	823	CLA	C6-C7-C8-C9
12	B	825	CLA	C14-C13-C15-C16
12	B	826	CLA	C6-C7-C8-C9
12	B	827	CLA	C11-C12-C13-C14
12	A	826	CLA	C3-C5-C6-C7
12	B	807	CLA	C3-C5-C6-C7
12	B	821	CLA	C5-C6-C7-C8
12	A	833	CLA	O1A-CGA-O2A-C1
12	A	809	CLA	C4B-C3B-CAB-CBB
12	A	819	CLA	C4B-C3B-CAB-CBB
12	A	820	CLA	C4B-C3B-CAB-CBB
12	A	825	CLA	C4B-C3B-CAB-CBB
12	B	803	CLA	C4B-C3B-CAB-CBB
12	B	820	CLA	C4B-C3B-CAB-CBB
12	B	828	CLA	C4B-C3B-CAB-CBB
12	B	831	CLA	C4B-C3B-CAB-CBB
12	B	834	CLA	C4B-C3B-CAB-CBB
12	F	301	CLA	C4B-C3B-CAB-CBB
12	L	201	CLA	C4B-C3B-CAB-CBB
12	B	826	CLA	C8-C10-C11-C12
12	B	806	CLA	C4-C3-C5-C6
12	A	837	CLA	C2-C3-C5-C6
12	B	806	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
12	B	825	CLA	C2A-CAA-CBA-CGA
12	A	804	CLA	CBA-CGA-O2A-C1
12	B	805	CLA	CBA-CGA-O2A-C1
12	B	834	CLA	C3A-C2A-CAA-CBA
12	B	803	CLA	C6-C7-C8-C10
12	B	807	CLA	C5-C6-C7-C8
12	A	824	CLA	C3-C5-C6-C7
12	A	828	CLA	C15-C16-C17-C18
12	A	809	CLA	C2B-C3B-CAB-CBB
12	A	816	CLA	C2B-C3B-CAB-CBB
12	A	820	CLA	C2B-C3B-CAB-CBB
12	A	825	CLA	C2B-C3B-CAB-CBB
12	B	803	CLA	C2B-C3B-CAB-CBB
12	B	820	CLA	C2B-C3B-CAB-CBB
12	B	822	CLA	C2B-C3B-CAB-CBB
12	B	825	CLA	C2B-C3B-CAB-CBB
12	B	828	CLA	C2B-C3B-CAB-CBB
12	B	830	CLA	C2B-C3B-CAB-CBB
12	B	834	CLA	C2B-C3B-CAB-CBB
12	L	201	CLA	C2B-C3B-CAB-CBB
12	A	808	CLA	O1A-CGA-O2A-C1
17	A	849	LMU	O5'-C1'-O1'-C1
12	B	801	CLA	C5-C6-C7-C8
14	A	843	LHG	O9-C7-O7-C5
12	A	810	CLA	C11-C12-C13-C14
12	A	801	CLA	C6-C7-C8-C9
12	A	804	CLA	C11-C10-C8-C9
12	A	832	CLA	C11-C10-C8-C9
12	B	806	CLA	C6-C7-C8-C9
12	B	813	CLA	C6-C7-C8-C9
13	A	840	PQN	C16-C17-C18-C19
12	L	201	CLA	C11-C12-C13-C15
12	B	823	CLA	C3-C5-C6-C7
15	J	101	BCR	C1-C6-C7-C8
15	J	101	BCR	C23-C24-C25-C26
12	A	801	CLA	CAA-CBA-CGA-O2A
12	B	816	CLA	C1A-C2A-CAA-CBA
15	B	804	BCR	C17-C18-C19-C20
12	A	801	CLA	C8-C10-C11-C12
18	B	844	DGD	O1B-C1B-O2G-C2G
12	A	801	CLA	C6-C7-C8-C10
12	A	820	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
12	A	822	CLA	C11-C10-C8-C7
12	A	838	CLA	C12-C13-C15-C16
12	B	801	CLA	C6-C7-C8-C10
12	B	803	CLA	C12-C13-C15-C16
12	B	813	CLA	C6-C7-C8-C10
12	B	813	CLA	C11-C10-C8-C7
12	B	823	CLA	C6-C7-C8-C10
12	B	826	CLA	C6-C7-C8-C10
12	B	839	CLA	C12-C13-C15-C16
13	A	840	PQN	C16-C17-C18-C20
12	B	809	CLA	C13-C15-C16-C17
12	B	806	CLA	C2A-CAA-CBA-CGA
18	B	844	DGD	C3A-C4A-C5A-C6A
12	A	804	CLA	C10-C11-C12-C13
12	A	811	CLA	CAD-CBD-CGD-O2D
12	A	815	CLA	CAD-CBD-CGD-O2D
12	A	816	CLA	CAD-CBD-CGD-O2D
12	A	817	CLA	CAD-CBD-CGD-O2D
12	A	821	CLA	CAD-CBD-CGD-O2D
12	A	824	CLA	CAD-CBD-CGD-O2D
12	A	833	CLA	CAD-CBD-CGD-O2D
12	B	801	CLA	CAD-CBD-CGD-O2D
12	B	806	CLA	CAD-CBD-CGD-O2D
12	B	820	CLA	CAD-CBD-CGD-O2D
12	B	822	CLA	CAD-CBD-CGD-O2D
12	B	828	CLA	CAD-CBD-CGD-O2D
12	B	838	CLA	CAD-CBD-CGD-O2D
12	B	837	CLA	O1D-CGD-O2D-CED
18	B	844	DGD	O6D-C1D-O3G-C3G
12	B	815	CLA	CAA-CBA-CGA-O2A
12	A	805	CLA	O2A-C1-C2-C3
12	A	812	CLA	O2A-C1-C2-C3
12	A	804	CLA	CHA-CBD-CGD-O1D
12	A	813	CLA	CHA-CBD-CGD-O1D
12	A	813	CLA	CHA-CBD-CGD-O2D
12	A	818	CLA	CHA-CBD-CGD-O1D
12	A	818	CLA	CHA-CBD-CGD-O2D
12	B	812	CLA	CHA-CBD-CGD-O1D
12	B	812	CLA	CHA-CBD-CGD-O2D
12	B	816	CLA	CHA-CBD-CGD-O1D
12	B	816	CLA	CHA-CBD-CGD-O2D
12	L	201	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
12	L	201	CLA	CHA-CBD-CGD-O2D
12	B	805	CLA	O1A-CGA-O2A-C1
12	B	803	CLA	O1D-CGD-O2D-CED
12	A	804	CLA	O1A-CGA-O2A-C1
12	A	838	CLA	O1D-CGD-O2D-CED
12	A	818	CLA	C11-C12-C13-C14
12	A	833	CLA	C11-C10-C8-C9
12	B	803	CLA	C14-C13-C15-C16
12	B	839	CLA	C14-C13-C15-C16
12	B	823	CLA	C11-C10-C8-C9
12	B	807	CLA	C1A-C2A-CAA-CBA
14	A	843	LHG	C4-O6-P-O3
12	A	829	CLA	C2-C3-C5-C6
14	A	843	LHG	C4-O6-P-O5
12	A	812	CLA	CBA-CGA-O2A-C1
12	A	804	CLA	CAD-CBD-CGD-O1D
12	A	813	CLA	CAD-CBD-CGD-O1D
12	A	814	CLA	CAD-CBD-CGD-O1D
12	A	819	CLA	CAD-CBD-CGD-O1D
12	A	837	CLA	CAD-CBD-CGD-O1D
12	J	102	CLA	CAD-CBD-CGD-O1D
12	B	816	CLA	O1D-CGD-O2D-CED
12	B	820	CLA	CBA-CGA-O2A-C1
12	K	203	CLA	C6-C7-C8-C9
12	A	818	CLA	C11-C12-C13-C15
12	A	832	CLA	C12-C13-C15-C16
12	A	841	CLA	CAD-CBD-CGD-O2D
12	B	807	CLA	C11-C12-C13-C15
12	B	809	CLA	C11-C10-C8-C7
12	B	827	CLA	C3A-C2A-CAA-CBA
12	L	201	CLA	C11-C12-C13-C14
12	A	841	CLA	CAD-CBD-CGD-O1D
12	A	828	CLA	C10-C11-C12-C13
12	B	815	CLA	C3-C5-C6-C7
12	B	822	CLA	C4-C3-C5-C6
12	B	813	CLA	C11-C10-C8-C9
12	A	812	CLA	O1A-CGA-O2A-C1
12	B	833	CLA	O1A-CGA-O2A-C1
12	A	812	CLA	C2B-C3B-CAB-CBB
12	A	819	CLA	C2B-C3B-CAB-CBB
12	A	828	CLA	C2B-C3B-CAB-CBB
12	A	833	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
12	A	837	CLA	C2B-C3B-CAB-CBB
12	B	831	CLA	C2B-C3B-CAB-CBB
12	B	833	CLA	C2B-C3B-CAB-CBB
12	F	301	CLA	C2B-C3B-CAB-CBB
12	B	825	CLA	C10-C11-C12-C13
12	B	801	CLA	C10-C11-C12-C13
12	A	816	CLA	C2A-CAA-CBA-CGA
12	A	836	CLA	C2A-CAA-CBA-CGA
12	B	805	CLA	C2-C1-O2A-CGA
12	B	832	CLA	C2-C1-O2A-CGA
12	A	817	CLA	CAA-CBA-CGA-O2A
12	A	824	CLA	CBA-CGA-O2A-C1
15	J	101	BCR	C23-C24-C25-C30
12	B	826	CLA	C5-C6-C7-C8
12	B	811	CLA	C11-C12-C13-C14
14	A	842	LHG	C3-O3-P-O6
14	A	842	LHG	C4-O6-P-O3
14	A	843	LHG	C3-O3-P-O6
12	A	833	CLA	C11-C10-C8-C7
12	B	822	CLA	C2-C3-C5-C6
13	A	840	PQN	C21-C22-C23-C25
12	B	810	CLA	C3-C5-C6-C7
12	A	823	CLA	C14-C13-C15-C16
12	B	810	CLA	C14-C13-C15-C16
12	A	823	CLA	C10-C11-C12-C13
15	B	804	BCR	C9-C10-C11-C12
15	L	204	BCR	C37-C22-C23-C24
12	A	822	CLA	C8-C10-C11-C12
12	B	838	CLA	C5-C6-C7-C8
17	A	849	LMU	O5'-C5'-C6'-O6'
12	B	811	CLA	CBD-CGD-O2D-CED
14	A	842	LHG	C1-C2-C3-O3
12	A	829	CLA	C10-C11-C12-C13
12	K	203	CLA	C6-C7-C8-C10
12	A	817	CLA	CBA-CGA-O2A-C1
14	A	843	LHG	C23-C24-C25-C26
12	A	806	CLA	C4B-C3B-CAB-CBB
12	A	822	CLA	C4B-C3B-CAB-CBB
12	A	828	CLA	C4B-C3B-CAB-CBB
12	A	833	CLA	C4B-C3B-CAB-CBB
12	A	837	CLA	C4B-C3B-CAB-CBB
12	B	833	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
12	A	817	CLA	O1A-CGA-O2A-C1
14	A	842	LHG	C31-C32-C33-C34
12	A	804	CLA	CBD-CGD-O2D-CED
12	B	834	CLA	C2A-CAA-CBA-CGA
12	A	819	CLA	C3A-C2A-CAA-CBA
12	A	828	CLA	C3A-C2A-CAA-CBA
12	B	815	CLA	C3A-C2A-CAA-CBA
12	B	838	CLA	C6-C7-C8-C10
12	B	839	CLA	CAA-CBA-CGA-O2A
12	B	836	CLA	C8-C10-C11-C12
12	A	817	CLA	C6-C7-C8-C9
12	A	832	CLA	C14-C13-C15-C16
12	B	839	CLA	C11-C12-C13-C14
13	A	840	PQN	C21-C22-C23-C24
12	B	811	CLA	O1D-CGD-O2D-CED
12	B	817	CLA	C2A-CAA-CBA-CGA
15	B	841	BCR	C11-C10-C9-C34
15	B	841	BCR	C20-C21-C22-C37
15	L	202	BCR	C20-C21-C22-C37
12	A	826	CLA	O1A-CGA-O2A-C1
12	A	819	CLA	C1A-C2A-CAA-CBA
12	A	824	CLA	C1A-C2A-CAA-CBA
12	B	803	CLA	C5-C6-C7-C8
12	B	833	CLA	CAA-CBA-CGA-O2A
12	B	803	CLA	C8-C10-C11-C12
12	A	804	CLA	O1D-CGD-O2D-CED
12	B	812	CLA	C13-C15-C16-C17
12	B	831	CLA	CAA-CBA-CGA-O1A
12	A	826	CLA	CBA-CGA-O2A-C1
12	B	820	CLA	C5-C6-C7-C8
12	A	824	CLA	CAA-CBA-CGA-O2A
12	B	820	CLA	CAA-CBA-CGA-O2A
12	B	827	CLA	C2-C3-C5-C6
12	A	806	CLA	C2B-C3B-CAB-CBB
12	A	811	CLA	C2B-C3B-CAB-CBB
12	A	822	CLA	C2B-C3B-CAB-CBB
12	B	813	CLA	C2B-C3B-CAB-CBB
15	B	841	BCR	C11-C10-C9-C8
15	B	841	BCR	C20-C21-C22-C23
15	L	202	BCR	C20-C21-C22-C23
17	A	849	LMU	C9-C10-C11-C12
15	I	201	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
12	A	815	CLA	CAA-CBA-CGA-O2A
15	K	202	BCR	C1-C6-C7-C8
12	B	831	CLA	CAA-CBA-CGA-O2A
12	A	837	CLA	C5-C6-C7-C8
17	A	849	LMU	O1'-C1-C2-C3
12	B	802	CLA	C4-C3-C5-C6
12	B	827	CLA	C4-C3-C5-C6
12	B	815	CLA	O1A-CGA-O2A-C1
12	A	829	CLA	C2A-CAA-CBA-CGA
12	A	811	CLA	C4B-C3B-CAB-CBB
12	A	812	CLA	C4B-C3B-CAB-CBB
12	A	841	CLA	C4B-C3B-CAB-CBB
12	B	813	CLA	C4B-C3B-CAB-CBB
12	B	835	CLA	C4B-C3B-CAB-CBB
12	B	839	CLA	C11-C12-C13-C15
12	B	815	CLA	CBA-CGA-O2A-C1
12	A	801	CLA	O1A-CGA-O2A-C1
12	A	801	CLA	CBA-CGA-O2A-C1
12	A	825	CLA	CBA-CGA-O2A-C1
12	A	816	CLA	C11-C12-C13-C15
12	A	807	CLA	CAA-CBA-CGA-O2A
12	B	807	CLA	C11-C12-C13-C14
12	B	809	CLA	C11-C10-C8-C9
12	B	810	CLA	C11-C10-C8-C9
12	B	821	CLA	C3A-C2A-CAA-CBA
14	A	842	LHG	O2-C2-C3-O3
12	A	825	CLA	O1A-CGA-O2A-C1
12	A	806	CLA	CAD-CBD-CGD-O2D
12	A	808	CLA	CAD-CBD-CGD-O2D
12	A	812	CLA	CAD-CBD-CGD-O2D
12	A	820	CLA	CAD-CBD-CGD-O2D
12	A	825	CLA	CAD-CBD-CGD-O2D
12	A	829	CLA	CAD-CBD-CGD-O2D
12	B	810	CLA	CAD-CBD-CGD-O2D
12	B	814	CLA	CAD-CBD-CGD-O2D
12	B	817	CLA	CAD-CBD-CGD-O2D
12	B	824	CLA	CAD-CBD-CGD-O2D
12	B	831	CLA	CAD-CBD-CGD-O2D
12	B	837	CLA	CAD-CBD-CGD-O2D
12	K	203	CLA	CAD-CBD-CGD-O2D
12	K	204	CLA	CAD-CBD-CGD-O2D
12	B	838	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
12	A	803	CLA	CAA-CBA-CGA-O2A
14	A	842	LHG	C24-C25-C26-C27
12	B	807	CLA	C4-C3-C5-C6
12	A	805	CLA	CAA-CBA-CGA-O2A
15	L	204	BCR	C21-C22-C23-C24
14	A	842	LHG	C17-C18-C19-C20
12	A	802	CLA	CHA-CBD-CGD-O2D
12	A	804	CLA	CHA-CBD-CGD-O2D
12	A	807	CLA	CHA-CBD-CGD-O1D
12	A	807	CLA	CHA-CBD-CGD-O2D
12	A	815	CLA	CHA-CBD-CGD-O2D
12	A	824	CLA	CHA-CBD-CGD-O2D
12	A	835	CLA	CHA-CBD-CGD-O1D
12	A	835	CLA	CHA-CBD-CGD-O2D
12	B	802	CLA	CHA-CBD-CGD-O1D
12	B	802	CLA	CHA-CBD-CGD-O2D
12	B	818	CLA	CHA-CBD-CGD-O1D
12	B	823	CLA	CHA-CBD-CGD-O1D
12	B	823	CLA	CHA-CBD-CGD-O2D
12	B	825	CLA	CHA-CBD-CGD-O1D
12	B	825	CLA	CHA-CBD-CGD-O2D
12	B	835	CLA	CHA-CBD-CGD-O1D
12	B	835	CLA	CHA-CBD-CGD-O2D
12	B	819	CLA	C2-C3-C5-C6
12	A	815	CLA	CAA-CBA-CGA-O1A
12	B	812	CLA	CAA-CBA-CGA-O2A
12	K	203	CLA	CAA-CBA-CGA-O2A
12	A	820	CLA	CAA-CBA-CGA-O2A
12	B	825	CLA	C4-C3-C5-C6
12	A	818	CLA	C16-C17-C18-C19
12	B	806	CLA	C16-C17-C18-C20
12	A	841	CLA	C2B-C3B-CAB-CBB
12	B	835	CLA	C2B-C3B-CAB-CBB
12	B	802	CLA	CBA-CGA-O2A-C1
12	A	801	CLA	CAA-CBA-CGA-O1A
12	B	802	CLA	O1A-CGA-O2A-C1
12	A	812	CLA	C8-C10-C11-C12
12	B	836	CLA	C4-C3-C5-C6
12	B	814	CLA	CBA-CGA-O2A-C1
12	A	802	CLA	C1A-C2A-CAA-CBA
12	A	820	CLA	C1A-C2A-CAA-CBA
12	A	825	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	B	803	CLA	C1A-C2A-CAA-CBA
12	B	821	CLA	C1A-C2A-CAA-CBA
12	B	822	CLA	C1A-C2A-CAA-CBA
12	B	823	CLA	C1A-C2A-CAA-CBA
12	A	807	CLA	CAA-CBA-CGA-O1A
12	A	819	CLA	C2C-C3C-CAC-CBC
12	A	829	CLA	C5-C6-C7-C8
12	A	832	CLA	C2A-CAA-CBA-CGA
12	B	824	CLA	CBD-CGD-O2D-CED
12	B	806	CLA	C5-C6-C7-C8
14	A	843	LHG	C2-C3-O3-P
12	A	824	CLA	C4B-C3B-CAB-CBB
14	A	842	LHG	C3-O3-P-O5
14	A	843	LHG	C3-O3-P-O5
12	K	203	CLA	CAA-CBA-CGA-O1A
12	A	803	CLA	CAA-CBA-CGA-O1A
12	A	828	CLA	C2A-CAA-CBA-CGA
12	B	806	CLA	CAA-CBA-CGA-O2A
12	A	805	CLA	CAA-CBA-CGA-O1A
12	A	816	CLA	C4-C3-C5-C6
12	B	802	CLA	CAD-CBD-CGD-O1D
12	A	823	CLA	CAA-CBA-CGA-O2A
14	A	842	LHG	O8-C23-C24-C25
12	B	827	CLA	C11-C10-C8-C9
12	A	822	CLA	CAA-CBA-CGA-O2A
12	B	813	CLA	CAA-CBA-CGA-O2A
12	A	804	CLA	CAA-CBA-CGA-O2A
13	A	840	PQN	C20-C21-C22-C23
12	B	819	CLA	C4-C3-C5-C6
12	A	823	CLA	C11-C10-C8-C7
12	B	803	CLA	C3A-C2A-CAA-CBA
12	B	815	CLA	CHA-CBD-CGD-O1D
12	A	829	CLA	CAA-CBA-CGA-O2A
15	L	202	BCR	C17-C18-C19-C20
12	A	820	CLA	CAA-CBA-CGA-O1A
12	B	813	CLA	CAA-CBA-CGA-O1A
12	B	810	CLA	CAA-CBA-CGA-O2A
12	B	825	CLA	C13-C15-C16-C17
12	A	804	CLA	CAA-CBA-CGA-O1A
12	A	822	CLA	CAA-CBA-CGA-O1A
12	A	823	CLA	CAA-CBA-CGA-O1A
12	B	806	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
12	A	818	CLA	C16-C17-C18-C20
12	A	828	CLA	C8-C10-C11-C12
12	B	827	CLA	C5-C6-C7-C8
14	A	842	LHG	O10-C23-C24-C25
12	B	824	CLA	O1D-CGD-O2D-CED

There are no ring outliers.

79 monomers are involved in 149 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	M	101	BCR	3	0
12	B	807	CLA	1	0
12	B	821	CLA	3	0
12	A	832	CLA	1	0
12	B	819	CLA	1	0
12	A	811	CLA	1	0
12	B	805	CLA	4	0
14	A	842	LHG	2	0
12	B	809	CLA	1	0
12	B	802	CLA	3	0
12	A	820	CLA	5	0
12	A	815	CLA	1	0
12	A	807	CLA	1	0
12	A	812	CLA	5	0
12	B	812	CLA	4	0
15	A	846	BCR	4	0
15	K	202	BCR	2	0
15	A	845	BCR	3	0
12	B	803	CLA	1	0
12	B	839	CLA	3	0
12	B	813	CLA	2	0
12	B	832	CLA	1	0
12	B	835	CLA	1	0
13	A	840	PQN	1	0
12	A	802	CLA	2	0
15	B	804	BCR	4	0
12	B	825	CLA	1	0
15	B	843	BCR	4	0
15	B	842	BCR	3	0
12	A	823	CLA	3	0
12	A	835	CLA	1	0
12	B	823	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	C	101	SF4	1	0
12	B	828	CLA	2	0
12	A	810	CLA	2	0
12	A	833	CLA	1	0
12	B	826	CLA	1	0
12	B	827	CLA	1	0
12	A	813	CLA	1	0
12	B	814	CLA	2	0
12	A	805	CLA	2	0
12	A	803	CLA	1	0
12	J	102	CLA	1	0
12	A	818	CLA	4	0
12	A	831	CLA	2	0
15	I	201	BCR	4	0
12	B	822	CLA	1	0
14	A	843	LHG	3	0
12	B	838	CLA	3	0
12	A	801	CLA	2	0
15	J	101	BCR	5	0
12	A	837	CLA	5	0
15	L	202	BCR	6	0
17	A	849	LMU	1	0
12	L	201	CLA	1	0
12	A	839	CLA	2	0
15	A	844	BCR	3	0
12	A	824	CLA	2	0
12	A	814	CLA	2	0
12	A	828	CLA	3	0
15	B	841	BCR	1	0
12	L	203	CLA	3	0
12	B	811	CLA	5	0
15	A	847	BCR	5	0
12	A	826	CLA	3	0
12	A	827	CLA	2	0
16	C	102	SF4	2	0
12	A	804	CLA	2	0
13	B	840	PQN	5	0
12	B	810	CLA	3	0
12	B	824	CLA	2	0
12	B	801	CLA	3	0
12	B	830	CLA	1	0
15	L	204	BCR	7	0

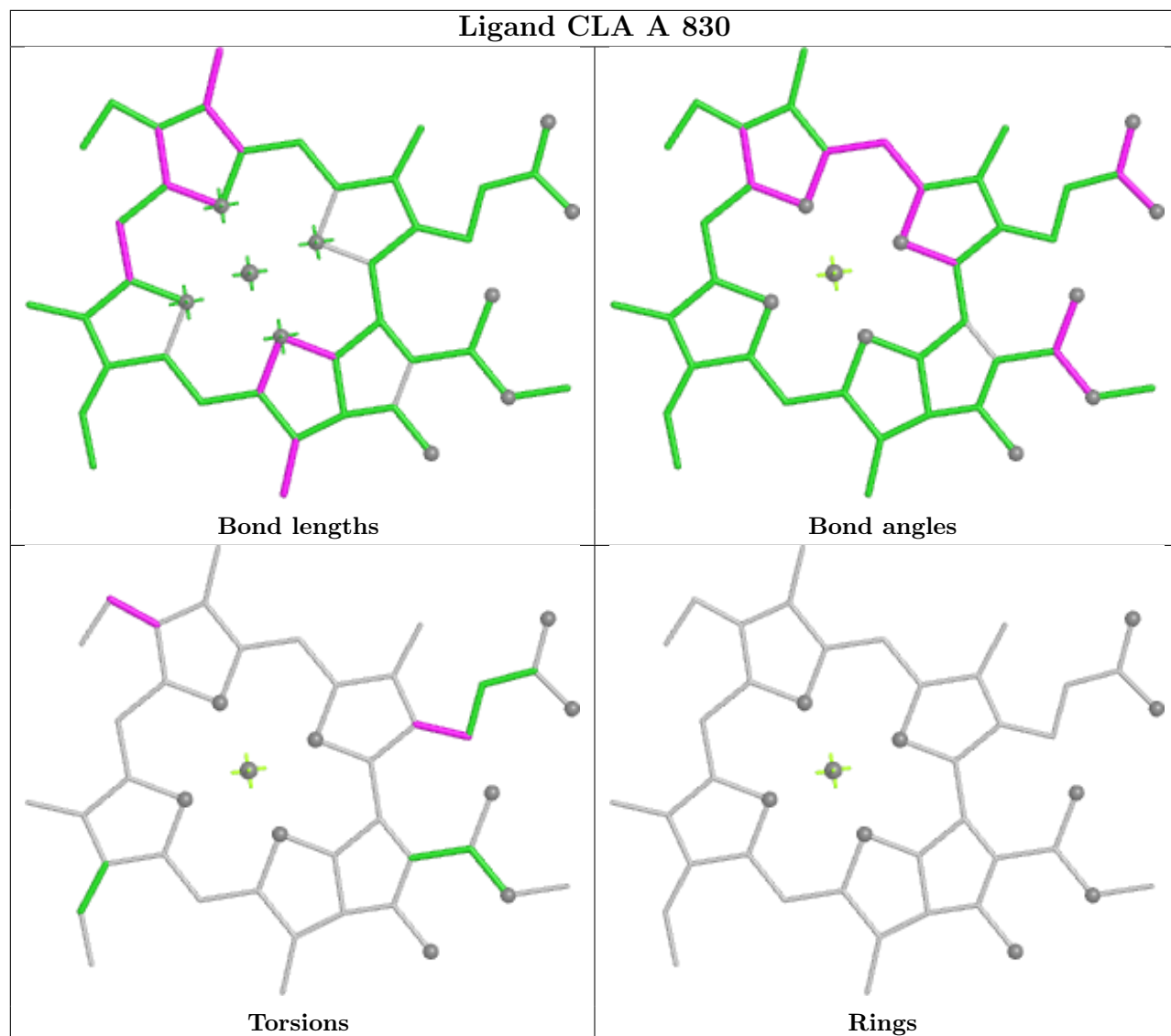
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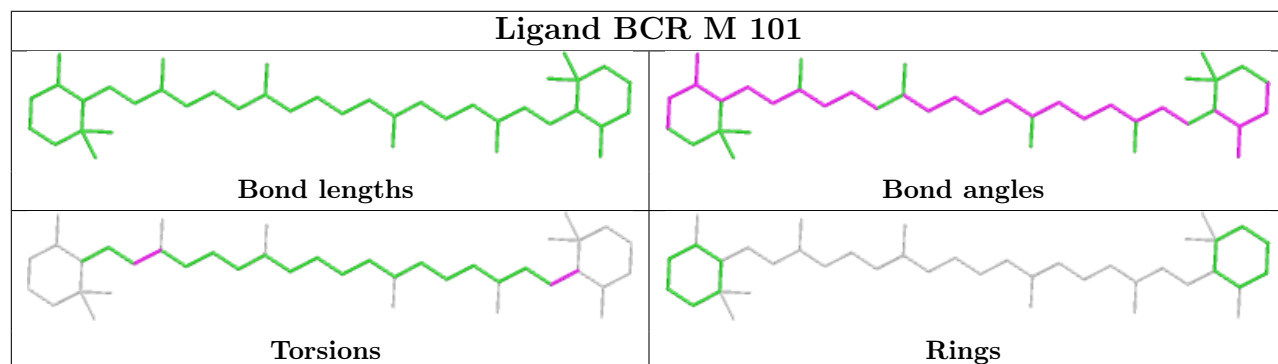
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	822	CLA	2	0
12	A	829	CLA	3	0
12	B	836	CLA	1	0
12	B	834	CLA	3	0
12	A	838	CLA	2	0

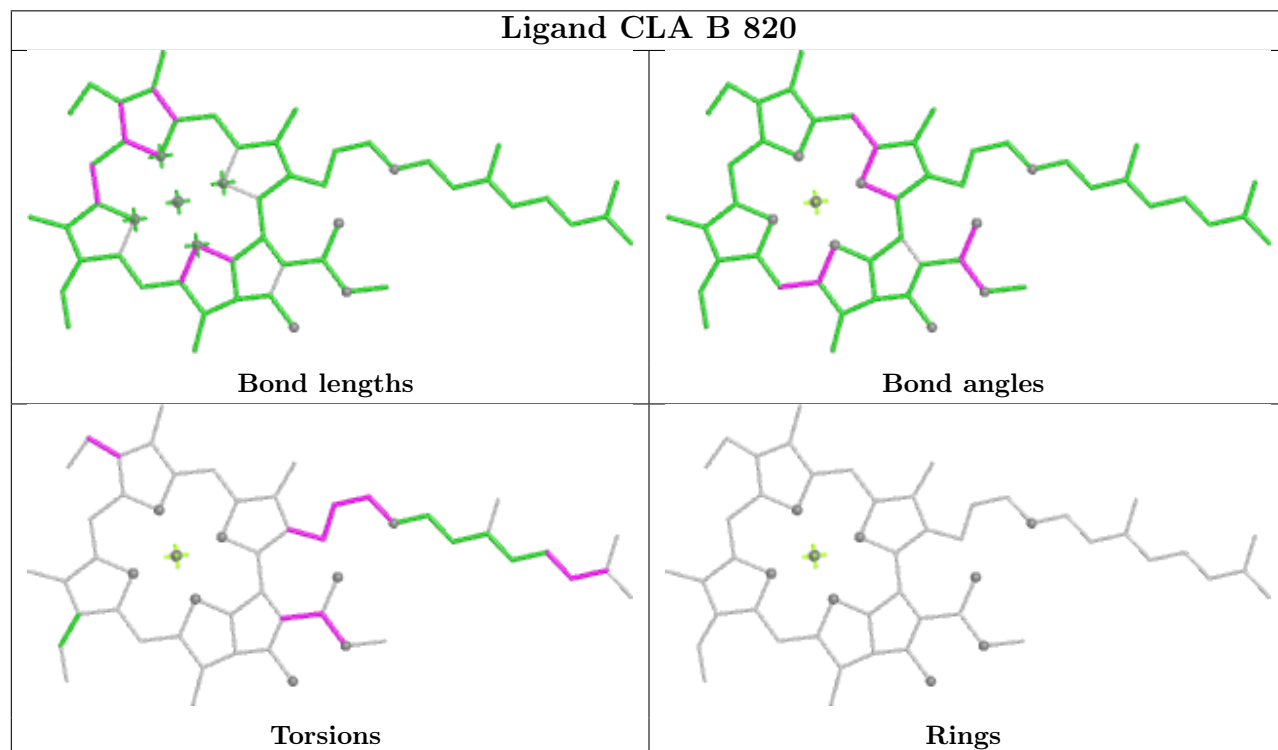
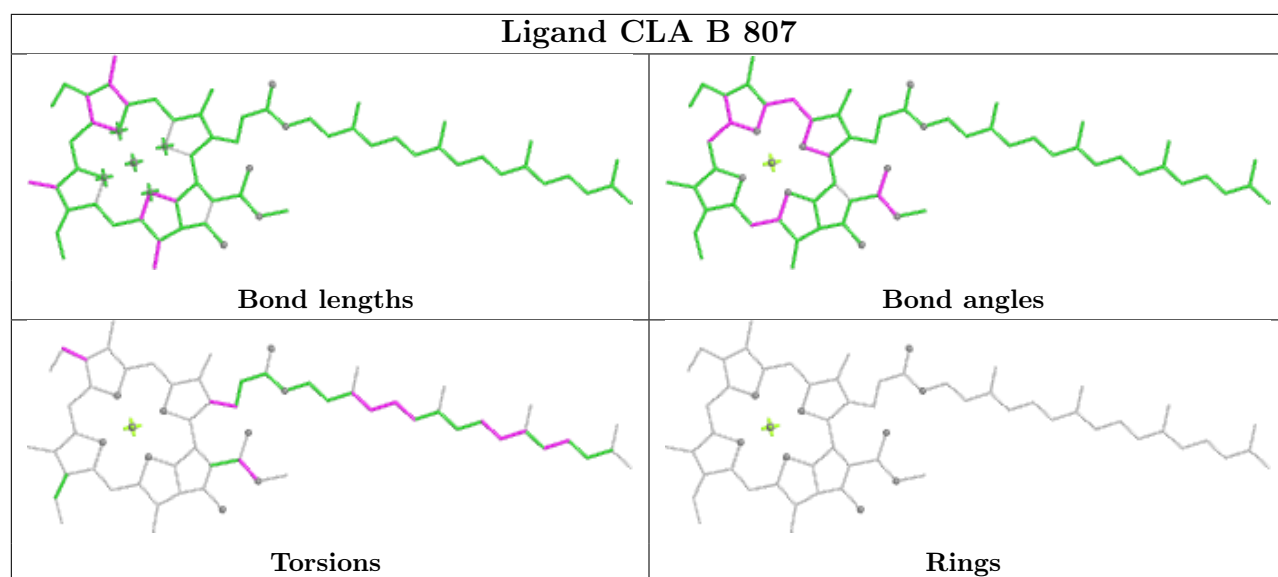
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 A 830

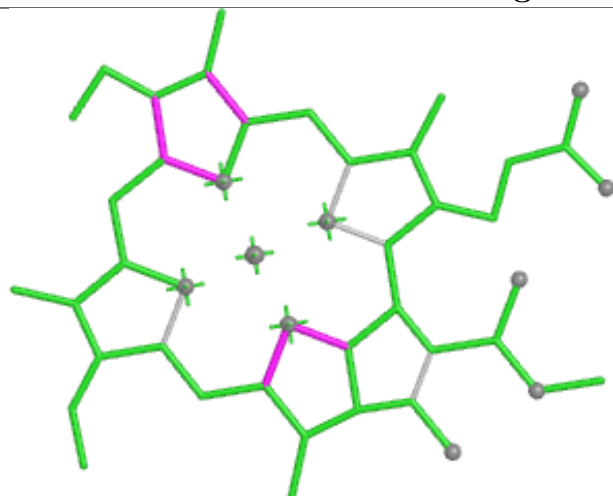


Ligand BCR M 101

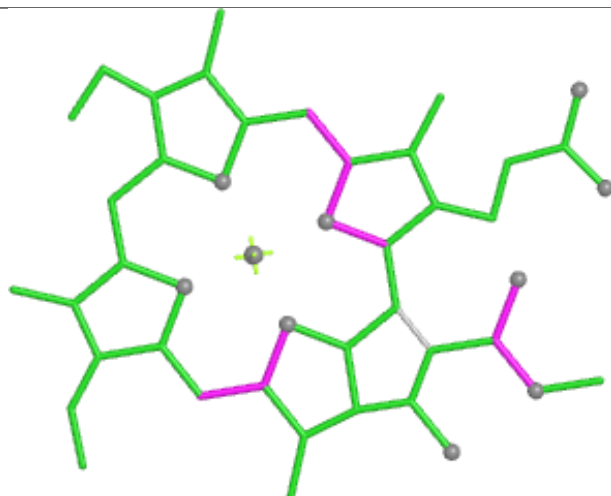




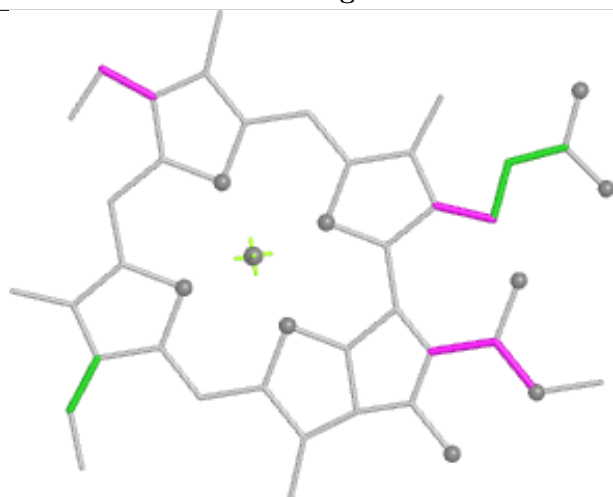
Ligand CLA A 806



Bond lengths



Bond angles

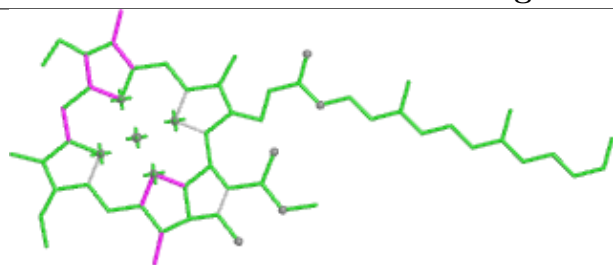


Torsions

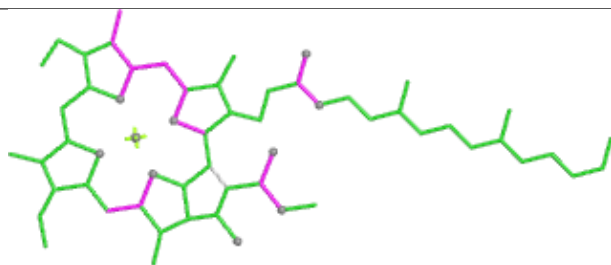


Rings

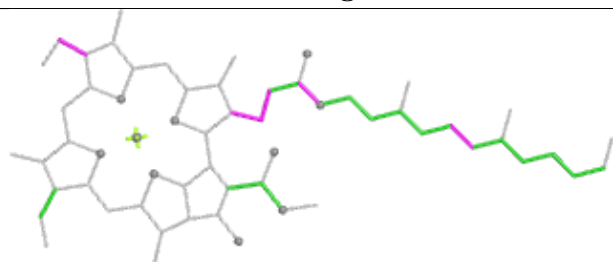
Ligand CLA B 821



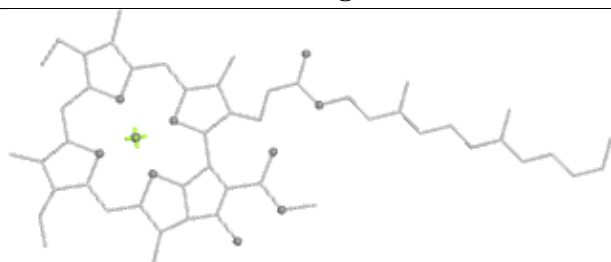
Bond lengths



Bond angles

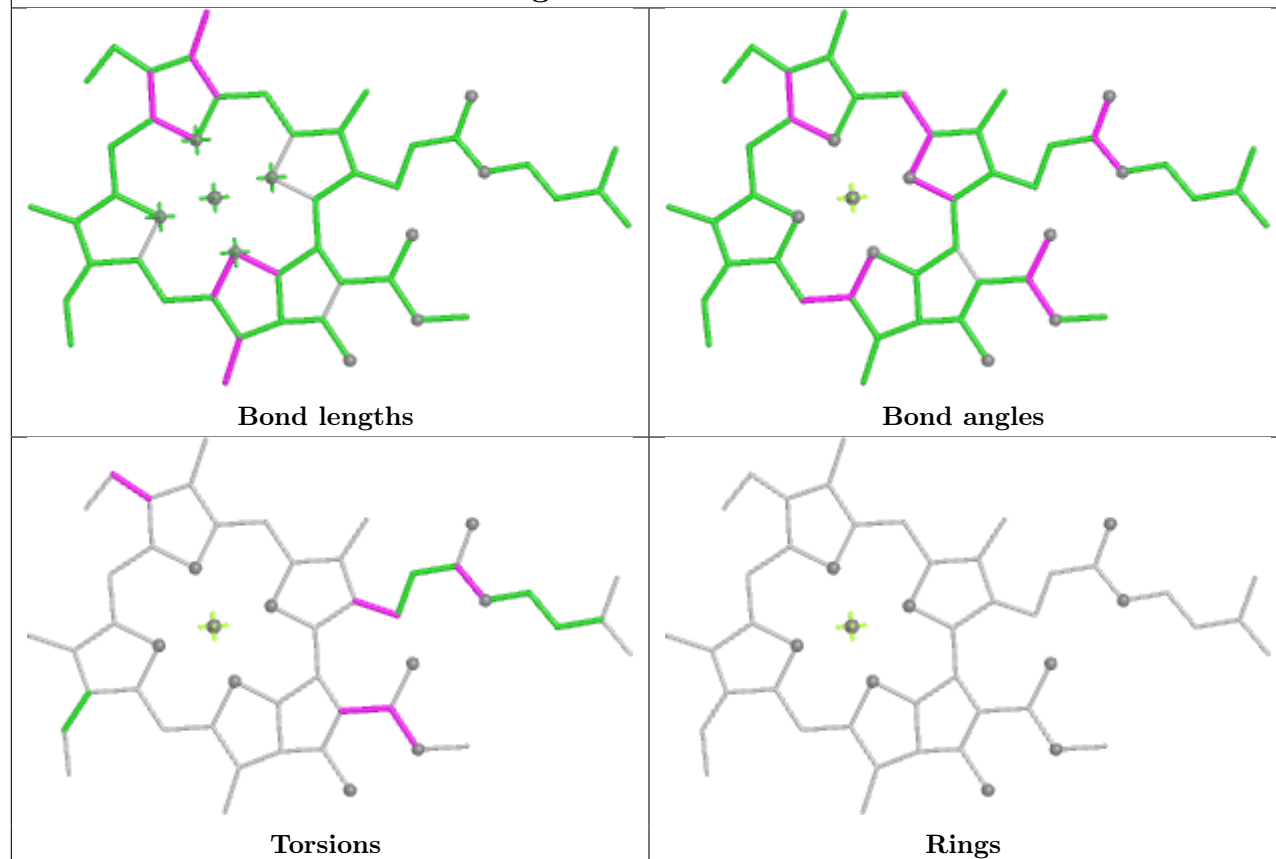


Torsions

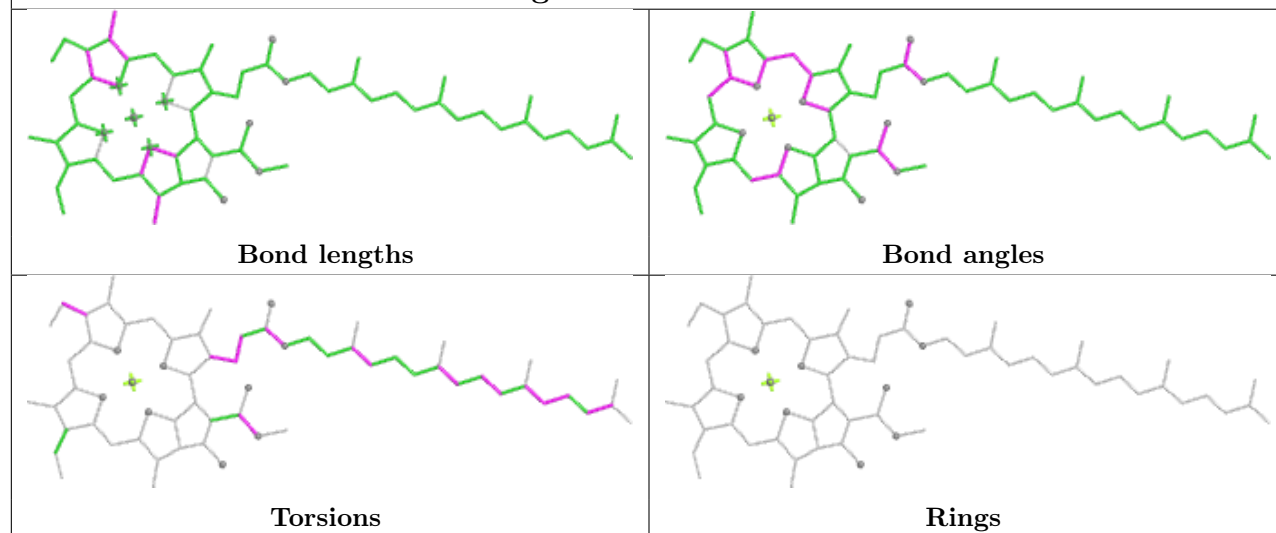


Rings

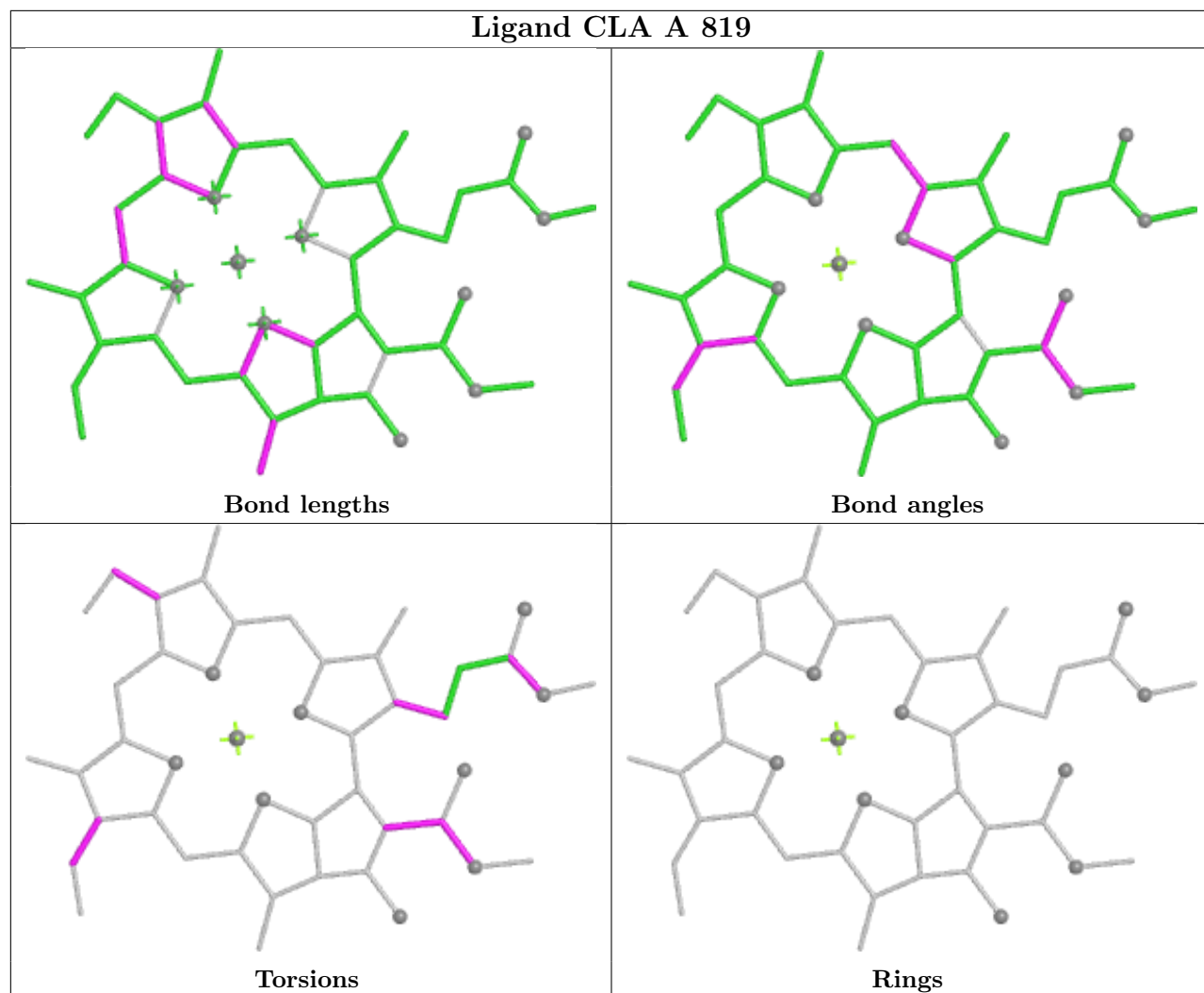
Ligand CLA A 825

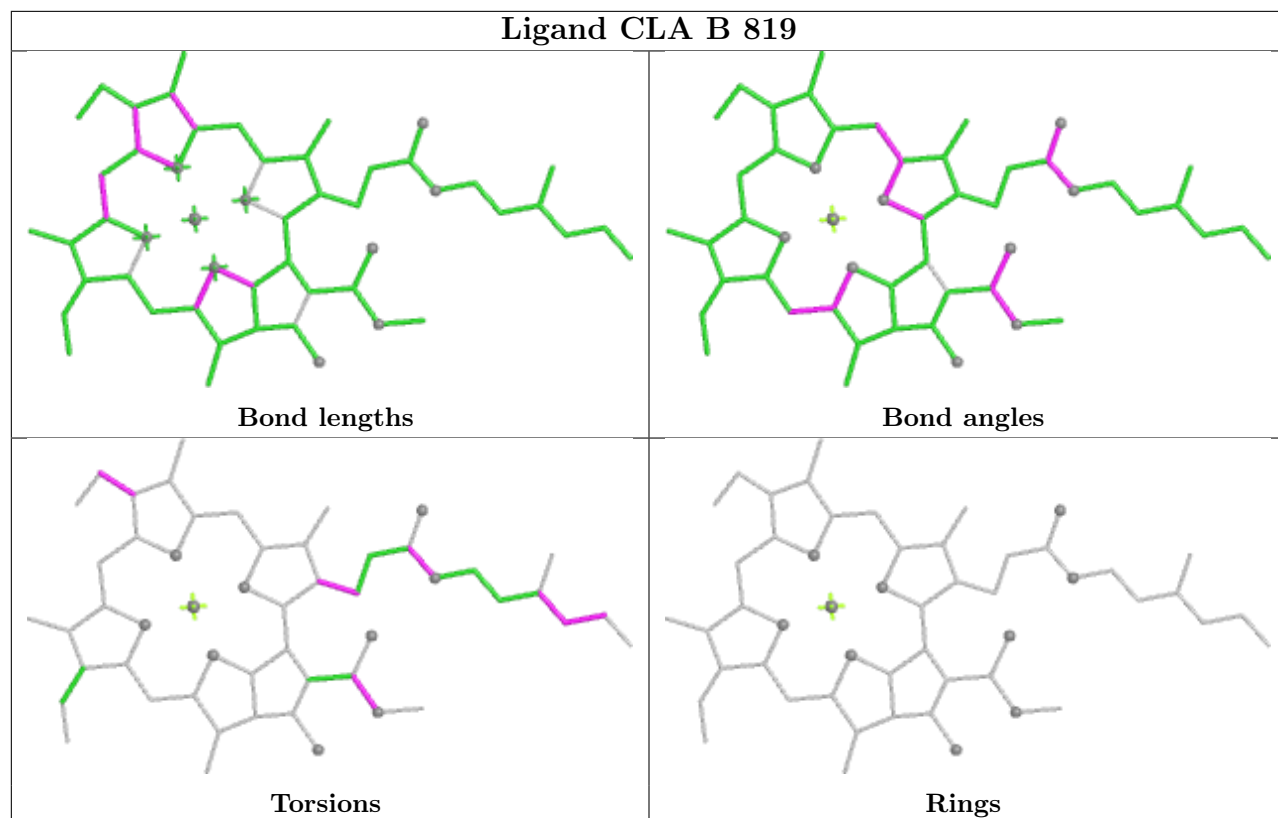


Ligand CLA A 832

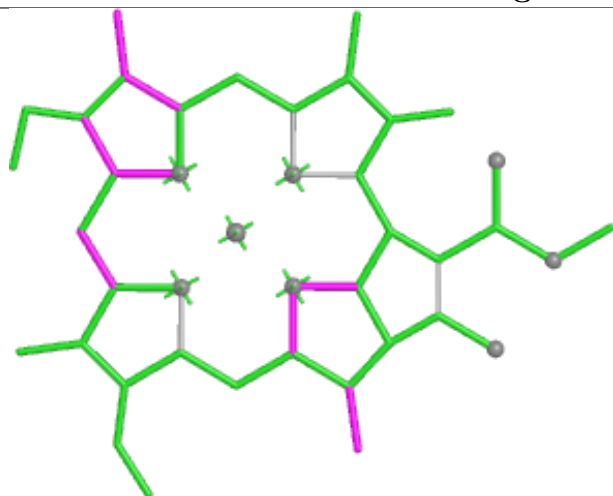


Ligand CLA A 819

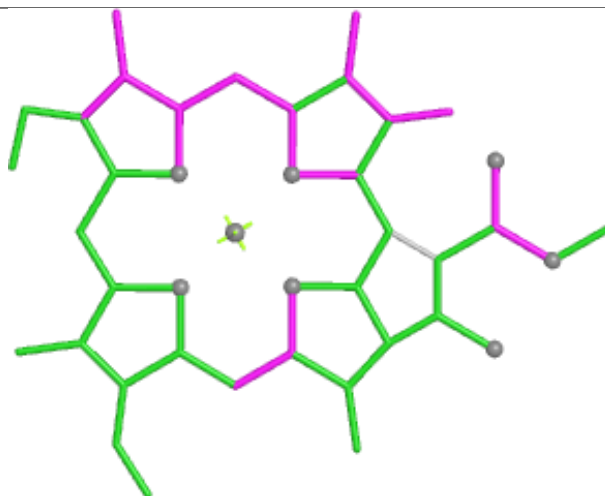




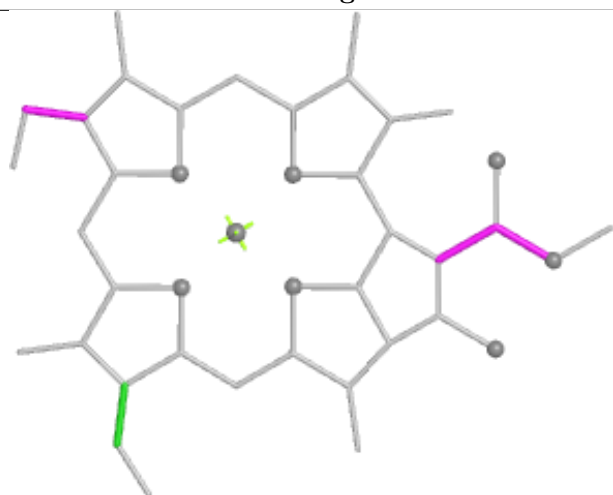
Ligand CLA A 811



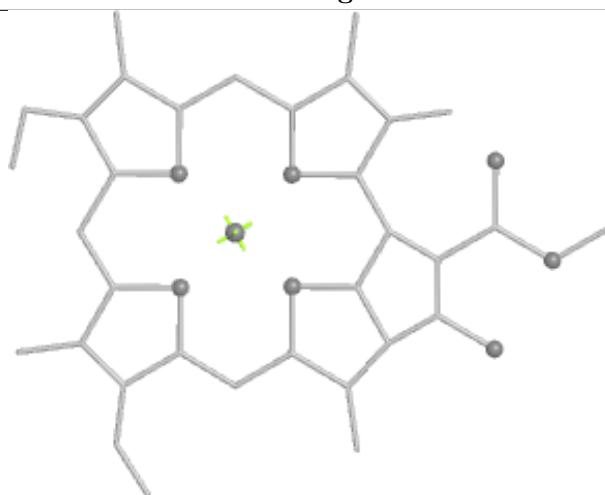
Bond lengths



Bond angles

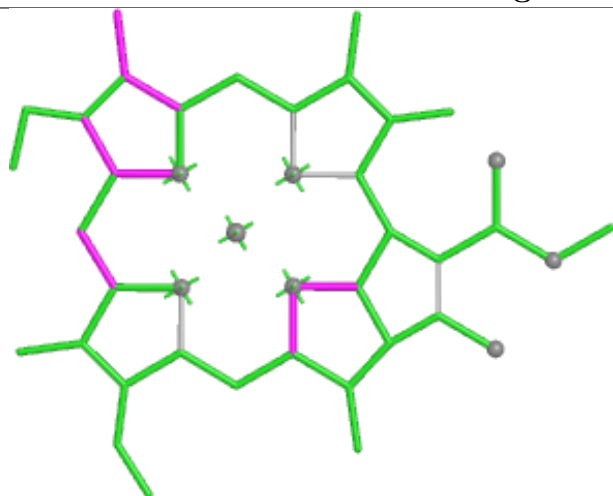


Torsions

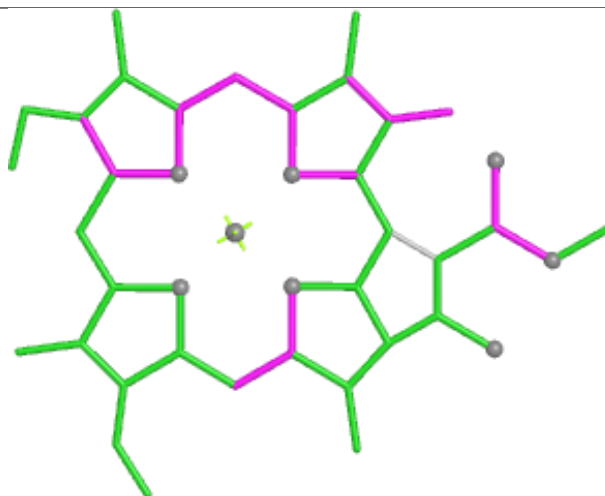


Rings

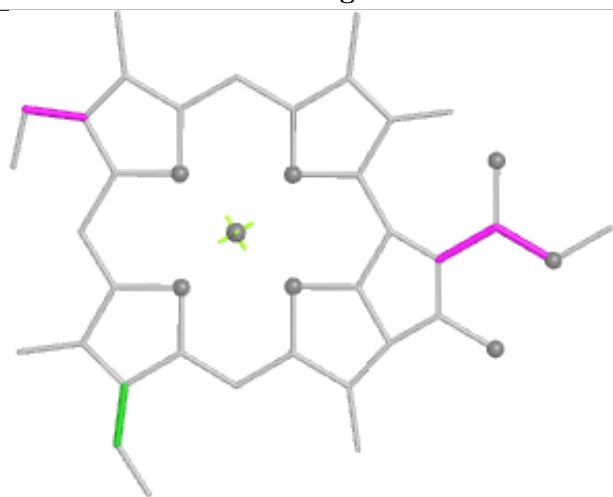
Ligand CLA A 834



Bond lengths



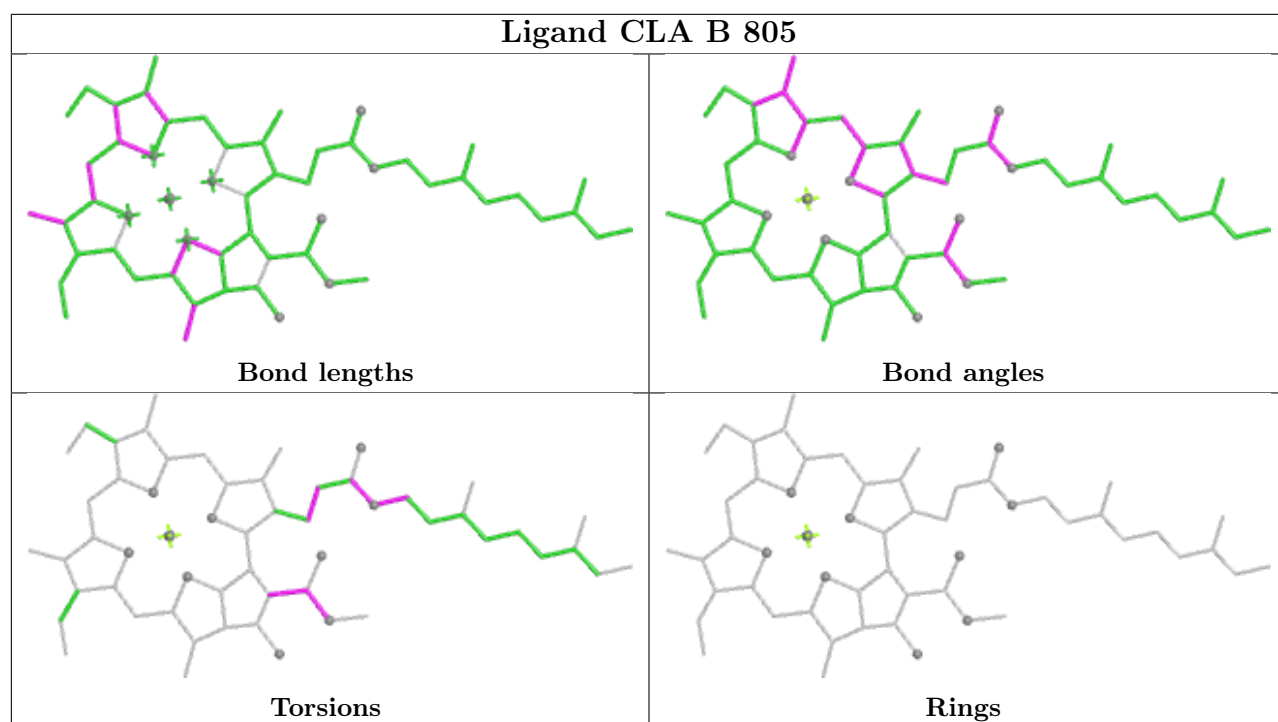
Bond angles

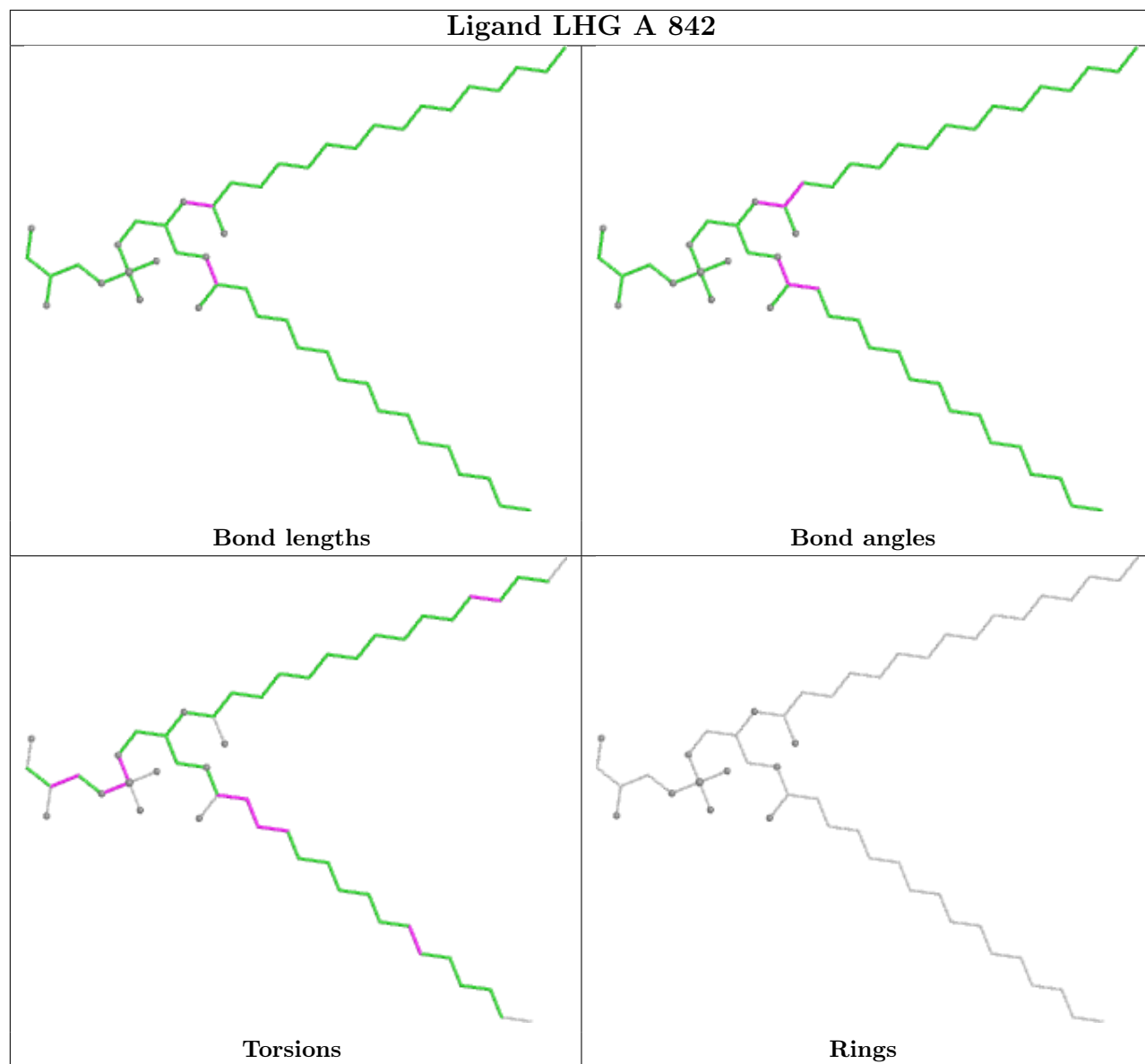


Torsions

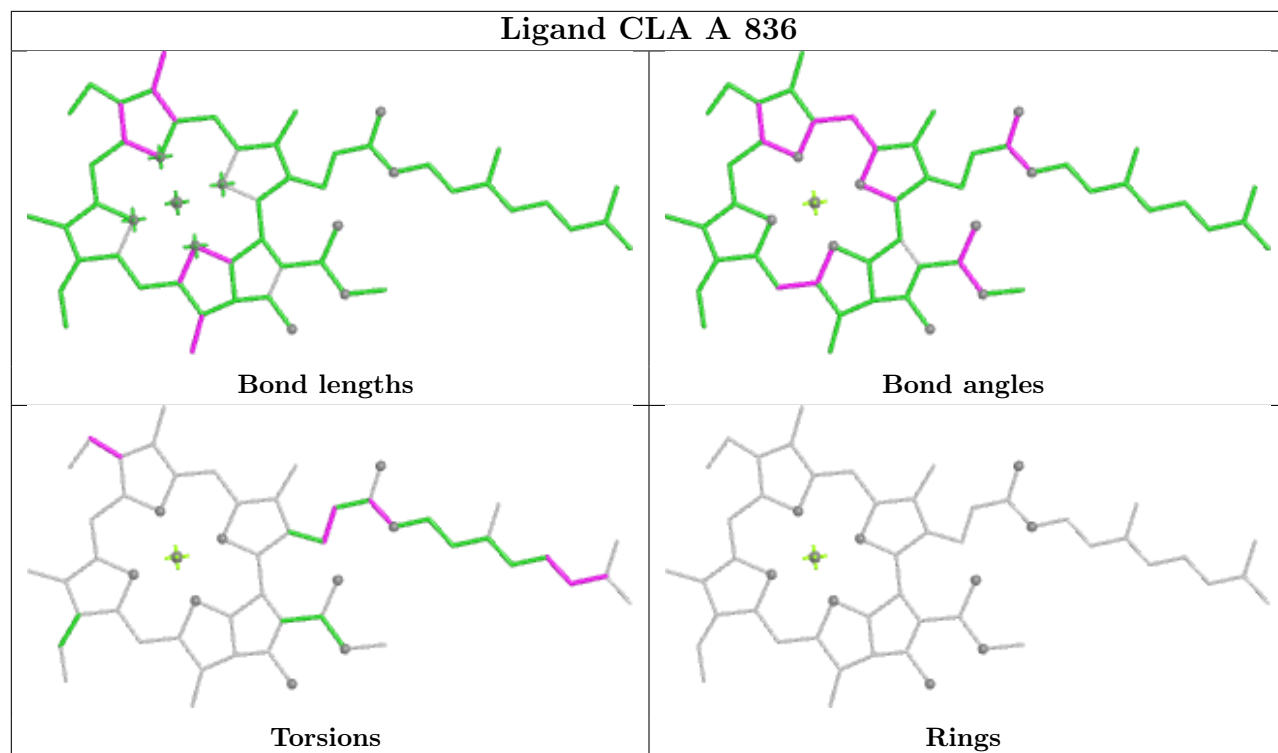


Rings

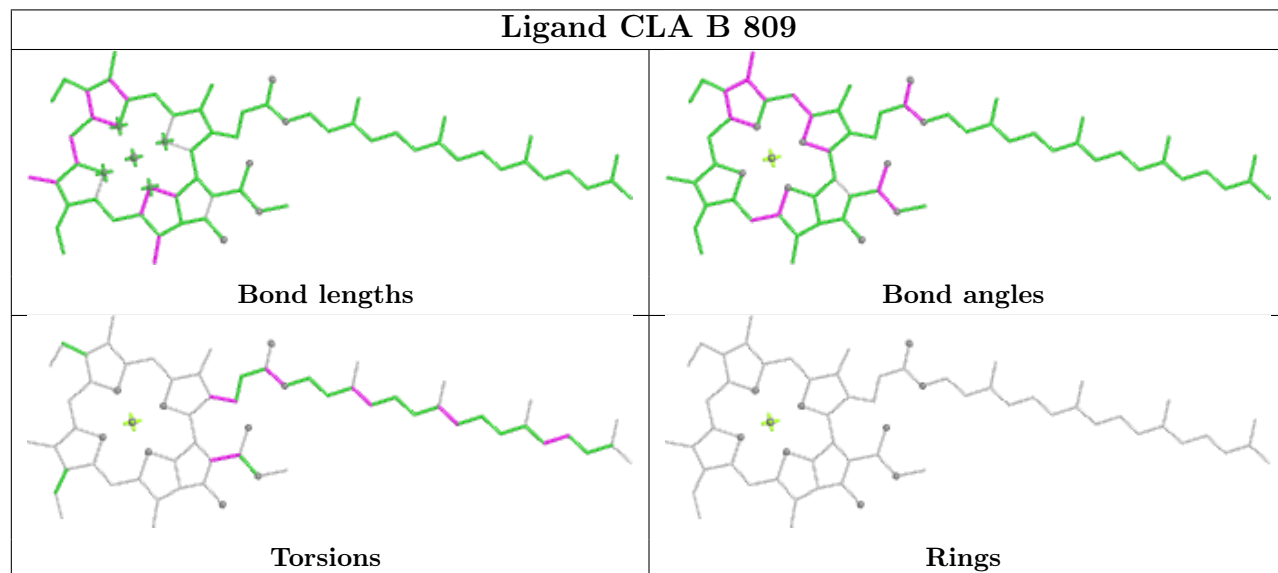


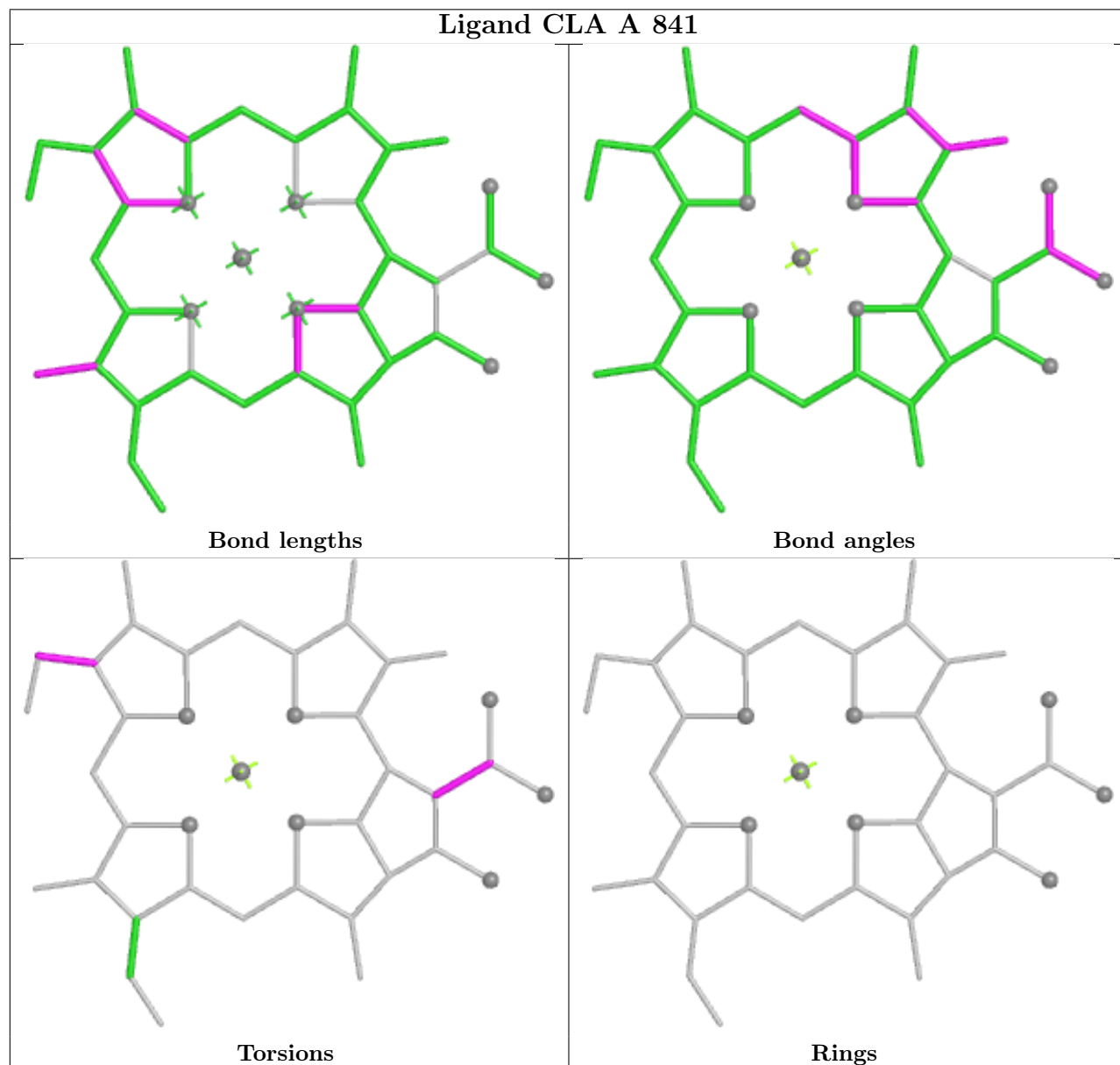
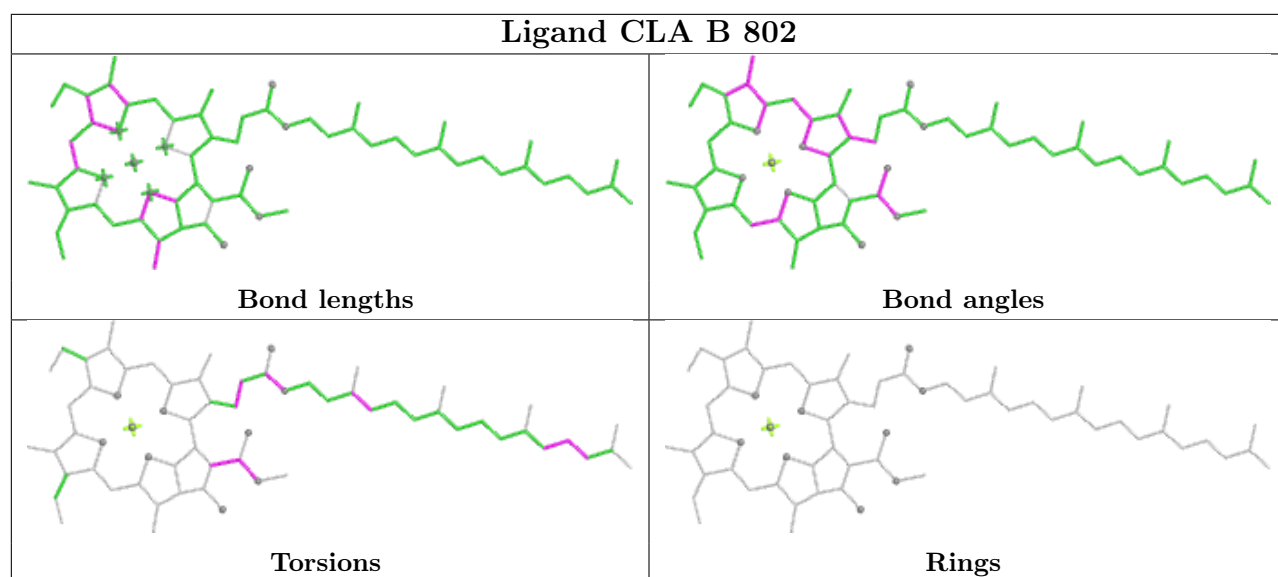


Ligand CLA A 836

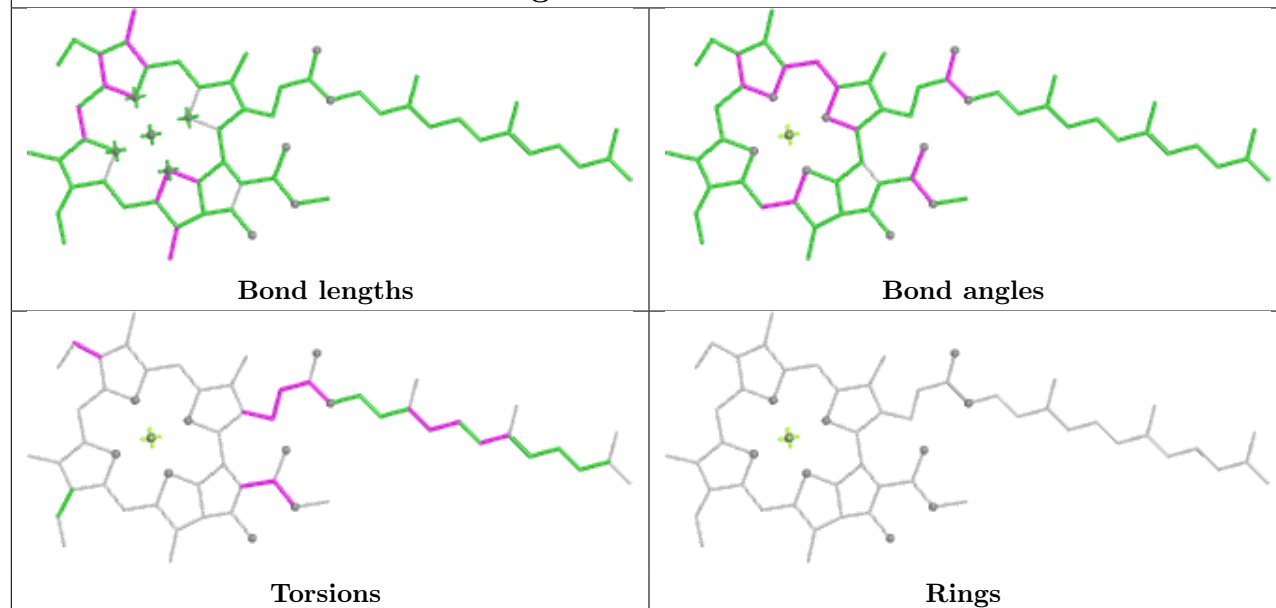


Ligand CLA B 809

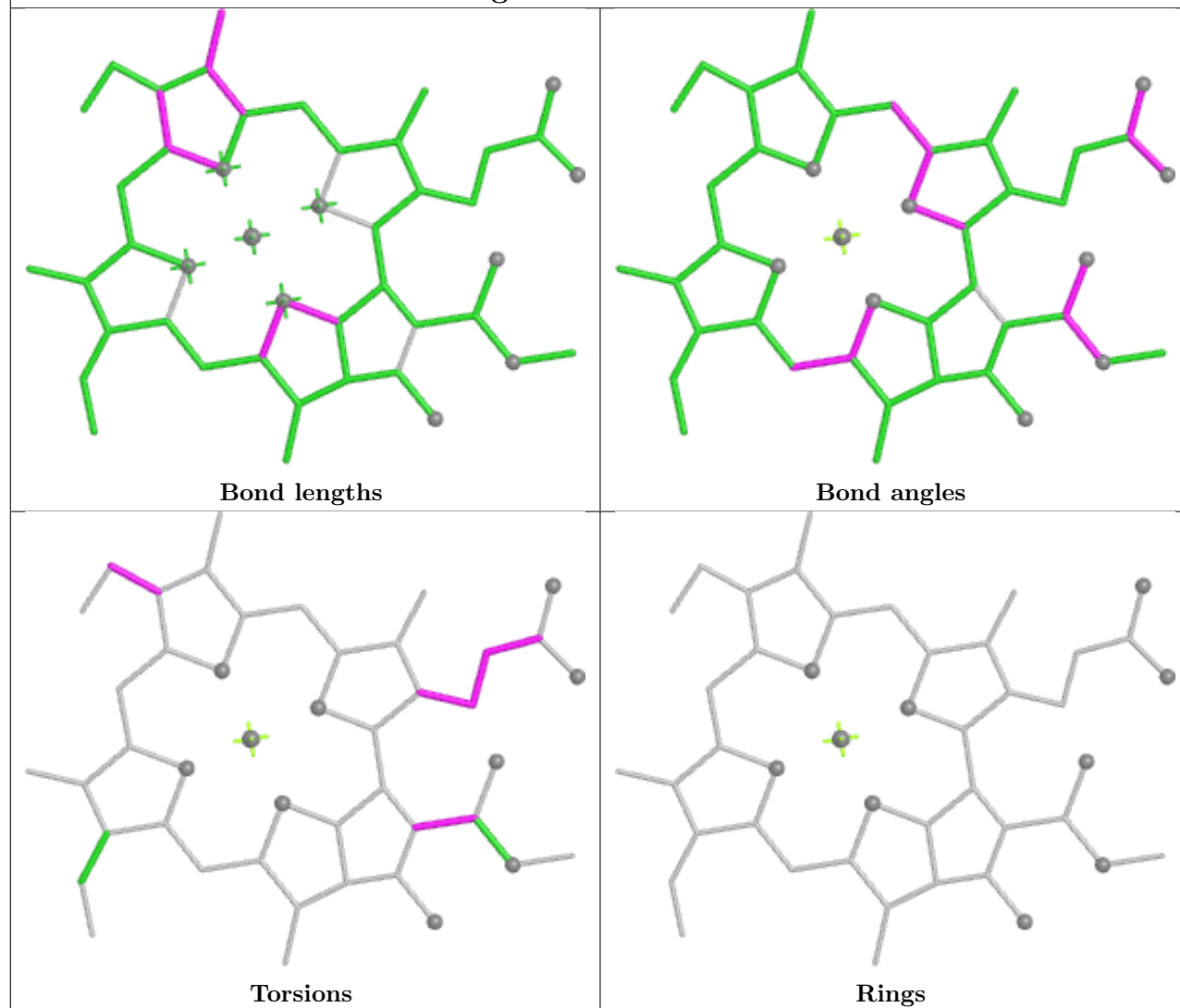




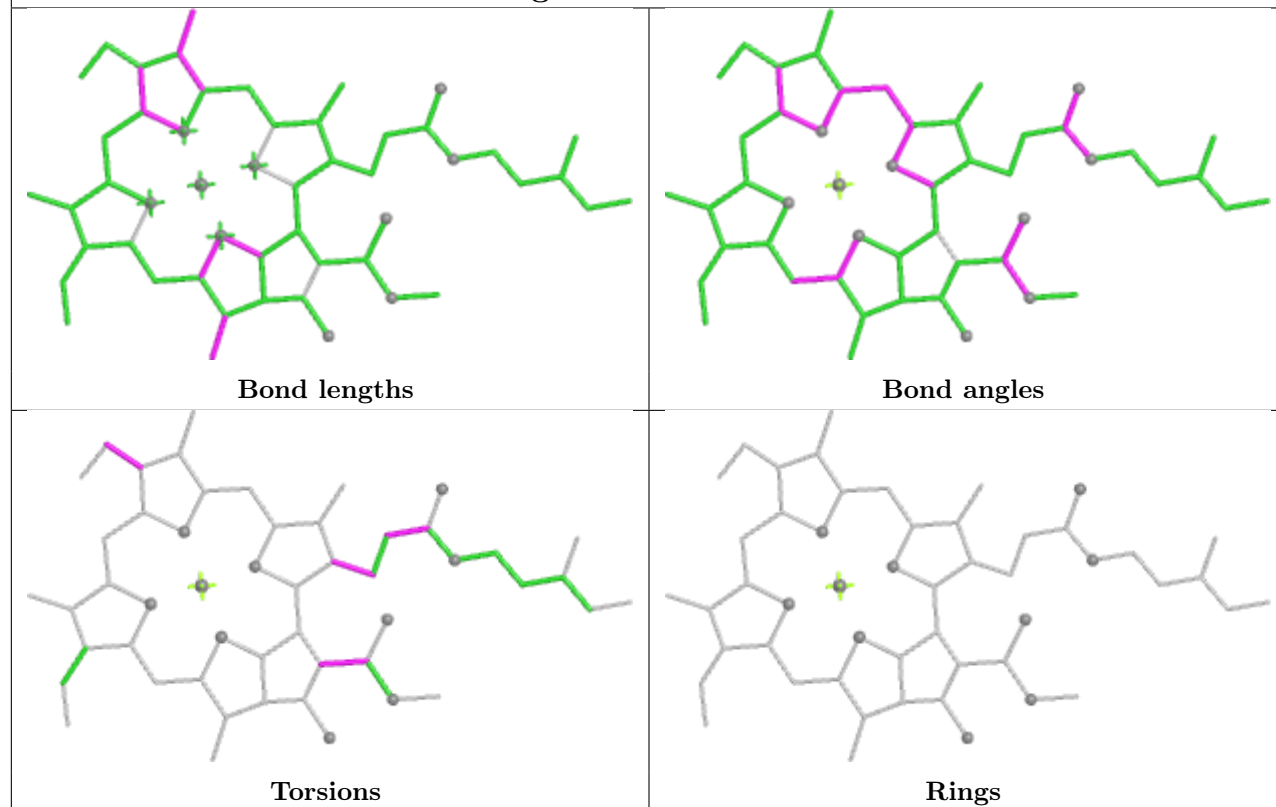
Ligand CLA A 820



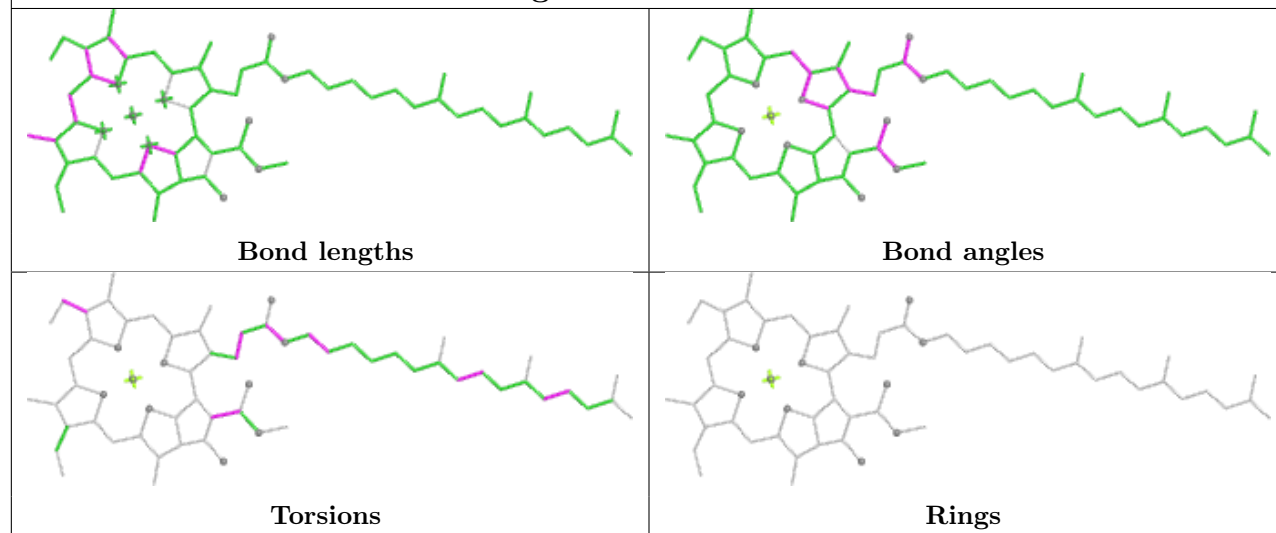
Ligand CLA A 815



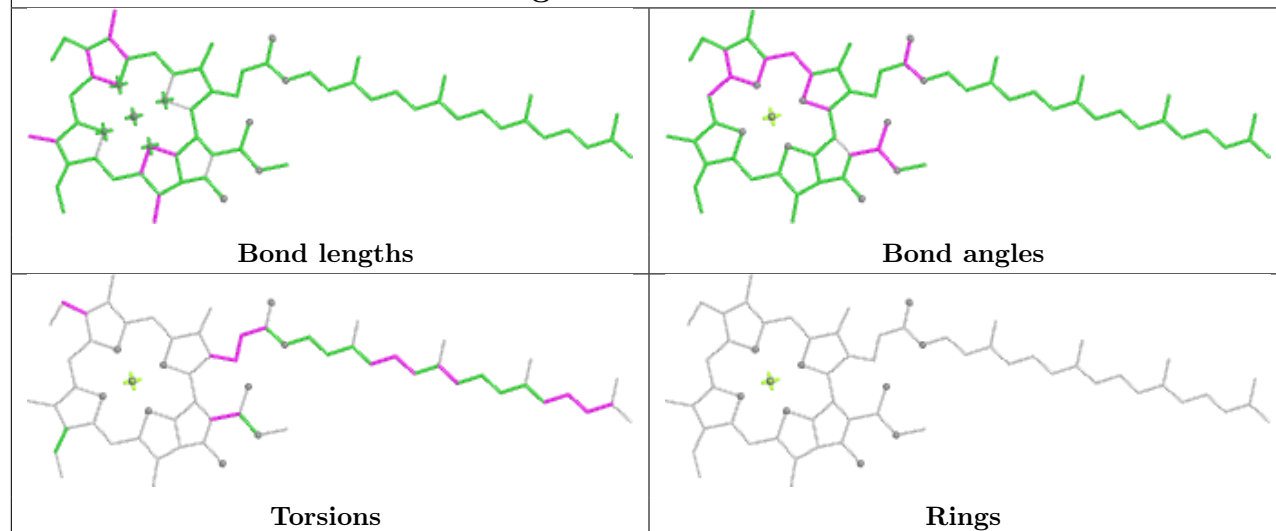
Ligand CLA A 807



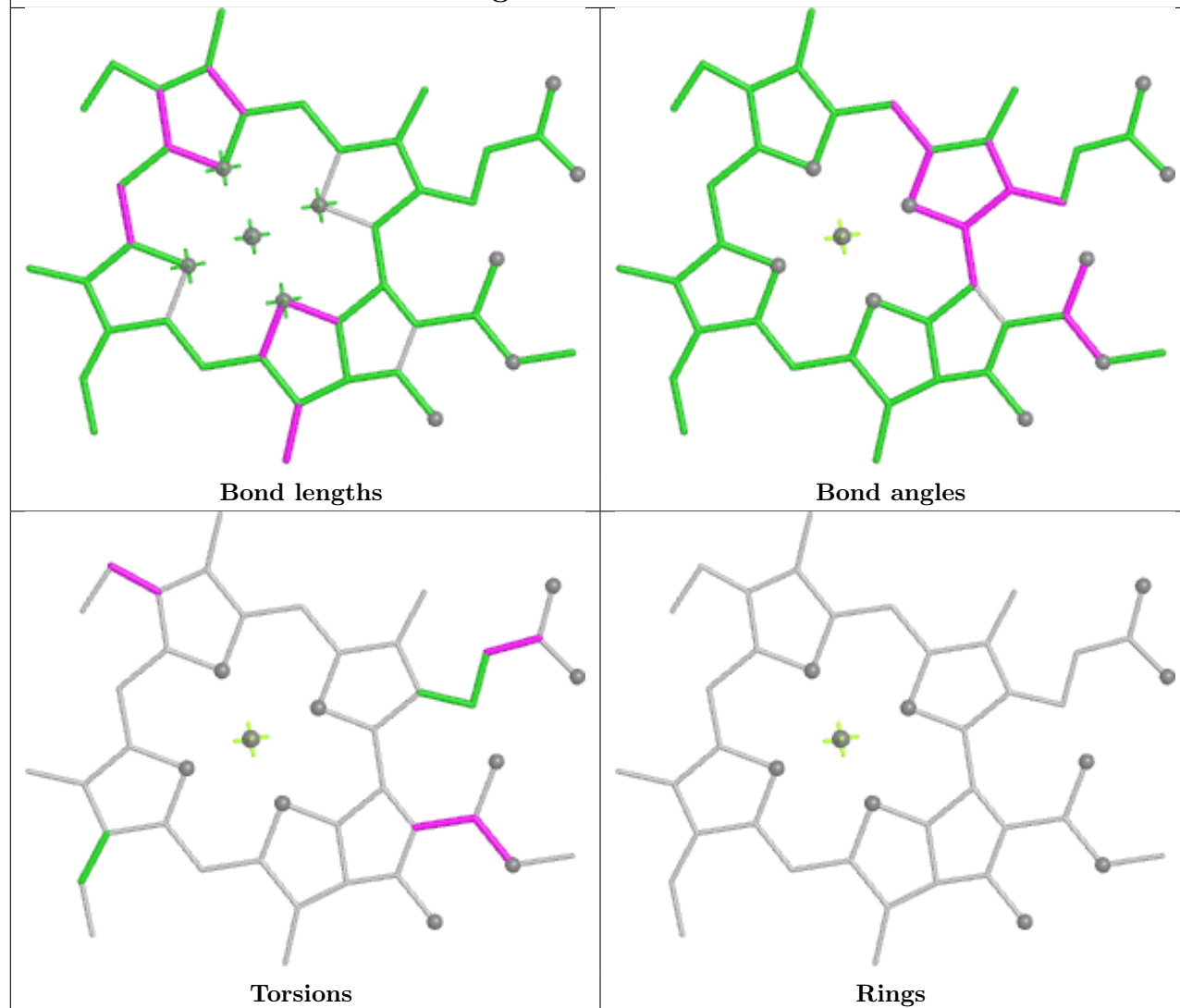
Ligand CLA A 812

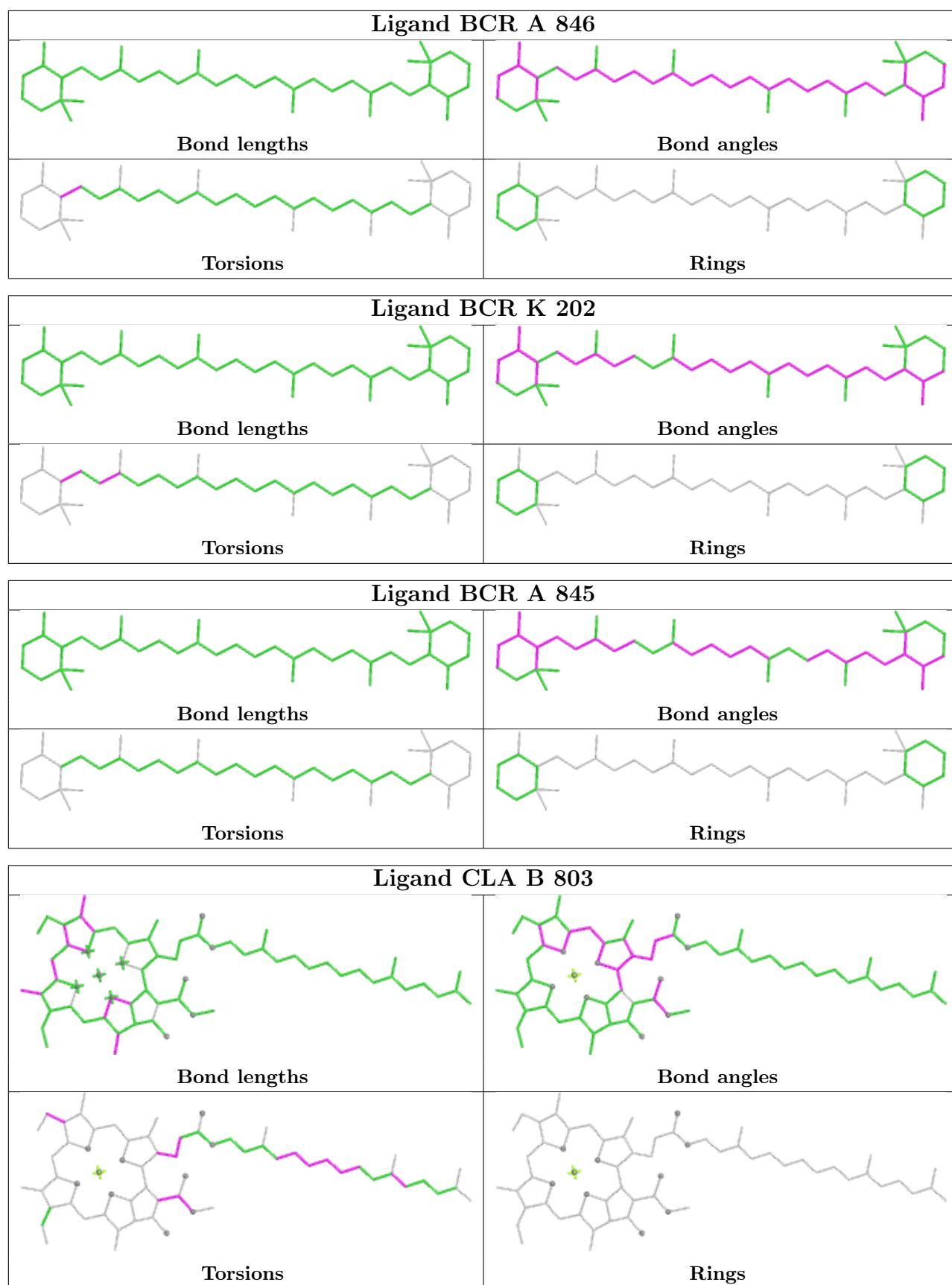


Ligand CLA B 812

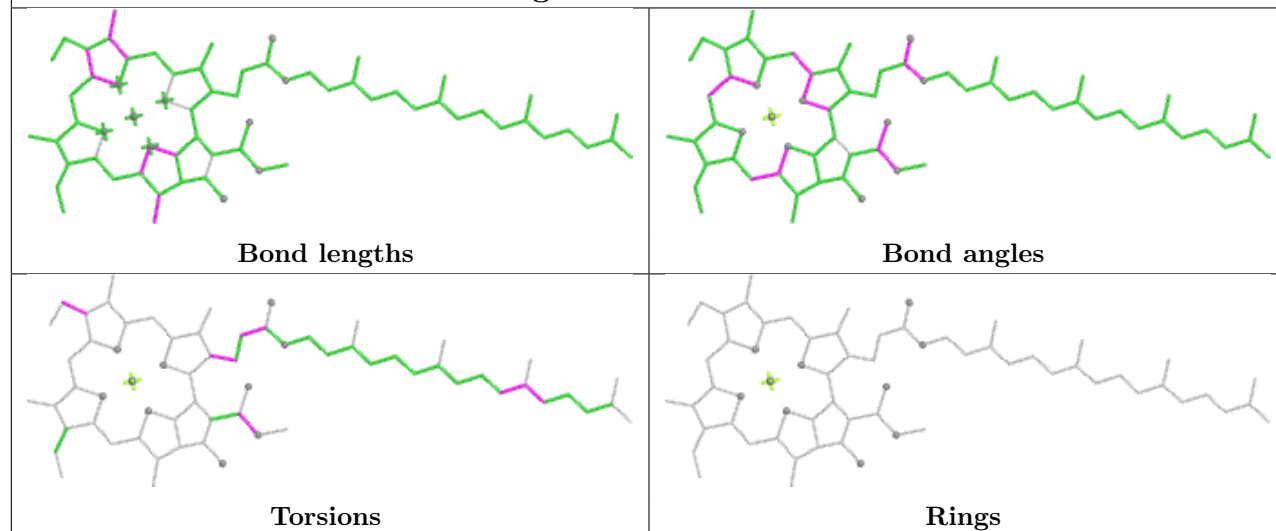


Ligand CLA B 831

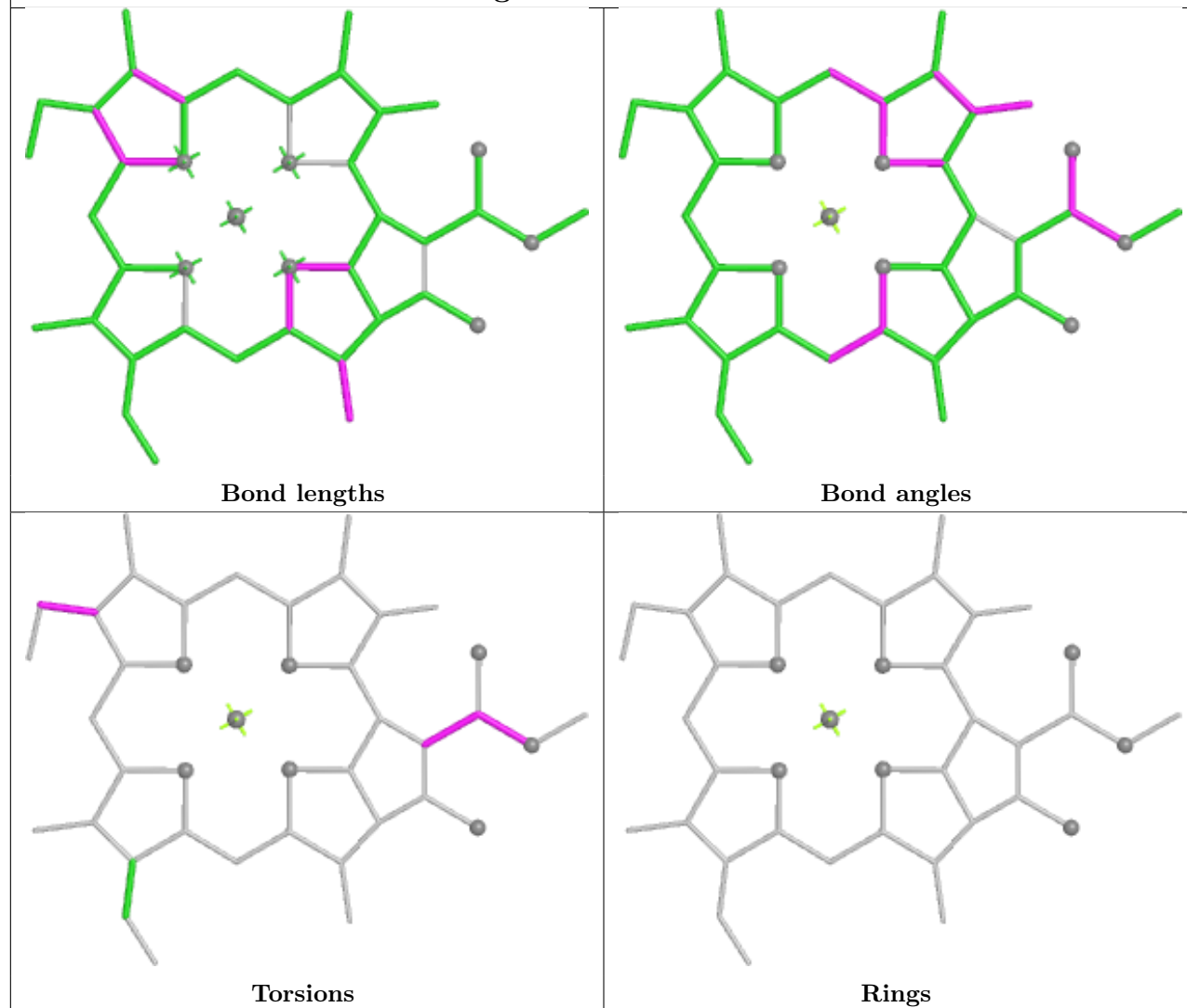


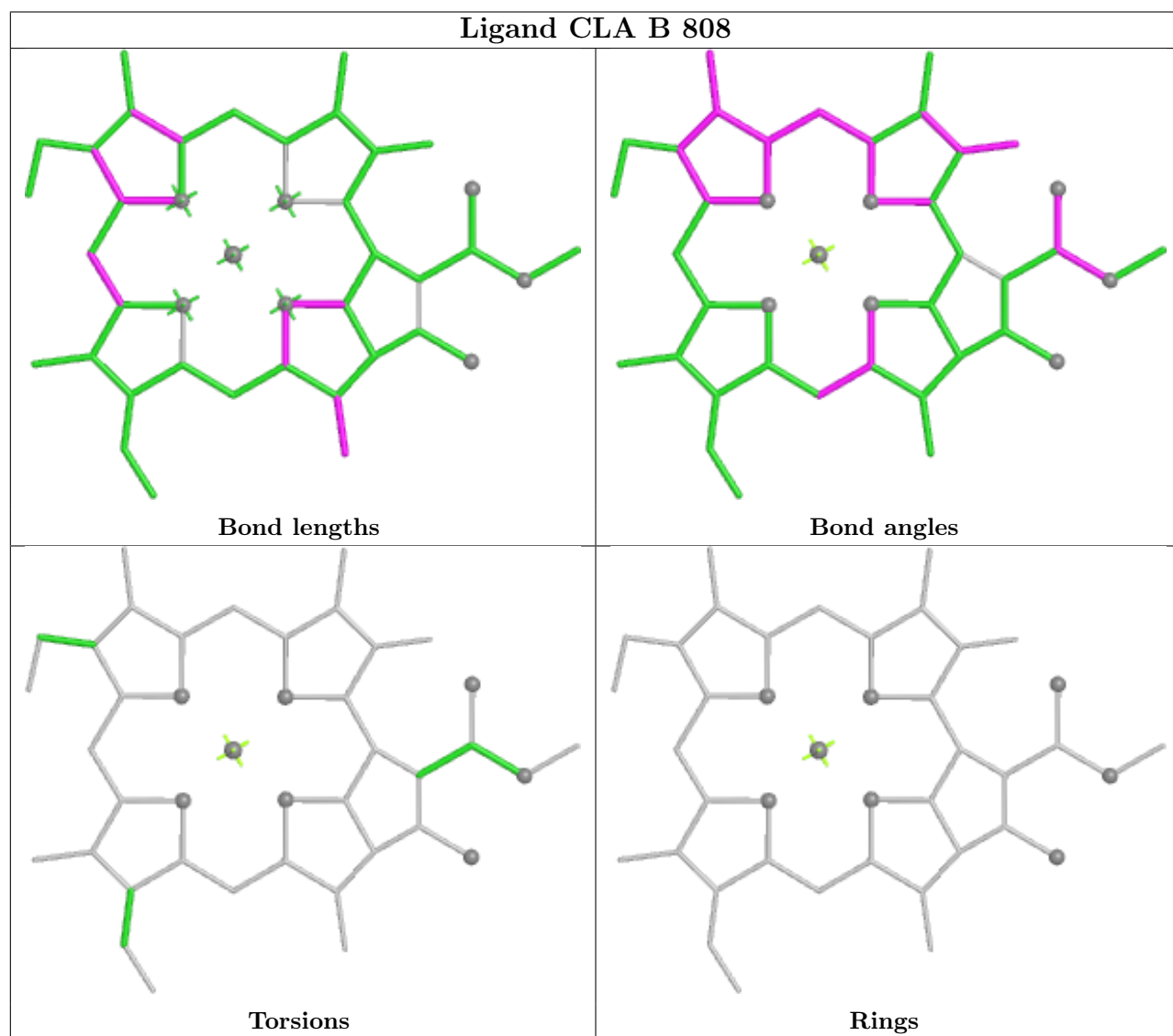
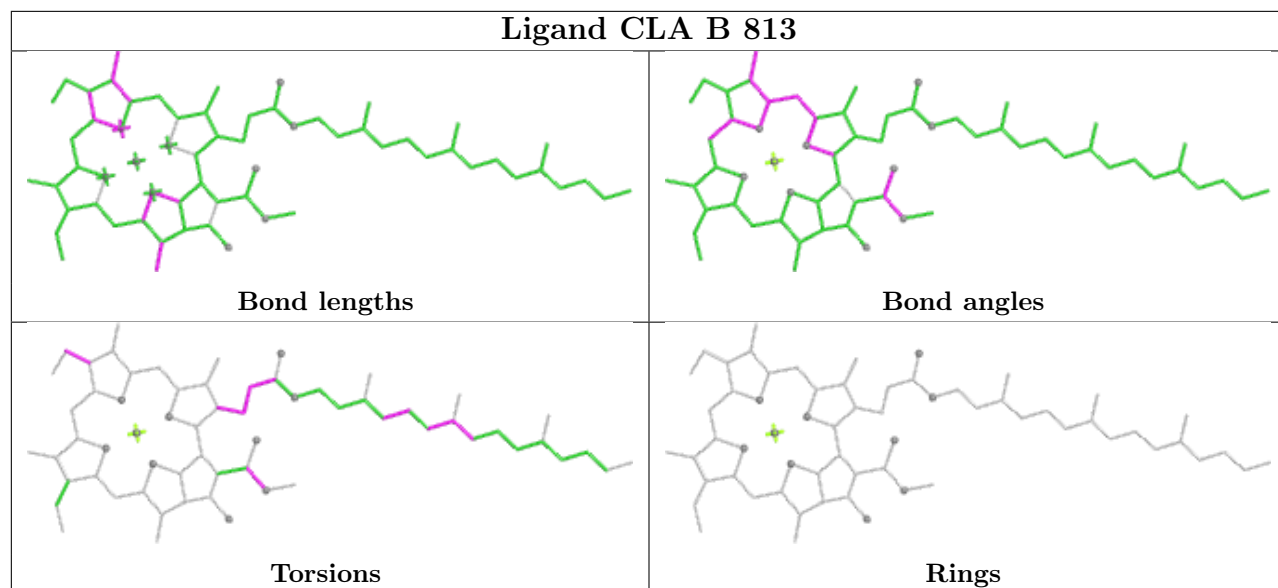


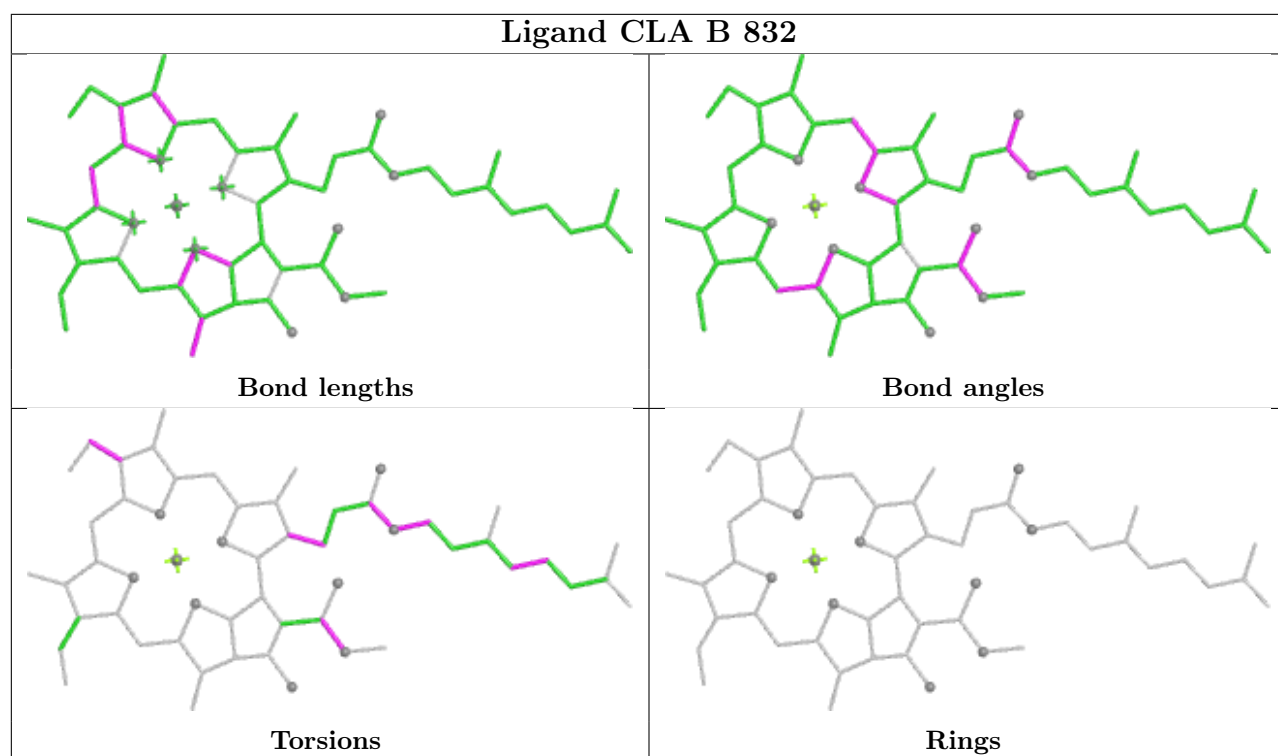
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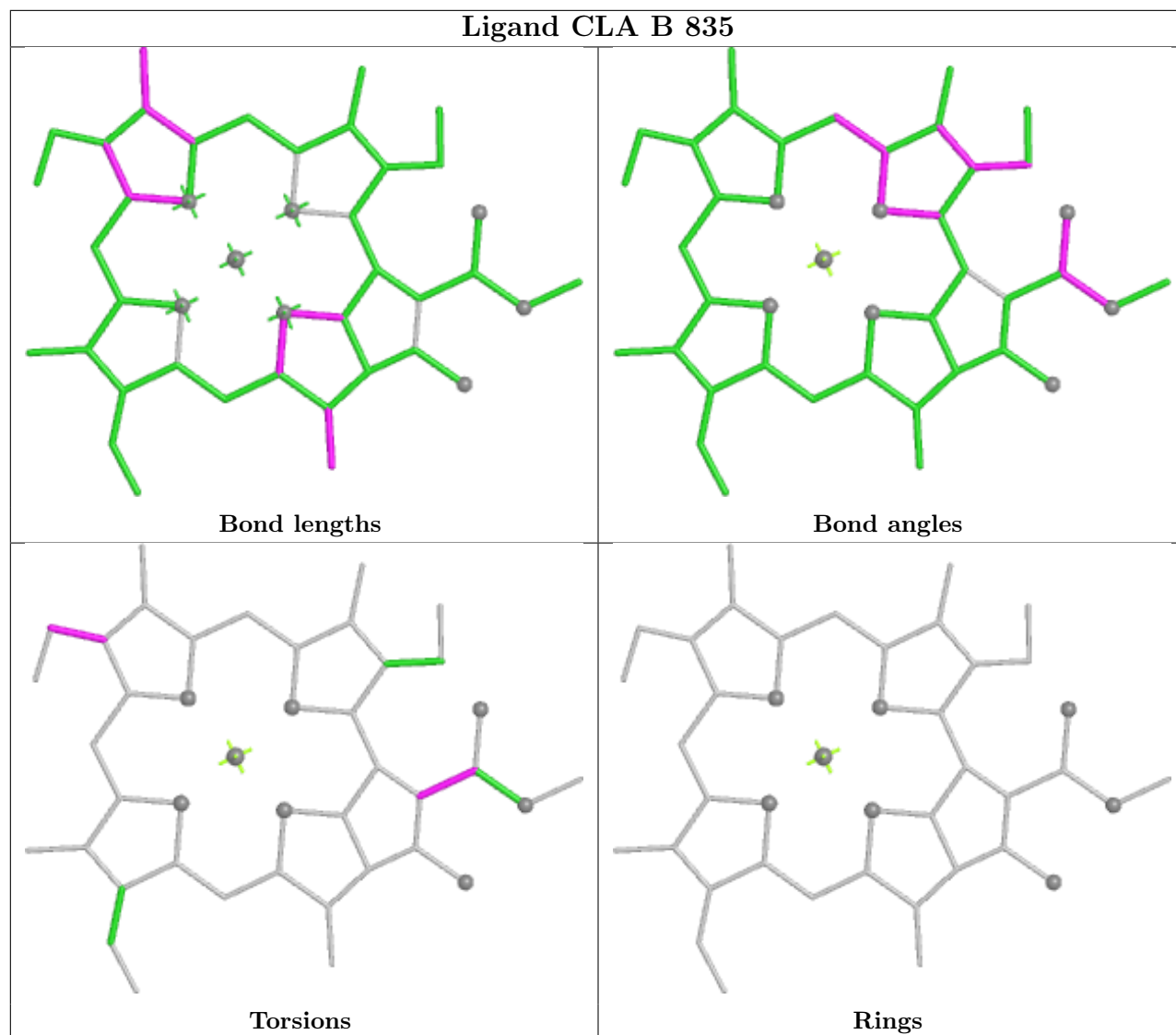
Ligand CLA K 201



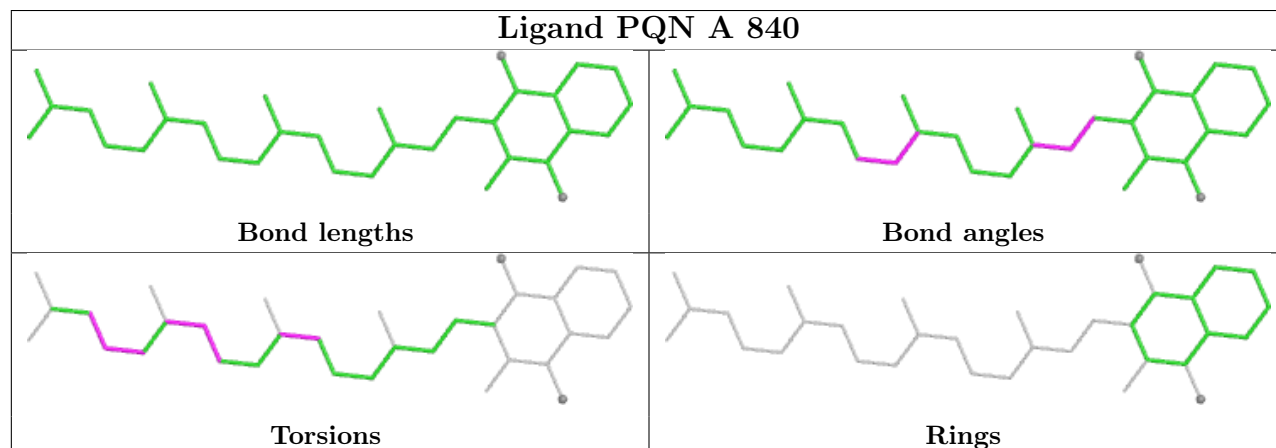


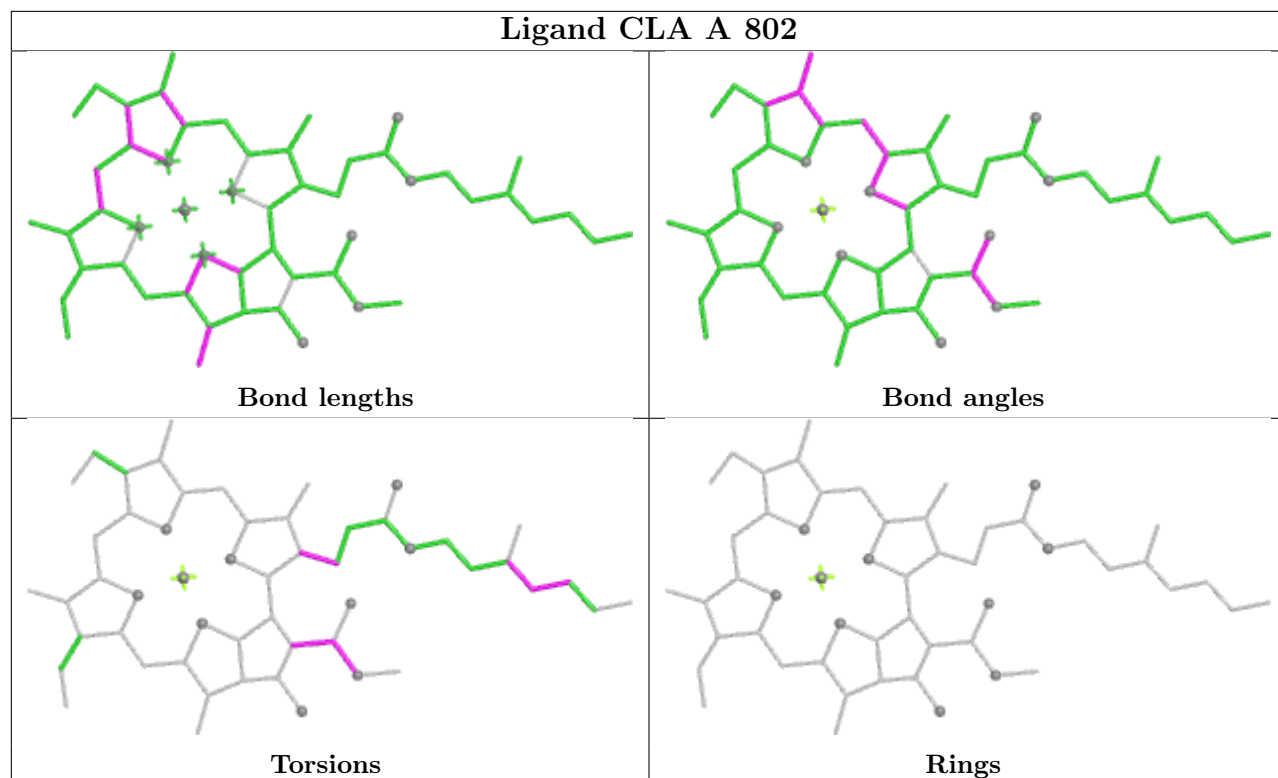


Ligand CLA B 835

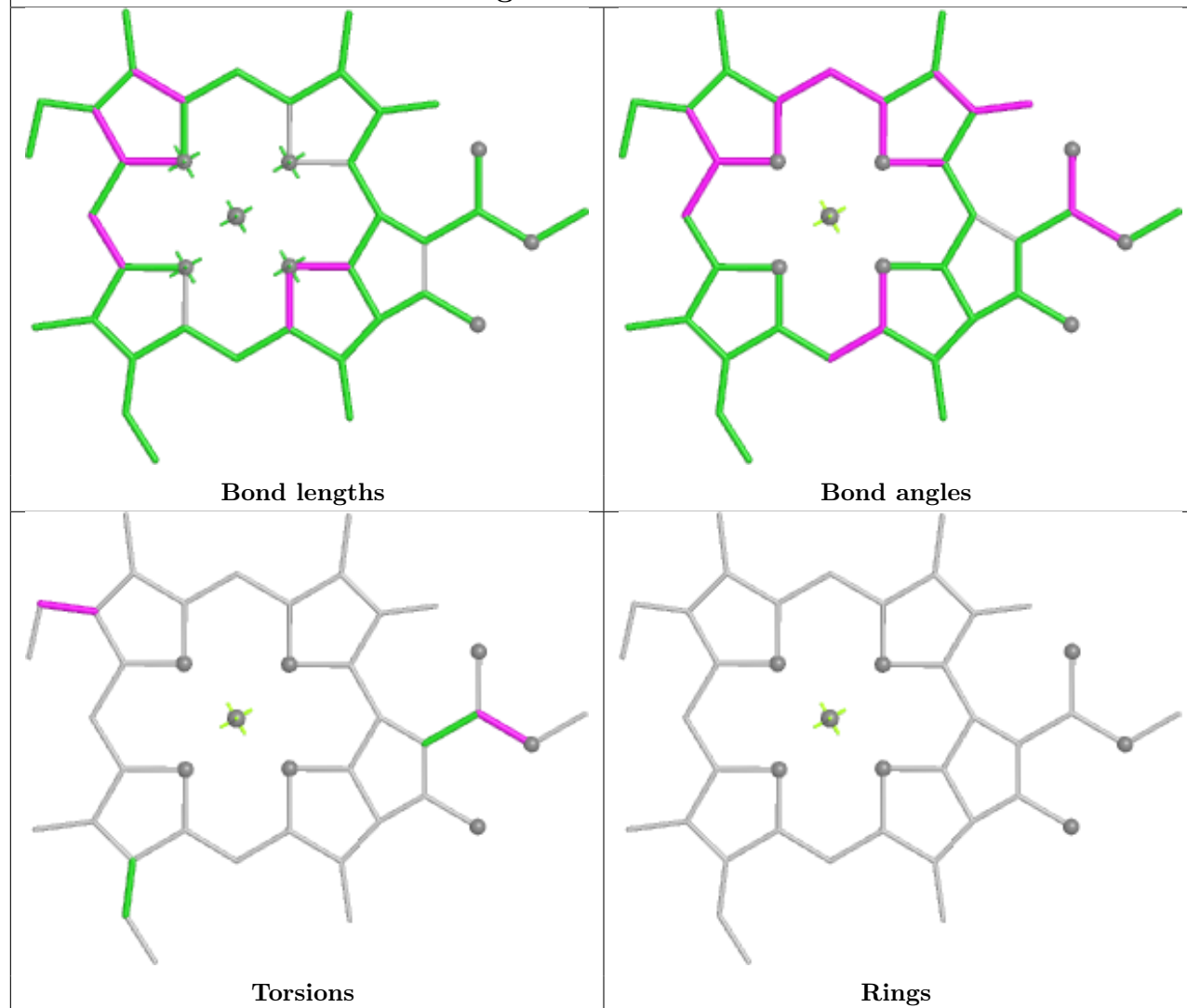


Ligand PQN A 840

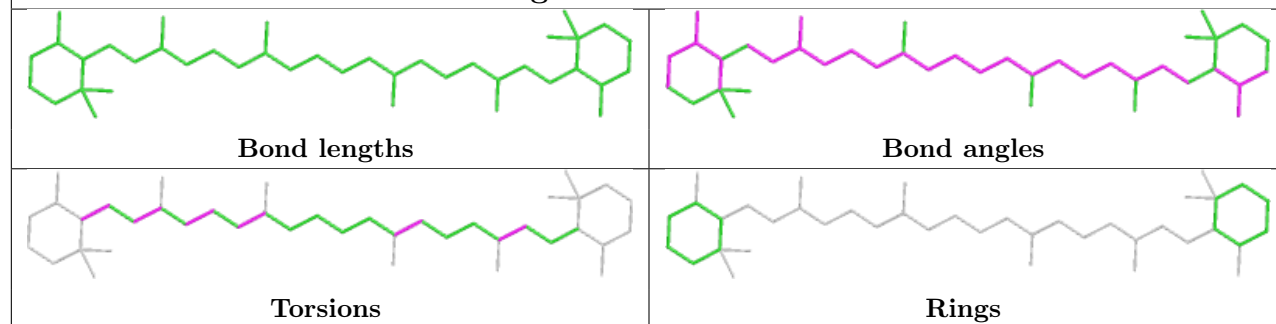




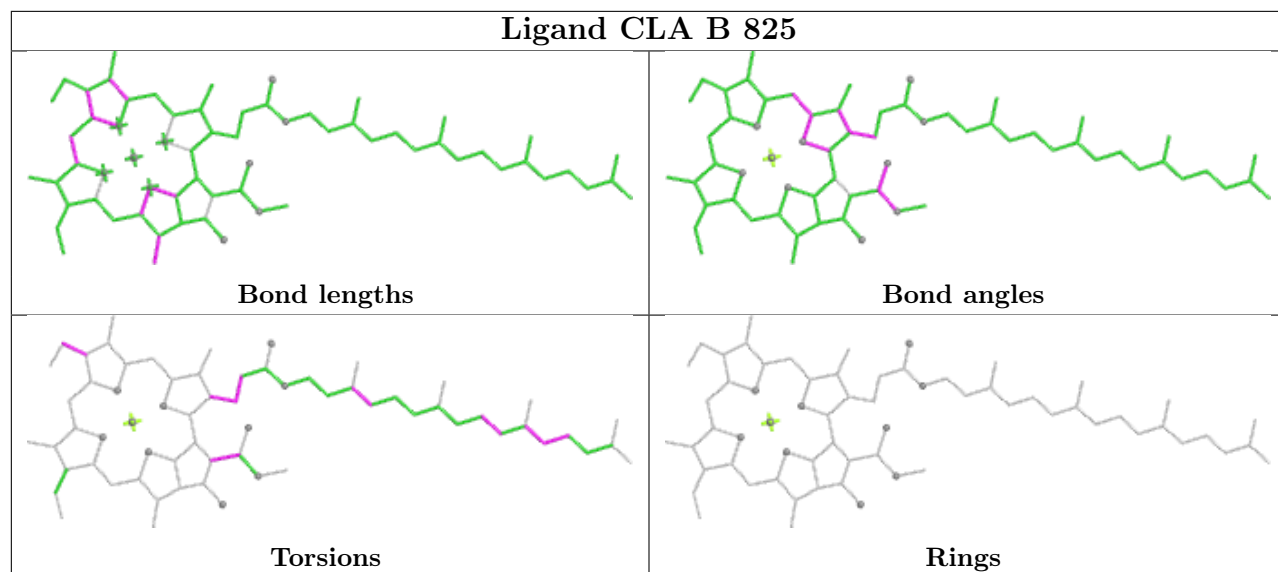
Ligand CLA F 301



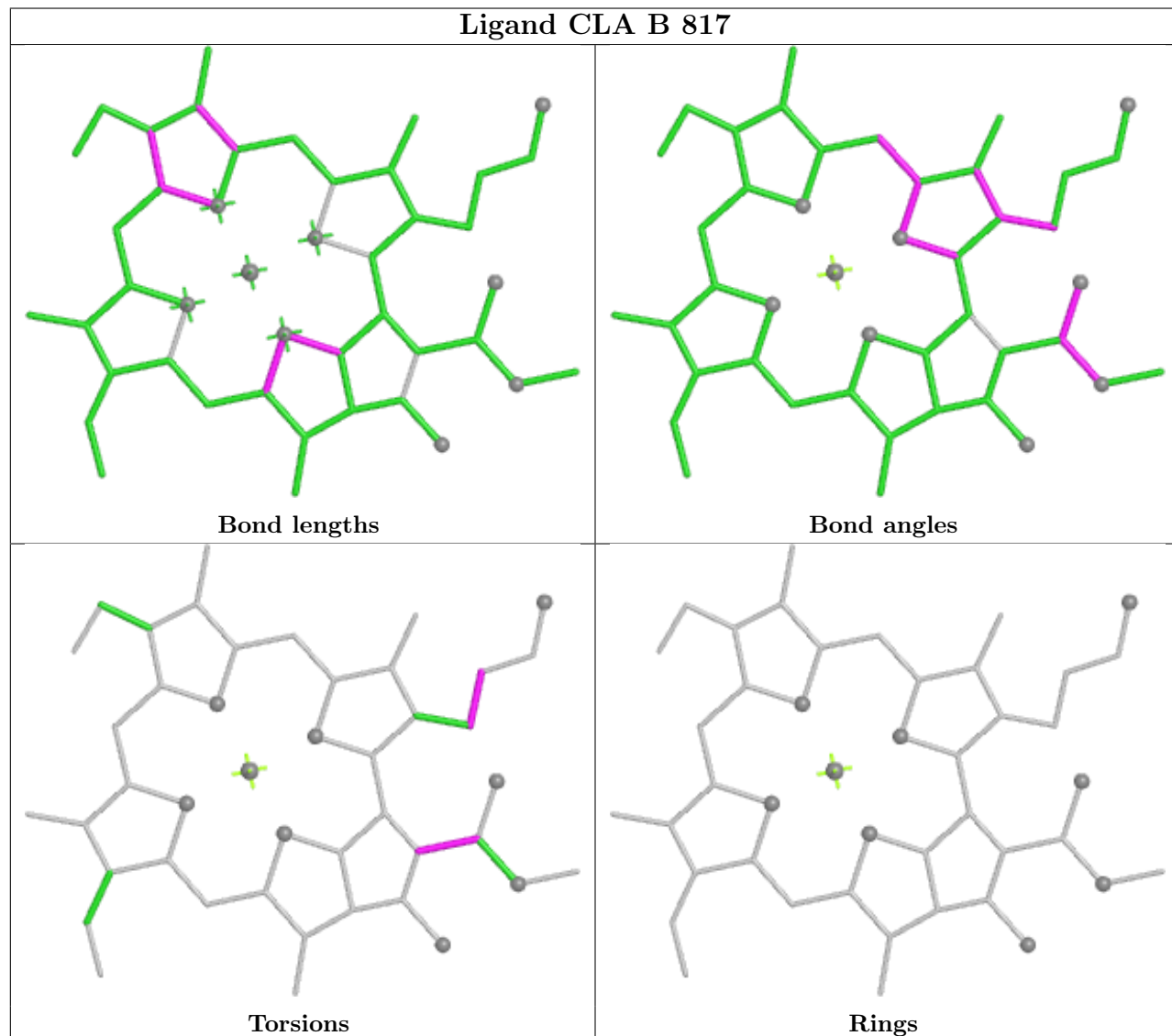
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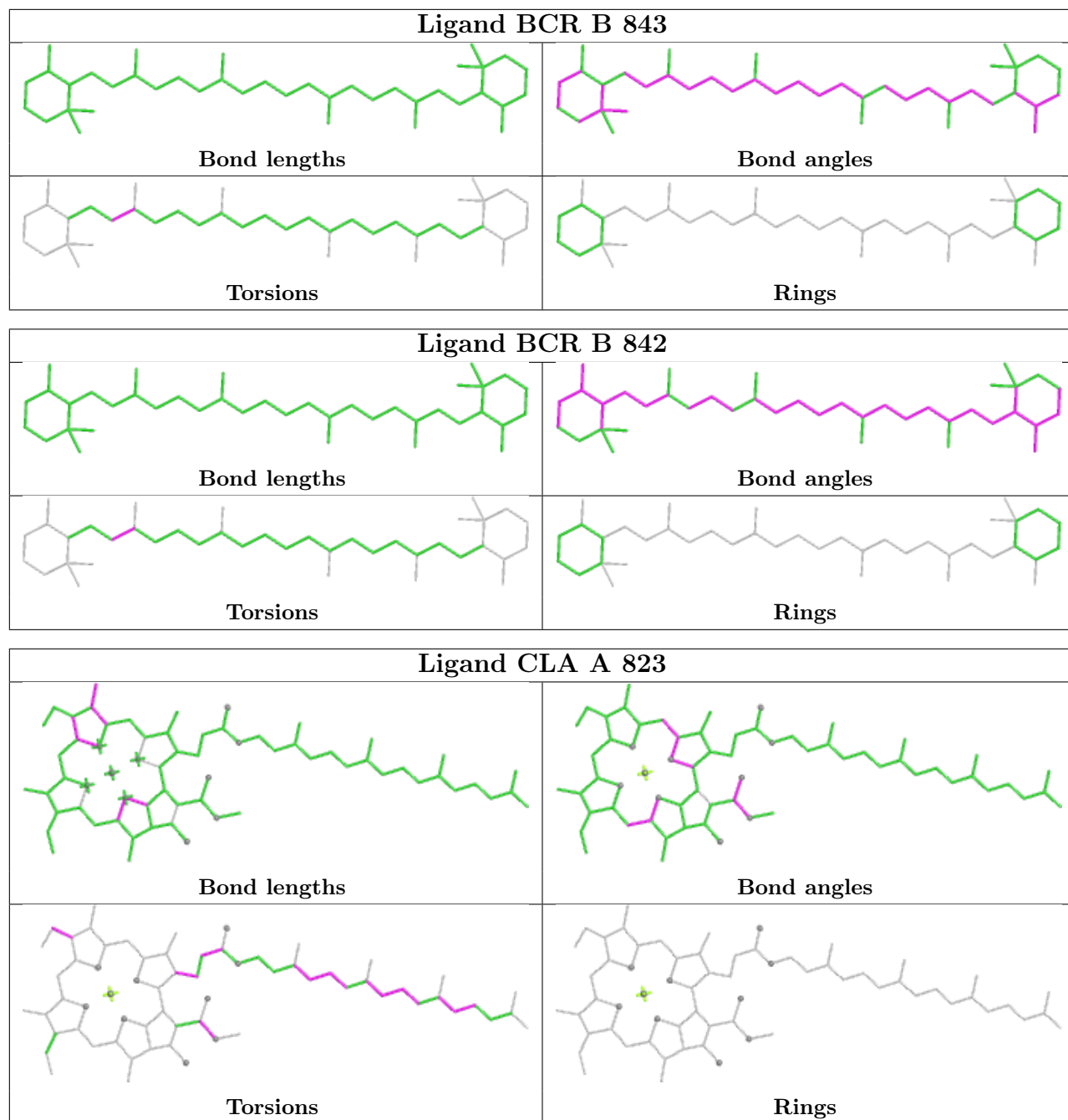


Ligand CLA B 825

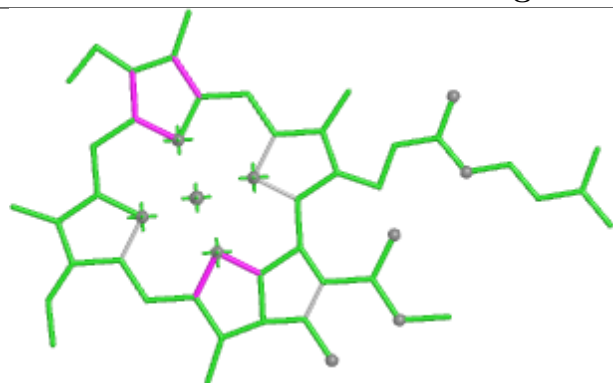


Ligand CLA B 817

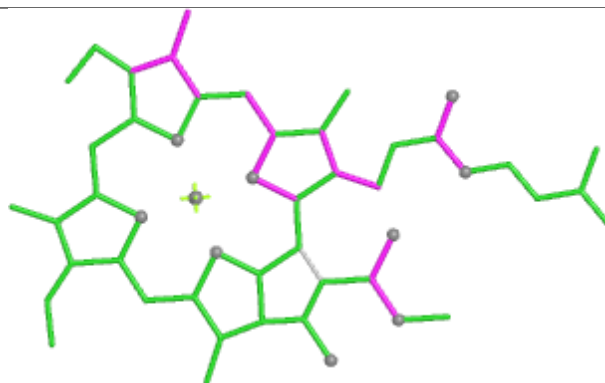




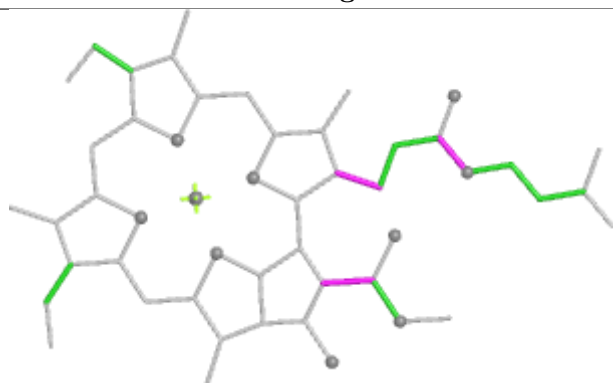
Ligand CLA A 835



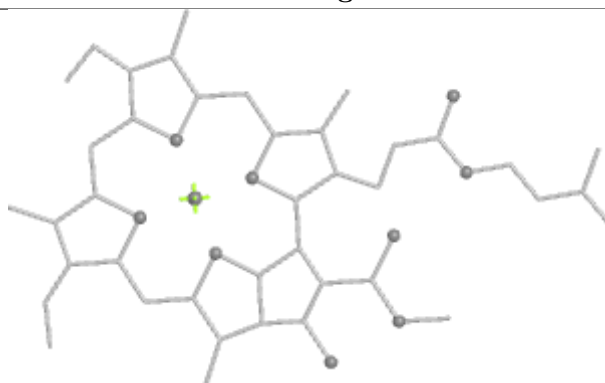
Bond lengths



Bond angles

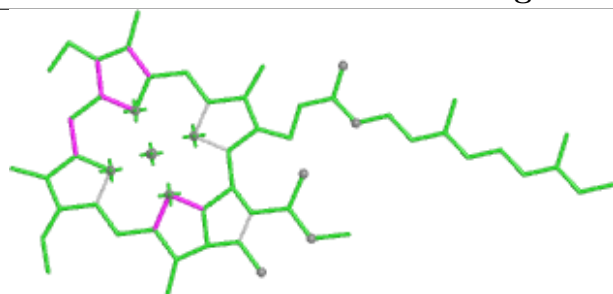


Torsions

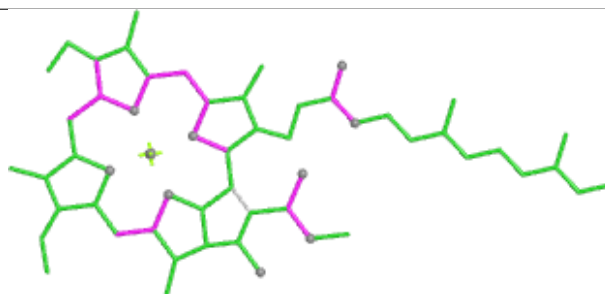


Rings

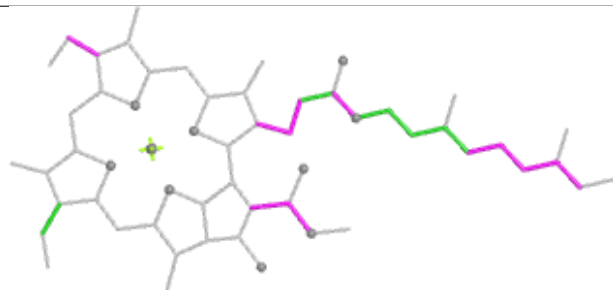
Ligand CLA B 823



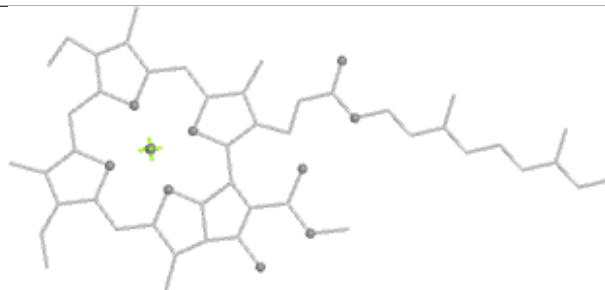
Bond lengths



Bond angles

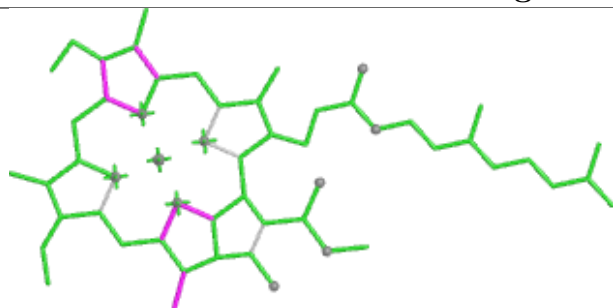


Torsions

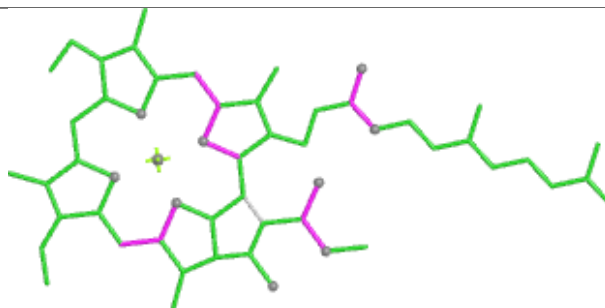


Rings

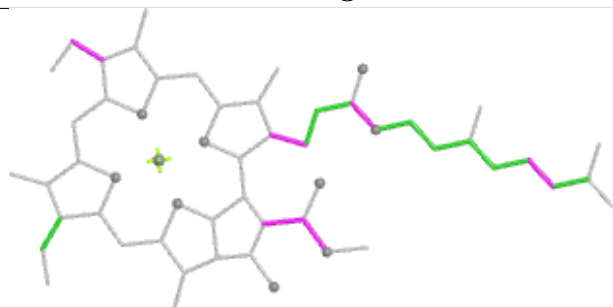
Ligand CLA B 828



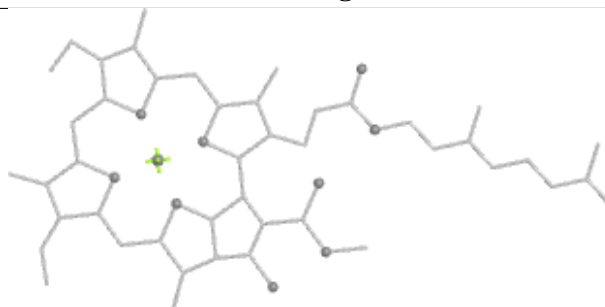
Bond lengths



Bond angles

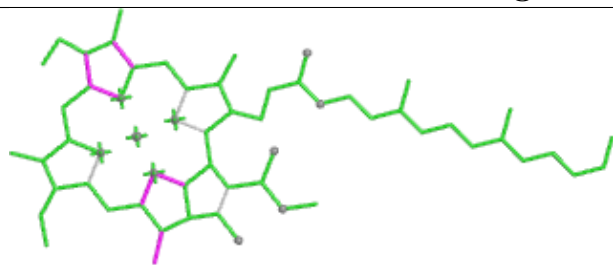


Torsions

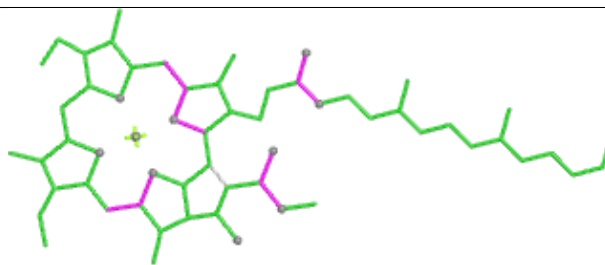


Rings

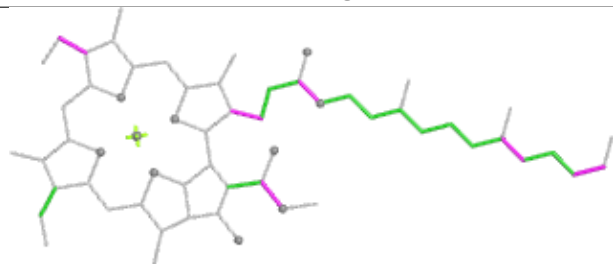
Ligand CLA A 810



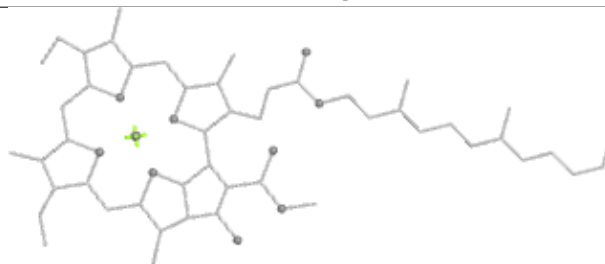
Bond lengths



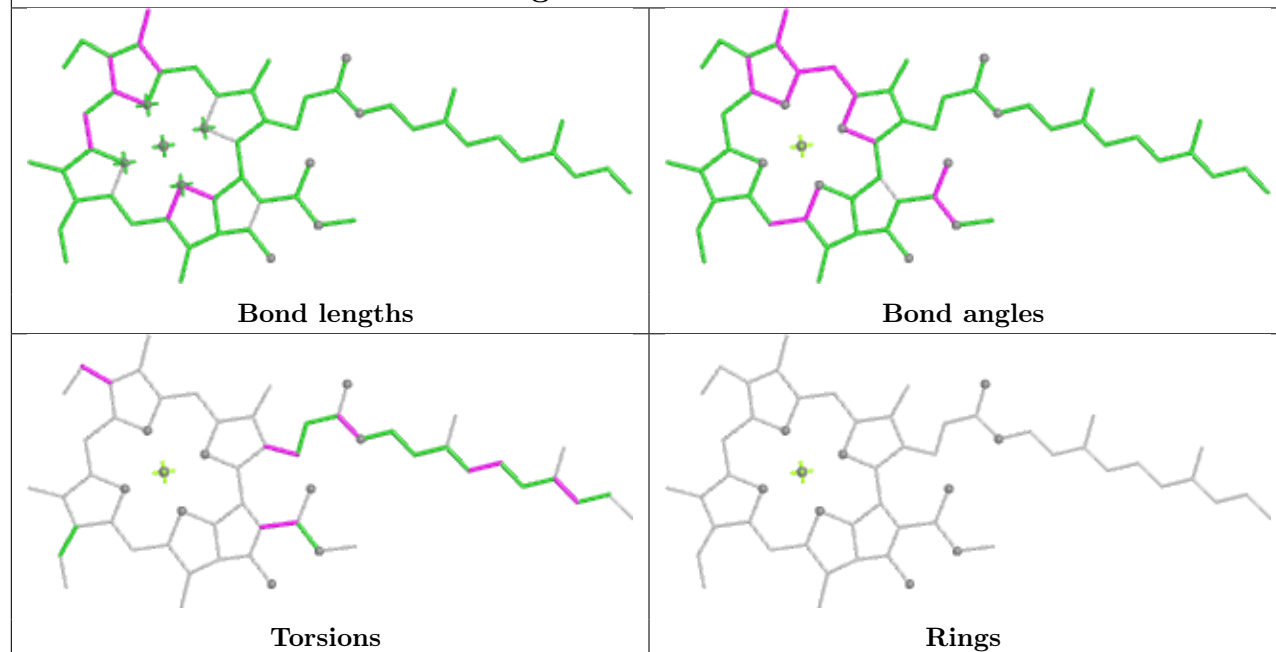
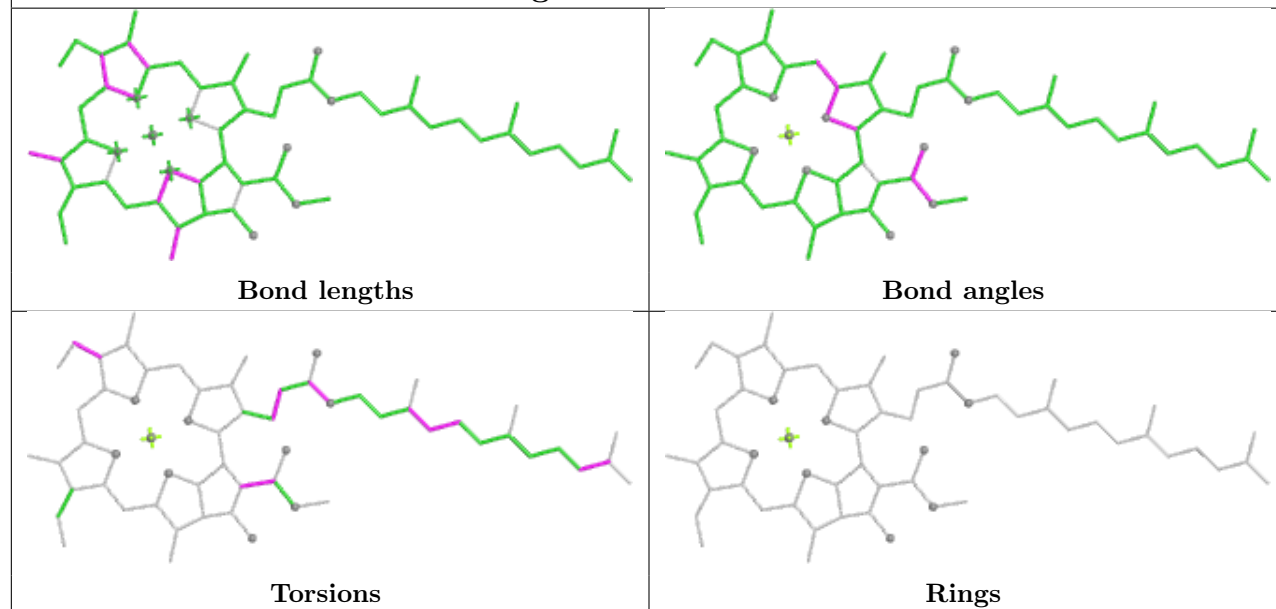
Bond angles

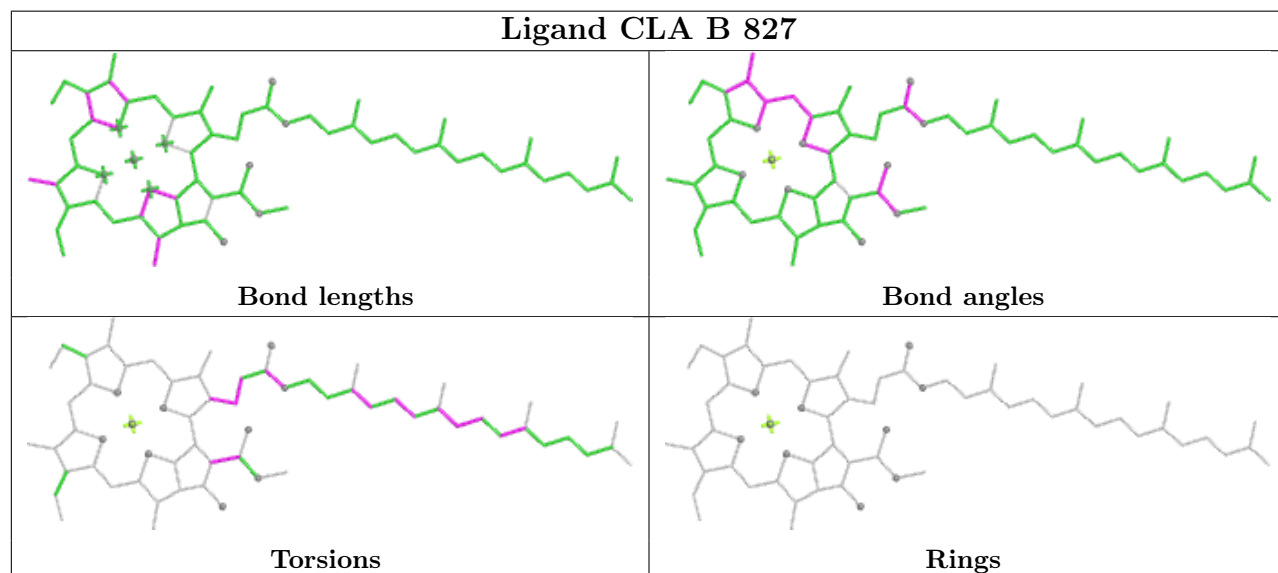
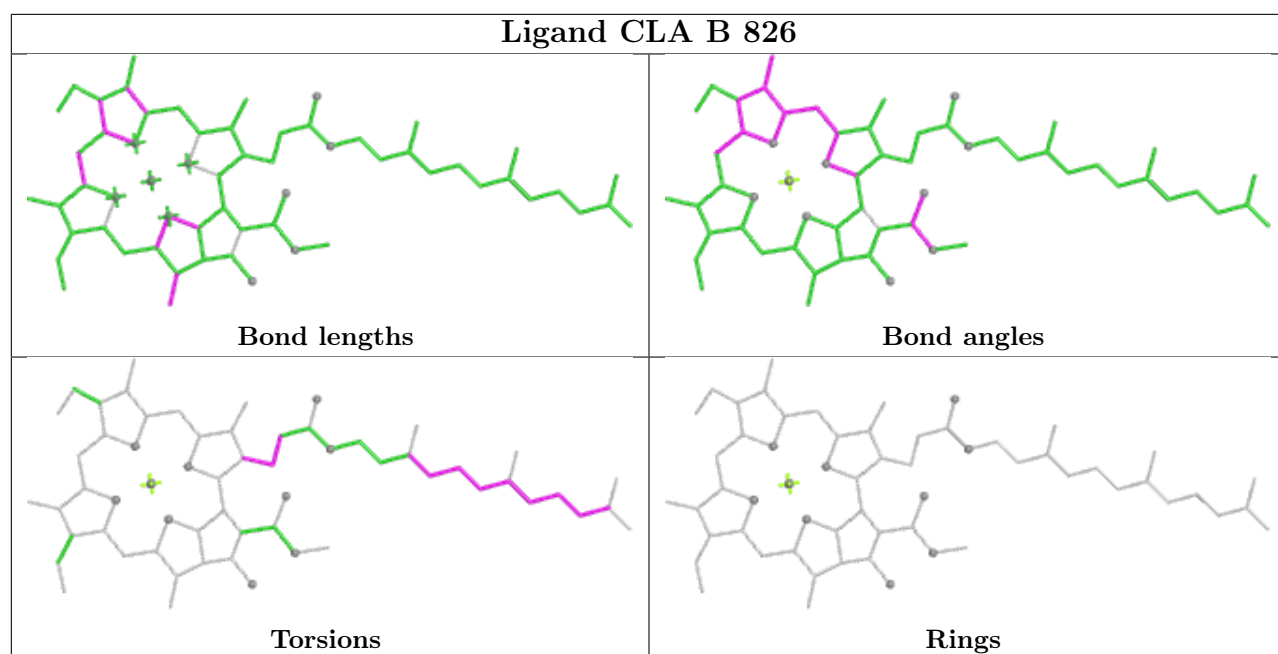


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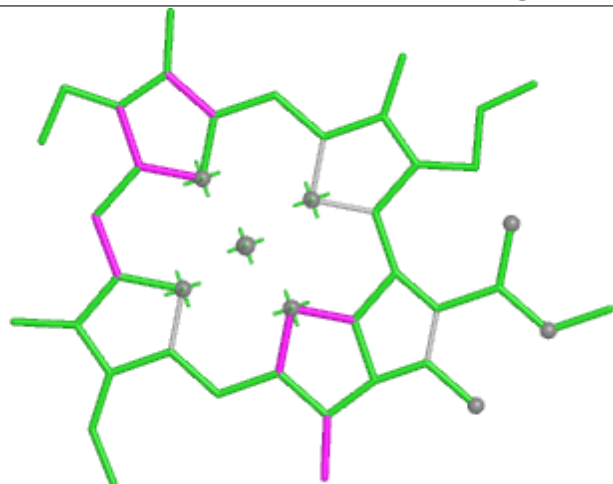


Rings

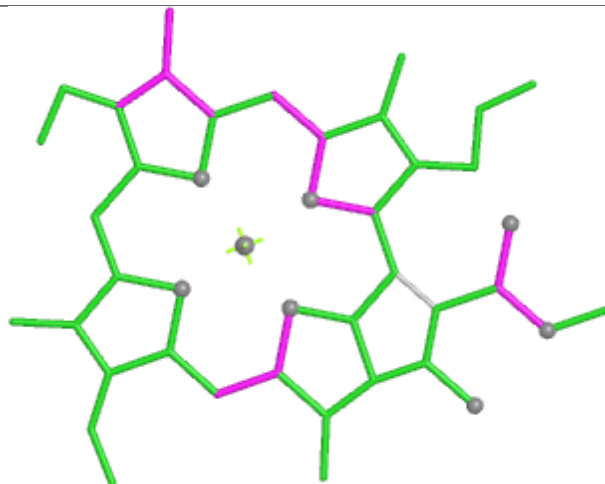
Ligand CLA A 833**Ligand CLA A 816**



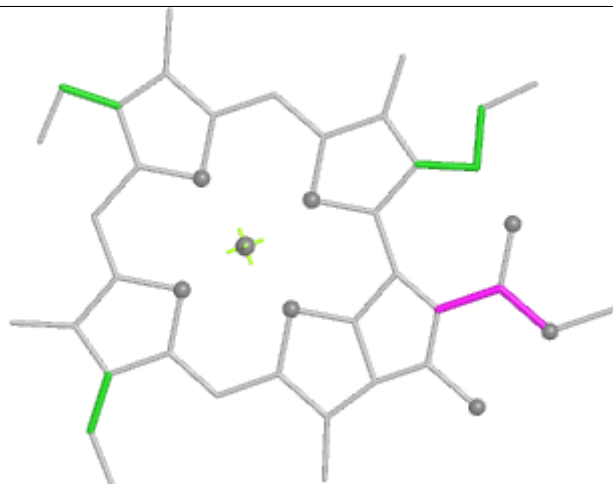
Ligand CLA A 813



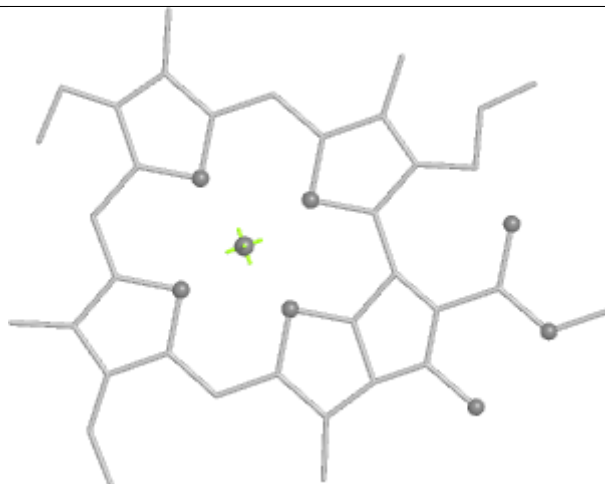
Bond lengths



Bond angles

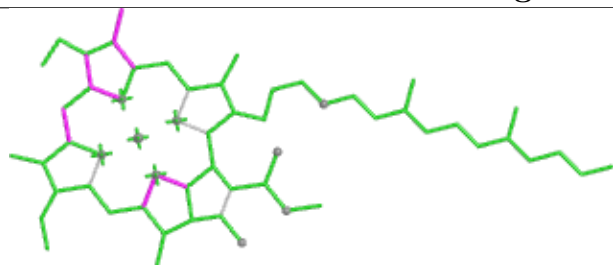


Torsions

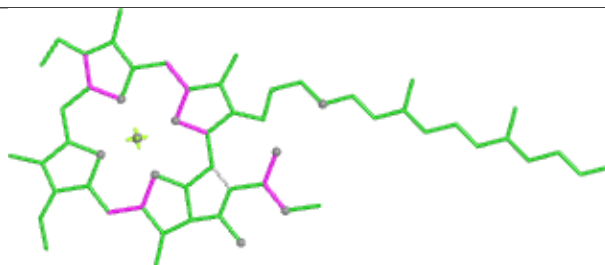


Rings

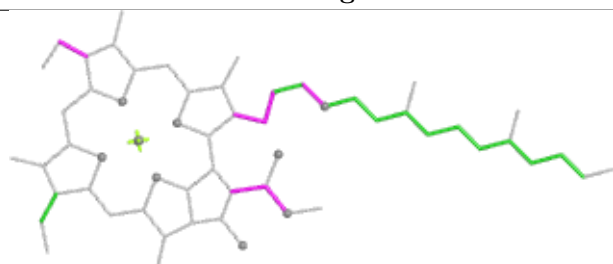
Ligand CLA B 814



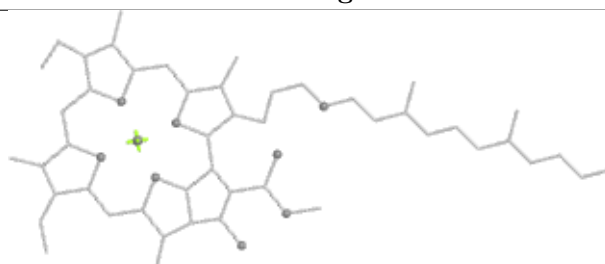
Bond lengths



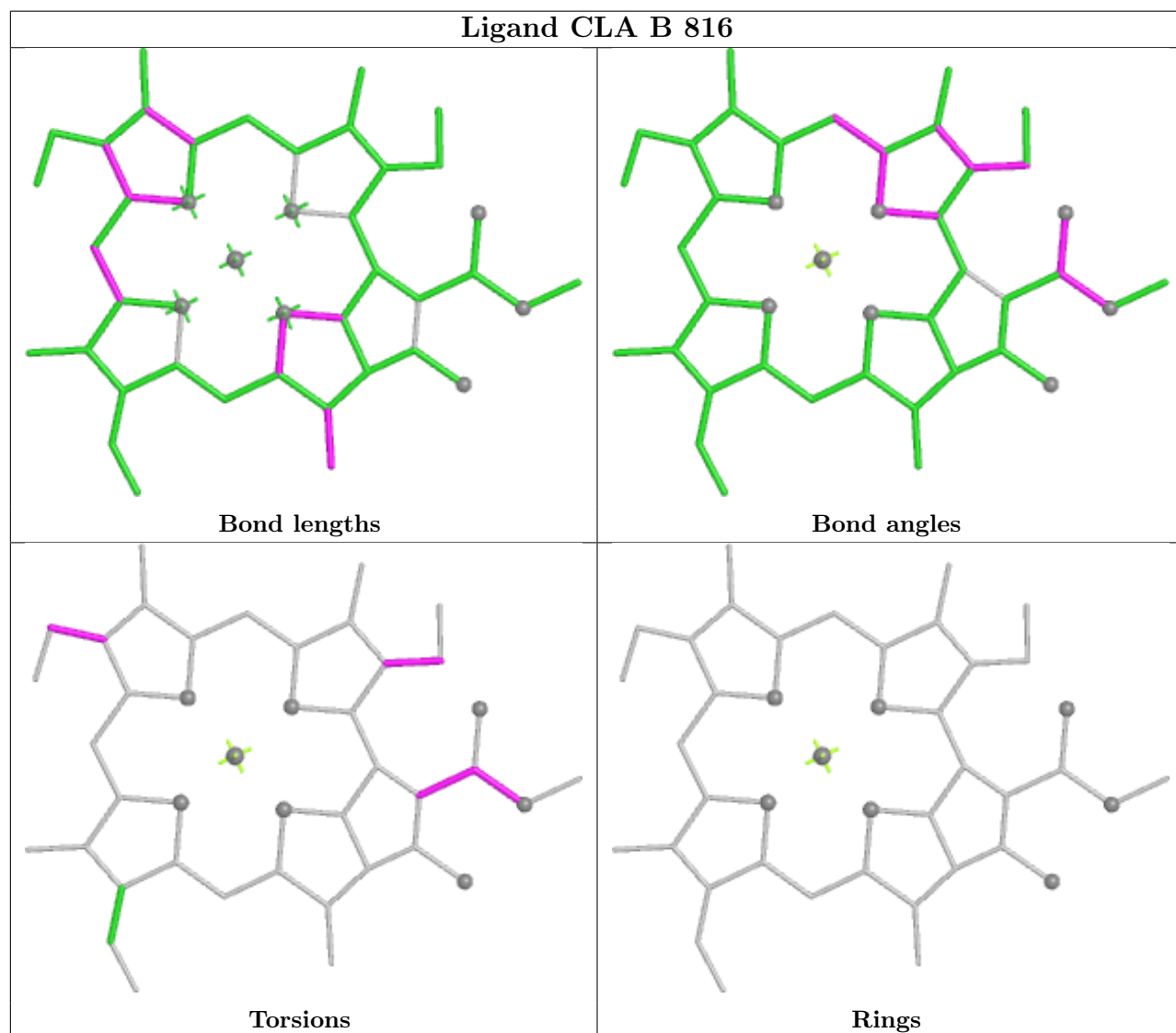
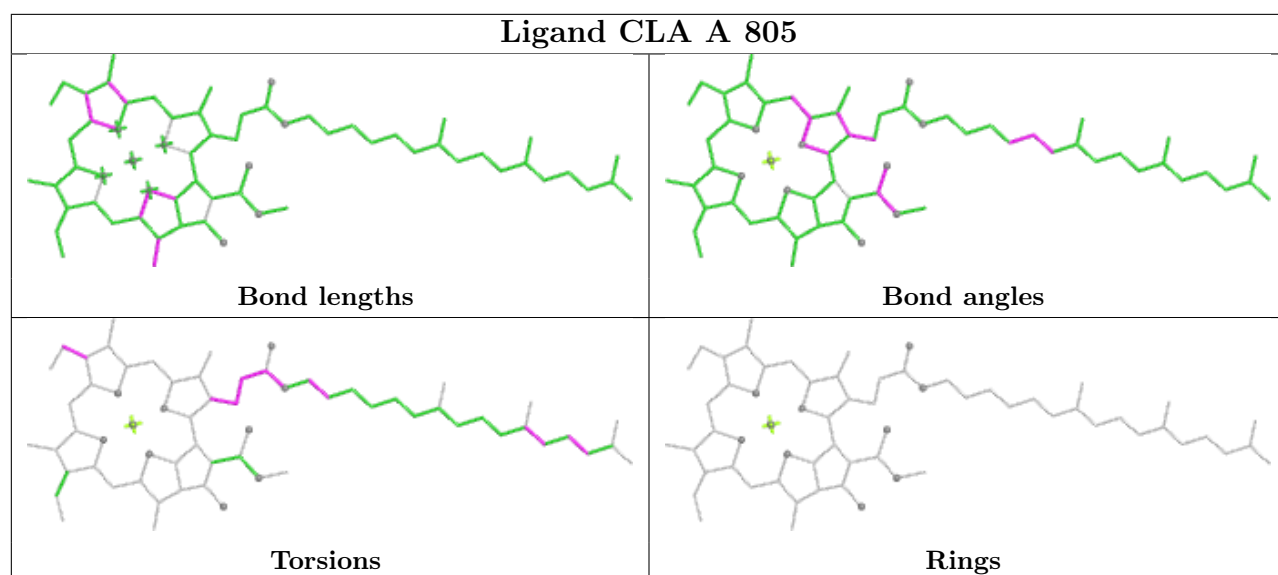
Bond angles



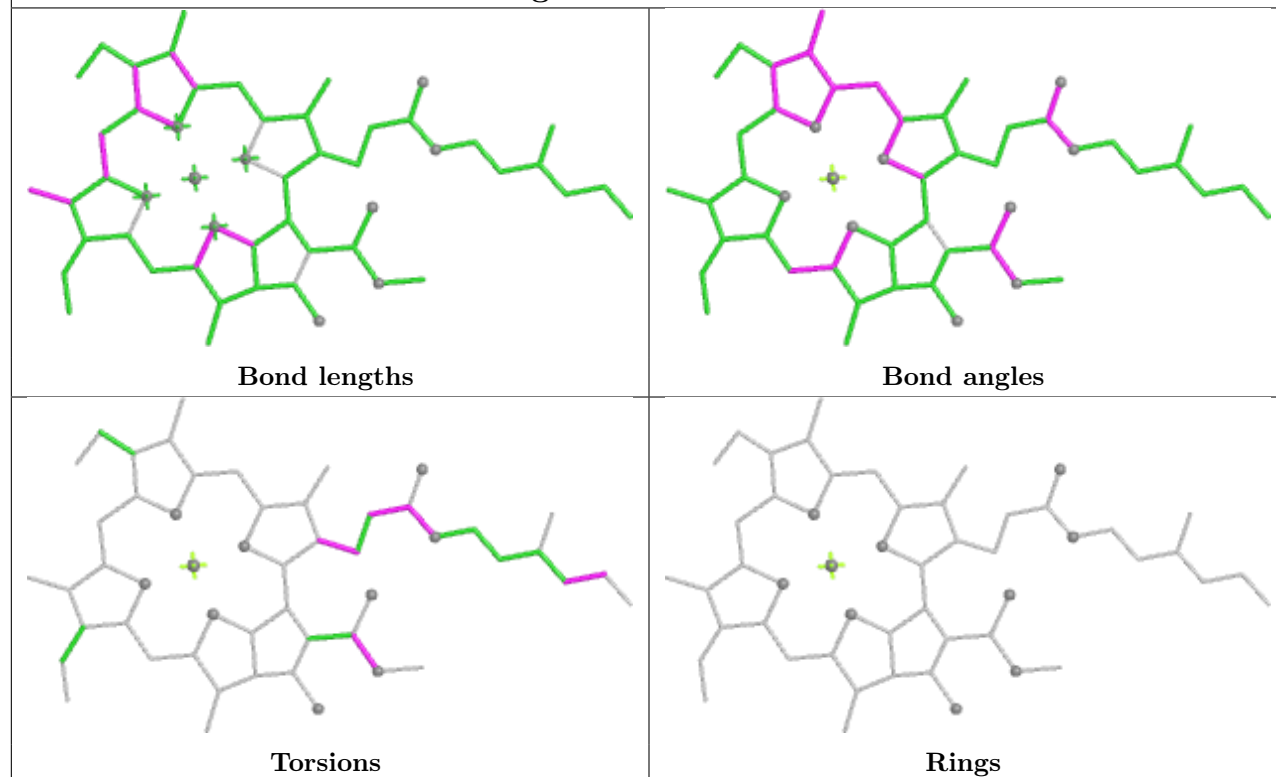
Torsions



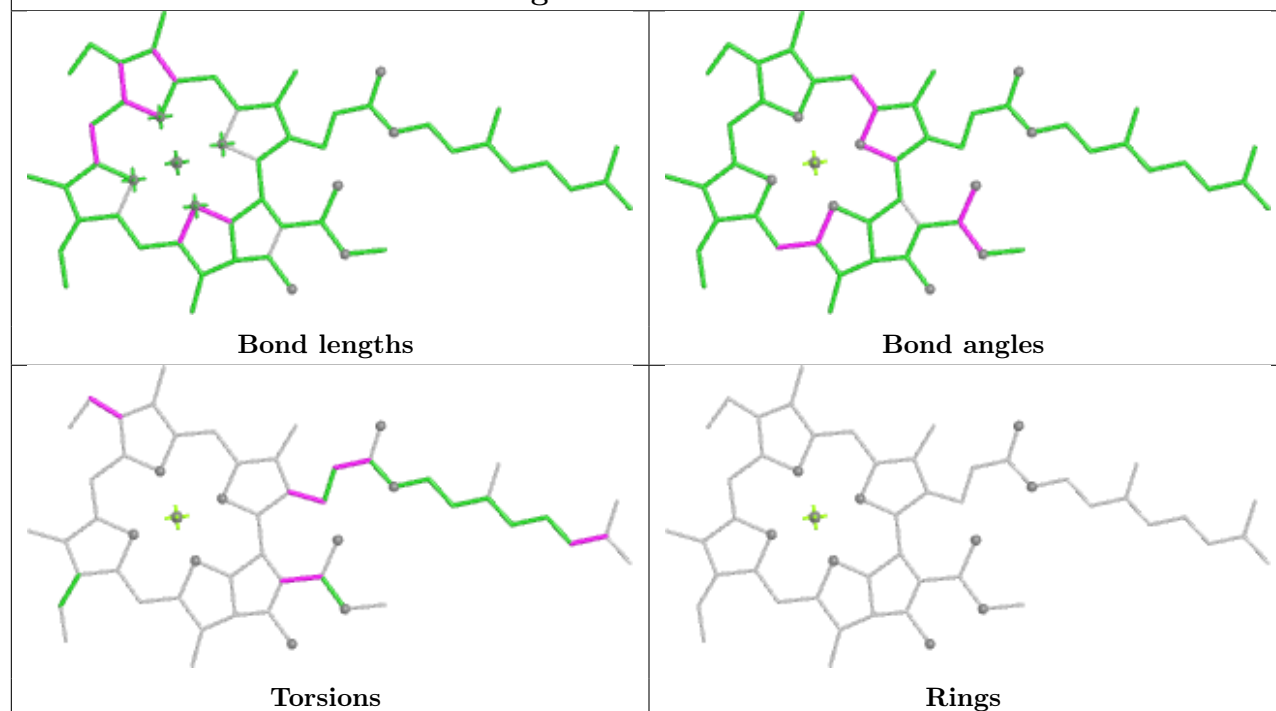
Rings



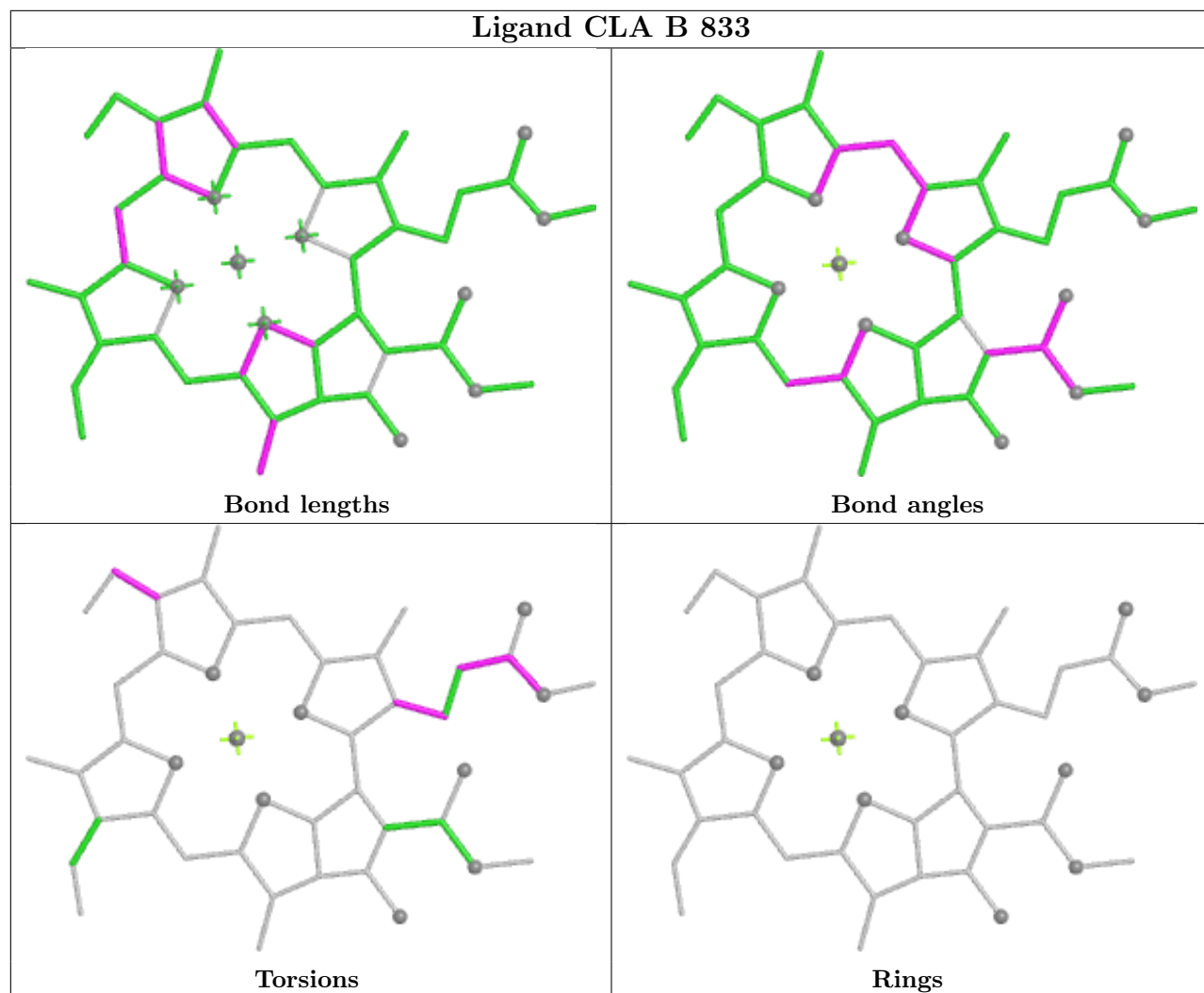
Ligand CLA A 803



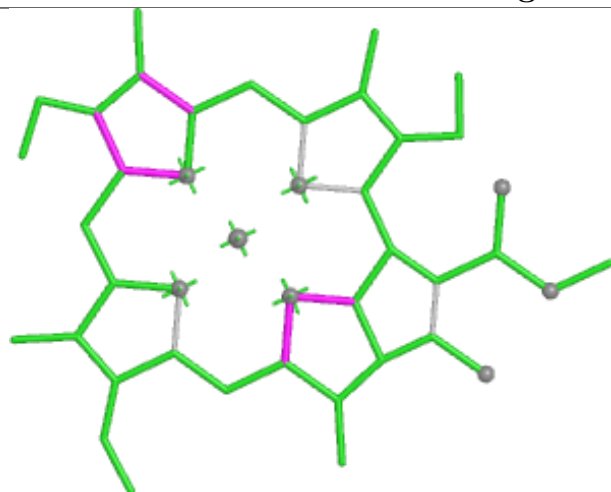
Ligand CLA K 203



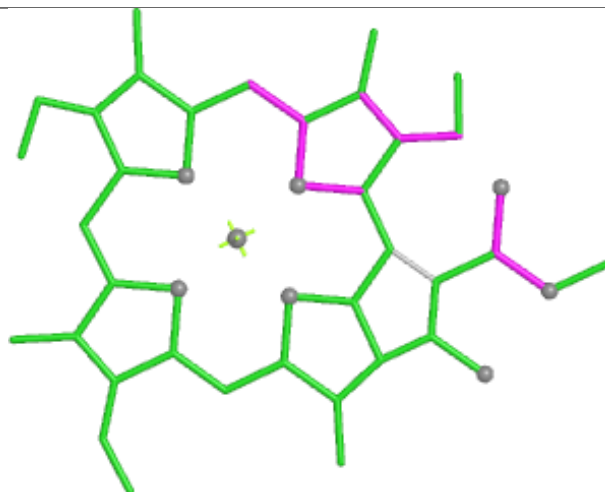
Ligand CLA B 833



Ligand CLA J 102



Bond lengths



Bond angles

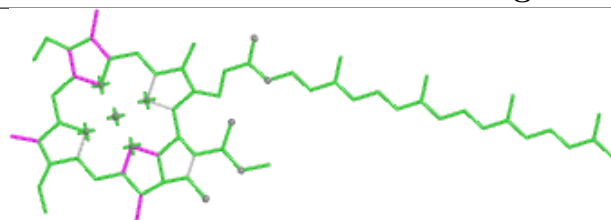


Torsions

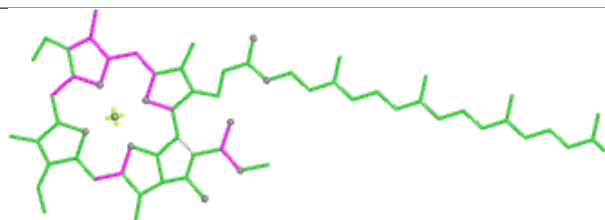


Rings

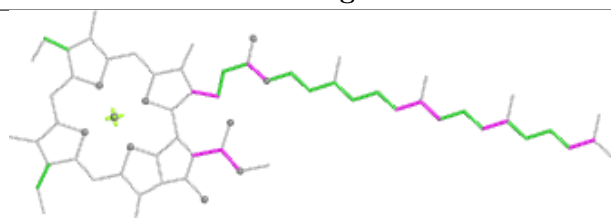
Ligand CLA A 818



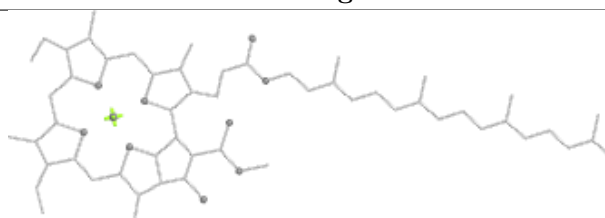
Bond lengths



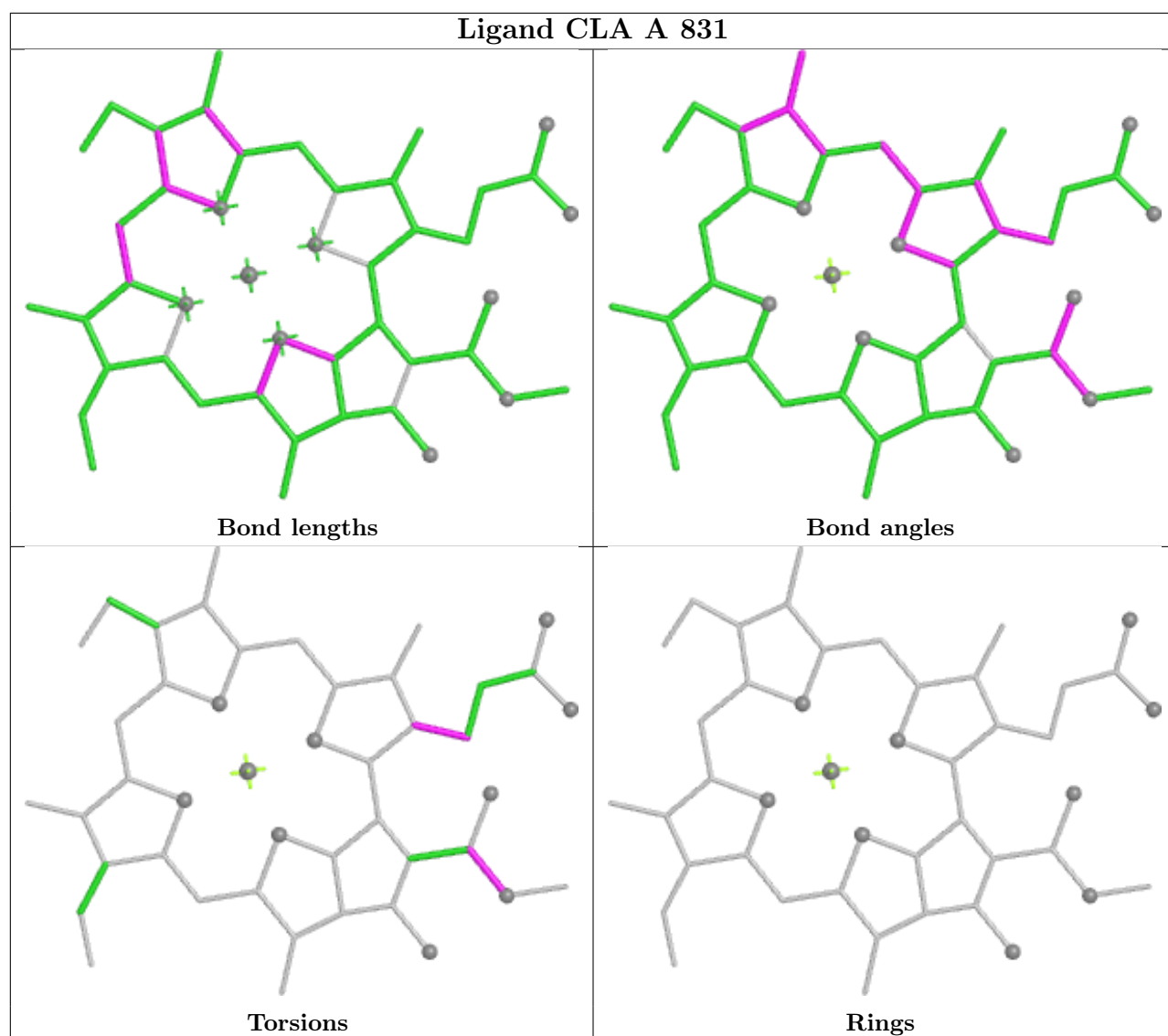
Bond angles



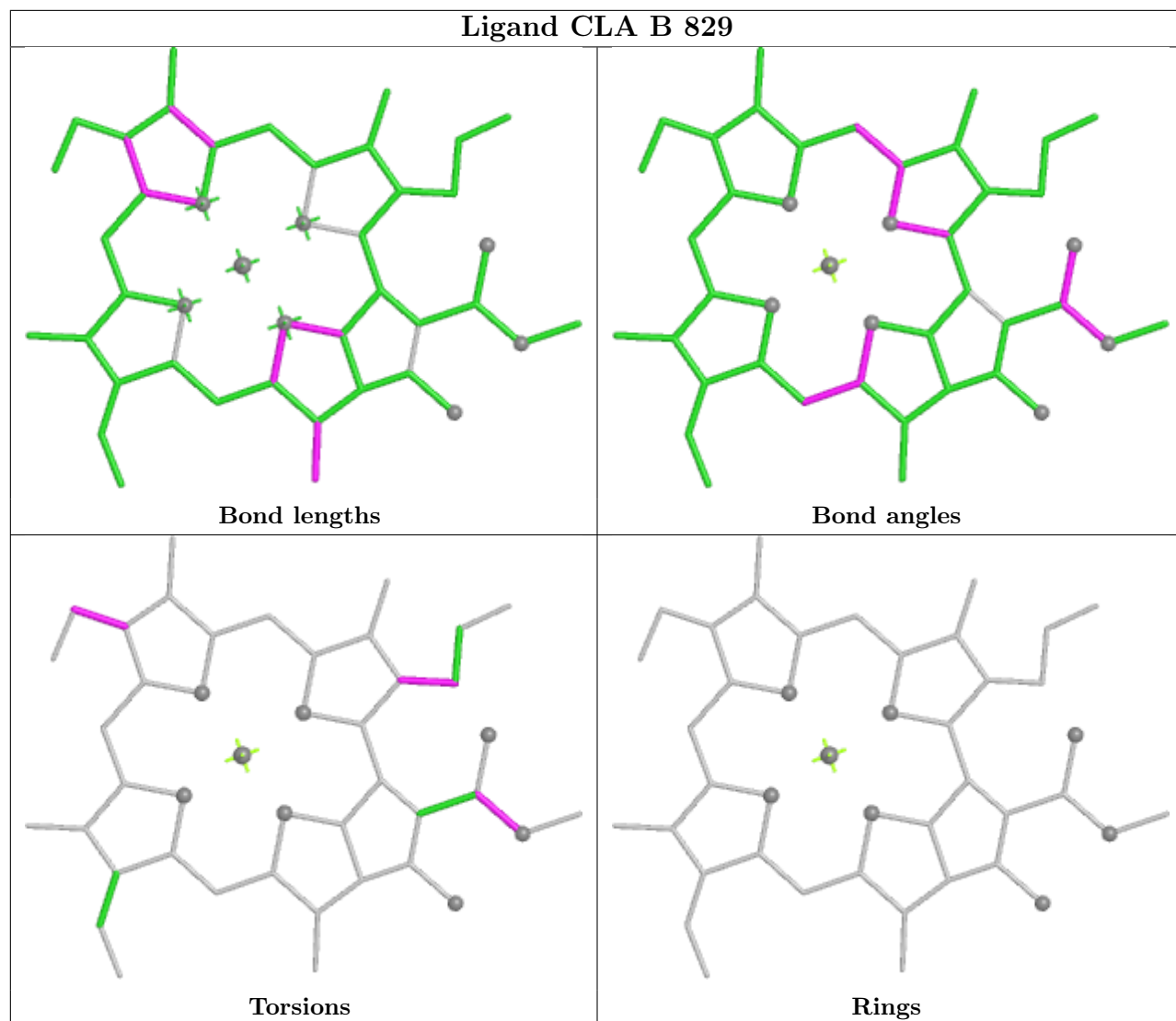
Torsions



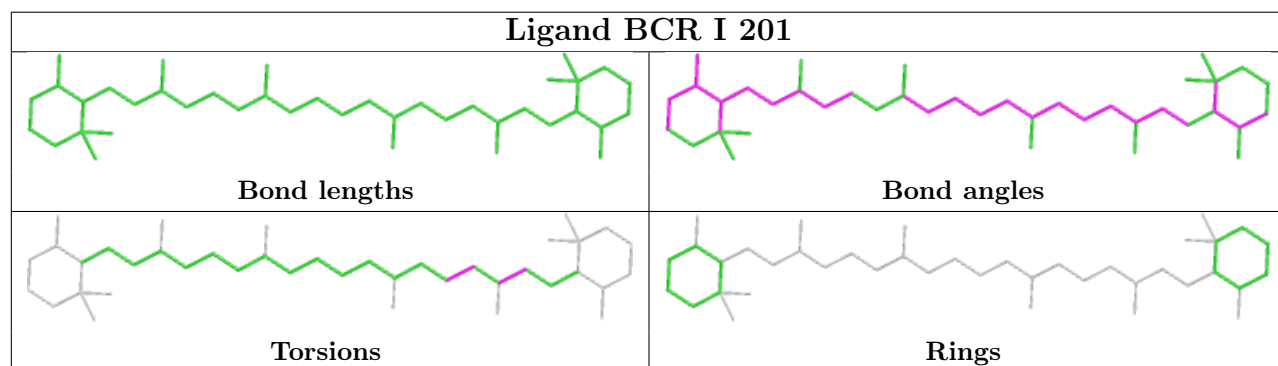
Rings



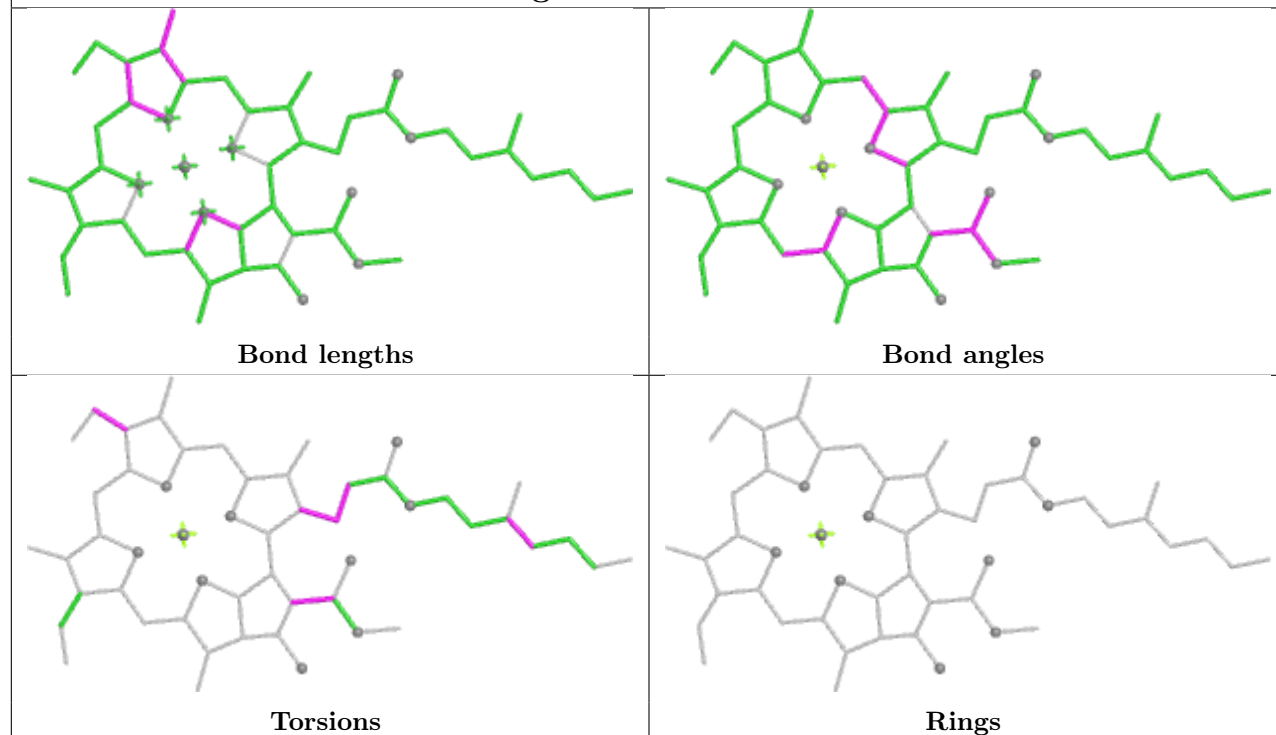
Ligand CLA B 829



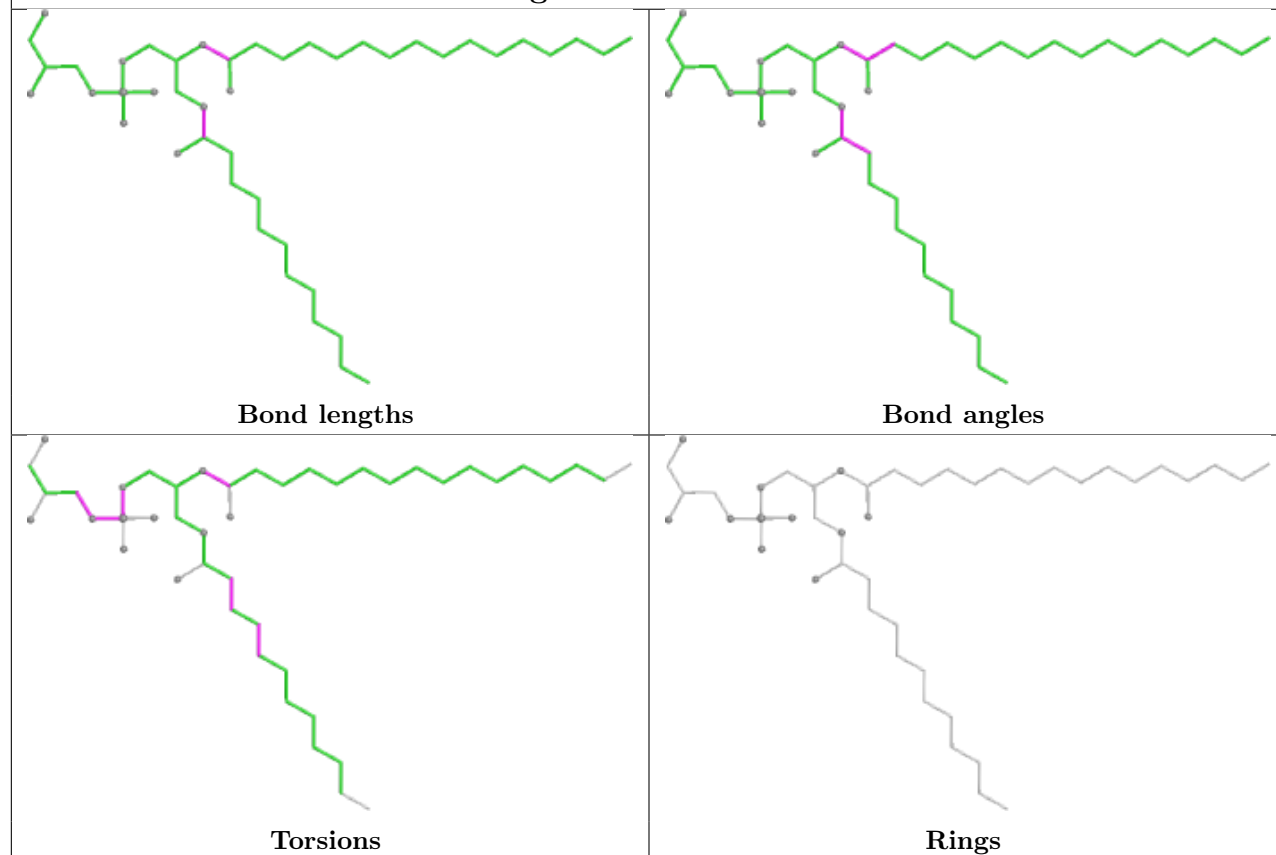
Ligand BCR I 201



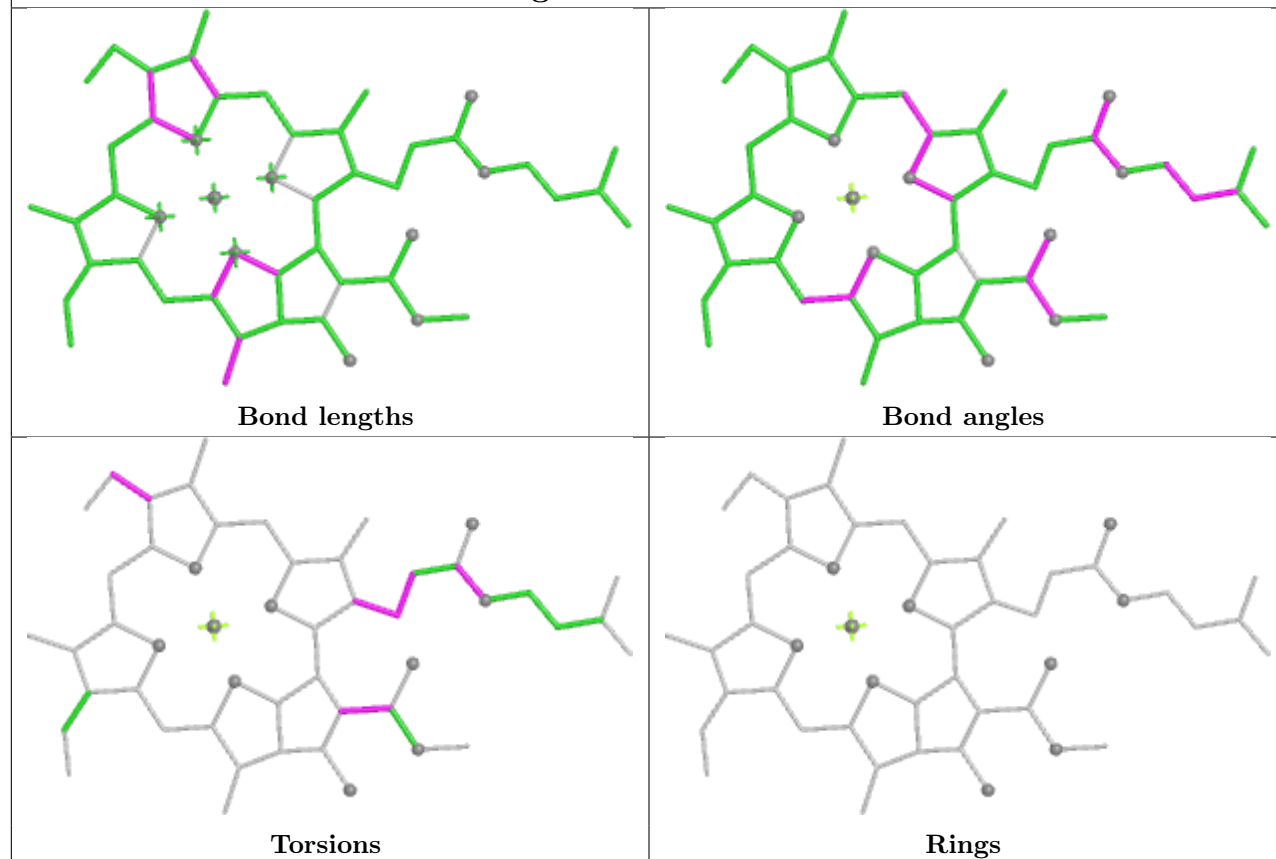
Ligand CLA B 822



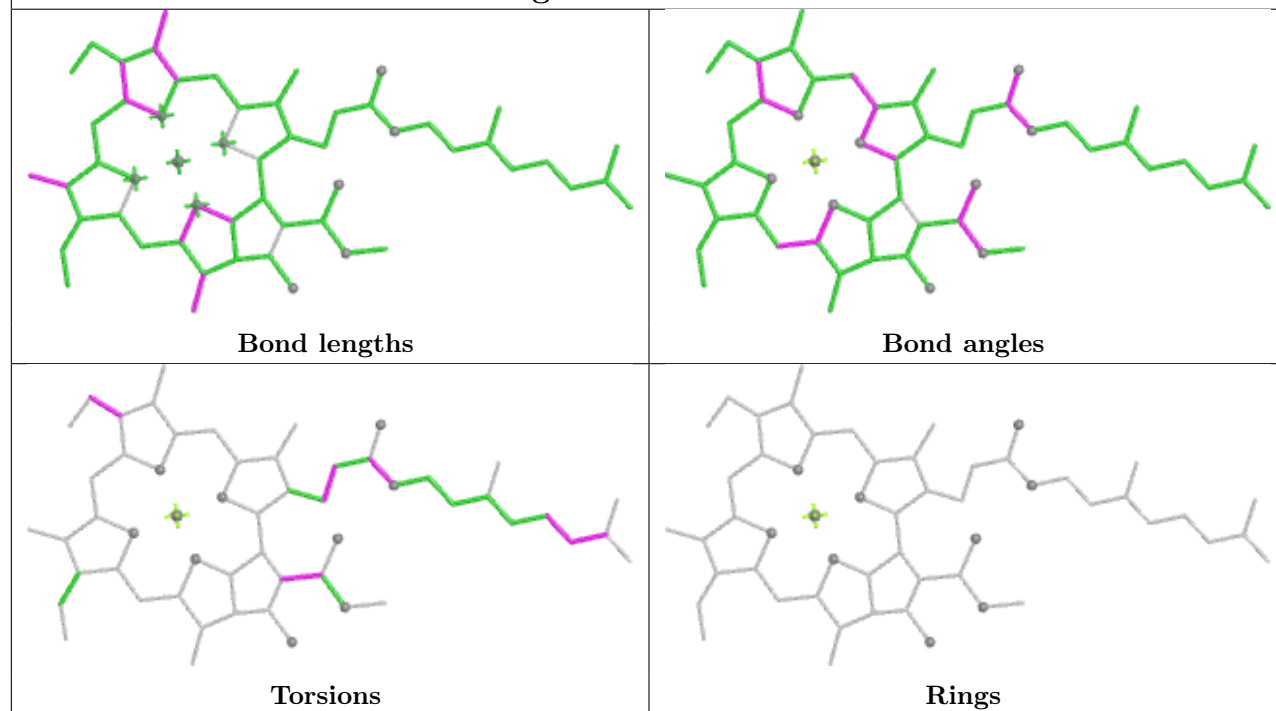
Ligand LHG A 843

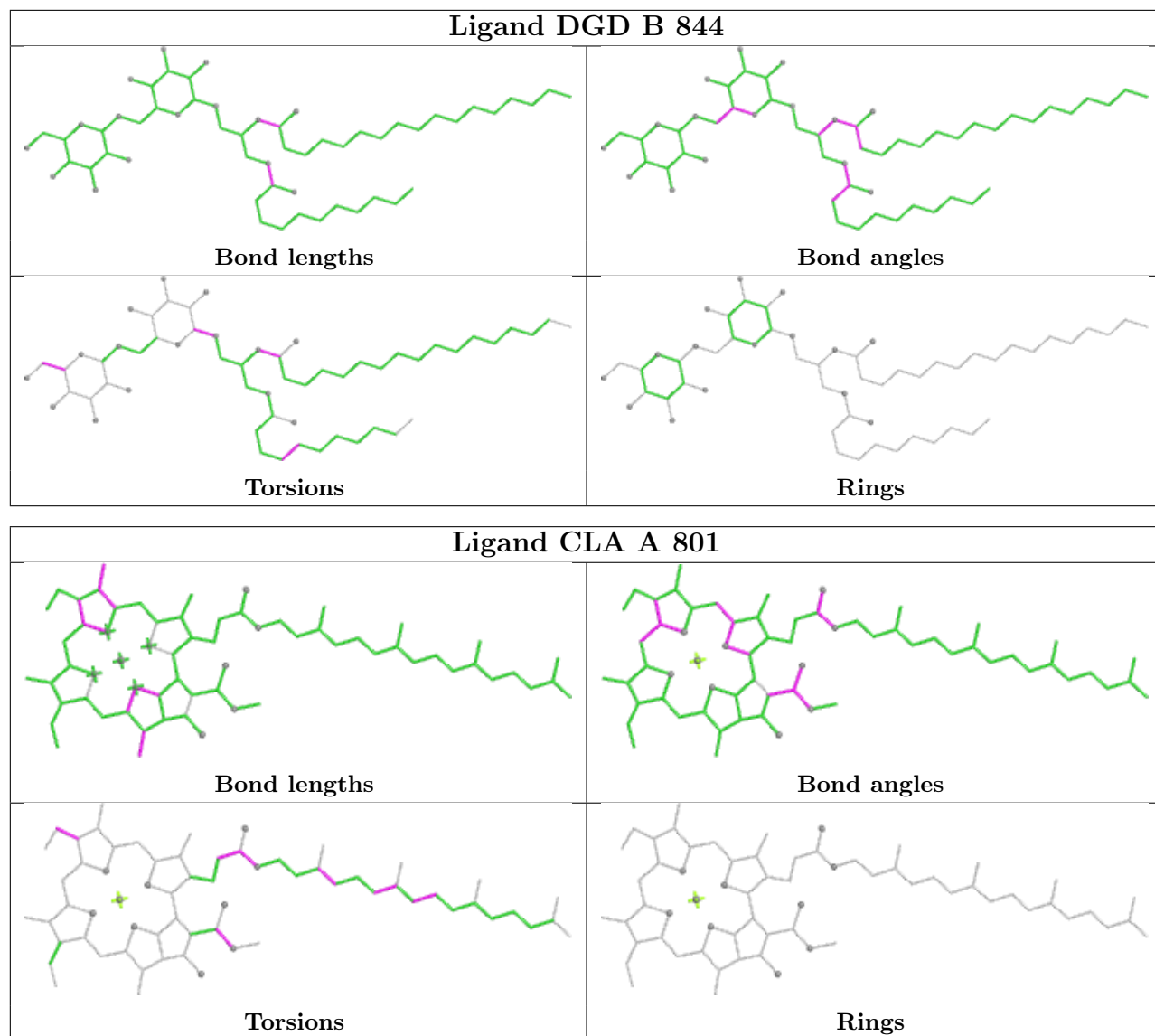


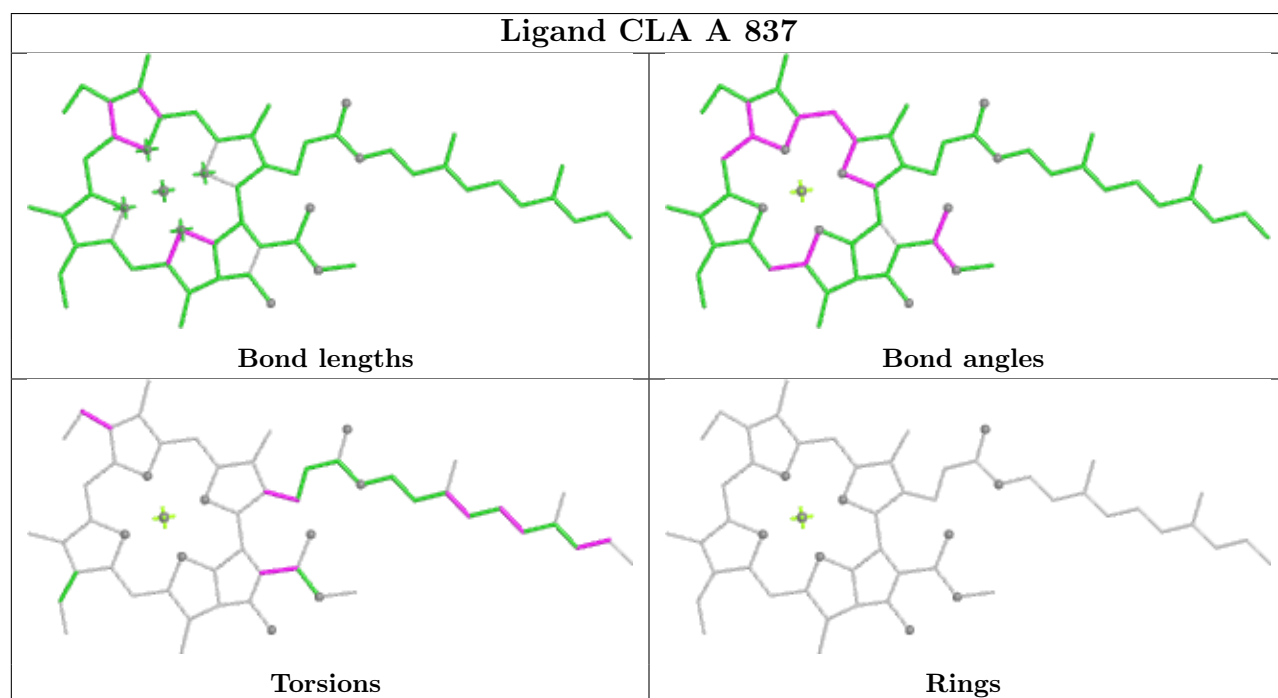
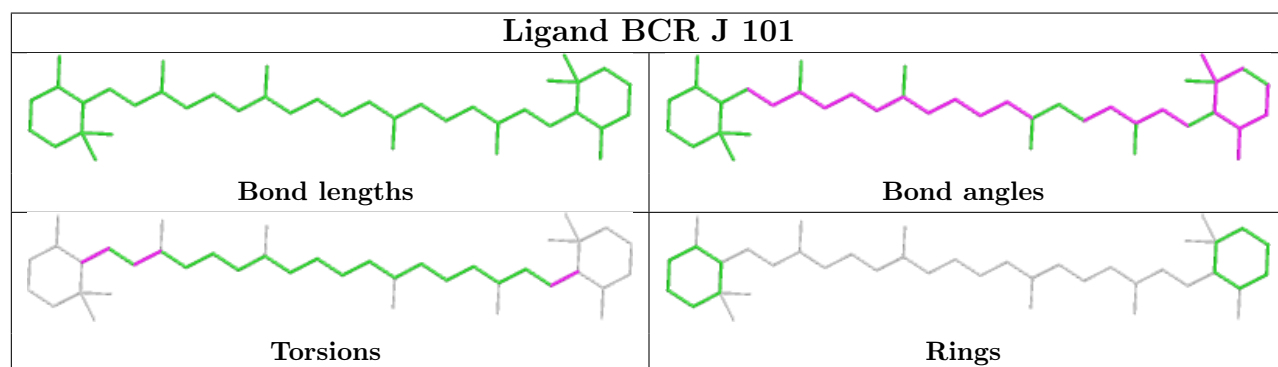
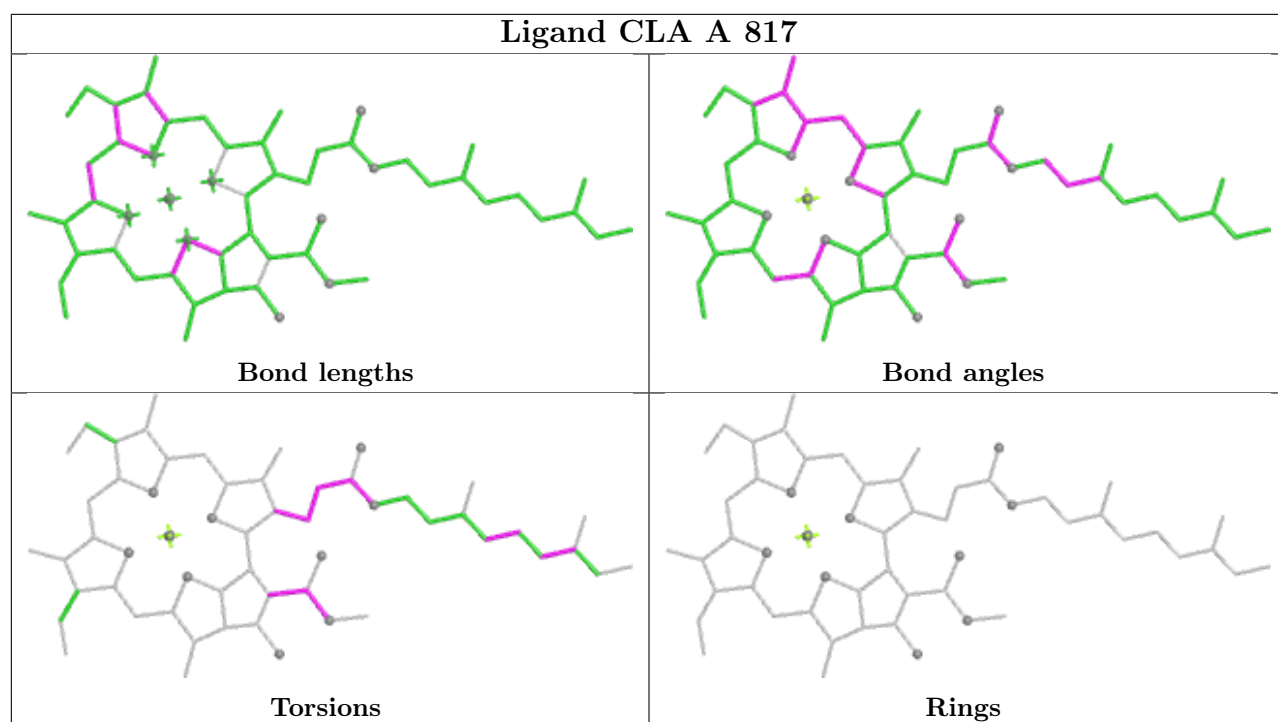
Ligand CLA A 808

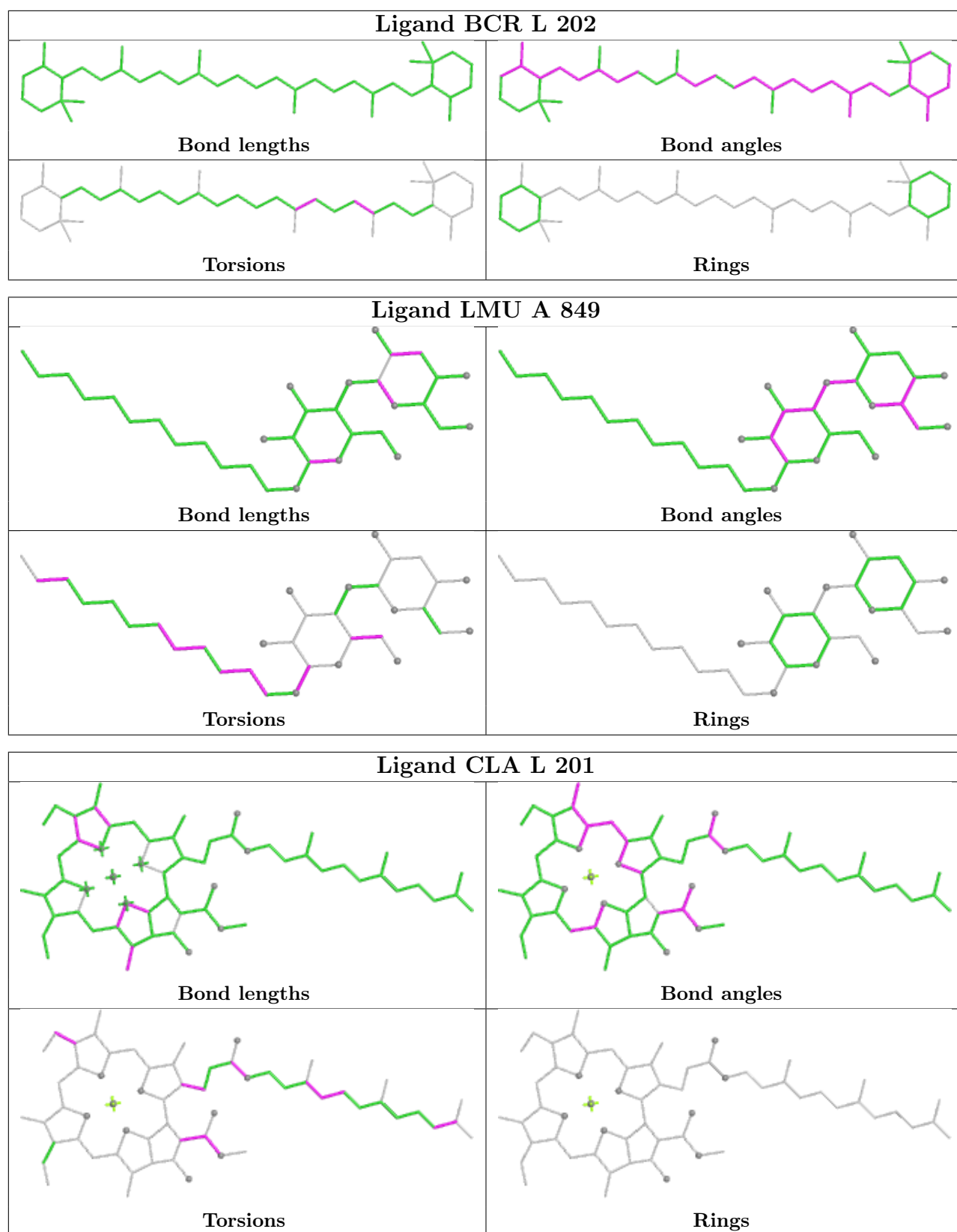


Ligand CLA B 838

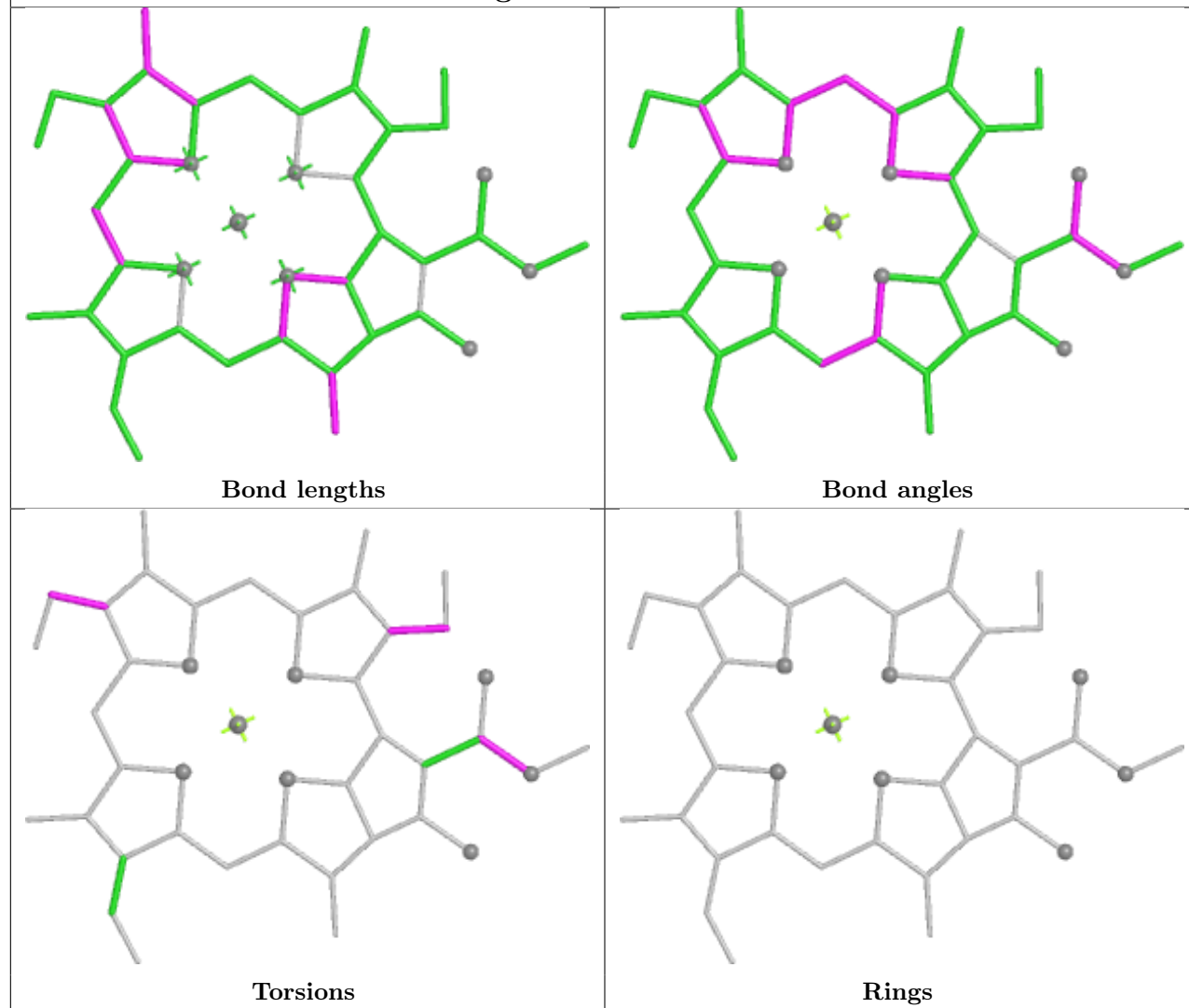




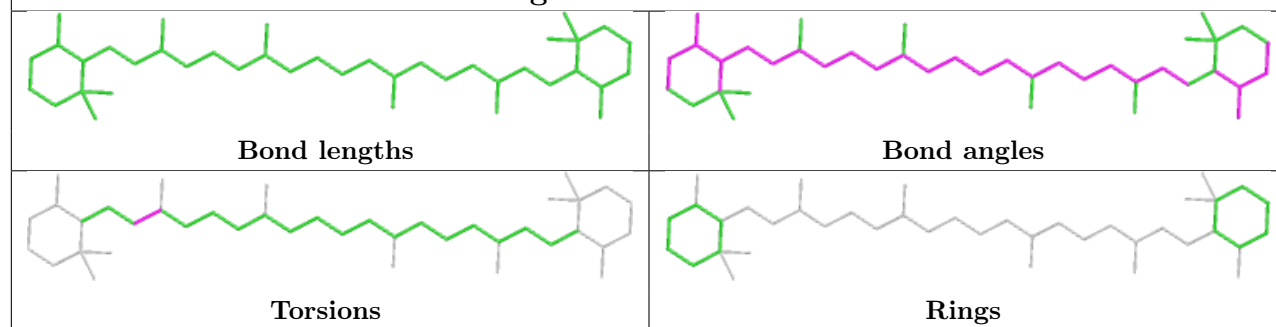


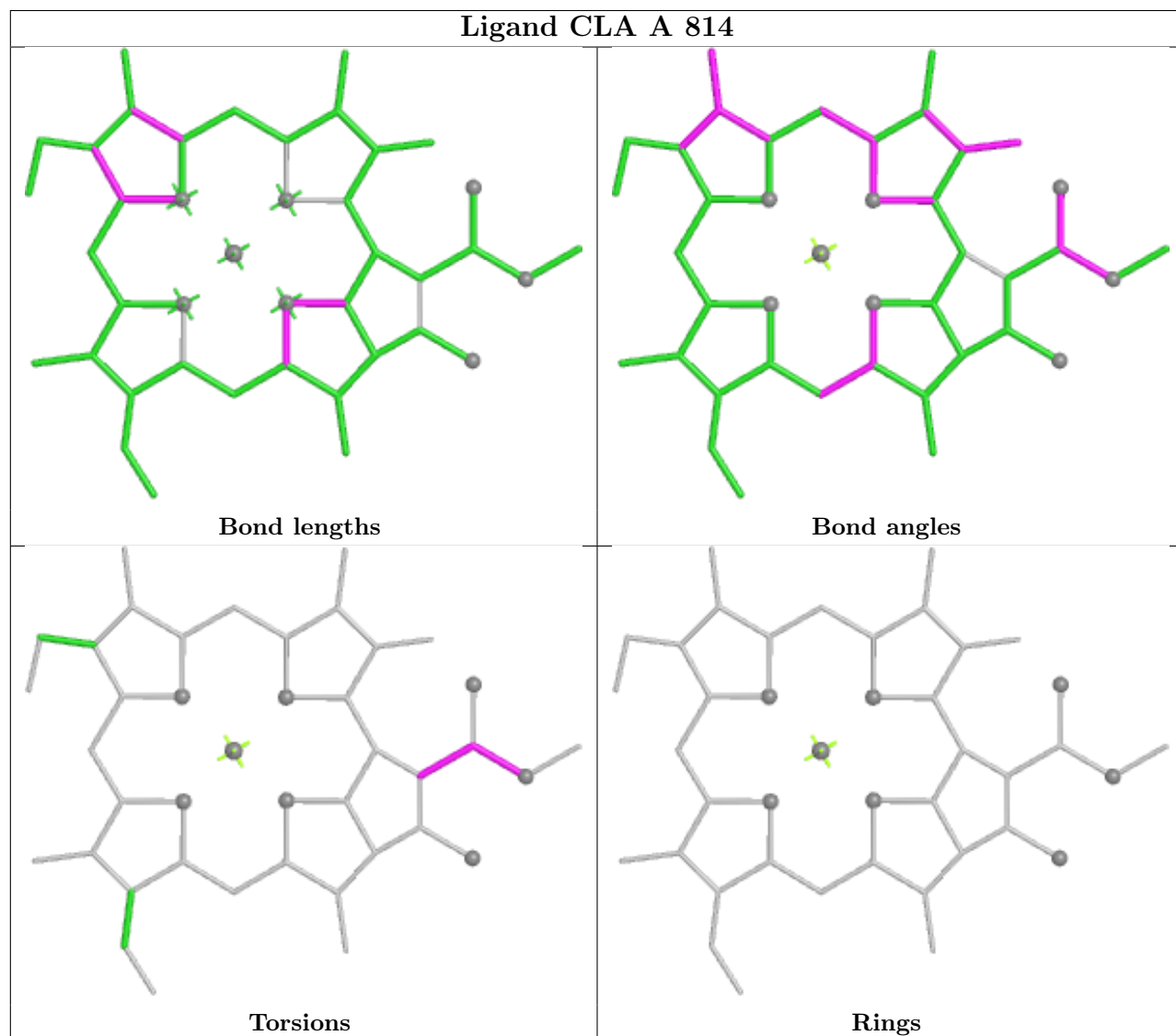
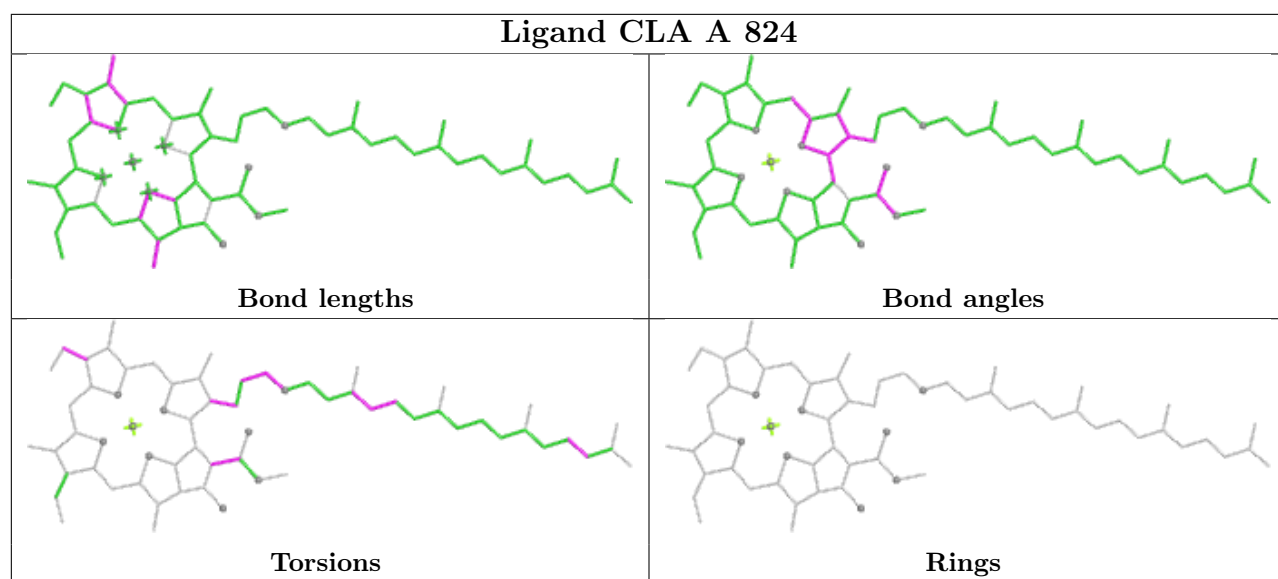


Ligand CLA A 839

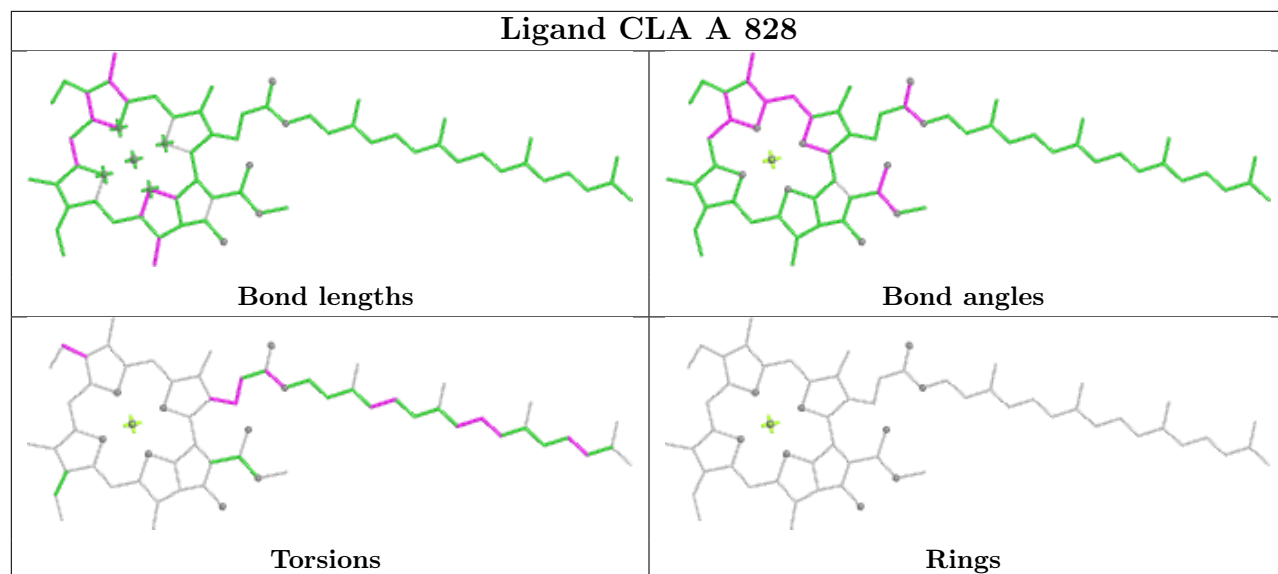


Ligand BCR A 844

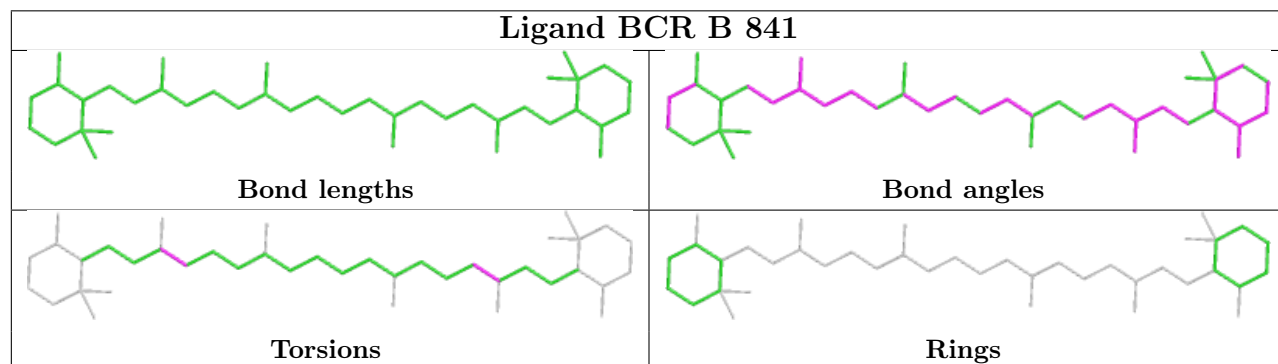




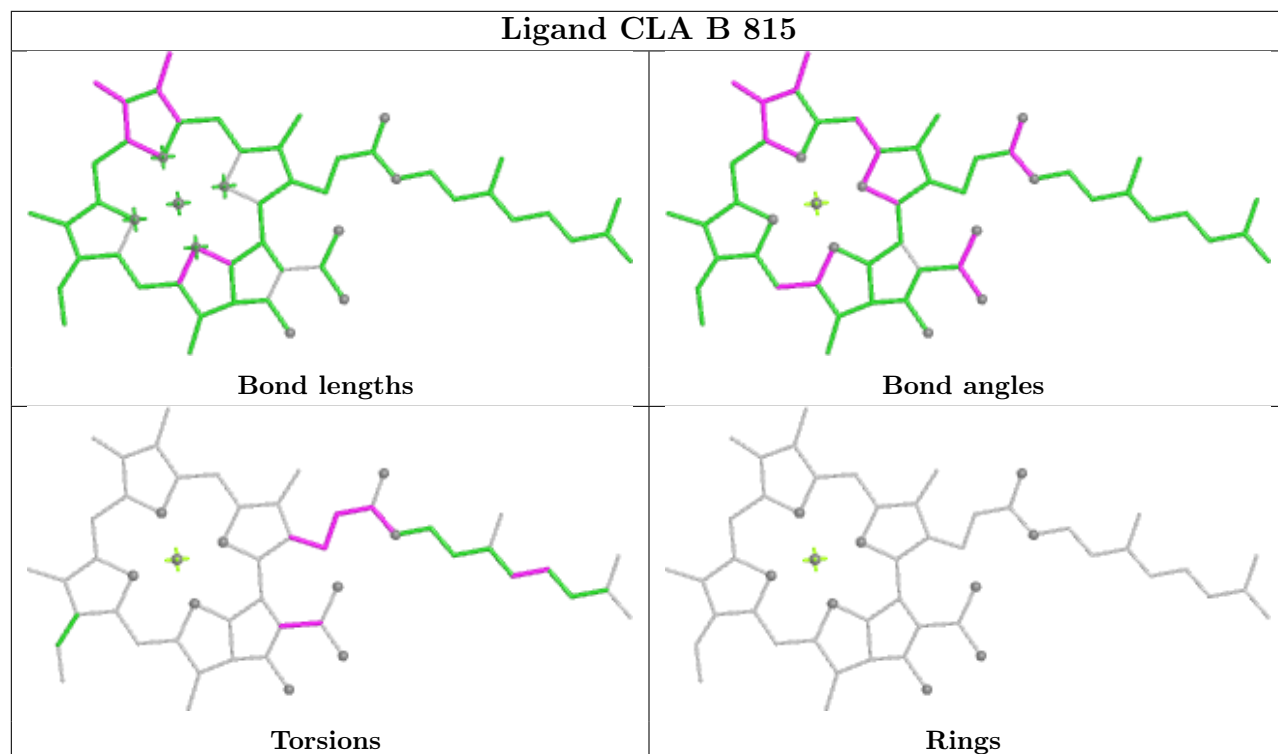
Ligand CLA A 828



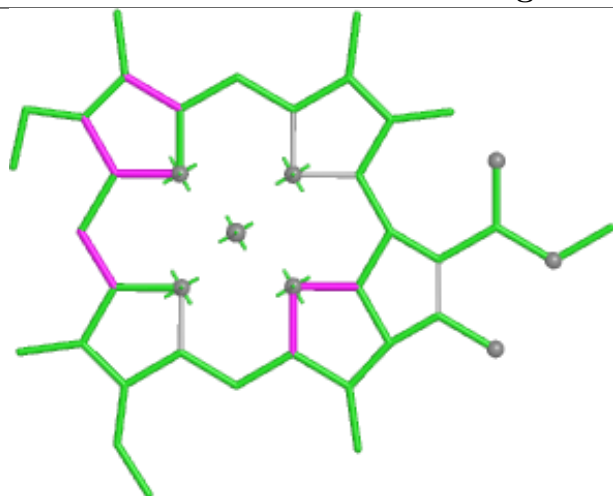
Ligand BCR B 841



Ligand CLA B 815



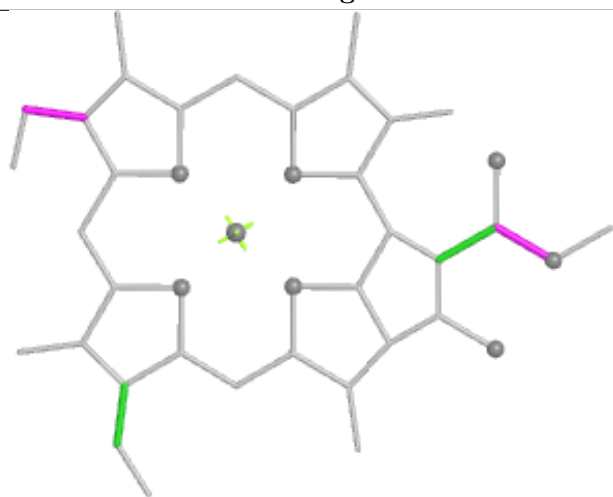
Ligand CLA L 203



Bond lengths



Bond angles

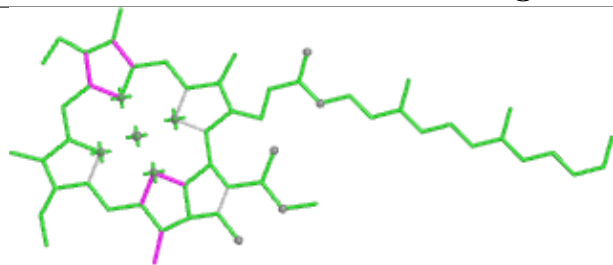


Torsions

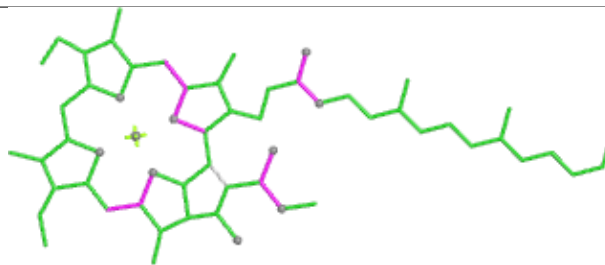


Rings

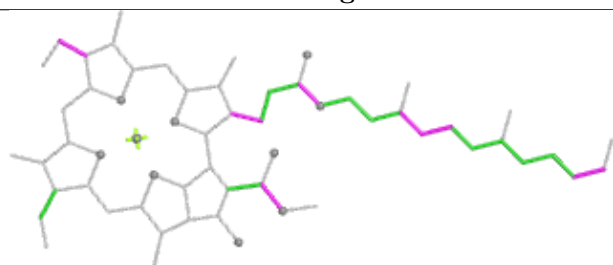
Ligand CLA B 811



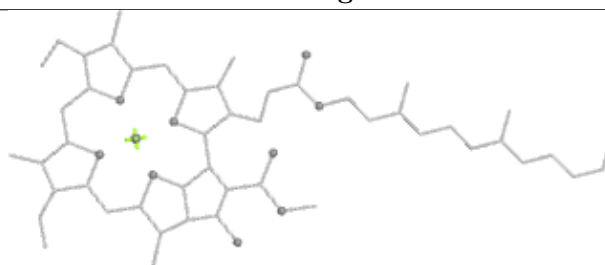
Bond lengths



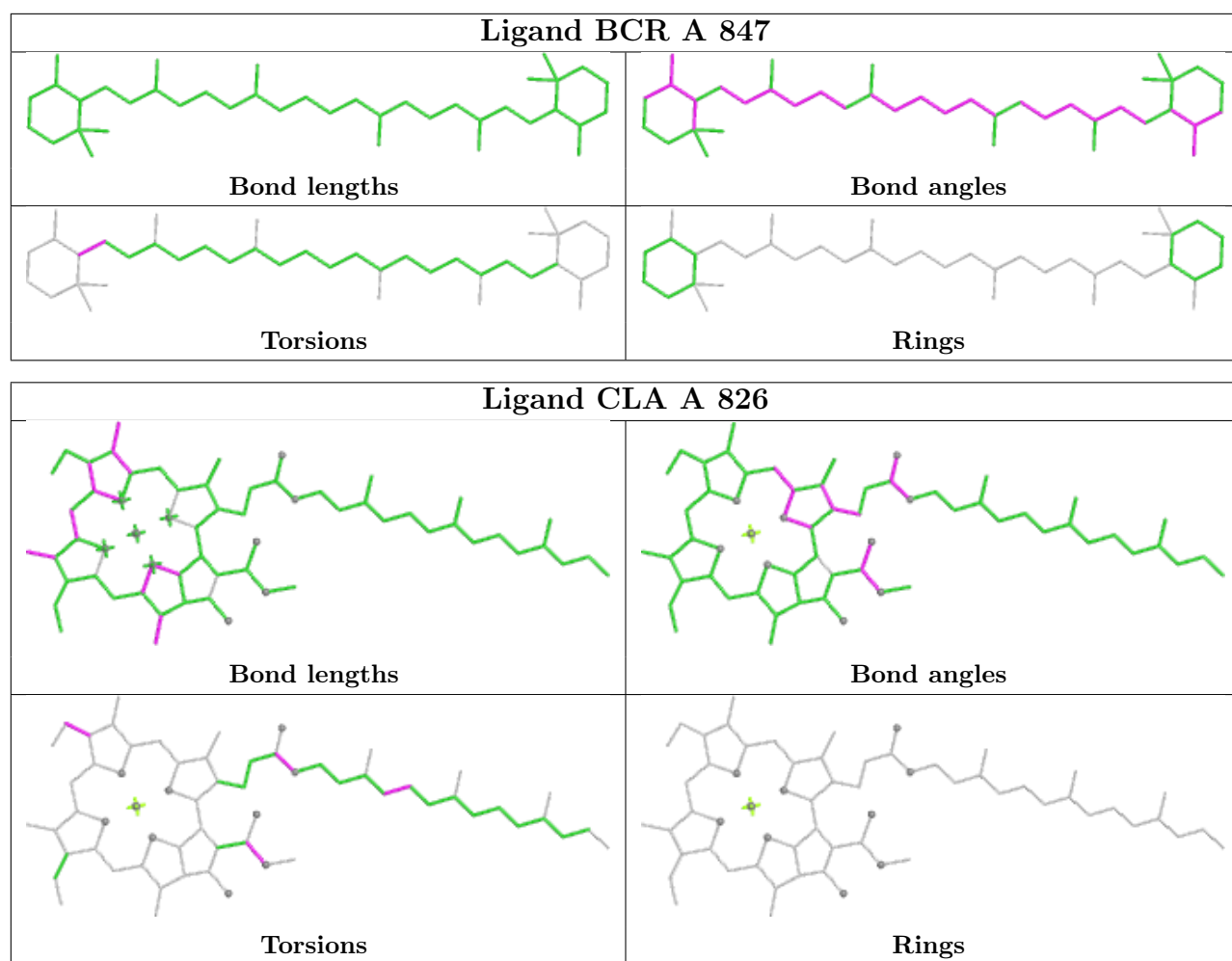
Bond angles



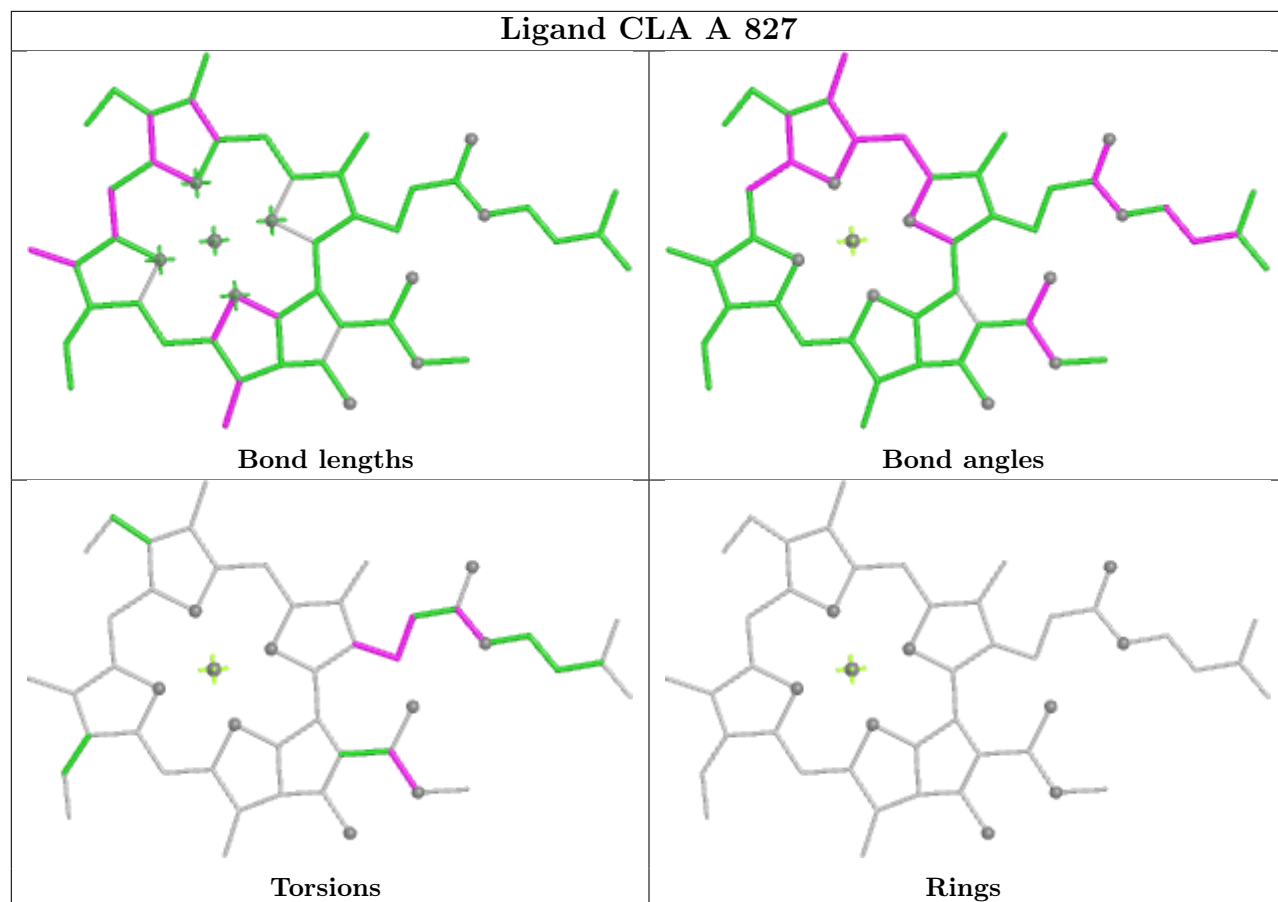
Torsions



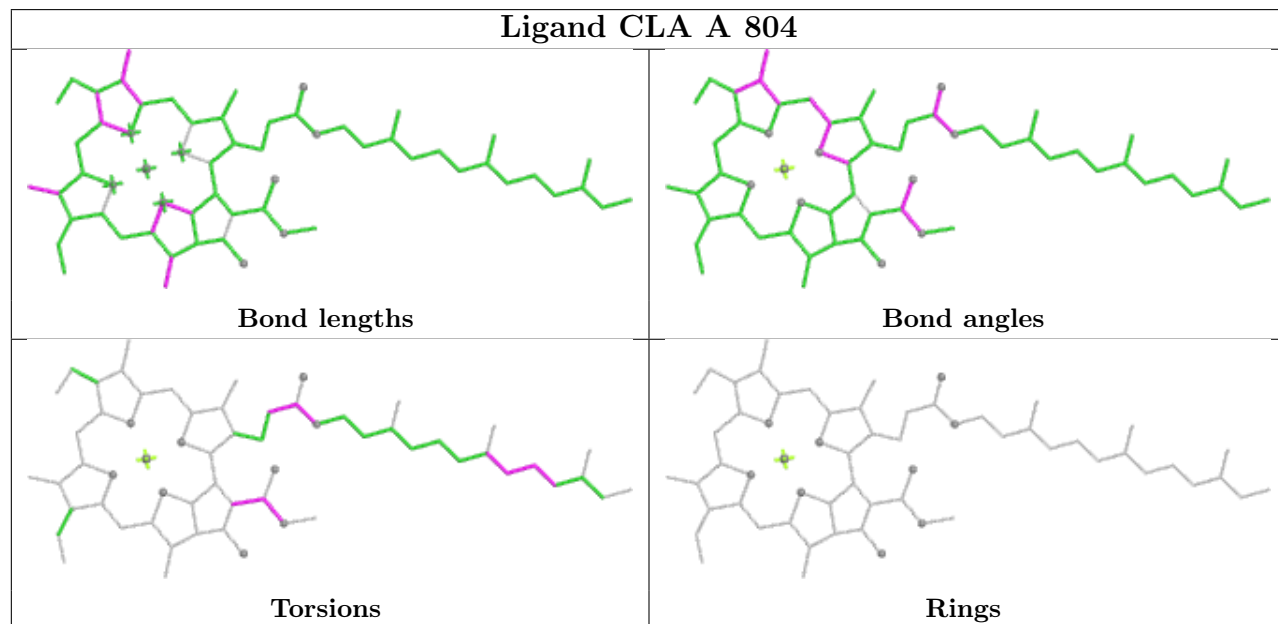
Rings



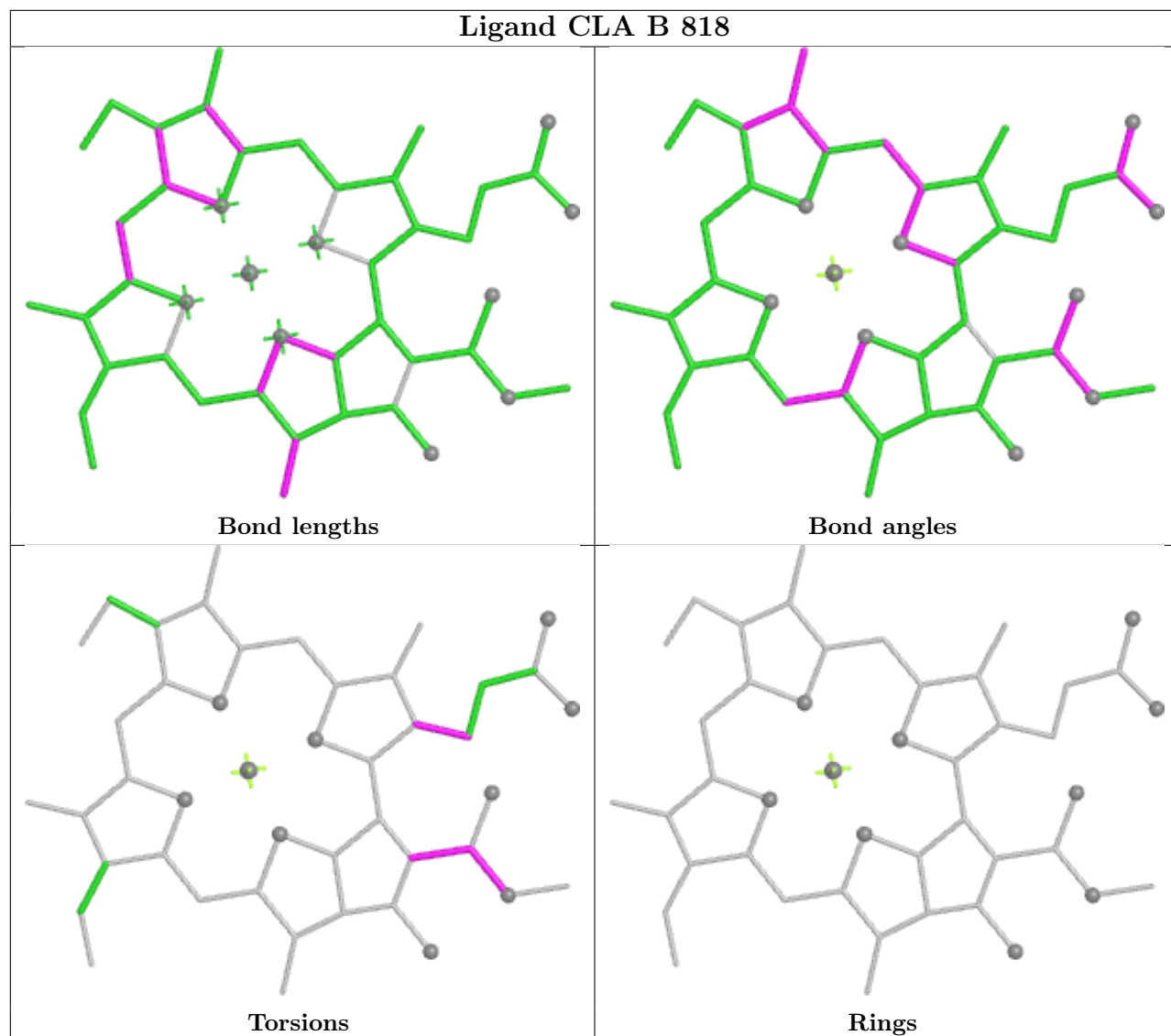
Ligand CLA A 827



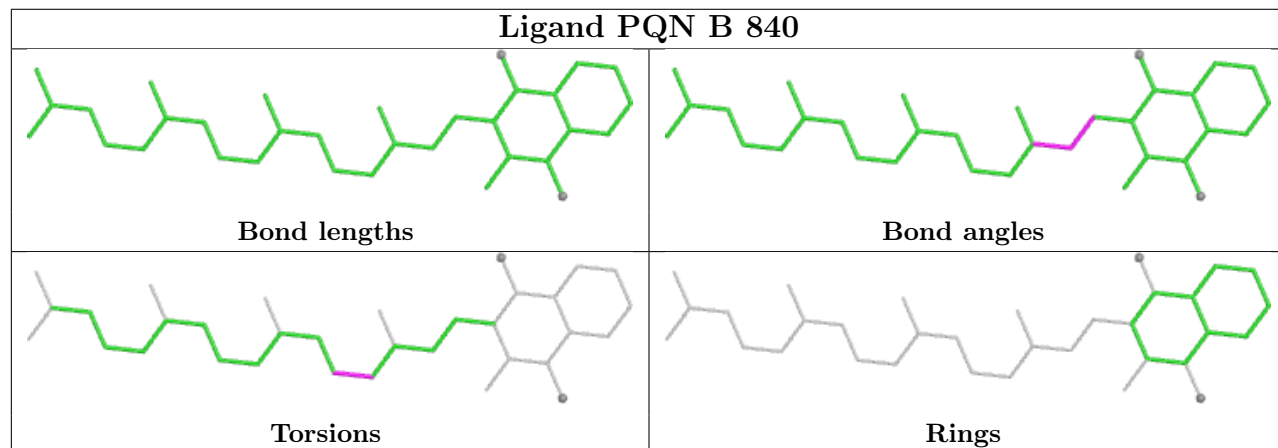
Ligand CLA A 804



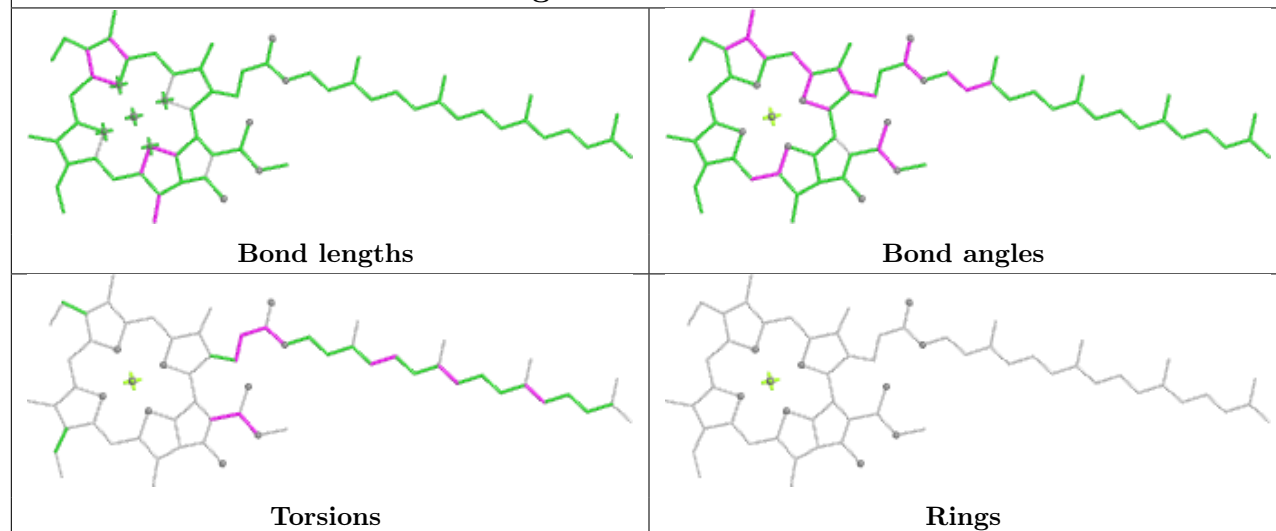
Ligand CLA B 818



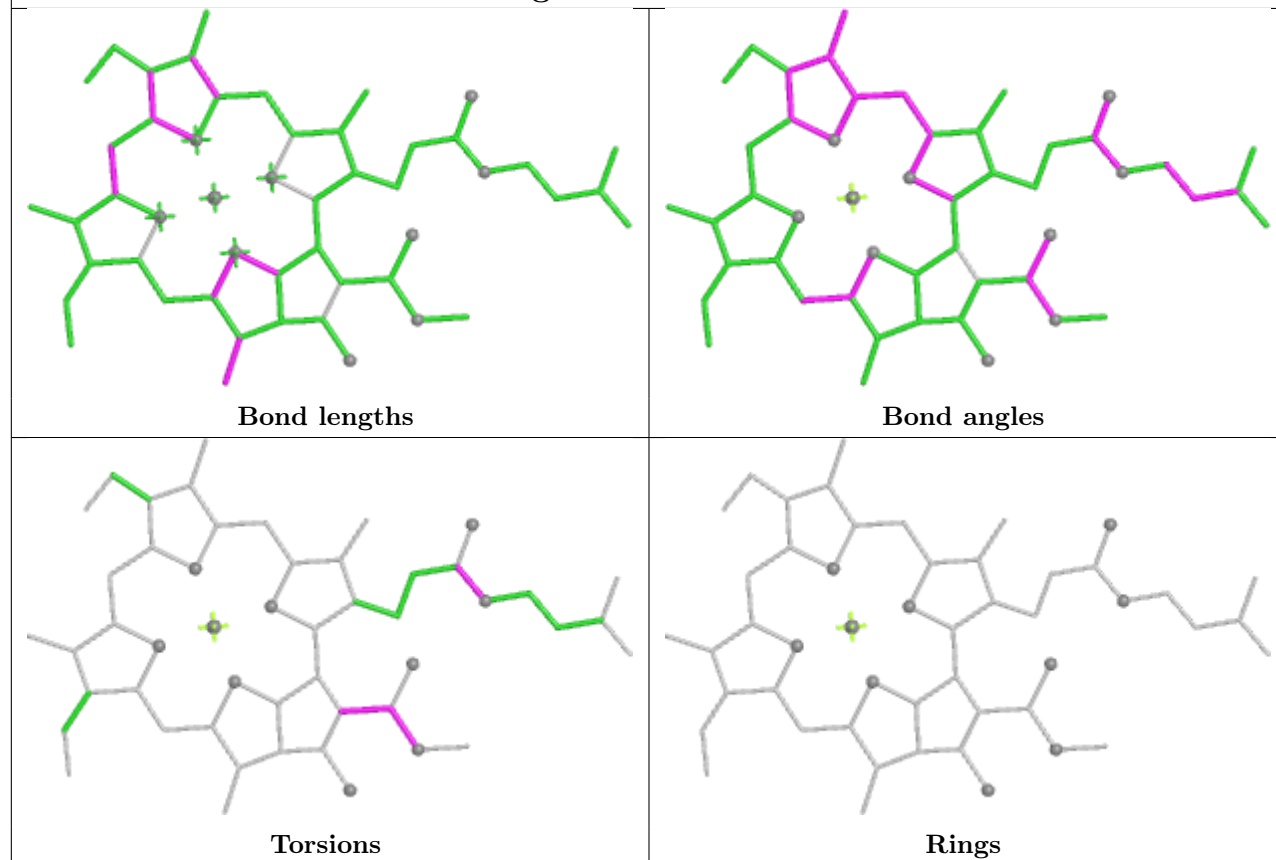
Ligand PQN B 840



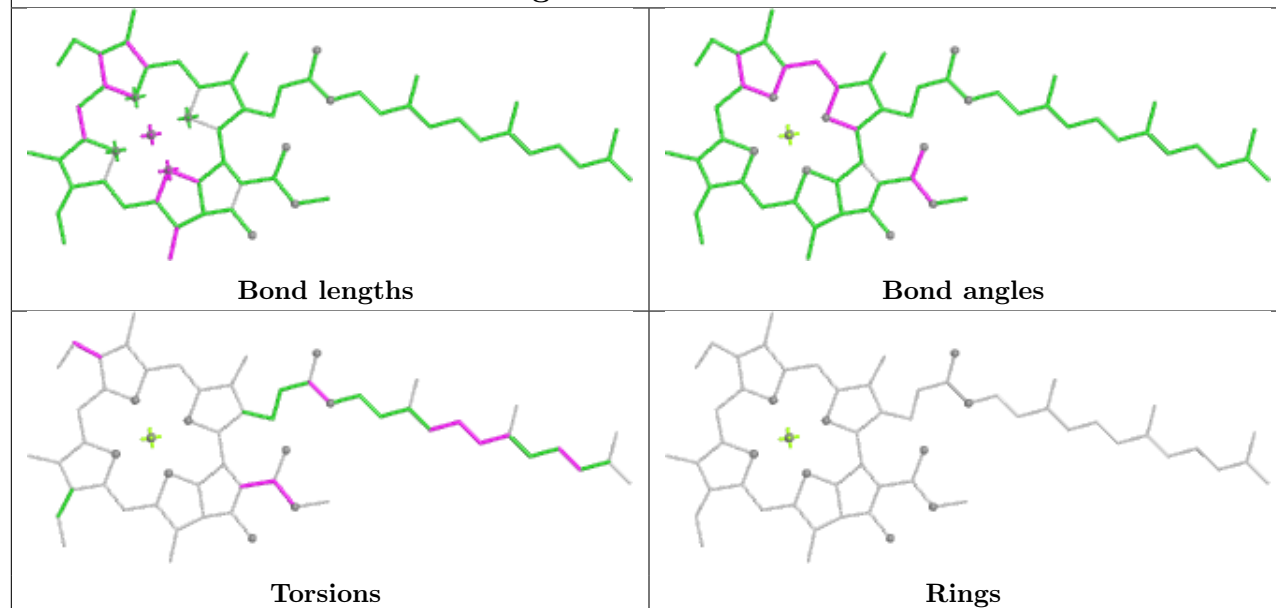
Ligand CLA B 810



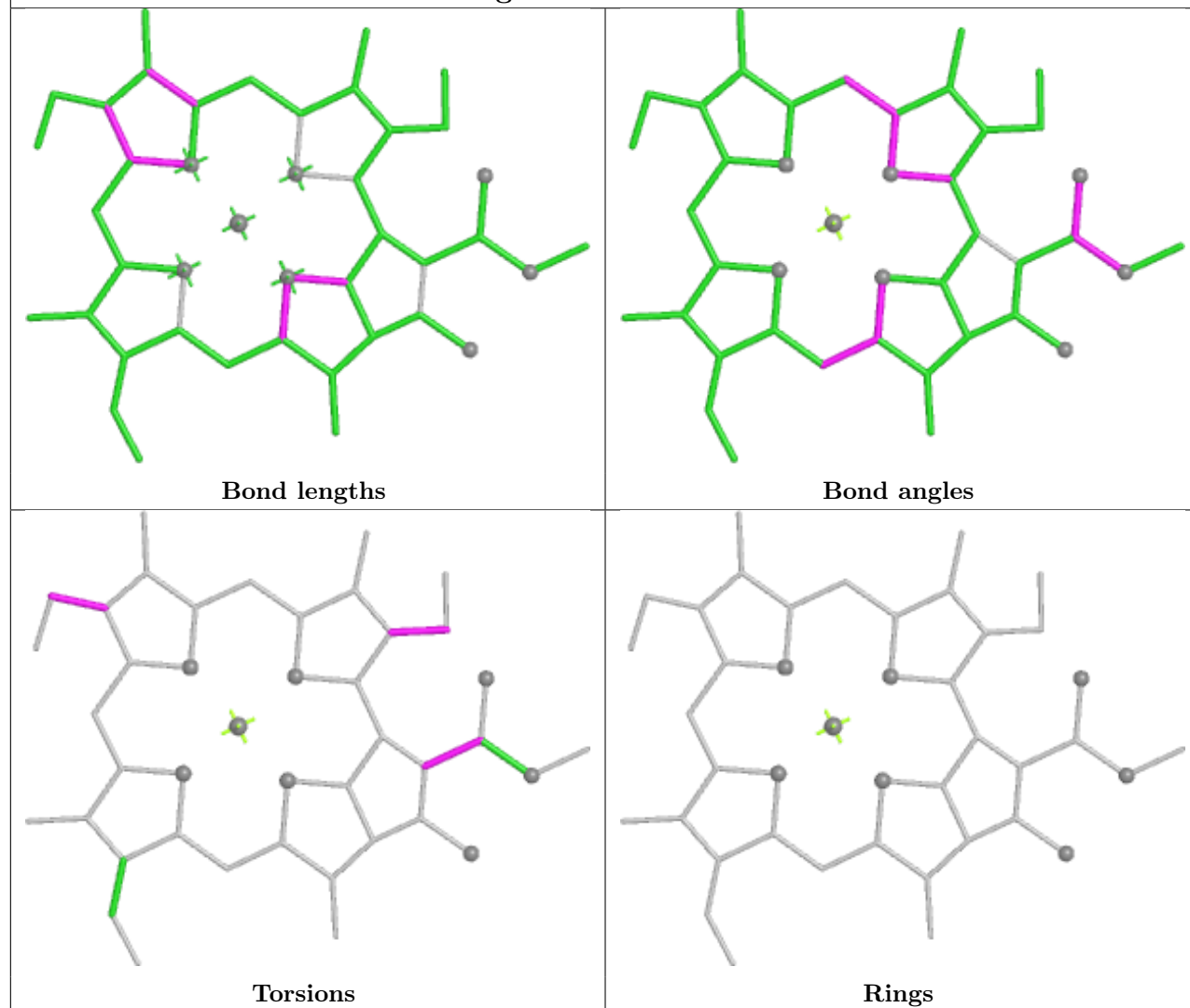
Ligand CLA B 824



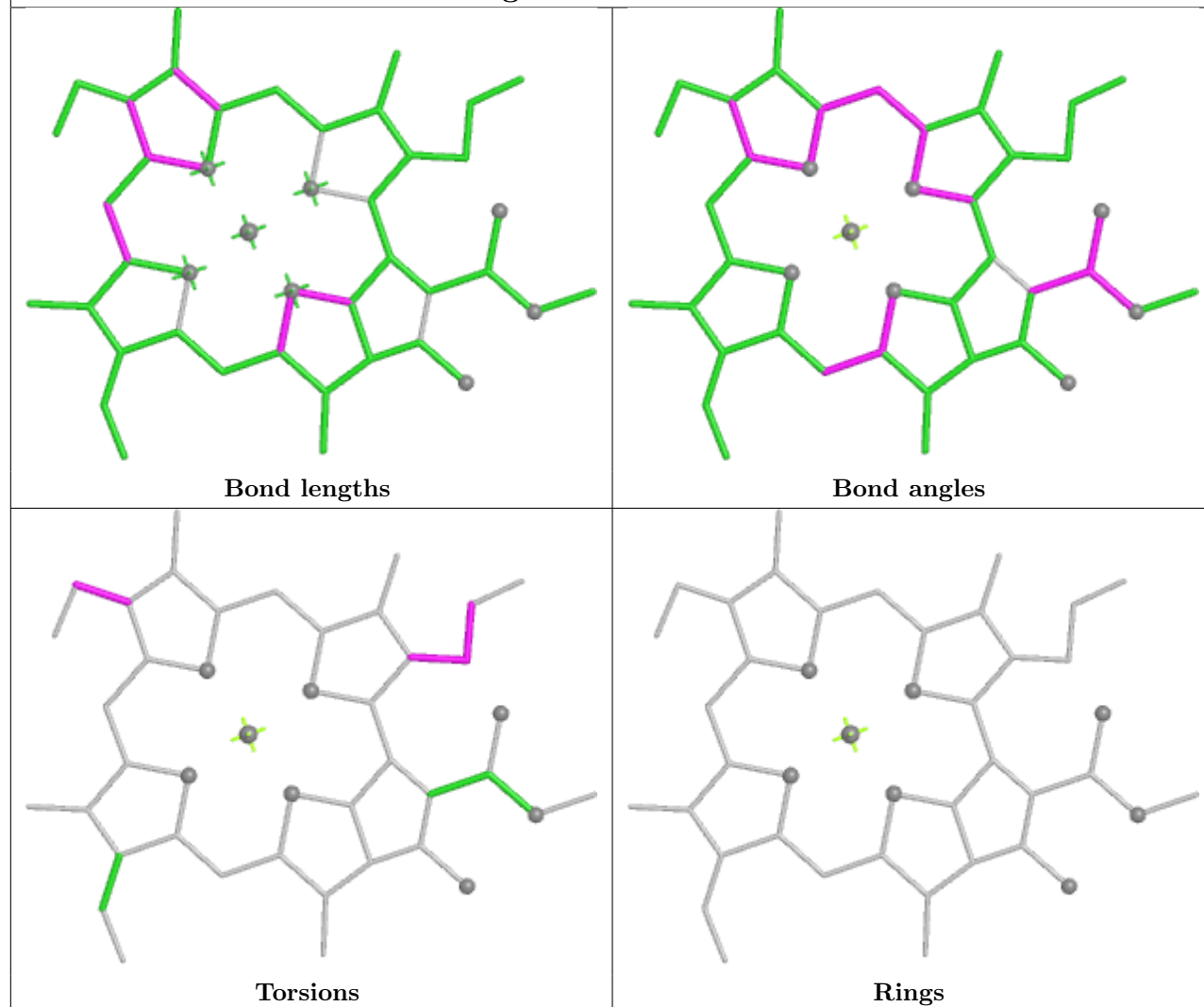
Ligand CLA B 801



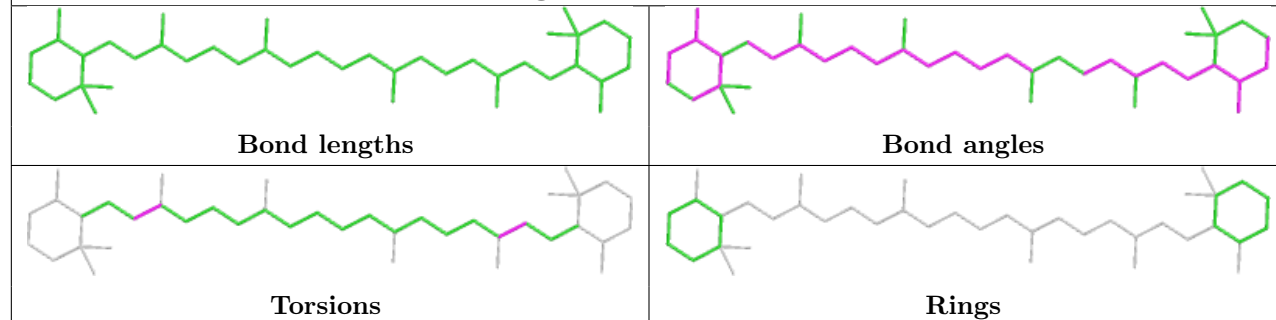
Ligand CLA A 821



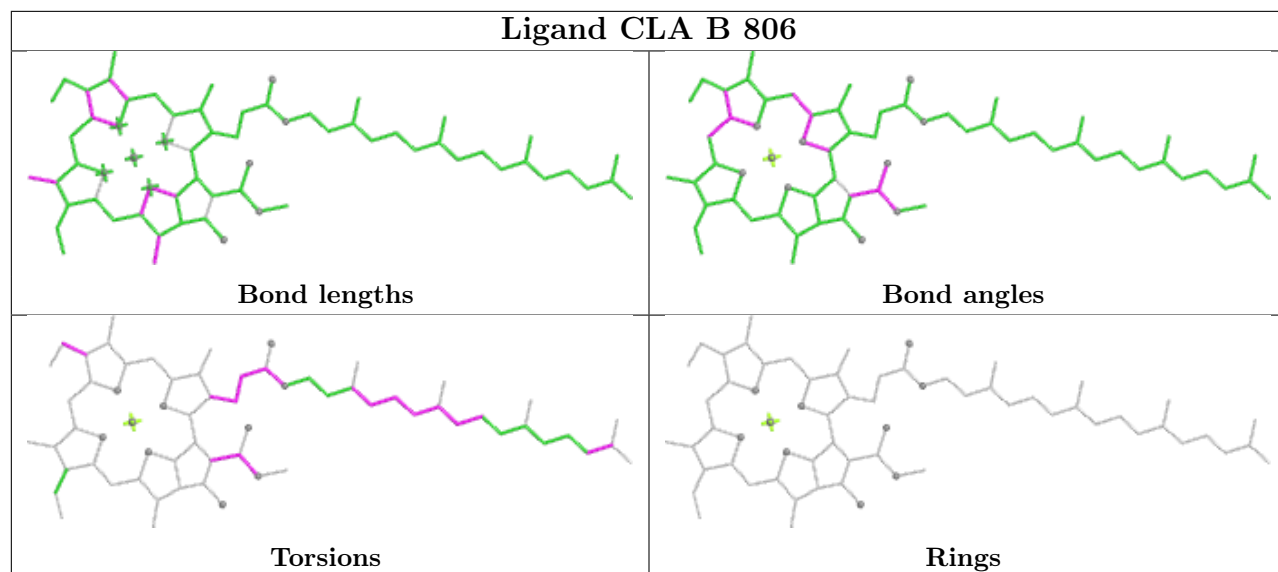
Ligand CLA B 830



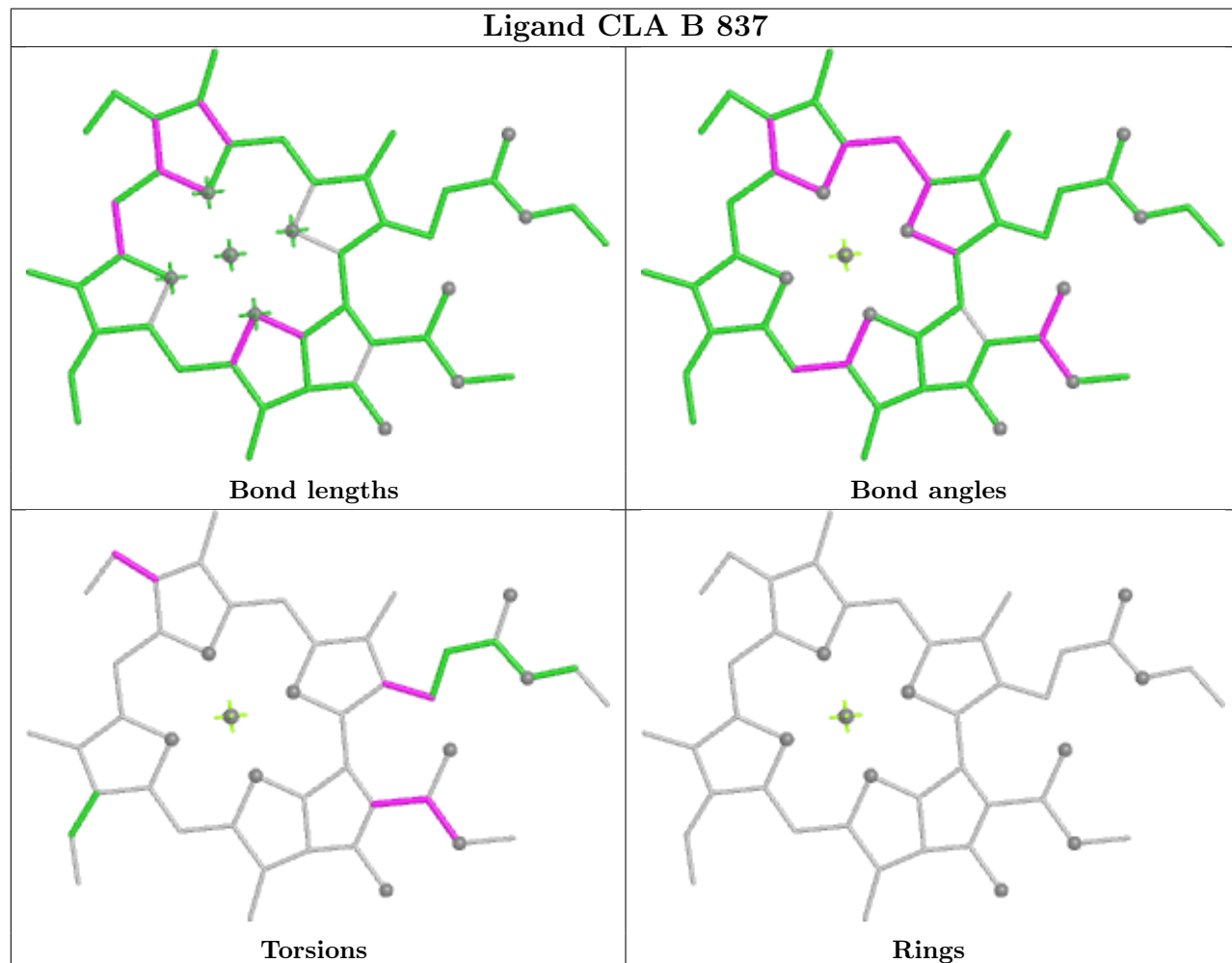
Ligand BCR L 204

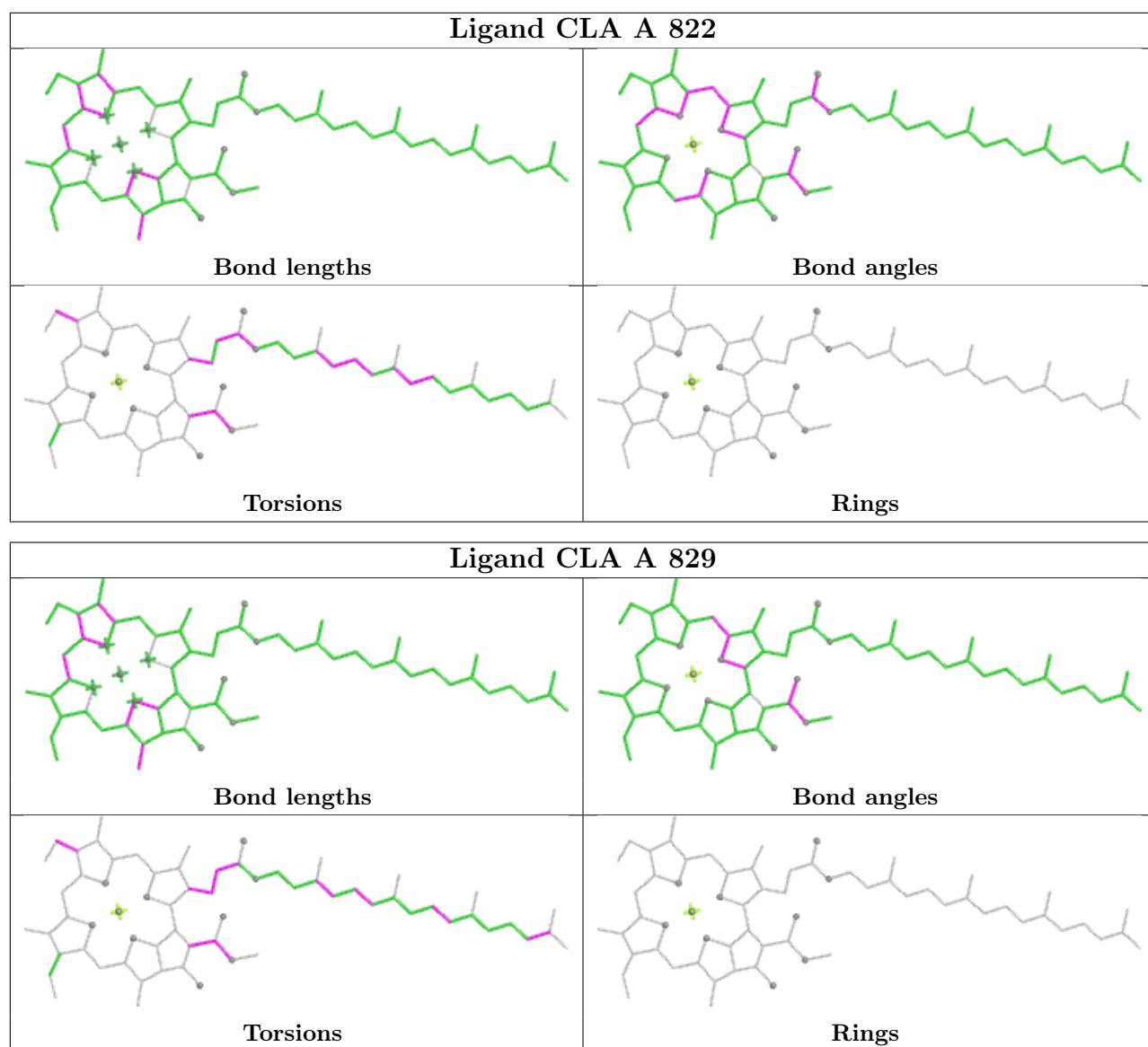


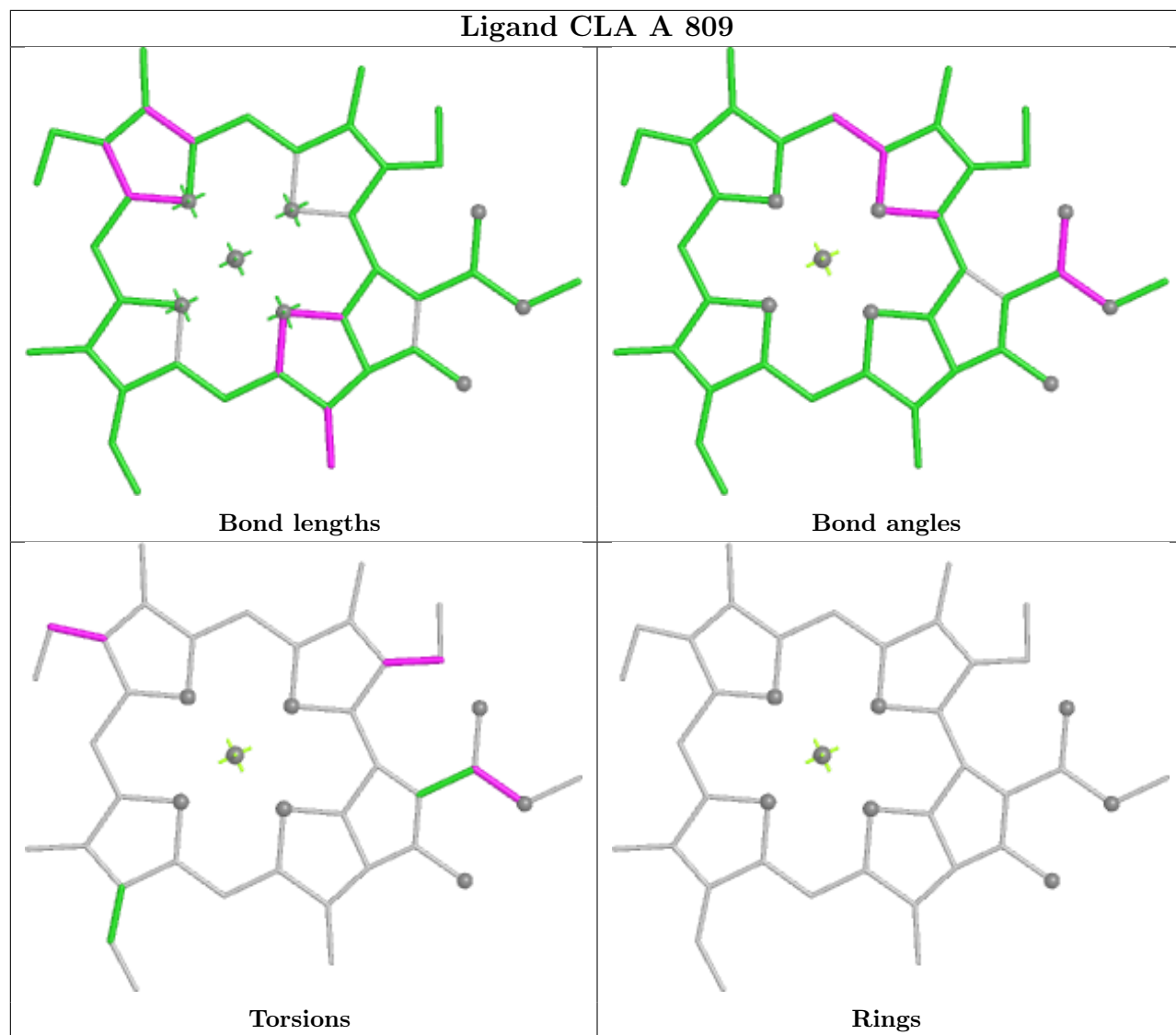
Ligand CLA B 806



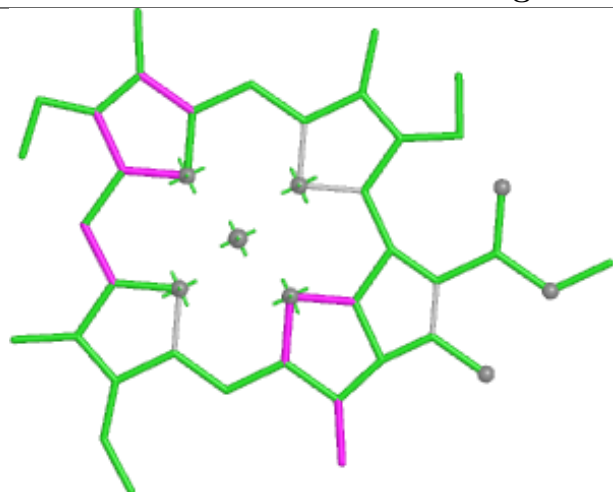
Ligand CLA B 837



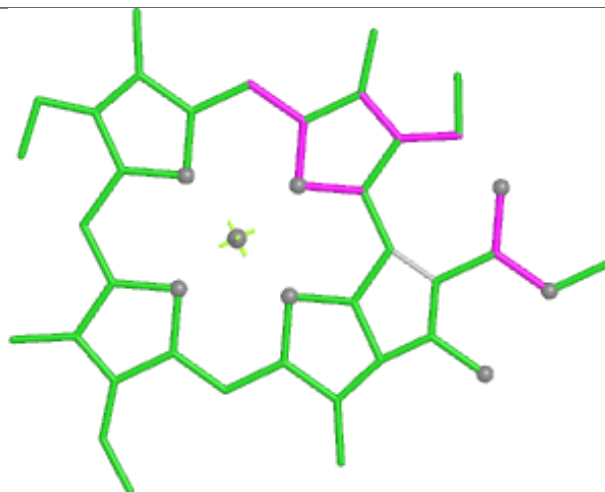




Ligand CLA K 204



Bond lengths



Bond angles

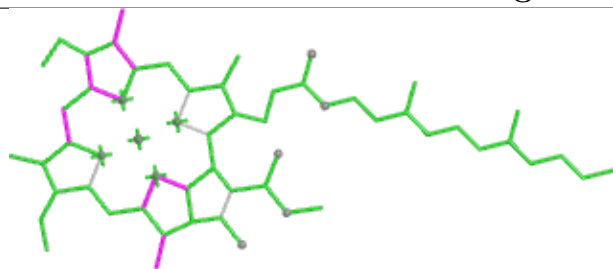


Torsions

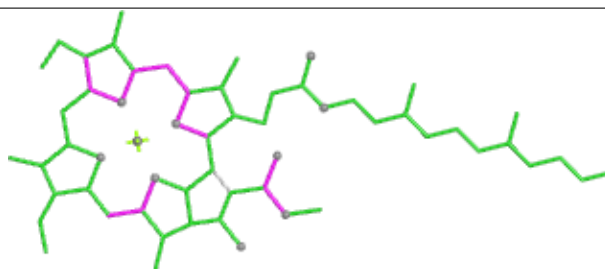


Rings

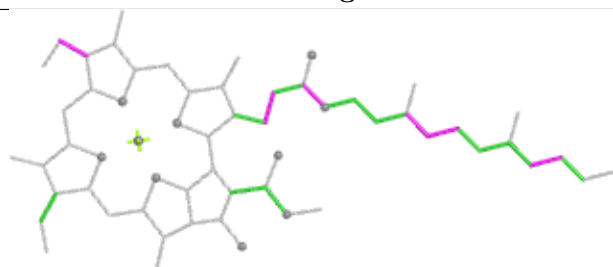
Ligand CLA B 836



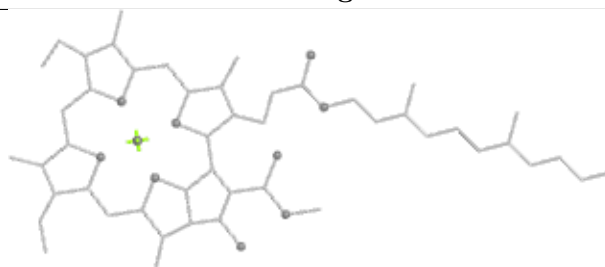
Bond lengths



Bond angles

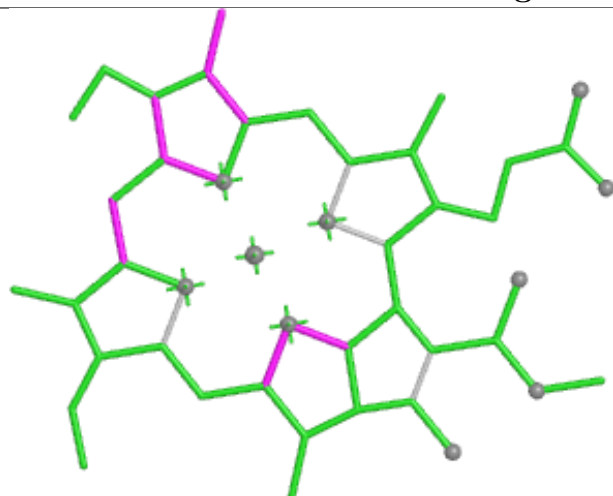


Torsions

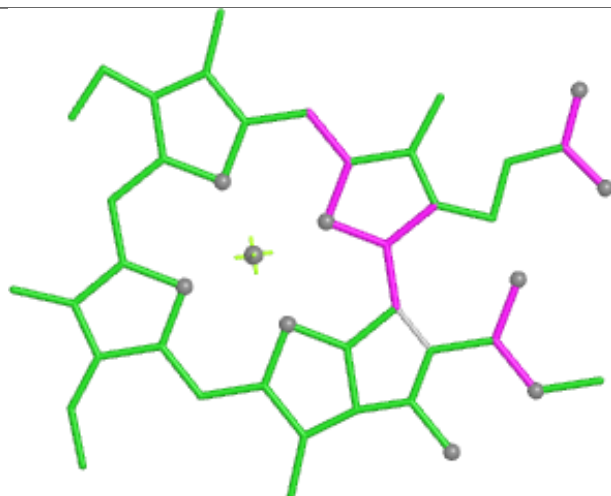


Rings

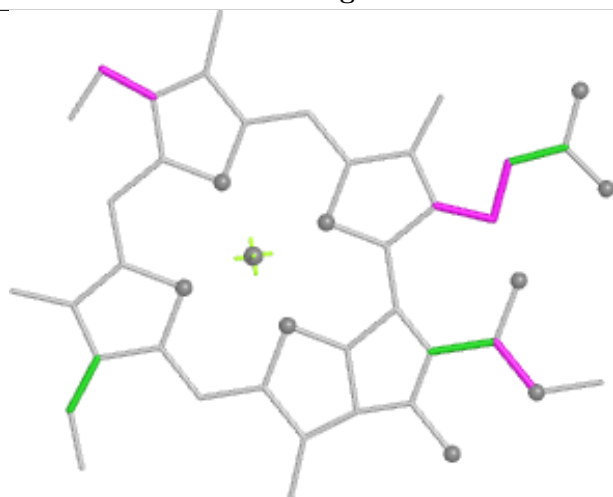
Ligand CLA B 834



Bond lengths



Bond angles

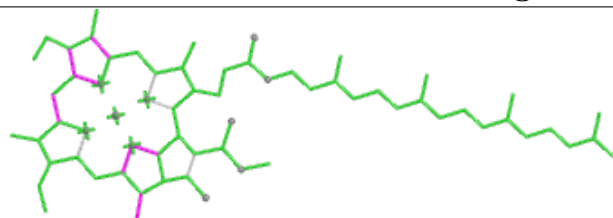


Torsions

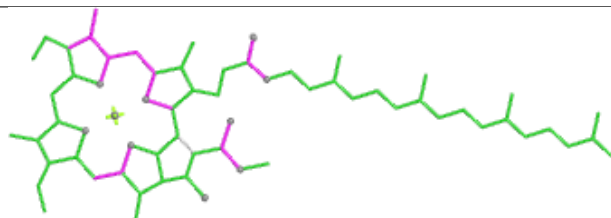


Rings

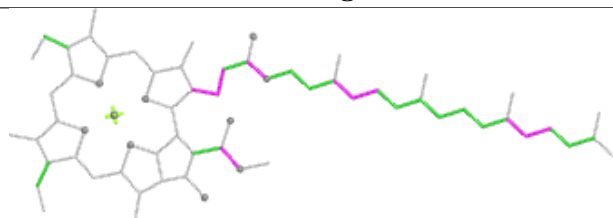
Ligand CLA A 838



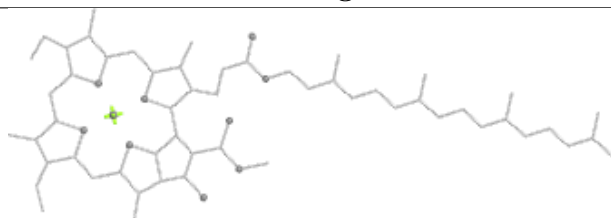
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

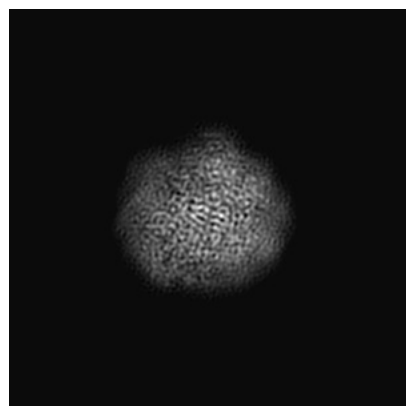
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66564. These allow visual inspection of the internal detail of the map and identification of artifacts.

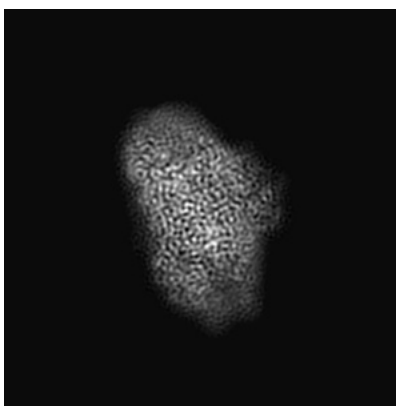
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

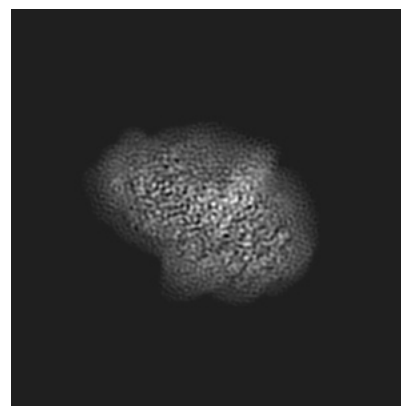
6.1.1 Primary map



X

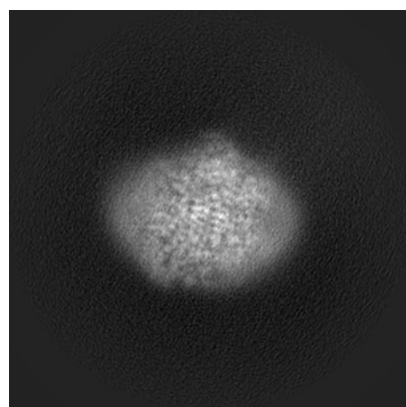


Y

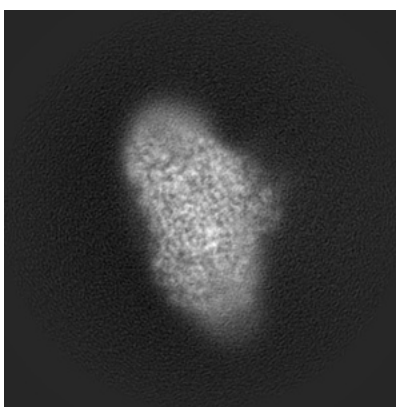


Z

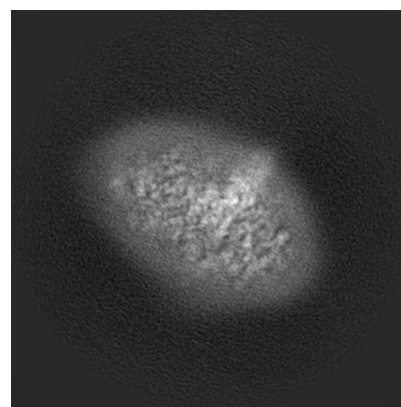
6.1.2 Raw map



X



Y

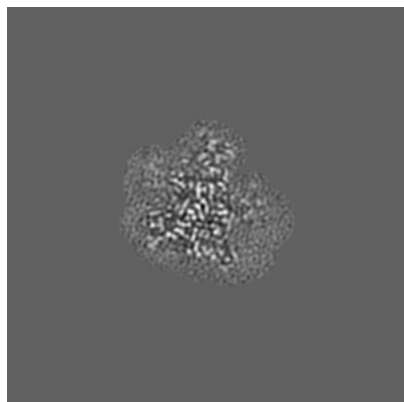


Z

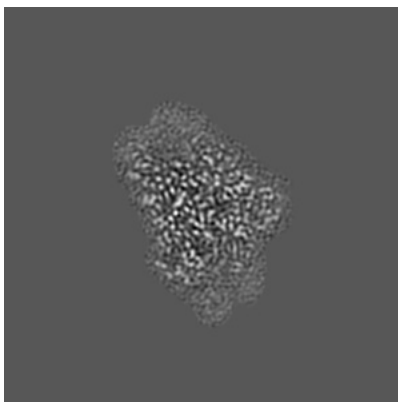
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

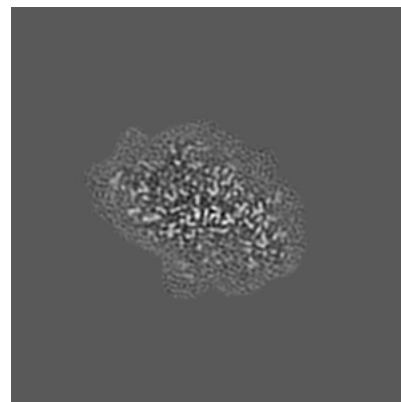
6.2.1 Primary map



X Index: 128

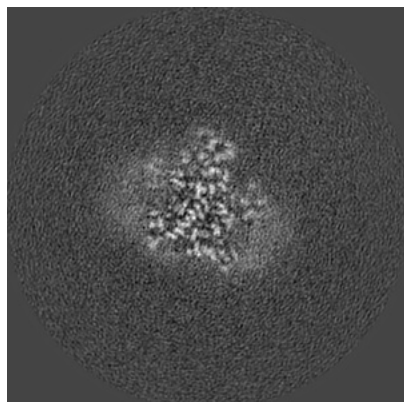


Y Index: 128

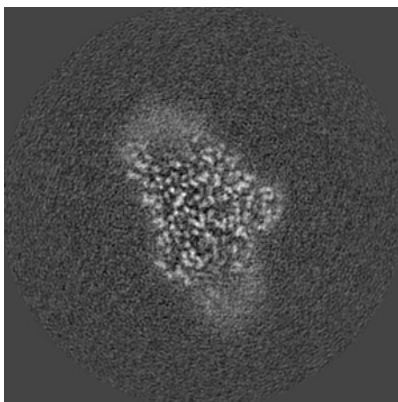


Z Index: 128

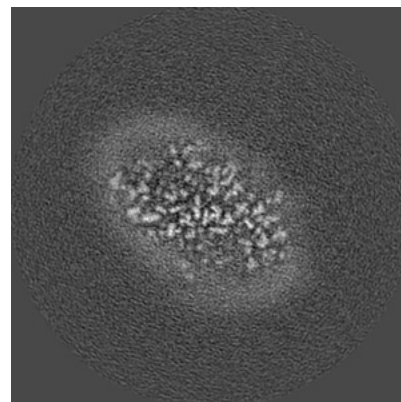
6.2.2 Raw map



X Index: 128



Y Index: 128

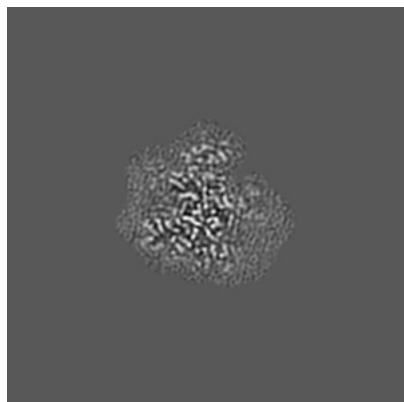


Z Index: 128

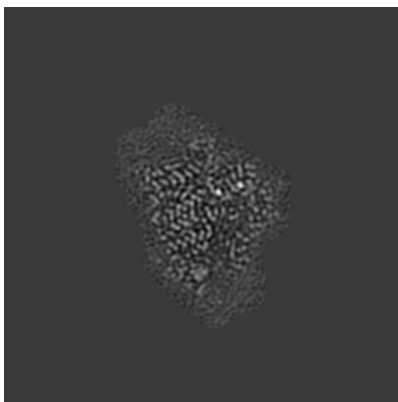
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

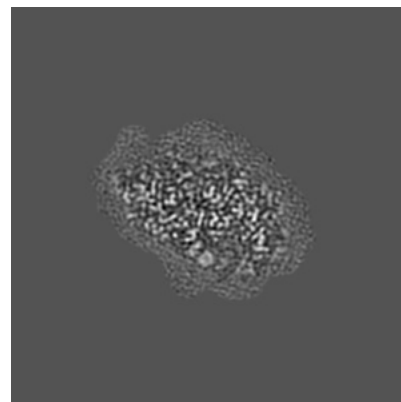
6.3.1 Primary map



X Index: 130

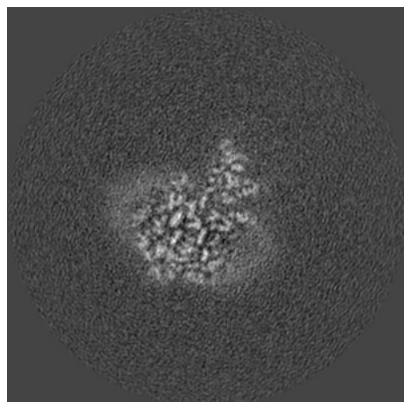


Y Index: 133

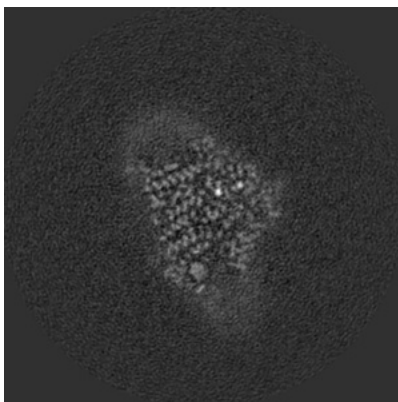


Z Index: 124

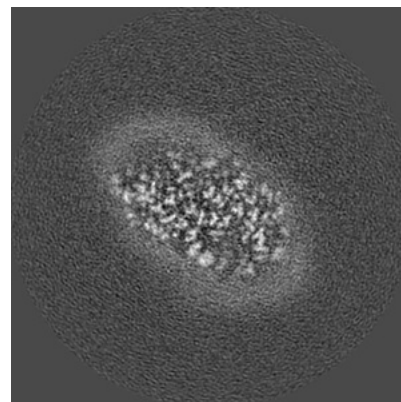
6.3.2 Raw map



X Index: 151



Y Index: 132

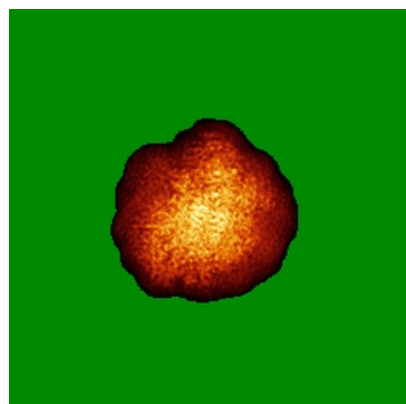


Z Index: 124

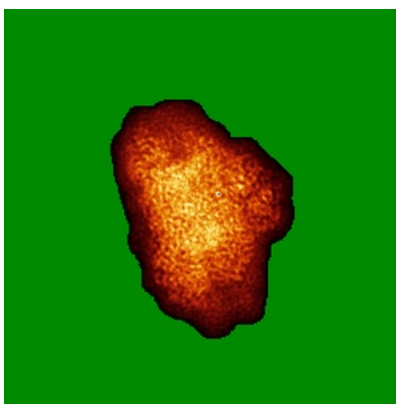
The images above show the largest variance slices of the map in three orthogonal directions.

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

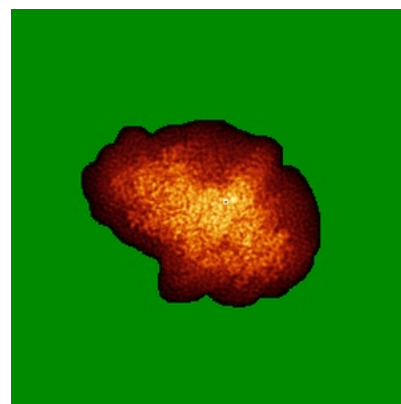
6.4.1 Primary map



X

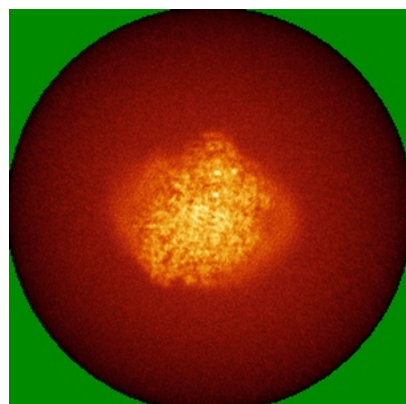


Y

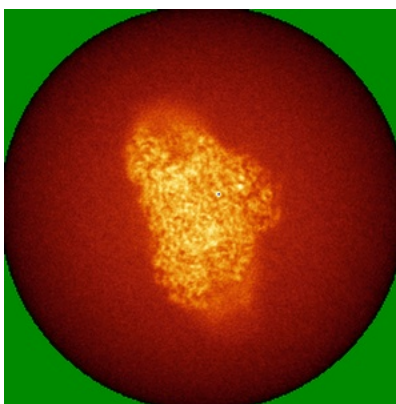


Z

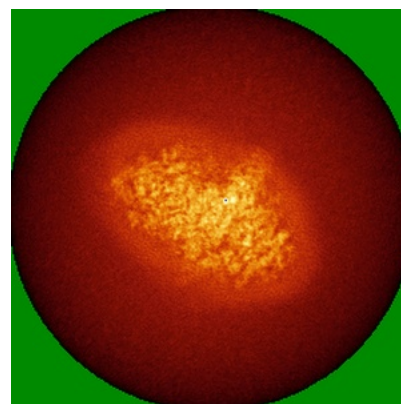
6.4.2 Raw map



X



Y

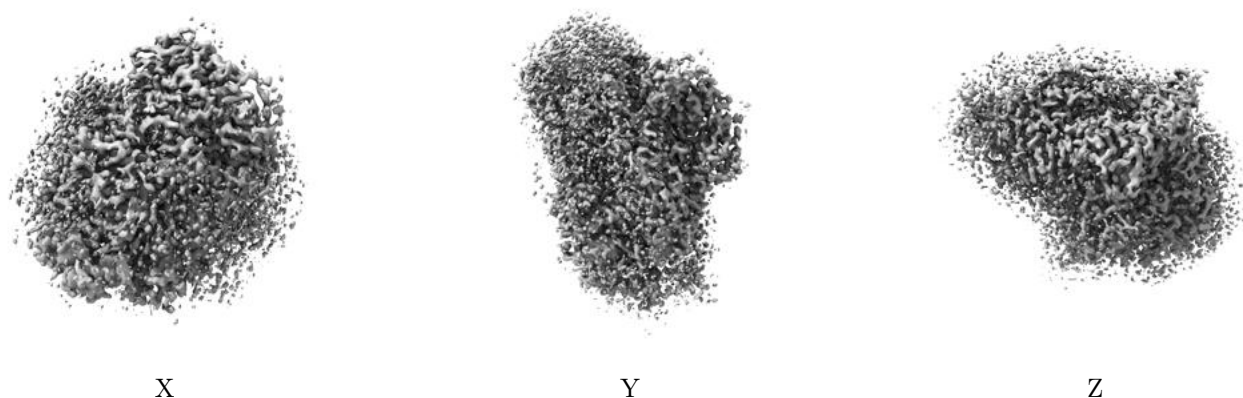


Z

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 0.03. 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.

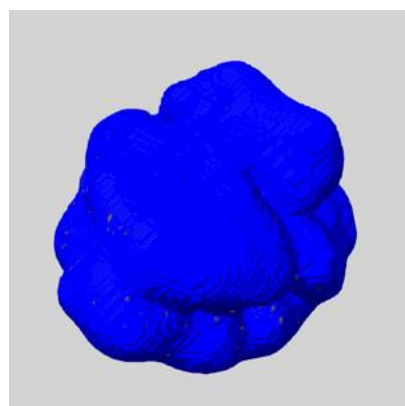
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

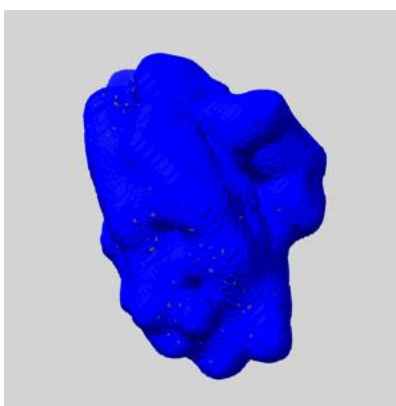
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

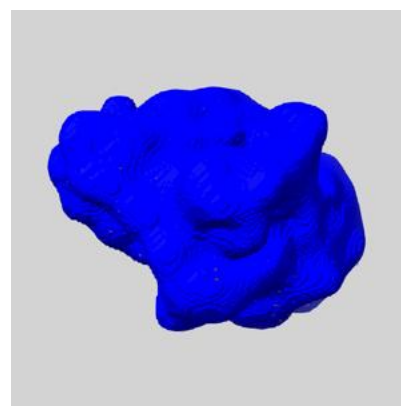
6.6.1 emd_66564_msk_1.map [i](#)



X



Y

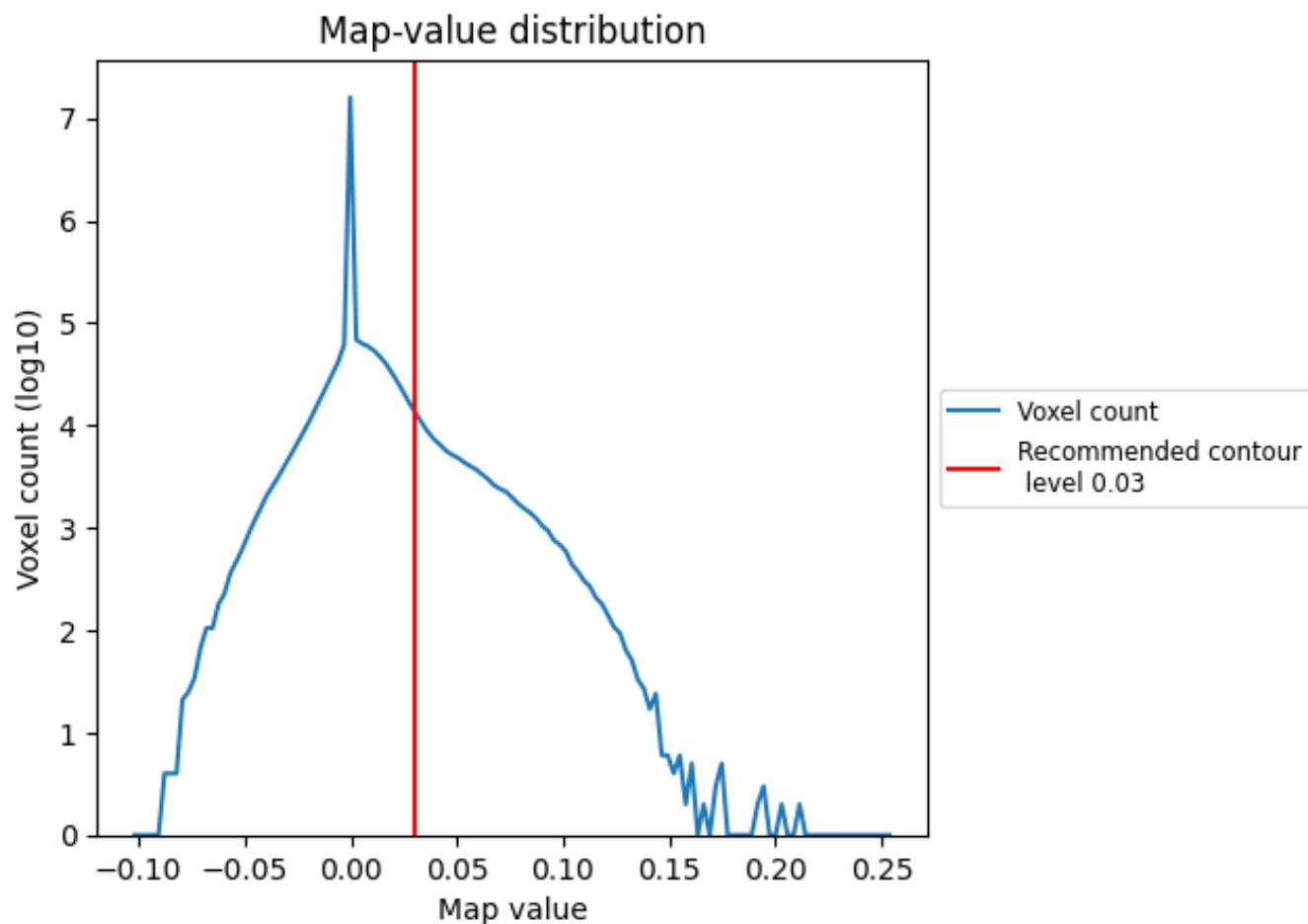


Z

7 Map analysis [i](#)

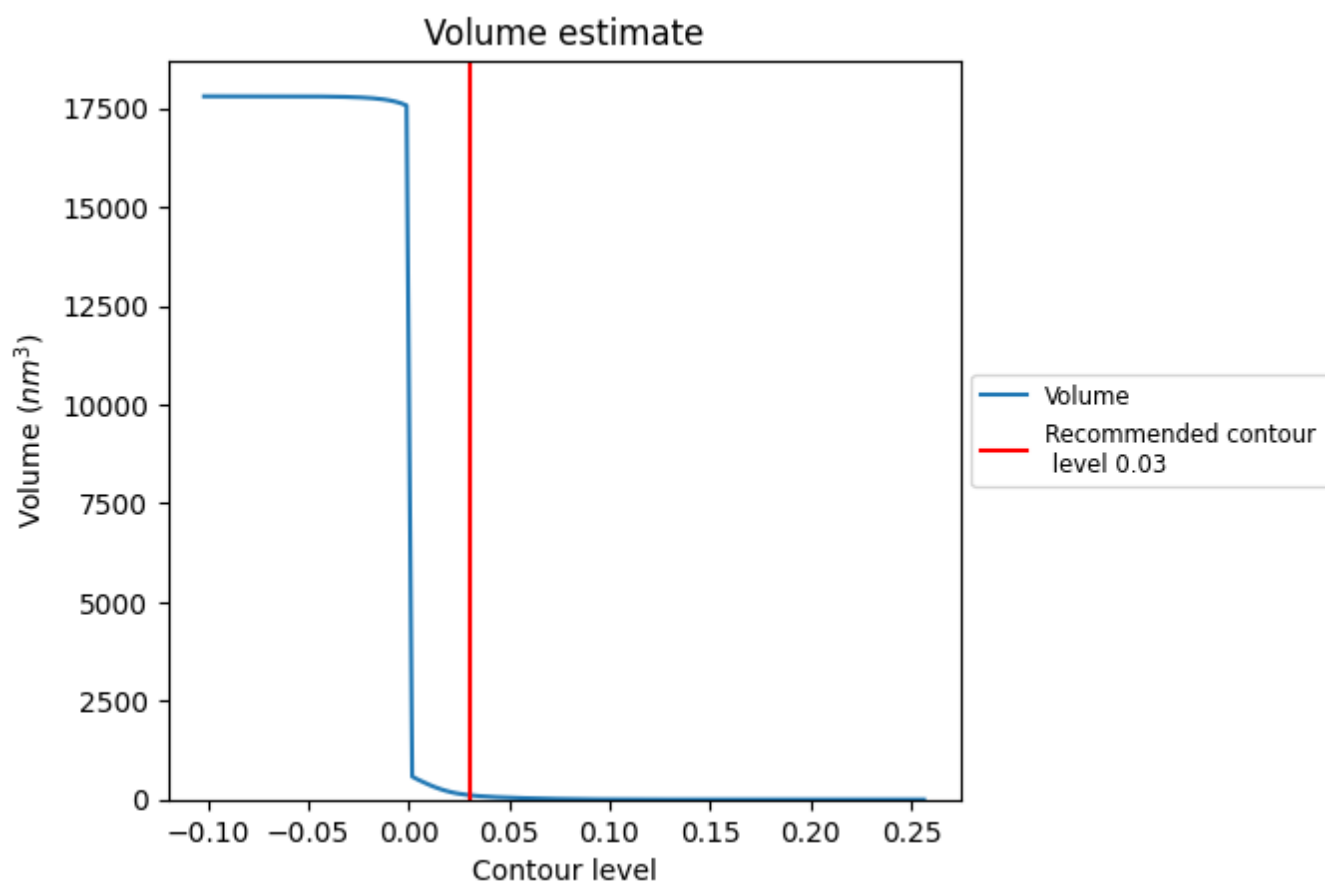
This section contains the results of statistical analysis of the map.

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.

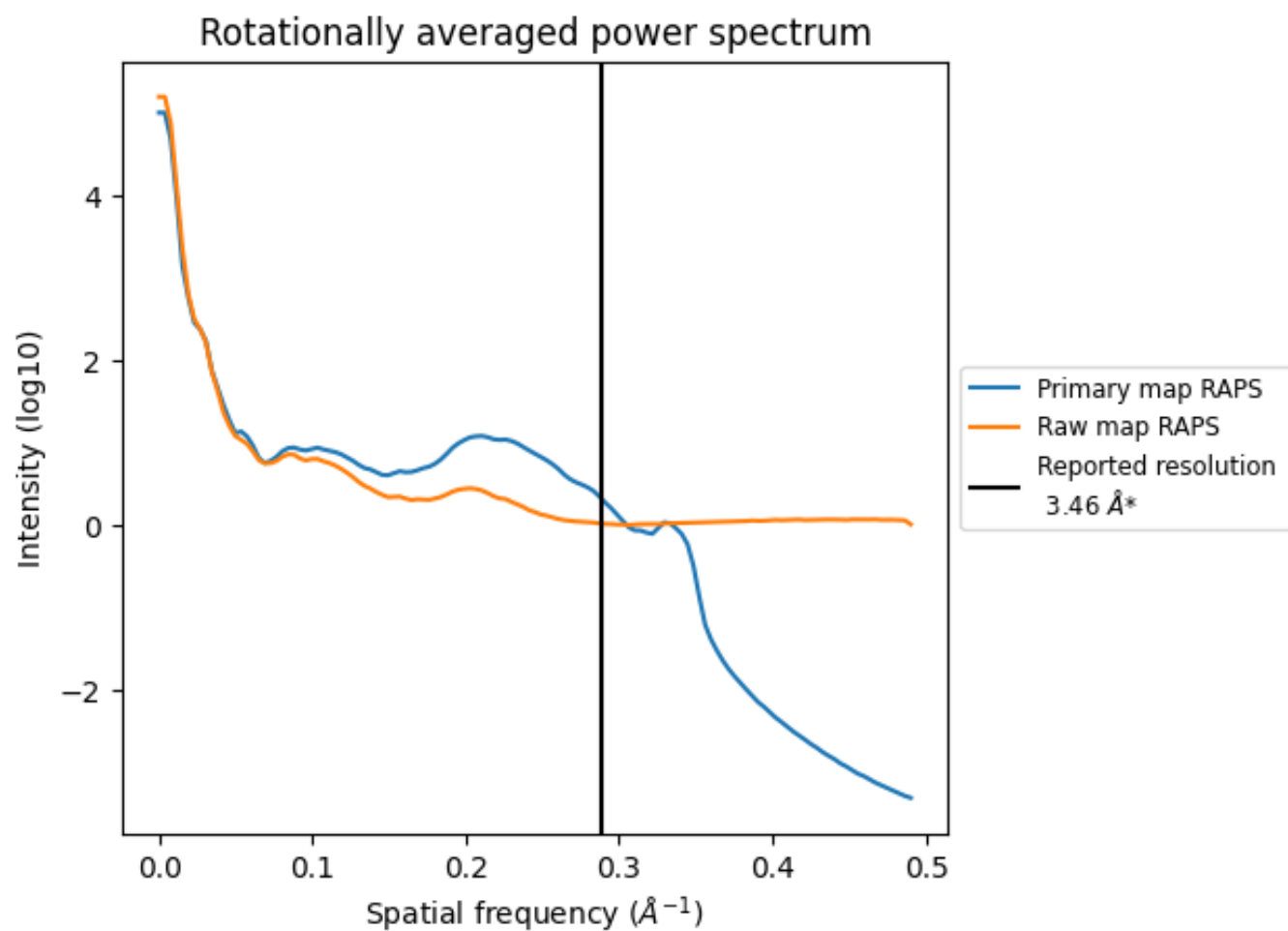
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 112 nm^3 ; this corresponds to an approximate mass of 101 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 ⓘ

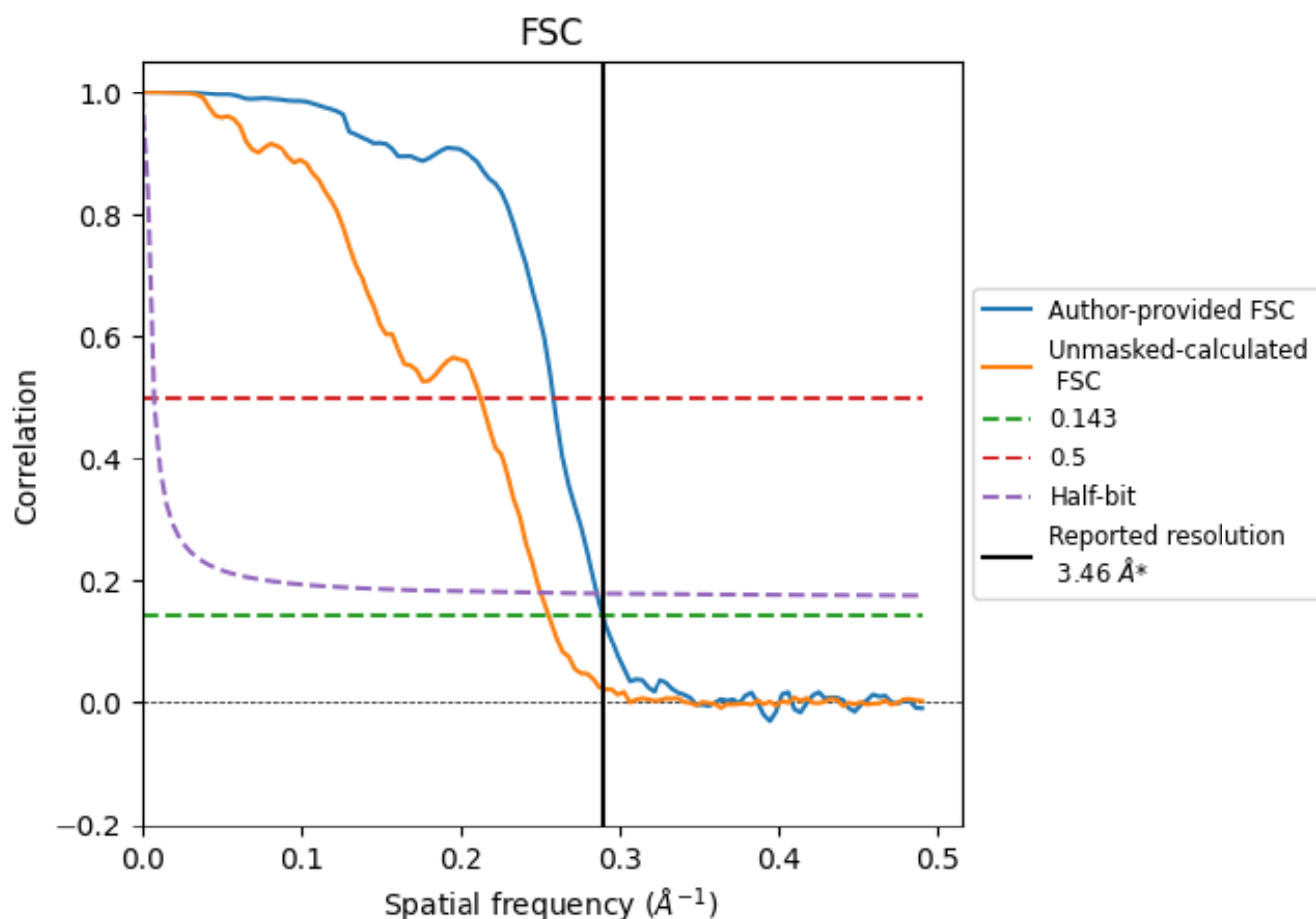


*Reported resolution corresponds to spatial frequency of $0.289 \text{ \AA}^{-1}$

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 0.289 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

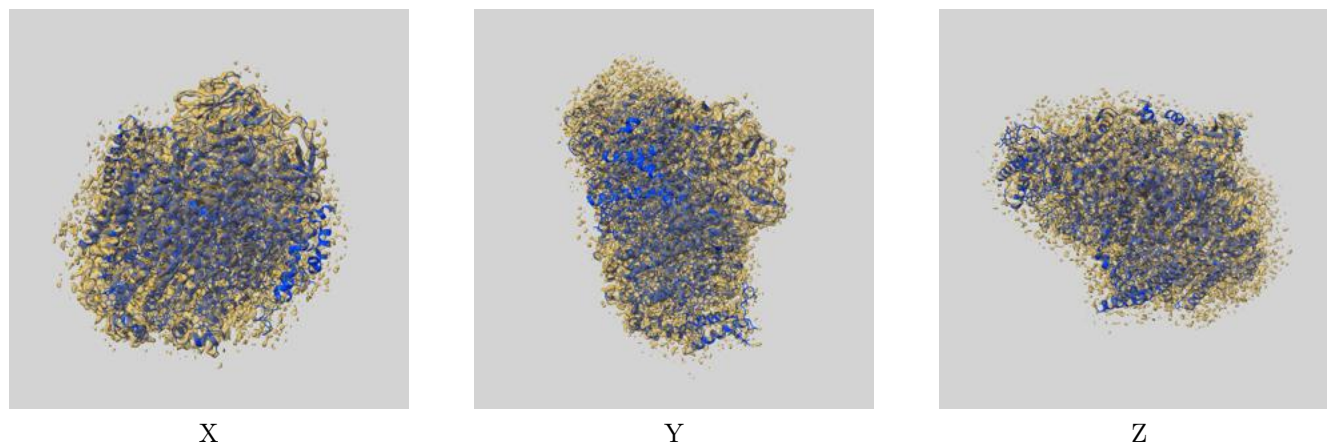
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.46	-	-
Author-provided FSC curve	3.46	3.87	3.50
Unmasked-calculated*	3.92	4.70	3.99

*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 3.92 differs from the reported value 3.46 by more than 10 %

9 Map-model fit [i](#)

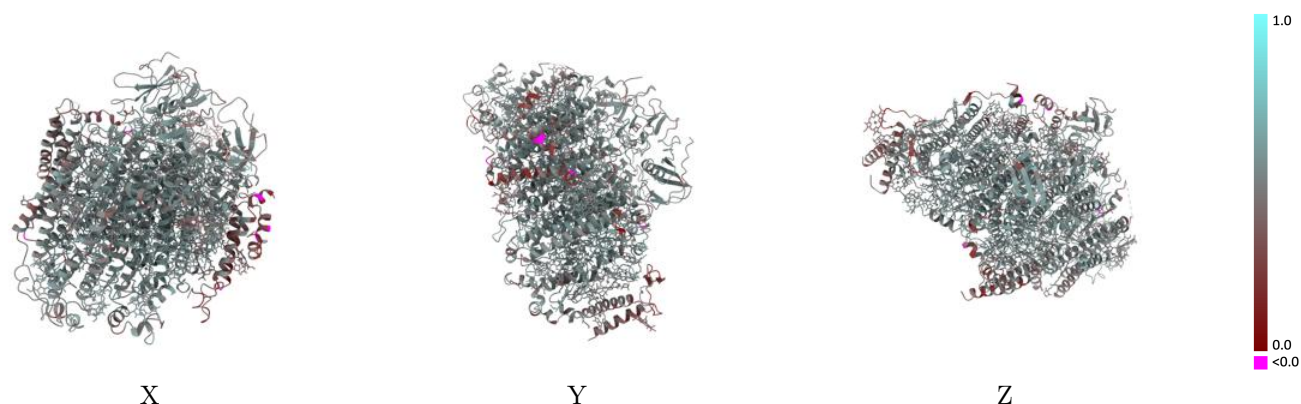
This section contains information regarding the fit between EMDB map EMD-66564 and PDB model 9X4R. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



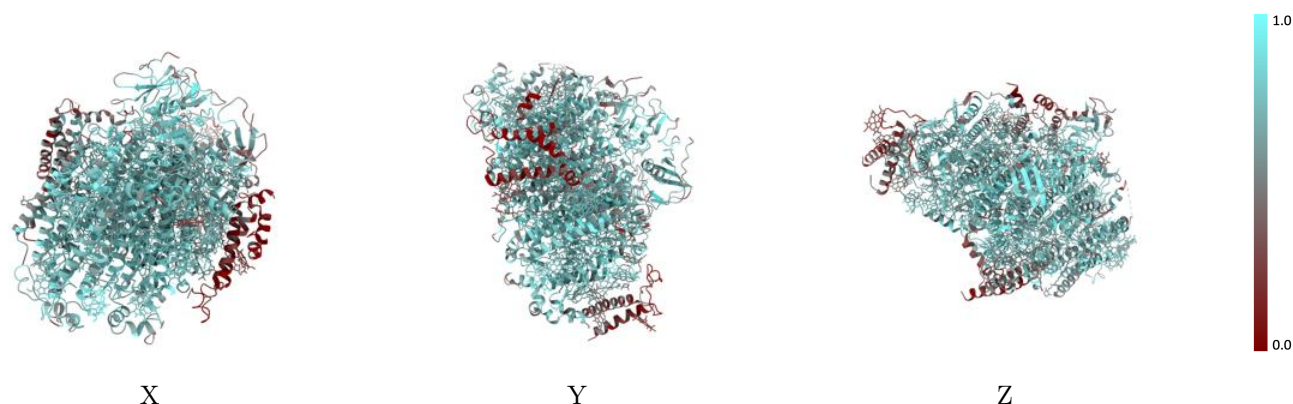
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



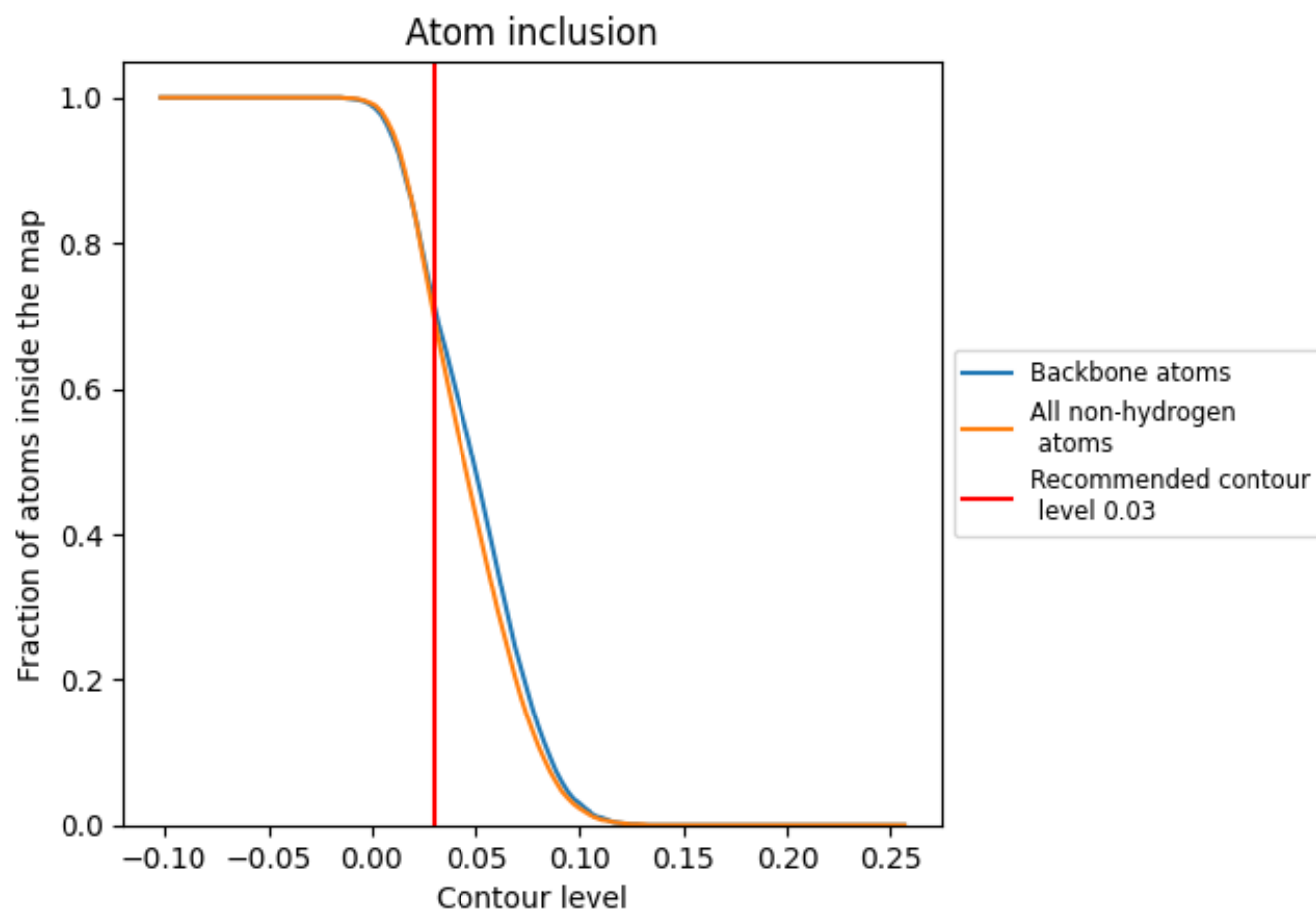
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 70% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6960	 0.5080
A	 0.7680	 0.5340
B	 0.7700	 0.5320
C	 0.7860	 0.5210
D	 0.6850	 0.5080
E	 0.6230	 0.5000
F	 0.1740	 0.3430
I	 0.5680	 0.4530
J	 0.1430	 0.2960
K	 0.2800	 0.3710
L	 0.4390	 0.4130
M	 0.5900	 0.4570

