



Full wwPDB EM Validation Report ⓘ

Oct 12, 2026 – 02:34 PM JST

PDB ID : 27GG / pdb_000027gg
EMDB ID : EMD-81136
Title : photosystem I with two LHCI from a green alga as lichen phycobiont
Authors : Su, X.D.; Wei, X.L.; Li, M.
Deposited on : 2026-05-29
Resolution : 3.84 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

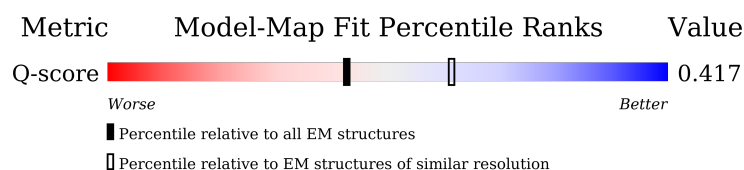
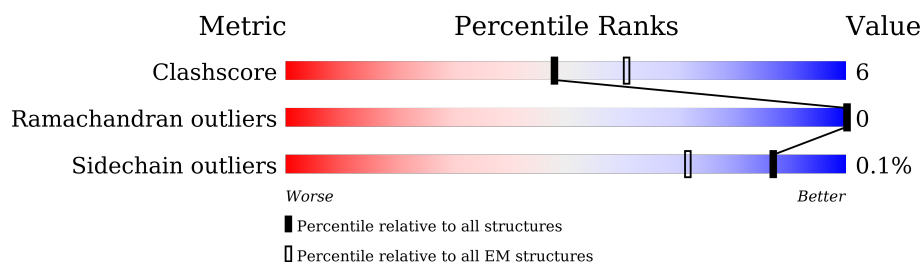
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.84 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.



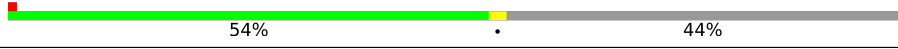
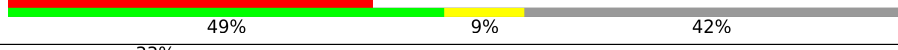
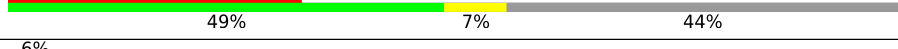
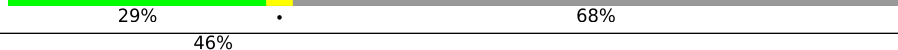
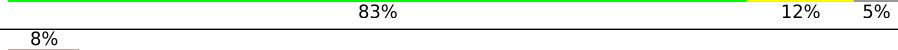
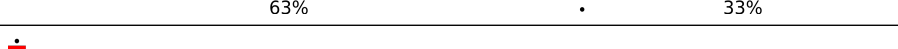
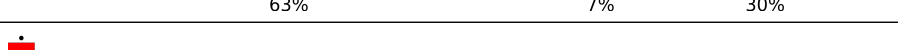
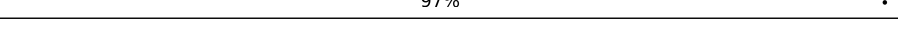
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	9033 (3.34 - 4.34)

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	2	270	
2	9	249	
3	A	751	
4	B	734	

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Mol	Chain	Length	Quality of chain
5	C	81	
6	D	239	
7	E	111	
8	F	251	
9	G	163	
10	H	126	
11	I	106	
12	J	41	
13	K	126	
14	L	176	
15	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
21	SF4	A	851	-	-	X	-

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 28453 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 Lhca2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	210	Total	C	N	O	S	0	0
			1590	1027	262	294	7		

- Molecule 2 is a protein called Lhca9.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	9	182	Total	C	N	O	S	0	0
			1427	925	240	258	4		

- Molecule 3 is a protein called PsaA.

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

- Molecule 4 is a protein called PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	734	Total	C	N	O	S	0	0
			5822	3823	984	1003	12		

- Molecule 5 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	81	Total	C	N	O	S	0	0
			608	374	104	117	13		

- Molecule 6 is a protein called PsaD.

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

- Molecule 7 is a protein called PsaE.

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

- Molecule 8 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	146	Total	C	N	O	S	0	0
			1124	726	199	197	2		

- Molecule 9 is a protein called PsaG.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	G	92	Total	C	N	O	0	0
			681	431	120	130		

- Molecule 10 is a protein called PsaH.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	H	54	Total	C	N	O	0	0
			412	266	77	69		

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

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

- Molecule 12 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	39	Total	C	N	O	S	0	0
			320	219	45	55	1		

- Molecule 13 is a protein called PsaK.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	K	84	Total	C	N	O	0	0
			595	380	100	115		

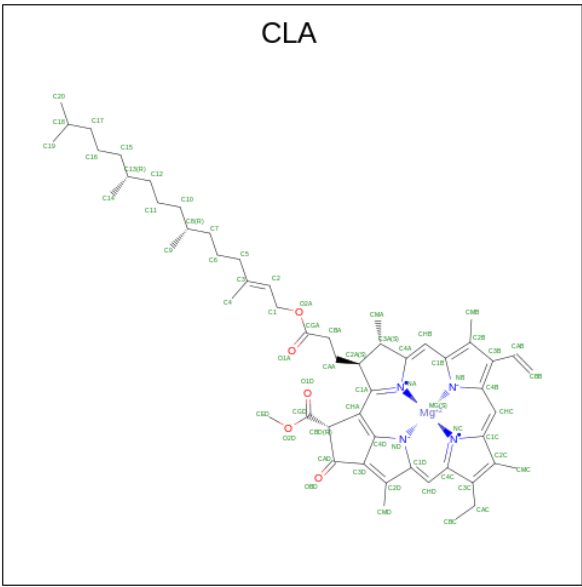
- Molecule 14 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	123	Total	C	N	O	S	0	0
			897	586	147	162	2		

- Molecule 15 is a protein called Photosystem I reaction center subunit XII.

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

- Molecule 16 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
16	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
16	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	2	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
16	2	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
16	2	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
16	2	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
16	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
16	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
16	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
16	2	1	Total 39	C 32	Mg 1	N 4	O 2	0
16	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
16	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
16	2	1	Total 40	C 32	Mg 1	N 4	O 3	0
16	9	1	Total 49	C 39	Mg 1	N 4	O 5	0
16	9	1	Total 51	C 41	Mg 1	N 4	O 5	0
16	9	1	Total 44	C 35	Mg 1	N 4	O 4	0
16	9	1	Total 45	C 36	Mg 1	N 4	O 4	0
16	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
16	9	1	Total 40	C 32	Mg 1	N 4	O 3	0
16	9	1	Total 35	C 29	Mg 1	N 4	O 1	0
16	9	1	Total 42	C 34	Mg 1	N 4	O 3	0
16	9	1	Total 42	C 34	Mg 1	N 4	O 3	0
16	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
16	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
16	A	1	Total 43	C 35	Mg 1	N 4	O 3	0
16	A	1	Total 61	C 51	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
16	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
16	A	1	Total	C	Mg	N	O	0
			49	41	1	4	3	
16	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
16	A	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
16	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
16	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
16	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
16	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
16	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
16	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
16	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
16	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
16	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			57	48	1	4	4	
16	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			54	45	1	4	4	
16	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
16	B	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
16	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
16	B	1	Total	C	Mg	N	O	0
			48	38	1	4	5	

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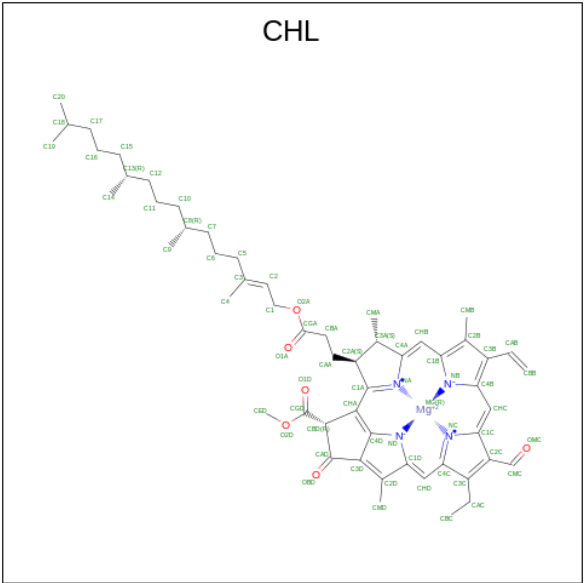
Mol	Chain	Residues	Atoms					AltConf
16	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
16	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
16	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	F	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
16	F	1	Total	C	Mg	N	O	0
			39	33	1	4	1	
16	G	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			35	29	1	4	1	
16	H	1	Total	C	Mg	N		0
			27	22	1	4		

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Mol	Chain	Residues	Atoms					AltConf
16	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
16	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
16	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	K	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
16	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
16	L	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
16	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	L	1	Total	C	Mg	N	O	0
			37	31	1	4	1	

- Molecule 17 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
17	9	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
17	9	1	Total	C	Mg	N	O	0
			41	32	1	4	4	

- Molecule 18 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms			AltCon
18	A	1	Total	C	O	0
			33	31	2	
18	B	1	Total	C	O	0
			33	31	2	

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $\text{C}_{38}\text{H}_{75}\text{O}_{10}\text{P}$).



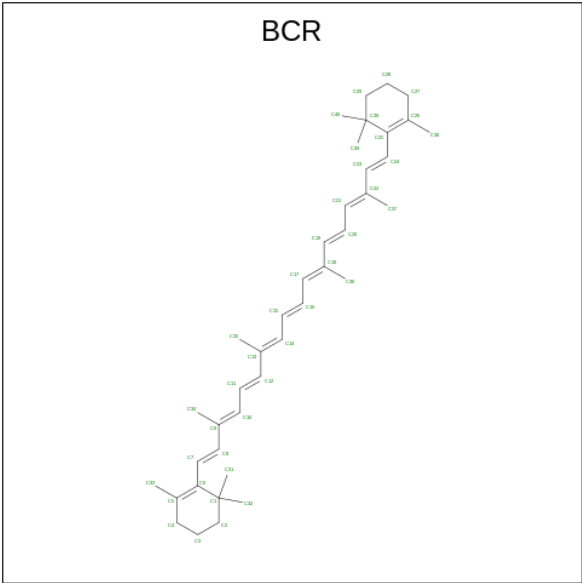
Mol	Chain	Residues	Atoms				AltCon
19	A	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
19	A	1	Total	C	O	P	0
			45	34	10	1	

- Molecule 20 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



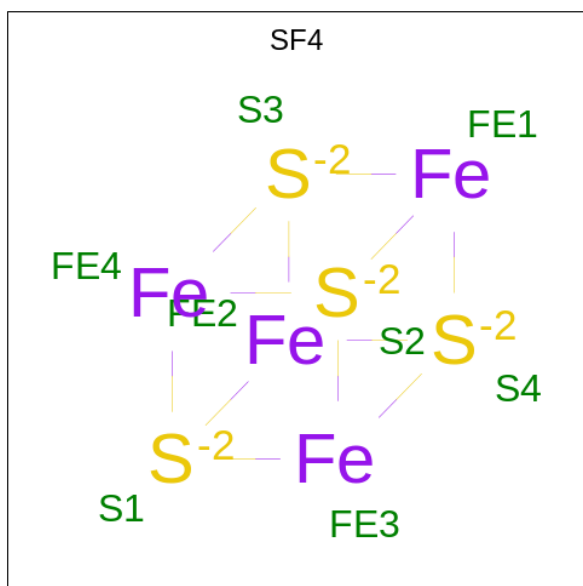
Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	A	1	Total	C	0
			40	40	
20	B	1	Total	C	0
			40	40	
20	B	1	Total	C	0
			40	40	
20	B	1	Total	C	0
			40	40	
20	B	1	Total	C	0
			40	40	
20	F	1	Total	C	0
			40	40	

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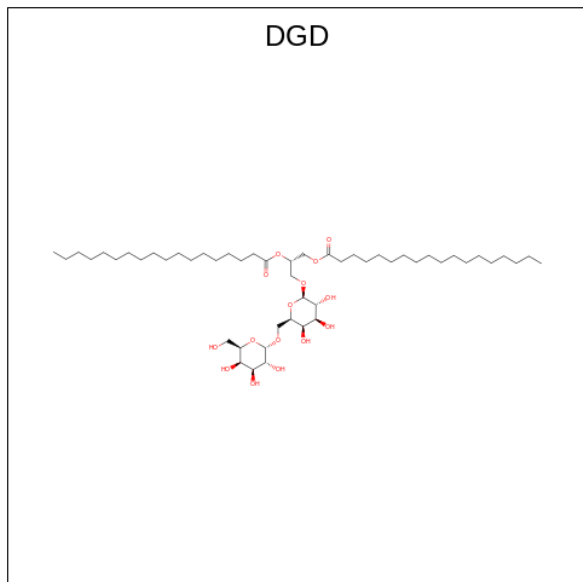
Mol	Chain	Residues	Atoms	AltConf
20	F	1	Total C 40 40	0
20	I	1	Total C 40 40	0
20	J	1	Total C 40 40	0
20	K	1	Total C 40 40	0
20	K	1	Total C 40 40	0
20	L	1	Total C 40 40	0
20	L	1	Total C 40 40	0
20	M	1	Total C 40 40	0

- Molecule 21 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 22 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).

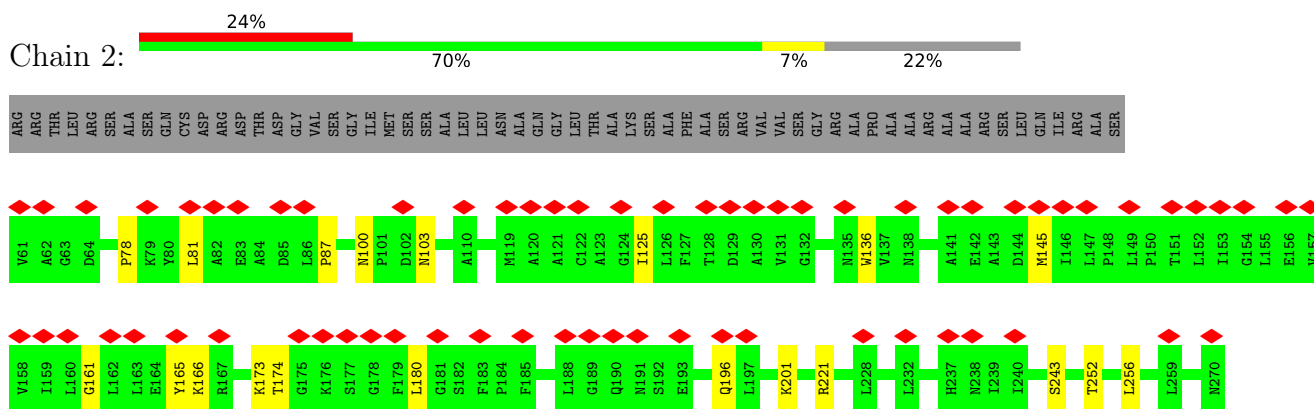


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
22	B	1	58	43	15	0

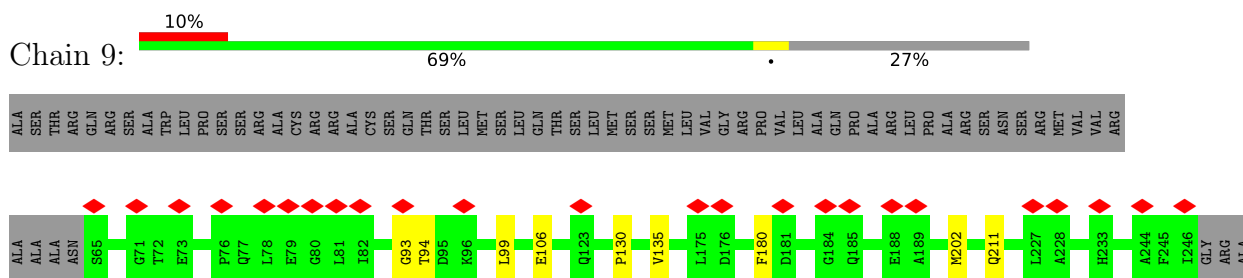
3 Residue-property plots

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.

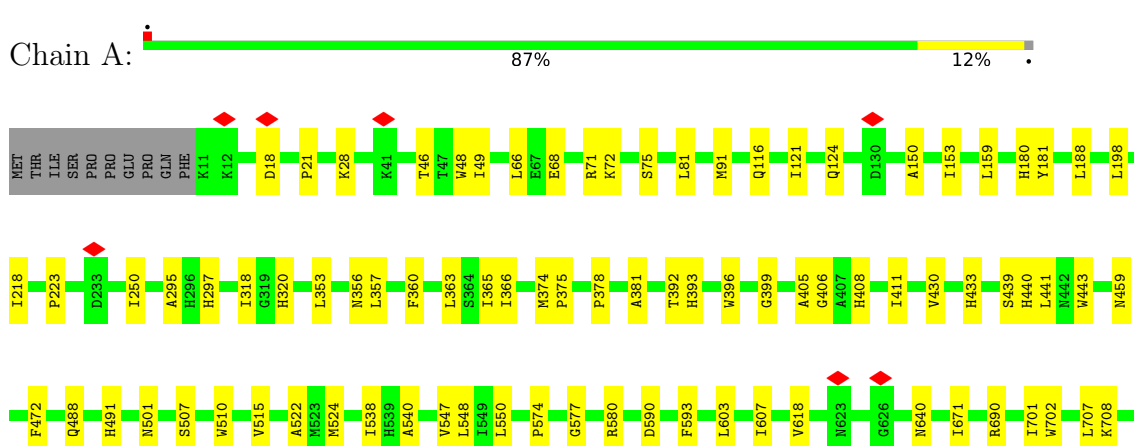
• Molecule 1: Lhca2



• Molecule 2: Lhca9



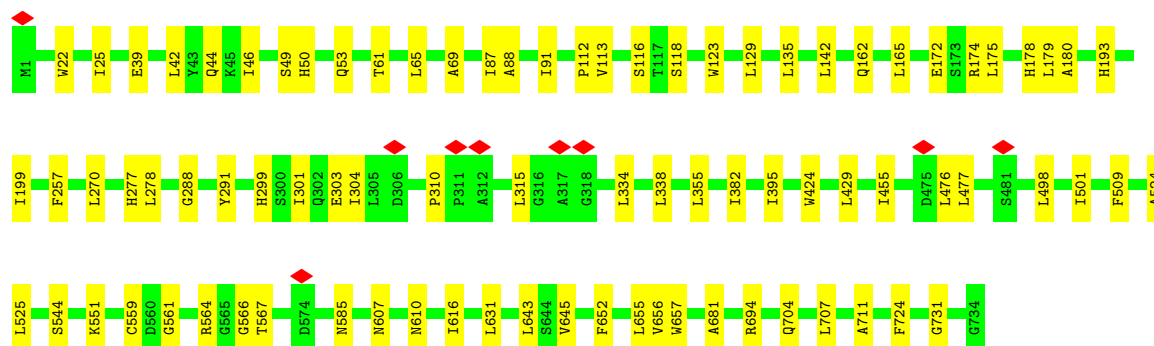
• Molecule 3: PsaA





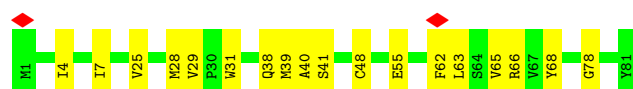
• Molecule 4: PsaB

Chain B: 88% 12%



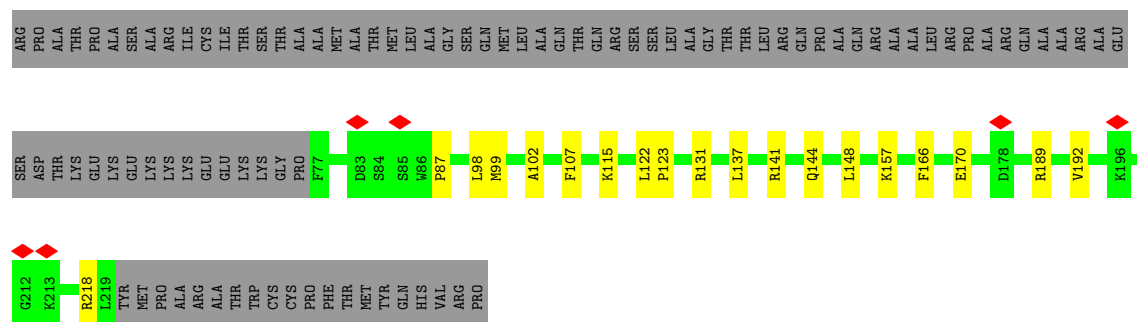
• Molecule 5: Photosystem I iron-sulfur center

Chain C: 78% 22%



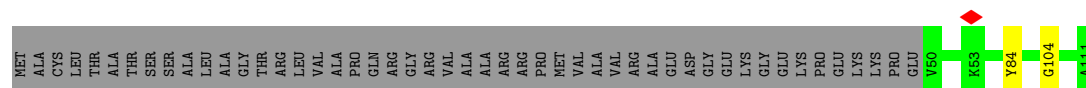
• Molecule 6: PsaD

Chain D: 52% 8% 40%



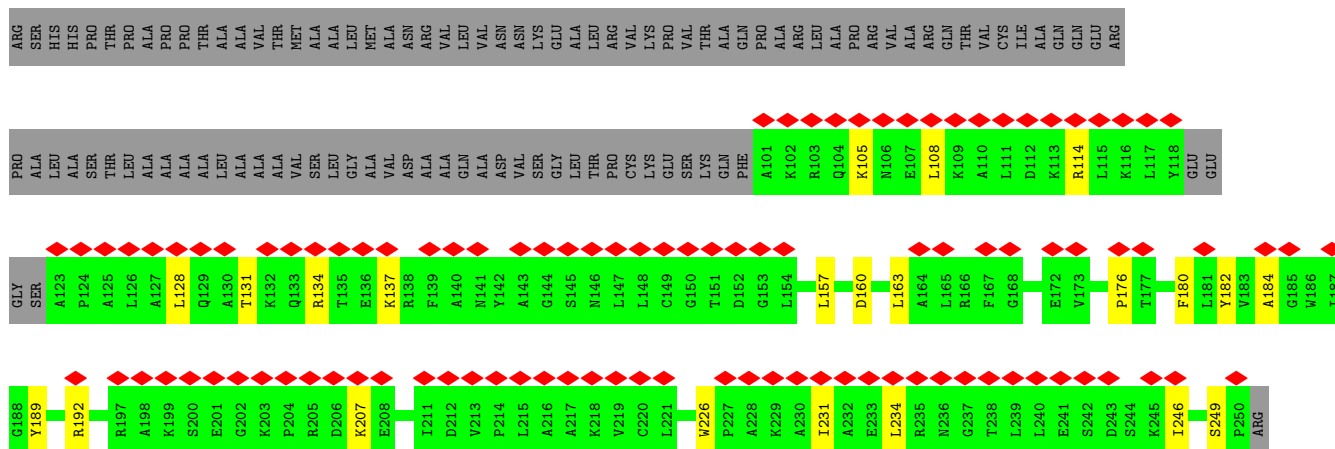
• Molecule 7: PsaE

Chain E: 54% 44%

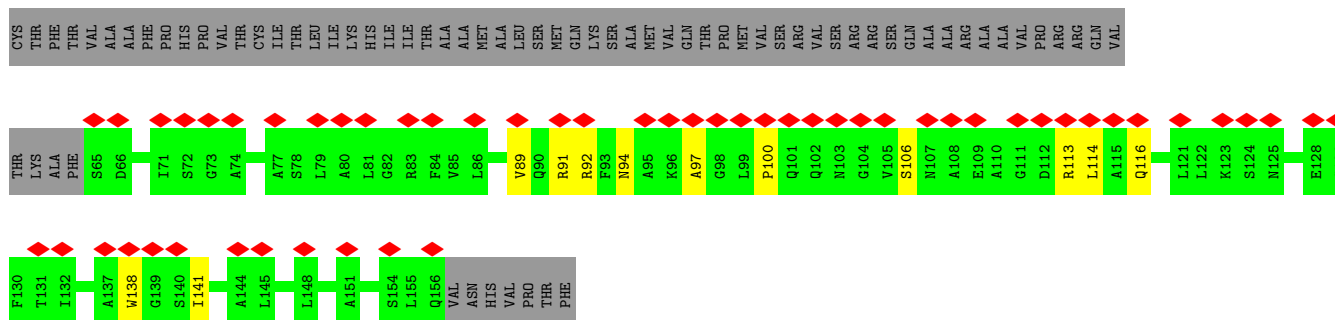


• Molecule 8: PsaF

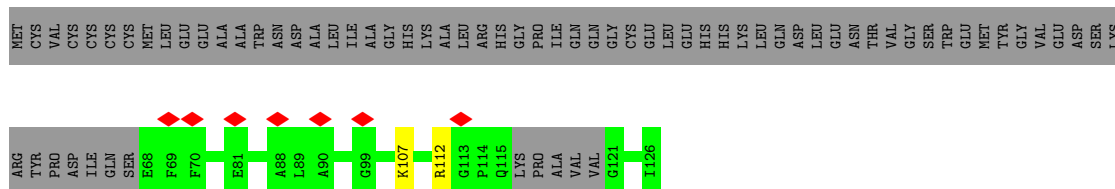
Chain F: 41% 49% 9% 42%



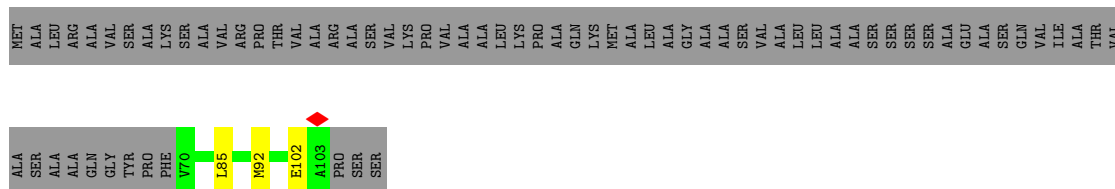
• Molecule 9: PsuG



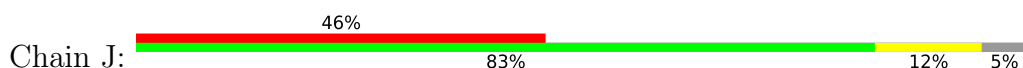
• Molecule 10: PsuH

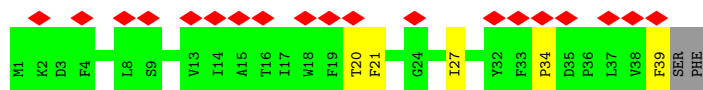


• Molecule 11: Photosystem I reaction center subunit VIII

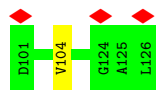
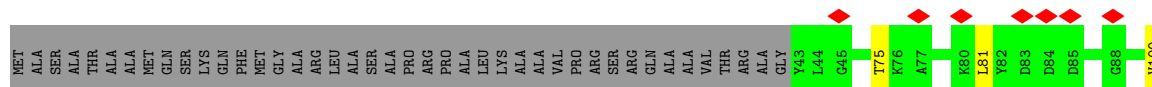


• Molecule 12: Photosystem I reaction center subunit IX

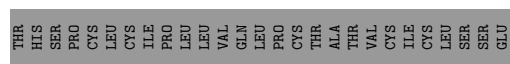
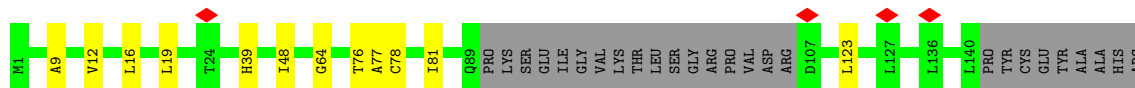




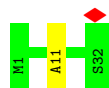
• Molecule 13: PsaK



• Molecule 14: PsaL



• Molecule 15: 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	20609	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI SPIRIT	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.201	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	2	0.25	0/1630	0.54	0/2225
2	9	0.23	0/1468	0.54	0/1997
3	A	0.20	0/6030	0.46	0/8224
4	B	0.20	0/6037	0.45	0/8252
5	C	0.20	0/618	0.53	0/836
6	D	0.19	0/1146	0.48	0/1545
7	E	0.20	0/495	0.45	0/674
8	F	0.25	0/1147	0.56	0/1547
9	G	0.24	0/693	0.55	0/943
10	H	0.20	0/421	0.52	0/563
11	I	0.30	0/265	0.63	0/367
12	J	0.26	0/331	0.50	0/454
13	K	0.23	0/605	0.55	0/823
14	L	0.24	0/916	0.55	0/1250
15	M	0.25	0/249	0.56	0/335
All	All	0.21	0/22051	0.49	0/30035

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2	1590	0	1588	13	0
2	9	1427	0	1398	6	0
3	A	5834	0	5700	72	0
4	B	5822	0	5577	66	0
5	C	608	0	593	13	0
6	D	1120	0	1137	14	0
7	E	484	0	481	1	0
8	F	1124	0	1165	18	0
9	G	681	0	678	9	0
10	H	412	0	422	1	0
11	I	256	0	268	3	0
12	J	320	0	322	6	0
13	K	595	0	605	4	0
14	L	897	0	930	8	0
15	M	246	0	260	1	0
16	2	522	0	352	6	0
16	9	434	0	318	5	0
16	A	2259	0	2034	68	0
16	B	2172	0	2003	71	0
16	F	91	0	71	3	0
16	G	92	0	68	0	0
16	H	62	0	20	0	0
16	J	42	0	31	1	0
16	K	179	0	138	0	0
16	L	138	0	112	3	0
17	9	84	0	55	1	0
18	A	33	0	46	1	0
18	B	33	0	46	2	0
19	A	94	0	137	2	0
20	A	200	0	280	17	0
20	B	160	0	224	13	0
20	F	80	0	112	7	0
20	I	40	0	56	4	0
20	J	40	0	56	1	0
20	K	80	0	112	4	0
20	L	80	0	112	6	0
20	M	40	0	56	5	0
21	A	8	0	0	2	0
21	C	16	0	0	0	0
22	B	58	0	74	3	0
All	All	28453	0	27637	330	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 6.

All (330) 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:A:393:HIS:HE1	16:A:827:CLA:ND	1.78	0.81
16:2:613:CLA:H3A	20:M:101:BCR:H281	1.66	0.77
3:A:393:HIS:CE1	16:A:827:CLA:ND	2.54	0.74
21:A:851:SF4:S4	4:B:559:CYS:CB	2.77	0.71
16:A:818:CLA:HAB	16:A:818:CLA:H8	1.72	0.71
3:A:690:ARG:HG3	3:A:720:ILE:HG13	1.76	0.68
16:A:803:CLA:HBB2	16:A:811:CLA:H102	1.75	0.68
16:A:827:CLA:ND	20:A:850:BCR:H281	2.08	0.68
3:A:393:HIS:ND1	16:A:827:CLA:NB	2.41	0.68
8:F:180:PHE:HE2	16:F:802:CLA:ND	1.92	0.68
3:A:68:GLU:HA	3:A:71:ARG:HD2	1.76	0.67
1:2:161:GLY:O	1:2:165:TYR:HB2	1.95	0.66
16:A:834:CLA:H71	20:A:849:BCR:H10C	1.78	0.66
16:B:826:CLA:HMA1	20:B:844:BCR:H17C	1.78	0.66
16:A:802:CLA:C1B	16:B:804:CLA:HBB1	2.15	0.65
3:A:441:LEU:HD22	16:A:838:CLA:HBB1	1.81	0.62
16:A:802:CLA:C4B	16:B:804:CLA:HBB1	2.15	0.62
4:B:310:PRO:HG2	4:B:315:LEU:H	1.65	0.62
4:B:544:SER:HA	8:F:249:SER:HB3	1.80	0.62
4:B:301:ILE:HG21	16:B:825:CLA:HAC1	1.82	0.62
16:B:806:CLA:H41	16:B:814:CLA:H61	1.82	0.62
16:B:837:CLA:H111	20:F:804:BCR:H23C	1.82	0.62
2:9:211:GLN:OE1	16:9:611:CLA:NA	2.33	0.61
16:A:820:CLA:H102	20:A:849:BCR:H21C	1.82	0.60
16:2:601:CLA:HBB2	16:2:602:CLA:HAC1	1.81	0.60
1:2:161:GLY:HA2	16:2:607:CLA:HAB	1.83	0.60
16:A:805:CLA:H121	20:A:846:BCR:H272	1.84	0.60
16:B:806:CLA:H122	16:B:806:CLA:HBD	1.83	0.60
2:9:93:GLY:HA3	2:9:99:LEU:HD13	1.84	0.59
4:B:694:ARG:HH22	11:I:102:GLU:HB2	1.66	0.59
4:B:616:ILE:HG21	16:B:802:CLA:HBA2	1.86	0.58
4:B:585:ASN:HB2	16:B:802:CLA:HBC2	1.85	0.58
4:B:53:GLN:HG2	16:B:806:CLA:H3A	1.84	0.58
1:2:173:LYS:HG3	1:2:174:THR:HG23	1.84	0.58
8:F:131:THR:HG22	8:F:134:ARG:HH12	1.69	0.58
3:A:720:ILE:HD11	4:B:566:GLY:HA3	1.87	0.57
4:B:53:GLN:HE21	16:B:806:CLA:HHB	1.67	0.57
3:A:538:ILE:HD12	16:A:801:CLA:H172	1.86	0.57
16:B:827:CLA:HED1	16:B:834:CLA:HAB	1.86	0.57
4:B:180:ALA:HB2	4:B:288:GLY:HA3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B:808:CLA:HBC1	15:M:11:ALA:HB1	1.88	0.56
16:B:802:CLA:HHB	16:B:803:CLA:H192	1.88	0.56
3:A:124:GLN:OE1	16:A:809:CLA:NC	2.39	0.56
4:B:199:ILE:HG12	4:B:270:LEU:HB3	1.87	0.56
16:F:803:CLA:HBB2	20:F:804:BCR:H382	1.88	0.56
16:B:807:CLA:H151	16:B:829:CLA:HBB2	1.88	0.56
16:B:824:CLA:HED3	16:B:824:CLA:H2A	1.87	0.56
3:A:733:LEU:HD22	16:A:840:CLA:HMA1	1.88	0.55
4:B:87:ILE:HD12	4:B:113:VAL:HG21	1.87	0.55
1:2:100:ASN:HB2	1:2:103:ASN:HB2	1.87	0.55
16:A:828:CLA:H12	20:A:847:BCR:H402	1.88	0.55
16:B:801:CLA:H3A	16:B:801:CLA:H11	1.89	0.55
3:A:671:ILE:HG22	3:A:741:ALA:HB2	1.88	0.55
6:D:87:PRO:HB2	6:D:131:ARG:HH21	1.72	0.55
3:A:375:PRO:HG2	3:A:381:ALA:HB2	1.88	0.54
5:C:7:ILE:HG12	5:C:65:VAL:HG12	1.88	0.54
20:K:202:BCR:H362	20:K:206:BCR:H403	1.88	0.54
3:A:81:LEU:HD11	16:A:813:CLA:HBA2	1.88	0.54
4:B:172:GLU:HG3	9:G:100:PRO:HB3	1.90	0.54
5:C:68:TYR:HB2	6:D:218:ARG:HH21	1.73	0.54
3:A:91:MET:HE1	16:A:808:CLA:H2A	1.90	0.54
3:A:491:HIS:HE1	16:A:834:CLA:NB	2.06	0.53
8:F:105:LYS:HD3	8:F:108:LEU:HD11	1.90	0.53
16:A:839:CLA:H2A	16:A:839:CLA:HED3	1.90	0.53
7:E:84:TYR:HA	7:E:104:GLY:HA2	1.90	0.53
1:2:145:MET:HE3	16:2:605:CLA:HAB	1.91	0.53
4:B:123:TRP:HH2	16:B:829:CLA:H2	1.73	0.52
16:B:801:CLA:HBB1	16:B:802:CLA:C4B	2.39	0.52
5:C:25:VAL:HG21	5:C:48:CYS:HB2	1.90	0.52
2:9:106:GLU:HG3	2:9:202:MET:HE1	1.90	0.52
4:B:303:GLU:HG3	9:G:97:ALA:HA	1.91	0.52
16:B:840:CLA:H2	18:B:841:PQN:H243	1.91	0.52
5:C:29:VAL:HG12	6:D:189:ARG:HB3	1.92	0.52
16:2:611:CLA:HED3	16:2:611:CLA:H2A	1.91	0.52
3:A:441:LEU:HD21	3:A:547:VAL:HG12	1.90	0.52
9:G:89:VAL:HA	9:G:92:ARG:HG2	1.92	0.52
8:F:114:ARG:HB3	8:F:128:LEU:HD13	1.92	0.52
8:F:137:LYS:HE2	12:J:34:PRO:HD2	1.92	0.52
3:A:547:VAL:HG21	16:A:838:CLA:HMA1	1.91	0.51
3:A:577:GLY:HA2	4:B:561:GLY:HA2	1.93	0.51
3:A:707:LEU:HD21	16:B:832:CLA:H3A	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:28:LYS:HB2	16:A:811:CLA:HAA2	1.92	0.51
3:A:121:ILE:HD11	12:J:27:ILE:HG12	1.93	0.51
3:A:408:HIS:HA	3:A:411:ILE:HG22	1.93	0.51
16:A:819:CLA:HBA1	13:K:100:VAL:HG12	1.93	0.51
16:B:804:CLA:H141	16:B:811:CLA:HBC1	1.93	0.51
3:A:363:LEU:HD11	16:A:818:CLA:H72	1.92	0.51
16:A:804:CLA:HAA1	16:A:811:CLA:H2	1.93	0.51
14:L:78:CYS:HB2	20:L:305:BCR:H12C	1.93	0.51
3:A:223:PRO:HG3	3:A:250:ILE:HD12	1.93	0.51
3:A:439:SER:HB2	4:B:681:ALA:HB2	1.93	0.51
3:A:443:TRP:CE2	16:A:831:CLA:HAB	2.47	0.50
4:B:50:HIS:NE2	16:B:806:CLA:NA	2.59	0.50
16:A:832:CLA:H11	16:A:841:CLA:H43	1.92	0.50
12:J:21:PHE:HA	16:J:102:CLA:HBB2	1.92	0.50
9:G:113:ARG:HA	9:G:116:GLN:HG2	1.93	0.50
4:B:174:ARG:HG2	16:B:825:CLA:HMD1	1.92	0.50
16:B:814:CLA:H171	20:B:842:BCR:HC42	1.93	0.50
5:C:4:ILE:HB	6:D:218:ARG:HH22	1.77	0.50
2:9:94:THR:HG21	9:G:113:ARG:HB2	1.94	0.50
4:B:178:HIS:HB3	16:B:825:CLA:HED2	1.93	0.50
4:B:564:ARG:HH21	4:B:567:THR:HG21	1.77	0.50
16:B:813:CLA:HBB1	16:B:821:CLA:C4D	2.10	0.50
3:A:150:ALA:HB2	3:A:378:PRO:HD2	1.94	0.49
4:B:88:ALA:HB2	4:B:116:SER:HB2	1.94	0.49
8:F:134:ARG:HD3	12:J:34:PRO:HG2	1.92	0.49
3:A:353:LEU:O	3:A:357:LEU:HB2	2.12	0.49
3:A:392:THR:HG23	3:A:607:ILE:HG21	1.94	0.49
3:A:459:ASN:HD22	3:A:640:ASN:HB2	1.77	0.49
20:A:850:BCR:HC7	16:B:801:CLA:H101	1.94	0.49
4:B:607:ASN:HA	4:B:610:ASN:HB2	1.95	0.49
14:L:76:THR:HG21	14:L:123:LEU:HD22	1.94	0.49
4:B:498:LEU:HA	4:B:501:ILE:HG22	1.93	0.49
3:A:320:HIS:NE2	16:A:821:CLA:C4D	2.74	0.49
3:A:488:GLN:HG3	3:A:510:TRP:HE3	1.78	0.49
3:A:356:ASN:O	3:A:360:PHE:HB2	2.11	0.49
6:D:166:PHE:HD2	6:D:170:GLU:HB3	1.77	0.49
16:B:801:CLA:H42	16:B:801:CLA:HBB	1.94	0.48
4:B:118:SER:HA	16:B:828:CLA:HMA2	1.94	0.48
3:A:707:LEU:HD13	20:F:804:BCR:HC7	1.93	0.48
16:A:805:CLA:H151	20:A:846:BCR:H23C	1.95	0.48
8:F:184:ALA:HB1	16:F:802:CLA:H2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:353:LEU:HD11	16:A:829:CLA:HBB1	1.95	0.48
16:A:818:CLA:H3A	16:A:818:CLA:HBA2	1.65	0.48
4:B:175:LEU:O	4:B:179:LEU:HB2	2.13	0.48
16:B:835:CLA:HBA2	16:B:835:CLA:H3A	1.55	0.48
16:A:840:CLA:HBB1	16:B:801:CLA:H121	1.96	0.48
3:A:702:TRP:HA	8:F:246:ILE:HG12	1.94	0.48
16:A:830:CLA:H3A	16:A:830:CLA:HBA2	1.43	0.48
3:A:75:SER:HB2	3:A:181:TYR:HB2	1.96	0.47
3:A:580:ARG:HG2	5:C:78:GLY:HA3	1.97	0.47
16:A:817:CLA:H3A	16:A:817:CLA:HBA2	1.54	0.47
4:B:142:LEU:HD21	20:B:843:BCR:H342	1.95	0.47
4:B:69:ALA:HB2	4:B:135:LEU:HB2	1.96	0.47
3:A:393:HIS:CE1	16:A:827:CLA:NC	2.82	0.47
6:D:98:LEU:HD23	6:D:102:ALA:HB2	1.96	0.47
4:B:49:SER:HB2	16:B:806:CLA:HBB1	1.97	0.47
4:B:22:TRP:CG	4:B:704:GLN:HE22	2.32	0.47
16:B:814:CLA:H143	16:B:819:CLA:H2	1.96	0.47
5:C:7:ILE:HG21	5:C:40:ALA:HB3	1.97	0.47
12:J:20:THR:HG23	20:J:101:BCR:H363	1.97	0.47
4:B:711:ALA:HA	22:B:846:DGD:HBN1	1.96	0.47
3:A:357:LEU:HB3	3:A:405:ALA:HB2	1.97	0.47
16:A:801:CLA:HBB1	16:B:802:CLA:HED2	1.97	0.46
4:B:395:ILE:HG23	4:B:551:LYS:HA	1.97	0.46
3:A:441:LEU:HG	3:A:548:LEU:HB2	1.97	0.46
3:A:66:LEU:HD23	3:A:188:LEU:HD21	1.98	0.46
16:A:833:CLA:HHH	16:B:810:CLA:HBB2	1.97	0.46
4:B:455:ILE:HD13	8:F:157:LEU:HB2	1.98	0.46
8:F:182:TYR:HA	8:F:226:TRP:HZ2	1.81	0.46
3:A:46:THR:HG21	16:A:852:CLA:HBB1	1.97	0.46
20:B:845:BCR:H15C	20:B:845:BCR:H351	1.71	0.46
8:F:105:LYS:HB2	8:F:105:LYS:HE2	1.77	0.46
5:C:28:MET:HE3	5:C:38:GLN:HB3	1.96	0.46
20:M:101:BCR:H20C	20:M:101:BCR:H361	1.73	0.46
3:A:180:HIS:HE1	16:A:810:CLA:NC	2.14	0.46
16:A:829:CLA:H152	19:A:844:LHG:H362	1.96	0.46
1:2:125:ILE:HD12	1:2:136:TRP:HB2	1.97	0.46
4:B:501:ILE:HD11	4:B:509:PHE:HB2	1.98	0.46
4:B:174:ARG:HE	16:B:814:CLA:HBC2	1.81	0.46
14:L:48:ILE:HG22	14:L:64:GLY:HA3	1.98	0.46
8:F:160:ASP:HB3	8:F:163:LEU:HB2	1.98	0.45
1:2:78:PRO:HD2	1:2:81:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:116:GLN:OE1	16:A:808:CLA:C4D	2.62	0.45
4:B:193:HIS:CE1	16:B:815:CLA:NA	2.85	0.45
16:B:828:CLA:H3A	16:B:828:CLA:HBA2	1.50	0.45
4:B:25:ILE:HG12	20:L:305:BCR:H272	1.97	0.45
20:F:801:BCR:H351	20:F:801:BCR:H15C	1.72	0.45
14:L:19:LEU:HD22	16:L:303:CLA:HBD	1.97	0.45
3:A:48:TRP:HE3	3:A:49:ILE:HD13	1.82	0.45
20:F:804:BCR:H11C	20:F:804:BCR:H341	1.83	0.45
2:9:130:PRO:HD2	2:9:135:VAL:HG22	1.98	0.45
3:A:524:MET:HG2	3:A:618:VAL:HG13	1.98	0.45
20:B:842:BCR:H24C	20:B:842:BCR:H371	1.74	0.45
2:9:180:PHE:HB3	16:9:608:CLA:HBD	1.98	0.45
3:A:399:GLY:HA3	3:A:603:LEU:HD11	1.98	0.45
4:B:476:LEU:HD12	4:B:477:LEU:HB2	1.98	0.45
16:A:818:CLA:HAB	16:A:818:CLA:H111	1.99	0.45
5:C:41:SER:HB2	6:D:192:VAL:H	1.81	0.45
8:F:192:ARG:HD2	20:F:804:BCR:H313	1.99	0.45
16:A:819:CLA:H3A	16:A:819:CLA:HBA2	1.47	0.45
20:A:848:BCR:H20C	20:A:848:BCR:H361	1.83	0.45
4:B:278:LEU:HD11	16:B:817:CLA:HAB	1.98	0.44
5:C:55:GLU:HB3	5:C:63:LEU:HD22	1.98	0.44
20:K:206:BCR:H15C	20:K:206:BCR:H351	1.75	0.44
20:B:843:BCR:H15C	20:B:843:BCR:H351	1.78	0.44
17:9:605:CHL:HHC	17:9:605:CHL:HBB1	1.98	0.44
16:A:812:CLA:HBB2	20:A:847:BCR:H342	1.99	0.44
16:A:839:CLA:H3A	16:A:839:CLA:HBA2	1.58	0.44
4:B:424:TRP:CE2	16:B:832:CLA:HAB	2.53	0.44
16:B:821:CLA:HBA2	16:B:821:CLA:H3A	1.44	0.44
16:B:839:CLA:H112	16:B:839:CLA:H72	1.74	0.44
20:B:843:BCR:H371	20:B:843:BCR:H24C	1.73	0.44
3:A:690:ARG:HD2	3:A:719:SER:HA	1.99	0.44
16:A:826:CLA:H12	20:A:849:BCR:H16C	2.00	0.44
4:B:61:THR:HG23	4:B:142:LEU:HD13	2.00	0.44
3:A:396:TRP:CD1	16:A:827:CLA:HAB	2.52	0.44
1:2:161:GLY:O	1:2:165:TYR:CB	2.64	0.44
16:A:832:CLA:H102	16:A:832:CLA:H62	1.79	0.44
16:B:818:CLA:HBA2	16:B:827:CLA:HBB2	1.99	0.44
16:B:808:CLA:H2	16:B:808:CLA:H61	1.63	0.44
6:D:123:PRO:HD3	6:D:148:LEU:HD13	1.99	0.44
3:A:459:ASN:HD21	3:A:472:PHE:HB2	1.82	0.43
20:I:201:BCR:H15C	20:I:201:BCR:H351	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:812:CLA:HED2	16:A:812:CLA:HBD	1.84	0.43
4:B:129:LEU:HD13	4:B:135:LEU:HD23	2.00	0.43
4:B:524:ALA:HB2	16:B:837:CLA:HMA1	2.00	0.43
16:B:829:CLA:H3A	16:B:829:CLA:HBA2	1.49	0.43
20:I:201:BCR:H11C	20:I:201:BCR:H341	1.84	0.43
20:M:101:BCR:H11C	20:M:101:BCR:H341	1.87	0.43
4:B:429:LEU:HB3	4:B:525:LEU:HB2	2.00	0.43
20:M:101:BCR:H15C	20:M:101:BCR:H351	1.90	0.43
16:9:603:CLA:H3A	16:9:603:CLA:HBA1	1.80	0.43
3:A:440:HIS:CE1	16:A:831:CLA:NA	2.87	0.43
3:A:701:ILE:HD11	3:A:715:PRO:HD2	2.00	0.43
4:B:42:LEU:O	4:B:46:ILE:HG12	2.18	0.43
16:B:807:CLA:H101	16:B:807:CLA:H13	1.82	0.43
8:F:231:ILE:HG22	8:F:234:LEU:H	1.83	0.43
16:B:804:CLA:HED2	16:B:804:CLA:HBD	1.76	0.43
16:B:813:CLA:HAA1	9:G:114:LEU:HG	1.99	0.43
16:B:839:CLA:HBB2	18:B:841:PQN:H141	2.01	0.43
11:I:92:MET:HG2	20:L:305:BCR:H373	1.99	0.43
20:K:206:BCR:H11C	20:K:206:BCR:H341	1.76	0.43
8:F:207:LYS:HA	8:F:207:LYS:HD3	1.78	0.43
4:B:39:GLU:HG2	4:B:165:LEU:HD11	2.01	0.43
4:B:707:LEU:HD22	22:B:846:DGD:HA22	2.01	0.43
6:D:141:ARG:HB2	6:D:144:GLN:HG3	2.00	0.43
21:A:851:SF4:S4	4:B:559:CYS:HB3	2.52	0.43
6:D:122:LEU:HD23	6:D:137:LEU:HD21	2.01	0.43
8:F:189:TYR:HA	8:F:192:ARG:HG2	2.00	0.43
16:A:822:CLA:HBB	16:A:843:CLA:HBC3	2.01	0.43
4:B:91:ILE:HB	4:B:112:PRO:HB2	2.00	0.43
20:B:842:BCR:H341	20:B:842:BCR:H11C	1.65	0.43
4:B:277:HIS:CE1	16:B:819:CLA:NA	2.86	0.43
16:B:809:CLA:H3A	16:B:809:CLA:HBA2	1.56	0.43
20:F:804:BCR:H16C	20:F:804:BCR:H19C	1.78	0.42
3:A:590:ASP:HA	3:A:593:PHE:HB3	2.01	0.42
16:A:801:CLA:HBA1	16:A:801:CLA:H3A	1.70	0.42
20:A:849:BCR:H15C	20:A:849:BCR:H351	1.75	0.42
20:A:849:BCR:H24C	20:A:849:BCR:H371	1.86	0.42
4:B:643:LEU:HD11	4:B:731:GLY:HA3	2.01	0.42
20:B:845:BCR:H11C	20:B:845:BCR:H341	1.74	0.42
16:9:602:CLA:HAB	16:9:603:CLA:HMB2	2.02	0.42
3:A:218:ILE:HD11	3:A:295:ALA:HB1	2.01	0.42
16:B:811:CLA:H2	16:B:811:CLA:H62	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:221:ARG:HH11	1:2:243:SER:HB3	1.84	0.42
3:A:374:MET:HE2	3:A:507:SER:HB2	2.02	0.42
16:A:802:CLA:C1B	16:B:804:CLA:CBB	2.93	0.42
20:A:848:BCR:H11C	20:A:848:BCR:H341	1.82	0.42
10:H:107:LYS:HA	10:H:112:ARG:HH21	1.84	0.42
16:L:303:CLA:H12	16:L:303:CLA:H51	1.91	0.42
3:A:297:HIS:HE2	16:A:818:CLA:C2B	2.33	0.42
4:B:257:PHE:CZ	16:B:818:CLA:H2	2.55	0.42
4:B:645:VAL:HG23	16:B:810:CLA:HAC1	2.02	0.42
3:A:68:GLU:O	3:A:72:LYS:HG3	2.20	0.42
3:A:406:GLY:HA3	3:A:550:LEU:HD13	2.01	0.42
20:A:847:BCR:H341	20:A:847:BCR:H11C	1.77	0.42
16:B:826:CLA:H43	16:B:837:CLA:HBA1	2.00	0.42
6:D:115:LYS:HB2	6:D:115:LYS:HE2	1.81	0.42
13:K:100:VAL:O	13:K:104:VAL:HG23	2.20	0.42
1:2:87:PRO:HG3	1:2:196:GLN:NE2	2.35	0.42
16:B:808:CLA:H122	20:I:201:BCR:H332	2.01	0.42
6:D:99:MET:HE3	6:D:99:MET:HB2	1.86	0.42
9:G:91:ARG:HH12	9:G:94:ASN:HD22	1.67	0.42
3:A:153:ILE:HG21	3:A:159:LEU:HG	2.01	0.42
16:A:802:CLA:H141	16:A:802:CLA:H162	1.86	0.42
4:B:334:LEU:HD11	16:B:830:CLA:HBB1	2.02	0.42
4:B:551:LYS:H	4:B:551:LYS:HG2	1.72	0.42
14:L:9:ALA:HB3	14:L:12:VAL:HG23	2.02	0.42
1:2:166:LYS:HB2	1:2:180:LEU:HB2	2.02	0.42
3:A:708:LYS:HD3	3:A:708:LYS:HA	1.92	0.42
16:A:806:CLA:H12	16:A:806:CLA:HBA2	1.89	0.42
20:A:847:BCR:H24C	20:A:847:BCR:H371	1.89	0.42
4:B:631:LEU:HD22	4:B:724:PHE:HA	2.01	0.42
16:B:808:CLA:H101	20:I:201:BCR:HC21	2.02	0.42
3:A:318:ILE:HG21	13:K:104:VAL:HG21	2.02	0.41
4:B:299:HIS:HB3	4:B:304:ILE:HD11	2.02	0.41
5:C:62:PHE:HB3	5:C:63:LEU:H	1.67	0.41
11:I:85:LEU:HD21	20:L:301:BCR:HC22	2.01	0.41
4:B:338:LEU:HD22	4:B:382:ILE:HG23	2.01	0.41
4:B:657:TRP:CZ3	16:B:803:CLA:HHB	2.55	0.41
16:B:812:CLA:HBA2	9:G:114:LEU:HD21	2.02	0.41
5:C:31:TRP:HB2	5:C:39:MET:HB2	2.02	0.41
20:K:202:BCR:H361	20:K:202:BCR:H20C	1.77	0.41
3:A:365:ILE:HG22	16:A:825:CLA:HED2	2.02	0.41
3:A:574:PRO:HB3	3:A:720:ILE:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:174:ARG:O	4:B:178:HIS:HB2	2.20	0.41
13:K:75:THR:HB	13:K:81:LEU:HD23	2.02	0.41
1:2:252:THR:O	1:2:256:LEU:HB2	2.20	0.41
16:A:832:CLA:H111	16:A:832:CLA:H143	1.82	0.41
20:A:848:BCR:H351	20:A:848:BCR:H15C	1.79	0.41
4:B:44:GLN:HG2	4:B:162:GLN:HG2	2.02	0.41
5:C:66:ARG:HA	5:C:66:ARG:HD3	1.80	0.41
8:F:176:PRO:HG3	12:J:39:PHE:HD2	1.84	0.41
4:B:291:TYR:HA	4:B:299:HIS:H	1.85	0.41
16:B:828:CLA:H2	16:B:828:CLA:H62	1.66	0.41
14:L:16:LEU:HA	14:L:19:LEU:HD12	2.02	0.41
1:2:201:LYS:HB3	16:2:609:CLA:HMD1	2.02	0.41
16:A:806:CLA:H52	19:A:844:LHG:H251	2.03	0.41
16:B:809:CLA:H192	16:B:809:CLA:H162	1.88	0.41
16:B:840:CLA:H61	16:B:840:CLA:H41	1.86	0.41
6:D:157:LYS:HB2	6:D:157:LYS:HE2	1.89	0.41
16:A:831:CLA:HBB2	20:L:301:BCR:H373	2.03	0.41
16:B:840:CLA:HED3	22:B:846:DGD:HA52	2.02	0.41
16:A:802:CLA:HAA1	4:B:655:LEU:HD13	2.02	0.41
16:B:815:CLA:HBA1	20:B:843:BCR:H332	2.02	0.41
16:B:824:CLA:HBA2	16:B:824:CLA:H3A	1.79	0.41
16:9:606:CLA:HBA1	16:9:606:CLA:H3A	1.76	0.40
3:A:18:ASP:HB3	3:A:21:PRO:HG3	2.02	0.40
3:A:515:VAL:HG13	3:A:522:ALA:HB3	2.03	0.40
4:B:65:LEU:HD11	20:B:843:BCR:HC32	2.02	0.40
16:B:806:CLA:HBC2	16:B:830:CLA:HMA1	2.03	0.40
9:G:138:TRP:HA	9:G:141:ILE:HG22	2.03	0.40
16:A:826:CLA:H61	16:A:826:CLA:H2	1.72	0.40
16:A:840:CLA:HAA1	18:A:842:PQN:H302	2.03	0.40
4:B:652:PHE:O	4:B:656:VAL:HG23	2.21	0.40
3:A:198:LEU:HD23	3:A:198:LEU:HA	1.94	0.40
3:A:430:VAL:HA	3:A:433:HIS:CE1	2.56	0.40
3:A:540:ALA:HB2	16:A:837:CLA:HMA1	2.01	0.40
20:B:842:BCR:H281	20:B:842:BCR:H393	1.90	0.40
6:D:102:ALA:HA	6:D:107:PHE:HB3	2.03	0.40
3:A:366:ILE:HD13	16:A:825:CLA:HED3	2.04	0.40
16:A:814:CLA:H3A	20:A:846:BCR:H382	2.02	0.40
16:B:808:CLA:H93	20:M:101:BCR:H353	2.03	0.40
14:L:39:HIS:CE1	16:L:303:CLA:NA	2.89	0.40
3:A:393:HIS:HE1	16:A:827:CLA:C1D	2.34	0.40
3:A:501:ASN:HB3	16:A:816:CLA:HED2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:845:BCR:H20C	20:B:845:BCR:H36I	1.94	0.40
14:L:77:ALA:O	14:L:81:ILE:HG13	2.22	0.40
20:L:301:BCR:H15C	20:L:301:BCR:H35I	1.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	208/270 (77%)	188 (90%)	20 (10%)	0	100	100
2	9	180/249 (72%)	171 (95%)	9 (5%)	0	100	100
3	A	739/751 (98%)	704 (95%)	35 (5%)	0	100	100
4	B	732/734 (100%)	693 (95%)	39 (5%)	0	100	100
5	C	79/81 (98%)	74 (94%)	5 (6%)	0	100	100
6	D	141/239 (59%)	134 (95%)	7 (5%)	0	100	100
7	E	60/111 (54%)	54 (90%)	6 (10%)	0	100	100
8	F	142/251 (57%)	133 (94%)	9 (6%)	0	100	100
9	G	90/163 (55%)	82 (91%)	8 (9%)	0	100	100
10	H	50/126 (40%)	47 (94%)	3 (6%)	0	100	100
11	I	32/106 (30%)	29 (91%)	3 (9%)	0	100	100
12	J	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
13	K	82/126 (65%)	78 (95%)	4 (5%)	0	100	100
14	L	119/176 (68%)	114 (96%)	5 (4%)	0	100	100
15	M	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
All	All	2721/3456 (79%)	2566 (94%)	155 (6%)	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	2	163/207 (79%)	163 (100%)	0	100	100
2	9	147/201 (73%)	147 (100%)	0	100	100
3	A	604/614 (98%)	604 (100%)	0	100	100
4	B	595/595 (100%)	594 (100%)	1 (0%)	87	87
5	C	70/70 (100%)	70 (100%)	0	100	100
6	D	119/194 (61%)	119 (100%)	0	100	100
7	E	53/89 (60%)	53 (100%)	0	100	100
8	F	113/190 (60%)	113 (100%)	0	100	100
9	G	69/129 (54%)	68 (99%)	1 (1%)	59	70
10	H	40/101 (40%)	40 (100%)	0	100	100
11	I	28/76 (37%)	28 (100%)	0	100	100
12	J	35/37 (95%)	35 (100%)	0	100	100
13	K	60/87 (69%)	60 (100%)	0	100	100
14	L	92/140 (66%)	92 (100%)	0	100	100
15	M	27/27 (100%)	27 (100%)	0	100	100
All	All	2215/2757 (80%)	2213 (100%)	2 (0%)	87	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	355	LEU
9	G	106	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	216	GLN
1	2	223	GLN

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Mol	Chain	Res	Type
2	9	84	ASN
3	A	216	HIS
3	A	217	GLN
3	A	225	ASN
3	A	268	ASN
3	A	458	HIS
3	A	459	ASN
3	A	637	GLN
4	B	10	GLN
4	B	64	ASN
4	B	294	ASN
4	B	302	GLN
4	B	504	ASN
4	B	607	ASN
4	B	704	GLN
6	D	151	GLN
6	D	186	ASN
9	G	125	ASN
9	G	156	GLN
14	L	18	ASN
15	M	18	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](#)

148 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
16	CLA	A	830	3	49,53,73	1.48	8 (16%)	59,89,113	1.27	7 (11%)
16	CLA	A	811	3	63,67,73	1.31	7 (11%)	75,105,113	1.12	6 (8%)
16	CLA	B	806	4	69,73,73	1.25	7 (10%)	83,113,113	1.25	5 (6%)
16	CLA	B	809	4	69,73,73	1.25	7 (10%)	83,113,113	1.16	6 (7%)
16	CLA	B	819	4	64,68,73	1.30	6 (9%)	77,107,113	1.26	3 (3%)
20	BCR	M	101	-	41,41,41	0.69	0	56,56,56	1.90	12 (21%)
16	CLA	B	818	4	63,67,73	1.33	8 (12%)	75,105,113	1.18	4 (5%)
16	CLA	A	832	3	69,73,73	1.26	6 (8%)	83,113,113	1.16	7 (8%)
16	CLA	A	836	3	54,58,73	1.40	6 (11%)	65,95,113	1.37	8 (12%)
18	PQN	B	841	-	34,34,34	0.48	0	42,45,45	0.95	1 (2%)
16	CLA	B	811	4	61,65,73	1.32	7 (11%)	72,102,113	1.24	5 (6%)
20	BCR	L	305	-	41,41,41	0.66	0	56,56,56	1.79	11 (19%)
16	CLA	A	843	19	43,48,73	1.55	6 (13%)	51,83,113	1.32	5 (9%)
16	CLA	B	830	4	59,63,73	1.34	6 (10%)	71,101,113	1.17	5 (7%)
16	CLA	B	824	4	47,51,73	1.49	8 (17%)	56,86,113	1.24	3 (5%)
16	CLA	A	826	3	66,70,73	1.29	9 (13%)	79,109,113	1.22	5 (6%)
16	CLA	2	611	1	45,49,73	1.53	6 (13%)	54,84,113	1.33	5 (9%)
16	CLA	B	839	-	69,73,73	1.26	8 (11%)	83,113,113	1.17	5 (6%)
16	CLA	F	803	8	42,47,73	1.55	6 (14%)	52,81,113	1.41	6 (11%)
16	CLA	A	816	3	64,68,73	1.30	6 (9%)	77,107,113	1.18	3 (3%)
16	CLA	A	829	3	69,73,73	1.26	8 (11%)	83,113,113	1.11	4 (4%)
20	BCR	A	850	-	41,41,41	0.69	0	56,56,56	2.26	15 (26%)
20	BCR	B	845	-	41,41,41	0.73	0	56,56,56	1.97	14 (25%)
16	CLA	B	821	4	52,56,73	1.44	7 (13%)	62,92,113	1.32	4 (6%)
16	CLA	A	841	-	68,72,73	1.26	8 (11%)	81,111,113	1.16	6 (7%)
16	CLA	B	801	4	64,68,73	1.29	9 (14%)	77,107,113	1.27	7 (9%)
16	CLA	L	302	14	45,49,73	1.53	6 (13%)	54,84,113	1.29	6 (11%)
16	CLA	2	610	1	43,47,73	1.56	5 (11%)	49,81,113	1.36	4 (8%)
16	CLA	A	824	-	68,72,73	1.26	7 (10%)	81,111,113	1.33	8 (9%)
16	CLA	B	817	4	58,62,73	1.36	5 (8%)	69,99,113	1.18	5 (7%)
20	BCR	F	801	-	41,41,41	0.67	0	56,56,56	2.17	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	K	205	13	45,49,73	1.52	6 (13%)	54,84,113	1.30	5 (9%)
16	CLA	A	822	3	45,49,73	1.52	7 (15%)	54,84,113	1.35	7 (12%)
16	CLA	B	813	4	49,53,73	1.50	8 (16%)	59,89,113	1.32	6 (10%)
20	BCR	K	206	-	41,41,41	0.69	0	56,56,56	1.90	13 (23%)
16	CLA	A	833	3	64,68,73	1.29	7 (10%)	77,107,113	1.23	8 (10%)
16	CLA	A	801	3	69,73,73	1.24	7 (10%)	83,113,113	1.11	8 (9%)
22	DGD	B	846	-	59,59,67	0.92	2 (3%)	73,73,81	1.03	5 (6%)
16	CLA	A	812	3	46,50,73	1.52	6 (13%)	55,85,113	1.35	5 (9%)
20	BCR	A	848	-	41,41,41	0.71	0	56,56,56	1.99	16 (28%)
16	CLA	A	804	3	47,51,73	1.49	7 (14%)	56,86,113	1.28	8 (14%)
16	CLA	G	202	9	49,53,73	1.49	7 (14%)	59,89,113	1.42	7 (11%)
16	CLA	B	829	4	69,73,73	1.26	7 (10%)	83,113,113	1.16	7 (8%)
20	BCR	A	849	-	41,41,41	0.71	0	56,56,56	1.82	12 (21%)
16	CLA	A	810	3	52,56,73	1.42	6 (11%)	62,92,113	1.26	8 (12%)
16	CLA	B	825	-	52,56,73	1.45	8 (15%)	62,92,113	1.32	6 (9%)
18	PQN	A	842	-	34,34,34	0.35	0	42,45,45	0.99	1 (2%)
21	SF4	A	851	3,4	0,12,12	-	-	-	-	-
16	CLA	B	804	-	69,73,73	1.25	9 (13%)	83,113,113	1.14	6 (7%)
16	CLA	2	613	-	43,48,73	1.55	8 (18%)	52,82,113	1.32	4 (7%)
16	CLA	B	816	4	49,53,73	1.49	6 (12%)	59,89,113	1.26	3 (5%)
16	CLA	B	810	4	67,71,73	1.27	7 (10%)	80,110,113	1.19	6 (7%)
16	CLA	G	201	9	51,55,73	1.46	5 (9%)	61,91,113	1.30	4 (6%)
16	CLA	H	201	-	37,43,73	1.73	7 (18%)	49,76,113	1.41	7 (14%)
16	CLA	9	602	2	53,57,73	1.42	5 (9%)	62,93,113	1.26	5 (8%)
16	CLA	2	601	1	45,49,73	1.52	7 (15%)	54,84,113	1.31	6 (11%)
20	BCR	F	804	-	41,41,41	0.68	0	56,56,56	1.97	14 (25%)
16	CLA	2	605	-	41,44,73	1.59	7 (17%)	49,77,113	1.29	6 (12%)
16	CLA	9	612	2	45,49,73	1.53	6 (13%)	54,84,113	1.30	5 (9%)
19	LHG	A	844	-	48,48,48	0.94	2 (4%)	51,54,54	1.01	2 (3%)
20	BCR	A	847	-	41,41,41	0.70	0	56,56,56	1.99	16 (28%)
16	CLA	B	832	4	47,51,73	1.49	6 (12%)	56,86,113	1.30	6 (10%)
16	CLA	B	822	4	42,46,73	1.70	7 (16%)	49,80,113	1.37	6 (12%)
16	CLA	9	609	2	40,42,73	2.64	7 (17%)	44,71,113	1.10	3 (6%)
16	CLA	A	835	3	49,53,73	1.48	6 (12%)	59,89,113	1.33	7 (11%)
16	CLA	A	806	3	68,72,73	1.26	7 (10%)	81,111,113	1.27	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	B	808	4	63,67,73	1.30	6 (9%)	75,105,113	1.26	6 (8%)
20	BCR	B	843	-	41,41,41	0.69	0	56,56,56	1.98	14 (25%)
16	CLA	9	611	2	46,50,73	1.51	5 (10%)	55,85,113	1.29	4 (7%)
16	CLA	A	820	-	64,68,73	1.30	8 (12%)	77,107,113	1.16	5 (6%)
16	CLA	A	839	3	60,64,73	1.34	7 (11%)	72,102,113	1.22	6 (8%)
16	CLA	K	203	-	59,63,73	1.36	6 (10%)	71,101,113	1.19	5 (7%)
16	CLA	A	825	-	54,58,73	1.41	6 (11%)	65,95,113	1.23	7 (10%)
16	CLA	2	607	1	45,49,73	1.52	7 (15%)	54,84,113	1.31	6 (11%)
16	CLA	2	606	-	42,45,73	1.56	8 (19%)	50,78,113	1.27	3 (6%)
16	CLA	9	606	-	48,52,73	1.48	7 (14%)	56,87,113	1.28	4 (7%)
16	CLA	9	607	2	49,53,73	1.49	7 (14%)	59,89,113	1.23	6 (10%)
16	CLA	A	817	3	60,64,73	1.34	8 (13%)	72,102,113	1.23	9 (12%)
16	CLA	A	805	3	65,69,73	1.30	8 (12%)	78,108,113	1.29	7 (8%)
16	CLA	2	612	1	46,50,73	1.51	6 (13%)	55,85,113	1.41	4 (7%)
16	CLA	B	834	4	55,59,73	1.40	7 (12%)	66,96,113	1.23	6 (9%)
20	BCR	B	842	-	41,41,41	0.71	0	56,56,56	3.09	19 (33%)
16	CLA	9	603	2	55,59,73	1.41	7 (12%)	66,96,113	1.23	4 (6%)
16	CLA	B	826	-	54,58,73	1.41	7 (12%)	65,95,113	1.33	10 (15%)
16	CLA	2	604	-	42,45,73	1.57	6 (14%)	50,78,113	1.39	4 (8%)
16	CLA	9	604	2	48,52,73	1.48	8 (16%)	56,87,113	1.26	5 (8%)
21	SF4	C	102	5	0,12,12	-	-	-	-	-
16	CLA	B	807	4	69,73,73	1.26	8 (11%)	83,113,113	1.21	7 (8%)
16	CLA	9	610	2	46,50,73	1.51	5 (10%)	55,85,113	1.34	4 (7%)
17	CHL	9	601	2	47,51,74	2.40	18 (38%)	52,86,114	2.68	23 (44%)
16	CLA	F	802	4	56,60,73	1.41	7 (12%)	67,97,113	1.32	5 (7%)
16	CLA	B	836	4	54,58,73	1.40	7 (12%)	65,95,113	1.36	8 (12%)
16	CLA	A	831	3	49,53,73	1.48	6 (12%)	59,89,113	1.30	4 (6%)
16	CLA	A	827	3	54,58,73	1.42	8 (14%)	65,95,113	1.48	7 (10%)
16	CLA	A	809	3	46,50,73	1.51	7 (15%)	55,85,113	1.52	7 (12%)
16	CLA	A	828	3	69,73,73	1.25	9 (13%)	83,113,113	1.20	7 (8%)
16	CLA	B	820	-	49,53,73	1.48	6 (12%)	59,89,113	1.30	6 (10%)
20	BCR	I	201	-	41,41,41	0.72	0	56,56,56	2.09	16 (28%)
16	CLA	A	852	-	46,50,73	1.50	8 (17%)	55,85,113	1.27	4 (7%)
16	CLA	B	831	4	47,51,73	1.50	6 (12%)	56,86,113	1.29	5 (8%)
16	CLA	B	828	4	64,68,73	1.29	7 (10%)	77,107,113	1.14	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	A	819	3	50,54,73	1.45	5 (10%)	60,90,113	1.25	4 (6%)
16	CLA	A	838	3	56,60,73	1.39	6 (10%)	67,97,113	1.34	6 (8%)
16	CLA	J	102	12	46,50,73	1.52	5 (10%)	55,85,113	1.30	4 (7%)
16	CLA	L	303	14	64,68,73	1.30	7 (10%)	77,107,113	1.25	4 (5%)
16	CLA	2	603	1	43,48,73	1.56	7 (16%)	51,83,113	1.46	5 (9%)
16	CLA	A	834	3	61,65,73	1.34	8 (13%)	73,103,113	1.27	3 (4%)
16	CLA	2	608	1	45,49,73	1.54	7 (15%)	54,84,113	1.34	5 (9%)
16	CLA	9	608	2	43,48,73	1.56	6 (13%)	52,82,113	1.32	5 (9%)
16	CLA	B	815	4	59,63,73	1.35	7 (11%)	71,101,113	1.22	4 (5%)
16	CLA	A	807	3	46,50,73	1.50	5 (10%)	55,85,113	1.30	4 (7%)
16	CLA	B	812	4	56,61,73	1.44	6 (10%)	70,99,113	1.24	10 (14%)
16	CLA	H	202	-	28,35,73	1.91	7 (25%)	32,60,113	1.40	4 (12%)
16	CLA	A	823	3	61,65,73	1.34	6 (9%)	73,103,113	1.20	3 (4%)
16	CLA	L	304	-	42,45,73	1.56	7 (16%)	50,78,113	1.28	4 (8%)
16	CLA	2	602	1	50,54,73	1.46	5 (10%)	60,90,113	1.25	4 (6%)
20	BCR	K	202	-	41,41,41	0.68	0	56,56,56	2.16	17 (30%)
16	CLA	B	835	-	49,53,73	1.50	5 (10%)	59,89,113	1.33	5 (8%)
20	BCR	B	844	-	41,41,41	0.70	0	56,56,56	2.00	22 (39%)
19	LHG	A	845	16	44,44,48	0.97	2 (4%)	47,50,54	1.00	3 (6%)
21	SF4	C	101	5	0,12,12	-	-	-	-	-
16	CLA	K	201	13	45,49,73	1.53	7 (15%)	54,84,113	1.30	4 (7%)
16	CLA	A	814	3	43,48,73	1.56	7 (16%)	52,82,113	1.31	5 (9%)
17	CHL	9	605	-	44,49,74	2.42	17 (38%)	49,83,114	3.08	23 (46%)
16	CLA	B	823	4	48,52,73	1.49	5 (10%)	56,87,113	1.25	4 (7%)
16	CLA	A	837	3	59,63,73	1.33	6 (10%)	71,101,113	1.26	9 (12%)
16	CLA	B	805	4	45,49,73	1.52	7 (15%)	54,84,113	1.31	8 (14%)
16	CLA	A	802	-	69,73,73	1.25	7 (10%)	83,113,113	1.23	8 (9%)
16	CLA	A	840	3	46,50,73	1.50	7 (15%)	55,85,113	1.26	3 (5%)
16	CLA	B	833	4	51,55,73	1.44	6 (11%)	61,91,113	1.32	5 (8%)
16	CLA	B	802	-	60,64,73	1.33	8 (13%)	72,102,113	1.26	7 (9%)
20	BCR	A	846	-	41,41,41	0.67	0	56,56,56	2.02	17 (30%)
16	CLA	2	609	1	45,49,73	1.59	7 (15%)	57,84,113	1.40	10 (17%)
16	CLA	A	803	3	54,58,73	1.40	6 (11%)	65,95,113	1.42	10 (15%)
16	CLA	A	815	-	45,49,73	1.52	6 (13%)	54,84,113	1.34	5 (9%)
16	CLA	B	814	4	69,73,73	1.26	7 (10%)	83,113,113	1.26	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	A	808	3	55,59,73	1.39	7 (12%)	66,96,113	1.25	6 (9%)
16	CLA	B	827	4	69,73,73	1.26	6 (8%)	83,113,113	1.19	4 (4%)
16	CLA	A	813	3	48,52,73	1.47	6 (12%)	56,87,113	1.42	5 (8%)
16	CLA	B	803	4	69,73,73	1.26	7 (10%)	83,113,113	1.07	5 (6%)
16	CLA	A	821	3	46,50,73	1.51	5 (10%)	55,85,113	1.26	3 (5%)
20	BCR	L	301	-	41,41,41	0.71	0	56,56,56	2.12	22 (39%)
16	CLA	B	837	4	62,66,73	1.33	7 (11%)	74,104,113	1.20	7 (9%)
16	CLA	B	838	4	51,55,73	1.45	7 (13%)	61,91,113	1.29	7 (11%)
16	CLA	A	818	3	69,73,73	1.25	8 (11%)	83,113,113	1.18	7 (8%)
16	CLA	B	840	4	69,73,73	1.26	7 (10%)	83,113,113	1.13	4 (4%)
16	CLA	K	204	13	46,50,73	1.51	6 (13%)	55,85,113	1.38	4 (7%)
20	BCR	J	101	-	41,41,41	0.67	0	56,56,56	2.11	12 (21%)

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
16	CLA	A	830	3	-	10/15/91/115	-
16	CLA	A	811	3	-	11/32/108/115	-
16	CLA	B	806	4	-	15/39/115/115	-
16	CLA	B	809	4	-	15/39/115/115	-
16	CLA	B	819	4	-	9/33/109/115	-
20	BCR	M	101	-	-	4/29/63/63	0/2/2/2
16	CLA	B	818	4	-	12/32/108/115	-
16	CLA	A	832	3	-	19/39/115/115	-
16	CLA	A	836	3	-	7/21/97/115	-
18	PQN	B	841	-	-	7/23/43/43	0/2/2/2
16	CLA	B	811	4	-	14/29/105/115	-
20	BCR	L	305	-	-	10/29/63/63	0/2/2/2
16	CLA	A	843	19	-	4/8/84/115	-
16	CLA	B	830	4	-	10/27/103/115	-
16	CLA	B	824	4	-	7/13/89/115	-
16	CLA	A	826	3	-	8/36/112/115	-
16	CLA	2	611	1	-	4/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	B	839	-	-	15/39/115/115	-
16	CLA	F	803	8	-	2/6/82/115	-
16	CLA	A	816	3	-	12/33/109/115	-
16	CLA	A	829	3	-	12/39/115/115	-
20	BCR	A	850	-	-	12/29/63/63	0/2/2/2
20	BCR	B	845	-	-	4/29/63/63	0/2/2/2
16	CLA	B	821	4	-	12/19/95/115	-
16	CLA	A	841	-	-	14/37/113/115	-
16	CLA	B	801	4	-	14/33/109/115	-
16	CLA	L	302	14	-	5/10/86/115	-
16	CLA	2	610	1	-	4/4/82/115	-
16	CLA	A	824	-	-	6/37/113/115	-
16	CLA	B	817	4	-	10/25/101/115	-
20	BCR	F	801	-	-	9/29/63/63	0/2/2/2
16	CLA	K	205	13	-	4/10/86/115	-
16	CLA	A	822	3	-	8/10/86/115	-
16	CLA	B	813	4	-	9/15/91/115	-
20	BCR	K	206	-	-	0/29/63/63	0/2/2/2
16	CLA	A	833	3	-	7/33/109/115	-
16	CLA	A	801	3	-	17/39/115/115	-
22	DGD	B	846	-	-	6/47/87/95	0/2/2/2
16	CLA	A	812	3	-	8/12/88/115	-
20	BCR	A	848	-	-	0/29/63/63	0/2/2/2
16	CLA	A	804	3	-	7/13/89/115	-
16	CLA	G	202	9	-	6/15/91/115	-
16	CLA	B	829	4	-	15/39/115/115	-
20	BCR	A	849	-	-	5/29/63/63	0/2/2/2
16	CLA	A	810	3	-	10/14/90/115	-
16	CLA	B	825	-	-	6/19/95/115	-
18	PQN	A	842	-	-	6/23/43/43	0/2/2/2
21	SF4	A	851	3,4	-	-	0/6/5/5
16	CLA	B	804	-	-	18/39/115/115	-
16	CLA	2	613	-	-	6/10/82/115	-
16	CLA	B	816	4	-	8/15/91/115	-
16	CLA	B	810	4	-	12/37/113/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	G	201	9	-	11/18/94/115	-
16	CLA	9	602	2	-	9/20/96/115	-
16	CLA	2	601	1	-	7/10/86/115	-
20	BCR	F	804	-	-	4/29/63/63	0/2/2/2
16	CLA	2	605	-	-	2/2/74/115	-
16	CLA	9	612	2	-	4/10/86/115	-
19	LHG	A	844	-	-	7/53/53/53	-
20	BCR	A	847	-	-	0/29/63/63	0/2/2/2
16	CLA	B	832	4	-	5/13/89/115	-
16	CLA	B	822	4	-	4/6/82/115	-
16	CLA	9	609	2	-	4/6/62/115	-
16	CLA	A	835	3	-	8/15/91/115	-
16	CLA	A	806	3	-	12/37/113/115	-
16	CLA	B	808	4	-	15/32/108/115	-
20	BCR	B	843	-	-	4/29/63/63	0/2/2/2
16	CLA	9	611	2	-	8/12/88/115	-
16	CLA	A	820	-	-	11/33/109/115	-
16	CLA	A	839	3	-	12/29/105/115	-
16	CLA	K	203	-	-	15/27/103/115	-
16	CLA	A	825	-	-	7/21/97/115	-
16	CLA	2	607	1	-	4/10/86/115	-
16	CLA	2	606	-	-	2/4/76/115	-
16	CLA	9	606	-	-	6/13/90/115	-
16	CLA	9	607	2	-	6/15/91/115	-
16	CLA	A	817	3	-	9/29/105/115	-
16	CLA	A	805	3	-	14/35/111/115	-
16	CLA	2	612	1	-	5/12/88/115	-
16	CLA	B	834	4	-	11/23/99/115	-
20	BCR	B	842	-	-	8/29/63/63	0/2/2/2
16	CLA	9	603	2	-	11/23/99/115	-
16	CLA	B	826	-	-	7/21/97/115	-
16	CLA	2	604	-	-	4/4/76/115	-
16	CLA	9	604	2	-	7/13/90/115	-
21	SF4	C	102	5	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	B	807	4	-	14/39/115/115	-
16	CLA	9	610	2	-	6/12/88/115	-
17	CHL	9	601	2	-	6/14/90/117	-
16	CLA	F	802	4	-	6/24/100/115	-
16	CLA	B	836	4	-	10/21/97/115	-
16	CLA	A	831	3	-	9/15/91/115	-
16	CLA	A	827	3	-	7/21/97/115	-
16	CLA	A	809	3	-	5/12/88/115	-
16	CLA	A	828	3	-	18/39/115/115	-
16	CLA	B	820	-	-	7/15/91/115	-
20	BCR	I	201	-	-	4/29/63/63	0/2/2/2
16	CLA	A	852	-	-	8/12/88/115	-
16	CLA	B	831	4	-	8/13/89/115	-
16	CLA	B	828	4	-	18/33/109/115	-
16	CLA	A	819	3	-	10/17/93/115	-
16	CLA	A	838	3	-	10/24/100/115	-
16	CLA	J	102	12	-	6/12/88/115	-
16	CLA	L	303	14	-	14/33/109/115	-
16	CLA	2	603	1	-	3/8/84/115	-
16	CLA	A	834	3	-	10/30/106/115	-
16	CLA	2	608	1	-	5/10/86/115	-
16	CLA	9	608	2	-	3/10/82/115	-
16	CLA	B	815	4	-	13/27/103/115	-
16	CLA	A	807	3	-	6/12/88/115	-
16	CLA	B	812	4	-	9/23/99/115	-
16	CLA	A	823	3	-	13/30/106/115	-
16	CLA	L	304	-	-	2/4/76/115	-
16	CLA	2	602	1	-	7/17/93/115	-
20	BCR	K	202	-	-	1/29/63/63	0/2/2/2
16	CLA	B	835	-	-	7/15/91/115	-
20	BCR	B	844	-	-	2/29/63/63	0/2/2/2
19	LHG	A	845	16	-	10/49/49/53	-
21	SF4	C	101	5	-	-	0/6/5/5
16	CLA	K	201	13	-	4/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	A	814	3	-	7/10/82/115	-
17	CHL	9	605	-	-	4/12/84/117	-
16	CLA	B	823	4	-	5/13/90/115	-
16	CLA	A	837	3	-	10/27/103/115	-
16	CLA	B	805	4	-	3/10/86/115	-
16	CLA	A	802	-	-	12/39/115/115	-
16	CLA	A	840	3	-	7/12/88/115	-
16	CLA	B	833	4	-	9/18/94/115	-
16	CLA	B	802	-	-	8/29/105/115	-
20	BCR	A	846	-	-	2/29/63/63	0/2/2/2
16	CLA	2	609	1	-	4/10/86/115	-
16	CLA	A	803	3	-	9/21/97/115	-
16	CLA	A	815	-	-	5/10/86/115	-
16	CLA	B	814	4	-	16/39/115/115	-
16	CLA	A	808	3	-	7/23/99/115	-
16	CLA	B	827	4	-	16/39/115/115	-
16	CLA	A	813	3	-	8/13/90/115	-
16	CLA	B	803	4	-	18/39/115/115	-
16	CLA	A	821	3	-	7/12/88/115	-
20	BCR	L	301	-	-	3/29/63/63	0/2/2/2
16	CLA	B	837	4	-	10/31/107/115	-
16	CLA	B	838	4	-	6/18/94/115	-
16	CLA	A	818	3	-	17/39/115/115	-
16	CLA	B	840	4	-	19/39/115/115	-
16	CLA	K	204	13	-	8/12/88/115	-
20	BCR	J	101	-	-	6/29/63/63	0/2/2/2

All (848) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	9	609	CLA	C1A-NA	13.08	1.41	1.29
17	9	605	CHL	O2D-CGD	5.20	1.45	1.33
17	9	601	CHL	O2D-CGD	5.19	1.45	1.33
17	9	601	CHL	C2C-C3C	5.06	1.47	1.36
17	9	605	CHL	C2C-C3C	4.95	1.47	1.36
17	9	601	CHL	CHD-C1D	4.77	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	9	601	CHL	CHC-C1C	4.70	1.48	1.38
16	A	827	CLA	C1D-ND	4.61	1.43	1.37
17	9	605	CHL	CHC-C1C	4.61	1.47	1.38
17	9	605	CHL	CHD-C1D	4.53	1.47	1.38
16	H	202	CLA	C2B-C1B	4.53	1.49	1.40
16	H	202	CLA	C3B-C4B	4.49	1.49	1.40
22	B	846	DGD	O1G-C1A	4.28	1.45	1.33
16	A	838	CLA	C1D-ND	4.24	1.43	1.37
19	A	845	LHG	O8-C23	4.23	1.45	1.33
19	A	844	LHG	O8-C23	4.21	1.45	1.33
22	B	846	DGD	O2G-C1B	4.15	1.46	1.34
16	F	802	CLA	C1D-ND	4.14	1.42	1.37
19	A	844	LHG	O7-C7	4.13	1.45	1.34
17	9	601	CHL	CHD-C4C	4.06	1.48	1.39
16	L	302	CLA	C1D-ND	4.06	1.42	1.37
16	B	829	CLA	C1D-ND	4.05	1.42	1.37
16	2	609	CLA	C1D-ND	4.04	1.42	1.37
16	2	610	CLA	C1D-ND	4.04	1.42	1.37
16	F	802	CLA	C4B-NB	4.01	1.42	1.37
19	A	845	LHG	O7-C7	4.01	1.45	1.34
16	J	102	CLA	C1D-ND	4.01	1.42	1.37
16	A	806	CLA	C1D-ND	4.00	1.42	1.37
16	A	812	CLA	C1D-ND	4.00	1.42	1.37
16	B	807	CLA	C1D-ND	4.00	1.42	1.37
16	2	603	CLA	C1D-ND	4.00	1.42	1.37
16	G	201	CLA	C1D-ND	4.00	1.42	1.37
16	9	610	CLA	C1D-ND	3.99	1.42	1.37
16	A	816	CLA	C1D-ND	3.99	1.42	1.37
16	2	604	CLA	C1D-ND	3.98	1.42	1.37
16	B	821	CLA	C1D-ND	3.98	1.42	1.37
16	B	835	CLA	C1D-ND	3.97	1.42	1.37
16	A	822	CLA	C1D-ND	3.96	1.42	1.37
16	2	611	CLA	C1D-ND	3.96	1.42	1.37
16	B	833	CLA	C1D-ND	3.95	1.42	1.37
16	2	607	CLA	C1D-ND	3.95	1.42	1.37
16	B	819	CLA	C1D-ND	3.94	1.42	1.37
16	B	823	CLA	C1D-ND	3.94	1.42	1.37
16	A	824	CLA	C1D-ND	3.94	1.42	1.37
16	A	832	CLA	C1D-ND	3.93	1.42	1.37
16	A	831	CLA	C1D-ND	3.92	1.42	1.37
16	A	805	CLA	C1D-ND	3.92	1.42	1.37
16	A	823	CLA	C1D-ND	3.92	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	9	605	CHL	CHD-C4C	3.92	1.48	1.39
16	B	814	CLA	C1D-ND	3.91	1.42	1.37
16	A	833	CLA	C1D-ND	3.91	1.42	1.37
16	B	837	CLA	C1D-ND	3.91	1.42	1.37
16	K	205	CLA	C1D-ND	3.91	1.42	1.37
16	9	606	CLA	C1D-ND	3.91	1.42	1.37
16	9	603	CLA	C1D-ND	3.91	1.42	1.37
16	9	609	CLA	C1D-ND	3.91	1.42	1.37
16	2	601	CLA	C1D-ND	3.91	1.42	1.37
17	9	601	CHL	C1D-ND	-3.91	1.33	1.37
16	2	612	CLA	C1D-ND	3.91	1.42	1.37
16	9	608	CLA	C1D-ND	3.91	1.42	1.37
16	B	813	CLA	C4B-NB	3.91	1.42	1.37
16	A	803	CLA	C1D-ND	3.91	1.42	1.37
16	A	809	CLA	C1D-ND	3.90	1.42	1.37
16	B	832	CLA	C1D-ND	3.90	1.42	1.37
16	9	612	CLA	C1D-ND	3.90	1.42	1.37
16	B	827	CLA	C1D-ND	3.90	1.42	1.37
16	A	810	CLA	C1D-ND	3.90	1.42	1.37
16	H	201	CLA	C1D-ND	3.90	1.42	1.37
16	B	818	CLA	C1D-ND	3.90	1.42	1.37
16	A	815	CLA	C1D-ND	3.89	1.42	1.37
16	A	834	CLA	C1D-ND	3.89	1.42	1.37
16	2	605	CLA	C1D-ND	3.89	1.42	1.37
16	9	607	CLA	C1D-ND	3.89	1.42	1.37
16	B	831	CLA	C1D-ND	3.89	1.42	1.37
16	A	835	CLA	C1D-ND	3.89	1.42	1.37
16	9	602	CLA	C1D-ND	3.89	1.42	1.37
16	A	802	CLA	C1D-ND	3.89	1.42	1.37
16	A	801	CLA	C1D-ND	3.88	1.42	1.37
16	K	203	CLA	C1D-ND	3.88	1.42	1.37
16	L	303	CLA	C1D-ND	3.88	1.42	1.37
16	B	838	CLA	C1D-ND	3.88	1.42	1.37
16	L	304	CLA	C1D-ND	3.88	1.42	1.37
16	A	828	CLA	C1D-ND	3.87	1.42	1.37
16	B	813	CLA	C1D-ND	3.87	1.42	1.37
16	A	804	CLA	C1D-ND	3.87	1.42	1.37
16	A	807	CLA	C1D-ND	3.87	1.42	1.37
16	A	836	CLA	C1D-ND	3.87	1.42	1.37
16	B	812	CLA	C1D-ND	3.87	1.42	1.37
16	B	817	CLA	C1D-ND	3.87	1.42	1.37
16	B	822	CLA	C3C-C4C	3.87	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	839	CLA	C1D-ND	3.86	1.42	1.37
16	K	204	CLA	C1D-ND	3.86	1.42	1.37
16	G	202	CLA	C1D-ND	3.86	1.42	1.37
16	B	811	CLA	C1D-ND	3.86	1.42	1.37
16	A	821	CLA	C1D-ND	3.85	1.42	1.37
16	B	840	CLA	C1D-ND	3.85	1.42	1.37
16	L	302	CLA	C4B-NB	3.85	1.42	1.37
16	B	805	CLA	C1D-ND	3.85	1.42	1.37
16	2	606	CLA	C1D-ND	3.84	1.42	1.37
17	9	605	CHL	C1D-ND	-3.84	1.33	1.37
16	2	608	CLA	C1D-ND	3.84	1.42	1.37
16	B	806	CLA	C1D-ND	3.84	1.42	1.37
16	B	824	CLA	C1D-ND	3.84	1.42	1.37
17	9	601	CHL	CHC-C4B	3.84	1.48	1.39
16	A	813	CLA	C1D-ND	3.84	1.42	1.37
16	B	825	CLA	C1D-ND	3.84	1.42	1.37
16	9	611	CLA	C1D-ND	3.84	1.42	1.37
16	A	826	CLA	C1D-ND	3.83	1.42	1.37
16	2	602	CLA	C1D-ND	3.83	1.42	1.37
16	A	843	CLA	C1D-ND	3.83	1.42	1.37
16	A	814	CLA	C1D-ND	3.83	1.42	1.37
16	B	809	CLA	C1D-ND	3.83	1.42	1.37
16	A	829	CLA	C1D-ND	3.82	1.42	1.37
16	A	830	CLA	C1D-ND	3.82	1.42	1.37
16	B	826	CLA	C1D-ND	3.82	1.42	1.37
16	B	816	CLA	C1D-ND	3.81	1.42	1.37
17	9	601	CHL	C3D-C2D	3.81	1.49	1.39
16	A	819	CLA	C1D-ND	3.81	1.42	1.37
16	A	820	CLA	C1D-ND	3.81	1.42	1.37
16	9	604	CLA	C1D-ND	3.81	1.42	1.37
16	B	815	CLA	C1D-ND	3.81	1.42	1.37
16	B	825	CLA	C4B-NB	3.80	1.42	1.37
16	B	820	CLA	C1D-ND	3.80	1.42	1.37
16	B	822	CLA	C1D-ND	3.80	1.42	1.37
16	A	825	CLA	C1D-ND	3.80	1.42	1.37
16	B	834	CLA	C1D-ND	3.79	1.42	1.37
16	F	803	CLA	C1D-ND	3.79	1.42	1.37
16	B	808	CLA	C1D-ND	3.78	1.42	1.37
16	A	841	CLA	C1D-ND	3.78	1.42	1.37
16	K	201	CLA	C1D-ND	3.78	1.42	1.37
16	B	839	CLA	C1D-ND	3.77	1.42	1.37
16	A	808	CLA	C1D-ND	3.76	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	837	CLA	C1D-ND	3.76	1.42	1.37
16	A	840	CLA	C1D-ND	3.76	1.42	1.37
16	B	830	CLA	C1D-ND	3.76	1.42	1.37
16	A	818	CLA	C1D-ND	3.75	1.42	1.37
16	B	836	CLA	C1D-ND	3.75	1.42	1.37
17	9	605	CHL	CHC-C4B	3.75	1.47	1.39
17	9	601	CHL	OBD-CAD	3.75	1.28	1.22
16	B	828	CLA	C1D-ND	3.75	1.42	1.37
16	2	610	CLA	C4B-NB	3.75	1.42	1.37
17	9	605	CHL	OBD-CAD	3.74	1.28	1.22
16	A	817	CLA	C1D-ND	3.74	1.42	1.37
16	B	818	CLA	C4B-NB	3.74	1.42	1.37
16	9	611	CLA	C4B-NB	3.73	1.42	1.37
16	2	608	CLA	C4B-NB	3.72	1.42	1.37
16	A	811	CLA	C1D-ND	3.72	1.42	1.37
16	B	803	CLA	C1D-ND	3.72	1.42	1.37
16	2	611	CLA	C4B-NB	3.72	1.42	1.37
16	A	852	CLA	C1D-ND	3.72	1.42	1.37
16	K	201	CLA	C4B-NB	3.72	1.42	1.37
16	B	810	CLA	C1D-ND	3.71	1.42	1.37
16	B	835	CLA	C4B-NB	3.69	1.42	1.37
17	9	605	CHL	C3D-C2D	3.69	1.49	1.39
16	G	201	CLA	C4B-NB	3.68	1.42	1.37
16	9	610	CLA	C4B-NB	3.68	1.42	1.37
16	L	304	CLA	C4B-NB	3.68	1.42	1.37
16	B	840	CLA	C4B-NB	3.68	1.42	1.37
16	9	603	CLA	C4B-NB	3.68	1.42	1.37
16	J	102	CLA	C4B-NB	3.67	1.42	1.37
16	2	604	CLA	C4B-NB	3.67	1.42	1.37
16	B	823	CLA	C4B-NB	3.66	1.42	1.37
16	B	803	CLA	C4B-NB	3.66	1.42	1.37
16	9	609	CLA	C4B-NB	3.66	1.42	1.37
16	B	831	CLA	C4B-NB	3.66	1.42	1.37
16	B	822	CLA	C4B-NB	3.65	1.42	1.37
16	B	821	CLA	C4B-NB	3.64	1.42	1.37
16	A	814	CLA	C4B-NB	3.64	1.42	1.37
16	A	840	CLA	C4B-NB	3.64	1.42	1.37
16	B	824	CLA	C4B-NB	3.63	1.42	1.37
16	B	816	CLA	C4B-NB	3.63	1.42	1.37
16	H	201	CLA	C4B-NB	3.63	1.42	1.37
16	A	852	CLA	C4B-NB	3.62	1.42	1.37
16	9	612	CLA	C4B-NB	3.62	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	K	204	CLA	C4B-NB	3.62	1.42	1.37
16	A	819	CLA	C4B-NB	3.62	1.42	1.37
16	2	613	CLA	C1D-ND	3.62	1.42	1.37
16	A	804	CLA	C4B-NB	3.62	1.42	1.37
16	A	805	CLA	C4B-NB	3.62	1.42	1.37
16	K	203	CLA	C4B-NB	3.61	1.42	1.37
16	A	821	CLA	C4B-NB	3.61	1.42	1.37
16	B	801	CLA	C4B-NB	3.61	1.42	1.37
16	2	601	CLA	C4B-NB	3.60	1.42	1.37
16	A	811	CLA	C4B-NB	3.60	1.42	1.37
16	B	802	CLA	C1D-ND	3.60	1.42	1.37
16	A	829	CLA	C4B-NB	3.60	1.42	1.37
16	B	804	CLA	C1D-ND	3.60	1.42	1.37
16	9	607	CLA	C4B-NB	3.60	1.42	1.37
16	2	603	CLA	C4B-NB	3.59	1.42	1.37
16	A	810	CLA	C4B-NB	3.59	1.42	1.37
16	A	843	CLA	C4B-NB	3.59	1.42	1.37
16	B	820	CLA	C4B-NB	3.59	1.42	1.37
16	2	606	CLA	C4B-NB	3.59	1.42	1.37
16	K	205	CLA	C4B-NB	3.58	1.42	1.37
16	B	838	CLA	C4B-NB	3.58	1.42	1.37
16	A	834	CLA	C4B-NB	3.57	1.42	1.37
16	2	612	CLA	C4B-NB	3.57	1.42	1.37
16	B	839	CLA	C4B-NB	3.57	1.42	1.37
16	2	613	CLA	C4B-NB	3.57	1.42	1.37
16	A	820	CLA	C4B-NB	3.57	1.42	1.37
16	F	803	CLA	C4B-NB	3.57	1.42	1.37
16	2	607	CLA	C4B-NB	3.57	1.42	1.37
16	9	608	CLA	C4B-NB	3.55	1.42	1.37
16	B	812	CLA	C4B-NB	3.55	1.42	1.37
16	A	816	CLA	C4B-NB	3.55	1.42	1.37
16	A	823	CLA	C4B-NB	3.54	1.42	1.37
16	2	609	CLA	C4B-NB	3.54	1.42	1.37
16	A	835	CLA	C4B-NB	3.54	1.42	1.37
16	A	826	CLA	C4B-NB	3.54	1.42	1.37
16	G	202	CLA	C4B-NB	3.53	1.42	1.37
17	9	601	CHL	CHB-C1B	3.53	1.47	1.39
16	2	602	CLA	C4B-NB	3.53	1.42	1.37
16	B	808	CLA	C4B-NB	3.53	1.42	1.37
16	B	806	CLA	C4B-NB	3.53	1.42	1.37
16	B	833	CLA	C4B-NB	3.53	1.42	1.37
16	A	832	CLA	C4B-NB	3.52	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	L	303	CLA	C4B-NB	3.52	1.42	1.37
16	A	839	CLA	C4B-NB	3.52	1.42	1.37
16	A	815	CLA	C4B-NB	3.52	1.42	1.37
16	B	834	CLA	C4B-NB	3.52	1.42	1.37
16	9	604	CLA	C4B-NB	3.51	1.42	1.37
16	B	805	CLA	C4B-NB	3.51	1.42	1.37
16	B	819	CLA	C4B-NB	3.51	1.42	1.37
16	B	837	CLA	C4B-NB	3.50	1.42	1.37
16	2	605	CLA	C4B-NB	3.50	1.42	1.37
16	B	817	CLA	C4B-NB	3.50	1.42	1.37
16	A	812	CLA	C4B-NB	3.50	1.42	1.37
16	A	818	CLA	C4B-NB	3.50	1.42	1.37
16	B	826	CLA	C4B-NB	3.49	1.42	1.37
16	A	822	CLA	C4B-NB	3.49	1.42	1.37
16	9	602	CLA	C4B-NB	3.49	1.42	1.37
16	A	807	CLA	C4B-NB	3.48	1.42	1.37
16	A	830	CLA	C4B-NB	3.48	1.42	1.37
16	9	606	CLA	C4B-NB	3.48	1.42	1.37
16	B	815	CLA	C4B-NB	3.48	1.42	1.37
16	A	831	CLA	C4B-NB	3.47	1.42	1.37
16	B	832	CLA	C4B-NB	3.47	1.42	1.37
16	A	817	CLA	C4B-NB	3.45	1.42	1.37
16	B	827	CLA	C4B-NB	3.45	1.42	1.37
16	A	809	CLA	C4B-NB	3.45	1.42	1.37
16	A	801	CLA	C4B-NB	3.44	1.42	1.37
16	B	830	CLA	C4B-NB	3.43	1.42	1.37
16	B	807	CLA	C4B-NB	3.43	1.42	1.37
16	A	838	CLA	C4B-NB	3.42	1.42	1.37
16	A	808	CLA	C4B-NB	3.42	1.42	1.37
16	B	802	CLA	C4B-NB	3.42	1.42	1.37
16	A	841	CLA	C4B-NB	3.41	1.42	1.37
16	B	811	CLA	C4B-NB	3.40	1.42	1.37
16	B	810	CLA	C4B-NB	3.40	1.42	1.37
16	B	809	CLA	C4B-NB	3.38	1.41	1.37
16	B	801	CLA	C1D-ND	3.37	1.41	1.37
16	A	803	CLA	C4B-NB	3.37	1.41	1.37
16	A	824	CLA	C4B-NB	3.37	1.41	1.37
16	A	806	CLA	C4B-NB	3.36	1.41	1.37
16	B	829	CLA	C4B-NB	3.35	1.41	1.37
16	A	836	CLA	C4B-NB	3.35	1.41	1.37
16	A	827	CLA	C4B-NB	3.32	1.41	1.37
16	B	836	CLA	C4B-NB	3.32	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	9	605	CHL	CHB-C1B	3.31	1.46	1.39
16	B	804	CLA	C4B-NB	3.31	1.41	1.37
16	A	833	CLA	C4B-NB	3.30	1.41	1.37
16	A	802	CLA	C4B-NB	3.29	1.41	1.37
16	A	837	CLA	C4B-NB	3.28	1.41	1.37
16	B	828	CLA	C4B-NB	3.27	1.41	1.37
16	A	828	CLA	C4B-NB	3.27	1.41	1.37
16	H	202	CLA	C2D-C1D	3.26	1.48	1.42
16	A	813	CLA	C4B-NB	3.26	1.41	1.37
16	B	814	CLA	C4B-NB	3.25	1.41	1.37
16	A	825	CLA	C4B-NB	3.25	1.41	1.37
17	9	605	CHL	C3B-C4B	3.25	1.50	1.42
16	B	813	CLA	C3B-C4B	3.18	1.50	1.42
16	A	802	CLA	C4D-ND	-3.15	1.33	1.37
16	B	804	CLA	C4D-ND	-3.14	1.33	1.37
16	A	825	CLA	C4D-ND	-3.14	1.33	1.37
16	B	840	CLA	C4D-ND	-3.09	1.33	1.37
16	B	812	CLA	CAB-C3B	-3.08	1.44	1.50
16	A	811	CLA	C4D-ND	-3.07	1.33	1.37
16	B	802	CLA	C3B-C4B	3.07	1.49	1.42
16	B	828	CLA	C4D-ND	-3.07	1.33	1.37
17	9	601	CHL	C3B-C4B	3.06	1.49	1.42
16	H	201	CLA	CAB-C3B	-3.06	1.44	1.50
16	B	829	CLA	C4D-ND	-3.06	1.33	1.37
16	2	609	CLA	CAB-C3B	-3.04	1.44	1.50
16	A	804	CLA	C3B-C4B	3.03	1.49	1.42
16	B	801	CLA	C3B-C4B	3.03	1.49	1.42
16	A	805	CLA	C3B-C4B	3.02	1.49	1.42
16	9	609	CLA	C4D-ND	-3.02	1.33	1.37
16	A	817	CLA	C4D-ND	-3.02	1.33	1.37
16	B	834	CLA	C4D-ND	-3.02	1.33	1.37
16	A	828	CLA	C4D-ND	-3.02	1.33	1.37
16	9	608	CLA	C4D-ND	-3.01	1.33	1.37
16	A	814	CLA	C4D-ND	-3.01	1.33	1.37
16	B	807	CLA	C4D-ND	-3.00	1.33	1.37
16	A	830	CLA	C4D-ND	-3.00	1.33	1.37
16	B	807	CLA	C3B-C4B	3.00	1.49	1.42
16	B	837	CLA	C4D-ND	-3.00	1.33	1.37
16	B	810	CLA	C4D-ND	-2.99	1.33	1.37
16	A	829	CLA	C4D-ND	-2.99	1.33	1.37
16	2	602	CLA	C4D-ND	-2.98	1.33	1.37
16	B	836	CLA	C4D-ND	-2.98	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	2	613	CLA	C4D-ND	-2.98	1.33	1.37
16	B	826	CLA	C3B-C4B	2.98	1.49	1.42
17	9	605	CHL	C1B-NB	-2.98	1.34	1.37
16	B	805	CLA	C3B-C4B	2.97	1.49	1.42
16	A	841	CLA	C4D-ND	-2.97	1.33	1.37
16	A	837	CLA	C4D-ND	-2.96	1.33	1.37
16	A	827	CLA	C3B-C4B	2.96	1.49	1.42
16	B	830	CLA	C4D-ND	-2.96	1.33	1.37
16	B	820	CLA	C4D-ND	-2.96	1.33	1.37
16	B	818	CLA	C4D-ND	-2.96	1.33	1.37
16	H	202	CLA	C4D-ND	-2.96	1.33	1.37
16	B	838	CLA	C3B-C4B	2.96	1.49	1.42
16	A	820	CLA	C4D-ND	-2.95	1.33	1.37
16	2	608	CLA	C4D-ND	-2.95	1.33	1.37
16	B	816	CLA	C4D-ND	-2.95	1.33	1.37
16	A	852	CLA	C4D-ND	-2.94	1.33	1.37
16	A	812	CLA	C3B-C4B	2.94	1.49	1.42
17	9	601	CHL	MG-NA	-2.94	1.99	2.06
16	A	810	CLA	C3B-C4B	2.94	1.49	1.42
16	B	812	CLA	C4D-ND	-2.94	1.33	1.37
16	A	809	CLA	C3B-C4B	2.94	1.49	1.42
16	2	601	CLA	C4D-ND	-2.94	1.33	1.37
16	A	813	CLA	C4D-ND	-2.93	1.33	1.37
16	B	839	CLA	C4D-ND	-2.93	1.33	1.37
16	K	203	CLA	C4D-ND	-2.93	1.33	1.37
16	B	838	CLA	C4D-ND	-2.93	1.33	1.37
16	H	201	CLA	C4D-ND	-2.93	1.33	1.37
16	B	809	CLA	C4D-ND	-2.93	1.33	1.37
16	B	820	CLA	C3B-C4B	2.93	1.49	1.42
16	2	605	CLA	C4D-ND	-2.93	1.33	1.37
16	2	604	CLA	C3B-C4B	2.93	1.49	1.42
16	A	821	CLA	C4D-ND	-2.92	1.33	1.37
16	B	819	CLA	C4D-ND	-2.92	1.33	1.37
16	B	824	CLA	C4D-ND	-2.92	1.33	1.37
16	A	816	CLA	C4D-ND	-2.92	1.33	1.37
16	A	807	CLA	C4D-ND	-2.92	1.33	1.37
16	A	831	CLA	C4D-ND	-2.92	1.33	1.37
16	B	815	CLA	C4D-ND	-2.92	1.33	1.37
16	A	843	CLA	C4D-ND	-2.91	1.33	1.37
16	B	801	CLA	C4D-ND	-2.91	1.33	1.37
16	A	835	CLA	C3B-C4B	2.91	1.49	1.42
16	B	817	CLA	C4D-ND	-2.91	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	840	CLA	C3B-C4B	2.91	1.49	1.42
16	A	815	CLA	C4D-ND	-2.91	1.33	1.37
16	9	606	CLA	C4D-ND	-2.90	1.33	1.37
16	B	808	CLA	C4D-ND	-2.90	1.33	1.37
16	J	102	CLA	C3B-C4B	2.90	1.49	1.42
16	A	852	CLA	C3B-C4B	2.90	1.49	1.42
16	B	832	CLA	C4D-ND	-2.90	1.33	1.37
16	B	822	CLA	C4D-ND	-2.90	1.33	1.37
16	K	205	CLA	C4D-ND	-2.90	1.33	1.37
16	A	839	CLA	C3B-C4B	2.90	1.49	1.42
16	2	607	CLA	C4D-ND	-2.90	1.33	1.37
16	A	840	CLA	C4D-ND	-2.90	1.33	1.37
16	A	817	CLA	C3B-C4B	2.89	1.49	1.42
16	2	611	CLA	C4D-ND	-2.89	1.33	1.37
16	9	607	CLA	C4D-ND	-2.89	1.33	1.37
16	A	808	CLA	C4D-ND	-2.89	1.33	1.37
16	A	822	CLA	C4D-ND	-2.89	1.33	1.37
16	A	833	CLA	C4D-ND	-2.89	1.33	1.37
16	2	606	CLA	C4D-ND	-2.89	1.33	1.37
16	B	825	CLA	C4D-ND	-2.89	1.33	1.37
16	2	605	CLA	C3B-C4B	2.89	1.49	1.42
16	A	832	CLA	C4D-ND	-2.88	1.33	1.37
16	9	603	CLA	C3B-C4B	2.88	1.49	1.42
16	9	612	CLA	C3B-C4B	2.88	1.49	1.42
16	9	608	CLA	C3B-C4B	2.88	1.49	1.42
16	F	802	CLA	C3B-C4B	2.88	1.49	1.42
16	A	811	CLA	C3B-C4B	2.88	1.49	1.42
16	9	612	CLA	C4D-ND	-2.88	1.33	1.37
16	B	815	CLA	C3B-C4B	2.88	1.49	1.42
16	L	304	CLA	C4D-ND	-2.88	1.33	1.37
16	A	820	CLA	C3B-C4B	2.88	1.49	1.42
16	B	811	CLA	C4D-ND	-2.88	1.33	1.37
16	B	824	CLA	C3B-C4B	2.88	1.49	1.42
16	B	814	CLA	C4D-ND	-2.88	1.33	1.37
16	B	826	CLA	C4D-ND	-2.88	1.33	1.37
16	B	834	CLA	C3B-C4B	2.88	1.49	1.42
16	B	830	CLA	C1B-C2B	2.87	1.50	1.43
16	2	603	CLA	C3B-C4B	2.87	1.49	1.42
16	A	826	CLA	C3B-C4B	2.87	1.49	1.42
16	F	803	CLA	C3B-C4B	2.87	1.49	1.42
16	9	602	CLA	C4D-ND	-2.87	1.33	1.37
16	2	612	CLA	C3B-C4B	2.87	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	804	CLA	C4D-ND	-2.87	1.33	1.37
16	A	825	CLA	C3B-C4B	2.87	1.49	1.42
16	B	823	CLA	C4D-ND	-2.87	1.33	1.37
16	2	608	CLA	C3B-C4B	2.87	1.49	1.42
16	G	201	CLA	C3B-C4B	2.87	1.49	1.42
16	B	831	CLA	C4D-ND	-2.87	1.33	1.37
16	9	611	CLA	C4D-ND	-2.86	1.33	1.37
16	2	609	CLA	C4D-ND	-2.86	1.33	1.37
16	B	835	CLA	C3B-C4B	2.86	1.49	1.42
16	9	604	CLA	C4D-ND	-2.86	1.33	1.37
16	A	826	CLA	C4D-ND	-2.86	1.33	1.37
16	K	201	CLA	C3B-C4B	2.86	1.49	1.42
16	B	833	CLA	C4D-ND	-2.86	1.33	1.37
16	2	601	CLA	C3B-C4B	2.86	1.49	1.42
16	B	803	CLA	C4D-ND	-2.86	1.33	1.37
16	B	835	CLA	C4D-ND	-2.86	1.33	1.37
16	A	801	CLA	C4D-ND	-2.86	1.33	1.37
16	A	819	CLA	C4D-ND	-2.86	1.33	1.37
16	A	834	CLA	C3B-C4B	2.86	1.49	1.42
16	9	606	CLA	C3B-C4B	2.86	1.49	1.42
16	A	814	CLA	C3B-C4B	2.86	1.49	1.42
16	G	202	CLA	C3B-C4B	2.86	1.49	1.42
16	A	818	CLA	C3B-C4B	2.85	1.49	1.42
17	9	601	CHL	C1B-NB	-2.85	1.34	1.37
16	K	205	CLA	C3B-C4B	2.85	1.49	1.42
16	A	818	CLA	C4D-ND	-2.85	1.33	1.37
16	B	823	CLA	C3B-C4B	2.85	1.49	1.42
16	L	302	CLA	C3B-C4B	2.85	1.49	1.42
16	A	806	CLA	C4D-ND	-2.85	1.33	1.37
16	A	835	CLA	C4D-ND	-2.85	1.33	1.37
16	A	809	CLA	C4D-ND	-2.85	1.33	1.37
16	B	805	CLA	C4D-ND	-2.85	1.33	1.37
16	A	839	CLA	C4D-ND	-2.85	1.33	1.37
16	9	611	CLA	C3B-C4B	2.85	1.49	1.42
16	A	823	CLA	C4D-ND	-2.85	1.33	1.37
16	A	806	CLA	C3B-C4B	2.84	1.49	1.42
16	2	610	CLA	C3B-C4B	2.84	1.49	1.42
16	2	606	CLA	C3B-C4B	2.84	1.49	1.42
16	L	304	CLA	C3B-C4B	2.84	1.49	1.42
16	9	609	CLA	C3B-C4B	2.84	1.49	1.42
16	B	827	CLA	C4D-ND	-2.84	1.33	1.37
16	A	819	CLA	C3B-C4B	2.84	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	803	CLA	C3B-C4B	2.84	1.49	1.42
16	K	203	CLA	C3B-C4B	2.84	1.49	1.42
16	9	610	CLA	C3B-C4B	2.84	1.49	1.42
16	A	808	CLA	C3B-C4B	2.84	1.49	1.42
16	B	832	CLA	C3B-C4B	2.84	1.49	1.42
16	A	803	CLA	C3B-C4B	2.84	1.49	1.42
16	A	815	CLA	C3B-C4B	2.84	1.49	1.42
16	K	201	CLA	C4D-ND	-2.84	1.33	1.37
16	A	838	CLA	C4D-ND	-2.83	1.33	1.37
16	A	810	CLA	C4D-ND	-2.83	1.33	1.37
16	A	836	CLA	C4D-ND	-2.83	1.33	1.37
16	B	839	CLA	C3B-C4B	2.83	1.49	1.42
16	K	204	CLA	C3B-C4B	2.83	1.49	1.42
16	B	806	CLA	C4D-ND	-2.82	1.33	1.37
16	A	830	CLA	C3B-C4B	2.82	1.49	1.42
16	2	611	CLA	C3B-C4B	2.82	1.49	1.42
16	B	829	CLA	C3B-C4B	2.82	1.49	1.42
16	A	822	CLA	C3B-C4B	2.82	1.49	1.42
16	J	102	CLA	C4D-ND	-2.82	1.33	1.37
16	A	812	CLA	C4D-ND	-2.82	1.33	1.37
16	B	822	CLA	C3B-C4B	2.81	1.49	1.42
16	B	816	CLA	C3B-C4B	2.81	1.49	1.42
16	B	825	CLA	C3B-C4B	2.81	1.49	1.42
16	A	828	CLA	C3B-C4B	2.81	1.49	1.42
16	2	607	CLA	C3B-C4B	2.81	1.49	1.42
16	9	603	CLA	C4D-ND	-2.81	1.33	1.37
16	B	837	CLA	C3B-C4B	2.80	1.49	1.42
16	B	808	CLA	C3B-C4B	2.80	1.49	1.42
16	B	811	CLA	C3B-C4B	2.80	1.49	1.42
16	B	836	CLA	C3B-C4B	2.80	1.49	1.42
16	A	821	CLA	C3B-C4B	2.80	1.49	1.42
16	A	843	CLA	C3B-C4B	2.79	1.49	1.42
16	2	610	CLA	C4D-ND	-2.79	1.33	1.37
16	9	604	CLA	C3B-C4B	2.79	1.49	1.42
16	A	841	CLA	C3B-C4B	2.79	1.49	1.42
16	2	613	CLA	C3B-C4B	2.78	1.49	1.42
16	B	806	CLA	C1B-C2B	2.78	1.49	1.43
16	A	832	CLA	C3B-C4B	2.78	1.49	1.42
16	B	830	CLA	C3B-C4B	2.78	1.49	1.42
16	B	802	CLA	C4D-ND	-2.78	1.33	1.37
16	B	821	CLA	C4D-ND	-2.78	1.33	1.37
16	A	824	CLA	C3B-C4B	2.78	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	804	CLA	C3B-C4B	2.78	1.49	1.42
16	K	204	CLA	C4D-ND	-2.78	1.33	1.37
16	B	833	CLA	C3B-C4B	2.78	1.49	1.42
16	2	602	CLA	C3B-C4B	2.77	1.49	1.42
16	B	827	CLA	C3B-C4B	2.77	1.49	1.42
16	A	838	CLA	C3B-C4B	2.77	1.49	1.42
16	B	817	CLA	C3B-C4B	2.77	1.49	1.42
16	9	602	CLA	C3B-C4B	2.76	1.49	1.42
16	B	818	CLA	C3B-C4B	2.76	1.49	1.42
16	A	834	CLA	C4D-ND	-2.76	1.33	1.37
16	A	807	CLA	C3B-C4B	2.76	1.49	1.42
16	B	828	CLA	C3B-C4B	2.76	1.49	1.42
16	B	803	CLA	C1B-C2B	2.75	1.49	1.43
16	A	803	CLA	C4D-ND	-2.75	1.33	1.37
16	9	607	CLA	C3B-C4B	2.75	1.49	1.42
16	A	831	CLA	C3B-C4B	2.75	1.49	1.42
16	2	603	CLA	C4D-ND	-2.74	1.33	1.37
16	A	802	CLA	C3B-C4B	2.74	1.49	1.42
16	B	821	CLA	C3B-C4B	2.74	1.49	1.42
16	B	831	CLA	C1B-C2B	2.74	1.49	1.43
16	9	610	CLA	C4D-ND	-2.74	1.33	1.37
16	L	303	CLA	C4D-ND	-2.74	1.33	1.37
16	A	816	CLA	C3B-C4B	2.74	1.49	1.42
16	B	813	CLA	C4D-ND	-2.73	1.33	1.37
16	F	803	CLA	C4D-ND	-2.73	1.33	1.37
16	2	604	CLA	C4D-ND	-2.73	1.33	1.37
16	G	201	CLA	C4D-ND	-2.73	1.33	1.37
16	A	801	CLA	C3B-C4B	2.73	1.49	1.42
16	L	303	CLA	C3B-C4B	2.72	1.49	1.42
16	A	823	CLA	C3B-C4B	2.72	1.49	1.42
16	9	607	CLA	C1B-C2B	2.71	1.49	1.43
16	K	205	CLA	C1B-C2B	2.71	1.49	1.43
16	B	809	CLA	C3B-C4B	2.70	1.49	1.42
16	A	824	CLA	C1B-C2B	2.70	1.49	1.43
16	A	813	CLA	C3B-C4B	2.70	1.49	1.42
16	B	819	CLA	C3B-C4B	2.70	1.49	1.42
17	9	605	CHL	MG-NA	-2.69	1.99	2.06
16	B	814	CLA	C3B-C4B	2.69	1.49	1.42
16	2	607	CLA	C1B-C2B	2.69	1.49	1.43
16	2	612	CLA	C4D-ND	-2.69	1.34	1.37
16	A	807	CLA	C1B-C2B	2.68	1.49	1.43
16	9	611	CLA	C1B-C2B	2.68	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	G	202	CLA	C4D-ND	-2.68	1.34	1.37
16	L	302	CLA	C4D-ND	-2.68	1.34	1.37
16	B	822	CLA	C1B-C2B	2.68	1.49	1.43
16	A	806	CLA	C1B-C2B	2.67	1.49	1.43
16	A	813	CLA	C1B-C2B	2.67	1.49	1.43
16	K	204	CLA	C1B-C2B	2.67	1.49	1.43
16	B	821	CLA	C1B-C2B	2.67	1.49	1.43
16	B	831	CLA	C3B-C4B	2.67	1.49	1.42
16	A	805	CLA	C4D-ND	-2.67	1.34	1.37
16	2	609	CLA	C1B-C2B	2.66	1.49	1.43
16	9	610	CLA	C1B-C2B	2.66	1.49	1.43
16	2	610	CLA	C1B-C2B	2.66	1.49	1.43
16	2	603	CLA	C1B-C2B	2.66	1.49	1.43
16	G	201	CLA	C1B-C2B	2.66	1.49	1.43
16	A	824	CLA	C4D-ND	-2.66	1.34	1.37
16	A	821	CLA	C1B-C2B	2.66	1.49	1.43
16	B	808	CLA	C1B-C2B	2.66	1.49	1.43
16	A	837	CLA	C3B-C4B	2.66	1.49	1.42
16	2	613	CLA	C1B-C2B	2.66	1.49	1.43
16	9	612	CLA	C1B-C2B	2.65	1.49	1.43
16	B	840	CLA	C3B-C4B	2.65	1.49	1.42
16	A	836	CLA	C3B-C4B	2.65	1.49	1.42
16	9	608	CLA	C1B-C2B	2.65	1.49	1.43
16	9	609	CLA	C1B-C2B	2.65	1.49	1.43
16	F	803	CLA	C1B-C2B	2.65	1.49	1.43
16	J	102	CLA	C1B-C2B	2.65	1.49	1.43
16	A	843	CLA	C1B-C2B	2.65	1.49	1.43
16	A	816	CLA	C1B-C2B	2.65	1.49	1.43
16	K	201	CLA	C1B-C2B	2.65	1.49	1.43
16	B	840	CLA	C1B-C2B	2.64	1.49	1.43
16	2	612	CLA	C1B-C2B	2.64	1.49	1.43
16	A	836	CLA	C1B-C2B	2.64	1.49	1.43
16	2	606	CLA	C1B-C2B	2.64	1.49	1.43
16	A	840	CLA	C1B-C2B	2.64	1.49	1.43
16	9	606	CLA	C1B-C2B	2.64	1.49	1.43
16	B	812	CLA	C1B-C2B	2.64	1.49	1.43
16	H	201	CLA	C1B-C2B	2.63	1.49	1.43
16	B	817	CLA	C1B-C2B	2.63	1.49	1.43
16	2	602	CLA	C1B-C2B	2.63	1.49	1.43
16	2	605	CLA	C1B-C2B	2.63	1.49	1.43
16	B	809	CLA	C1B-C2B	2.63	1.49	1.43
16	A	823	CLA	C1B-C2B	2.63	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	833	CLA	C1B-C2B	2.63	1.49	1.43
16	2	611	CLA	C1B-C2B	2.63	1.49	1.43
16	B	827	CLA	C1B-C2B	2.63	1.49	1.43
16	B	823	CLA	C1B-C2B	2.63	1.49	1.43
16	A	829	CLA	C3B-C4B	2.63	1.48	1.42
16	A	852	CLA	C1B-C2B	2.63	1.49	1.43
17	9	601	CHL	C4D-CHA	2.62	1.47	1.38
16	A	819	CLA	C1B-C2B	2.62	1.49	1.43
16	B	810	CLA	C3B-C4B	2.62	1.48	1.42
16	B	806	CLA	C3B-C4B	2.62	1.48	1.42
16	A	815	CLA	C1B-C2B	2.62	1.49	1.43
16	A	838	CLA	C1B-C2B	2.62	1.49	1.43
16	2	609	CLA	C4B-C3B	2.62	1.49	1.43
16	B	816	CLA	C1B-C2B	2.62	1.49	1.43
16	B	811	CLA	C1B-C2B	2.62	1.49	1.43
16	B	824	CLA	C1B-C2B	2.62	1.49	1.43
16	H	201	CLA	C4B-C3B	2.62	1.49	1.43
16	K	203	CLA	C1B-C2B	2.62	1.49	1.43
16	A	833	CLA	C3B-C4B	2.62	1.48	1.42
16	A	822	CLA	C1B-C2B	2.62	1.49	1.43
16	A	803	CLA	C1B-C2B	2.61	1.49	1.43
16	A	839	CLA	C1B-C2B	2.61	1.49	1.43
16	9	603	CLA	C1B-C2B	2.61	1.49	1.43
16	L	304	CLA	C1B-C2B	2.61	1.49	1.43
16	L	303	CLA	C1B-C2B	2.61	1.49	1.43
16	A	810	CLA	C1B-C2B	2.61	1.49	1.43
16	B	814	CLA	C1B-C2B	2.61	1.49	1.43
16	B	819	CLA	C1B-C2B	2.61	1.49	1.43
16	A	805	CLA	C1B-C2B	2.60	1.49	1.43
16	A	814	CLA	C1B-C2B	2.60	1.49	1.43
16	A	841	CLA	C1B-C2B	2.60	1.49	1.43
16	A	809	CLA	C1B-C2B	2.60	1.49	1.43
16	B	832	CLA	C1B-C2B	2.60	1.49	1.43
16	A	811	CLA	C1B-C2B	2.59	1.49	1.43
16	A	835	CLA	C1B-C2B	2.59	1.49	1.43
16	B	834	CLA	C1B-C2B	2.59	1.49	1.43
16	A	832	CLA	C1B-C2B	2.59	1.49	1.43
16	F	802	CLA	C1B-C2B	2.59	1.49	1.43
16	A	812	CLA	C1B-C2B	2.59	1.49	1.43
16	B	838	CLA	C1B-C2B	2.59	1.49	1.43
16	B	828	CLA	C1B-C2B	2.59	1.49	1.43
16	L	302	CLA	C1B-C2B	2.59	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	808	CLA	C1B-C2B	2.58	1.49	1.43
16	A	801	CLA	C1B-C2B	2.58	1.49	1.43
16	9	602	CLA	C1B-C2B	2.58	1.49	1.43
16	H	202	CLA	CAD-C3D	-2.58	1.45	1.50
16	A	834	CLA	C1B-C2B	2.58	1.49	1.43
16	A	837	CLA	C1B-C2B	2.57	1.49	1.43
16	B	812	CLA	C4B-C3B	2.57	1.49	1.43
16	2	604	CLA	C1B-C2B	2.56	1.49	1.43
16	B	815	CLA	C1B-C2B	2.56	1.49	1.43
16	B	810	CLA	C1B-C2B	2.56	1.49	1.43
17	9	605	CHL	C4D-CHA	2.56	1.47	1.38
16	9	604	CLA	C1B-C2B	2.55	1.49	1.43
16	B	837	CLA	C1B-C2B	2.55	1.49	1.43
16	B	835	CLA	C1B-C2B	2.55	1.49	1.43
16	F	802	CLA	C4D-ND	-2.54	1.34	1.37
16	B	829	CLA	C1B-C2B	2.53	1.49	1.43
16	A	833	CLA	C1B-C2B	2.53	1.49	1.43
16	A	827	CLA	C1B-C2B	2.53	1.49	1.43
16	B	836	CLA	C1B-C2B	2.53	1.49	1.43
16	2	601	CLA	C1B-C2B	2.53	1.49	1.43
16	A	825	CLA	C1B-C2B	2.52	1.49	1.43
16	G	202	CLA	C1B-C2B	2.52	1.49	1.43
16	B	807	CLA	C1B-C2B	2.52	1.49	1.43
16	B	813	CLA	C1B-C2B	2.51	1.49	1.43
16	B	820	CLA	C1B-C2B	2.51	1.49	1.43
16	B	805	CLA	C1B-C2B	2.50	1.49	1.43
16	A	829	CLA	C1B-C2B	2.50	1.49	1.43
16	A	826	CLA	C1B-C2B	2.49	1.49	1.43
16	2	608	CLA	C1B-C2B	2.49	1.49	1.43
16	A	820	CLA	C1B-C2B	2.48	1.49	1.43
16	B	826	CLA	C1B-C2B	2.46	1.49	1.43
16	A	828	CLA	C1B-C2B	2.46	1.49	1.43
17	9	601	CHL	C1B-C2B	2.46	1.49	1.43
16	B	825	CLA	C1B-C2B	2.44	1.49	1.43
16	A	831	CLA	C1B-C2B	2.44	1.49	1.43
16	A	827	CLA	C4D-ND	-2.44	1.34	1.37
16	A	804	CLA	C1B-C2B	2.44	1.49	1.43
16	A	829	CLA	CMB-C2B	-2.43	1.45	1.50
16	B	839	CLA	C1B-C2B	2.43	1.49	1.43
16	A	830	CLA	C1B-C2B	2.42	1.49	1.43
16	B	802	CLA	CHC-C1C	2.42	1.43	1.38
17	9	601	CHL	C4C-C3C	2.42	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	817	CLA	C1B-C2B	2.41	1.48	1.43
16	B	804	CLA	C1B-C2B	2.41	1.48	1.43
16	B	801	CLA	C1B-C2B	2.39	1.48	1.43
16	B	818	CLA	C1B-C2B	2.37	1.48	1.43
16	A	802	CLA	C1B-C2B	2.36	1.48	1.43
16	A	818	CLA	C1B-C2B	2.35	1.48	1.43
16	B	840	CLA	CMB-C2B	-2.35	1.45	1.50
16	B	802	CLA	C1B-C2B	2.33	1.48	1.43
17	9	605	CHL	C1B-C2B	2.32	1.48	1.43
16	K	201	CLA	CMD-C2D	-2.30	1.45	1.50
16	A	804	CLA	CHC-C1C	2.29	1.43	1.38
17	9	605	CHL	C2C-C1C	2.29	1.49	1.44
17	9	605	CHL	C4C-C3C	2.28	1.49	1.45
16	B	810	CLA	CMB-C2B	-2.27	1.46	1.50
16	B	803	CLA	CMD-C2D	-2.25	1.46	1.50
16	B	802	CLA	CMC-C2C	-2.21	1.46	1.50
16	B	805	CLA	CHC-C1C	2.21	1.43	1.38
16	B	818	CLA	CMB-C2B	-2.21	1.46	1.50
17	9	601	CHL	C4B-NB	-2.20	1.35	1.37
16	B	801	CLA	CMD-C2D	-2.20	1.46	1.50
16	A	818	CLA	CMB-C2B	-2.19	1.46	1.50
17	9	601	CHL	C2C-C1C	2.19	1.49	1.44
16	9	609	CLA	CBD-CAD	2.18	1.56	1.51
16	B	813	CLA	CHC-C1C	2.18	1.43	1.38
16	B	839	CLA	CMD-C2D	-2.17	1.46	1.50
16	B	830	CLA	CMD-C2D	-2.17	1.46	1.50
16	A	801	CLA	CMB-C2B	-2.16	1.46	1.50
16	B	806	CLA	CMB-C2B	-2.16	1.46	1.50
16	B	825	CLA	CMB-C2B	-2.16	1.46	1.50
16	A	817	CLA	CHC-C1C	2.16	1.42	1.38
16	B	826	CLA	CHC-C1C	2.15	1.42	1.38
16	A	826	CLA	CHC-C1C	2.14	1.42	1.38
16	A	828	CLA	CMD-C2D	-2.14	1.46	1.50
16	A	852	CLA	CMC-C2C	-2.14	1.46	1.50
16	F	803	CLA	CMD-C2D	-2.14	1.46	1.50
16	A	830	CLA	CMB-C2B	-2.13	1.46	1.50
16	A	809	CLA	CHC-C1C	2.13	1.42	1.38
16	B	815	CLA	CMD-C2D	-2.13	1.46	1.50
16	2	613	CLA	CMD-C2D	-2.13	1.46	1.50
16	B	804	CLA	CHC-C1C	2.13	1.42	1.38
16	B	827	CLA	CMD-C2D	-2.12	1.46	1.50
16	2	605	CLA	CBD-CAD	2.12	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	811	CLA	CMD-C2D	-2.12	1.46	1.50
16	B	824	CLA	CMC-C2C	-2.12	1.46	1.50
16	B	802	CLA	CMD-C2D	-2.12	1.46	1.50
16	B	804	CLA	CMD-C2D	-2.12	1.46	1.50
16	2	608	CLA	CMB-C2B	-2.12	1.46	1.50
16	A	841	CLA	CMD-C2D	-2.12	1.46	1.50
16	B	820	CLA	CHC-C1C	2.11	1.42	1.38
16	A	834	CLA	CMB-C2B	-2.11	1.46	1.50
16	B	837	CLA	CMB-C2B	-2.11	1.46	1.50
16	B	831	CLA	CMB-C2B	-2.11	1.46	1.50
16	H	202	CLA	CHC-C1C	2.11	1.42	1.38
16	A	808	CLA	CHC-C1C	2.11	1.42	1.38
16	A	827	CLA	CMD-C2D	-2.11	1.46	1.50
16	A	814	CLA	CHC-C1C	2.10	1.42	1.38
16	B	809	CLA	CMD-C2D	-2.10	1.46	1.50
16	B	801	CLA	CHC-C1C	2.10	1.42	1.38
16	A	805	CLA	CMC-C2C	-2.10	1.46	1.50
16	A	825	CLA	CMD-C2D	-2.10	1.46	1.50
16	B	826	CLA	CMD-C2D	-2.10	1.46	1.50
16	L	302	CLA	CMD-C2D	-2.10	1.46	1.50
16	A	801	CLA	CMD-C2D	-2.10	1.46	1.50
16	B	803	CLA	CMB-C2B	-2.10	1.46	1.50
16	2	613	CLA	CMC-C2C	-2.10	1.46	1.50
16	B	805	CLA	CMD-C2D	-2.10	1.46	1.50
16	A	852	CLA	CMD-C2D	-2.10	1.46	1.50
16	9	608	CLA	CHC-C1C	2.10	1.42	1.38
16	L	303	CLA	CHC-C1C	2.10	1.42	1.38
16	9	603	CLA	CMD-C2D	-2.10	1.46	1.50
16	2	606	CLA	CBD-CAD	2.09	1.56	1.51
16	A	828	CLA	CMC-C2C	-2.09	1.46	1.50
16	A	834	CLA	CMD-C2D	-2.09	1.46	1.50
16	L	304	CLA	CBD-CAD	2.09	1.56	1.51
16	A	837	CLA	CMD-C2D	-2.09	1.46	1.50
16	A	827	CLA	CHC-C1C	2.09	1.42	1.38
16	A	831	CLA	CHC-C1C	2.09	1.42	1.38
16	B	825	CLA	CMD-C2D	-2.08	1.46	1.50
16	B	804	CLA	CMB-C2B	-2.08	1.46	1.50
16	K	204	CLA	CMD-C2D	-2.08	1.46	1.50
16	B	821	CLA	CMD-C2D	-2.08	1.46	1.50
16	A	810	CLA	CHC-C1C	2.08	1.42	1.38
16	H	201	CLA	CHC-C1C	2.08	1.42	1.38
16	B	814	CLA	CMD-C2D	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	802	CLA	CHC-C1C	2.08	1.42	1.38
16	A	824	CLA	CMD-C2D	-2.08	1.46	1.50
16	2	605	CLA	CHC-C1C	2.07	1.42	1.38
16	A	820	CLA	CMB-C2B	-2.07	1.46	1.50
16	A	840	CLA	CMD-C2D	-2.07	1.46	1.50
16	A	838	CLA	CHC-C1C	2.07	1.42	1.38
16	A	818	CLA	CMD-C2D	-2.07	1.46	1.50
16	B	828	CLA	CMD-C2D	-2.07	1.46	1.50
16	A	839	CLA	CMD-C2D	-2.07	1.46	1.50
16	9	604	CLA	CMB-C2B	-2.07	1.46	1.50
16	G	202	CLA	CMB-C2B	-2.07	1.46	1.50
16	2	604	CLA	CHC-C1C	2.07	1.42	1.38
16	2	609	CLA	CHC-C1C	2.07	1.42	1.38
16	B	815	CLA	CHC-C1C	2.07	1.42	1.38
16	A	817	CLA	CMD-C2D	-2.07	1.46	1.50
16	A	805	CLA	CMD-C2D	-2.07	1.46	1.50
16	B	814	CLA	CMB-C2B	-2.06	1.46	1.50
16	A	832	CLA	CMB-C2B	-2.06	1.46	1.50
16	9	604	CLA	CMD-C2D	-2.06	1.46	1.50
16	A	808	CLA	CMD-C2D	-2.06	1.46	1.50
16	B	836	CLA	CHC-C1C	2.06	1.42	1.38
16	H	202	CLA	C3C-C2C	2.06	1.39	1.35
16	B	829	CLA	CMD-C2D	-2.06	1.46	1.50
16	B	836	CLA	CMD-C2D	-2.06	1.46	1.50
16	B	809	CLA	CMB-C2B	-2.06	1.46	1.50
16	B	822	CLA	CMD-C2D	-2.06	1.46	1.50
16	A	820	CLA	CHC-C1C	2.06	1.42	1.38
16	A	809	CLA	CMD-C2D	-2.06	1.46	1.50
16	B	813	CLA	CMB-C2B	-2.06	1.46	1.50
16	2	613	CLA	CHC-C1C	2.06	1.42	1.38
16	B	801	CLA	CMB-C2B	-2.06	1.46	1.50
16	B	808	CLA	CMB-C2B	-2.06	1.46	1.50
16	A	830	CLA	CHC-C1C	2.06	1.42	1.38
16	L	303	CLA	CMB-C2B	-2.05	1.46	1.50
16	2	611	CLA	CHC-C1C	2.05	1.42	1.38
16	B	832	CLA	CHC-C1C	2.05	1.42	1.38
16	9	606	CLA	CMC-C2C	-2.05	1.46	1.50
16	A	806	CLA	CMC-C2C	-2.05	1.46	1.50
16	A	839	CLA	CHC-C1C	2.05	1.42	1.38
16	A	834	CLA	CHC-C1C	2.05	1.42	1.38
16	A	829	CLA	CMD-C2D	-2.05	1.46	1.50
16	2	612	CLA	CHC-C1C	2.05	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	811	CLA	CMD-C2D	-2.05	1.46	1.50
16	A	828	CLA	CHC-C1C	2.05	1.42	1.38
16	A	822	CLA	CMD-C2D	-2.05	1.46	1.50
16	B	825	CLA	CMC-C2C	-2.05	1.46	1.50
16	A	833	CLA	CMB-C2B	-2.05	1.46	1.50
16	9	603	CLA	CHC-C1C	2.05	1.42	1.38
16	A	835	CLA	CHC-C1C	2.05	1.42	1.38
16	B	801	CLA	CMC-C2C	-2.04	1.46	1.50
16	L	304	CLA	CHC-C1C	2.04	1.42	1.38
16	2	606	CLA	CHC-C1C	2.04	1.42	1.38
16	B	839	CLA	CMB-C2B	-2.04	1.46	1.50
16	2	603	CLA	CMC-C2C	-2.04	1.46	1.50
16	A	841	CLA	CMC-C2C	-2.04	1.46	1.50
16	A	806	CLA	CMD-C2D	-2.04	1.46	1.50
16	B	807	CLA	CMC-C2C	-2.04	1.46	1.50
16	K	205	CLA	CHC-C1C	2.04	1.42	1.38
16	A	805	CLA	CMB-C2B	-2.04	1.46	1.50
16	B	816	CLA	CMD-C2D	-2.04	1.46	1.50
16	A	826	CLA	CMB-C2B	-2.04	1.46	1.50
16	G	202	CLA	CMD-C2D	-2.04	1.46	1.50
16	A	814	CLA	CMD-C2D	-2.04	1.46	1.50
16	K	201	CLA	CHC-C1C	2.04	1.42	1.38
16	A	840	CLA	CMB-C2B	-2.03	1.46	1.50
16	9	606	CLA	CHC-C1C	2.03	1.42	1.38
16	9	607	CLA	CMB-C2B	-2.03	1.46	1.50
16	A	802	CLA	CMD-C2D	-2.03	1.46	1.50
16	A	812	CLA	CMD-C2D	-2.03	1.46	1.50
16	B	810	CLA	CMD-C2D	-2.03	1.46	1.50
16	A	820	CLA	CMD-C2D	-2.03	1.46	1.50
16	A	813	CLA	CMC-C2C	-2.03	1.46	1.50
16	A	826	CLA	CMD-C2D	-2.03	1.46	1.50
16	B	818	CLA	CMD-C2D	-2.03	1.46	1.50
16	B	833	CLA	CMC-C2C	-2.03	1.46	1.50
16	A	841	CLA	CMB-C2B	-2.03	1.46	1.50
16	B	828	CLA	CHC-C1C	2.03	1.42	1.38
16	2	606	CLA	CMD-C2D	-2.03	1.46	1.50
16	A	818	CLA	CHC-C1C	2.03	1.42	1.38
16	A	833	CLA	CMD-C2D	-2.03	1.46	1.50
16	A	815	CLA	CHC-C1C	2.03	1.42	1.38
16	2	607	CLA	CMD-C2D	-2.03	1.46	1.50
16	B	807	CLA	CHC-C1C	2.03	1.42	1.38
16	A	804	CLA	CMC-C2C	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	830	CLA	CMD-C2D	-2.02	1.46	1.50
16	F	802	CLA	CMD-C2D	-2.02	1.46	1.50
16	A	827	CLA	CMC-C2C	-2.02	1.46	1.50
16	A	829	CLA	CMC-C2C	-2.02	1.46	1.50
16	B	807	CLA	CMD-C2D	-2.02	1.46	1.50
16	B	819	CLA	CMB-C2B	-2.02	1.46	1.50
16	B	838	CLA	CMD-C2D	-2.02	1.46	1.50
16	9	604	CLA	CHC-C1C	2.02	1.42	1.38
16	2	603	CLA	CHC-C1C	2.02	1.42	1.38
16	A	817	CLA	CMC-C2C	-2.02	1.46	1.50
16	A	822	CLA	CHC-C1C	2.02	1.42	1.38
16	A	823	CLA	CMB-C2B	-2.02	1.46	1.50
16	B	804	CLA	CMC-C2C	-2.02	1.46	1.50
16	2	601	CLA	CMD-C2D	-2.02	1.46	1.50
16	B	834	CLA	CMB-C2B	-2.02	1.46	1.50
16	A	824	CLA	CMB-C2B	-2.02	1.46	1.50
16	B	829	CLA	CHC-C1C	2.02	1.42	1.38
16	K	203	CLA	CHC-C1C	2.01	1.42	1.38
16	2	608	CLA	CHC-C1C	2.01	1.42	1.38
16	B	806	CLA	CMD-C2D	-2.01	1.46	1.50
16	A	803	CLA	CMD-C2D	-2.01	1.46	1.50
16	A	836	CLA	CMD-C2D	-2.01	1.46	1.50
16	F	802	CLA	CMB-C2B	-2.01	1.46	1.50
16	B	818	CLA	CHC-C1C	2.01	1.42	1.38
16	B	837	CLA	CHC-C1C	2.01	1.42	1.38
16	9	607	CLA	CMD-C2D	-2.01	1.46	1.50
16	A	811	CLA	CMB-C2B	-2.01	1.46	1.50
16	B	824	CLA	CMD-C2D	-2.01	1.46	1.50
16	B	839	CLA	CHC-C1C	2.01	1.42	1.38
16	A	828	CLA	CMB-C2B	-2.01	1.46	1.50
16	9	612	CLA	CHC-C1C	2.01	1.42	1.38
16	A	816	CLA	CMD-C2D	-2.01	1.46	1.50
16	A	826	CLA	CMC-C2C	-2.01	1.46	1.50
16	B	840	CLA	CMD-C2D	-2.01	1.46	1.50
16	2	601	CLA	CHC-C1C	2.01	1.42	1.38
16	2	607	CLA	CHC-C1C	2.01	1.42	1.38
16	B	824	CLA	CHC-C1C	2.01	1.42	1.38
16	B	811	CLA	CHC-C1C	2.00	1.42	1.38
16	B	821	CLA	CMB-C2B	-2.00	1.46	1.50
16	B	834	CLA	CHC-C1C	2.00	1.42	1.38
16	A	843	CLA	CMB-C2B	-2.00	1.46	1.50
16	B	813	CLA	CMD-C2D	-2.00	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	852	CLA	CHC-C1C	2.00	1.42	1.38
16	B	838	CLA	CHC-C1C	2.00	1.42	1.38

All (1004) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	842	BCR	C39-C30-C25	-9.94	94.17	110.30
20	B	842	BCR	C40-C30-C39	-9.23	80.20	108.53
17	9	605	CHL	CBD-CHA-C1A	8.68	138.74	128.50
20	A	850	BCR	C24-C23-C22	-7.29	115.22	126.23
17	9	601	CHL	C4D-CHA-C1A	-7.16	112.53	121.25
17	9	605	CHL	C4D-CHA-C1A	-7.16	112.53	121.25
20	I	201	BCR	C24-C23-C22	-6.91	115.80	126.23
16	B	806	CLA	C4A-NA-C1A	6.80	109.76	106.71
20	B	842	BCR	C11-C10-C9	-6.75	117.67	127.31
20	B	842	BCR	C7-C8-C9	-6.66	116.18	126.23
20	F	801	BCR	C7-C8-C9	-6.65	116.19	126.23
16	A	834	CLA	C4A-NA-C1A	6.58	109.66	106.71
20	J	101	BCR	C7-C8-C9	-6.50	116.42	126.23
20	F	801	BCR	C11-C10-C9	-6.42	118.15	127.31
16	L	303	CLA	C4A-NA-C1A	6.40	109.58	106.71
16	A	827	CLA	C4A-NA-C1A	6.35	109.56	106.71
16	B	819	CLA	C4A-NA-C1A	6.16	109.47	106.71
16	A	813	CLA	C4A-NA-C1A	6.13	109.46	106.71
16	A	824	CLA	C4A-NA-C1A	6.08	109.44	106.71
17	9	601	CHL	C1D-ND-C4D	5.98	110.58	106.33
16	A	809	CLA	C4A-NA-C1A	5.94	109.38	106.71
16	A	806	CLA	C4A-NA-C1A	5.93	109.37	106.71
16	2	612	CLA	C4A-NA-C1A	5.84	109.33	106.71
20	L	301	BCR	C28-C27-C26	-5.80	103.73	114.08
20	F	804	BCR	C16-C17-C18	-5.79	119.04	127.31
16	B	808	CLA	C4A-NA-C1A	5.76	109.30	106.71
16	G	201	CLA	C4A-NA-C1A	5.73	109.28	106.71
20	B	842	BCR	C39-C30-C29	-5.71	86.07	108.91
20	J	101	BCR	C11-C10-C9	-5.70	119.18	127.31
16	B	814	CLA	C4A-NA-C1A	5.68	109.26	106.71
16	F	802	CLA	C4A-NA-C1A	5.67	109.25	106.71
16	A	812	CLA	C4A-NA-C1A	5.64	109.24	106.71
16	A	836	CLA	C4A-NA-C1A	5.64	109.24	106.71
16	A	805	CLA	C4A-NA-C1A	5.63	109.24	106.71
17	9	601	CHL	O2D-CGD-CBD	5.62	121.25	111.27
20	B	842	BCR	C40-C30-C25	5.61	119.40	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	833	CLA	C4A-NA-C1A	5.60	109.22	106.71
16	B	835	CLA	C4A-NA-C1A	5.59	109.22	106.71
16	B	827	CLA	C4A-NA-C1A	5.55	109.20	106.71
16	G	202	CLA	C4A-NA-C1A	5.54	109.19	106.71
20	A	850	BCR	C7-C8-C9	-5.53	117.88	126.23
16	B	811	CLA	C4A-NA-C1A	5.52	109.19	106.71
16	B	821	CLA	C4A-NA-C1A	5.51	109.18	106.71
16	J	102	CLA	C4A-NA-C1A	5.45	109.16	106.71
20	A	850	BCR	C28-C27-C26	-5.45	104.34	114.08
20	B	845	BCR	C11-C10-C9	-5.43	119.55	127.31
16	B	836	CLA	C4A-NA-C1A	5.42	109.14	106.71
16	A	838	CLA	C4A-NA-C1A	5.40	109.13	106.71
16	A	826	CLA	C4A-NA-C1A	5.39	109.13	106.71
20	M	101	BCR	C16-C17-C18	-5.38	119.63	127.31
16	K	204	CLA	C4A-NA-C1A	5.38	109.12	106.71
20	B	845	BCR	C15-C14-C13	-5.37	119.64	127.31
16	2	604	CLA	C4A-NA-C1A	5.36	109.12	106.71
16	2	610	CLA	C4A-NA-C1A	5.32	109.10	106.71
16	9	611	CLA	C4A-NA-C1A	5.32	109.10	106.71
16	A	816	CLA	C4A-NA-C1A	5.27	109.08	106.71
16	B	825	CLA	C4A-NA-C1A	5.27	109.08	106.71
16	A	803	CLA	C4A-NA-C1A	5.25	109.07	106.71
20	I	201	BCR	C20-C21-C22	-5.25	119.82	127.31
16	B	801	CLA	C4A-NA-C1A	5.22	109.05	106.71
16	A	808	CLA	C4A-NA-C1A	5.21	109.05	106.71
16	9	610	CLA	C4A-NA-C1A	5.20	109.05	106.71
16	2	603	CLA	C4A-NA-C1A	5.20	109.05	106.71
20	F	801	BCR	C15-C14-C13	-5.18	119.91	127.31
16	A	837	CLA	C4A-NA-C1A	5.17	109.03	106.71
17	9	605	CHL	CHD-C4C-C3C	-5.16	117.26	124.84
20	K	202	BCR	C3-C4-C5	-5.15	104.88	114.08
16	B	815	CLA	C4A-NA-C1A	5.14	109.02	106.71
20	M	101	BCR	C20-C21-C22	-5.14	119.97	127.31
17	9	605	CHL	O2D-CGD-CBD	5.13	120.38	111.27
20	J	101	BCR	C15-C14-C13	-5.12	120.01	127.31
17	9	605	CHL	C1D-ND-C4D	5.10	109.96	106.33
20	A	850	BCR	C20-C21-C22	-5.08	120.05	127.31
20	A	850	BCR	C11-C10-C9	-5.07	120.07	127.31
16	B	831	CLA	C4A-NA-C1A	5.07	108.98	106.71
16	A	833	CLA	C4A-NA-C1A	5.06	108.98	106.71
16	A	819	CLA	C4A-NA-C1A	5.05	108.98	106.71
16	A	807	CLA	C4A-NA-C1A	5.05	108.98	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	813	CLA	C4A-NA-C1A	5.03	108.97	106.71
16	B	809	CLA	C4A-NA-C1A	5.02	108.96	106.71
16	B	838	CLA	C4A-NA-C1A	4.99	108.95	106.71
16	A	852	CLA	C4A-NA-C1A	4.98	108.94	106.71
20	L	305	BCR	C24-C23-C22	-4.96	118.74	126.23
20	B	843	BCR	C7-C8-C9	-4.96	118.75	126.23
16	A	832	CLA	C4A-NA-C1A	4.95	108.93	106.71
16	9	603	CLA	C4A-NA-C1A	4.91	108.91	106.71
16	A	839	CLA	C4A-NA-C1A	4.90	108.91	106.71
16	B	823	CLA	C4A-NA-C1A	4.90	108.91	106.71
16	B	839	CLA	C4A-NA-C1A	4.90	108.91	106.71
17	9	601	CHL	OBD-CAD-C3D	-4.88	116.77	128.52
17	9	605	CHL	OBD-CAD-C3D	-4.88	116.78	128.52
16	B	837	CLA	C4A-NA-C1A	4.88	108.90	106.71
16	A	823	CLA	C4A-NA-C1A	4.87	108.90	106.71
16	A	821	CLA	C4A-NA-C1A	4.87	108.89	106.71
16	9	606	CLA	C4A-NA-C1A	4.85	108.89	106.71
16	9	602	CLA	C4A-NA-C1A	4.84	108.88	106.71
20	A	849	BCR	C7-C8-C9	-4.84	118.93	126.23
16	2	613	CLA	C4A-NA-C1A	4.82	108.87	106.71
16	A	831	CLA	C4A-NA-C1A	4.81	108.87	106.71
20	L	305	BCR	C15-C14-C13	-4.81	120.45	127.31
16	A	835	CLA	C4A-NA-C1A	4.80	108.86	106.71
16	2	602	CLA	C4A-NA-C1A	4.79	108.86	106.71
16	B	820	CLA	C4A-NA-C1A	4.79	108.86	106.71
16	B	832	CLA	C4A-NA-C1A	4.79	108.86	106.71
20	A	849	BCR	C15-C14-C13	-4.79	120.48	127.31
16	B	824	CLA	C4A-NA-C1A	4.77	108.85	106.71
16	B	816	CLA	C4A-NA-C1A	4.76	108.85	106.71
20	K	202	BCR	C7-C8-C9	-4.76	119.05	126.23
20	A	846	BCR	C15-C14-C13	-4.74	120.55	127.31
20	K	206	BCR	C15-C14-C13	-4.73	120.56	127.31
16	B	817	CLA	C4A-NA-C1A	4.70	108.82	106.71
16	K	201	CLA	C4A-NA-C1A	4.70	108.82	106.71
20	B	845	BCR	C7-C8-C9	-4.70	119.13	126.23
16	A	840	CLA	C4A-NA-C1A	4.70	108.82	106.71
16	A	820	CLA	C4A-NA-C1A	4.70	108.82	106.71
16	B	818	CLA	C4A-NA-C1A	4.68	108.81	106.71
20	B	843	BCR	C24-C23-C22	-4.68	119.17	126.23
16	H	202	CLA	C4A-NA-C1A	4.66	108.80	106.71
20	L	301	BCR	C24-C23-C22	-4.65	119.21	126.23
20	K	202	BCR	C11-C10-C9	-4.64	120.69	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	K	203	CLA	C4A-NA-C1A	4.64	108.79	106.71
16	A	802	CLA	C4A-NA-C1A	4.61	108.78	106.71
16	A	815	CLA	C4A-NA-C1A	4.61	108.78	106.71
16	L	304	CLA	C4A-NA-C1A	4.60	108.78	106.71
16	9	604	CLA	C4A-NA-C1A	4.60	108.77	106.71
16	2	609	CLA	C4A-NA-C1A	4.58	108.77	106.71
16	B	802	CLA	C4A-NA-C1A	4.58	108.77	106.71
20	A	847	BCR	C16-C17-C18	-4.57	120.78	127.31
16	F	803	CLA	C4A-NA-C1A	4.57	108.76	106.71
20	I	201	BCR	C15-C14-C13	-4.57	120.79	127.31
16	B	822	CLA	C4A-NA-C1A	4.57	108.76	106.71
16	B	834	CLA	C4A-NA-C1A	4.56	108.76	106.71
17	9	601	CHL	C1D-CHD-C4C	-4.56	116.22	126.06
16	H	201	CLA	C4A-NA-C1A	4.56	108.76	106.71
20	A	850	BCR	C15-C14-C13	-4.55	120.82	127.31
17	9	601	CHL	CHD-C4C-C3C	-4.54	118.17	124.84
17	9	605	CHL	C2C-C3C-C4C	-4.53	103.26	106.49
16	A	843	CLA	C4A-NA-C1A	4.53	108.74	106.71
20	A	849	BCR	C11-C10-C9	-4.52	120.86	127.31
16	B	830	CLA	C4A-NA-C1A	4.52	108.74	106.71
16	B	810	CLA	C4A-NA-C1A	4.52	108.74	106.71
16	9	608	CLA	C4A-NA-C1A	4.51	108.73	106.71
16	B	829	CLA	C4A-NA-C1A	4.51	108.73	106.71
20	K	206	BCR	C11-C10-C9	-4.51	120.88	127.31
16	K	205	CLA	C4A-NA-C1A	4.46	108.71	106.71
16	2	608	CLA	C4A-NA-C1A	4.46	108.71	106.71
17	9	601	CHL	C2C-C3C-C4C	-4.45	103.32	106.49
20	A	847	BCR	C11-C10-C9	-4.44	120.97	127.31
20	I	201	BCR	C16-C17-C18	-4.44	120.97	127.31
16	2	605	CLA	C4A-NA-C1A	4.42	108.69	106.71
16	2	611	CLA	C4A-NA-C1A	4.41	108.69	106.71
20	K	202	BCR	C16-C17-C18	-4.41	121.01	127.31
20	B	842	BCR	C20-C21-C22	-4.38	121.05	127.31
17	9	605	CHL	C1D-CHD-C4C	-4.38	116.60	126.06
16	2	603	CLA	CAA-C2A-C3A	-4.37	105.91	116.10
16	2	607	CLA	C4A-NA-C1A	4.37	108.67	106.71
20	B	843	BCR	C15-C14-C13	-4.34	121.12	127.31
16	2	606	CLA	C4A-NA-C1A	4.34	108.66	106.71
16	9	612	CLA	C4A-NA-C1A	4.34	108.66	106.71
20	M	101	BCR	C24-C23-C22	-4.33	119.69	126.23
20	I	201	BCR	C7-C8-C9	-4.32	119.70	126.23
16	A	822	CLA	C4A-NA-C1A	4.31	108.64	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	9	607	CLA	C4A-NA-C1A	4.30	108.64	106.71
20	A	847	BCR	C7-C8-C9	-4.29	119.76	126.23
20	A	848	BCR	C20-C21-C22	-4.28	121.20	127.31
16	A	818	CLA	C4A-NA-C1A	4.28	108.63	106.71
16	A	814	CLA	C4A-NA-C1A	4.27	108.63	106.71
20	A	848	BCR	C15-C14-C13	-4.27	121.22	127.31
16	A	830	CLA	C4A-NA-C1A	4.26	108.62	106.71
20	A	846	BCR	C24-C23-C22	-4.26	119.79	126.23
20	A	848	BCR	C24-C23-C22	-4.26	119.80	126.23
20	B	842	BCR	C24-C23-C22	-4.25	119.81	126.23
20	K	202	BCR	C20-C21-C22	-4.24	121.25	127.31
16	B	828	CLA	C4A-NA-C1A	4.24	108.61	106.71
20	A	846	BCR	C11-C10-C9	-4.22	121.29	127.31
16	A	828	CLA	C4A-NA-C1A	4.22	108.60	106.71
20	B	844	BCR	C16-C17-C18	-4.21	121.30	127.31
20	A	846	BCR	C20-C21-C22	-4.21	121.30	127.31
17	9	605	CHL	CHB-C4A-NA	4.21	130.33	124.51
16	A	829	CLA	C4A-NA-C1A	4.21	108.60	106.71
20	B	842	BCR	C35-C13-C12	4.20	124.69	118.08
16	A	810	CLA	C4A-NA-C1A	4.18	108.59	106.71
22	B	846	DGD	O2G-C1B-C2B	4.18	120.51	111.50
20	A	848	BCR	C7-C8-C9	-4.14	119.98	126.23
16	A	804	CLA	C4A-NA-C1A	4.13	108.56	106.71
16	A	817	CLA	C4A-NA-C1A	4.13	108.56	106.71
20	A	848	BCR	C16-C17-C18	-4.13	121.42	127.31
20	A	847	BCR	C15-C14-C13	-4.11	121.45	127.31
16	A	825	CLA	C4A-NA-C1A	4.10	108.55	106.71
20	A	847	BCR	C20-C21-C22	-4.10	121.46	127.31
19	A	844	LHG	O7-C7-C8	4.10	120.34	111.50
16	B	840	CLA	C4A-NA-C1A	4.09	108.55	106.71
20	B	844	BCR	C20-C21-C22	-4.07	121.50	127.31
20	A	849	BCR	C16-C17-C18	-4.06	121.51	127.31
16	B	807	CLA	C4A-NA-C1A	4.06	108.53	106.71
16	2	601	CLA	C4A-NA-C1A	4.05	108.53	106.71
20	F	804	BCR	C24-C23-C22	-4.05	120.11	126.23
17	9	605	CHL	C2B-C1B-NB	4.04	112.94	110.23
16	B	804	CLA	C4A-NA-C1A	4.04	108.52	106.71
20	K	206	BCR	C7-C8-C9	-4.04	120.13	126.23
16	B	826	CLA	O2D-CGD-O1D	-4.03	115.97	123.84
20	L	301	BCR	C20-C21-C22	-4.00	121.60	127.31
20	A	846	BCR	C16-C17-C18	-4.00	121.61	127.31
20	B	842	BCR	C30-C25-C26	-3.99	117.00	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	841	CLA	C4A-NA-C1A	3.97	108.49	106.71
20	K	202	BCR	C15-C14-C13	-3.94	121.68	127.31
20	F	801	BCR	C11-C12-C13	-3.91	115.43	126.42
20	J	101	BCR	C3-C4-C5	-3.91	107.09	114.08
20	F	804	BCR	C20-C21-C22	-3.91	121.73	127.31
16	A	811	CLA	C4A-NA-C1A	3.90	108.46	106.71
16	F	803	CLA	CBD-CHA-C1A	3.89	133.67	127.43
20	B	845	BCR	C24-C23-C22	-3.89	120.36	126.23
20	A	848	BCR	C11-C10-C9	-3.88	121.77	127.31
17	9	605	CHL	CHD-C4C-NC	3.87	130.30	124.20
20	K	206	BCR	C24-C23-C22	-3.85	120.42	126.23
20	I	201	BCR	C11-C10-C9	-3.83	121.85	127.31
20	B	843	BCR	C16-C17-C18	-3.83	121.85	127.31
20	A	846	BCR	C7-C8-C9	-3.81	120.48	126.23
20	K	202	BCR	C24-C23-C22	-3.80	120.49	126.23
20	B	842	BCR	C29-C30-C25	3.80	116.33	110.48
16	B	805	CLA	C4A-NA-C1A	3.79	108.41	106.71
20	M	101	BCR	C7-C8-C9	-3.78	120.52	126.23
20	J	101	BCR	C38-C26-C25	-3.77	120.29	124.53
20	J	101	BCR	C20-C21-C22	-3.77	121.93	127.31
20	F	804	BCR	C28-C27-C26	-3.77	107.34	114.08
20	L	301	BCR	C15-C14-C13	-3.74	121.97	127.31
17	9	601	CHL	CHB-C4A-NA	3.73	129.67	124.51
20	K	206	BCR	C16-C17-C18	-3.70	122.02	127.31
20	B	843	BCR	C11-C10-C9	-3.70	122.03	127.31
20	B	844	BCR	C24-C23-C22	-3.70	120.65	126.23
16	B	812	CLA	C4A-NA-C1A	3.70	108.37	106.71
20	J	101	BCR	C16-C17-C18	-3.70	122.03	127.31
20	L	305	BCR	C28-C27-C26	-3.68	107.50	114.08
16	A	809	CLA	CAA-C2A-C3A	-3.68	105.06	114.26
20	A	848	BCR	C38-C26-C25	-3.66	120.41	124.53
20	A	847	BCR	C24-C23-C22	-3.65	120.72	126.23
20	L	301	BCR	C16-C17-C18	-3.64	122.12	127.31
20	F	804	BCR	C11-C10-C9	-3.64	122.12	127.31
20	F	804	BCR	C7-C8-C9	-3.63	120.75	126.23
17	9	601	CHL	C3B-C2B-C1B	-3.63	102.78	107.16
20	K	206	BCR	C20-C21-C22	-3.62	122.14	127.31
20	A	847	BCR	C38-C26-C25	-3.60	120.48	124.53
20	B	843	BCR	C20-C21-C22	-3.60	122.17	127.31
20	L	301	BCR	C33-C5-C6	-3.60	120.49	124.53
16	B	826	CLA	C4A-NA-C1A	3.59	108.32	106.71
20	A	850	BCR	C15-C16-C17	-3.59	116.13	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	842	BCR	C40-C30-C29	3.58	123.24	108.91
17	9	601	CHL	CHD-C4C-NC	3.57	129.83	124.20
16	H	201	CLA	CBD-CHA-C1A	3.56	131.83	128.06
20	B	845	BCR	C38-C26-C25	-3.52	120.58	124.53
17	9	605	CHL	C3B-C2B-C1B	-3.50	102.94	107.16
20	B	844	BCR	C33-C5-C6	-3.49	120.61	124.53
20	K	202	BCR	C4-C5-C6	-3.47	117.70	122.73
20	L	305	BCR	C20-C21-C22	-3.43	122.41	127.31
20	B	844	BCR	C33-C5-C4	3.43	120.20	113.62
20	J	101	BCR	C24-C23-C22	-3.43	121.06	126.23
20	A	848	BCR	C33-C5-C6	-3.42	120.69	124.53
20	B	844	BCR	C8-C7-C6	-3.41	117.62	127.20
17	9	601	CHL	C4B-CHC-C1C	-3.40	118.28	126.34
20	B	844	BCR	C28-C27-C26	-3.39	108.02	114.08
16	B	813	CLA	O2D-CGD-O1D	-3.38	117.23	123.84
16	B	803	CLA	C4A-NA-C1A	3.37	108.22	106.71
16	A	810	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
17	9	605	CHL	C2A-C1A-CHA	-3.35	117.52	122.71
16	2	609	CLA	O2D-CGD-O1D	-3.34	117.32	123.84
20	L	305	BCR	C16-C17-C18	-3.33	122.56	127.31
20	F	801	BCR	C20-C21-C22	-3.32	122.57	127.31
20	B	845	BCR	C15-C16-C17	-3.32	116.68	123.47
20	A	846	BCR	C33-C5-C6	-3.31	120.81	124.53
20	K	202	BCR	C28-C27-C26	-3.31	108.17	114.08
20	A	846	BCR	C28-C27-C26	-3.30	108.19	114.08
17	9	601	CHL	C2B-C1B-NB	3.29	112.44	110.23
20	F	804	BCR	C15-C14-C13	-3.27	122.64	127.31
20	K	206	BCR	C38-C26-C25	-3.27	120.86	124.53
20	A	846	BCR	C3-C4-C5	-3.25	108.27	114.08
17	9	605	CHL	C4B-CHC-C1C	-3.25	118.63	126.34
20	B	844	BCR	C10-C11-C12	-3.25	113.09	123.22
20	B	843	BCR	C28-C27-C26	-3.24	108.28	114.08
20	B	845	BCR	C20-C21-C22	-3.24	122.69	127.31
20	L	305	BCR	C3-C4-C5	-3.23	108.31	114.08
20	K	206	BCR	C3-C4-C5	-3.23	108.31	114.08
20	K	202	BCR	C38-C26-C25	-3.23	120.90	124.53
20	M	101	BCR	C16-C15-C14	-3.23	116.86	123.47
20	F	801	BCR	C16-C17-C18	-3.23	122.70	127.31
16	K	204	CLA	CAA-C2A-C3A	-3.22	106.21	114.26
19	A	845	LHG	O7-C7-C8	3.22	118.44	111.50
16	H	202	CLA	C3A-C4A-CHB	-3.22	119.97	123.91
20	M	101	BCR	C11-C10-C9	-3.21	122.73	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	K	202	BCR	C33-C5-C4	3.21	119.78	113.62
20	F	801	BCR	C28-C27-C26	-3.20	108.36	114.08
20	F	804	BCR	C33-C5-C6	-3.19	120.94	124.53
16	2	611	CLA	CAA-C2A-C3A	-3.19	108.65	116.10
16	2	612	CLA	CAA-C2A-C3A	-3.18	106.31	114.26
16	F	803	CLA	CAA-C2A-C3A	-3.18	106.32	114.26
16	B	803	CLA	O2D-CGD-O1D	-3.17	117.63	123.84
20	A	849	BCR	C38-C26-C25	-3.17	120.97	124.53
16	B	808	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
20	L	301	BCR	C8-C7-C6	-3.17	118.31	127.20
16	A	802	CLA	CMB-C2B-C1B	-3.17	120.55	125.37
16	2	604	CLA	CAA-C2A-C3A	-3.16	106.37	114.26
16	A	840	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
17	9	605	CHL	C3A-C4A-CHB	-3.15	115.72	124.01
16	A	824	CLA	CAA-C2A-C3A	-3.14	104.18	112.78
16	B	838	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
20	B	843	BCR	C38-C26-C25	-3.12	121.02	124.53
16	9	610	CLA	CAA-C2A-C3A	-3.12	106.47	114.26
16	A	838	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
20	L	301	BCR	C1-C6-C5	-3.08	118.27	122.61
16	A	803	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
20	L	301	BCR	C37-C22-C21	-3.07	118.62	122.92
20	B	844	BCR	C16-C15-C14	-3.05	117.23	123.47
16	2	608	CLA	CAA-C2A-C3A	-3.05	108.99	116.10
20	B	842	BCR	C16-C15-C14	-3.04	117.25	123.47
20	B	845	BCR	C16-C17-C18	-3.04	122.98	127.31
16	B	840	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
16	B	834	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
20	F	801	BCR	C38-C26-C27	3.02	119.42	113.62
16	A	817	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
16	B	805	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
16	A	803	CLA	CMB-C2B-C1B	-3.02	120.77	125.37
17	9	601	CHL	CHC-C1C-NC	3.02	128.78	124.20
20	J	101	BCR	C11-C12-C13	-3.01	117.95	126.42
16	A	827	CLA	CHB-C4A-NA	3.01	128.67	124.51
20	L	301	BCR	C38-C26-C27	3.00	119.38	113.62
16	A	822	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
17	9	605	CHL	CHC-C1C-NC	2.99	128.74	124.20
16	A	801	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
16	B	831	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
20	K	206	BCR	C33-C5-C6	-2.98	121.19	124.53
16	A	833	CLA	O2D-CGD-O1D	-2.97	118.03	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	802	CLA	CMB-C2B-C1B	-2.97	120.84	125.37
16	A	815	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
17	9	605	CHL	CHB-C1B-NB	2.96	127.39	124.26
20	B	844	BCR	C38-C26-C25	-2.96	121.21	124.53
20	A	847	BCR	C33-C5-C6	-2.95	121.21	124.53
20	L	301	BCR	C33-C5-C4	2.95	119.28	113.62
16	A	824	CLA	CHB-C4A-NA	2.95	128.59	124.51
17	9	601	CHL	CAC-C3C-C4C	2.94	128.63	124.81
16	A	803	CLA	CAA-C2A-C3A	-2.94	104.73	112.78
20	A	846	BCR	C33-C5-C4	2.94	119.26	113.62
16	L	302	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
20	B	842	BCR	C33-C5-C6	-2.94	121.23	124.53
16	A	828	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
16	B	832	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
16	A	835	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
16	B	833	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
16	B	801	CLA	CHB-C4A-NA	2.92	128.55	124.51
16	A	805	CLA	CHB-C4A-NA	2.92	128.55	124.51
16	2	610	CLA	CAA-C2A-C3A	-2.92	106.97	114.26
16	A	820	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
20	F	801	BCR	C38-C26-C25	-2.91	121.25	124.53
20	B	844	BCR	C7-C8-C9	-2.91	121.83	126.23
16	A	838	CLA	CHD-C1D-ND	-2.91	121.78	124.45
20	A	849	BCR	C24-C23-C22	-2.90	121.85	126.23
16	A	806	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
16	A	812	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
16	B	804	CLA	C3B-C4B-NB	-2.89	107.83	110.52
16	K	203	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
16	A	824	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
16	B	828	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
16	B	817	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
20	B	843	BCR	C38-C26-C27	2.88	119.15	113.62
16	B	804	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
16	2	613	CLA	CBD-CHA-C1A	2.88	131.89	128.50
20	A	848	BCR	C38-C26-C27	2.88	119.15	113.62
20	L	301	BCR	C38-C26-C25	-2.88	121.30	124.53
20	B	844	BCR	C38-C26-C27	2.87	119.14	113.62
17	9	605	CHL	CHA-C4D-ND	2.87	138.50	132.50
16	9	611	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
16	A	832	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
20	F	801	BCR	C24-C23-C22	-2.87	121.90	126.23
16	9	602	CLA	O2D-CGD-O1D	-2.87	118.23	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	805	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
16	L	303	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
17	9	601	CHL	C2A-C1A-CHA	-2.86	118.85	123.86
16	A	834	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
16	9	612	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
16	B	823	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
16	K	205	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
16	2	601	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
16	B	816	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
16	B	830	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
20	B	843	BCR	C34-C9-C10	-2.85	118.92	122.92
16	9	610	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
20	B	844	BCR	C3-C4-C5	-2.85	108.98	114.08
16	A	837	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
20	M	101	BCR	C28-C27-C26	-2.85	108.99	114.08
16	A	811	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
16	A	831	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
16	9	606	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
16	B	825	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
16	B	839	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
16	A	818	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
16	B	821	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
20	B	843	BCR	C37-C22-C21	-2.84	118.95	122.92
16	F	802	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
16	B	810	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
17	9	601	CHL	CHA-C4D-ND	2.84	138.44	132.50
16	B	813	CLA	O2D-CGD-CBD	2.84	116.31	111.27
16	B	807	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
16	9	604	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
16	B	807	CLA	CHB-C4A-NA	2.83	128.43	124.51
20	B	842	BCR	C10-C11-C12	2.83	132.05	123.22
16	A	804	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
16	A	836	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
16	J	102	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
16	L	304	CLA	CAA-C2A-C3A	-2.83	109.50	116.10
16	A	816	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
16	A	806	CLA	CHB-C4A-NA	2.83	128.42	124.51
16	A	807	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
16	B	814	CLA	CHB-C4A-NA	2.82	128.41	124.51
16	B	811	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
20	F	804	BCR	C16-C15-C14	-2.82	117.70	123.47
16	A	813	CLA	CHB-C4A-NA	2.82	128.41	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	814	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
16	B	836	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
16	B	827	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
20	F	804	BCR	C33-C5-C4	2.81	119.01	113.62
16	A	809	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
16	K	204	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
16	G	201	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
20	M	101	BCR	C15-C14-C13	-2.80	123.31	127.31
20	F	801	BCR	C15-C16-C17	-2.80	117.74	123.47
16	9	603	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
17	9	605	CHL	CAC-C3C-C4C	2.80	128.44	124.81
16	A	809	CLA	CHB-C4A-NA	2.80	128.38	124.51
16	A	839	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
16	B	824	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
20	M	101	BCR	C20-C19-C18	-2.80	118.56	126.42
16	A	813	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
16	2	611	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
16	2	603	CLA	CHB-C4A-NA	2.79	128.38	124.51
16	B	802	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
16	B	801	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
16	A	823	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
20	A	846	BCR	C38-C26-C25	-2.79	121.40	124.53
16	A	802	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
16	A	829	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
16	B	819	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
16	B	818	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
16	B	820	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
16	2	607	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
16	9	607	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
20	K	206	BCR	C33-C5-C4	2.78	118.95	113.62
16	A	802	CLA	CMB-C2B-C3B	2.78	133.32	126.59
16	A	830	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
16	G	202	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
16	2	613	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
16	A	803	CLA	CHB-C4A-NA	2.77	128.35	124.51
16	A	841	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
16	A	816	CLA	CHB-C4A-NA	2.77	128.34	124.51
20	L	305	BCR	C11-C10-C9	-2.76	123.36	127.31
16	A	852	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
16	K	201	CLA	CAA-C2A-C3A	-2.76	109.65	116.10
16	F	803	CLA	CHB-C4A-NA	2.76	128.33	124.51
16	B	809	CLA	O2D-CGD-O1D	-2.76	118.45	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	810	CLA	O2D-CGD-CBD	2.75	116.16	111.27
16	A	819	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
16	A	838	CLA	CHB-C4A-NA	2.75	128.32	124.51
16	K	204	CLA	CHB-C4A-NA	2.75	128.32	124.51
16	A	827	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
20	A	850	BCR	C16-C17-C18	-2.74	123.40	127.31
20	A	848	BCR	C33-C5-C4	2.74	118.88	113.62
16	B	815	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
20	B	842	BCR	C11-C12-C13	2.74	134.10	126.42
20	I	201	BCR	C33-C5-C6	-2.73	121.46	124.53
16	B	815	CLA	CHB-C4A-NA	2.73	128.29	124.51
16	2	612	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
16	A	836	CLA	CHB-C4A-NA	2.73	128.28	124.51
16	K	201	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
20	A	847	BCR	C38-C26-C27	2.72	118.84	113.62
16	G	202	CLA	CHB-C4A-NA	2.72	128.27	124.51
16	A	827	CLA	CHD-C1D-ND	-2.72	121.96	124.45
20	A	850	BCR	C38-C26-C25	-2.72	121.48	124.53
17	9	601	CHL	CHC-C4B-NB	2.71	127.13	124.26
16	A	814	CLA	CBD-CHA-C1A	2.71	131.70	128.50
20	I	201	BCR	C33-C5-C4	2.71	118.82	113.62
16	A	808	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
17	9	601	CHL	O2D-CGD-O1D	-2.71	118.54	123.84
20	B	842	BCR	C12-C13-C14	-2.71	114.78	118.94
20	K	202	BCR	C38-C26-C27	2.71	118.82	113.62
20	J	101	BCR	C15-C16-C17	-2.71	117.93	123.47
16	A	825	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
18	A	842	PQN	C11-C12-C13	-2.71	122.29	126.79
16	A	833	CLA	CHB-C4A-NA	2.70	128.25	124.51
16	F	802	CLA	CHB-C4A-NA	2.70	128.25	124.51
16	A	801	CLA	C4A-NA-C1A	2.70	107.92	106.71
16	2	608	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
16	A	815	CLA	CAA-C2A-C3A	-2.70	109.79	116.10
20	I	201	BCR	C15-C16-C17	-2.70	117.94	123.47
16	B	822	CLA	CAA-C2A-C3A	-2.70	109.80	116.10
16	B	806	CLA	CHB-C4A-NA	2.70	128.24	124.51
17	9	605	CHL	C1C-C2C-C3C	-2.70	104.97	107.11
16	A	819	CLA	CHB-C4A-NA	2.69	128.24	124.51
16	A	814	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
16	L	302	CLA	C4A-NA-C1A	2.69	107.92	106.71
16	B	837	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
16	G	202	CLA	CMB-C2B-C1B	-2.69	121.28	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	9	608	CLA	CBD-CHA-C1A	2.68	131.66	128.50
16	A	839	CLA	CHB-C4A-NA	2.68	128.22	124.51
17	9	605	CHL	CHB-C1B-C2B	-2.68	119.67	127.24
16	A	834	CLA	CHB-C4A-NA	2.68	128.22	124.51
16	A	826	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
20	B	845	BCR	C11-C12-C13	-2.67	118.91	126.42
16	B	836	CLA	CHB-C4A-NA	2.67	128.21	124.51
16	A	826	CLA	CAA-C2A-C3A	-2.67	105.46	112.78
16	A	808	CLA	CHB-C4A-NA	2.67	128.21	124.51
16	B	808	CLA	CHB-C4A-NA	2.67	128.21	124.51
16	B	804	CLA	CHB-C4A-NA	2.66	128.19	124.51
22	B	846	DGD	C2G-O2G-C1B	-2.66	111.24	117.79
20	F	801	BCR	C23-C24-C25	-2.66	119.73	127.20
20	B	845	BCR	C1-C6-C5	-2.66	118.87	122.61
16	B	802	CLA	CMB-C2B-C3B	2.66	133.03	126.59
18	B	841	PQN	C11-C12-C13	-2.65	122.37	126.79
16	B	835	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
16	9	602	CLA	CHB-C4A-NA	2.64	128.16	124.51
16	2	612	CLA	CHB-C4A-NA	2.64	128.16	124.51
16	A	835	CLA	CHB-C4A-NA	2.63	128.15	124.51
16	A	821	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
16	2	610	CLA	CHB-C4A-NA	2.63	128.15	124.51
16	A	804	CLA	CHB-C4A-NA	2.63	128.14	124.51
20	A	850	BCR	C30-C25-C26	-2.62	118.92	122.61
16	A	812	CLA	CHB-C4A-NA	2.62	128.13	124.51
16	B	806	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
20	A	847	BCR	C30-C25-C26	-2.62	118.93	122.61
16	A	806	CLA	CAA-C2A-C3A	-2.61	105.62	112.78
16	2	602	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
16	B	829	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
16	B	821	CLA	CHB-C4A-NA	2.61	128.13	124.51
16	B	812	CLA	CHB-C4A-NA	2.61	128.12	124.51
17	9	601	CHL	C1C-C2C-C3C	-2.61	105.04	107.11
16	A	826	CLA	CHB-C4A-NA	2.61	128.12	124.51
16	9	612	CLA	CAA-C2A-C3A	-2.61	110.01	116.10
16	A	817	CLA	CHB-C4A-NA	2.60	128.11	124.51
16	B	822	CLA	CHC-C1C-C2C	-2.60	123.58	129.77
16	B	811	CLA	CHB-C4A-NA	2.60	128.11	124.51
22	B	846	DGD	O1G-C1A-C2A	2.60	120.07	111.91
16	B	822	CLA	O2D-CGD-O1D	-2.60	118.19	124.09
16	B	829	CLA	CHB-C4A-NA	2.60	128.10	124.51
16	2	604	CLA	CHB-C4A-NA	2.60	128.10	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	825	CLA	CHB-C4A-NA	2.60	128.10	124.51
16	A	818	CLA	CHB-C1B-NB	2.59	127.00	124.26
16	B	809	CLA	CHB-C4A-NA	2.59	128.10	124.51
16	G	201	CLA	CHB-C4A-NA	2.59	128.10	124.51
16	A	852	CLA	CHB-C4A-NA	2.59	128.09	124.51
16	B	826	CLA	CHD-C1D-ND	-2.58	122.08	124.45
16	B	817	CLA	CHB-C4A-NA	2.58	128.09	124.51
16	9	608	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
20	A	847	BCR	C33-C5-C4	2.58	118.57	113.62
16	2	603	CLA	O2D-CGD-O1D	-2.58	118.24	124.09
16	A	803	CLA	CMB-C2B-C3B	2.58	132.83	126.59
16	9	606	CLA	CHB-C4A-NA	2.58	128.07	124.51
16	9	603	CLA	CHB-C4A-NA	2.57	128.07	124.51
16	B	839	CLA	CHB-C4A-NA	2.57	128.07	124.51
16	2	602	CLA	CHD-C1D-ND	-2.57	122.09	124.45
16	A	807	CLA	CHB-C4A-NA	2.57	128.07	124.51
16	B	834	CLA	CHB-C4A-NA	2.57	128.07	124.51
16	B	812	CLA	O2D-CGD-O1D	-2.57	118.25	124.09
20	A	849	BCR	C20-C21-C22	-2.57	123.65	127.31
16	2	606	CLA	CAA-C2A-C3A	-2.56	110.11	116.10
19	A	844	LHG	O8-C23-C24	2.56	119.93	111.91
16	L	302	CLA	CAA-C2A-C3A	-2.55	110.14	116.10
16	2	607	CLA	CHB-C4A-NA	2.55	128.04	124.51
16	9	604	CLA	CHB-C4A-NA	2.55	128.04	124.51
16	L	303	CLA	CHB-C4A-NA	2.55	128.04	124.51
16	9	609	CLA	C3A-C4A-CHB	-2.55	117.53	124.50
20	A	848	BCR	C30-C25-C26	-2.55	119.02	122.61
16	A	837	CLA	CHB-C4A-NA	2.55	128.04	124.51
16	B	827	CLA	CHB-C4A-NA	2.55	128.03	124.51
20	M	101	BCR	C33-C5-C6	-2.54	121.67	124.53
16	H	201	CLA	CAB-C3B-C2B	2.54	130.18	123.59
16	2	601	CLA	CHB-C4A-NA	2.54	128.03	124.51
16	A	843	CLA	O2D-CGD-O1D	-2.54	118.32	124.09
16	A	801	CLA	CHC-C4B-NB	2.54	126.95	124.26
16	B	830	CLA	CHB-C4A-NA	2.54	128.03	124.51
20	L	305	BCR	C15-C16-C17	-2.54	118.28	123.47
16	A	832	CLA	CHB-C4A-NA	2.53	128.02	124.51
16	2	605	CLA	CAA-C2A-C3A	-2.53	110.19	116.10
16	B	812	CLA	CAB-C3B-C2B	2.53	130.15	123.59
16	A	843	CLA	CAA-C2A-C3A	-2.53	110.20	116.10
16	A	830	CLA	CHB-C4A-NA	2.53	128.00	124.51
16	B	832	CLA	CHB-C4A-NA	2.53	128.00	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	841	CLA	CHB-C4A-NA	2.52	128.00	124.51
16	A	810	CLA	CHB-C4A-NA	2.52	128.00	124.51
20	B	843	BCR	C3-C4-C5	-2.52	109.57	114.08
16	A	828	CLA	CMB-C2B-C1B	-2.52	121.54	125.37
16	B	840	CLA	CHB-C4A-NA	2.51	127.99	124.51
16	H	201	CLA	CMB-C2B-C3B	2.51	130.10	123.59
16	9	610	CLA	CHB-C4A-NA	2.51	127.98	124.51
16	A	818	CLA	CHB-C4A-NA	2.51	127.98	124.51
16	A	821	CLA	CHB-C4A-NA	2.51	127.98	124.51
16	2	601	CLA	CAA-C2A-C3A	-2.50	110.25	116.10
16	B	838	CLA	CHB-C4A-NA	2.50	127.97	124.51
16	2	609	CLA	CAB-C3B-C2B	2.50	130.07	123.59
16	A	828	CLA	CHB-C4A-NA	2.50	127.97	124.51
16	2	602	CLA	CHB-C4A-NA	2.50	127.96	124.51
16	9	611	CLA	CHB-C4A-NA	2.50	127.96	124.51
16	A	815	CLA	CHB-C4A-NA	2.49	127.96	124.51
16	B	816	CLA	CHB-C4A-NA	2.49	127.96	124.51
16	A	811	CLA	CHD-C1D-ND	-2.49	122.17	124.45
16	2	609	CLA	C3B-C4B-NB	-2.49	108.56	110.23
16	A	813	CLA	CAA-C2A-C3A	-2.49	105.96	112.78
16	J	102	CLA	CHB-C4A-NA	2.49	127.95	124.51
16	A	820	CLA	CHB-C4A-NA	2.49	127.95	124.51
16	K	205	CLA	CHB-C4A-NA	2.49	127.95	124.51
16	K	205	CLA	CAA-C2A-C3A	-2.49	110.30	116.10
16	B	826	CLA	CHB-C4A-NA	2.49	127.95	124.51
16	B	833	CLA	CHB-C4A-NA	2.48	127.94	124.51
16	B	805	CLA	CAA-C2A-C3A	-2.48	110.31	116.10
16	A	823	CLA	CHB-C4A-NA	2.48	127.94	124.51
16	B	824	CLA	CHB-C4A-NA	2.48	127.94	124.51
20	B	845	BCR	C38-C26-C27	2.48	118.38	113.62
22	B	846	DGD	O6D-C5D-C6D	2.48	111.67	106.67
16	A	843	CLA	CHB-C4A-NA	2.47	127.93	124.51
16	A	840	CLA	CHB-C4A-NA	2.47	127.93	124.51
16	B	837	CLA	CHB-C4A-NA	2.47	127.92	124.51
20	B	844	BCR	C15-C14-C13	-2.46	123.80	127.31
16	2	605	CLA	CHB-C4A-NA	2.46	127.91	124.51
16	B	812	CLA	CAA-C2A-C3A	-2.46	106.05	112.78
16	B	803	CLA	CHC-C4B-NB	2.46	126.86	124.26
16	A	822	CLA	CHB-C4A-NA	2.46	127.91	124.51
16	A	831	CLA	CHB-C4A-NA	2.46	127.91	124.51
16	A	804	CLA	C3B-C4B-NB	-2.45	108.24	110.52
16	B	807	CLA	CAA-C2A-C3A	-2.45	106.06	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	810	CLA	CHC-C4B-NB	2.45	126.85	124.26
20	A	850	BCR	C33-C5-C6	-2.45	121.78	124.53
20	F	801	BCR	C30-C25-C26	-2.45	119.16	122.61
17	9	605	CHL	O2D-CGD-O1D	-2.45	119.05	123.84
16	9	612	CLA	CHB-C4A-NA	2.45	127.90	124.51
16	B	812	CLA	CMB-C2B-C3B	2.45	129.93	123.59
16	A	825	CLA	CHD-C1D-ND	-2.45	122.20	124.45
16	B	831	CLA	CHB-C4A-NA	2.45	127.90	124.51
16	A	835	CLA	CMB-C2B-C1B	-2.44	121.65	125.37
20	B	844	BCR	C4-C5-C6	-2.44	119.19	122.73
16	B	823	CLA	CHB-C4A-NA	2.44	127.89	124.51
16	B	808	CLA	O2D-CGD-CBD	2.44	115.60	111.27
16	B	807	CLA	CMB-C2B-C1B	-2.44	121.66	125.37
16	B	835	CLA	CHB-C4A-NA	2.44	127.88	124.51
16	A	817	CLA	CMB-C2B-C1B	-2.44	121.66	125.37
20	A	849	BCR	C11-C12-C13	-2.43	119.58	126.42
16	B	820	CLA	CMB-C2B-C1B	-2.43	121.66	125.37
16	B	820	CLA	CHB-C4A-NA	2.43	127.87	124.51
20	L	305	BCR	C33-C5-C6	-2.42	121.81	124.53
16	B	822	CLA	CHB-C4A-NA	2.42	127.86	124.51
16	A	825	CLA	CHB-C4A-NA	2.42	127.86	124.51
17	9	605	CHL	CHC-C4B-NB	2.42	126.82	124.26
16	9	607	CLA	CHB-C4A-NA	2.42	127.86	124.51
16	A	802	CLA	C2B-C1B-NB	2.42	111.85	110.23
20	F	801	BCR	C3-C4-C5	-2.42	109.76	114.08
20	I	201	BCR	C20-C19-C18	-2.41	119.63	126.42
16	2	606	CLA	CHB-C4A-NA	2.41	127.85	124.51
16	9	608	CLA	CHD-C1D-ND	-2.41	122.24	124.45
20	F	804	BCR	C29-C30-C25	2.41	114.19	110.48
22	B	846	DGD	C4D-C3D-C2D	2.41	115.03	110.82
16	2	609	CLA	CHB-C4A-NA	2.41	127.85	124.51
16	2	609	CLA	CMB-C2B-C3B	2.41	129.84	123.59
19	A	845	LHG	O8-C23-C24	2.41	119.47	111.91
16	A	801	CLA	O1D-CGD-CBD	2.41	129.41	124.48
16	G	202	CLA	CAA-C2A-C3A	-2.40	106.19	112.78
16	B	813	CLA	CHB-C4A-NA	2.40	127.83	124.51
16	B	805	CLA	CHB-C4A-NA	2.40	127.83	124.51
16	A	817	CLA	CHB-C1B-NB	2.40	126.79	124.26
16	B	834	CLA	CHD-C1D-ND	-2.40	122.25	124.45
20	A	846	BCR	C15-C16-C17	-2.39	118.57	123.47
20	A	849	BCR	C1-C6-C5	-2.39	119.25	122.61
20	L	301	BCR	C10-C11-C12	-2.39	115.76	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	845	LHG	C20-C19-C18	-2.39	102.30	114.42
16	K	201	CLA	CHB-C4A-NA	2.39	127.81	124.51
16	K	203	CLA	CHB-C4A-NA	2.39	127.81	124.51
16	B	813	CLA	CMB-C2B-C1B	-2.39	121.74	125.37
16	B	812	CLA	C3B-C4B-NB	-2.39	108.63	110.23
16	L	302	CLA	CHB-C4A-NA	2.38	127.81	124.51
16	A	837	CLA	CHC-C4B-NB	2.38	126.78	124.26
20	B	845	BCR	C4-C5-C6	-2.38	119.27	122.73
16	A	804	CLA	CHB-C1B-NB	2.38	126.78	124.26
16	A	824	CLA	C2A-C1A-CHA	2.38	128.02	123.86
16	A	822	CLA	CHD-C1D-ND	-2.38	122.27	124.45
16	F	802	CLA	CAA-C2A-C3A	-2.37	106.28	112.78
20	L	301	BCR	C27-C26-C25	-2.37	119.28	122.73
16	B	828	CLA	CHB-C4A-NA	2.37	127.79	124.51
16	L	304	CLA	CHB-C4A-NA	2.37	127.79	124.51
16	B	836	CLA	CAA-C2A-C3A	-2.37	106.28	112.78
16	2	611	CLA	CHB-C4A-NA	2.37	127.79	124.51
20	B	842	BCR	C20-C19-C18	-2.37	119.76	126.42
20	K	206	BCR	C11-C12-C13	-2.37	119.77	126.42
20	J	101	BCR	C38-C26-C27	2.37	118.16	113.62
20	A	848	BCR	C8-C7-C6	-2.36	120.56	127.20
20	B	844	BCR	C1-C6-C5	-2.36	119.28	122.61
20	F	801	BCR	C27-C26-C25	-2.36	119.30	122.73
16	A	822	CLA	CAA-C2A-C3A	-2.36	110.58	116.10
16	A	841	CLA	CHC-C4B-NB	2.36	126.76	124.26
20	L	301	BCR	C11-C10-C9	-2.35	123.96	127.31
20	F	804	BCR	C1-C6-C5	-2.35	119.31	122.61
16	2	607	CLA	CAA-C2A-C3A	-2.35	110.62	116.10
20	M	101	BCR	C33-C5-C4	2.34	118.11	113.62
16	B	805	CLA	CMB-C2B-C1B	-2.34	121.81	125.37
20	L	305	BCR	C29-C30-C25	2.34	114.08	110.48
20	B	842	BCR	C38-C26-C25	-2.34	121.90	124.53
16	B	804	CLA	CHB-C1B-NB	2.34	126.73	124.26
16	B	839	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
16	B	810	CLA	CHB-C4A-NA	2.33	127.73	124.51
16	B	819	CLA	CHB-C4A-NA	2.32	127.72	124.51
16	B	806	CLA	CHC-C4B-NB	2.32	126.71	124.26
20	K	206	BCR	C15-C16-C17	-2.32	118.73	123.47
16	B	814	CLA	CAA-C2A-C3A	-2.31	106.45	112.78
20	B	844	BCR	C23-C24-C25	-2.31	120.71	127.20
16	B	826	CLA	CHB-C1B-NB	2.31	126.70	124.26
16	B	832	CLA	CHD-C1D-ND	-2.31	122.33	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	824	CLA	CMB-C2B-C1B	-2.31	121.86	125.37
16	A	805	CLA	CAA-C2A-C3A	-2.31	106.47	112.78
16	A	830	CLA	CHB-C1B-NB	2.30	126.69	124.26
16	A	802	CLA	CAA-C2A-C3A	-2.30	106.49	112.78
16	A	818	CLA	CMB-C2B-C1B	-2.29	121.88	125.37
16	B	828	CLA	C3B-C4B-NB	-2.29	108.39	110.52
16	B	827	CLA	CAA-C2A-C3A	-2.29	106.52	112.78
17	9	601	CHL	CHB-C1B-NB	2.29	126.68	124.26
16	9	609	CLA	CHD-C1D-ND	-2.29	122.35	124.45
16	A	807	CLA	CHD-C1D-ND	-2.29	122.35	124.45
16	A	811	CLA	CHB-C4A-NA	2.28	127.67	124.51
20	A	850	BCR	C10-C11-C12	-2.28	116.10	123.22
20	A	846	BCR	C8-C7-C6	-2.28	120.80	127.20
16	B	829	CLA	CMB-C2B-C1B	-2.28	121.90	125.37
16	A	833	CLA	CHD-C1D-ND	-2.27	122.36	124.45
16	L	302	CLA	CMA-C3A-C2A	-2.27	110.80	116.10
20	L	301	BCR	C29-C30-C25	2.27	113.98	110.48
20	A	846	BCR	C11-C12-C13	-2.27	120.05	126.42
16	B	820	CLA	CHD-C1D-ND	-2.27	122.37	124.45
16	A	827	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
16	2	609	CLA	CHC-C4B-NB	2.26	126.65	124.26
16	A	833	CLA	CHC-C4B-NB	2.26	126.65	124.26
16	B	828	CLA	CHC-C4B-NB	2.26	126.65	124.26
16	A	802	CLA	CHB-C4A-NA	2.25	127.63	124.51
16	A	841	CLA	CAA-C2A-C3A	-2.25	106.60	112.78
16	B	840	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
20	J	101	BCR	C2-C1-C6	2.25	113.94	110.48
17	9	601	CHL	CHB-C1B-C2B	-2.25	120.89	127.24
20	K	202	BCR	C20-C19-C18	-2.25	120.10	126.42
20	A	847	BCR	C23-C24-C25	-2.25	120.89	127.20
16	2	607	CLA	CMA-C3A-C2A	-2.24	110.87	116.10
20	A	849	BCR	C15-C16-C17	-2.24	118.89	123.47
20	B	845	BCR	C21-C20-C19	-2.24	116.23	123.22
16	A	817	CLA	C3B-C4B-NB	-2.24	108.44	110.52
16	B	832	CLA	C3B-C4B-NB	-2.24	108.44	110.52
16	B	837	CLA	CHB-C1B-NB	2.24	126.63	124.26
16	B	818	CLA	CHB-C4A-NA	2.24	127.61	124.51
16	B	837	CLA	CHD-C1D-ND	-2.24	122.40	124.45
16	B	807	CLA	CMB-C2B-C3B	2.24	132.00	126.59
16	B	811	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
20	K	202	BCR	C2-C1-C6	2.23	113.92	110.48
16	A	826	CLA	C3B-C4B-NB	-2.23	108.45	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	801	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
16	B	826	CLA	O2D-CGD-CBD	2.23	115.23	111.27
16	A	804	CLA	CHD-C1D-ND	-2.23	122.41	124.45
17	9	601	CHL	CMB-C2B-C1B	2.23	128.76	125.37
16	B	809	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
16	A	817	CLA	CMB-C2B-C3B	2.23	131.98	126.59
16	A	814	CLA	CHD-C1D-ND	-2.23	122.41	124.45
16	2	609	CLA	CHD-C1D-ND	-2.22	122.41	124.45
16	B	802	CLA	C2B-C1B-NB	2.22	111.72	110.23
16	A	828	CLA	CHB-C1B-NB	2.22	126.61	124.26
16	A	829	CLA	CHB-C4A-NA	2.22	127.58	124.51
16	B	830	CLA	CHD-C1D-ND	-2.22	122.41	124.45
16	B	825	CLA	O2D-CGD-CBD	2.22	115.21	111.27
16	B	801	CLA	CMD-C2D-C3D	2.22	132.71	127.61
16	2	607	CLA	C3B-C4B-NB	-2.21	108.46	110.52
16	A	836	CLA	CMB-C2B-C1B	-2.21	122.00	125.37
16	B	802	CLA	CHB-C4A-NA	2.21	127.57	124.51
20	L	301	BCR	C3-C4-C5	-2.21	110.13	114.08
20	F	804	BCR	C8-C7-C6	-2.21	121.00	127.20
16	H	202	CLA	CHD-C1D-ND	-2.21	122.38	124.52
16	A	831	CLA	CAA-C2A-C3A	-2.20	106.74	112.78
16	A	833	CLA	C3B-C4B-NB	-2.20	108.47	110.52
16	A	832	CLA	C3B-C4B-NB	-2.20	108.47	110.52
16	B	828	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
16	9	604	CLA	C3B-C4B-NB	-2.20	108.47	110.52
20	K	206	BCR	C1-C6-C5	-2.20	119.52	122.61
16	B	801	CLA	CMD-C2D-C1D	-2.20	120.84	124.71
16	A	801	CLA	CHB-C4A-NA	2.20	127.55	124.51
16	A	814	CLA	CHB-C4A-NA	2.20	127.55	124.51
16	B	826	CLA	C3B-C4B-NB	-2.19	108.48	110.52
20	A	847	BCR	C16-C15-C14	-2.19	118.98	123.47
16	2	608	CLA	CHB-C4A-NA	2.19	127.54	124.51
16	A	841	CLA	C3B-C4B-NB	-2.19	108.48	110.52
16	H	201	CLA	CHB-C4A-NA	2.19	127.54	124.51
16	A	835	CLA	CHD-C1D-ND	-2.19	122.44	124.45
20	F	804	BCR	C3-C4-C5	-2.18	110.18	114.08
20	I	201	BCR	C8-C7-C6	-2.18	121.07	127.20
16	2	605	CLA	C3B-C4B-NB	-2.18	108.49	110.52
16	A	804	CLA	CMB-C2B-C1B	-2.18	122.05	125.37
16	G	202	CLA	CMB-C2B-C3B	2.18	131.87	126.59
16	A	832	CLA	CHC-C4B-NB	2.18	126.56	124.26
16	B	810	CLA	CHB-C1B-NB	2.18	126.56	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	807	CLA	CHD-C1D-ND	-2.17	122.46	124.45
16	A	801	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
16	A	837	CLA	CMB-C2B-C1B	-2.17	122.06	125.37
16	A	810	CLA	C3B-C4B-NB	-2.17	108.50	110.52
16	A	812	CLA	C2A-C1A-CHA	2.17	127.65	123.86
16	9	609	CLA	C1A-CHA-C4D	-2.17	121.47	125.32
16	B	812	CLA	CHD-C1D-ND	-2.17	122.46	124.45
16	A	803	CLA	O2D-CGD-CBD	2.16	115.11	111.27
16	A	833	CLA	O2D-CGD-CBD	2.16	115.11	111.27
20	A	850	BCR	C21-C20-C19	-2.16	116.47	123.22
16	A	839	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
16	B	825	CLA	C2A-C1A-CHA	2.16	127.64	123.86
16	A	801	CLA	C3B-C4B-NB	-2.16	108.51	110.52
16	A	809	CLA	C3B-C4B-NB	-2.16	108.51	110.52
16	A	832	CLA	CHB-C1B-NB	2.16	126.54	124.26
16	B	805	CLA	CHB-C1B-NB	2.16	126.54	124.26
16	A	828	CLA	CMB-C2B-C3B	2.16	131.81	126.59
16	A	839	CLA	CHD-C1D-ND	-2.16	122.47	124.45
16	B	829	CLA	CHB-C1B-NB	2.16	126.54	124.26
16	A	803	CLA	C1-C2-C3	-2.15	123.27	126.75
16	B	803	CLA	CHB-C4A-NA	2.15	127.49	124.51
16	B	838	CLA	C3B-C4B-NB	-2.15	108.52	110.52
16	2	608	CLA	CHD-C1D-ND	-2.15	122.48	124.45
20	A	847	BCR	C11-C12-C13	-2.15	120.38	126.42
16	A	836	CLA	CAA-C2A-C3A	-2.15	106.90	112.78
16	A	805	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
16	B	834	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
20	K	202	BCR	C1-C6-C5	-2.14	119.59	122.61
16	F	803	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
20	A	846	BCR	C38-C26-C27	2.14	117.73	113.62
16	A	837	CLA	CHB-C1B-NB	2.14	126.52	124.26
16	B	809	CLA	CHC-C4B-NB	2.14	126.52	124.26
16	B	818	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
16	B	837	CLA	C3B-C4B-NB	-2.14	108.53	110.52
16	A	809	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
16	B	832	CLA	CHB-C1B-NB	2.14	126.52	124.26
20	I	201	BCR	C1-C6-C5	-2.14	119.60	122.61
16	B	823	CLA	CHD-C1D-ND	-2.13	122.49	124.45
16	B	831	CLA	CHD-C1D-ND	-2.13	122.49	124.45
16	2	609	CLA	CHB-C1B-NB	2.13	126.52	124.26
16	B	838	CLA	CHB-C1B-NB	2.13	126.52	124.26
16	B	809	CLA	C3B-C4B-NB	-2.13	108.54	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	844	BCR	C27-C26-C25	-2.13	119.64	122.73
16	K	203	CLA	CHD-C1D-ND	-2.13	122.50	124.45
16	A	830	CLA	O2A-CGA-O1A	-2.13	117.99	123.30
20	A	847	BCR	C28-C27-C26	-2.13	110.27	114.08
16	B	804	CLA	CHC-C4B-NB	2.13	126.51	124.26
16	A	833	CLA	CHB-C1B-NB	2.13	126.51	124.26
16	A	809	CLA	C2A-C1A-CHA	2.13	127.58	123.86
16	A	843	CLA	CHD-C1D-ND	-2.12	122.50	124.45
16	A	835	CLA	CHB-C1B-NB	2.12	126.50	124.26
16	A	837	CLA	CHD-C1D-ND	-2.12	122.50	124.45
16	L	304	CLA	CHD-C1D-ND	-2.12	122.50	124.45
16	B	820	CLA	CMB-C2B-C3B	2.12	131.73	126.59
16	A	808	CLA	CHD-C1D-ND	-2.12	122.50	124.45
16	A	810	CLA	CAA-C2A-C3A	-2.12	111.15	116.10
16	9	602	CLA	CHD-C1D-ND	-2.12	122.51	124.45
16	K	205	CLA	CHD-C1D-ND	-2.12	122.51	124.45
20	L	301	BCR	C7-C8-C9	-2.12	123.03	126.23
16	B	826	CLA	CMB-C2B-C1B	-2.12	122.15	125.37
16	9	607	CLA	CHC-C4B-NB	2.12	126.50	124.26
20	B	843	BCR	C30-C25-C26	-2.12	119.63	122.61
16	B	806	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
16	B	826	CLA	O1D-CGD-CBD	2.11	128.81	124.48
16	A	805	CLA	CHD-C1D-ND	-2.11	122.51	124.45
16	A	835	CLA	CMB-C2B-C3B	2.11	131.70	126.59
16	9	607	CLA	CHD-C1D-ND	-2.11	122.52	124.45
20	I	201	BCR	C3-C4-C5	-2.11	110.31	114.08
16	9	612	CLA	CHD-C1D-ND	-2.11	122.52	124.45
16	A	852	CLA	C3B-C4B-NB	-2.11	108.56	110.52
16	B	836	CLA	C3B-C4B-NB	-2.11	108.56	110.52
16	A	811	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
16	2	611	CLA	CMA-C3A-C2A	-2.11	111.18	116.10
20	B	844	BCR	C35-C13-C12	2.11	121.40	118.08
16	9	611	CLA	CHD-C1D-ND	-2.11	122.52	124.45
16	A	805	CLA	C3B-C4B-NB	-2.11	108.56	110.52
16	A	827	CLA	C1-C2-C3	-2.11	123.35	126.75
20	A	848	BCR	C23-C24-C25	-2.10	121.29	127.20
16	2	610	CLA	C2B-C1B-NB	2.10	111.64	110.23
16	B	808	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
16	A	827	CLA	CAA-C2A-C3A	-2.10	107.02	112.78
16	9	604	CLA	CHB-C1B-NB	2.10	126.48	124.26
16	A	836	CLA	CMB-C2B-C3B	2.10	131.67	126.59
16	2	613	CLA	CHB-C4A-NA	2.10	127.42	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	H	201	CLA	CHD-C1D-ND	-2.10	122.53	124.45
16	2	609	CLA	O2D-CGD-CBD	2.10	115.00	111.27
20	I	201	BCR	C4-C5-C6	-2.09	119.69	122.73
16	9	606	CLA	CHD-C1D-ND	-2.09	122.53	124.45
16	B	805	CLA	C3B-C4B-NB	-2.09	108.57	110.52
16	B	829	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
20	A	848	BCR	C20-C19-C18	-2.09	120.54	126.42
20	K	202	BCR	C11-C12-C13	-2.09	120.54	126.42
16	A	822	CLA	CHB-C1B-NB	2.09	126.47	124.26
16	B	814	CLA	C2A-C1A-CHA	2.09	127.51	123.86
16	A	808	CLA	C3B-C4B-NB	-2.09	108.58	110.52
16	B	805	CLA	CMB-C2B-C3B	2.09	131.65	126.59
16	A	825	CLA	CHB-C1B-NB	2.09	126.47	124.26
16	A	830	CLA	C3B-C4B-NB	-2.09	108.58	110.52
16	B	802	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
17	9	601	CHL	O1D-CGD-CBD	-2.09	120.21	124.48
16	B	831	CLA	O2D-CGD-CBD	2.09	114.98	111.27
20	A	846	BCR	C1-C6-C5	-2.08	119.68	122.61
16	A	815	CLA	CHD-C1D-ND	-2.08	122.54	124.45
16	A	829	CLA	CMB-C2B-C1B	-2.08	122.20	125.37
16	A	822	CLA	C3B-C4B-NB	-2.08	108.58	110.52
20	A	847	BCR	C1-C6-C5	-2.08	119.69	122.61
16	9	608	CLA	CHB-C4A-NA	2.08	127.39	124.51
16	B	812	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
16	B	821	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
16	A	838	CLA	C3B-C4B-NB	-2.08	108.59	110.52
20	A	850	BCR	C36-C18-C19	2.08	121.35	118.08
20	B	844	BCR	C30-C25-C26	-2.08	119.69	122.61
16	B	817	CLA	CHD-C1D-ND	-2.08	122.55	124.45
16	B	830	CLA	O2A-CGA-O1A	-2.08	118.36	123.59
16	B	822	CLA	C4C-C3C-C2C	-2.07	106.59	108.89
16	2	605	CLA	CHB-C1B-NB	2.07	126.45	124.26
16	J	102	CLA	CAA-C2A-C3A	-2.07	109.08	114.26
20	F	801	BCR	C8-C9-C10	2.07	122.12	118.94
16	B	803	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
16	B	835	CLA	C2B-C1B-NB	2.07	111.62	110.23
20	L	301	BCR	C15-C16-C17	-2.07	119.23	123.47
20	A	848	BCR	C11-C12-C13	-2.07	120.60	126.42
20	K	202	BCR	C30-C25-C26	-2.07	119.70	122.61
16	B	813	CLA	O2A-CGA-O1A	-2.07	118.14	123.30
16	B	833	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
16	A	820	CLA	O2A-CGA-O1A	-2.07	118.37	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	I	201	BCR	C10-C11-C12	-2.07	116.77	123.22
16	B	810	CLA	CHD-C1D-ND	-2.07	122.56	124.45
16	A	828	CLA	C3B-C4B-NB	-2.07	108.60	110.52
16	B	836	CLA	CMB-C2B-C1B	-2.06	122.22	125.37
16	A	830	CLA	CHD-C1D-ND	-2.06	122.56	124.45
16	B	808	CLA	CHD-C1D-ND	-2.06	122.56	124.45
20	A	846	BCR	C20-C19-C18	-2.06	120.62	126.42
16	B	829	CLA	CMB-C2B-C3B	2.06	131.58	126.59
16	B	825	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
16	A	810	CLA	CHB-C1B-NB	2.06	126.44	124.26
16	B	838	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
16	A	824	CLA	CHC-C4B-NB	2.06	126.44	124.26
16	H	201	CLA	C3B-C4B-NB	-2.06	108.85	110.23
20	L	301	BCR	C1-C6-C7	2.05	121.59	115.78
20	B	845	BCR	C23-C24-C25	-2.05	121.43	127.20
16	A	817	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
20	A	850	BCR	C38-C26-C27	2.05	117.56	113.62
16	A	836	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
16	A	837	CLA	C3B-C4B-NB	-2.05	108.61	110.52
16	L	303	CLA	C3B-C4B-NB	-2.05	108.61	110.52
20	I	201	BCR	C30-C25-C26	-2.05	119.73	122.61
16	B	811	CLA	CMB-C2B-C1B	-2.05	122.25	125.37
16	H	202	CLA	CHB-C4A-NA	2.05	127.47	124.34
16	B	839	CLA	CHD-C1D-ND	-2.05	122.57	124.45
16	A	812	CLA	CHA-C1A-NA	-2.05	121.71	126.40
20	B	844	BCR	C34-C9-C8	2.04	121.30	118.08
16	F	802	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
16	L	302	CLA	C2B-C1B-NB	2.04	111.60	110.23
16	A	810	CLA	CHD-C1D-ND	-2.04	122.58	124.45
16	A	819	CLA	CHD-C1D-ND	-2.04	122.58	124.45
20	B	844	BCR	C8-C9-C10	-2.04	115.81	118.94
16	K	203	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
16	2	604	CLA	CAD-CBD-CHA	2.04	107.43	105.14
16	A	811	CLA	C3B-C4B-NB	-2.04	108.62	110.52
16	A	803	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
20	M	101	BCR	C10-C11-C12	-2.04	116.86	123.22
16	9	602	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
16	B	833	CLA	CHD-C1D-ND	-2.04	122.58	124.45
16	A	839	CLA	CHB-C1B-NB	2.04	126.41	124.26
16	A	825	CLA	C3B-C4B-NB	-2.03	108.63	110.52
16	A	838	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
16	B	828	CLA	CHB-C1B-NB	2.03	126.41	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	808	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
16	2	601	CLA	CHB-C1B-NB	2.03	126.41	124.26
16	A	817	CLA	CHD-C1D-ND	-2.03	122.59	124.45
16	A	801	CLA	CHB-C1B-NB	2.03	126.41	124.26
16	A	818	CLA	CHC-C4B-NB	2.03	126.40	124.26
16	B	826	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
16	G	202	CLA	C2A-C1A-CHA	2.03	127.40	123.86
16	A	825	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
16	B	834	CLA	C3B-C4B-NB	-2.03	108.64	110.52
16	B	812	CLA	CHC-C4B-NB	2.03	126.40	124.26
16	G	201	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
16	2	601	CLA	CHD-C1D-ND	-2.02	122.59	124.45
16	A	806	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
16	B	815	CLA	C3B-C4B-NB	-2.02	108.64	110.52
16	B	801	CLA	C3B-C4B-NB	-2.02	108.64	110.52
16	A	818	CLA	C3B-C4B-NB	-2.02	108.64	110.52
20	B	843	BCR	C27-C26-C25	-2.02	119.80	122.73
16	2	605	CLA	CHD-C1D-ND	-2.02	122.60	124.45
16	A	804	CLA	CMB-C2B-C3B	2.02	131.47	126.59
16	F	803	CLA	CMB-C2B-C3B	2.02	131.47	126.59
16	A	813	CLA	C2A-C1A-CHA	2.02	127.38	123.86
16	A	803	CLA	C2A-C1A-CHA	2.02	127.38	123.86
16	9	607	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
16	2	603	CLA	C2A-C1A-CHA	2.01	127.37	123.85
16	A	832	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
16	9	603	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
20	A	849	BCR	C21-C20-C19	-2.01	116.94	123.22
16	A	820	CLA	CHD-C1D-ND	-2.01	122.61	124.45
16	A	837	CLA	CMB-C2B-C3B	2.01	131.46	126.59
20	A	848	BCR	C28-C27-C26	-2.01	110.49	114.08
16	B	836	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
16	B	838	CLA	CHD-C1D-ND	-2.01	122.61	124.45
20	L	305	BCR	C33-C5-C4	2.01	117.47	113.62
20	L	301	BCR	C34-C9-C8	2.01	121.24	118.08
16	A	802	CLA	CHD-C1D-ND	-2.01	122.61	124.45
20	L	301	BCR	C16-C15-C14	-2.01	119.36	123.47
16	B	835	CLA	O2A-CGA-O1A	-2.01	118.30	123.30
16	A	836	CLA	C1-C2-C3	-2.01	123.51	126.75
16	A	824	CLA	CAC-C3C-C4C	2.01	127.41	124.81
16	B	814	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
16	B	817	CLA	C3B-C4B-NB	-2.00	108.66	110.52
20	A	849	BCR	C3-C4-C5	-2.00	110.50	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	836	CLA	CMB-C2B-C3B	2.00	131.44	126.59
16	B	837	CLA	CHC-C4B-NB	2.00	126.38	124.26

There are no chirality outliers.

All (1185) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	2	601	CLA	C2B-C3B-CAB-CBB
16	2	601	CLA	C4B-C3B-CAB-CBB
16	2	601	CLA	CHA-CBD-CGD-O1D
16	2	602	CLA	C2B-C3B-CAB-CBB
16	2	602	CLA	C4B-C3B-CAB-CBB
16	2	604	CLA	C1A-C2A-CAA-CBA
16	2	607	CLA	C2B-C3B-CAB-CBB
16	2	607	CLA	C4B-C3B-CAB-CBB
16	2	607	CLA	CBD-CGD-O2D-CED
16	2	608	CLA	C2B-C3B-CAB-CBB
16	2	608	CLA	C4B-C3B-CAB-CBB
16	2	610	CLA	C1A-C2A-CAA-CBA
16	2	612	CLA	CHA-CBD-CGD-O1D
16	2	612	CLA	CHA-CBD-CGD-O2D
16	2	613	CLA	CHA-CBD-CGD-O1D
16	2	613	CLA	CHA-CBD-CGD-O2D
16	9	604	CLA	C2A-CAA-CBA-CGA
16	9	604	CLA	CBD-CGD-O2D-CED
16	9	606	CLA	CHA-CBD-CGD-O1D
16	9	606	CLA	CHA-CBD-CGD-O2D
16	9	609	CLA	CMA-C3A-C4A-CHB
16	9	610	CLA	C1A-C2A-CAA-CBA
16	9	610	CLA	C3A-C2A-CAA-CBA
16	9	611	CLA	C2B-C3B-CAB-CBB
16	9	611	CLA	C4B-C3B-CAB-CBB
16	9	611	CLA	CHA-CBD-CGD-O1D
16	9	611	CLA	CHA-CBD-CGD-O2D
16	9	611	CLA	CAD-CBD-CGD-O1D
16	9	612	CLA	C2B-C3B-CAB-CBB
16	9	612	CLA	C4B-C3B-CAB-CBB
16	A	801	CLA	C1A-C2A-CAA-CBA
16	A	801	CLA	C2B-C3B-CAB-CBB
16	A	801	CLA	C4B-C3B-CAB-CBB
16	A	801	CLA	CBD-CGD-O2D-CED
16	A	802	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
16	A	802	CLA	CHA-CBD-CGD-O2D
16	A	802	CLA	CBD-CGD-O2D-CED
16	A	803	CLA	CHA-CBD-CGD-O2D
16	A	804	CLA	C3A-C2A-CAA-CBA
16	A	805	CLA	CHA-CBD-CGD-O1D
16	A	805	CLA	CHA-CBD-CGD-O2D
16	A	807	CLA	C1A-C2A-CAA-CBA
16	A	810	CLA	CHA-CBD-CGD-O2D
16	A	810	CLA	CBD-CGD-O2D-CED
16	A	811	CLA	C4B-C3B-CAB-CBB
16	A	811	CLA	CBD-CGD-O2D-CED
16	A	812	CLA	C1A-C2A-CAA-CBA
16	A	812	CLA	C3A-C2A-CAA-CBA
16	A	812	CLA	CBD-CGD-O2D-CED
16	A	813	CLA	C2A-CAA-CBA-CGA
16	A	814	CLA	CHA-CBD-CGD-O1D
16	A	817	CLA	C1A-C2A-CAA-CBA
16	A	817	CLA	C3A-C2A-CAA-CBA
16	A	818	CLA	C1A-C2A-CAA-CBA
16	A	818	CLA	C3A-C2A-CAA-CBA
16	A	818	CLA	CHA-CBD-CGD-O1D
16	A	818	CLA	CHA-CBD-CGD-O2D
16	A	819	CLA	C1A-C2A-CAA-CBA
16	A	819	CLA	C3A-C2A-CAA-CBA
16	A	819	CLA	CBD-CGD-O2D-CED
16	A	821	CLA	C1A-C2A-CAA-CBA
16	A	821	CLA	C3A-C2A-CAA-CBA
16	A	822	CLA	C2B-C3B-CAB-CBB
16	A	822	CLA	C4B-C3B-CAB-CBB
16	A	822	CLA	CHA-CBD-CGD-O1D
16	A	822	CLA	CHA-CBD-CGD-O2D
16	A	822	CLA	CAD-CBD-CGD-O1D
16	A	822	CLA	CBD-CGD-O2D-CED
16	A	823	CLA	C2B-C3B-CAB-CBB
16	A	823	CLA	C4B-C3B-CAB-CBB
16	A	826	CLA	CHA-CBD-CGD-O1D
16	A	826	CLA	CHA-CBD-CGD-O2D
16	A	828	CLA	C1A-C2A-CAA-CBA
16	A	830	CLA	C3A-C2A-CAA-CBA
16	A	832	CLA	C2B-C3B-CAB-CBB
16	A	832	CLA	C4B-C3B-CAB-CBB
16	A	832	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	A	833	CLA	C2B-C3B-CAB-CBB
16	A	833	CLA	C4B-C3B-CAB-CBB
16	A	834	CLA	C1A-C2A-CAA-CBA
16	A	834	CLA	C2B-C3B-CAB-CBB
16	A	834	CLA	C4B-C3B-CAB-CBB
16	A	834	CLA	CBD-CGD-O2D-CED
16	A	835	CLA	C1A-C2A-CAA-CBA
16	A	835	CLA	C3A-C2A-CAA-CBA
16	A	835	CLA	CHA-CBD-CGD-O1D
16	A	835	CLA	CHA-CBD-CGD-O2D
16	A	837	CLA	CHA-CBD-CGD-O1D
16	A	837	CLA	CHA-CBD-CGD-O2D
16	A	838	CLA	C1A-C2A-CAA-CBA
16	A	838	CLA	CHA-CBD-CGD-O1D
16	A	838	CLA	CHA-CBD-CGD-O2D
16	A	838	CLA	CAD-CBD-CGD-O1D
16	A	839	CLA	C1A-C2A-CAA-CBA
16	A	839	CLA	C3A-C2A-CAA-CBA
16	A	839	CLA	CBD-CGD-O2D-CED
16	A	840	CLA	C1A-C2A-CAA-CBA
16	A	840	CLA	C3A-C2A-CAA-CBA
16	A	840	CLA	CBD-CGD-O2D-CED
16	A	841	CLA	C1A-C2A-CAA-CBA
16	A	841	CLA	C4B-C3B-CAB-CBB
16	A	843	CLA	CAD-CBD-CGD-O2D
16	A	852	CLA	C1A-C2A-CAA-CBA
16	A	852	CLA	C3A-C2A-CAA-CBA
16	A	852	CLA	C4B-C3B-CAB-CBB
16	A	852	CLA	CHA-CBD-CGD-O1D
16	A	852	CLA	CHA-CBD-CGD-O2D
16	B	801	CLA	C1A-C2A-CAA-CBA
16	B	801	CLA	C3A-C2A-CAA-CBA
16	B	802	CLA	CBD-CGD-O2D-CED
16	B	803	CLA	CBD-CGD-O2D-CED
16	B	803	CLA	O1D-CGD-O2D-CED
16	B	804	CLA	C2B-C3B-CAB-CBB
16	B	804	CLA	C4B-C3B-CAB-CBB
16	B	804	CLA	CHA-CBD-CGD-O1D
16	B	804	CLA	CHA-CBD-CGD-O2D
16	B	804	CLA	CBD-CGD-O2D-CED
16	B	806	CLA	C1A-C2A-CAA-CBA
16	B	806	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
16	B	806	CLA	CHA-CBD-CGD-O1D
16	B	806	CLA	CHA-CBD-CGD-O2D
16	B	806	CLA	CAD-CBD-CGD-O1D
16	B	807	CLA	CBD-CGD-O2D-CED
16	B	808	CLA	C1A-C2A-CAA-CBA
16	B	808	CLA	C2B-C3B-CAB-CBB
16	B	808	CLA	C4B-C3B-CAB-CBB
16	B	809	CLA	C1A-C2A-CAA-CBA
16	B	809	CLA	C3A-C2A-CAA-CBA
16	B	809	CLA	C2B-C3B-CAB-CBB
16	B	809	CLA	C4B-C3B-CAB-CBB
16	B	810	CLA	C1A-C2A-CAA-CBA
16	B	810	CLA	C2A-CAA-CBA-CGA
16	B	811	CLA	CHA-CBD-CGD-O1D
16	B	811	CLA	CHA-CBD-CGD-O2D
16	B	812	CLA	C1A-C2A-CAA-CBA
16	B	813	CLA	CHA-CBD-CGD-O1D
16	B	813	CLA	CHA-CBD-CGD-O2D
16	B	814	CLA	CBD-CGD-O2D-CED
16	B	815	CLA	CBD-CGD-O2D-CED
16	B	816	CLA	CBD-CGD-O2D-CED
16	B	817	CLA	C2B-C3B-CAB-CBB
16	B	817	CLA	C4B-C3B-CAB-CBB
16	B	818	CLA	C2A-CAA-CBA-CGA
16	B	818	CLA	CBD-CGD-O2D-CED
16	B	821	CLA	C1A-C2A-CAA-CBA
16	B	821	CLA	C3A-C2A-CAA-CBA
16	B	823	CLA	C4B-C3B-CAB-CBB
16	B	824	CLA	C3A-C2A-CAA-CBA
16	B	825	CLA	CHA-CBD-CGD-O1D
16	B	825	CLA	CHA-CBD-CGD-O2D
16	B	828	CLA	C1A-C2A-CAA-CBA
16	B	828	CLA	C3A-C2A-CAA-CBA
16	B	829	CLA	C1A-C2A-CAA-CBA
16	B	829	CLA	C3A-C2A-CAA-CBA
16	B	829	CLA	CHA-CBD-CGD-O1D
16	B	829	CLA	CHA-CBD-CGD-O2D
16	B	831	CLA	C2B-C3B-CAB-CBB
16	B	831	CLA	C4B-C3B-CAB-CBB
16	B	831	CLA	CHA-CBD-CGD-O1D
16	B	831	CLA	CHA-CBD-CGD-O2D
16	B	834	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
16	B	835	CLA	C1A-C2A-CAA-CBA
16	B	835	CLA	CBD-CGD-O2D-CED
16	B	835	CLA	O1D-CGD-O2D-CED
16	B	836	CLA	C1A-C2A-CAA-CBA
16	B	839	CLA	CBD-CGD-O2D-CED
16	B	840	CLA	C1A-C2A-CAA-CBA
16	B	840	CLA	C2B-C3B-CAB-CBB
16	B	840	CLA	C4B-C3B-CAB-CBB
16	B	840	CLA	CHA-CBD-CGD-O1D
16	B	840	CLA	CHA-CBD-CGD-O2D
16	B	840	CLA	CAD-CBD-CGD-O1D
16	B	840	CLA	CBD-CGD-O2D-CED
16	F	802	CLA	C4B-C3B-CAB-CBB
16	F	803	CLA	C1A-C2A-CAA-CBA
16	G	201	CLA	C2B-C3B-CAB-CBB
16	G	201	CLA	C4B-C3B-CAB-CBB
16	G	201	CLA	CHA-CBD-CGD-O1D
16	G	201	CLA	CHA-CBD-CGD-O2D
16	G	201	CLA	CAD-CBD-CGD-O1D
16	G	202	CLA	CBD-CGD-O2D-CED
16	J	102	CLA	C2B-C3B-CAB-CBB
16	J	102	CLA	C4B-C3B-CAB-CBB
16	K	201	CLA	C2B-C3B-CAB-CBB
16	K	201	CLA	C4B-C3B-CAB-CBB
16	K	201	CLA	CBD-CGD-O2D-CED
16	K	203	CLA	C1A-C2A-CAA-CBA
16	K	203	CLA	C3A-C2A-CAA-CBA
16	L	302	CLA	CBD-CGD-O2D-CED
16	L	303	CLA	C2B-C3B-CAB-CBB
16	L	303	CLA	C4B-C3B-CAB-CBB
17	9	601	CHL	C1A-C2A-CAA-CBA
17	9	601	CHL	C3A-C2A-CAA-CBA
19	A	844	LHG	C3-O3-P-O5
19	A	844	LHG	C3-O3-P-O6
19	A	844	LHG	C4-O6-P-O5
19	A	845	LHG	C3-O3-P-O5
19	A	845	LHG	C4-O6-P-O4
20	A	846	BCR	C7-C8-C9-C34
20	A	849	BCR	C1-C6-C7-C8
20	A	849	BCR	C7-C8-C9-C10
20	A	849	BCR	C7-C8-C9-C34
20	A	850	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
20	A	850	BCR	C7-C8-C9-C34
20	A	850	BCR	C19-C20-C21-C22
20	A	850	BCR	C21-C22-C23-C24
20	A	850	BCR	C37-C22-C23-C24
20	B	842	BCR	C7-C8-C9-C34
20	B	842	BCR	C11-C12-C13-C14
20	B	842	BCR	C11-C12-C13-C35
20	B	842	BCR	C17-C18-C19-C20
20	B	842	BCR	C36-C18-C19-C20
20	B	844	BCR	C7-C8-C9-C10
20	B	844	BCR	C7-C8-C9-C34
20	B	845	BCR	C7-C8-C9-C10
20	B	845	BCR	C7-C8-C9-C34
20	F	801	BCR	C7-C8-C9-C10
20	F	801	BCR	C7-C8-C9-C34
20	F	801	BCR	C11-C12-C13-C14
20	F	801	BCR	C11-C12-C13-C35
20	F	801	BCR	C21-C22-C23-C24
20	F	801	BCR	C37-C22-C23-C24
20	I	201	BCR	C21-C22-C23-C24
20	I	201	BCR	C37-C22-C23-C24
20	J	101	BCR	C7-C8-C9-C10
20	J	101	BCR	C7-C8-C9-C34
20	L	305	BCR	C5-C6-C7-C8
20	L	305	BCR	C7-C8-C9-C34
20	L	305	BCR	C21-C22-C23-C24
20	L	305	BCR	C37-C22-C23-C24
20	M	101	BCR	C21-C22-C23-C24
20	M	101	BCR	C37-C22-C23-C24
16	2	609	CLA	O1D-CGD-O2D-CED
16	9	610	CLA	O1D-CGD-O2D-CED
16	A	810	CLA	O1D-CGD-O2D-CED
16	A	814	CLA	O1D-CGD-O2D-CED
16	A	815	CLA	O1D-CGD-O2D-CED
16	B	804	CLA	O1D-CGD-O2D-CED
16	G	201	CLA	O1D-CGD-O2D-CED
16	G	202	CLA	O1D-CGD-O2D-CED
16	J	102	CLA	O1D-CGD-O2D-CED
16	A	801	CLA	O1D-CGD-O2D-CED
16	A	811	CLA	O1D-CGD-O2D-CED
16	A	812	CLA	O1D-CGD-O2D-CED
16	A	830	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	L	302	CLA	O1D-CGD-O2D-CED
16	2	609	CLA	CBD-CGD-O2D-CED
16	2	611	CLA	CBD-CGD-O2D-CED
16	9	608	CLA	CBD-CGD-O2D-CED
16	9	610	CLA	CBD-CGD-O2D-CED
16	9	611	CLA	CBD-CGD-O2D-CED
16	9	612	CLA	CBD-CGD-O2D-CED
16	A	803	CLA	CBD-CGD-O2D-CED
16	A	813	CLA	CBD-CGD-O2D-CED
16	A	814	CLA	CBD-CGD-O2D-CED
16	A	815	CLA	CBD-CGD-O2D-CED
16	A	816	CLA	CBD-CGD-O2D-CED
16	A	827	CLA	CBD-CGD-O2D-CED
16	A	828	CLA	CBD-CGD-O2D-CED
16	A	830	CLA	CBD-CGD-O2D-CED
16	A	831	CLA	CBD-CGD-O2D-CED
16	B	810	CLA	CBD-CGD-O2D-CED
16	B	817	CLA	CBD-CGD-O2D-CED
16	B	821	CLA	CBD-CGD-O2D-CED
16	B	824	CLA	CBD-CGD-O2D-CED
16	B	826	CLA	CBD-CGD-O2D-CED
16	B	830	CLA	CBD-CGD-O2D-CED
16	B	836	CLA	CBD-CGD-O2D-CED
16	G	201	CLA	CBD-CGD-O2D-CED
16	J	102	CLA	CBD-CGD-O2D-CED
16	K	204	CLA	CBD-CGD-O2D-CED
16	K	205	CLA	CBD-CGD-O2D-CED
16	B	801	CLA	O1A-CGA-O2A-C1
16	A	802	CLA	O1D-CGD-O2D-CED
16	A	822	CLA	O1D-CGD-O2D-CED
16	B	802	CLA	O1D-CGD-O2D-CED
16	B	807	CLA	O1D-CGD-O2D-CED
16	B	817	CLA	O1D-CGD-O2D-CED
16	K	201	CLA	O1D-CGD-O2D-CED
16	2	607	CLA	O1D-CGD-O2D-CED
16	9	604	CLA	O1D-CGD-O2D-CED
16	A	816	CLA	O1D-CGD-O2D-CED
16	A	819	CLA	O1D-CGD-O2D-CED
16	A	834	CLA	O1D-CGD-O2D-CED
16	A	839	CLA	O1D-CGD-O2D-CED
16	B	814	CLA	O1D-CGD-O2D-CED
16	B	815	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	B	840	CLA	O1D-CGD-O2D-CED
16	B	801	CLA	CBA-CGA-O2A-C1
16	9	602	CLA	CBD-CGD-O2D-CED
16	9	607	CLA	CBD-CGD-O2D-CED
16	A	809	CLA	CBD-CGD-O2D-CED
16	A	817	CLA	CBD-CGD-O2D-CED
16	A	820	CLA	CBD-CGD-O2D-CED
16	A	823	CLA	CBD-CGD-O2D-CED
16	A	836	CLA	CBD-CGD-O2D-CED
16	A	838	CLA	CBD-CGD-O2D-CED
16	B	801	CLA	CBD-CGD-O2D-CED
16	B	805	CLA	CBD-CGD-O2D-CED
16	B	813	CLA	CBD-CGD-O2D-CED
16	B	823	CLA	CBD-CGD-O2D-CED
16	B	828	CLA	CBD-CGD-O2D-CED
16	B	833	CLA	CBD-CGD-O2D-CED
16	K	203	CLA	CBD-CGD-O2D-CED
16	A	806	CLA	O1A-CGA-O2A-C1
16	B	808	CLA	O1A-CGA-O2A-C1
16	A	832	CLA	O1D-CGD-O2D-CED
16	A	840	CLA	O1D-CGD-O2D-CED
16	B	816	CLA	O1D-CGD-O2D-CED
16	B	818	CLA	O1D-CGD-O2D-CED
16	B	839	CLA	O1D-CGD-O2D-CED
16	A	833	CLA	CBD-CGD-O2D-CED
16	A	827	CLA	O1D-CGD-O2D-CED
16	9	611	CLA	O1D-CGD-O2D-CED
16	A	834	CLA	C3-C5-C6-C7
16	A	837	CLA	C3-C5-C6-C7
16	A	839	CLA	C3-C5-C6-C7
16	B	802	CLA	C3-C5-C6-C7
16	B	829	CLA	C3-C5-C6-C7
16	A	806	CLA	CBA-CGA-O2A-C1
16	B	808	CLA	CBA-CGA-O2A-C1
16	B	830	CLA	O1D-CGD-O2D-CED
16	2	601	CLA	CBD-CGD-O2D-CED
16	A	804	CLA	CBD-CGD-O2D-CED
16	A	829	CLA	CBD-CGD-O2D-CED
16	A	835	CLA	CBD-CGD-O2D-CED
16	B	831	CLA	CBD-CGD-O2D-CED
16	A	824	CLA	CBD-CGD-O2D-CED
16	B	811	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	A	841	CLA	C2A-CAA-CBA-CGA
16	B	812	CLA	C2A-CAA-CBA-CGA
16	B	828	CLA	C2A-CAA-CBA-CGA
16	B	839	CLA	C2A-CAA-CBA-CGA
16	L	303	CLA	C2A-CAA-CBA-CGA
16	B	810	CLA	O1D-CGD-O2D-CED
16	A	801	CLA	C3-C5-C6-C7
16	A	841	CLA	C3-C5-C6-C7
16	B	808	CLA	C3-C5-C6-C7
16	L	303	CLA	C3-C5-C6-C7
16	A	818	CLA	CBA-CGA-O2A-C1
16	A	837	CLA	CBA-CGA-O2A-C1
16	B	806	CLA	CBA-CGA-O2A-C1
16	B	807	CLA	CBA-CGA-O2A-C1
16	B	830	CLA	CBA-CGA-O2A-C1
16	2	611	CLA	O1D-CGD-O2D-CED
16	9	612	CLA	O1D-CGD-O2D-CED
16	A	813	CLA	O1D-CGD-O2D-CED
16	A	828	CLA	O1D-CGD-O2D-CED
16	B	821	CLA	O1D-CGD-O2D-CED
16	B	826	CLA	O1D-CGD-O2D-CED
16	B	836	CLA	O1D-CGD-O2D-CED
16	B	834	CLA	CBD-CGD-O2D-CED
16	9	608	CLA	O1D-CGD-O2D-CED
16	A	831	CLA	O1D-CGD-O2D-CED
16	B	824	CLA	O1D-CGD-O2D-CED
16	A	832	CLA	O1A-CGA-O2A-C1
16	A	837	CLA	O1A-CGA-O2A-C1
16	B	807	CLA	O1A-CGA-O2A-C1
20	A	850	BCR	C9-C10-C11-C12
16	2	613	CLA	CBD-CGD-O2D-CED
16	9	606	CLA	CBD-CGD-O2D-CED
16	A	805	CLA	CBD-CGD-O2D-CED
16	A	825	CLA	CBD-CGD-O2D-CED
16	A	837	CLA	CBD-CGD-O2D-CED
16	F	802	CLA	CBD-CGD-O2D-CED
17	9	605	CHL	CBD-CGD-O2D-CED
16	B	810	CLA	C3-C5-C6-C7
16	A	832	CLA	CBA-CGA-O2A-C1
16	K	205	CLA	O1D-CGD-O2D-CED
16	A	819	CLA	CBA-CGA-O2A-C1
16	L	303	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	B	828	CLA	C3-C5-C6-C7
16	A	811	CLA	CBA-CGA-O2A-C1
16	B	818	CLA	CBA-CGA-O2A-C1
16	A	803	CLA	O1D-CGD-O2D-CED
16	B	806	CLA	O1A-CGA-O2A-C1
16	B	830	CLA	O1A-CGA-O2A-C1
16	2	608	CLA	CBD-CGD-O2D-CED
16	A	801	CLA	C2A-CAA-CBA-CGA
16	A	802	CLA	C2A-CAA-CBA-CGA
16	A	808	CLA	C2A-CAA-CBA-CGA
16	A	817	CLA	C2A-CAA-CBA-CGA
16	G	201	CLA	C2A-CAA-CBA-CGA
16	A	818	CLA	O1A-CGA-O2A-C1
16	K	204	CLA	O1D-CGD-O2D-CED
16	B	834	CLA	CBA-CGA-O2A-C1
16	B	823	CLA	O1D-CGD-O2D-CED
16	K	203	CLA	O1D-CGD-O2D-CED
16	B	818	CLA	O1A-CGA-O2A-C1
16	9	602	CLA	O1D-CGD-O2D-CED
16	A	811	CLA	O1A-CGA-O2A-C1
16	B	809	CLA	C3-C5-C6-C7
16	A	817	CLA	O1D-CGD-O2D-CED
16	A	827	CLA	CBA-CGA-O2A-C1
16	B	828	CLA	CBA-CGA-O2A-C1
16	K	203	CLA	CBA-CGA-O2A-C1
16	L	303	CLA	CBA-CGA-O2A-C1
16	K	203	CLA	O1A-CGA-O2A-C1
16	9	607	CLA	O1D-CGD-O2D-CED
16	A	809	CLA	O1D-CGD-O2D-CED
16	A	820	CLA	O1D-CGD-O2D-CED
16	A	838	CLA	O1D-CGD-O2D-CED
16	B	801	CLA	O1D-CGD-O2D-CED
16	B	813	CLA	O1D-CGD-O2D-CED
16	B	833	CLA	O1D-CGD-O2D-CED
16	B	802	CLA	C2A-CAA-CBA-CGA
16	B	830	CLA	C2A-CAA-CBA-CGA
20	J	101	BCR	C11-C12-C13-C35
16	L	303	CLA	O1A-CGA-O2A-C1
16	A	832	CLA	C5-C6-C7-C8
16	B	832	CLA	C2A-CAA-CBA-CGA
16	A	803	CLA	CBA-CGA-O2A-C1
16	B	814	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	A	828	CLA	C8-C10-C11-C12
16	B	814	CLA	C8-C10-C11-C12
16	A	829	CLA	C8-C10-C11-C12
16	B	803	CLA	C8-C10-C11-C12
16	B	806	CLA	C15-C16-C17-C18
16	B	837	CLA	C5-C6-C7-C8
16	9	603	CLA	CBD-CGD-O2D-CED
16	B	820	CLA	CBD-CGD-O2D-CED
16	A	823	CLA	O1D-CGD-O2D-CED
16	B	804	CLA	C5-C6-C7-C8
16	B	825	CLA	O2A-C1-C2-C3
16	A	819	CLA	O1A-CGA-O2A-C1
16	B	827	CLA	C5-C6-C7-C8
16	A	802	CLA	C11-C10-C8-C7
16	A	823	CLA	C6-C7-C8-C10
16	A	829	CLA	C11-C10-C8-C7
16	B	803	CLA	C12-C13-C15-C16
16	B	811	CLA	C3-C5-C6-C7
16	A	827	CLA	O1A-CGA-O2A-C1
20	A	850	BCR	C13-C14-C15-C16
20	A	850	BCR	C15-C16-C17-C18
16	2	602	CLA	C2A-CAA-CBA-CGA
16	B	834	CLA	C2A-CAA-CBA-CGA
16	A	833	CLA	O1D-CGD-O2D-CED
16	A	836	CLA	O1D-CGD-O2D-CED
16	B	805	CLA	O1D-CGD-O2D-CED
16	B	828	CLA	O1D-CGD-O2D-CED
16	B	828	CLA	O1A-CGA-O2A-C1
16	A	816	CLA	C3-C5-C6-C7
16	B	818	CLA	C3-C5-C6-C7
16	A	828	CLA	CBA-CGA-O2A-C1
16	B	814	CLA	O1A-CGA-O2A-C1
16	B	834	CLA	O1A-CGA-O2A-C1
16	A	811	CLA	C5-C6-C7-C8
16	A	841	CLA	C15-C16-C17-C18
16	A	829	CLA	O1D-CGD-O2D-CED
16	A	835	CLA	O1D-CGD-O2D-CED
16	B	829	CLA	CBD-CGD-O2D-CED
16	A	803	CLA	O1A-CGA-O2A-C1
16	B	804	CLA	C13-C15-C16-C17
19	A	845	LHG	C4-O6-P-O3
16	A	820	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	2	601	CLA	O1D-CGD-O2D-CED
16	A	804	CLA	O1D-CGD-O2D-CED
16	B	831	CLA	O1D-CGD-O2D-CED
16	A	820	CLA	C4-C3-C5-C6
16	B	802	CLA	C4-C3-C5-C6
16	B	828	CLA	C8-C10-C11-C12
16	L	303	CLA	C10-C11-C12-C13
16	A	806	CLA	C2A-CAA-CBA-CGA
16	A	819	CLA	C2A-CAA-CBA-CGA
16	A	839	CLA	C2A-CAA-CBA-CGA
16	B	807	CLA	C2A-CAA-CBA-CGA
16	B	815	CLA	C2A-CAA-CBA-CGA
16	B	829	CLA	C2A-CAA-CBA-CGA
16	A	810	CLA	C14-C13-C15-C16
16	A	839	CLA	CBA-CGA-O2A-C1
16	B	809	CLA	CBA-CGA-O2A-C1
20	B	842	BCR	C15-C16-C17-C18
16	A	824	CLA	O1D-CGD-O2D-CED
16	B	817	CLA	C2A-CAA-CBA-CGA
16	B	811	CLA	O1D-CGD-O2D-CED
16	B	817	CLA	C6-C7-C8-C10
16	K	203	CLA	C6-C7-C8-C10
16	A	836	CLA	CBA-CGA-O2A-C1
16	B	836	CLA	CBA-CGA-O2A-C1
16	A	824	CLA	C10-C11-C12-C13
16	B	834	CLA	O1D-CGD-O2D-CED
16	B	801	CLA	C3-C5-C6-C7
16	A	805	CLA	O1D-CGD-O2D-CED
16	B	830	CLA	C5-C6-C7-C8
16	A	820	CLA	O1A-CGA-O2A-C1
16	B	840	CLA	C16-C17-C18-C19
16	A	839	CLA	C4-C3-C5-C6
16	B	818	CLA	C10-C11-C12-C13
16	A	820	CLA	C2-C3-C5-C6
16	A	839	CLA	C2-C3-C5-C6
16	A	825	CLA	O1D-CGD-O2D-CED
16	B	809	CLA	C15-C16-C17-C18
16	A	823	CLA	C2A-CAA-CBA-CGA
16	A	828	CLA	O1A-CGA-O2A-C1
16	2	605	CLA	C4B-C3B-CAB-CBB
16	2	610	CLA	C4B-C3B-CAB-CBB
16	2	611	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
16	2	612	CLA	C4B-C3B-CAB-CBB
16	2	613	CLA	C4B-C3B-CAB-CBB
16	9	604	CLA	C4B-C3B-CAB-CBB
16	9	607	CLA	C4B-C3B-CAB-CBB
16	A	807	CLA	C4B-C3B-CAB-CBB
16	A	810	CLA	C4B-C3B-CAB-CBB
16	A	812	CLA	C4B-C3B-CAB-CBB
16	A	815	CLA	C4B-C3B-CAB-CBB
16	A	820	CLA	C4B-C3B-CAB-CBB
16	A	821	CLA	C4B-C3B-CAB-CBB
16	A	825	CLA	C4B-C3B-CAB-CBB
16	A	826	CLA	C4B-C3B-CAB-CBB
16	A	830	CLA	C4B-C3B-CAB-CBB
16	A	831	CLA	C4B-C3B-CAB-CBB
16	A	840	CLA	C4B-C3B-CAB-CBB
16	A	843	CLA	C4B-C3B-CAB-CBB
16	B	803	CLA	C4B-C3B-CAB-CBB
16	B	810	CLA	C4B-C3B-CAB-CBB
16	B	816	CLA	C4B-C3B-CAB-CBB
16	B	818	CLA	C4B-C3B-CAB-CBB
16	B	819	CLA	C4B-C3B-CAB-CBB
16	B	821	CLA	C4B-C3B-CAB-CBB
16	B	822	CLA	C4B-C3B-CAB-CBB
16	B	827	CLA	C4B-C3B-CAB-CBB
16	B	832	CLA	C4B-C3B-CAB-CBB
16	B	833	CLA	C4B-C3B-CAB-CBB
16	B	837	CLA	C4B-C3B-CAB-CBB
16	B	838	CLA	C4B-C3B-CAB-CBB
16	K	205	CLA	C4B-C3B-CAB-CBB
16	L	304	CLA	C4B-C3B-CAB-CBB
16	A	810	CLA	C12-C13-C15-C16
16	B	815	CLA	C6-C7-C8-C9
16	B	817	CLA	C6-C7-C8-C9
16	2	613	CLA	O1D-CGD-O2D-CED
17	9	605	CHL	O1D-CGD-O2D-CED
19	A	844	LHG	C16-C17-C18-C19
16	B	815	CLA	CBA-CGA-O2A-C1
16	9	606	CLA	O1D-CGD-O2D-CED
16	A	837	CLA	O1D-CGD-O2D-CED
16	F	802	CLA	O1D-CGD-O2D-CED
16	A	801	CLA	C3A-C2A-CAA-CBA
16	A	806	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
16	A	824	CLA	C3A-C2A-CAA-CBA
16	A	831	CLA	C3A-C2A-CAA-CBA
16	A	832	CLA	C3A-C2A-CAA-CBA
16	A	836	CLA	C3A-C2A-CAA-CBA
16	A	838	CLA	C3A-C2A-CAA-CBA
16	B	804	CLA	C3A-C2A-CAA-CBA
16	B	808	CLA	C3A-C2A-CAA-CBA
16	B	810	CLA	C3A-C2A-CAA-CBA
16	B	827	CLA	C3A-C2A-CAA-CBA
16	B	831	CLA	C3A-C2A-CAA-CBA
16	B	836	CLA	C3A-C2A-CAA-CBA
16	B	840	CLA	C3A-C2A-CAA-CBA
16	B	811	CLA	C4-C3-C5-C6
16	B	815	CLA	C4-C3-C5-C6
16	A	817	CLA	CBA-CGA-O2A-C1
16	B	811	CLA	C2-C3-C5-C6
16	B	815	CLA	C2-C3-C5-C6
16	2	602	CLA	CBA-CGA-O2A-C1
16	B	809	CLA	O1A-CGA-O2A-C1
16	B	840	CLA	C16-C17-C18-C20
16	K	203	CLA	C6-C7-C8-C9
16	2	605	CLA	C2B-C3B-CAB-CBB
16	2	611	CLA	C2B-C3B-CAB-CBB
16	2	612	CLA	C2B-C3B-CAB-CBB
16	2	613	CLA	C2B-C3B-CAB-CBB
16	9	602	CLA	C2B-C3B-CAB-CBB
16	9	603	CLA	C2B-C3B-CAB-CBB
16	9	604	CLA	C2B-C3B-CAB-CBB
16	9	607	CLA	C2B-C3B-CAB-CBB
16	9	609	CLA	C2B-C3B-CAB-CBB
16	9	610	CLA	C2B-C3B-CAB-CBB
16	A	807	CLA	C2B-C3B-CAB-CBB
16	A	810	CLA	C2B-C3B-CAB-CBB
16	A	811	CLA	C2B-C3B-CAB-CBB
16	A	812	CLA	C2B-C3B-CAB-CBB
16	A	815	CLA	C2B-C3B-CAB-CBB
16	A	820	CLA	C2B-C3B-CAB-CBB
16	A	821	CLA	C2B-C3B-CAB-CBB
16	A	826	CLA	C2B-C3B-CAB-CBB
16	A	830	CLA	C2B-C3B-CAB-CBB
16	A	831	CLA	C2B-C3B-CAB-CBB
16	A	840	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
16	A	841	CLA	C2B-C3B-CAB-CBB
16	A	852	CLA	C2B-C3B-CAB-CBB
16	B	801	CLA	C2B-C3B-CAB-CBB
16	B	803	CLA	C2B-C3B-CAB-CBB
16	B	810	CLA	C2B-C3B-CAB-CBB
16	B	816	CLA	C2B-C3B-CAB-CBB
16	B	821	CLA	C2B-C3B-CAB-CBB
16	B	822	CLA	C2B-C3B-CAB-CBB
16	B	823	CLA	C2B-C3B-CAB-CBB
16	B	827	CLA	C2B-C3B-CAB-CBB
16	B	832	CLA	C2B-C3B-CAB-CBB
16	B	833	CLA	C2B-C3B-CAB-CBB
16	B	834	CLA	C2B-C3B-CAB-CBB
16	B	835	CLA	C2B-C3B-CAB-CBB
16	B	837	CLA	C2B-C3B-CAB-CBB
16	B	838	CLA	C2B-C3B-CAB-CBB
16	F	802	CLA	C2B-C3B-CAB-CBB
16	K	205	CLA	C2B-C3B-CAB-CBB
16	F	802	CLA	CBA-CGA-O2A-C1
16	A	839	CLA	O1A-CGA-O2A-C1
22	B	846	DGD	C1A-C2A-C3A-C4A
16	A	823	CLA	C5-C6-C7-C8
16	A	818	CLA	C5-C6-C7-C8
16	A	836	CLA	O1A-CGA-O2A-C1
16	B	836	CLA	O1A-CGA-O2A-C1
16	A	826	CLA	C3-C5-C6-C7
20	A	849	BCR	C5-C6-C7-C8
20	A	850	BCR	C23-C24-C25-C26
20	A	850	BCR	C23-C24-C25-C30
20	F	801	BCR	C1-C6-C7-C8
20	F	801	BCR	C5-C6-C7-C8
20	L	305	BCR	C1-C6-C7-C8
20	M	101	BCR	C23-C24-C25-C26
20	M	101	BCR	C23-C24-C25-C30
16	A	816	CLA	CBA-CGA-O2A-C1
16	A	834	CLA	CBA-CGA-O2A-C1
16	B	838	CLA	CBA-CGA-O2A-C1
16	B	821	CLA	O2A-C1-C2-C3
16	B	814	CLA	C10-C11-C12-C13
16	A	817	CLA	O1A-CGA-O2A-C1
16	B	815	CLA	O1A-CGA-O2A-C1
16	B	809	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
16	B	813	CLA	C2A-CAA-CBA-CGA
16	L	303	CLA	O1D-CGD-O2D-CED
16	9	603	CLA	CBA-CGA-O2A-C1
16	2	608	CLA	O1D-CGD-O2D-CED
16	F	802	CLA	O1A-CGA-O2A-C1
16	A	816	CLA	O1A-CGA-O2A-C1
16	B	838	CLA	O1A-CGA-O2A-C1
16	A	832	CLA	C16-C17-C18-C20
16	B	802	CLA	C2-C3-C5-C6
16	A	802	CLA	C11-C10-C8-C9
16	A	818	CLA	C6-C7-C8-C9
16	A	823	CLA	C6-C7-C8-C9
16	A	829	CLA	C11-C10-C8-C9
16	B	803	CLA	C14-C13-C15-C16
16	A	829	CLA	C3-C5-C6-C7
16	9	603	CLA	C2A-CAA-CBA-CGA
16	A	827	CLA	C2A-CAA-CBA-CGA
20	L	305	BCR	C11-C12-C13-C35
20	L	305	BCR	C7-C8-C9-C10
16	A	834	CLA	O1A-CGA-O2A-C1
16	9	604	CLA	C1A-C2A-CAA-CBA
16	9	607	CLA	C1A-C2A-CAA-CBA
16	A	804	CLA	C1A-C2A-CAA-CBA
16	A	806	CLA	C1A-C2A-CAA-CBA
16	A	811	CLA	C1A-C2A-CAA-CBA
16	A	824	CLA	C1A-C2A-CAA-CBA
16	A	829	CLA	C1A-C2A-CAA-CBA
16	A	830	CLA	C1A-C2A-CAA-CBA
16	A	831	CLA	C1A-C2A-CAA-CBA
16	A	832	CLA	C1A-C2A-CAA-CBA
16	A	836	CLA	C1A-C2A-CAA-CBA
16	B	817	CLA	C1A-C2A-CAA-CBA
16	B	819	CLA	C1A-C2A-CAA-CBA
16	B	824	CLA	C1A-C2A-CAA-CBA
16	B	827	CLA	C1A-C2A-CAA-CBA
16	B	830	CLA	C1A-C2A-CAA-CBA
16	B	831	CLA	C1A-C2A-CAA-CBA
16	B	834	CLA	C1A-C2A-CAA-CBA
16	A	816	CLA	C11-C12-C13-C15
16	B	815	CLA	C6-C7-C8-C10
16	B	828	CLA	C10-C11-C12-C13
16	B	829	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
16	B	839	CLA	C15-C16-C17-C18
22	B	846	DGD	O6E-C5E-C6E-O5E
16	2	604	CLA	C3A-C2A-CAA-CBA
16	2	610	CLA	C3A-C2A-CAA-CBA
16	F	803	CLA	C3A-C2A-CAA-CBA
19	A	845	LHG	C11-C12-C13-C14
16	B	809	CLA	C5-C6-C7-C8
16	B	803	CLA	C2A-CAA-CBA-CGA
16	B	828	CLA	C11-C12-C13-C14
16	A	808	CLA	CBA-CGA-O2A-C1
19	A	845	LHG	C16-C17-C18-C19
16	B	820	CLA	O1D-CGD-O2D-CED
16	A	832	CLA	C16-C17-C18-C19
16	9	602	CLA	CBA-CGA-O2A-C1
16	B	812	CLA	CBA-CGA-O2A-C1
16	B	821	CLA	CBA-CGA-O2A-C1
16	B	811	CLA	C8-C10-C11-C12
16	A	830	CLA	C2A-CAA-CBA-CGA
16	A	837	CLA	C2A-CAA-CBA-CGA
16	B	804	CLA	C3-C5-C6-C7
16	9	603	CLA	O1D-CGD-O2D-CED
16	B	839	CLA	CBA-CGA-O2A-C1
16	A	816	CLA	C11-C12-C13-C14
16	L	303	CLA	C11-C12-C13-C14
16	B	829	CLA	C8-C10-C11-C12
16	B	829	CLA	O1D-CGD-O2D-CED
16	9	603	CLA	O1A-CGA-O2A-C1
16	A	828	CLA	C4-C3-C5-C6
16	B	830	CLA	C4-C3-C5-C6
16	A	828	CLA	C10-C11-C12-C13
16	A	801	CLA	C11-C12-C13-C15
16	A	805	CLA	C11-C10-C8-C7
16	A	811	CLA	C6-C7-C8-C10
16	A	818	CLA	C6-C7-C8-C10
16	A	818	CLA	C11-C10-C8-C7
16	A	828	CLA	C12-C13-C15-C16
16	B	803	CLA	C11-C10-C8-C7
16	B	807	CLA	C12-C13-C15-C16
16	B	809	CLA	C11-C10-C8-C7
16	B	811	CLA	C6-C7-C8-C10
16	B	818	CLA	C11-C10-C8-C7
16	B	827	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
16	B	839	CLA	C6-C7-C8-C10
16	B	840	CLA	C12-C13-C15-C16
16	A	801	CLA	C11-C12-C13-C14
16	A	805	CLA	C11-C10-C8-C9
16	A	828	CLA	C14-C13-C15-C16
16	B	801	CLA	C11-C10-C8-C9
16	B	803	CLA	C6-C7-C8-C9
16	B	803	CLA	C11-C10-C8-C9
16	B	807	CLA	C14-C13-C15-C16
16	B	809	CLA	C11-C10-C8-C9
16	B	811	CLA	C6-C7-C8-C9
16	B	811	CLA	C11-C10-C8-C9
16	B	827	CLA	C11-C10-C8-C9
16	B	827	CLA	C14-C13-C15-C16
16	B	839	CLA	C6-C7-C8-C9
16	B	840	CLA	C14-C13-C15-C16
16	B	833	CLA	CBA-CGA-O2A-C1
16	A	808	CLA	O1A-CGA-O2A-C1
20	A	850	BCR	C11-C12-C13-C35
20	B	845	BCR	C37-C22-C23-C24
20	A	846	BCR	C7-C8-C9-C10
20	A	850	BCR	C11-C12-C13-C14
20	B	842	BCR	C7-C8-C9-C10
20	J	101	BCR	C11-C12-C13-C14
16	2	606	CLA	C4B-C3B-CAB-CBB
16	9	602	CLA	C4B-C3B-CAB-CBB
16	9	603	CLA	C4B-C3B-CAB-CBB
16	9	606	CLA	C4B-C3B-CAB-CBB
16	9	609	CLA	C4B-C3B-CAB-CBB
16	9	610	CLA	C4B-C3B-CAB-CBB
16	A	805	CLA	C4B-C3B-CAB-CBB
16	A	808	CLA	C4B-C3B-CAB-CBB
16	A	813	CLA	C4B-C3B-CAB-CBB
16	A	814	CLA	C4B-C3B-CAB-CBB
16	A	816	CLA	C4B-C3B-CAB-CBB
16	A	819	CLA	C4B-C3B-CAB-CBB
16	B	801	CLA	C4B-C3B-CAB-CBB
16	B	824	CLA	C4B-C3B-CAB-CBB
16	B	825	CLA	C4B-C3B-CAB-CBB
16	B	828	CLA	C4B-C3B-CAB-CBB
16	B	835	CLA	C4B-C3B-CAB-CBB
16	B	839	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
16	K	203	CLA	C4B-C3B-CAB-CBB
16	K	204	CLA	C4B-C3B-CAB-CBB
16	L	302	CLA	C4B-C3B-CAB-CBB
16	A	832	CLA	C13-C15-C16-C17
16	B	838	CLA	C2-C1-O2A-CGA
16	A	816	CLA	C4-C3-C5-C6
16	B	803	CLA	C4-C3-C5-C6
16	A	828	CLA	C2-C3-C5-C6
16	B	803	CLA	C2-C3-C5-C6
16	B	830	CLA	C2-C3-C5-C6
16	G	201	CLA	CBA-CGA-O2A-C1
16	A	852	CLA	CBD-CGD-O2D-CED
16	A	828	CLA	C3A-C2A-CAA-CBA
16	A	834	CLA	C3A-C2A-CAA-CBA
16	B	835	CLA	C3A-C2A-CAA-CBA
16	A	841	CLA	C16-C17-C18-C19
16	9	602	CLA	O1A-CGA-O2A-C1
16	B	812	CLA	O1A-CGA-O2A-C1
17	9	601	CHL	C3C-C2C-CMC-OMC
16	B	807	CLA	C3-C5-C6-C7
16	B	821	CLA	O1A-CGA-O2A-C1
16	L	303	CLA	C11-C12-C13-C15
16	B	807	CLA	C15-C16-C17-C18
16	B	840	CLA	CAA-CBA-CGA-O2A
16	2	606	CLA	C2B-C3B-CAB-CBB
16	2	610	CLA	C2B-C3B-CAB-CBB
16	9	606	CLA	C2B-C3B-CAB-CBB
16	A	808	CLA	C2B-C3B-CAB-CBB
16	A	813	CLA	C2B-C3B-CAB-CBB
16	A	814	CLA	C2B-C3B-CAB-CBB
16	A	816	CLA	C2B-C3B-CAB-CBB
16	A	825	CLA	C2B-C3B-CAB-CBB
16	A	843	CLA	C2B-C3B-CAB-CBB
16	B	818	CLA	C2B-C3B-CAB-CBB
16	B	819	CLA	C2B-C3B-CAB-CBB
16	B	839	CLA	C2B-C3B-CAB-CBB
16	K	203	CLA	C2B-C3B-CAB-CBB
16	K	204	CLA	C2B-C3B-CAB-CBB
16	L	302	CLA	C2B-C3B-CAB-CBB
16	L	304	CLA	C2B-C3B-CAB-CBB
19	A	845	LHG	C12-C13-C14-C15
16	A	841	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
16	B	828	CLA	C11-C12-C13-C15
16	A	818	CLA	C4-C3-C5-C6
16	B	804	CLA	C2-C1-O2A-CGA
16	B	812	CLA	C2-C1-O2A-CGA
16	B	833	CLA	O1A-CGA-O2A-C1
16	A	818	CLA	C11-C12-C13-C14
16	B	808	CLA	C6-C7-C8-C9
16	B	814	CLA	C11-C10-C8-C9
16	B	818	CLA	C11-C10-C8-C9
16	B	839	CLA	C11-C12-C13-C14
16	B	808	CLA	C11-C12-C13-C14
16	B	811	CLA	C5-C6-C7-C8
16	B	839	CLA	O1A-CGA-O2A-C1
16	B	825	CLA	C2A-CAA-CBA-CGA
16	B	819	CLA	C11-C12-C13-C15
20	I	201	BCR	C23-C24-C25-C26
20	L	305	BCR	C23-C24-C25-C26
20	L	305	BCR	C23-C24-C25-C30
16	2	612	CLA	C1A-C2A-CAA-CBA
16	9	611	CLA	C1A-C2A-CAA-CBA
16	K	204	CLA	C1A-C2A-CAA-CBA
16	A	818	CLA	C11-C12-C13-C15
16	A	832	CLA	C12-C13-C15-C16
16	B	801	CLA	C11-C10-C8-C7
16	B	803	CLA	C6-C7-C8-C10
16	B	804	CLA	C11-C12-C13-C15
16	B	808	CLA	C6-C7-C8-C10
16	B	811	CLA	C11-C10-C8-C7
16	B	814	CLA	C11-C10-C8-C7
16	B	827	CLA	C11-C10-C8-C7
18	B	841	PQN	C16-C17-C18-C20
16	K	203	CLA	C5-C6-C7-C8
20	A	849	BCR	C9-C10-C11-C12
20	L	301	BCR	C19-C20-C21-C22
16	A	801	CLA	CBA-CGA-O2A-C1
16	A	810	CLA	C13-C15-C16-C17
16	A	841	CLA	C13-C15-C16-C17
16	B	816	CLA	C2A-CAA-CBA-CGA
16	A	802	CLA	C15-C16-C17-C18
16	A	841	CLA	C11-C10-C8-C7
16	A	838	CLA	CBA-CGA-O2A-C1
16	B	817	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	2	602	CLA	CAD-CBD-CGD-O2D
16	9	604	CLA	CAD-CBD-CGD-O2D
16	A	806	CLA	CAD-CBD-CGD-O2D
16	A	809	CLA	CAD-CBD-CGD-O2D
16	A	817	CLA	CAD-CBD-CGD-O2D
16	A	819	CLA	CAD-CBD-CGD-O2D
16	A	822	CLA	CAD-CBD-CGD-O2D
16	A	823	CLA	CAD-CBD-CGD-O2D
16	A	832	CLA	CAD-CBD-CGD-O2D
16	B	803	CLA	CAD-CBD-CGD-O2D
16	B	818	CLA	CAD-CBD-CGD-O2D
16	B	827	CLA	CAD-CBD-CGD-O2D
16	B	832	CLA	CAD-CBD-CGD-O2D
16	G	201	CLA	CAD-CBD-CGD-O2D
16	K	203	CLA	CAD-CBD-CGD-O2D
16	B	810	CLA	C8-C10-C11-C12
16	A	841	CLA	CBA-CGA-O2A-C1
16	B	829	CLA	CBA-CGA-O2A-C1
16	A	832	CLA	C4-C3-C5-C6
16	A	818	CLA	C2-C3-C5-C6
16	2	601	CLA	CHA-CBD-CGD-O2D
16	2	609	CLA	CHA-CBD-CGD-O1D
16	2	609	CLA	CHA-CBD-CGD-O2D
16	A	803	CLA	CHA-CBD-CGD-O1D
16	A	810	CLA	CHA-CBD-CGD-O1D
16	A	813	CLA	CHA-CBD-CGD-O1D
16	A	813	CLA	CHA-CBD-CGD-O2D
16	A	814	CLA	CHA-CBD-CGD-O2D
16	A	821	CLA	CHA-CBD-CGD-O1D
16	A	821	CLA	CHA-CBD-CGD-O2D
16	A	828	CLA	CHA-CBD-CGD-O1D
16	A	828	CLA	CHA-CBD-CGD-O2D
16	A	830	CLA	CHA-CBD-CGD-O1D
16	A	830	CLA	CHA-CBD-CGD-O2D
16	A	833	CLA	CHA-CBD-CGD-O1D
16	A	833	CLA	CHA-CBD-CGD-O2D
16	B	808	CLA	CHA-CBD-CGD-O1D
16	B	808	CLA	CHA-CBD-CGD-O2D
16	B	820	CLA	CHA-CBD-CGD-O1D
16	B	836	CLA	CHA-CBD-CGD-O1D
16	K	203	CLA	CHA-CBD-CGD-O1D
16	K	204	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
17	9	601	CHL	CHA-CBD-CGD-O1D
17	9	601	CHL	CHA-CBD-CGD-O2D
17	9	605	CHL	CHA-CBD-CGD-O1D
17	9	605	CHL	CHA-CBD-CGD-O2D
20	F	801	BCR	C9-C10-C11-C12
16	G	201	CLA	O1A-CGA-O2A-C1
16	A	832	CLA	C14-C13-C15-C16
16	B	806	CLA	C6-C7-C8-C9
16	A	801	CLA	O1A-CGA-O2A-C1
16	B	804	CLA	C1A-C2A-CAA-CBA
16	B	816	CLA	C1A-C2A-CAA-CBA
16	B	820	CLA	C1A-C2A-CAA-CBA
16	B	822	CLA	CHA-CBD-CGD-O2D
16	B	832	CLA	C1A-C2A-CAA-CBA
16	B	826	CLA	CBA-CGA-O2A-C1
16	B	808	CLA	O1D-CGD-O2D-CED
16	A	838	CLA	O1A-CGA-O2A-C1
16	B	829	CLA	O1A-CGA-O2A-C1
16	2	602	CLA	O1A-CGA-O2A-C1
19	A	845	LHG	C4-O6-P-O5
16	B	803	CLA	C16-C17-C18-C20
16	2	601	CLA	CAD-CBD-CGD-O1D
16	9	603	CLA	C2-C3-C5-C6
16	A	805	CLA	CAD-CBD-CGD-O1D
16	A	813	CLA	CAD-CBD-CGD-O1D
16	A	814	CLA	CAD-CBD-CGD-O1D
16	A	821	CLA	CAD-CBD-CGD-O1D
16	A	830	CLA	CAD-CBD-CGD-O1D
16	B	826	CLA	CAD-CBD-CGD-O1D
16	B	836	CLA	CAD-CBD-CGD-O1D
16	K	204	CLA	CAD-CBD-CGD-O1D
16	A	841	CLA	O1A-CGA-O2A-C1
16	A	801	CLA	C11-C10-C8-C7
16	B	839	CLA	C11-C12-C13-C15
16	L	303	CLA	C6-C7-C8-C10
20	K	202	BCR	C9-C10-C11-C12
16	A	801	CLA	C8-C10-C11-C12
16	B	808	CLA	CBD-CGD-O2D-CED
16	A	828	CLA	C2A-CAA-CBA-CGA
16	B	819	CLA	C11-C12-C13-C14
16	A	843	CLA	CAD-CBD-CGD-O1D
17	9	601	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
16	B	826	CLA	O1A-CGA-O2A-C1
16	B	806	CLA	C4-C3-C5-C6
16	B	809	CLA	C10-C11-C12-C13
16	B	804	CLA	C11-C12-C13-C14
16	B	812	CLA	C3-C5-C6-C7
20	B	842	BCR	C10-C11-C12-C13
16	A	852	CLA	O1D-CGD-O2D-CED
20	F	804	BCR	C37-C22-C23-C24
18	B	841	PQN	C25-C26-C27-C28
20	B	845	BCR	C21-C22-C23-C24
16	2	603	CLA	C2B-C3B-CAB-CBB
16	A	804	CLA	C2B-C3B-CAB-CBB
16	A	818	CLA	C2B-C3B-CAB-CBB
16	A	819	CLA	C2B-C3B-CAB-CBB
16	A	839	CLA	C2B-C3B-CAB-CBB
16	B	806	CLA	C2B-C3B-CAB-CBB
16	B	813	CLA	C2B-C3B-CAB-CBB
16	B	814	CLA	C2B-C3B-CAB-CBB
16	B	815	CLA	C2B-C3B-CAB-CBB
16	B	824	CLA	C2B-C3B-CAB-CBB
16	B	825	CLA	C2B-C3B-CAB-CBB
16	B	828	CLA	C2B-C3B-CAB-CBB
16	A	802	CLA	C10-C11-C12-C13
16	B	801	CLA	C8-C10-C11-C12
16	9	602	CLA	C1-C2-C3-C4
16	9	602	CLA	C2A-CAA-CBA-CGA
16	B	801	CLA	C2A-CAA-CBA-CGA
16	B	827	CLA	C2A-CAA-CBA-CGA
16	A	837	CLA	C2-C1-O2A-CGA
16	B	814	CLA	C2-C1-O2A-CGA
16	A	801	CLA	CAA-CBA-CGA-O2A
16	A	807	CLA	CBD-CGD-O2D-CED
16	9	609	CLA	CMA-C3A-C4A-NA
16	A	805	CLA	O1A-CGA-O2A-C1
20	I	201	BCR	C23-C24-C25-C30
16	B	827	CLA	C16-C17-C18-C19
16	A	805	CLA	CBA-CGA-O2A-C1
19	A	844	LHG	C4-O6-P-O3
19	A	845	LHG	C3-O3-P-O6
16	A	832	CLA	C2-C3-C5-C6
16	A	801	CLA	C11-C10-C8-C9
16	A	811	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
16	A	818	CLA	C11-C10-C8-C9
16	L	303	CLA	C6-C7-C8-C9
18	B	841	PQN	C16-C17-C18-C19
16	A	828	CLA	C15-C16-C17-C18
16	B	803	CLA	C16-C17-C18-C19
22	B	846	DGD	C8B-C9B-CAB-CBB
16	2	602	CLA	CAA-CBA-CGA-O2A
16	B	814	CLA	C5-C6-C7-C8
16	A	816	CLA	C2-C3-C5-C6
16	2	603	CLA	C4B-C3B-CAB-CBB
16	2	604	CLA	C4B-C3B-CAB-CBB
16	A	804	CLA	C4B-C3B-CAB-CBB
16	A	818	CLA	C4B-C3B-CAB-CBB
16	A	837	CLA	C4B-C3B-CAB-CBB
16	A	839	CLA	C4B-C3B-CAB-CBB
16	B	806	CLA	C4B-C3B-CAB-CBB
16	B	813	CLA	C4B-C3B-CAB-CBB
16	B	814	CLA	C4B-C3B-CAB-CBB
16	B	815	CLA	C4B-C3B-CAB-CBB
16	B	803	CLA	CAA-CBA-CGA-O2A
16	A	807	CLA	O1D-CGD-O2D-CED
16	B	802	CLA	C2-C1-O2A-CGA
16	B	837	CLA	C2-C1-O2A-CGA
16	B	839	CLA	C13-C15-C16-C17
16	A	803	CLA	C2A-CAA-CBA-CGA
16	A	816	CLA	C2A-CAA-CBA-CGA
16	B	819	CLA	C2A-CAA-CBA-CGA
16	A	802	CLA	C3A-C2A-CAA-CBA
16	A	803	CLA	C3A-C2A-CAA-CBA
16	A	841	CLA	C3A-C2A-CAA-CBA
16	L	303	CLA	C5-C6-C7-C8
16	A	826	CLA	C14-C13-C15-C16
16	B	804	CLA	C11-C10-C8-C9
20	B	843	BCR	C11-C10-C9-C34
20	B	843	BCR	C20-C21-C22-C37
20	F	804	BCR	C16-C17-C18-C36
20	L	301	BCR	C20-C21-C22-C37
16	B	827	CLA	C16-C17-C18-C20
16	B	840	CLA	C13-C15-C16-C17
16	A	802	CLA	C13-C15-C16-C17
16	A	802	CLA	C1A-C2A-CAA-CBA
16	A	803	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
16	B	838	CLA	C1A-C2A-CAA-CBA
16	A	806	CLA	C12-C13-C15-C16
16	A	829	CLA	C2A-CAA-CBA-CGA
16	B	814	CLA	C2A-CAA-CBA-CGA
16	B	807	CLA	C5-C6-C7-C8
16	A	834	CLA	C5-C6-C7-C8
16	B	804	CLA	C4-C3-C5-C6
16	2	604	CLA	C2B-C3B-CAB-CBB
16	9	608	CLA	C2B-C3B-CAB-CBB
16	A	805	CLA	C2B-C3B-CAB-CBB
16	A	806	CLA	C2B-C3B-CAB-CBB
16	A	829	CLA	C2B-C3B-CAB-CBB
16	B	826	CLA	C2B-C3B-CAB-CBB
16	A	835	CLA	CAA-CBA-CGA-O1A
20	B	843	BCR	C11-C10-C9-C8
20	B	843	BCR	C20-C21-C22-C23
20	F	804	BCR	C16-C17-C18-C19
20	L	301	BCR	C20-C21-C22-C23
20	J	101	BCR	C9-C10-C11-C12
16	A	835	CLA	CAA-CBA-CGA-O2A
16	B	806	CLA	C13-C15-C16-C17
18	B	841	PQN	C14-C13-C15-C16
16	A	829	CLA	C2-C1-O2A-CGA
16	B	807	CLA	C2-C1-O2A-CGA
16	B	811	CLA	C2A-CAA-CBA-CGA
16	B	819	CLA	C10-C11-C12-C13
16	A	809	CLA	C1A-C2A-CAA-CBA
18	B	841	PQN	C15-C16-C17-C18
16	B	806	CLA	C2-C3-C5-C6
16	B	836	CLA	C2A-CAA-CBA-CGA
16	A	817	CLA	CAA-CBA-CGA-O2A
16	B	812	CLA	CAA-CBA-CGA-O2A
16	A	829	CLA	C4B-C3B-CAB-CBB
16	B	826	CLA	C4B-C3B-CAB-CBB
16	B	810	CLA	C4-C3-C5-C6
16	A	832	CLA	C6-C7-C8-C10
16	B	804	CLA	C11-C10-C8-C7
16	B	806	CLA	C6-C7-C8-C10
16	B	828	CLA	C6-C7-C8-C10
16	A	806	CLA	CAA-CBA-CGA-O2A
22	B	846	DGD	C7B-C8B-C9B-CAB
16	B	840	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
16	G	202	CLA	CAA-CBA-CGA-O2A
16	B	807	CLA	CAA-CBA-CGA-O2A
16	A	806	CLA	C14-C13-C15-C16
16	A	823	CLA	O1A-CGA-O2A-C1
16	B	829	CLA	CAA-CBA-CGA-O2A
16	B	816	CLA	CAA-CBA-CGA-O2A
16	2	608	CLA	CAD-CBD-CGD-O2D
16	A	807	CLA	CAD-CBD-CGD-O2D
16	A	820	CLA	CAD-CBD-CGD-O2D
16	A	824	CLA	CAD-CBD-CGD-O2D
16	A	825	CLA	CAD-CBD-CGD-O2D
16	A	829	CLA	CAD-CBD-CGD-O2D
16	A	831	CLA	CAD-CBD-CGD-O2D
16	A	836	CLA	CAD-CBD-CGD-O2D
16	A	838	CLA	CAD-CBD-CGD-O2D
16	A	840	CLA	CAD-CBD-CGD-O2D
16	A	841	CLA	CAD-CBD-CGD-O2D
16	B	801	CLA	CAD-CBD-CGD-O2D
16	B	802	CLA	CAD-CBD-CGD-O2D
16	B	814	CLA	CAD-CBD-CGD-O2D
16	B	815	CLA	CAD-CBD-CGD-O2D
16	B	817	CLA	CAD-CBD-CGD-O2D
16	B	830	CLA	CAD-CBD-CGD-O2D
16	B	834	CLA	CAD-CBD-CGD-O2D
16	B	839	CLA	CAD-CBD-CGD-O2D
16	L	302	CLA	CAD-CBD-CGD-O2D
16	A	825	CLA	CBA-CGA-O2A-C1
22	B	846	DGD	O1B-C1B-O2G-C2G
16	B	814	CLA	C15-C16-C17-C18
16	B	820	CLA	CAA-CBA-CGA-O2A
18	A	842	PQN	C14-C13-C15-C16
16	B	804	CLA	C2-C3-C5-C6
16	B	828	CLA	CAA-CBA-CGA-O2A
20	F	804	BCR	C21-C22-C23-C24
20	L	305	BCR	C11-C12-C13-C14
16	A	828	CLA	CAA-CBA-CGA-O2A
16	B	834	CLA	CAA-CBA-CGA-O2A
16	K	203	CLA	CAA-CBA-CGA-O2A
19	A	844	LHG	O8-C23-C24-C25
16	B	840	CLA	CAA-CBA-CGA-O1A
16	B	820	CLA	CAA-CBA-CGA-O1A
16	9	602	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
16	9	603	CLA	CHA-CBD-CGD-O1D
16	9	603	CLA	CHA-CBD-CGD-O2D
16	A	804	CLA	CHA-CBD-CGD-O2D
16	A	808	CLA	CHA-CBD-CGD-O1D
16	A	808	CLA	CHA-CBD-CGD-O2D
16	A	812	CLA	CHA-CBD-CGD-O1D
16	A	812	CLA	CHA-CBD-CGD-O2D
16	A	815	CLA	CHA-CBD-CGD-O1D
16	A	827	CLA	CHA-CBD-CGD-O1D
16	A	827	CLA	CHA-CBD-CGD-O2D
16	B	805	CLA	CHA-CBD-CGD-O1D
16	B	807	CLA	CHA-CBD-CGD-O2D
16	B	809	CLA	CHA-CBD-CGD-O2D
16	B	820	CLA	CHA-CBD-CGD-O2D
16	B	824	CLA	CHA-CBD-CGD-O2D
16	B	828	CLA	CHA-CBD-CGD-O2D
16	B	833	CLA	CHA-CBD-CGD-O1D
16	B	836	CLA	CHA-CBD-CGD-O2D
16	B	837	CLA	CHA-CBD-CGD-O1D
16	B	837	CLA	CHA-CBD-CGD-O2D
16	G	202	CLA	CHA-CBD-CGD-O1D
16	G	202	CLA	CHA-CBD-CGD-O2D
16	J	102	CLA	CHA-CBD-CGD-O1D
16	J	102	CLA	CHA-CBD-CGD-O2D
16	K	204	CLA	CHA-CBD-CGD-O2D
16	B	816	CLA	CAA-CBA-CGA-O1A
16	G	202	CLA	CAA-CBA-CGA-O1A
16	A	820	CLA	CAA-CBA-CGA-O2A
16	A	823	CLA	CAA-CBA-CGA-O2A
16	B	813	CLA	CAA-CBA-CGA-O2A
16	A	825	CLA	O1A-CGA-O2A-C1
16	B	833	CLA	CAA-CBA-CGA-O2A
16	B	827	CLA	C6-C7-C8-C10
16	B	837	CLA	C6-C7-C8-C10
18	A	842	PQN	C12-C13-C15-C16
16	A	810	CLA	C16-C17-C18-C20
16	B	828	CLA	C6-C7-C8-C9
16	B	837	CLA	C6-C7-C8-C9
18	A	842	PQN	C16-C17-C18-C19
16	A	823	CLA	CBA-CGA-O2A-C1
16	B	821	CLA	CAA-CBA-CGA-O2A
22	B	846	DGD	C2B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
16	A	826	CLA	C1A-C2A-CAA-CBA
16	B	812	CLA	CHA-CBD-CGD-O2D
16	B	815	CLA	C1A-C2A-CAA-CBA
16	A	806	CLA	CAA-CBA-CGA-O1A
16	B	827	CLA	C13-C15-C16-C17
16	B	839	CLA	C5-C6-C7-C8
16	A	801	CLA	C2-C1-O2A-CGA
16	B	807	CLA	CAA-CBA-CGA-O1A
16	B	829	CLA	CAA-CBA-CGA-O1A
19	A	845	LHG	C10-C11-C12-C13
16	A	831	CLA	CAA-CBA-CGA-O2A
16	B	840	CLA	O1A-CGA-O2A-C1
16	B	837	CLA	CAA-CBA-CGA-O2A
16	A	823	CLA	CAA-CBA-CGA-O1A
16	A	809	CLA	C4B-C3B-CAB-CBB
16	A	820	CLA	CAA-CBA-CGA-O1A
16	A	828	CLA	CAA-CBA-CGA-O1A
16	K	203	CLA	CAA-CBA-CGA-O1A
19	A	844	LHG	O10-C23-C24-C25
16	B	810	CLA	C10-C11-C12-C13
16	B	834	CLA	CAA-CBA-CGA-O1A
16	B	808	CLA	CAA-CBA-CGA-O2A
16	B	840	CLA	CBA-CGA-O2A-C1
16	B	821	CLA	C2A-CAA-CBA-CGA
16	A	833	CLA	C5-C6-C7-C8
16	B	823	CLA	CAD-CBD-CGD-O1D
16	B	809	CLA	C8-C10-C11-C12
18	B	841	PQN	C20-C21-C22-C23
16	B	827	CLA	C6-C7-C8-C9
16	B	829	CLA	C11-C10-C8-C9
18	A	842	PQN	C21-C22-C23-C24
16	B	813	CLA	CAA-CBA-CGA-O1A
16	A	805	CLA	CAA-CBA-CGA-O2A
16	B	819	CLA	CAA-CBA-CGA-O2A
16	B	821	CLA	CAA-CBA-CGA-O1A
16	B	833	CLA	CAA-CBA-CGA-O1A
16	A	806	CLA	C15-C16-C17-C18
16	B	837	CLA	C2A-CAA-CBA-CGA
16	B	835	CLA	CAA-CBA-CGA-O2A
16	2	603	CLA	CHA-CBD-CGD-O1D
16	A	826	CLA	C12-C13-C15-C16
16	B	812	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
16	B	822	CLA	CHA-CBD-CGD-O1D
18	A	842	PQN	C16-C17-C18-C20
18	A	842	PQN	C21-C22-C23-C25
18	B	841	PQN	C12-C13-C15-C16
16	9	607	CLA	CAA-CBA-CGA-O2A
16	9	603	CLA	CAA-CBA-CGA-O2A
19	A	845	LHG	O7-C7-C8-C9
16	A	811	CLA	C11-C12-C13-C14
20	J	101	BCR	C17-C18-C19-C20
16	B	819	CLA	CAA-CBA-CGA-O1A
16	A	831	CLA	CAA-CBA-CGA-O1A
16	B	810	CLA	CAA-CBA-CGA-O2A
16	B	814	CLA	CAA-CBA-CGA-O2A
16	A	805	CLA	C8-C10-C11-C12
16	A	805	CLA	CAA-CBA-CGA-O1A
16	A	832	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

108 monomers are involved in 193 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	830	CLA	1	0
16	A	811	CLA	3	0
16	B	806	CLA	7	0
16	B	809	CLA	2	0
16	B	819	CLA	2	0
20	M	101	BCR	5	0
16	B	818	CLA	2	0
16	A	832	CLA	3	0
18	B	841	PQN	2	0
16	B	811	CLA	2	0
20	L	305	BCR	3	0
16	A	843	CLA	1	0
16	B	830	CLA	2	0
16	B	824	CLA	2	0
16	A	826	CLA	2	0
16	2	611	CLA	1	0
16	B	839	CLA	2	0
16	F	803	CLA	1	0
16	A	816	CLA	1	0
16	A	829	CLA	2	0
20	A	850	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	845	BCR	3	0
16	B	821	CLA	2	0
16	A	841	CLA	1	0
16	B	801	CLA	5	0
16	B	817	CLA	1	0
20	F	801	BCR	1	0
16	A	822	CLA	1	0
16	B	813	CLA	2	0
20	K	206	BCR	3	0
16	A	833	CLA	1	0
16	A	801	CLA	3	0
22	B	846	DGD	3	0
16	A	812	CLA	2	0
20	A	848	BCR	3	0
16	A	804	CLA	1	0
16	B	829	CLA	3	0
20	A	849	BCR	5	0
16	A	810	CLA	1	0
16	B	825	CLA	3	0
18	A	842	PQN	1	0
21	A	851	SF4	2	0
16	B	804	CLA	5	0
16	2	613	CLA	1	0
16	B	810	CLA	2	0
16	9	602	CLA	1	0
16	2	601	CLA	1	0
20	F	804	BCR	6	0
16	2	605	CLA	1	0
19	A	844	LHG	2	0
20	A	847	BCR	4	0
16	B	832	CLA	2	0
16	A	806	CLA	2	0
16	B	808	CLA	5	0
20	B	843	BCR	5	0
16	9	611	CLA	1	0
16	A	820	CLA	1	0
16	A	839	CLA	2	0
16	A	825	CLA	2	0
16	2	607	CLA	1	0
16	9	606	CLA	1	0
16	A	817	CLA	1	0
16	A	805	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	834	CLA	1	0
20	B	842	BCR	4	0
16	9	603	CLA	2	0
16	B	826	CLA	2	0
16	B	807	CLA	2	0
16	F	802	CLA	2	0
16	A	831	CLA	3	0
16	A	827	CLA	7	0
16	A	809	CLA	1	0
16	A	828	CLA	1	0
20	I	201	BCR	4	0
16	A	852	CLA	1	0
16	B	828	CLA	3	0
16	A	819	CLA	2	0
16	A	838	CLA	2	0
16	J	102	CLA	1	0
16	L	303	CLA	3	0
16	A	834	CLA	2	0
16	9	608	CLA	1	0
16	B	815	CLA	2	0
16	B	812	CLA	1	0
16	2	602	CLA	1	0
20	K	202	BCR	2	0
16	B	835	CLA	1	0
20	B	844	BCR	1	0
16	A	814	CLA	1	0
17	9	605	CHL	1	0
16	A	837	CLA	1	0
16	A	802	CLA	5	0
16	A	840	CLA	3	0
16	B	802	CLA	5	0
20	A	846	BCR	3	0
16	2	609	CLA	1	0
16	A	803	CLA	1	0
16	B	814	CLA	4	0
16	A	808	CLA	2	0
16	B	827	CLA	2	0
16	A	813	CLA	1	0
16	B	803	CLA	2	0
16	A	821	CLA	1	0
20	L	301	BCR	3	0
16	B	837	CLA	3	0

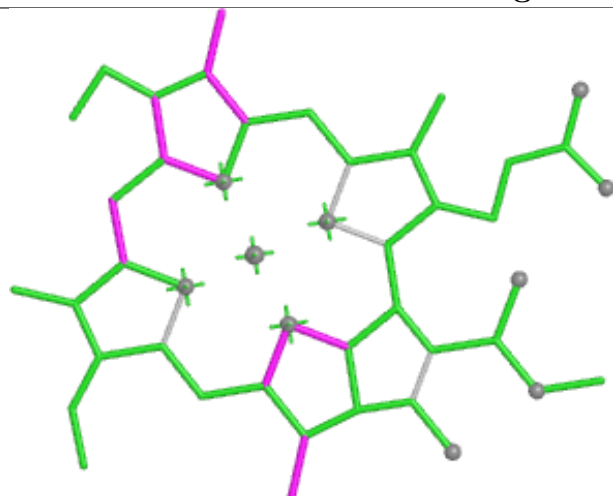
Continued on next page...

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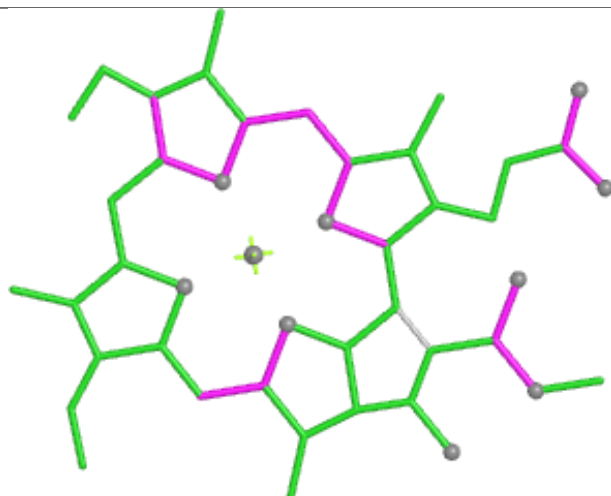
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	818	CLA	5	0
16	B	840	CLA	3	0
20	J	101	BCR	1	0

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

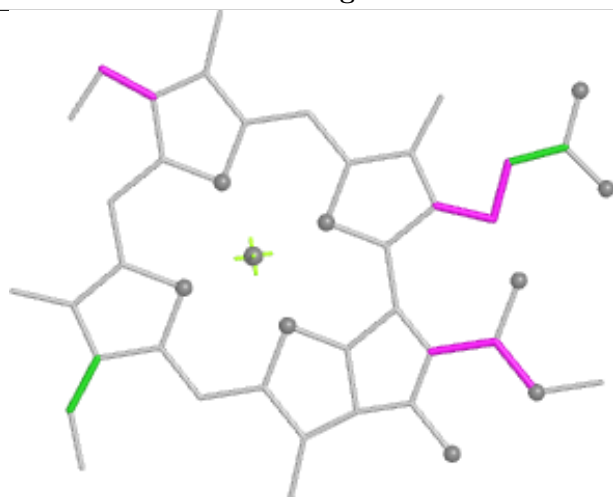
Ligand CLA A 830



Bond lengths



Bond angles

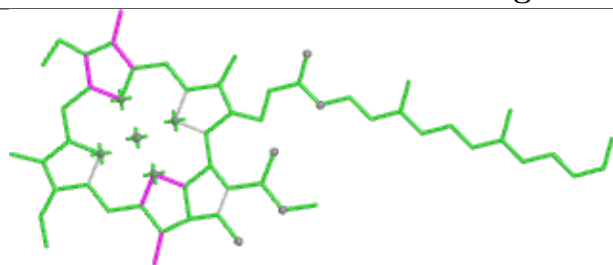


Torsions

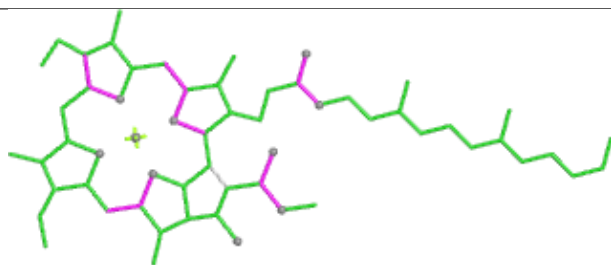


Rings

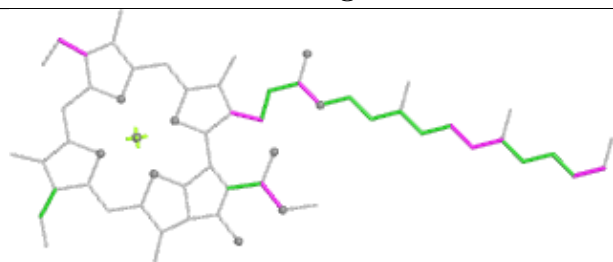
Ligand CLA A 811



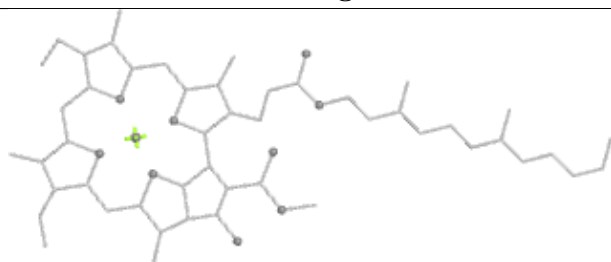
Bond lengths



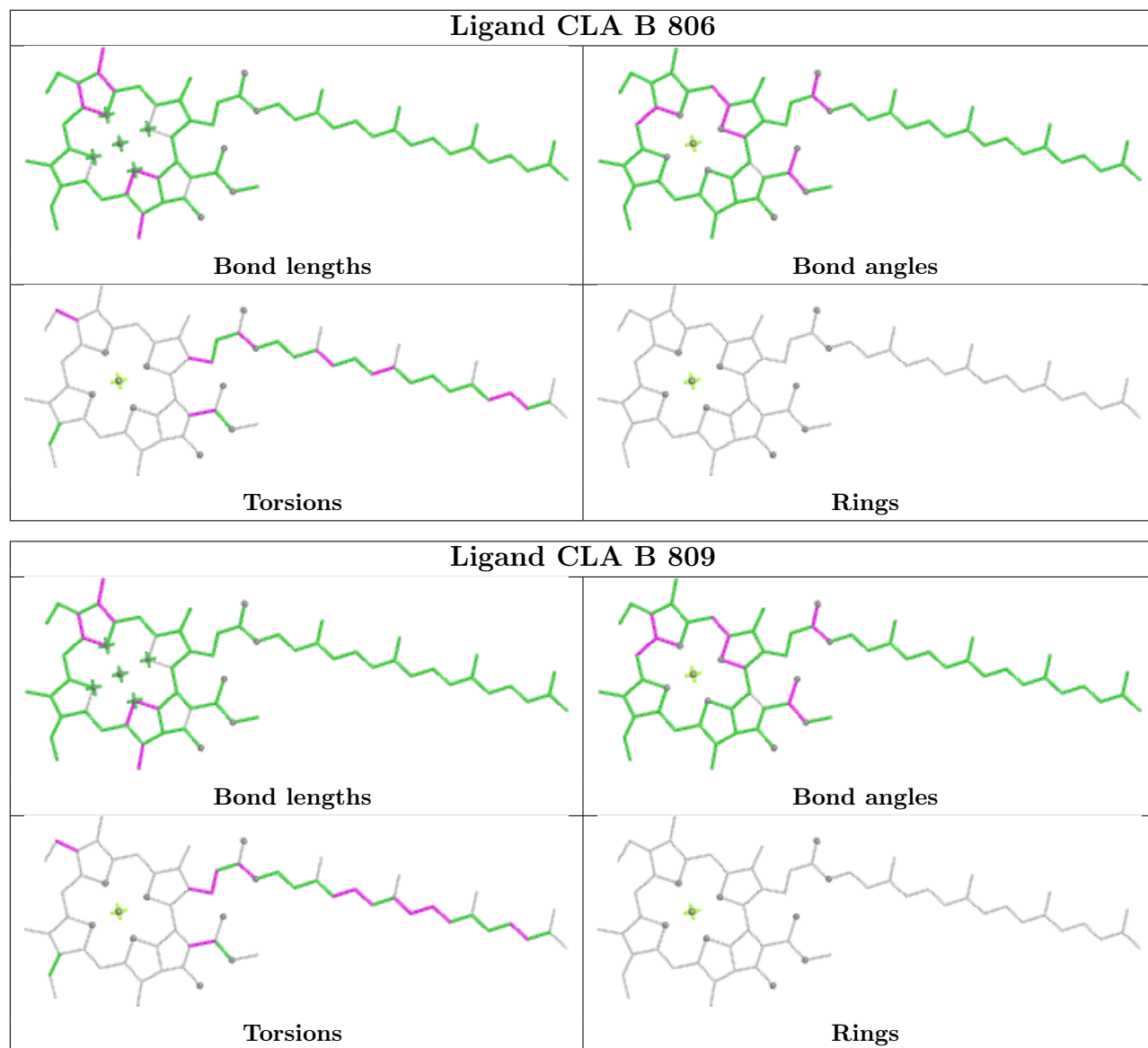
Bond angles

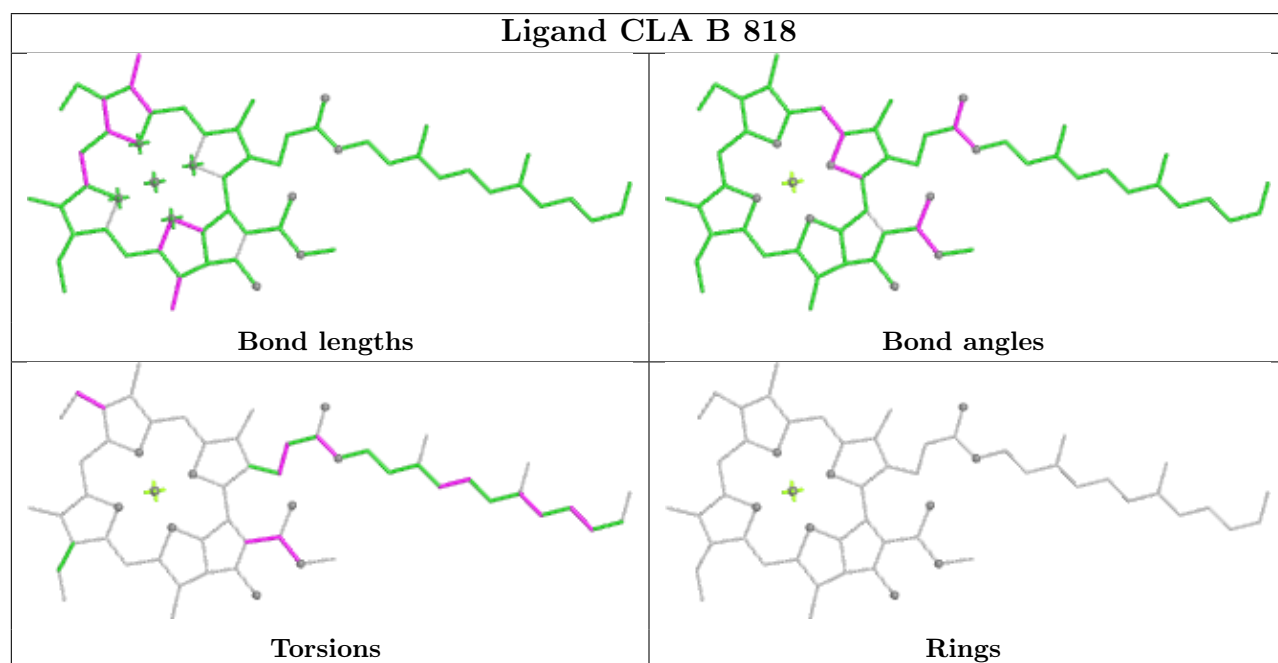
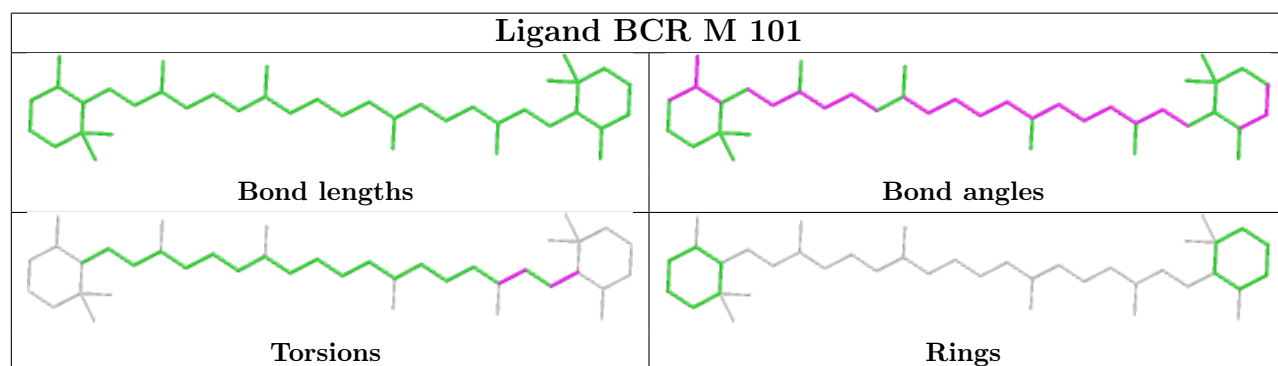
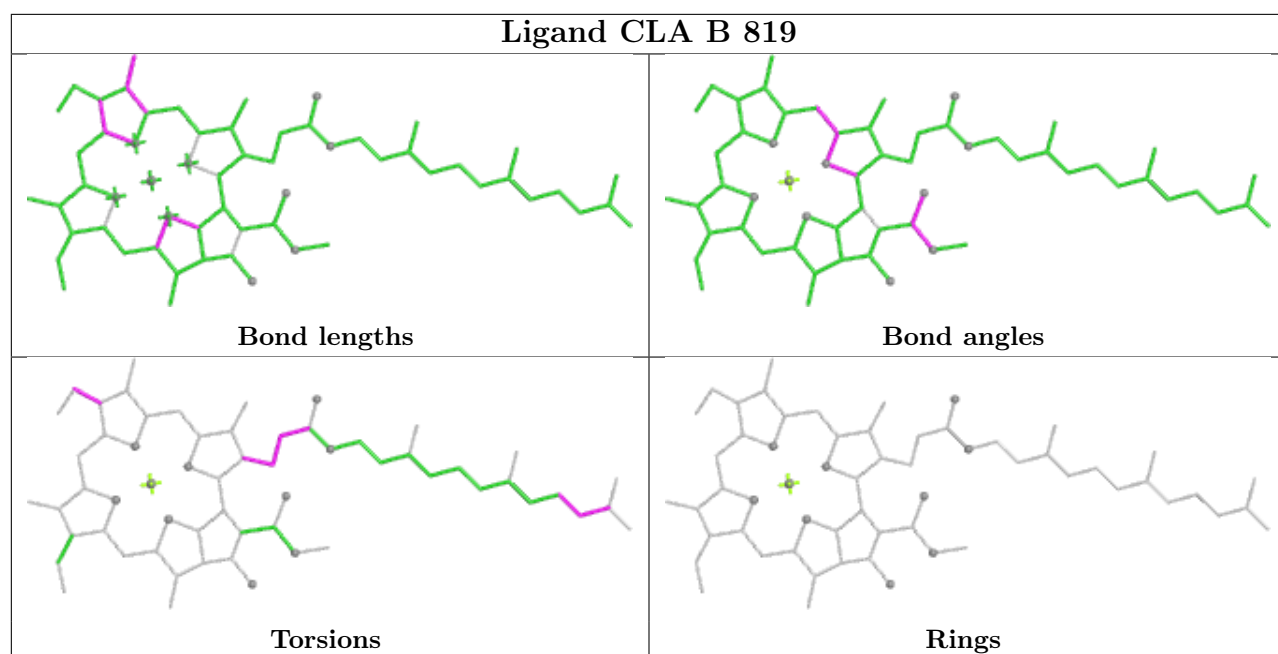


Torsions

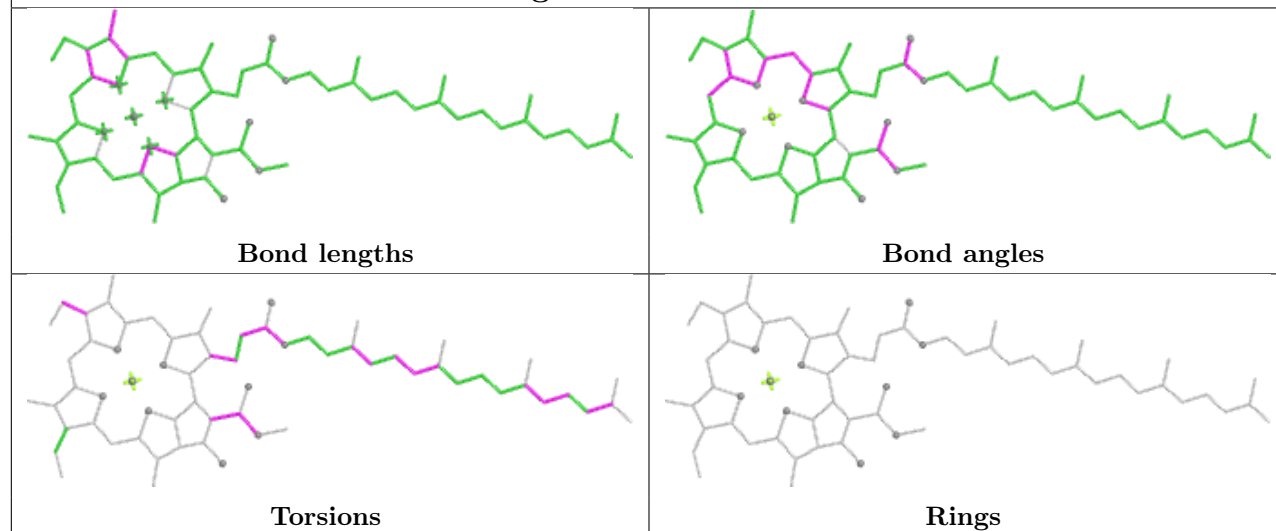


Rings

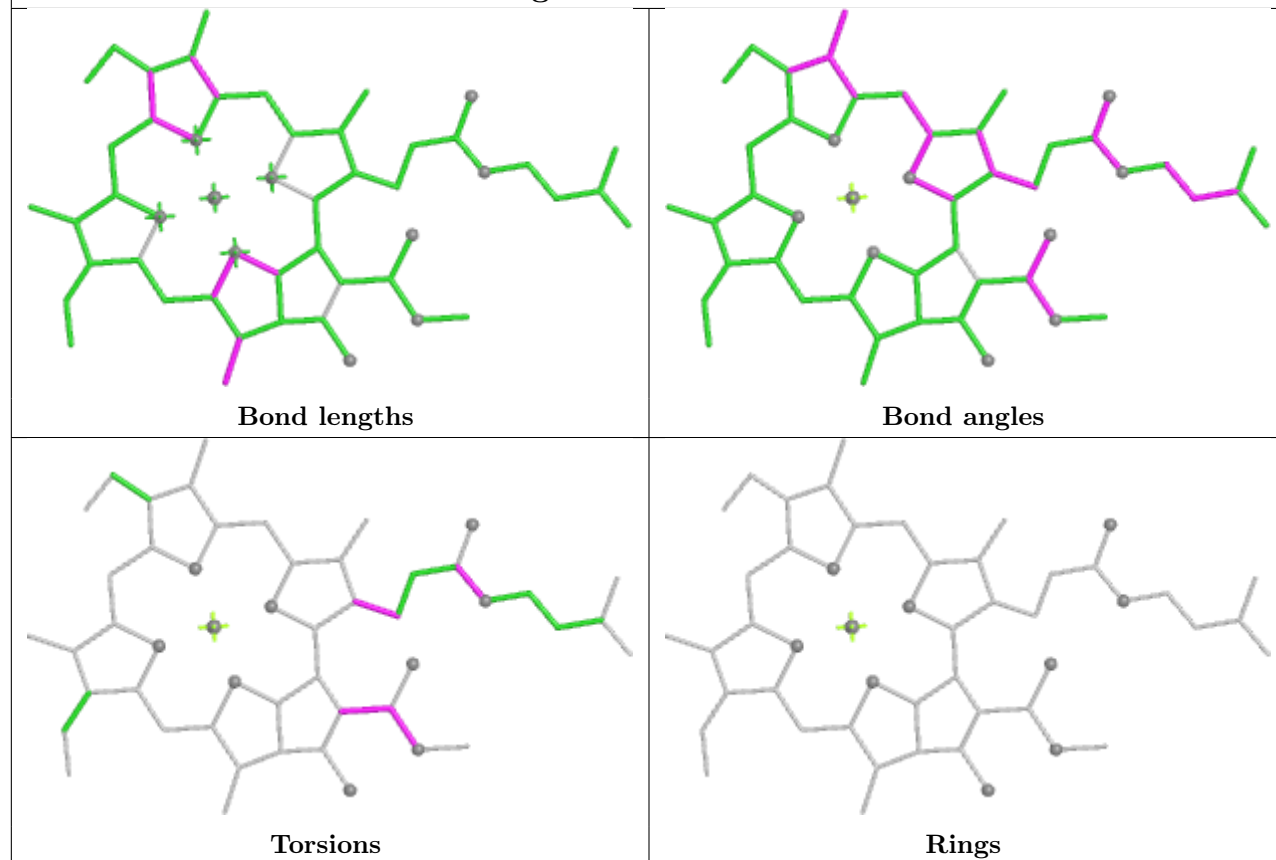


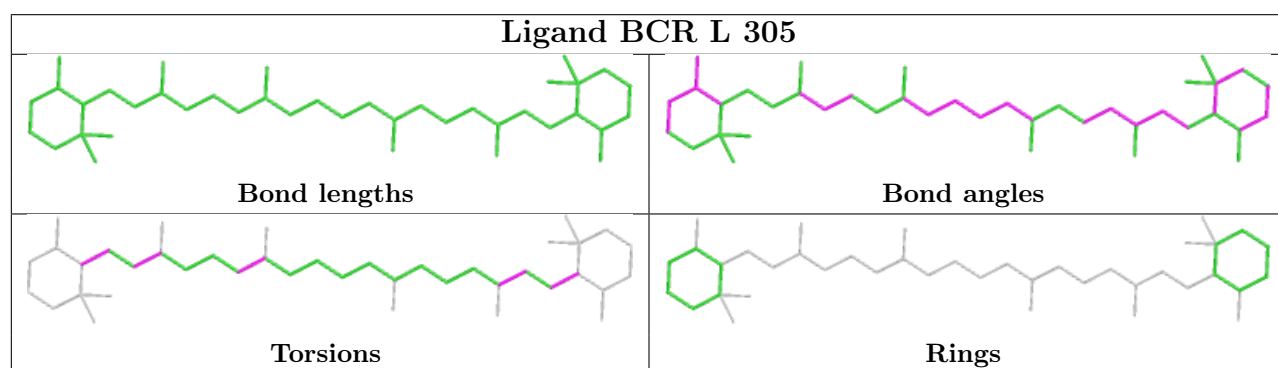
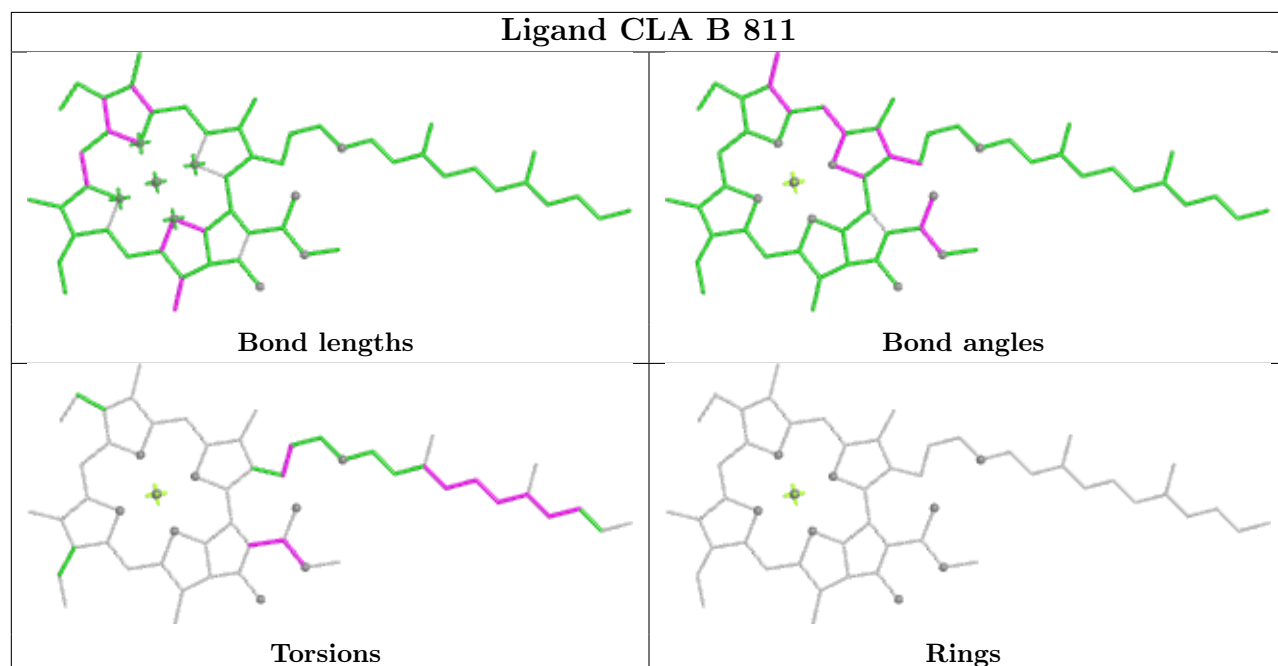
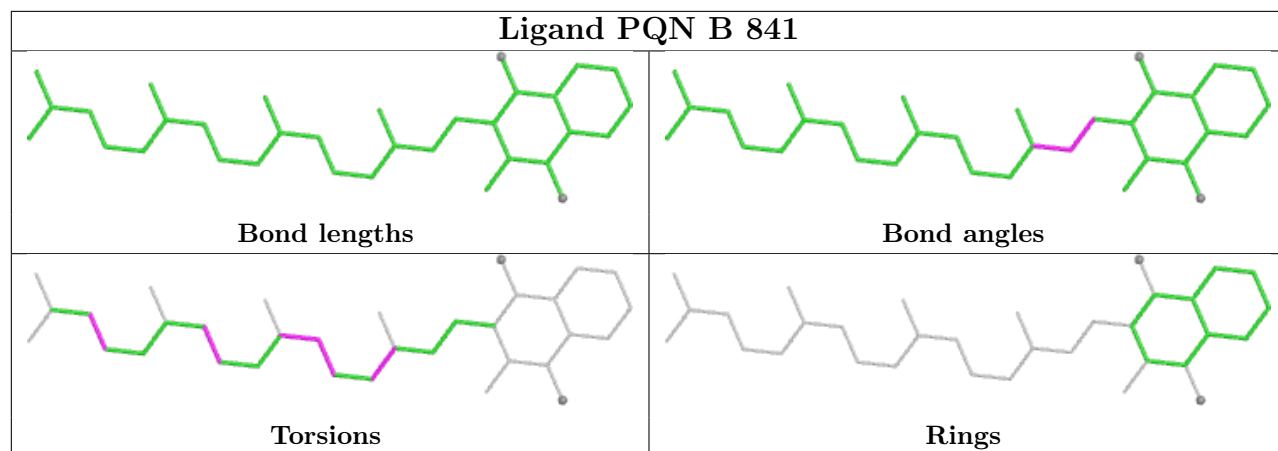


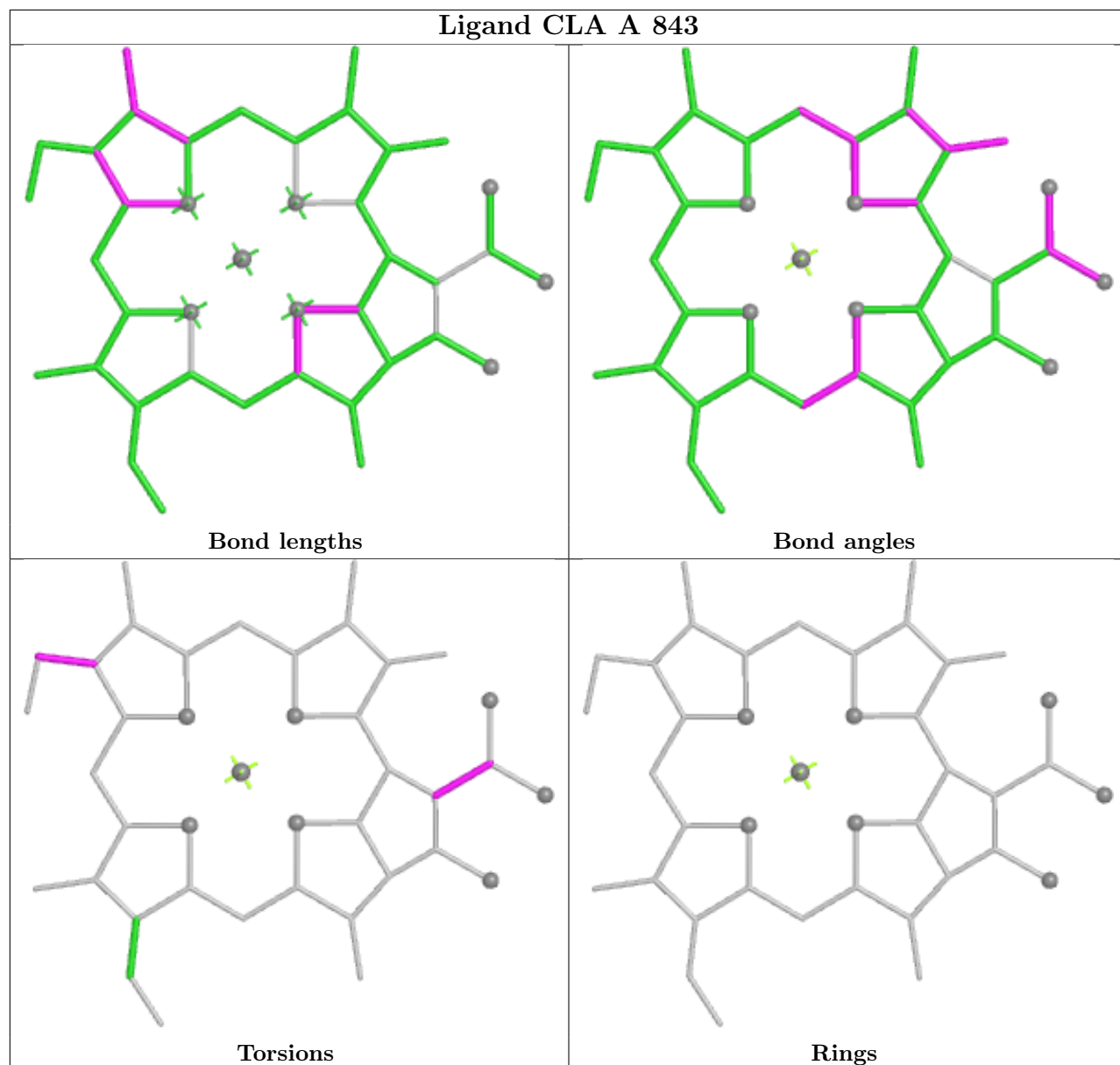
Ligand CLA A 832

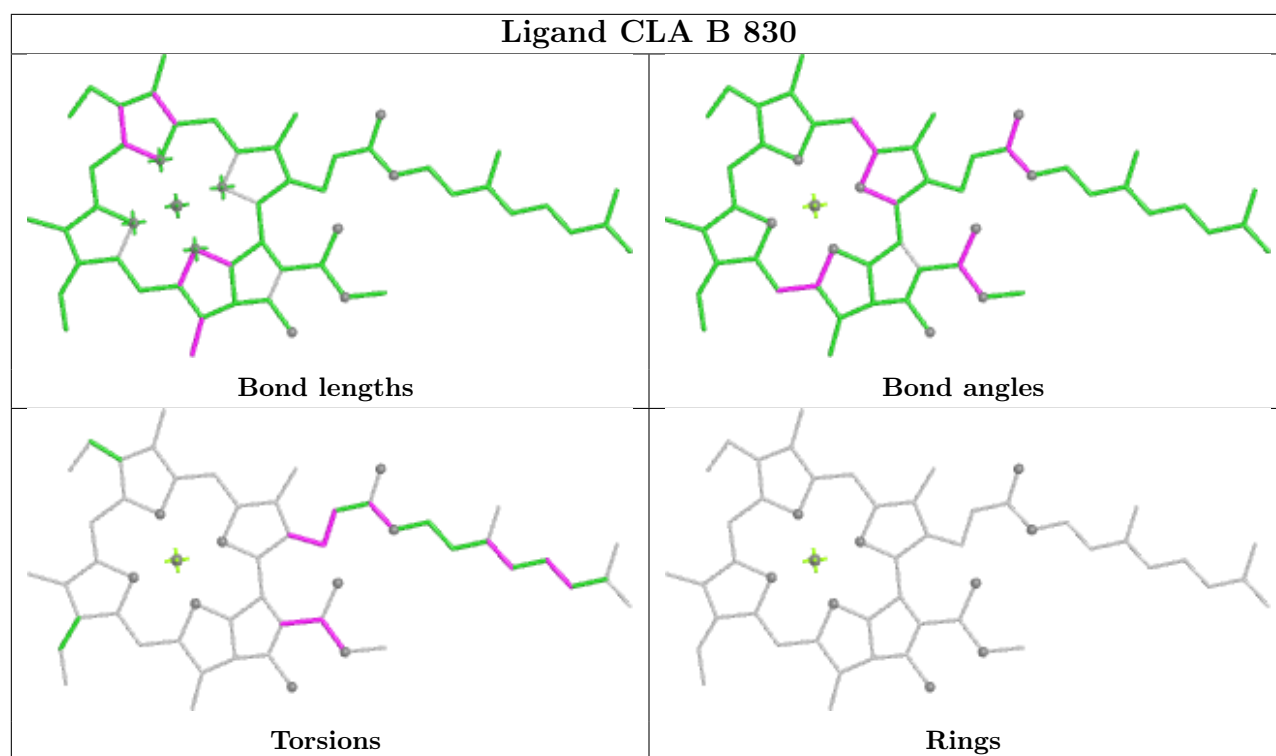


Ligand CLA A 836

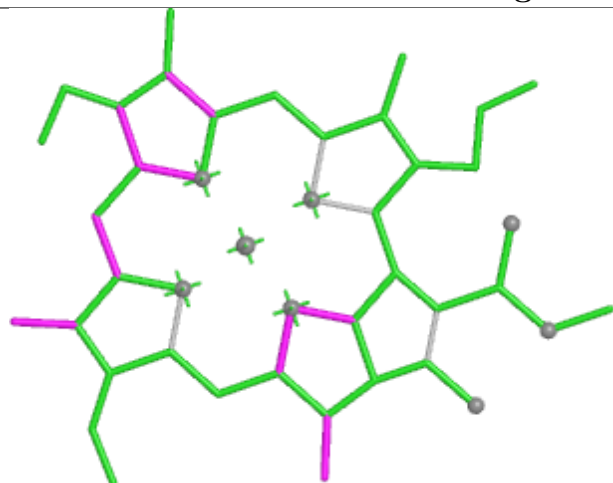




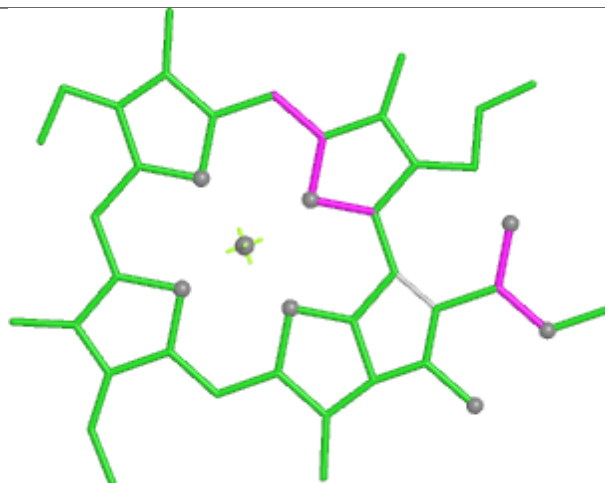




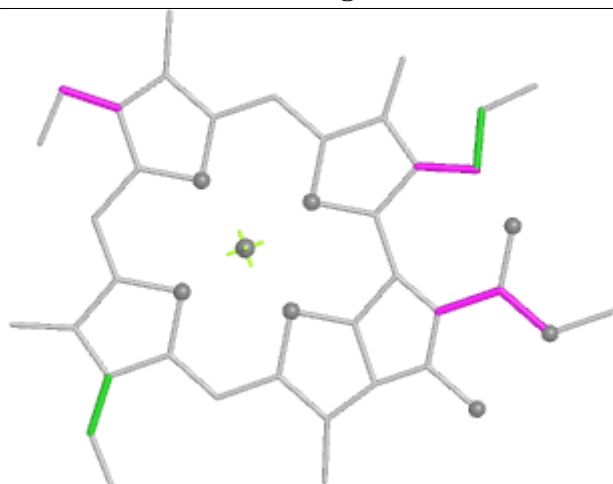
Ligand CLA B 824



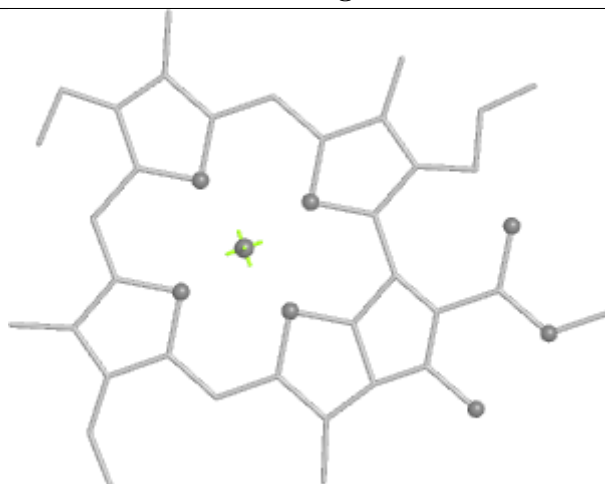
Bond lengths



Bond angles

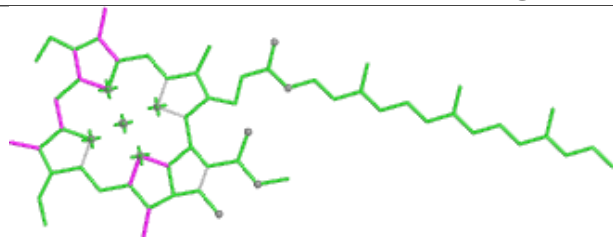


Torsions

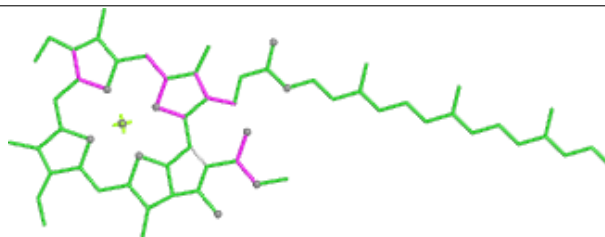


Rings

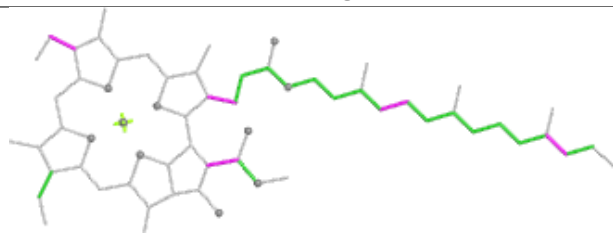
Ligand CLA A 826



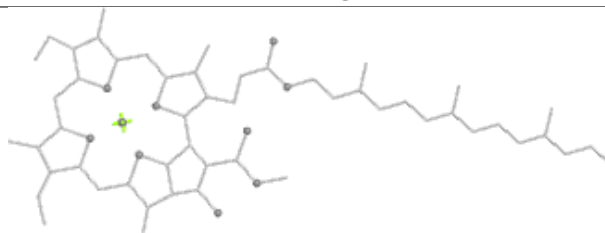
Bond lengths



Bond angles

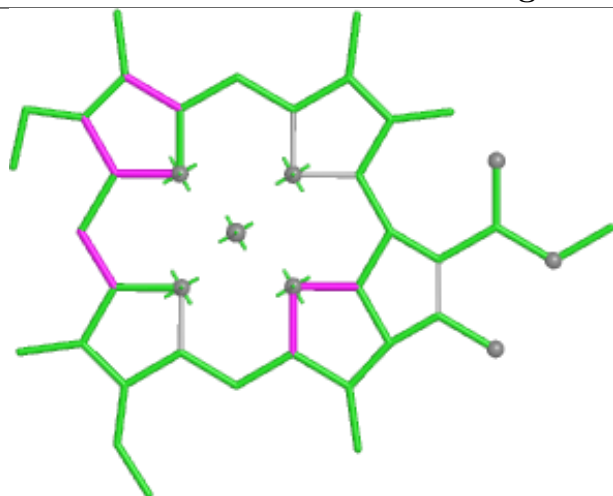


Torsions



Rings

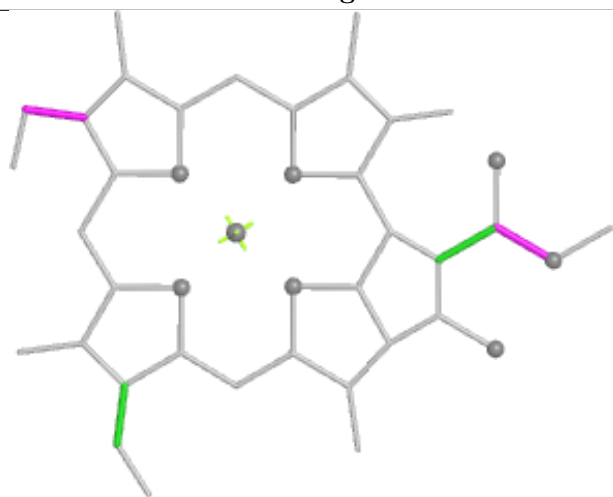
Ligand CLA 2 611



Bond lengths



Bond angles

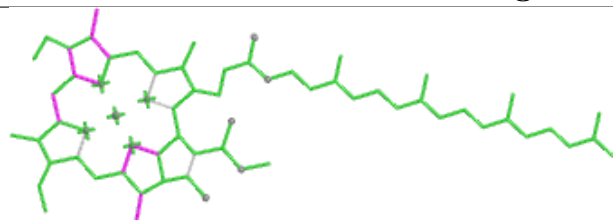


Torsions

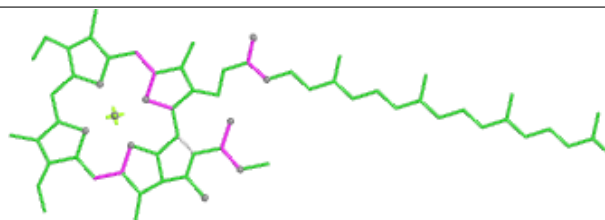


Rings

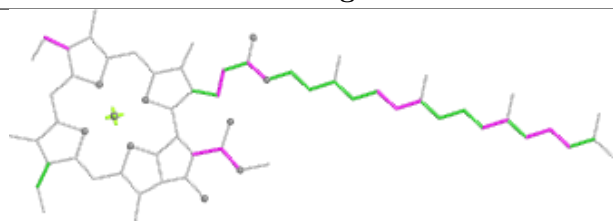
Ligand CLA B 839



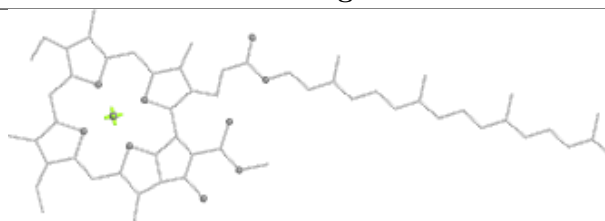
Bond lengths



Bond angles

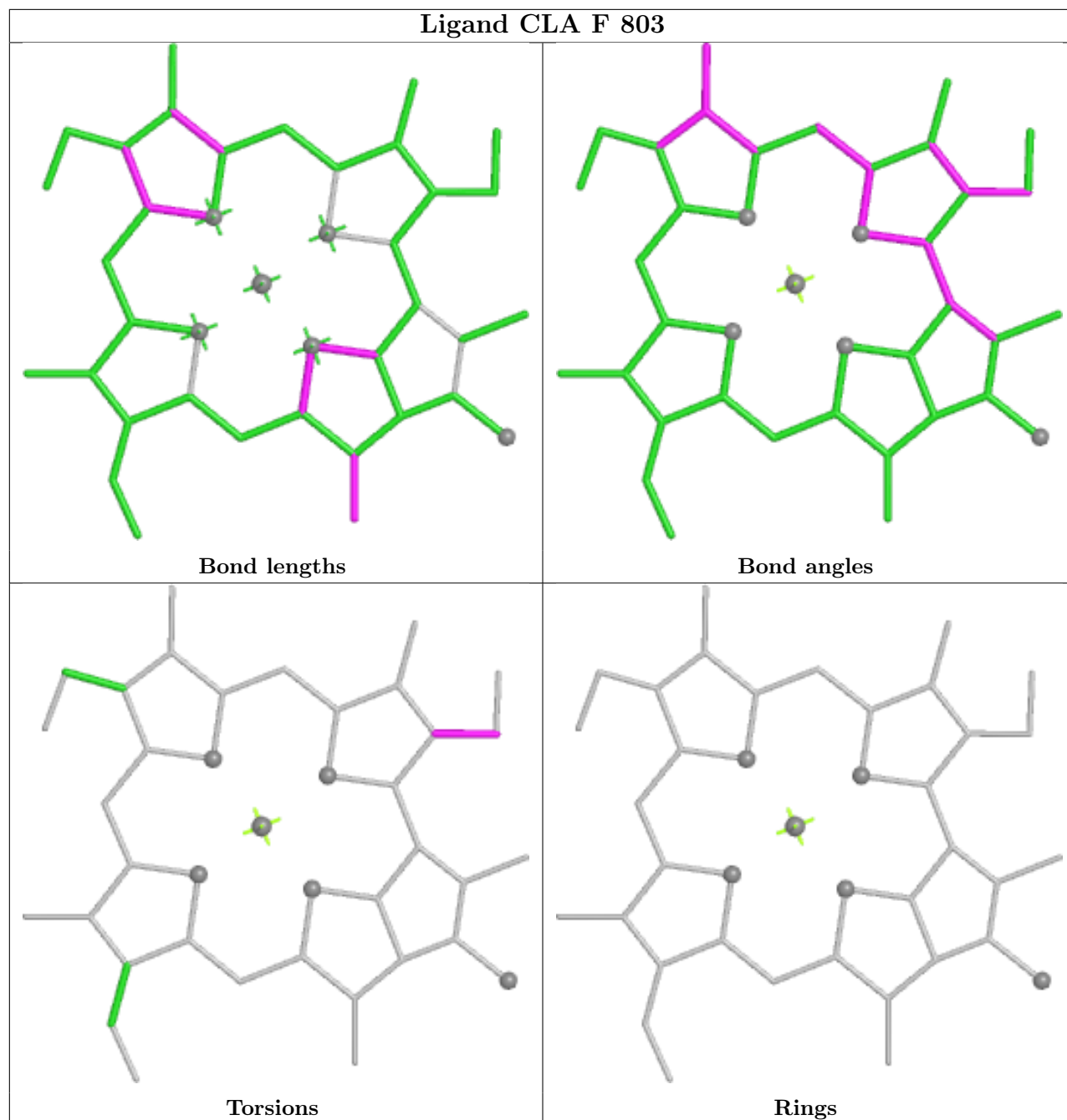


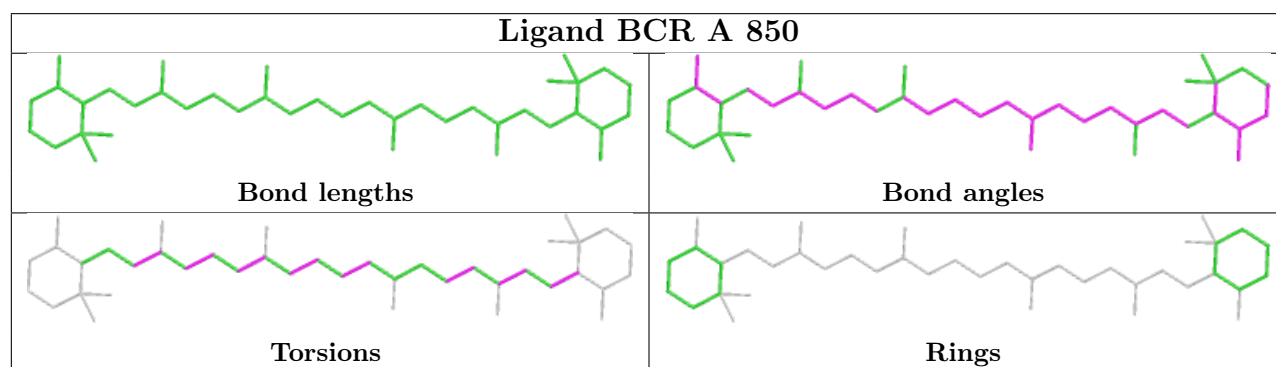
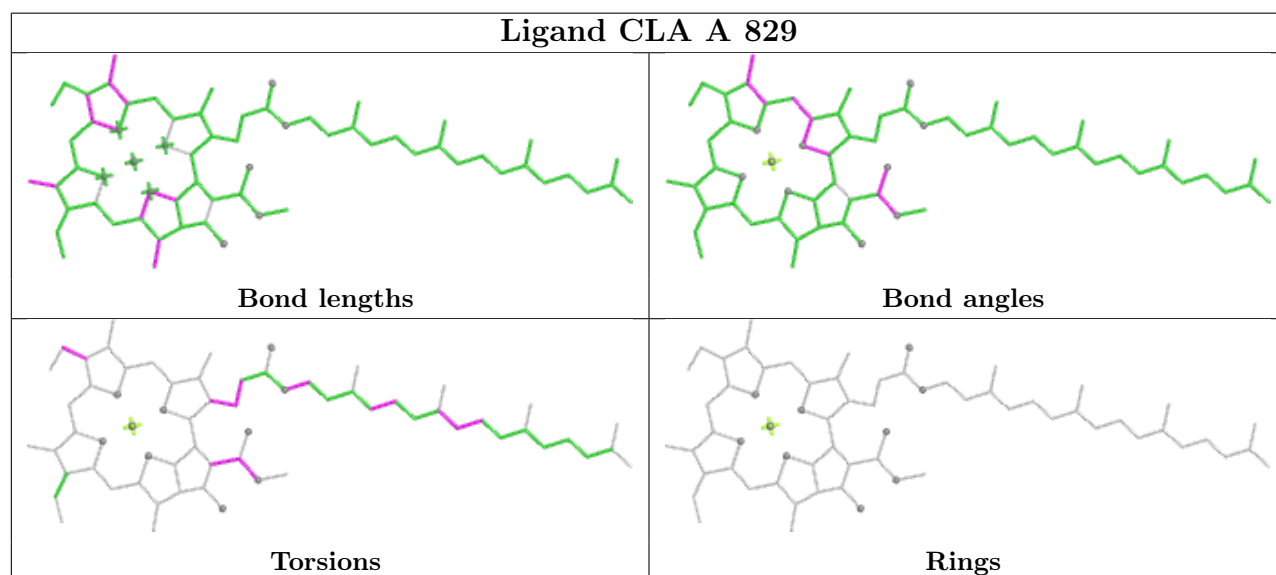
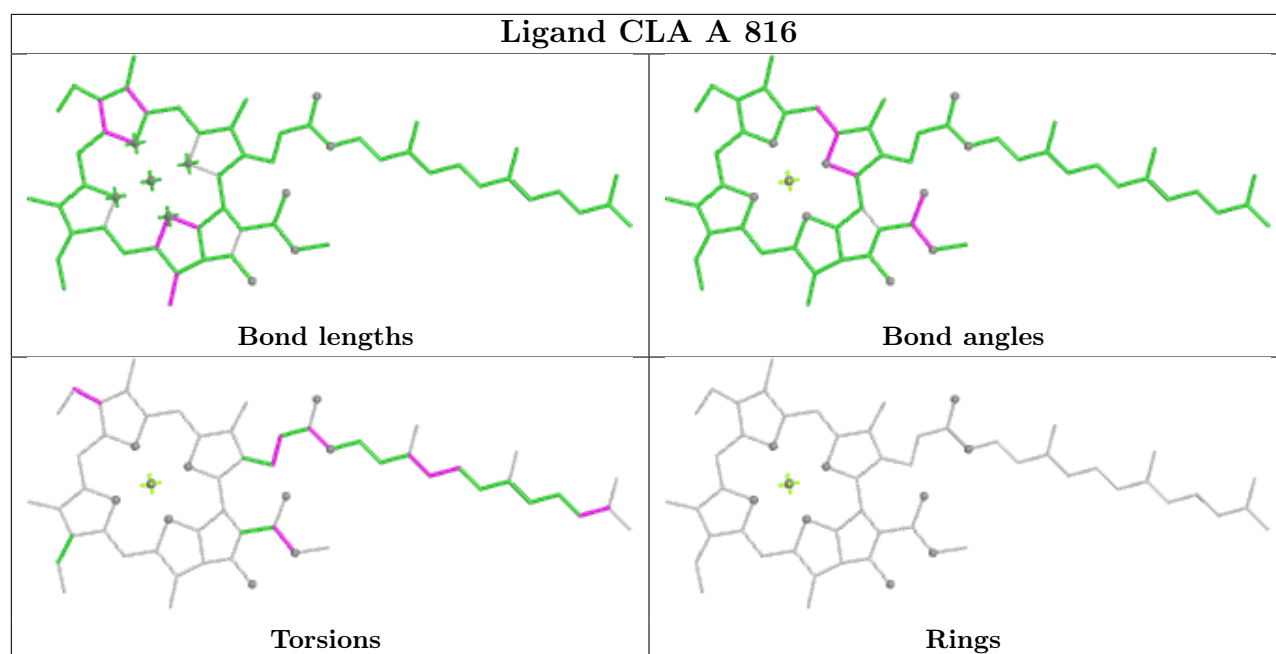
Torsions

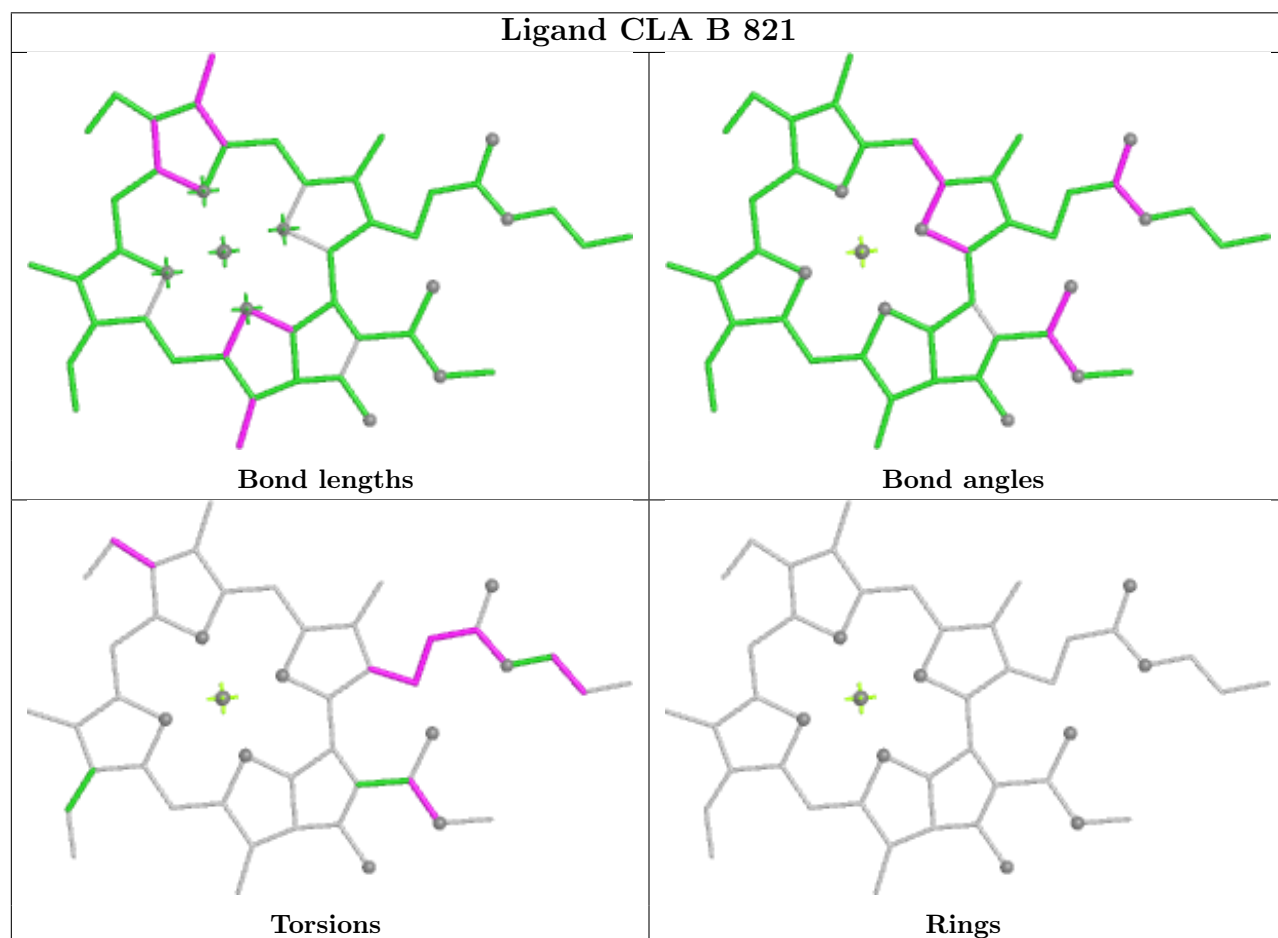
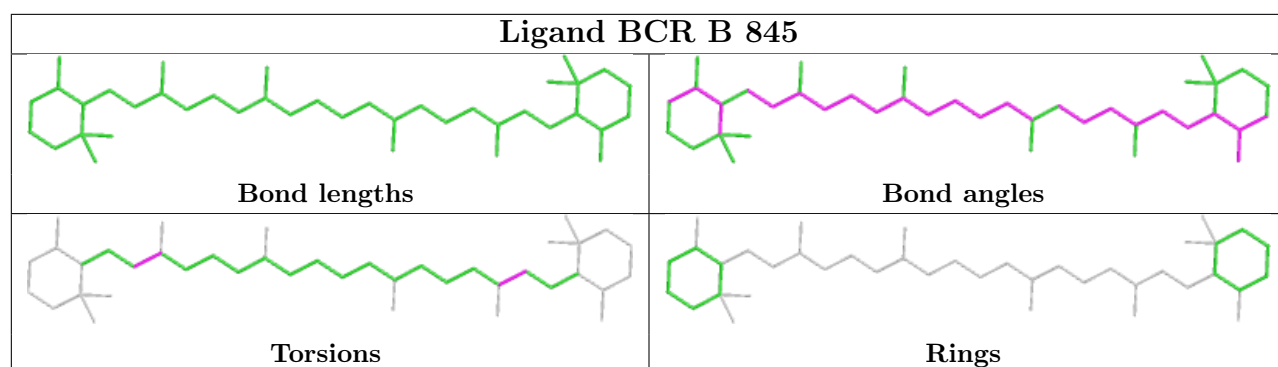


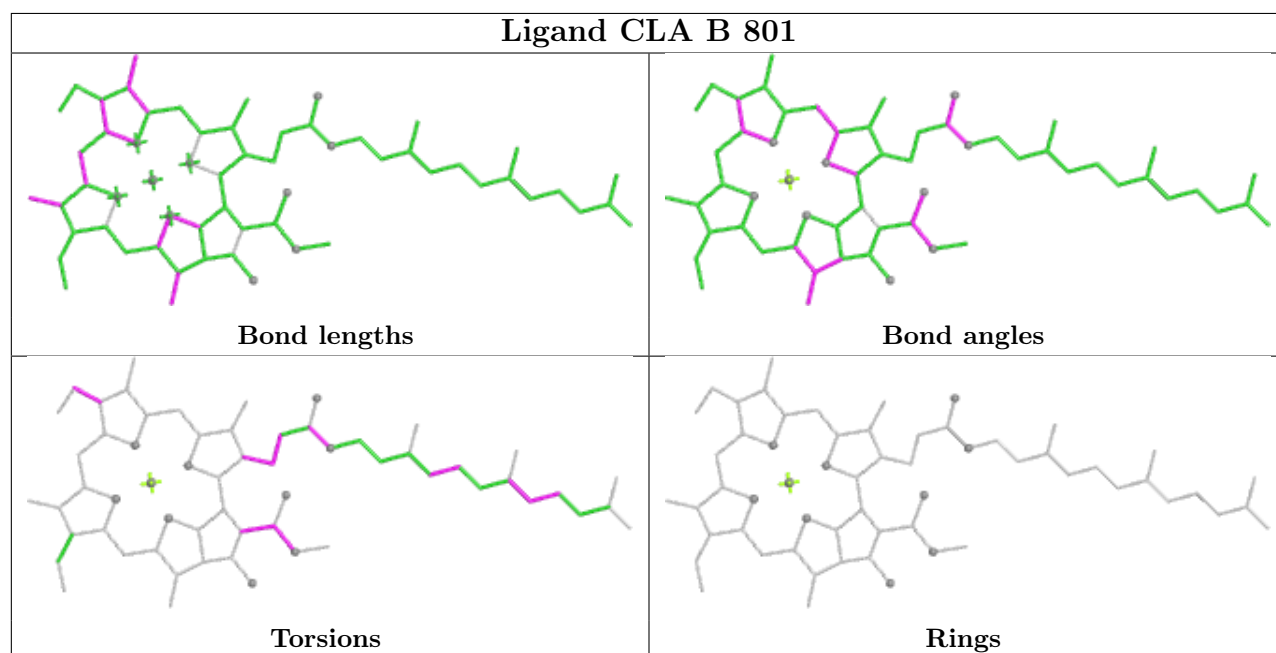
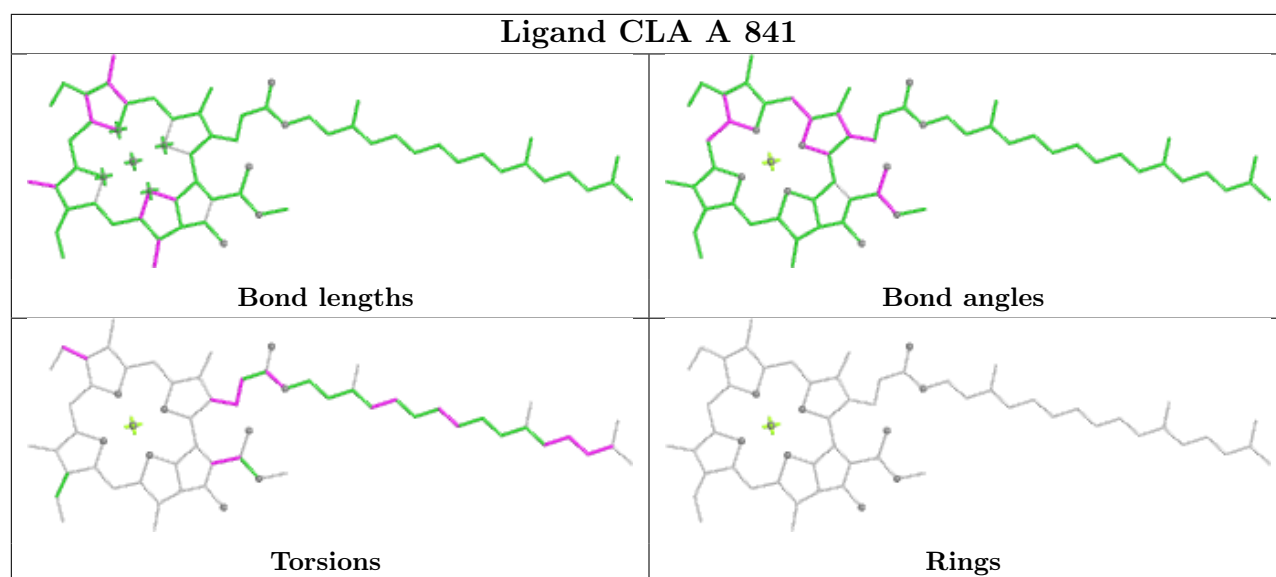
Rings

Ligand CLA F 803

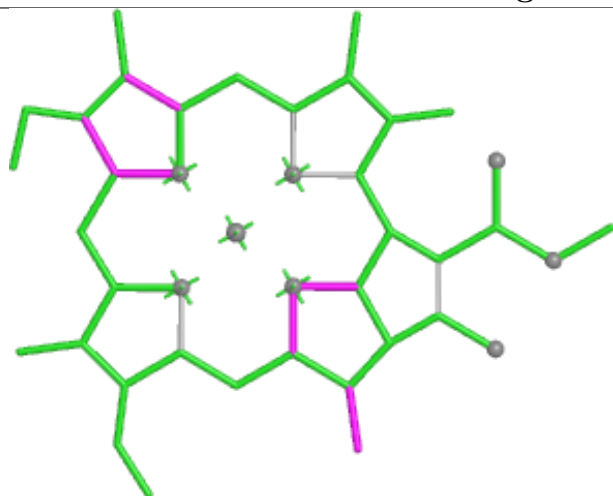




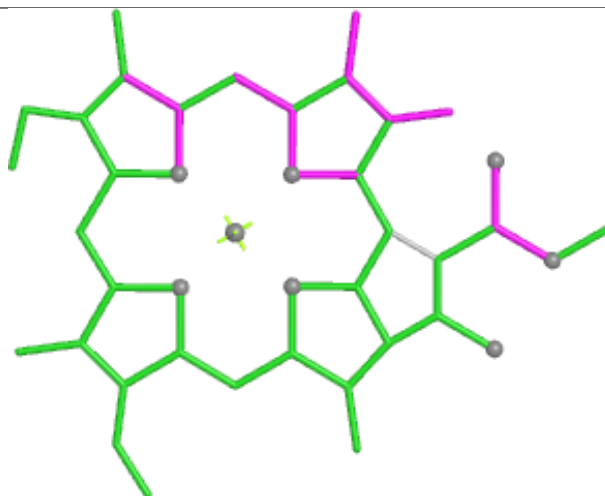




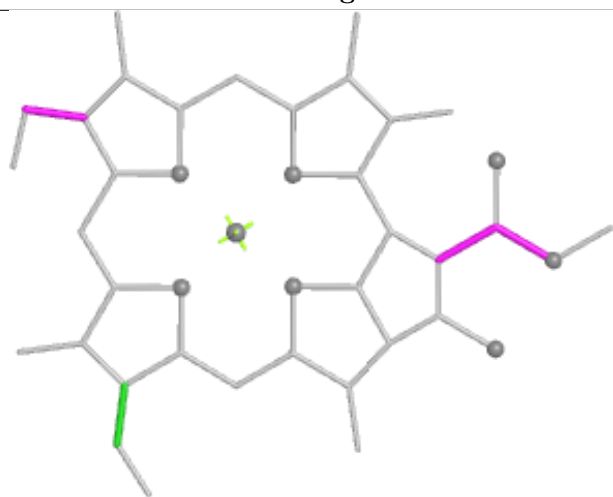
Ligand CLA L 302



Bond lengths



Bond angles

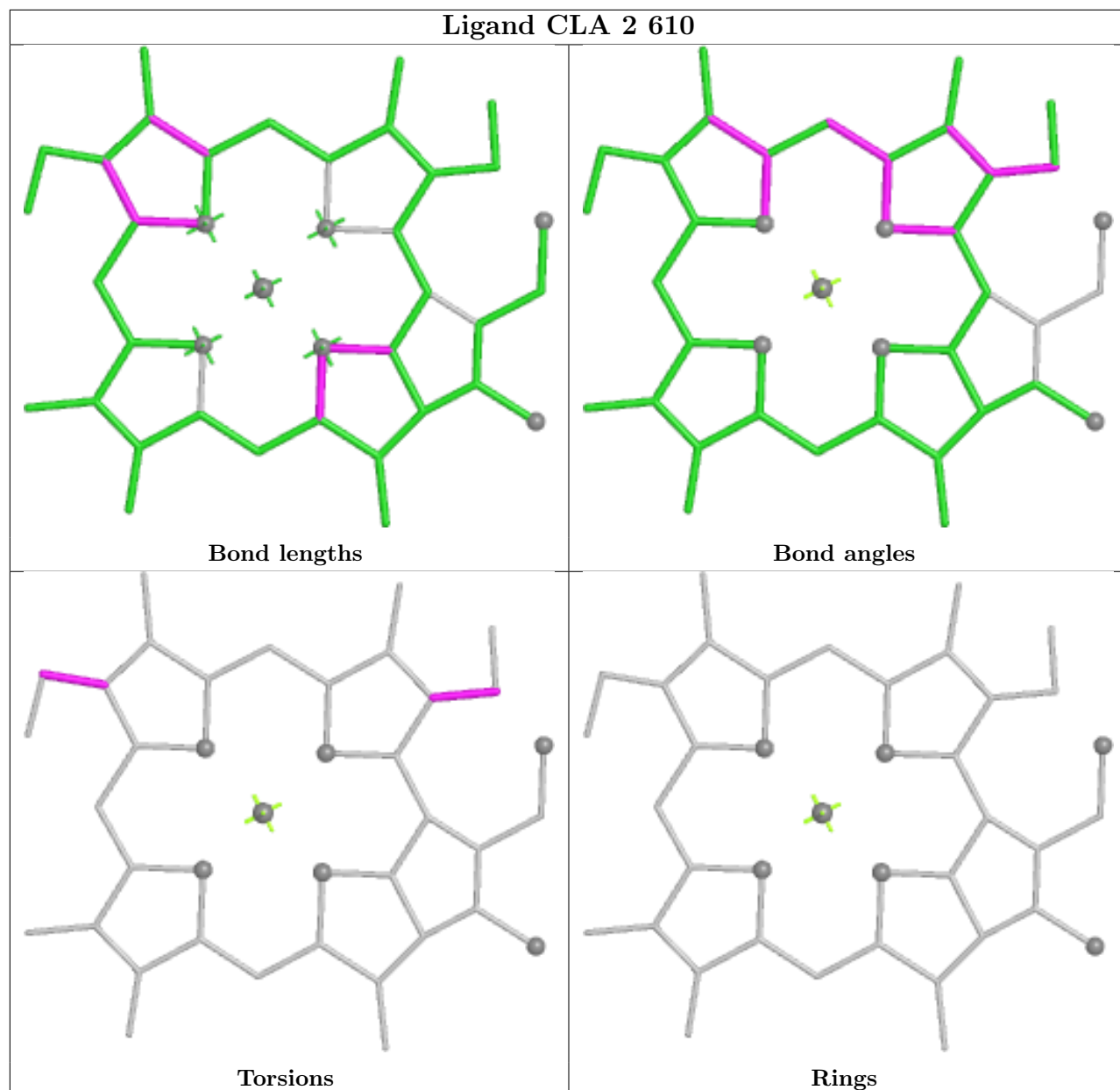


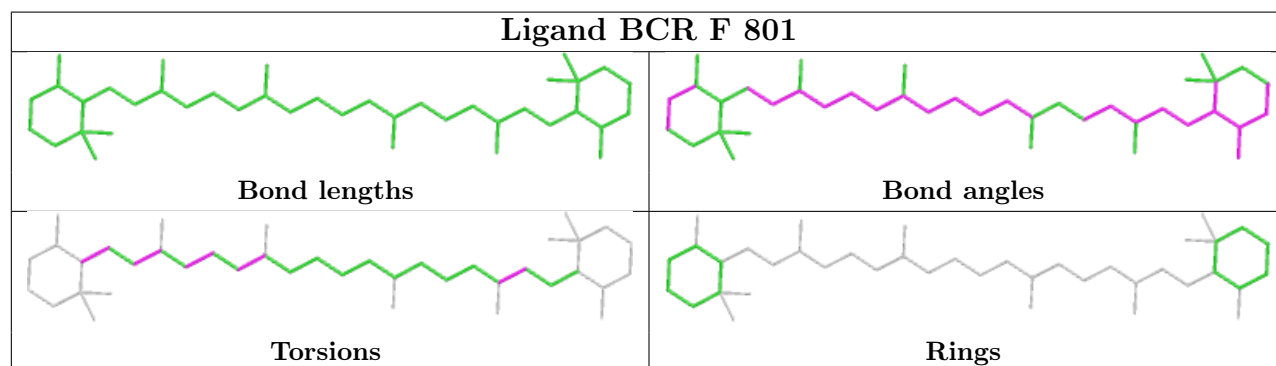
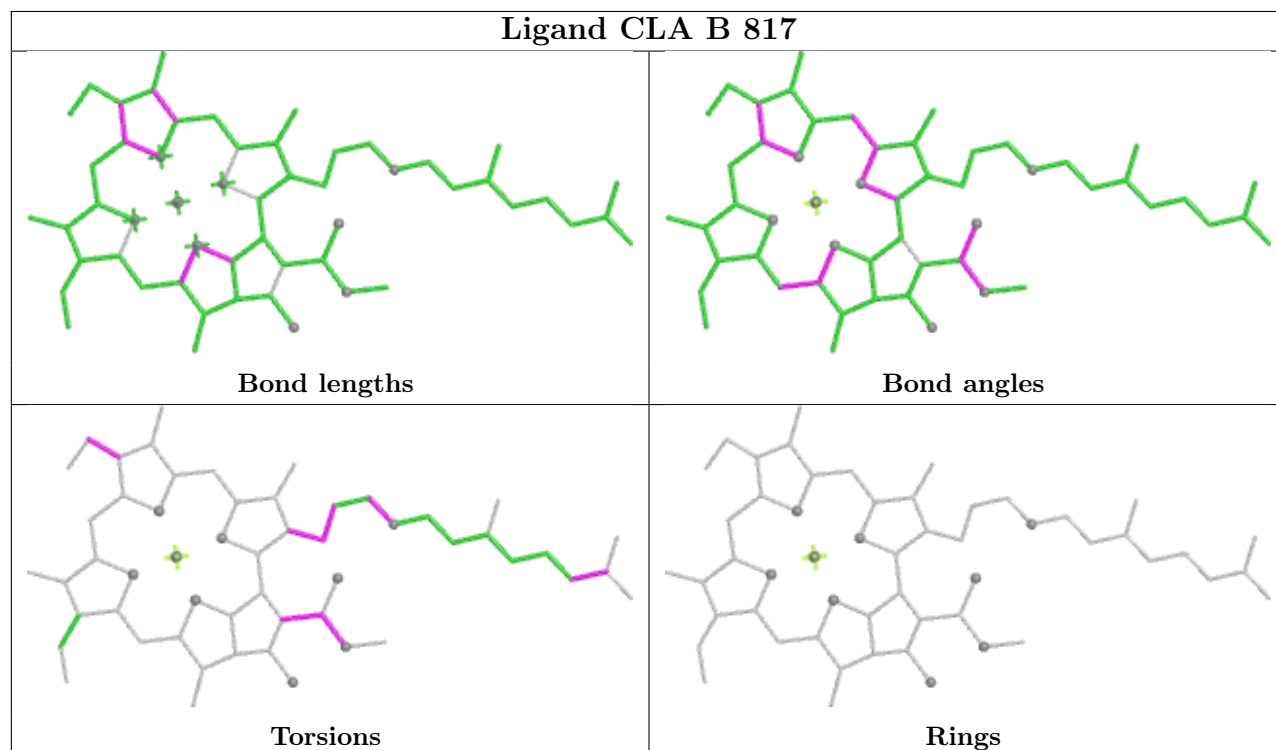
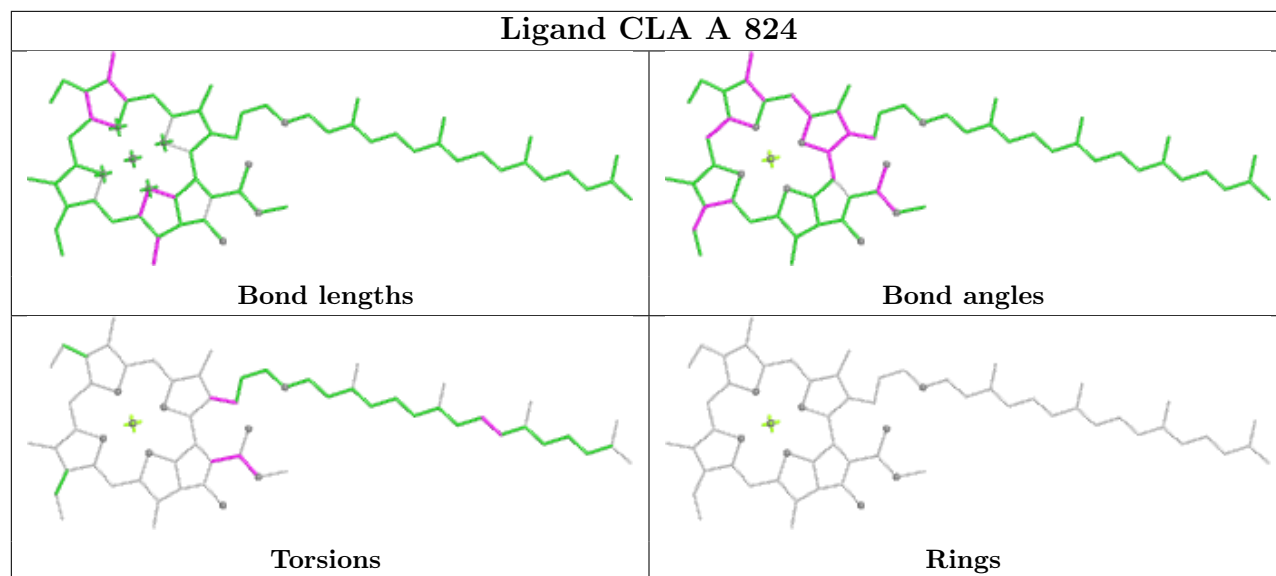
Torsions



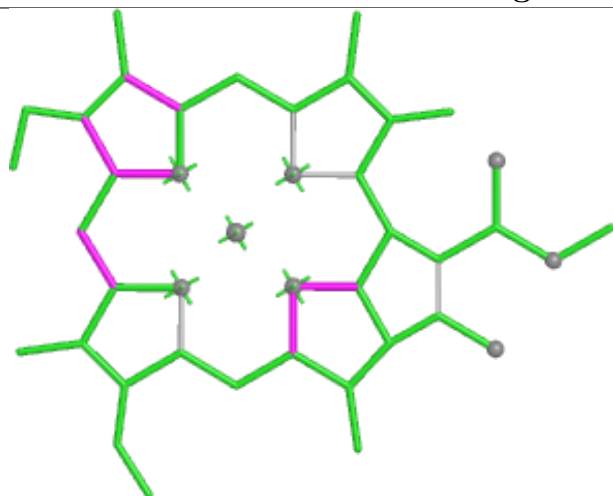
Rings

Ligand CLA 2 610





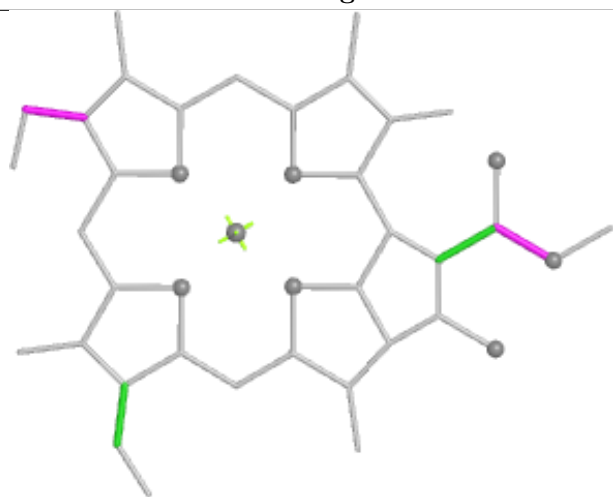
Ligand CLA K 205



Bond lengths



Bond angles

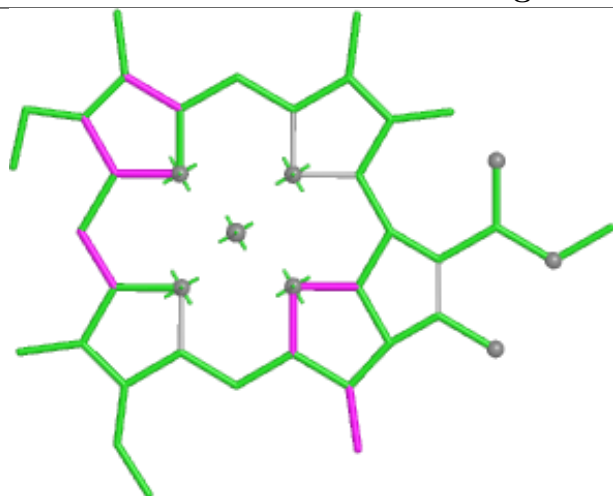


Torsions

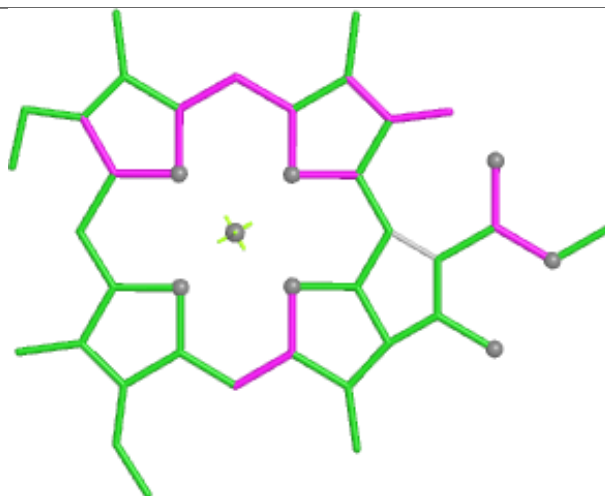


Rings

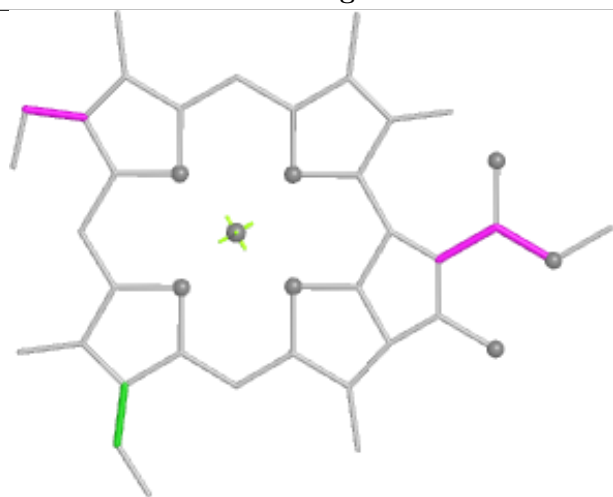
Ligand CLA A 822



Bond lengths



Bond angles

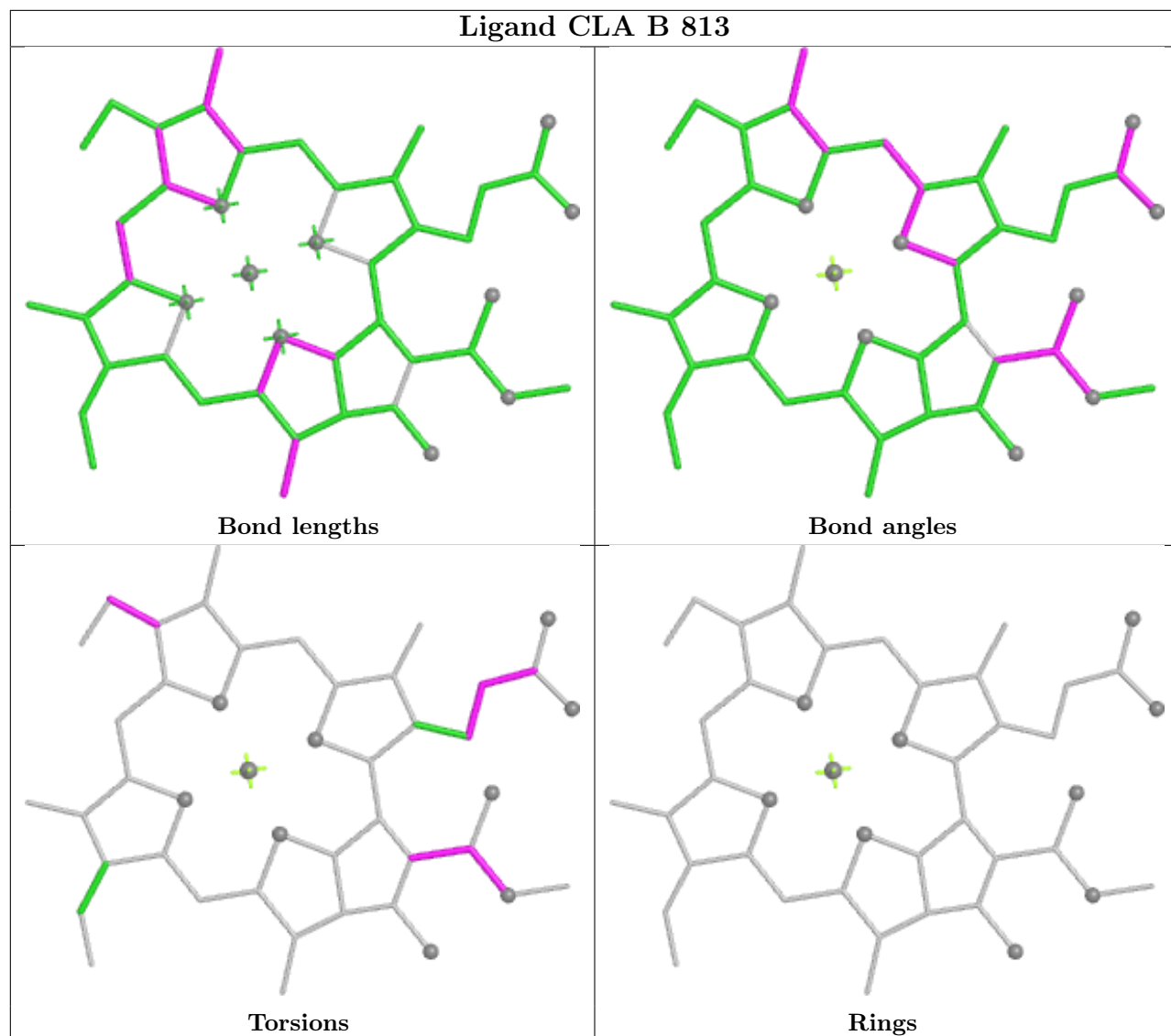


Torsions

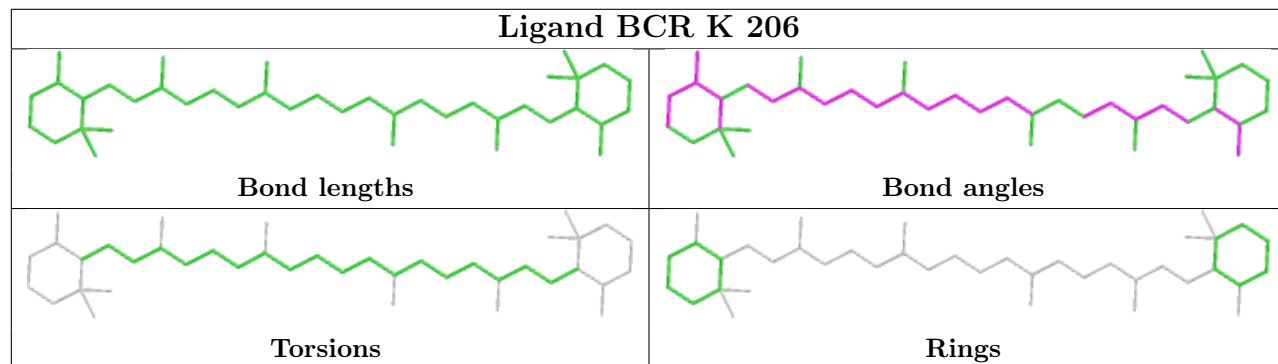


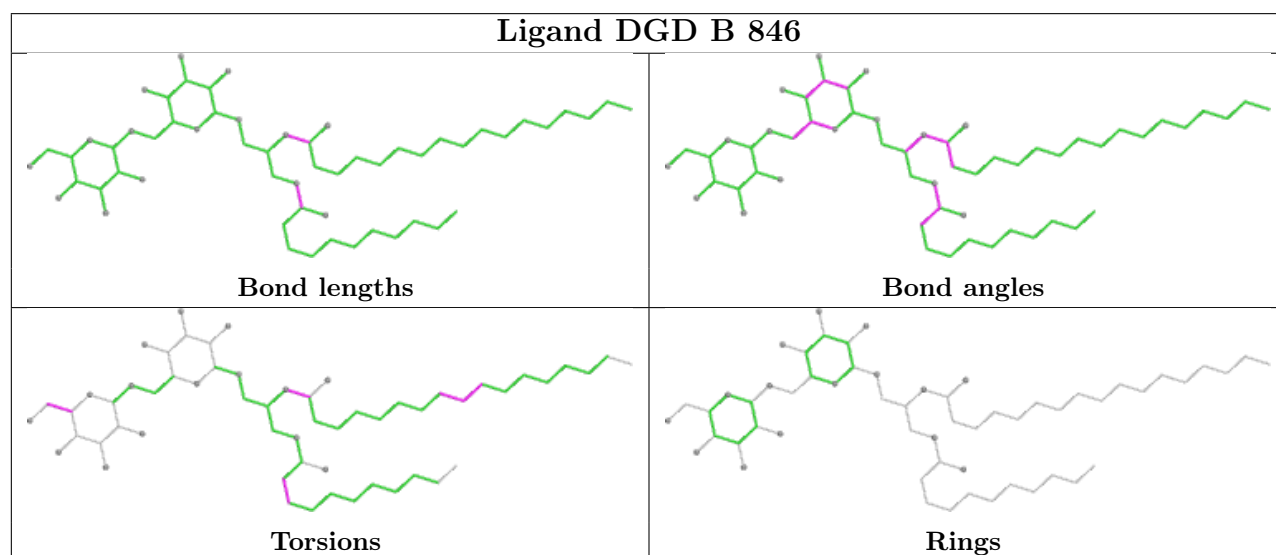
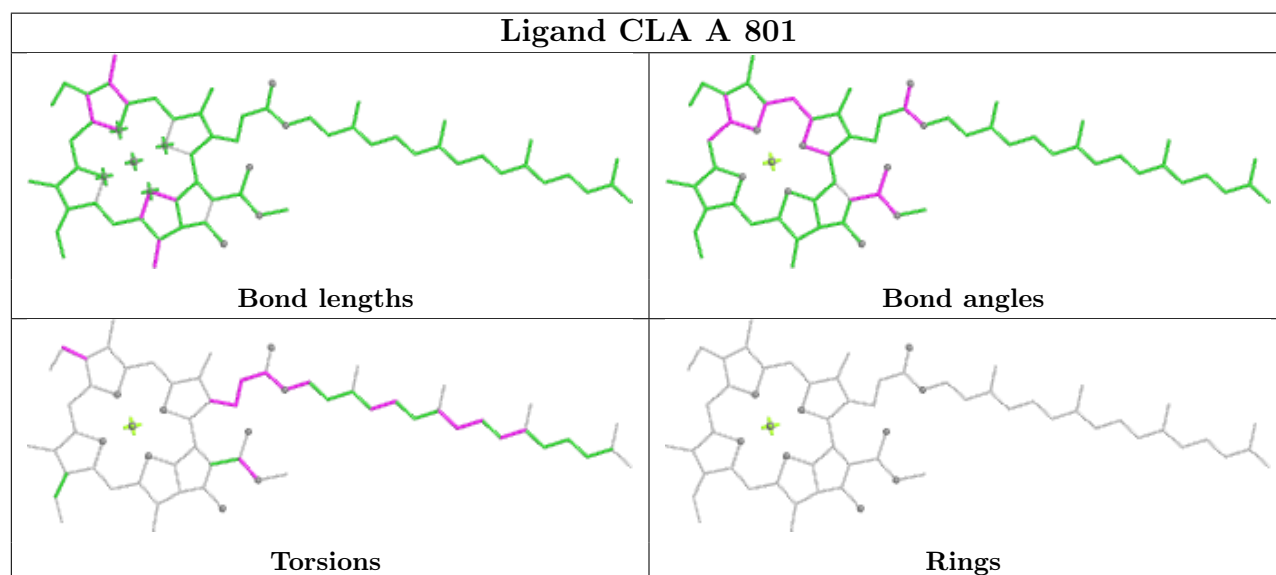
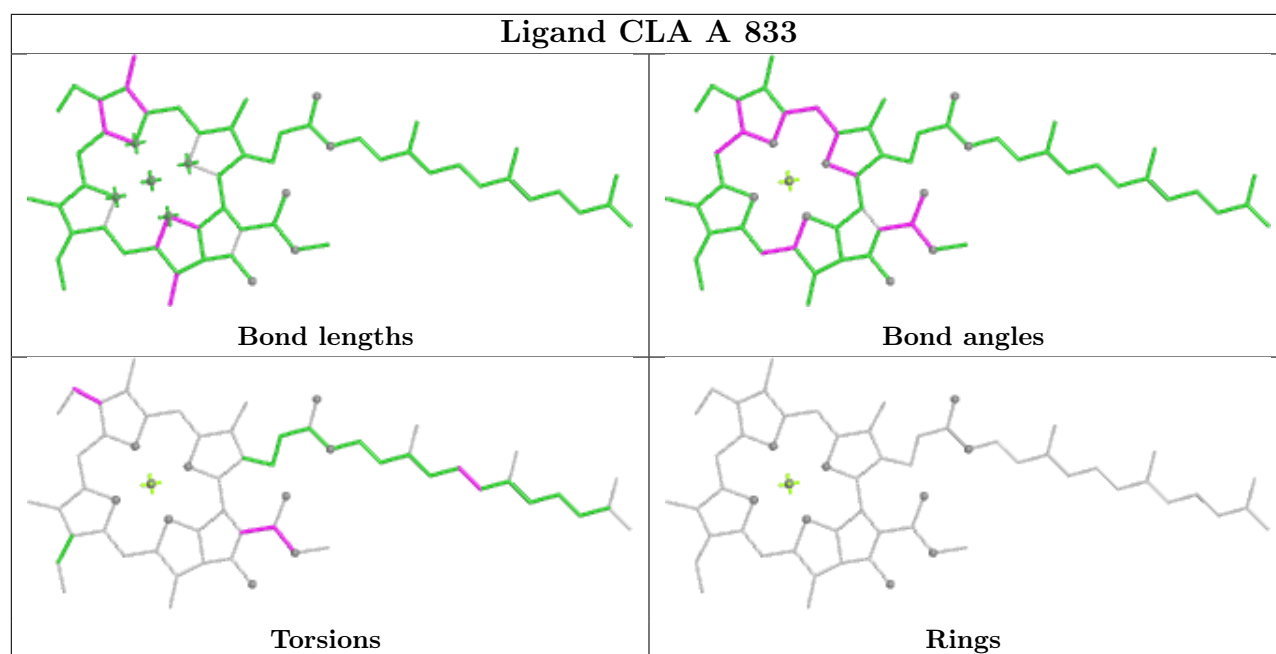
Rings

Ligand CLA B 813

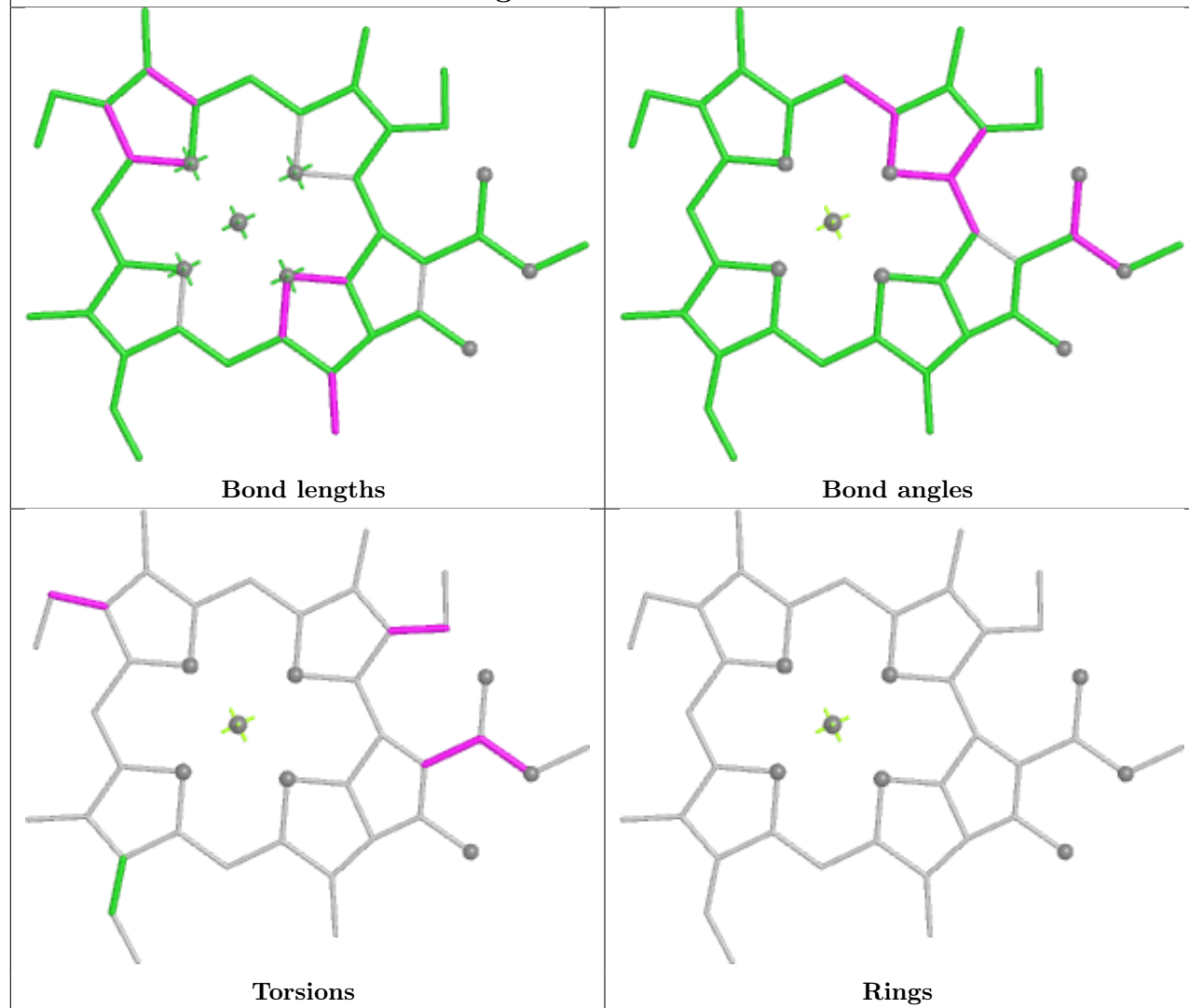


Ligand BCR K 206

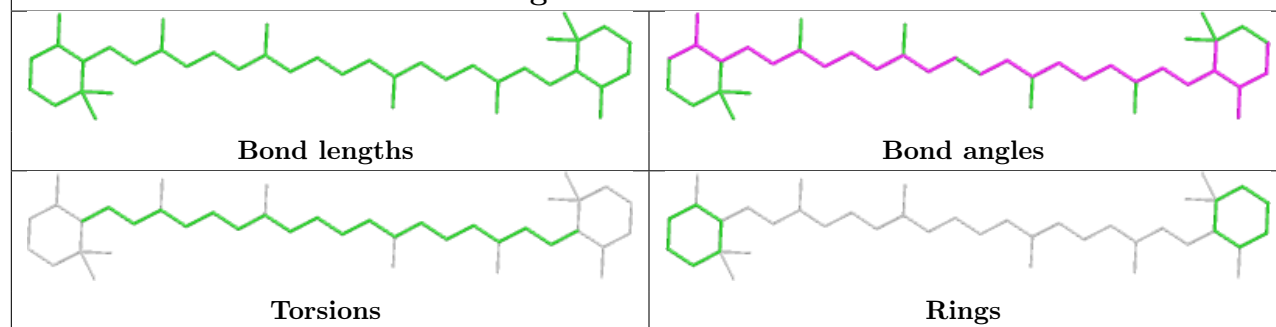




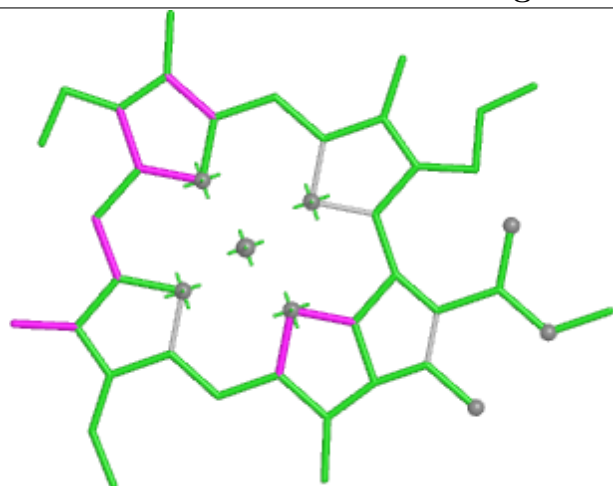
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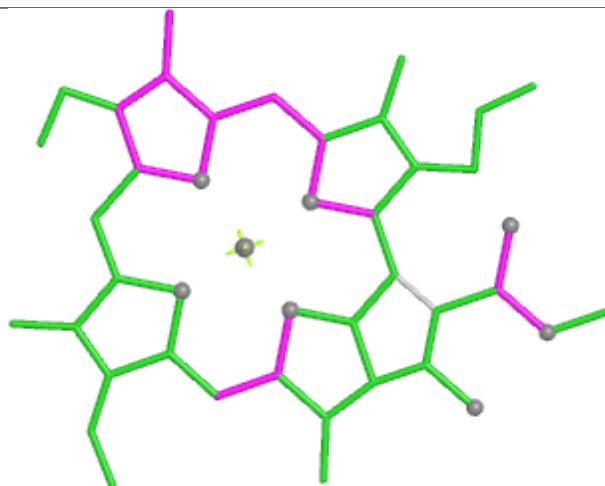
Ligand BCR A 848



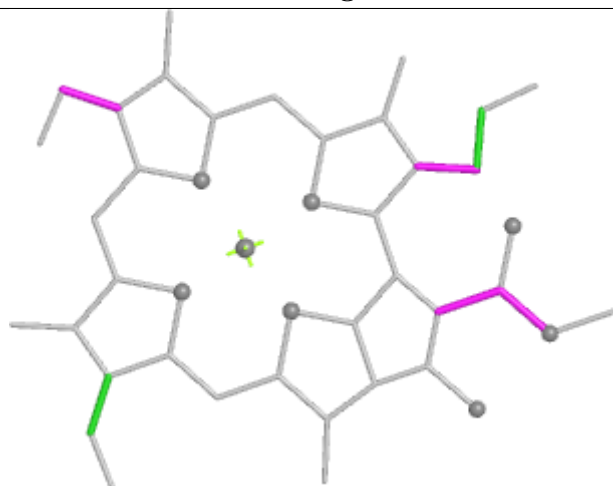
Ligand CLA A 804



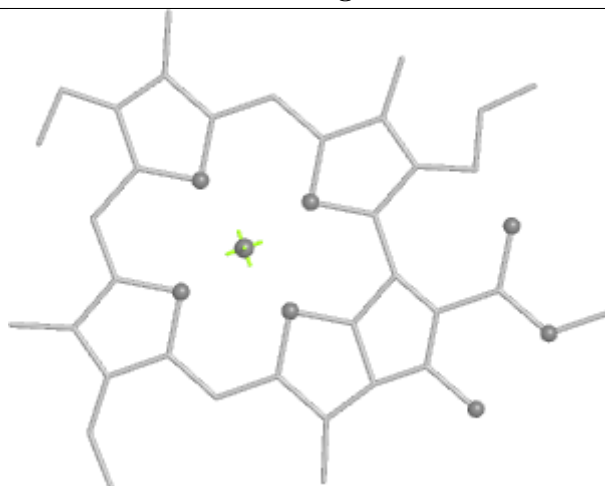
Bond lengths



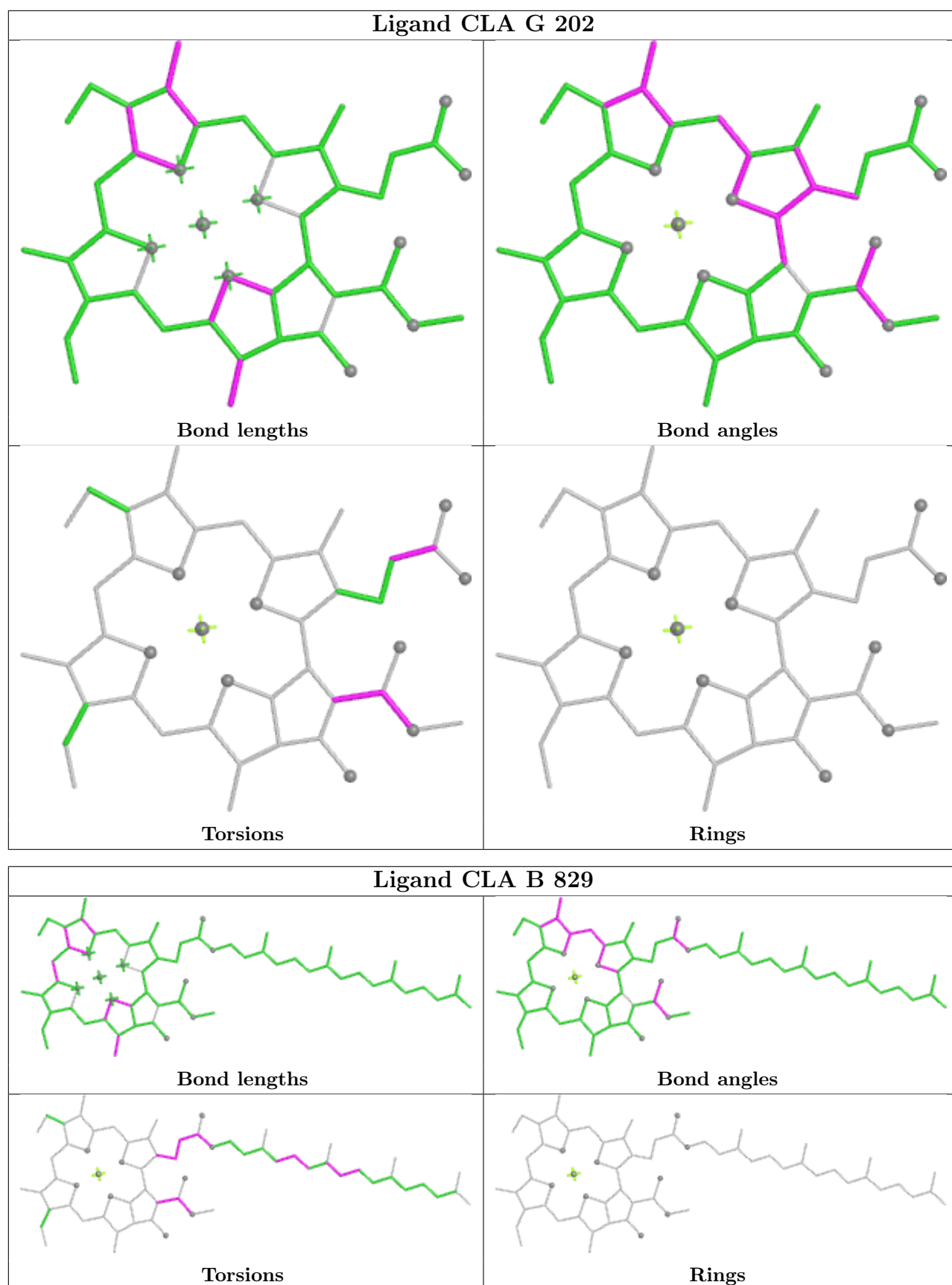
Bond angles

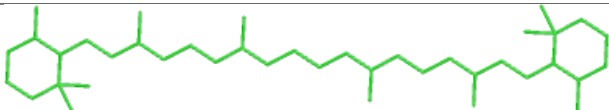
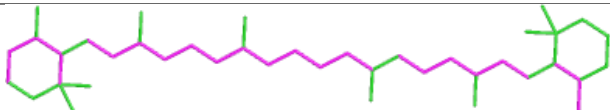
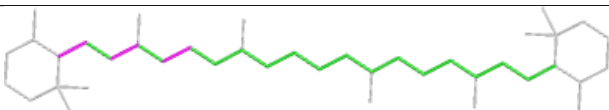
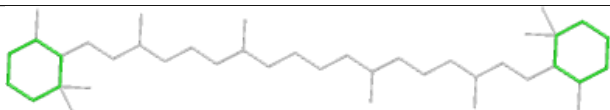


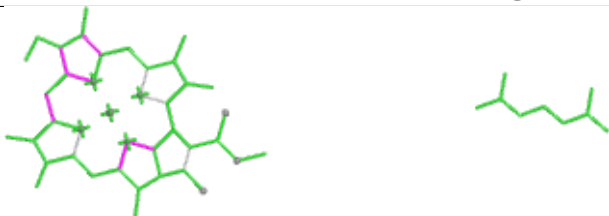
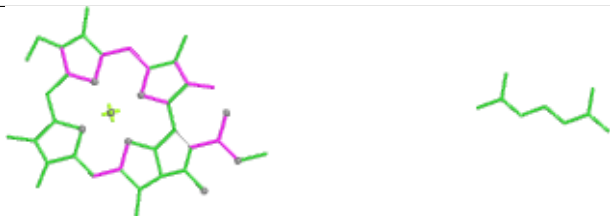
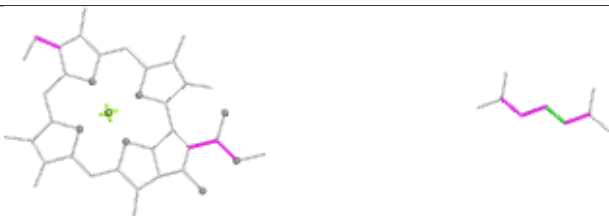
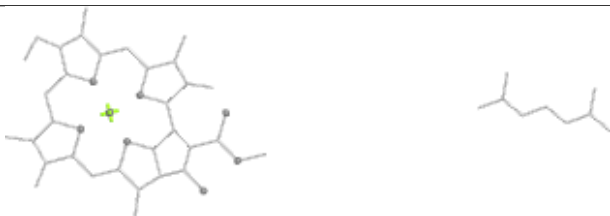
Torsions

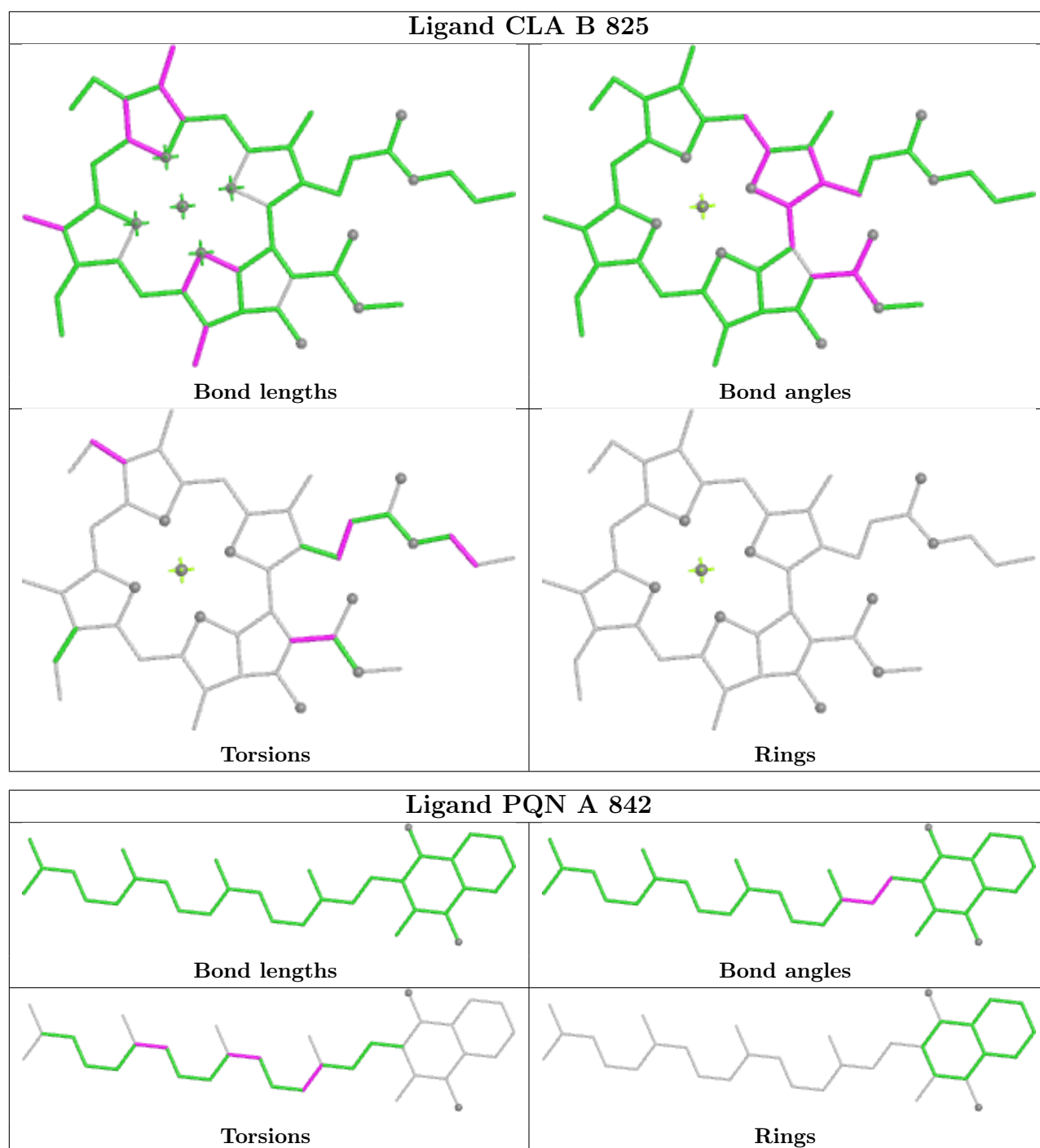


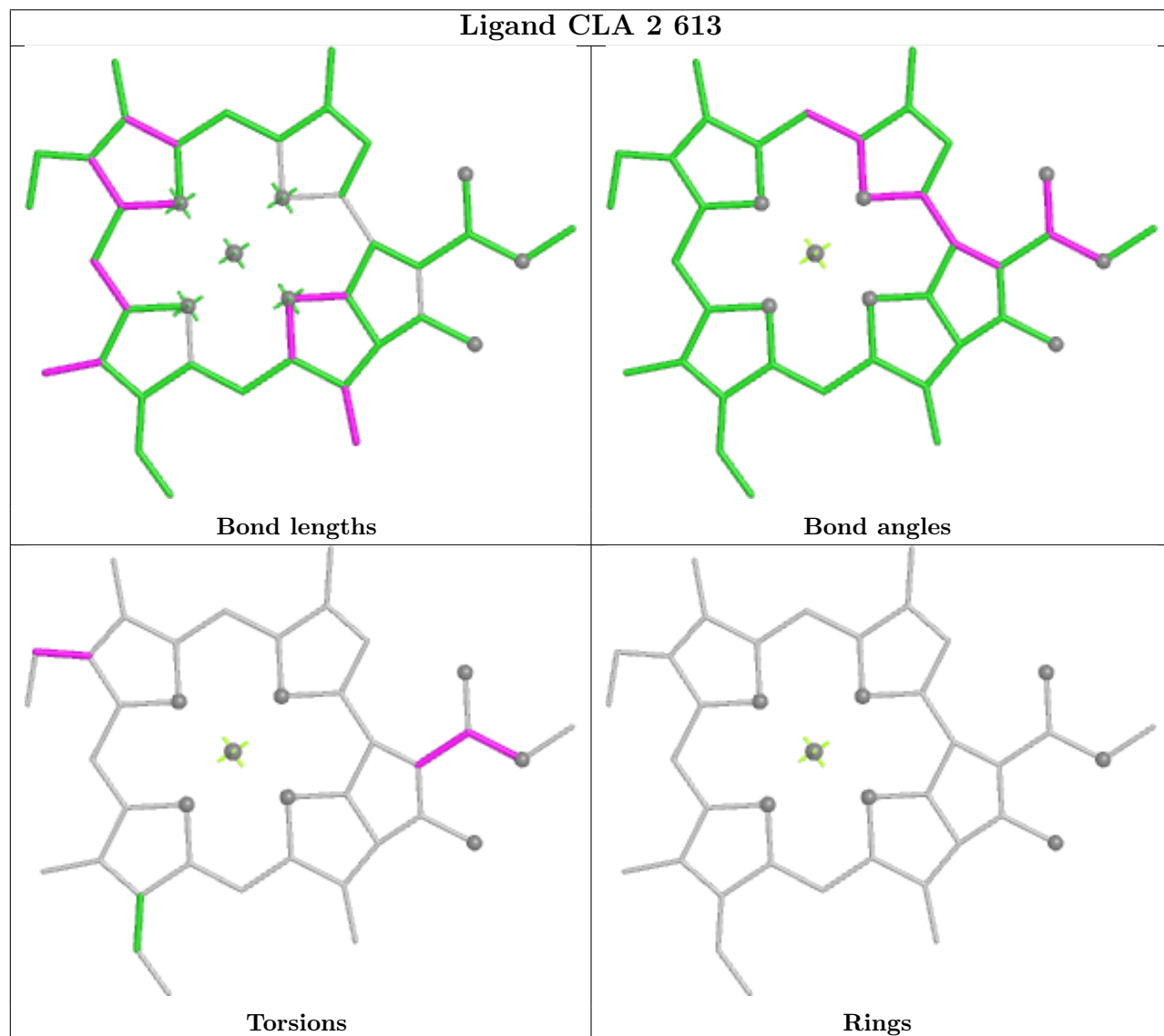
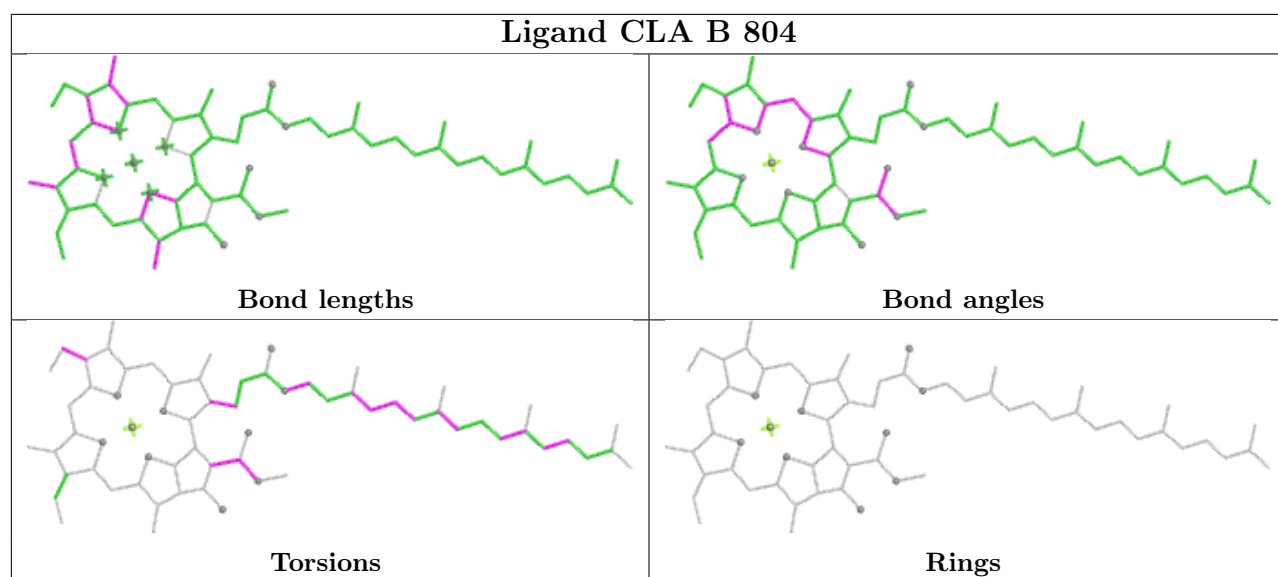
Rings

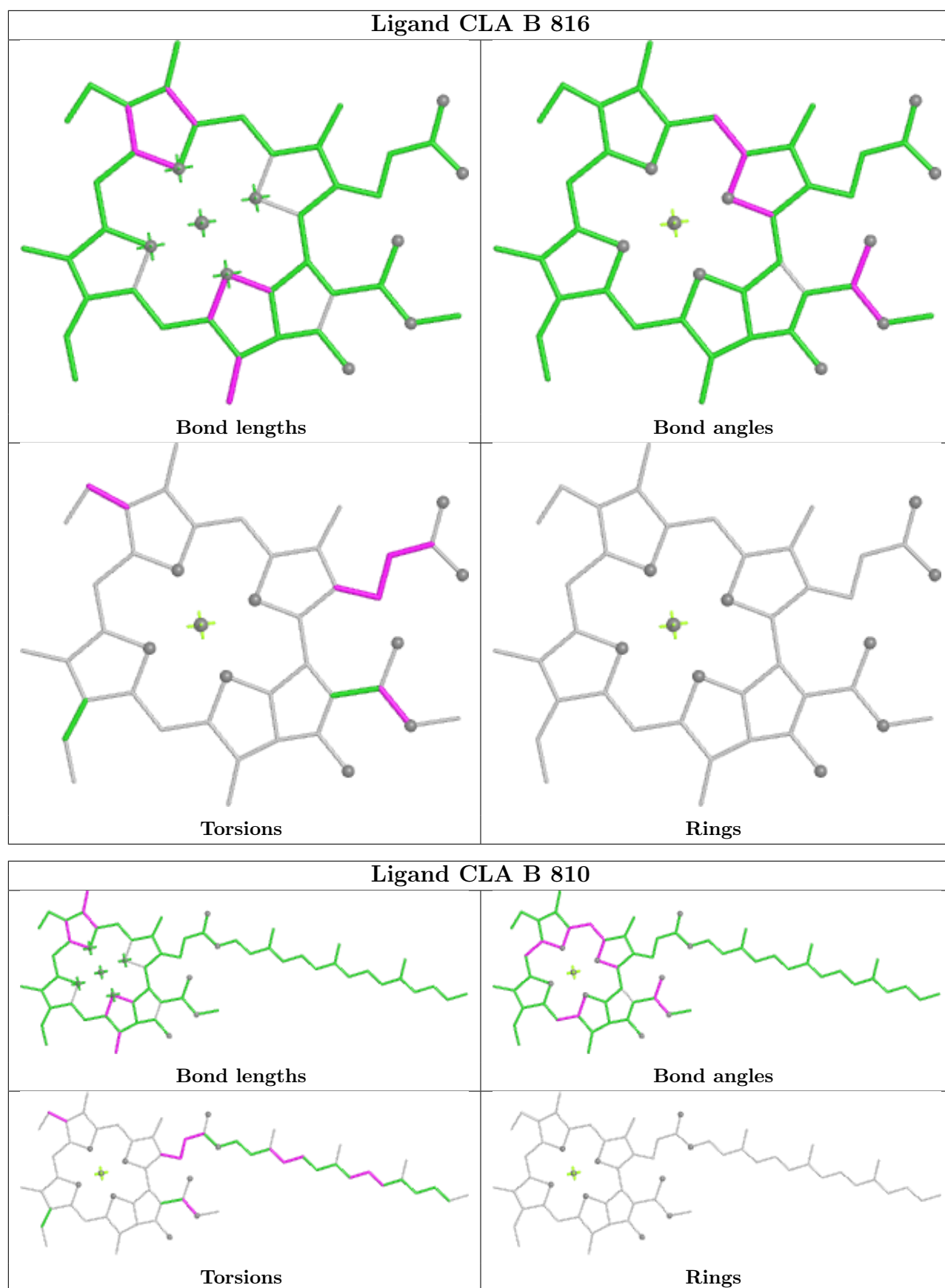


Ligand BCR A 849	
	
Bond lengths	Bond angles
	
Torsions	Rings

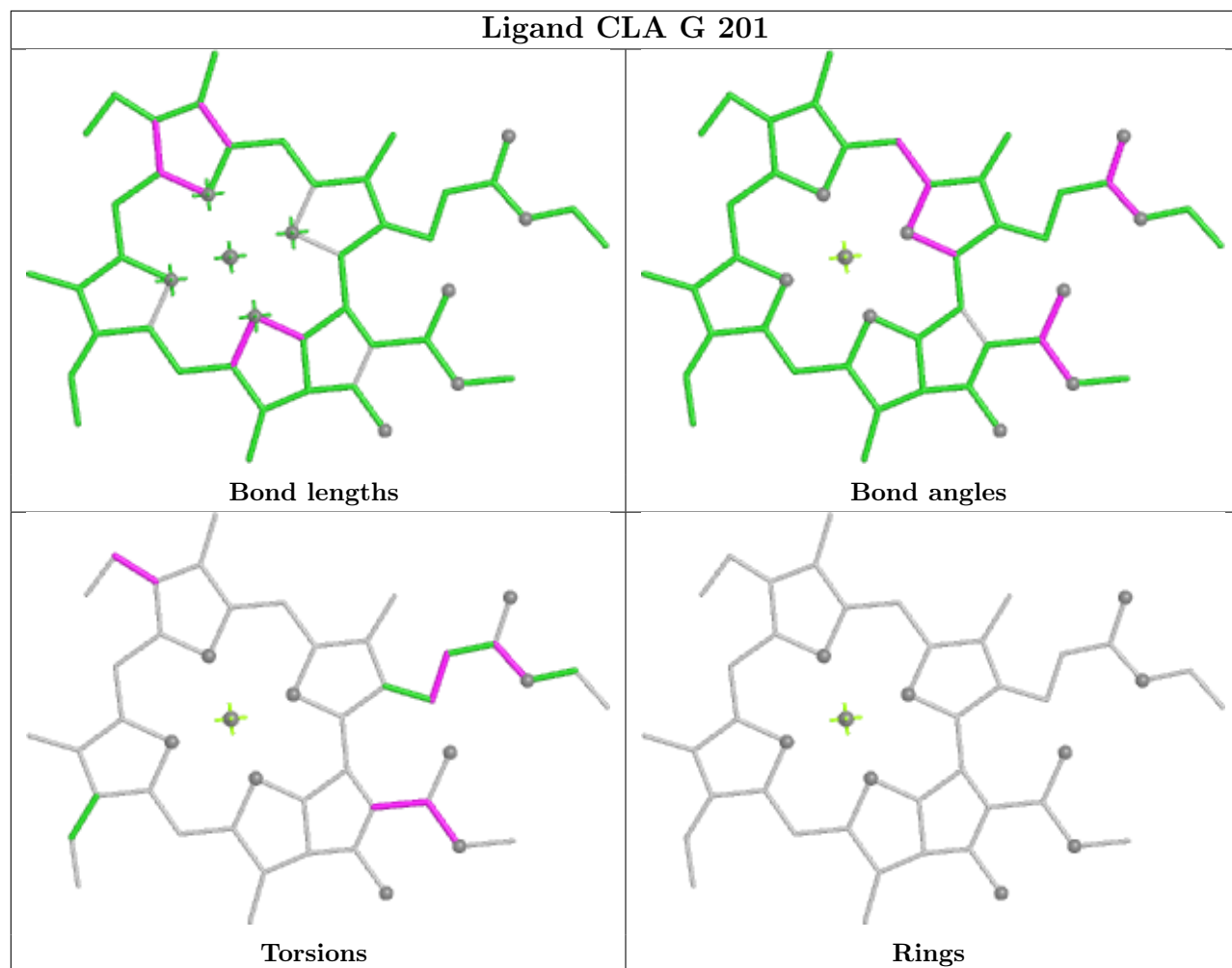
Ligand CLA A 810	
	
Bond lengths	Bond angles
	
Torsions	Rings

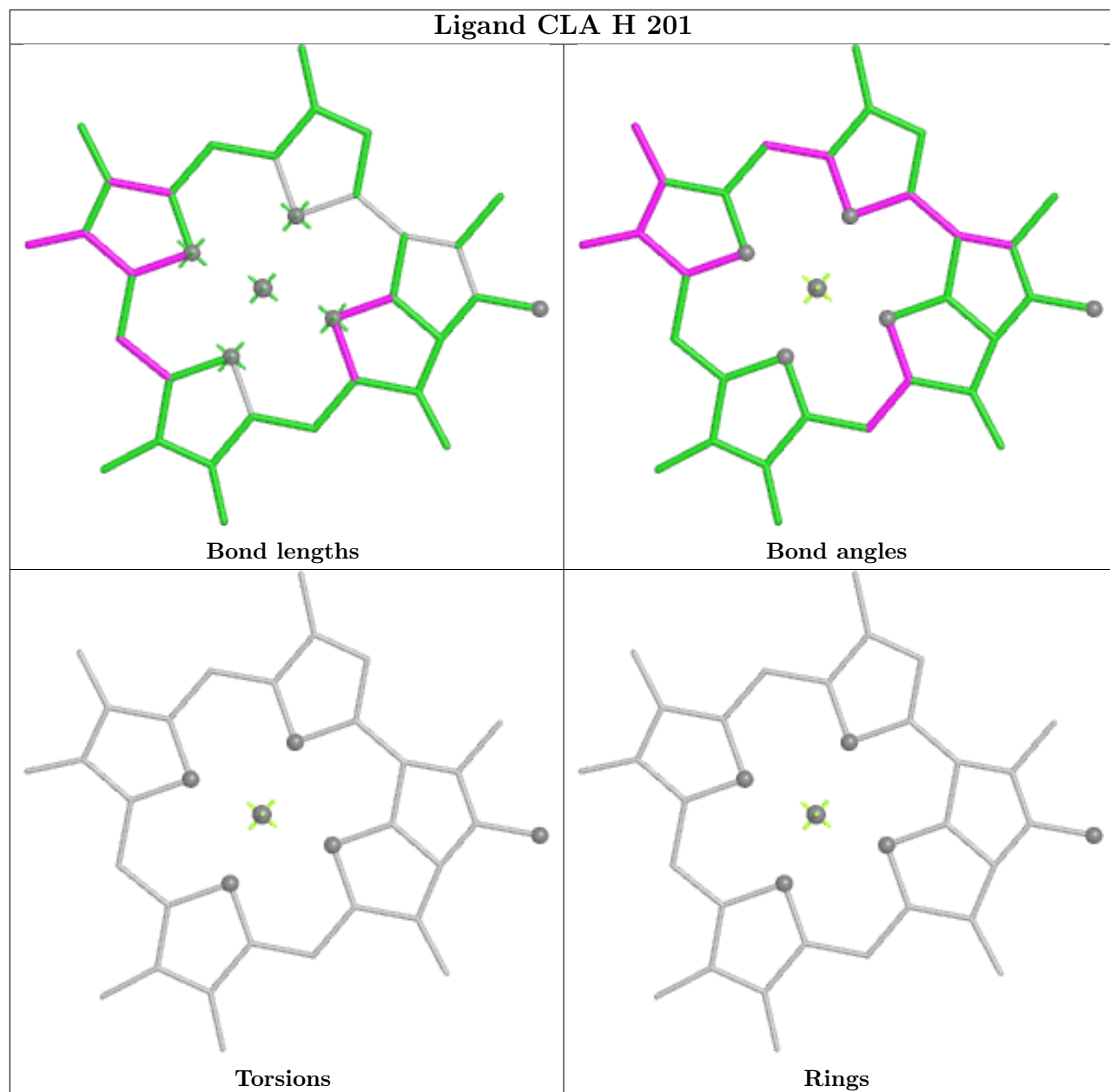


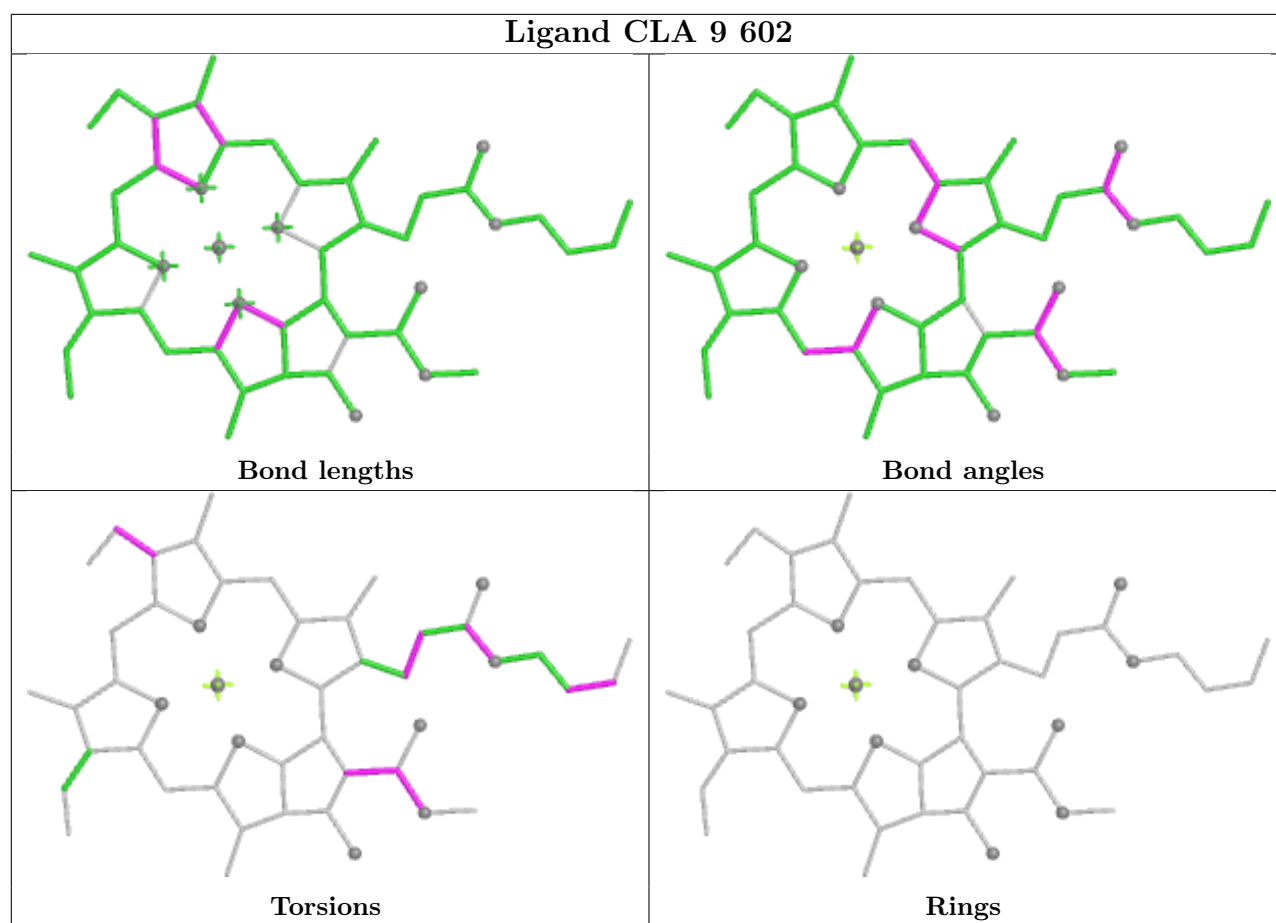




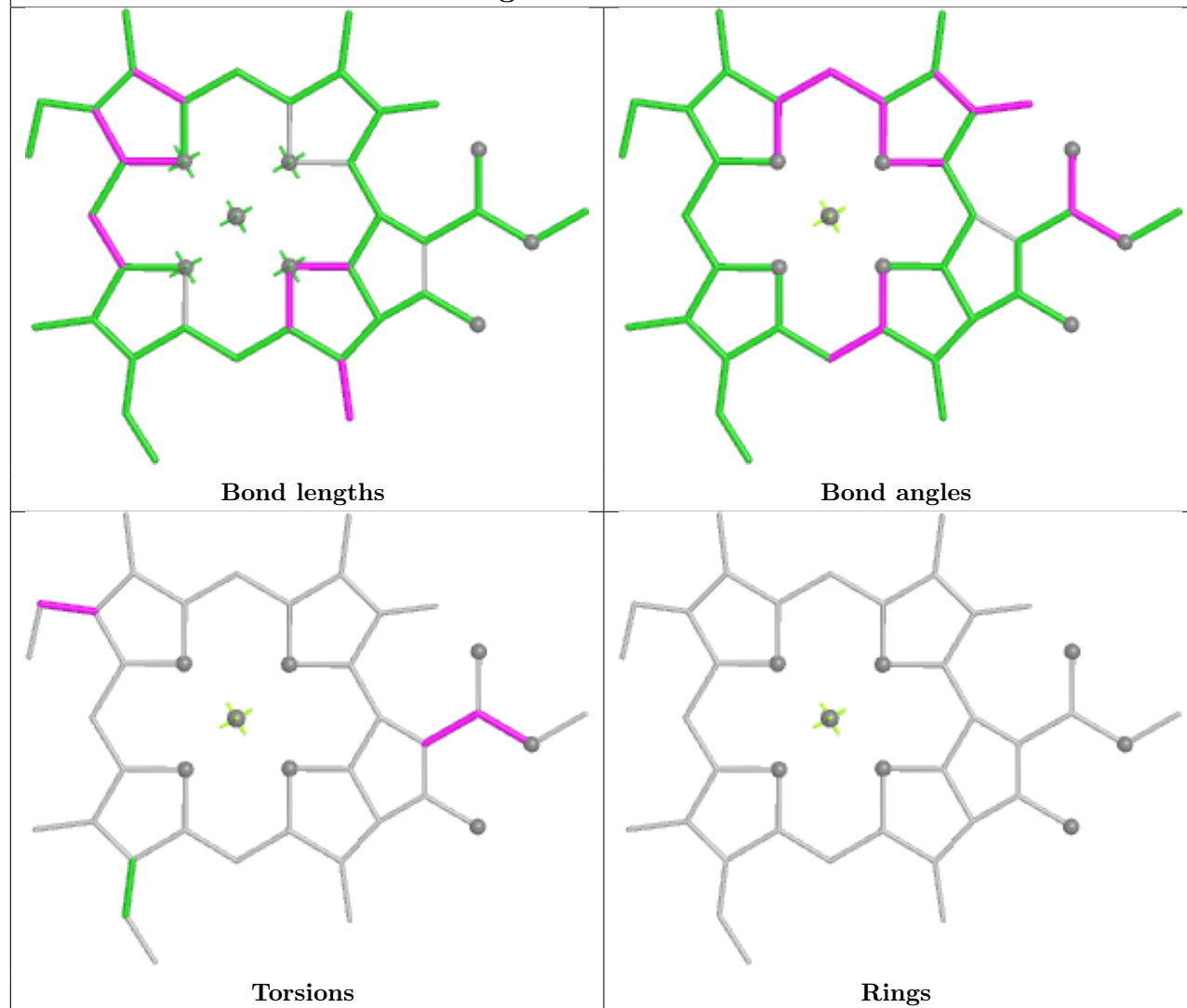
Ligand CLA G 201



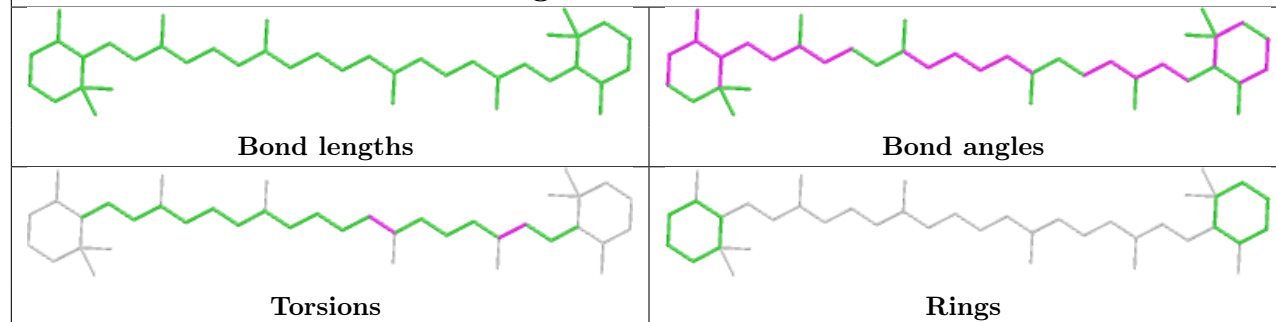




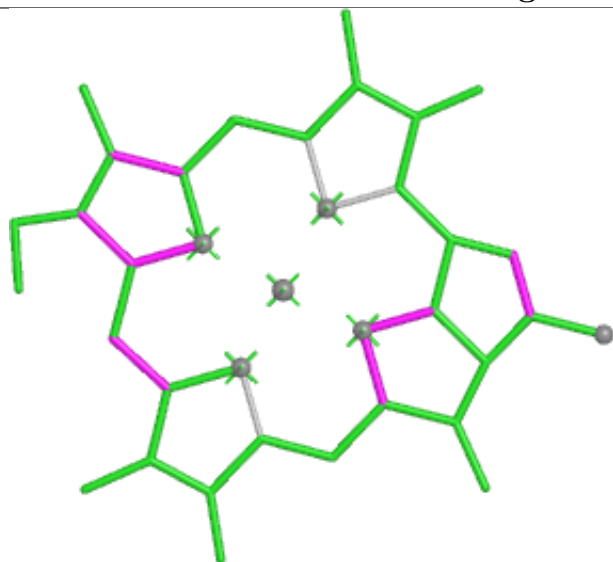
Ligand CLA 2 601



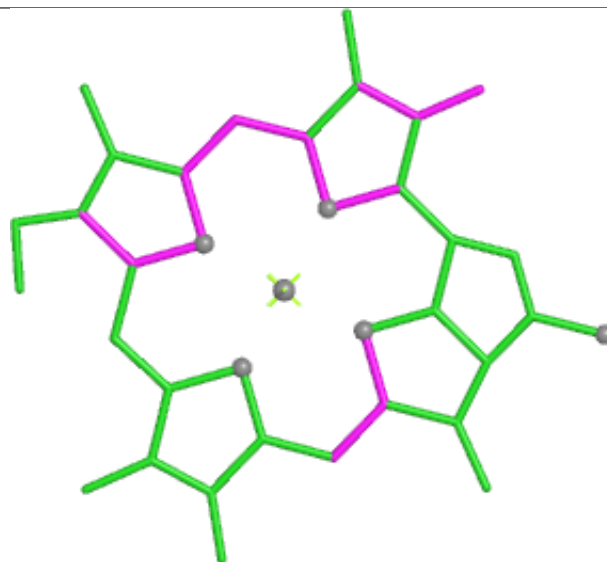
Ligand BCR F 804



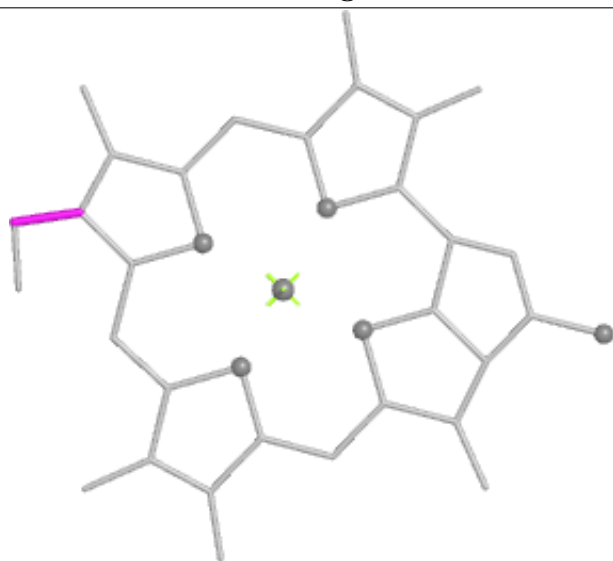
Ligand CLA 2 605



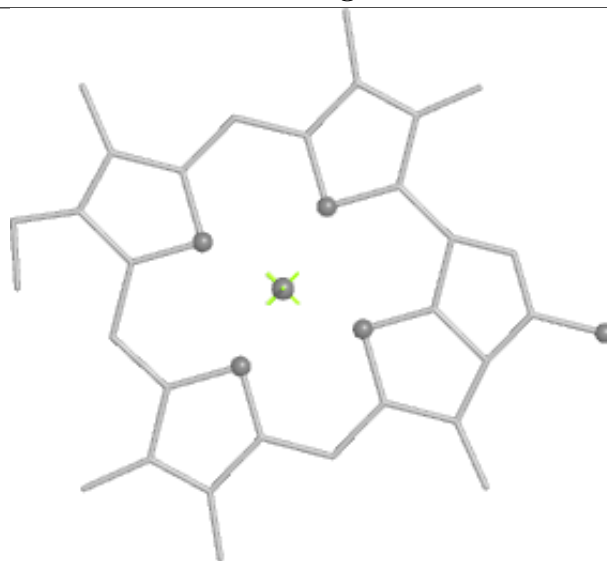
Bond lengths



Bond angles

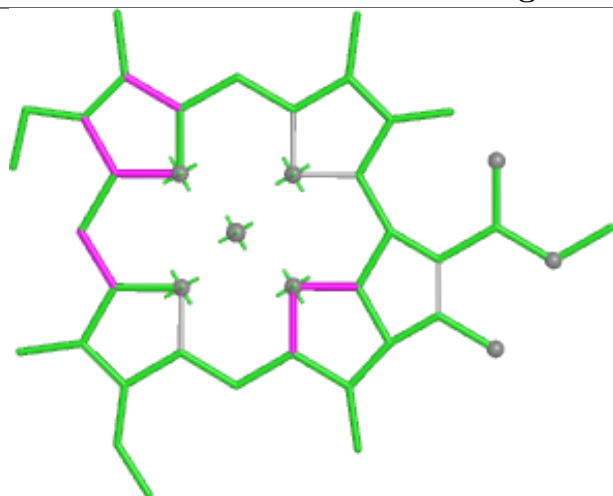


Torsions



Rings

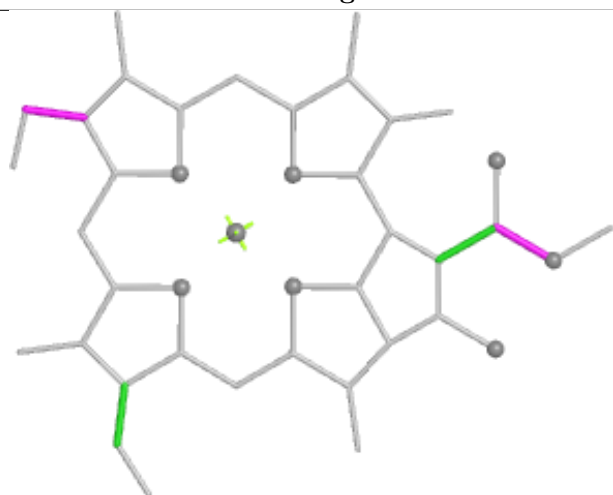
Ligand CLA 9 612



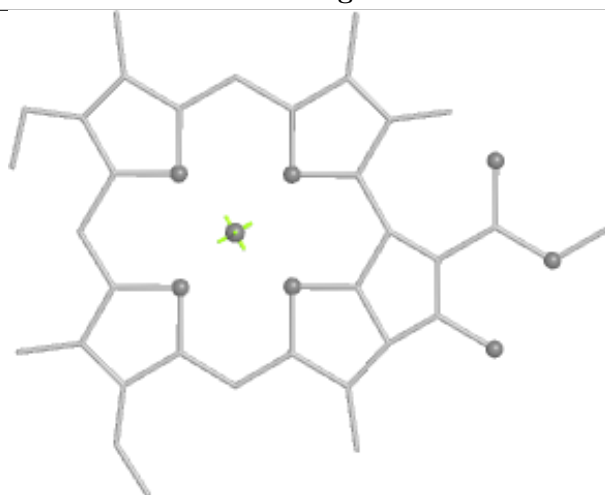
Bond lengths



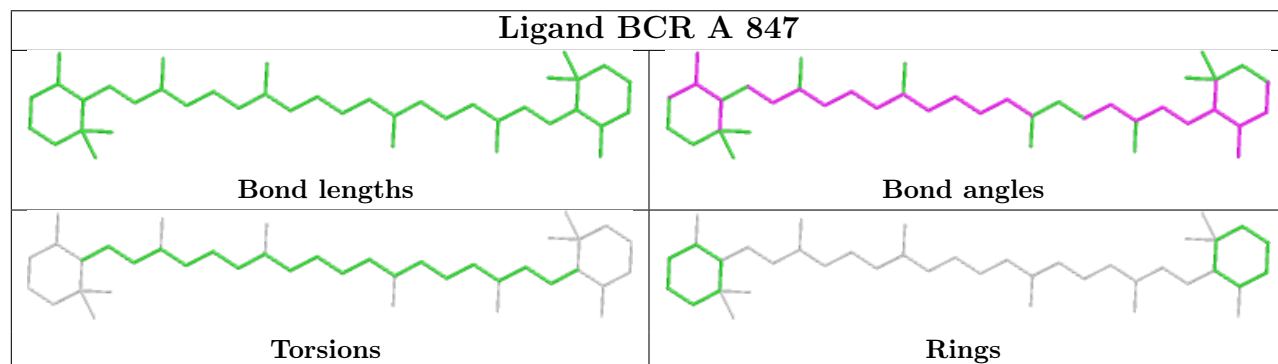
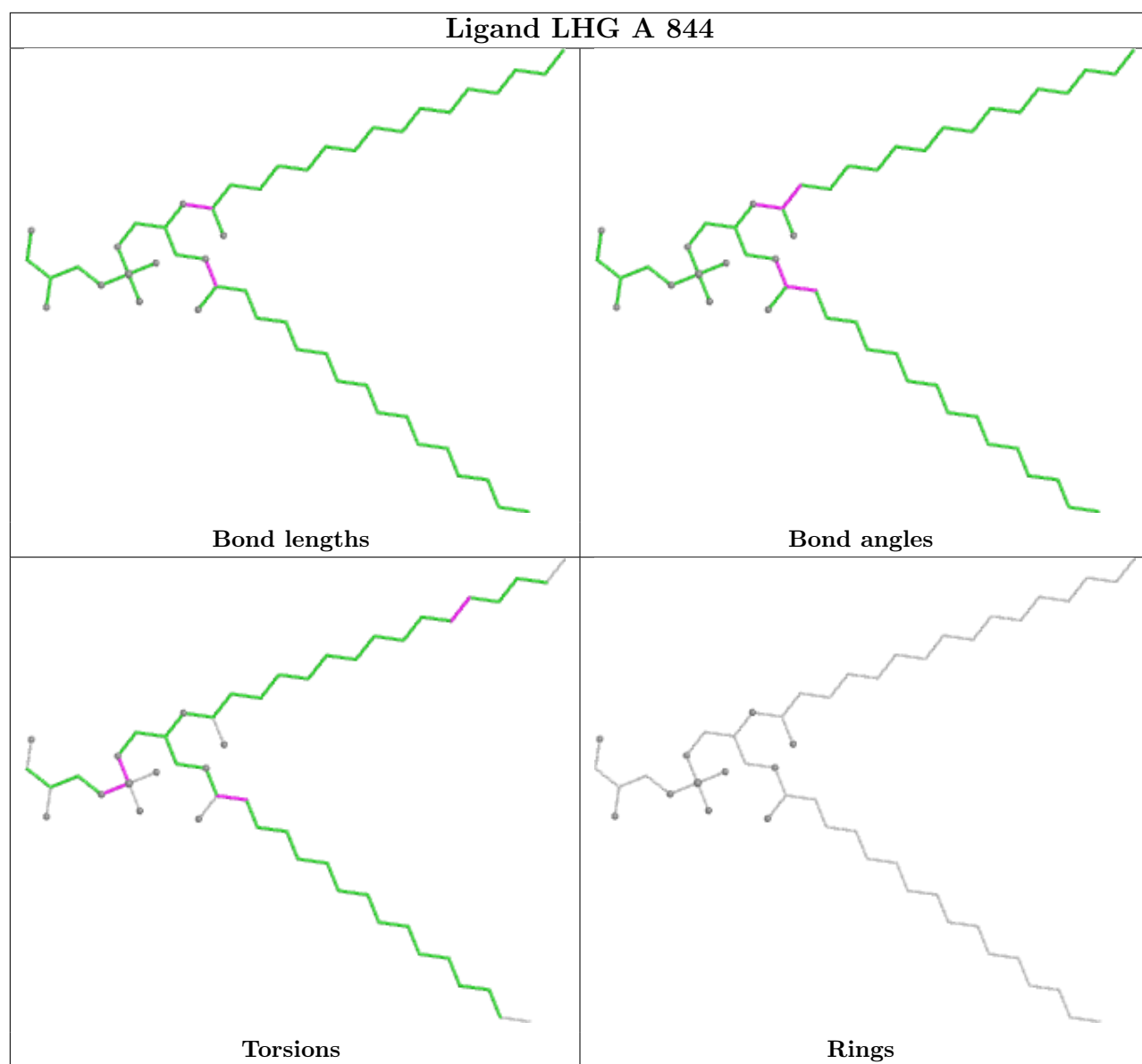
Bond angles



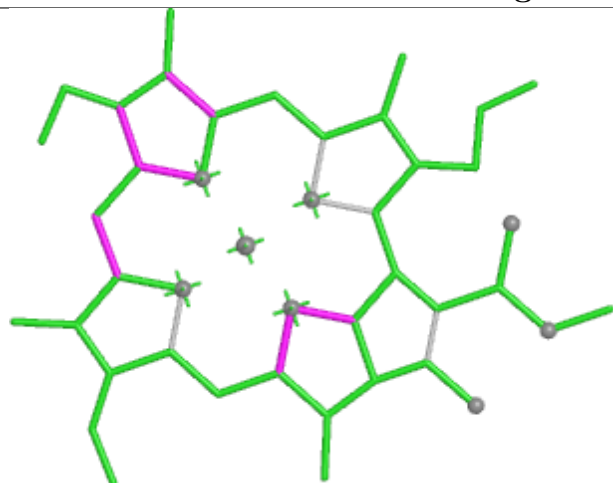
Torsions



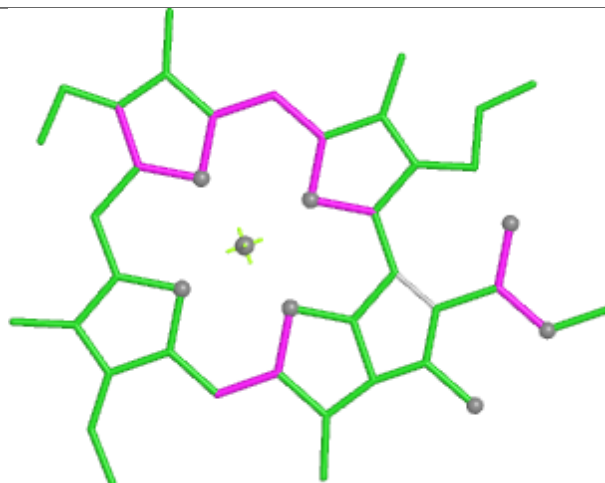
Rings



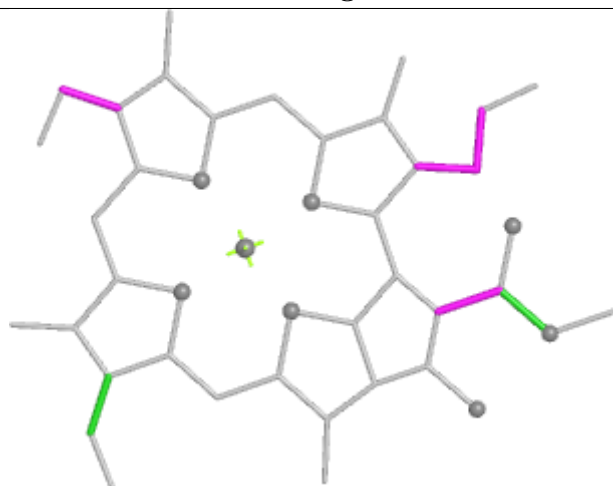
Ligand CLA B 832



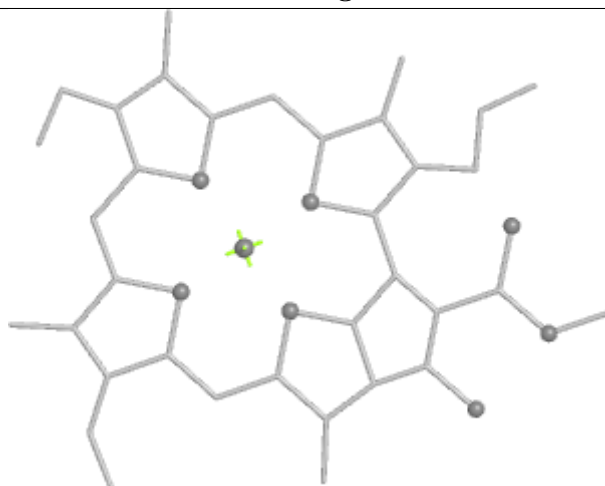
Bond lengths



Bond angles

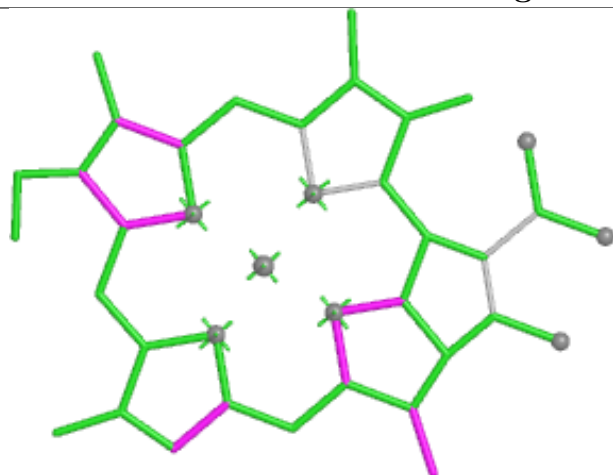


Torsions

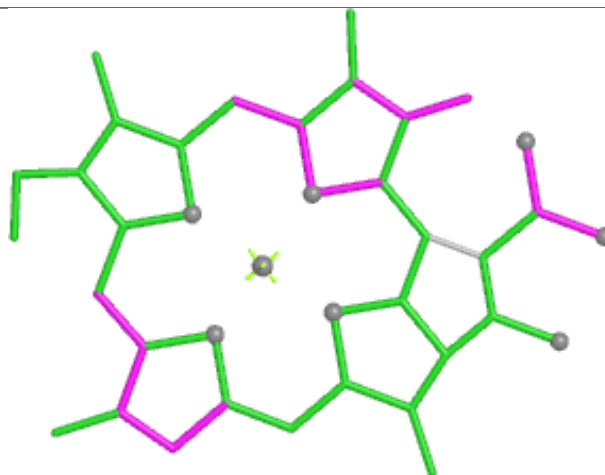


Rings

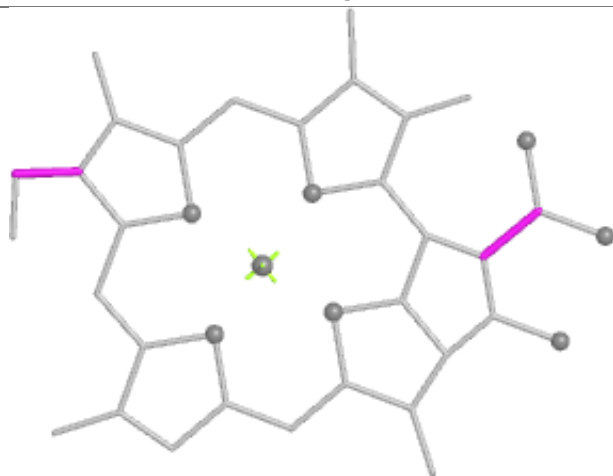
Ligand CLA B 822



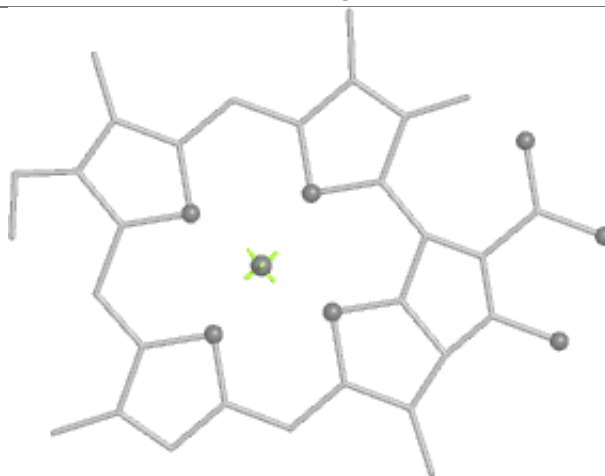
Bond lengths



Bond angles

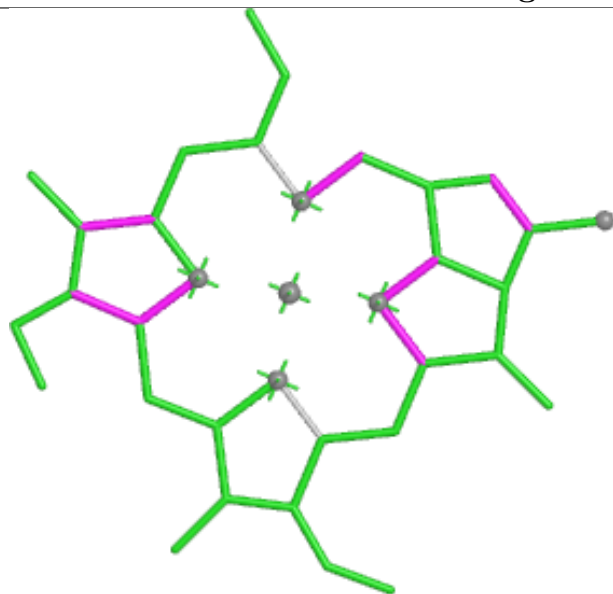


Torsions

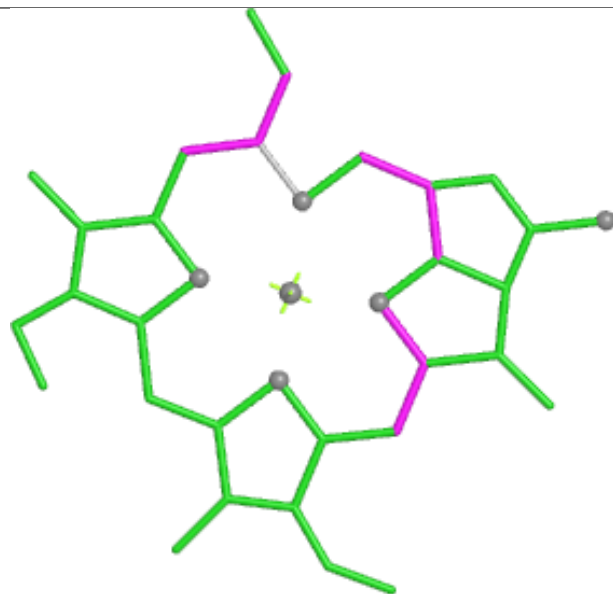


Rings

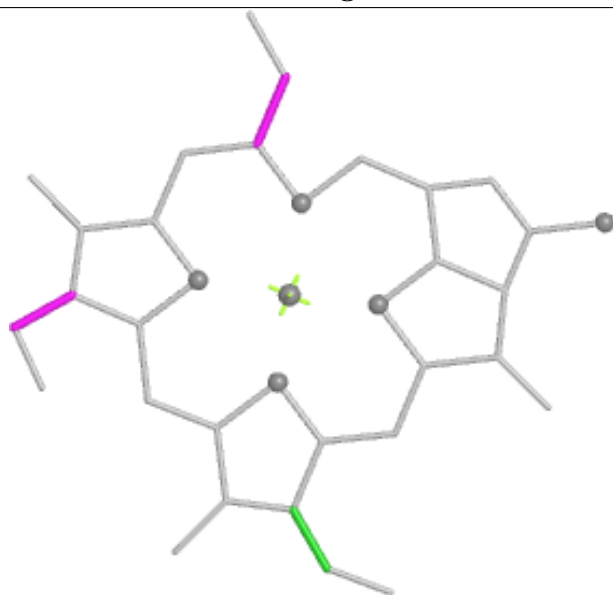
Ligand CLA 9 609



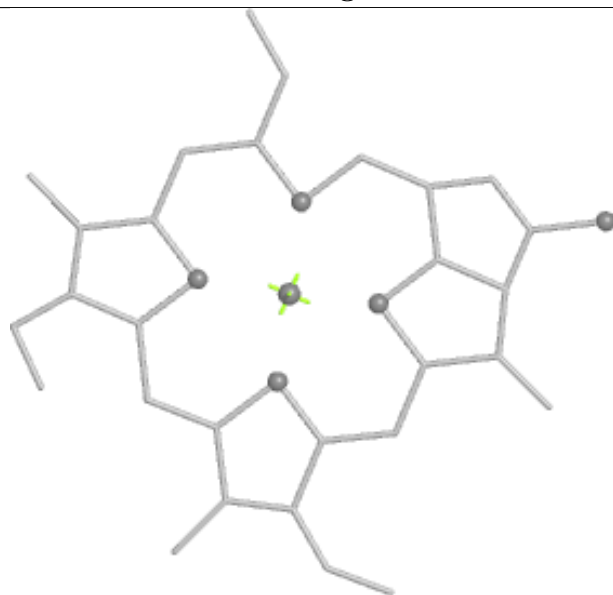
Bond lengths



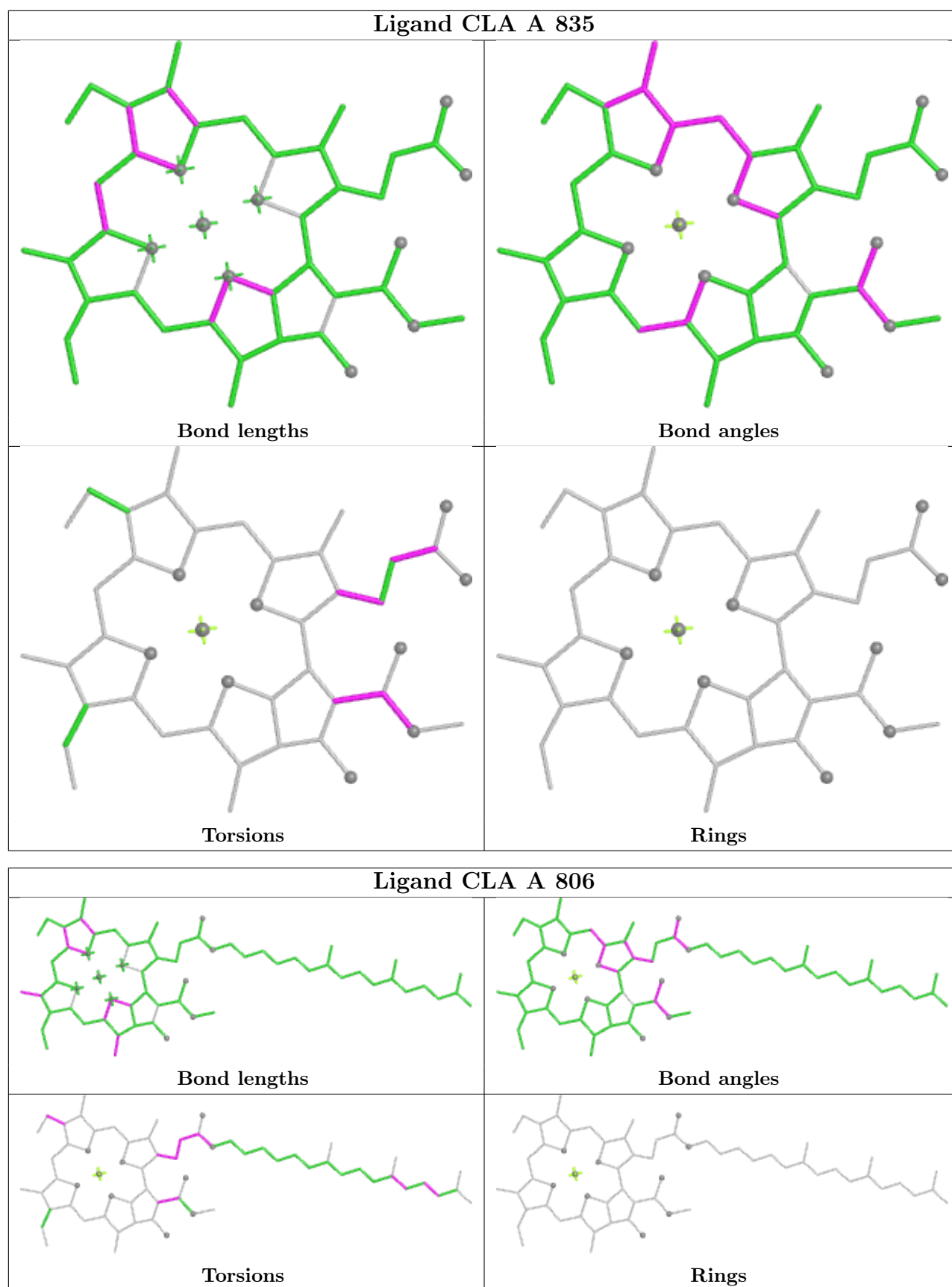
Bond angles

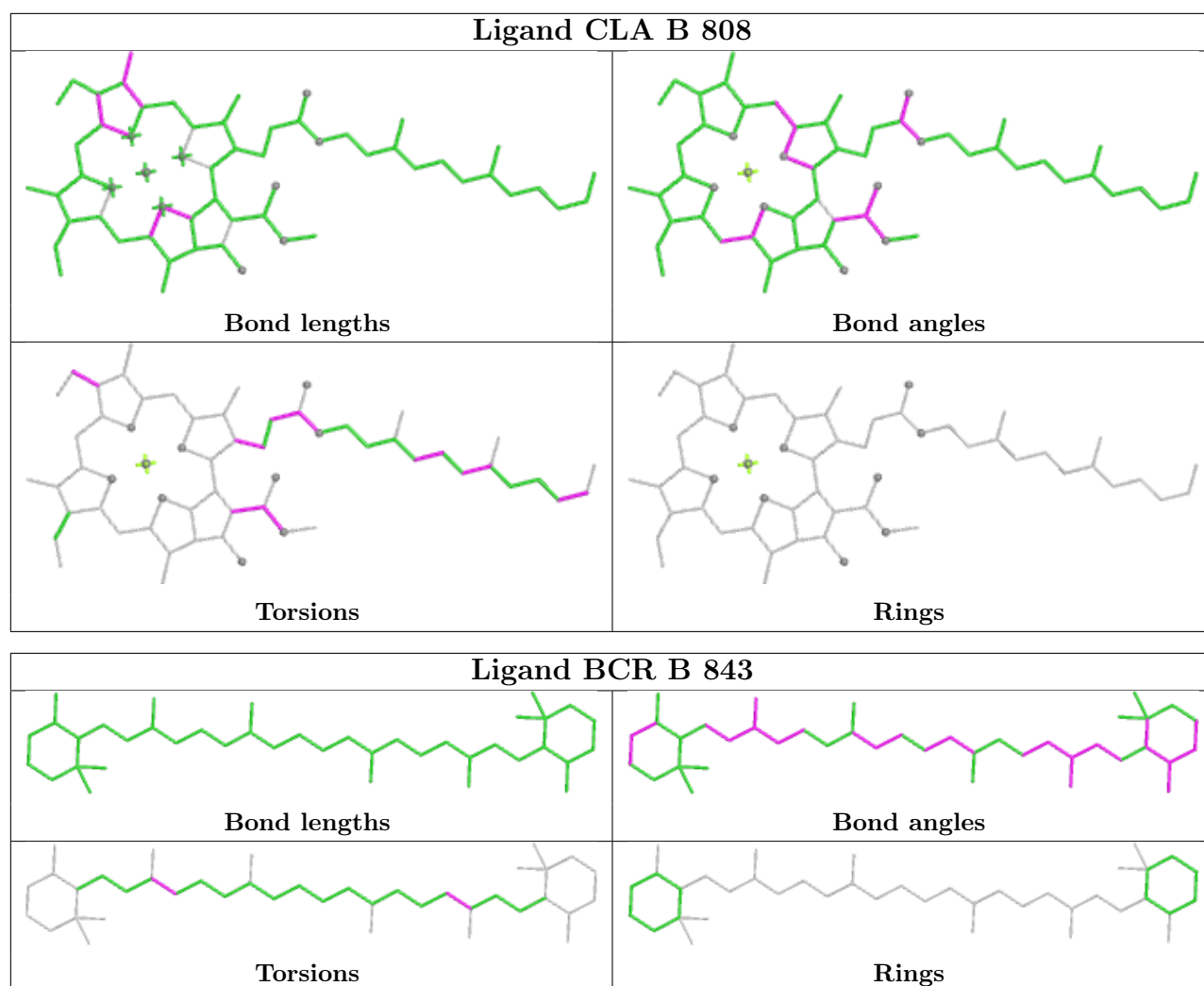


Torsions

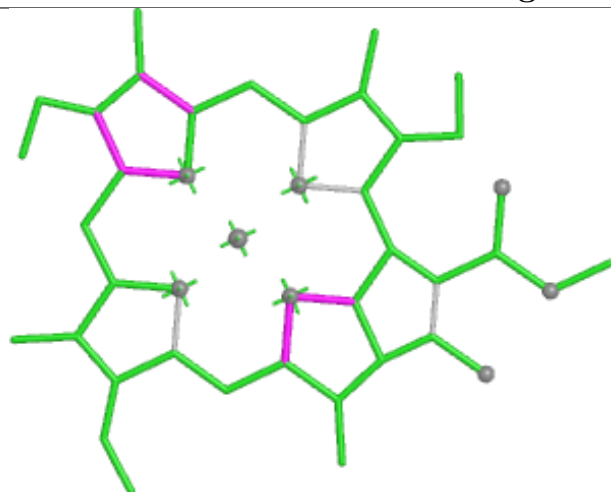


Rings

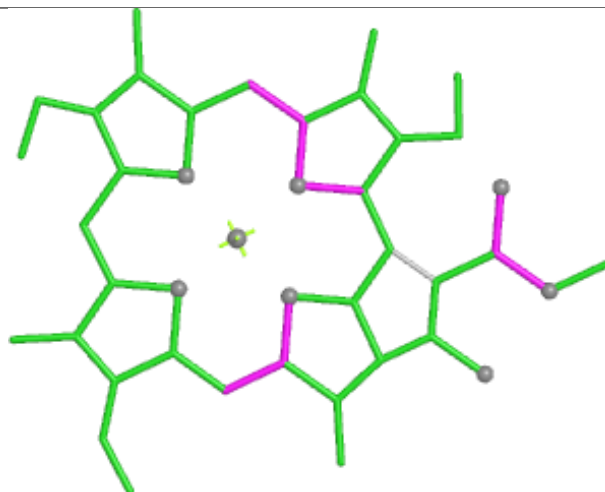




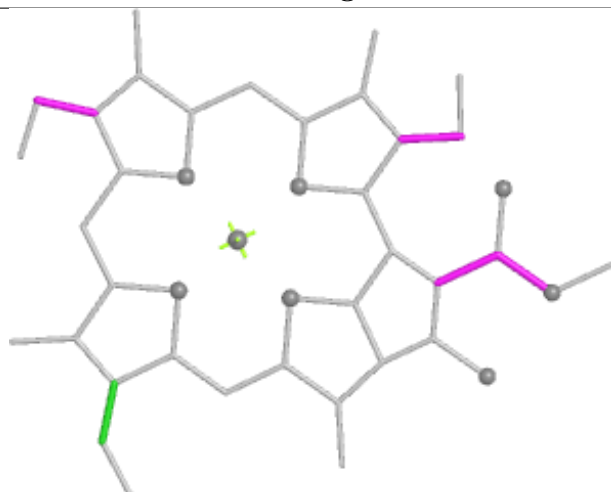
Ligand CLA 9 611



Bond lengths



Bond angles

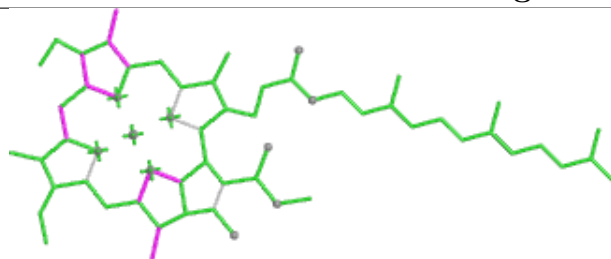


Torsions

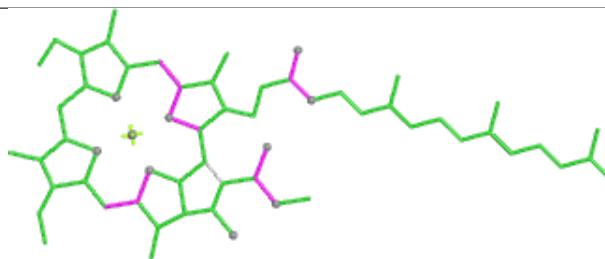


Rings

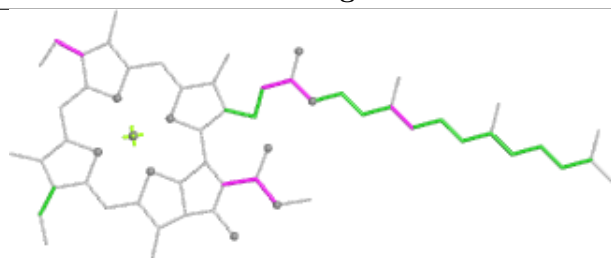
Ligand CLA A 820



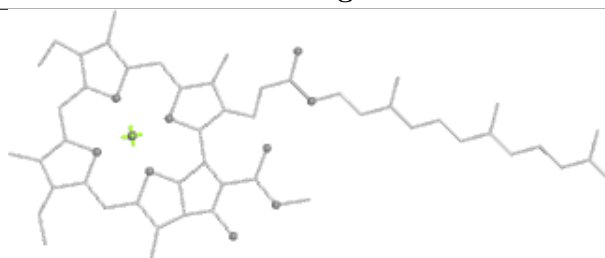
Bond lengths



Bond angles

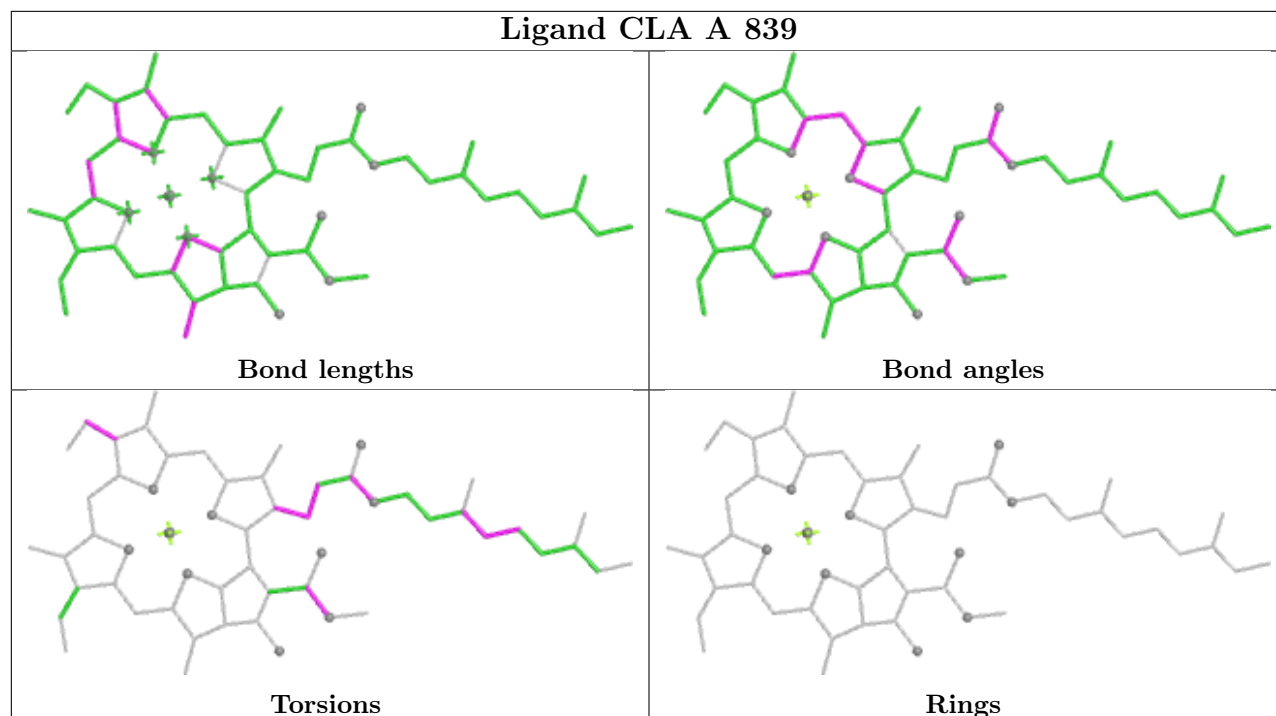


Torsions

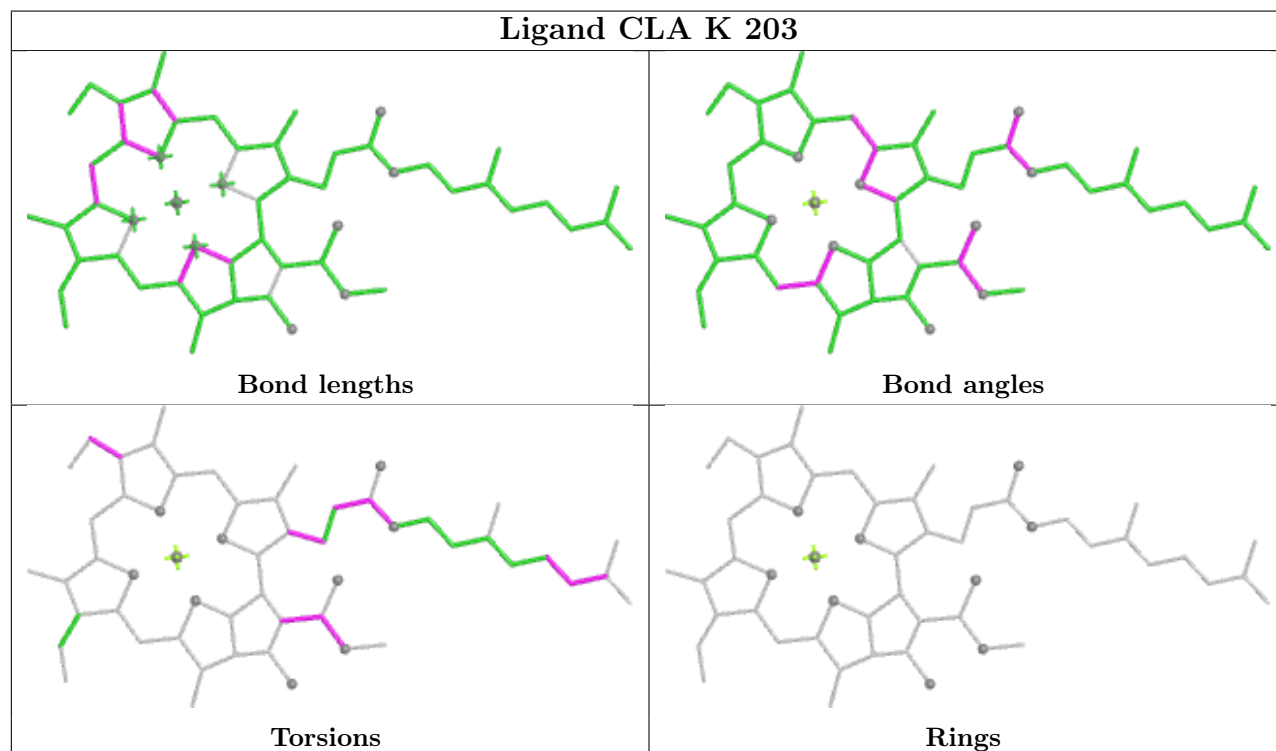


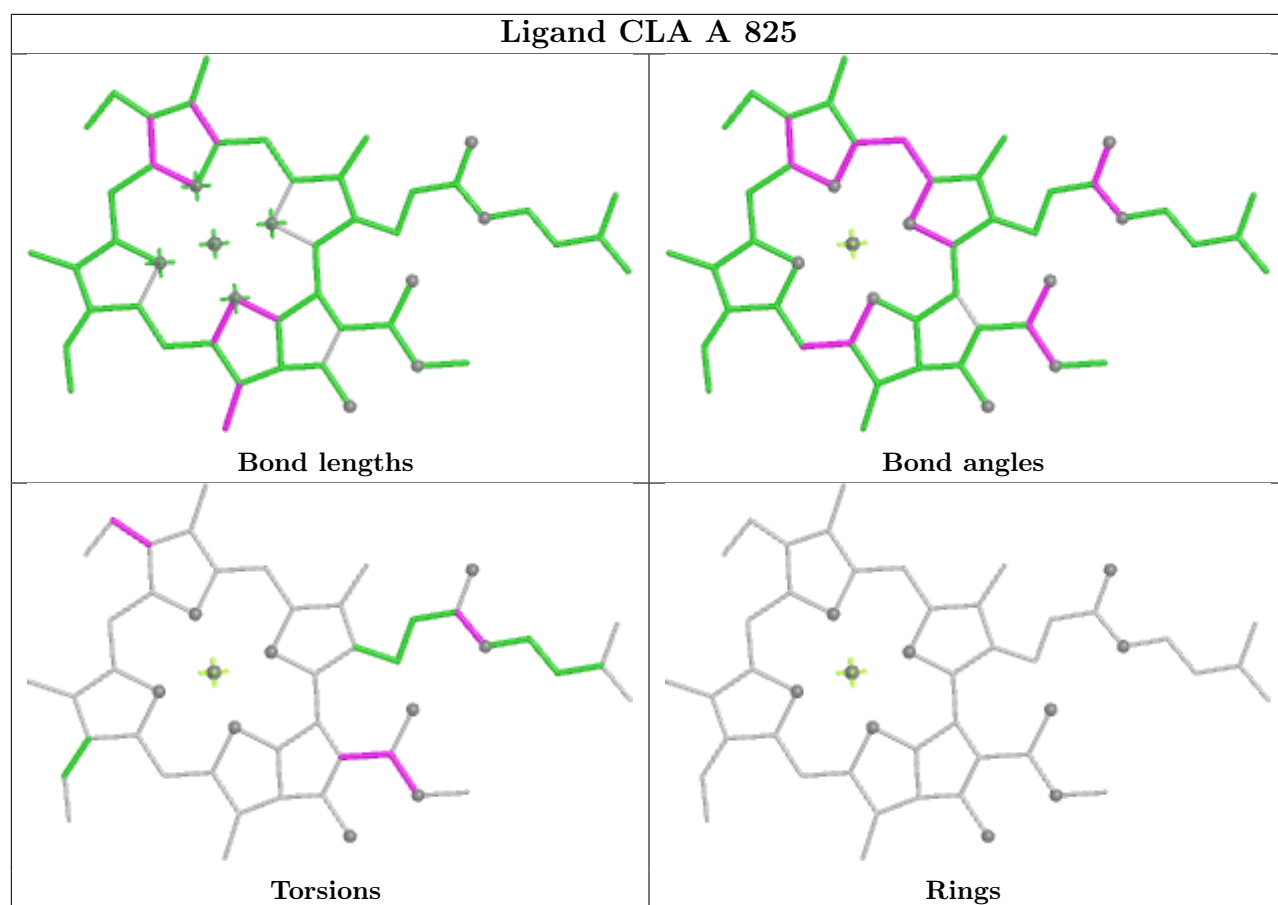
Rings

Ligand CLA A 839

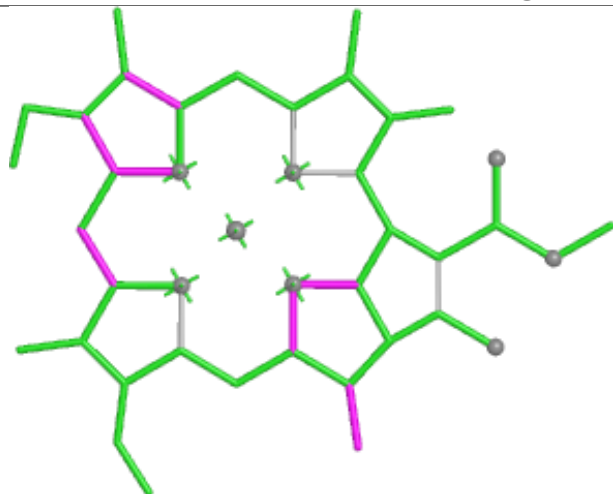


Ligand CLA K 203

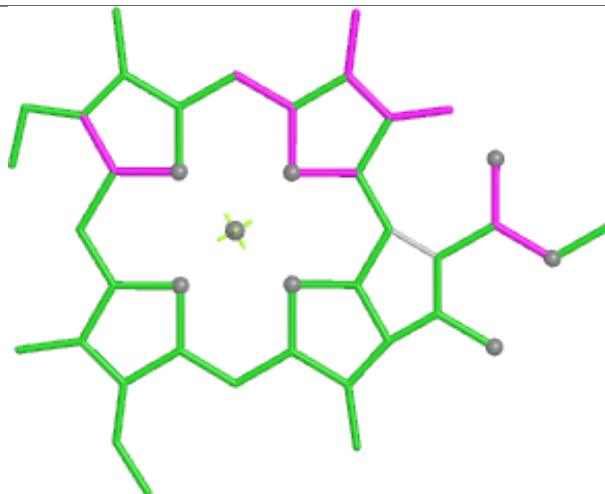




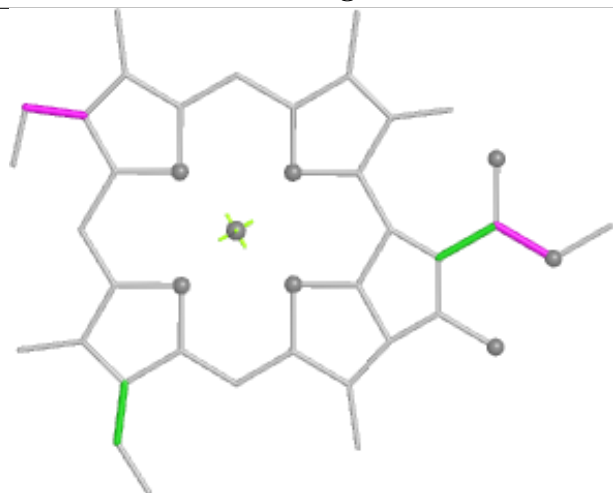
Ligand CLA 2 607



Bond lengths



Bond angles

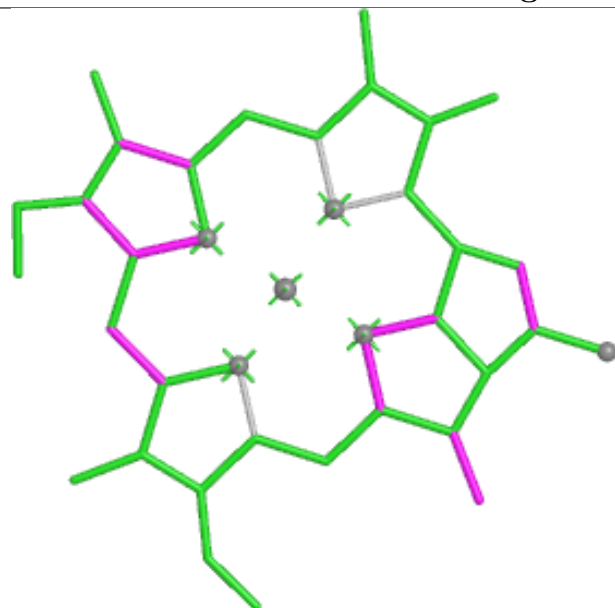


Torsions

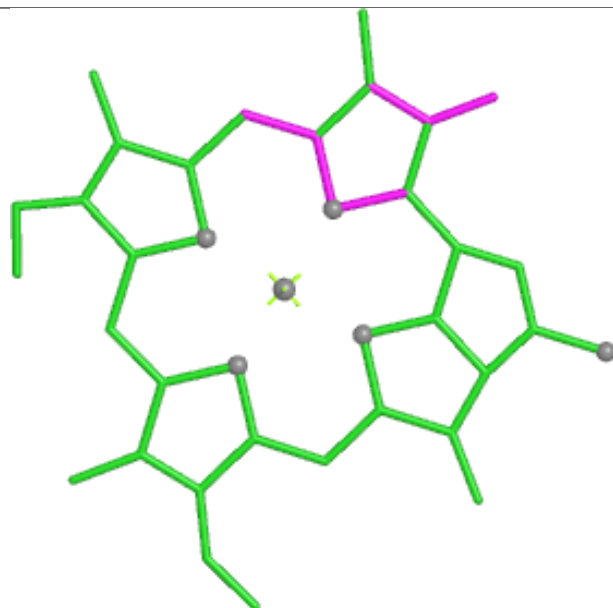


Rings

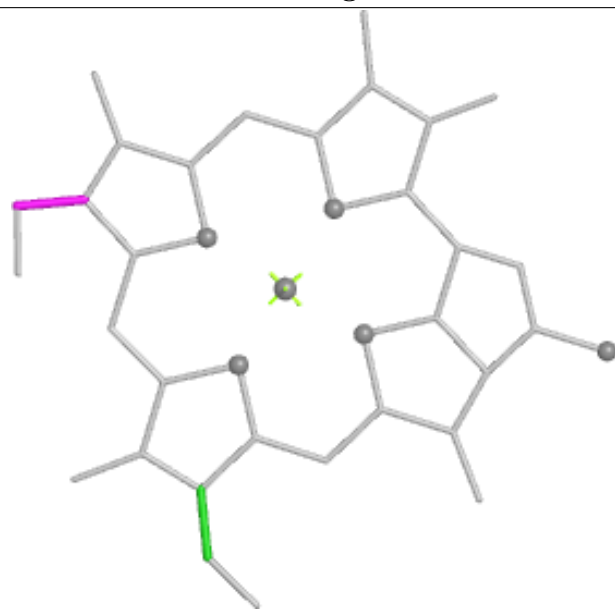
Ligand CLA 2 606



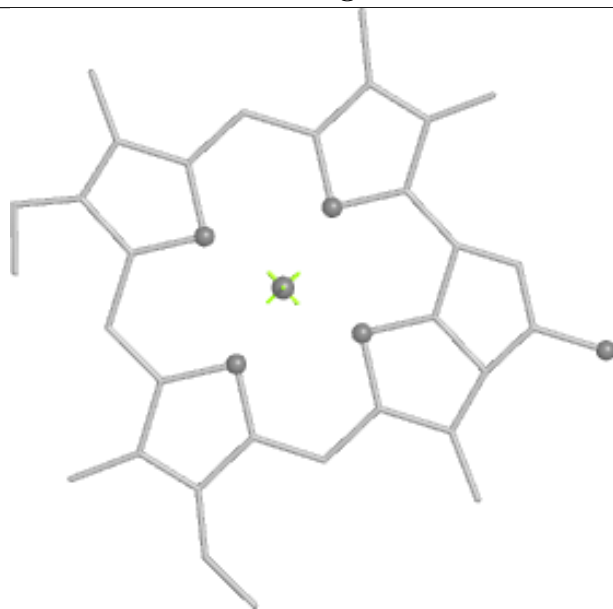
Bond lengths



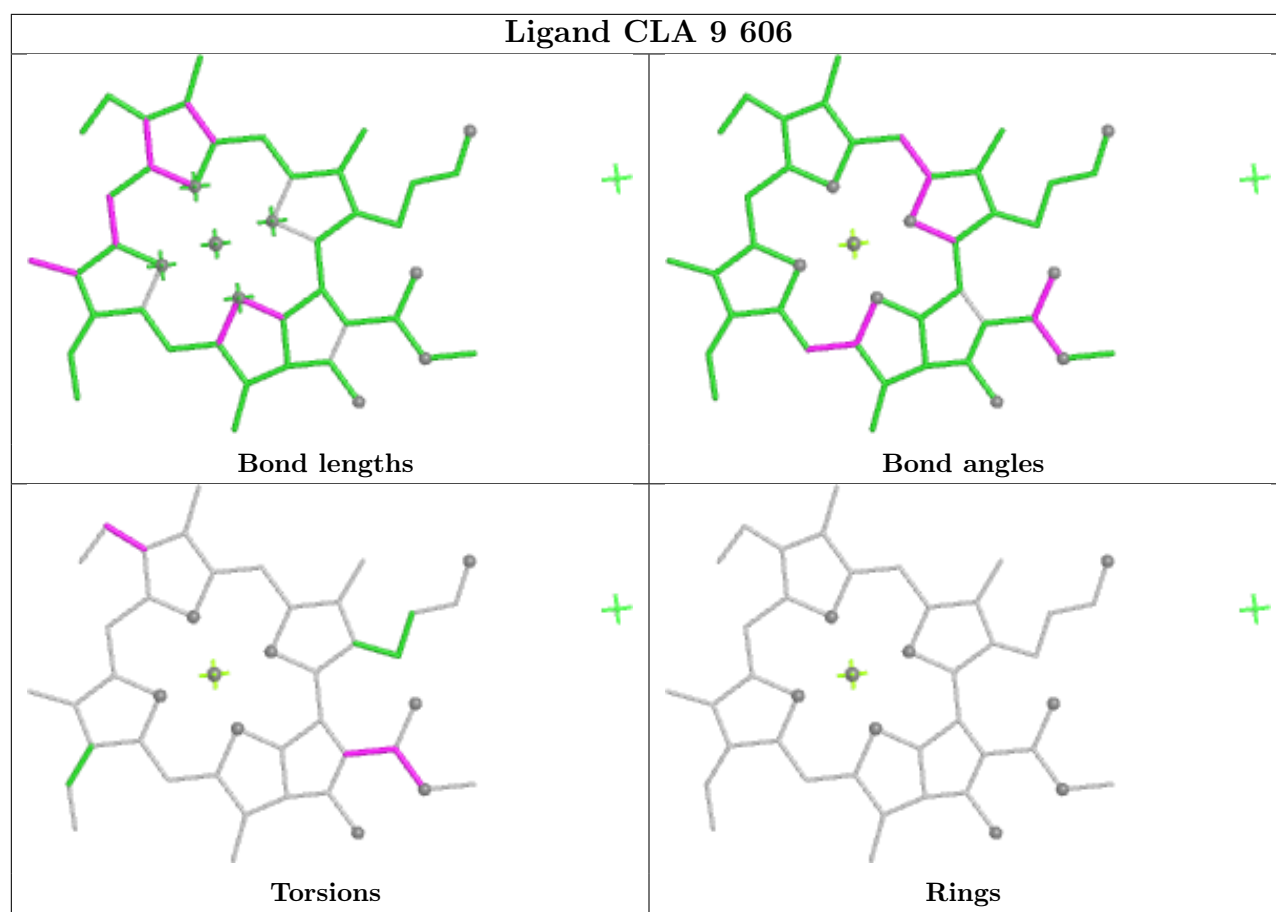
Bond angles



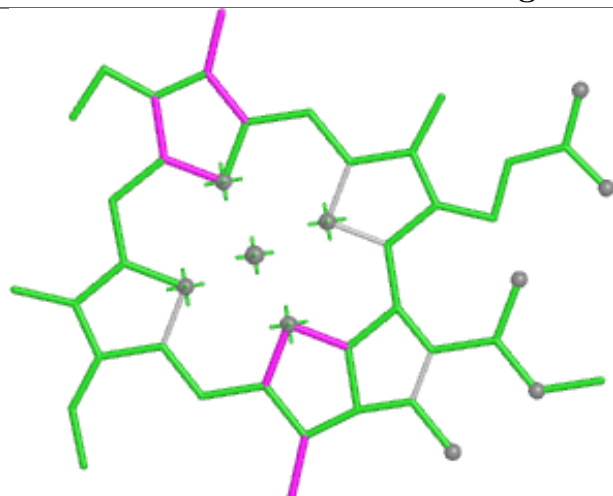
Torsions



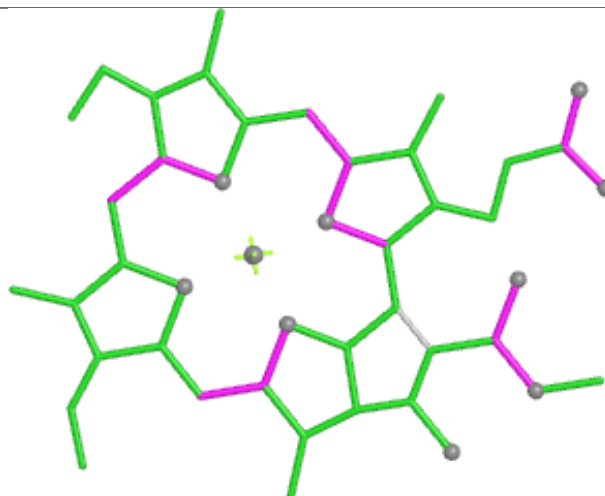
Rings



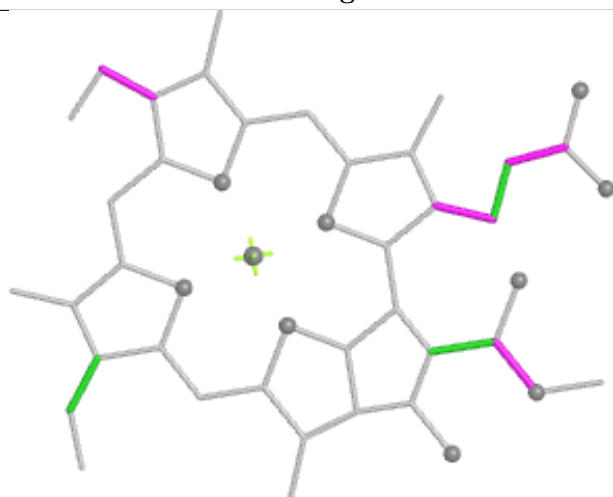
Ligand CLA 9 607



Bond lengths



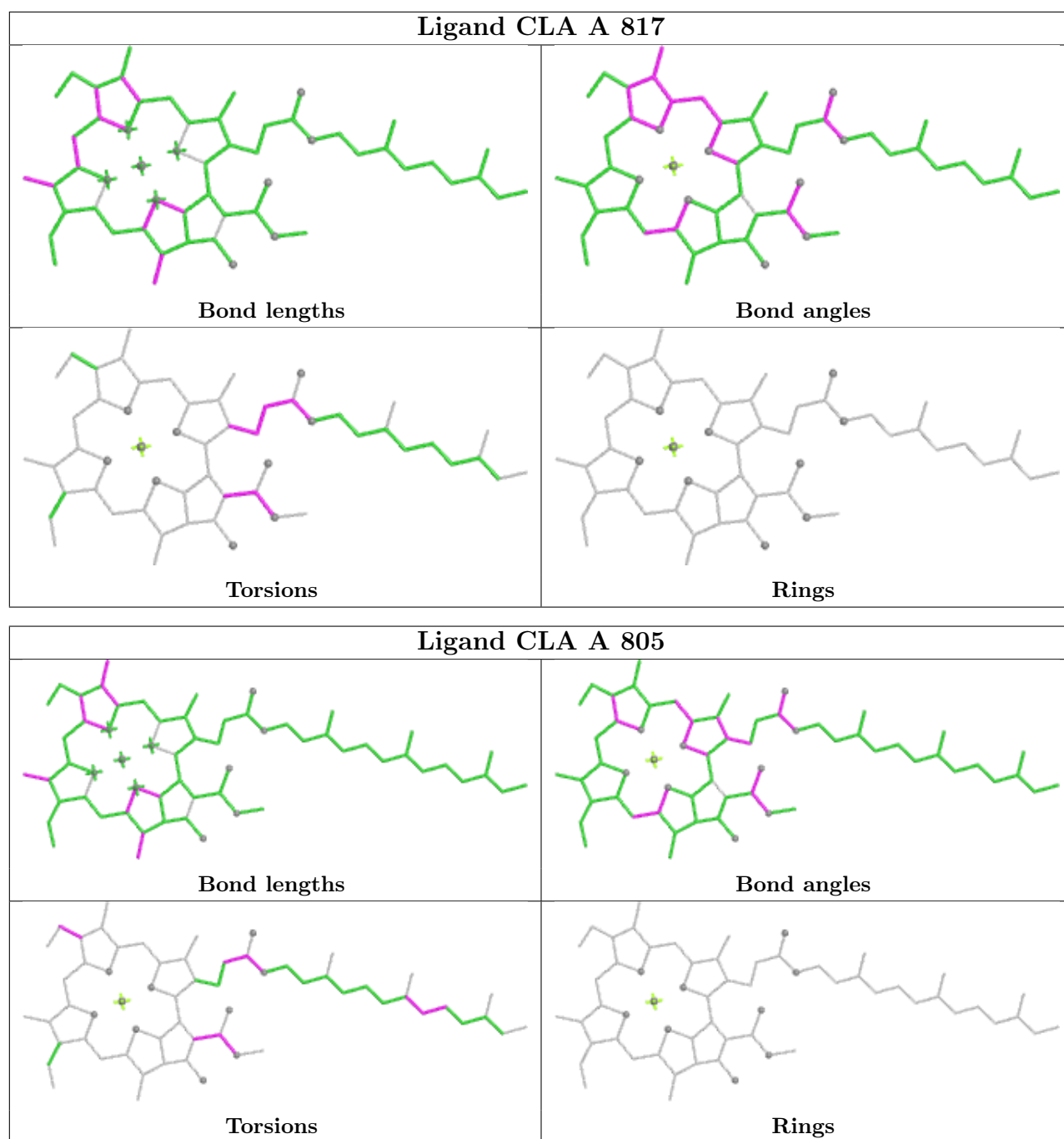
Bond angles



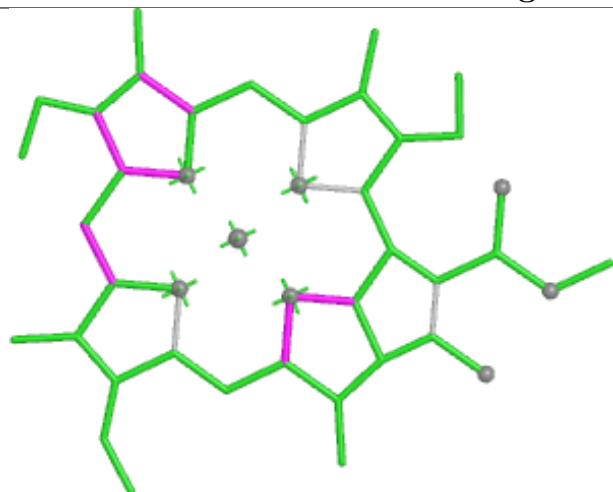
Torsions



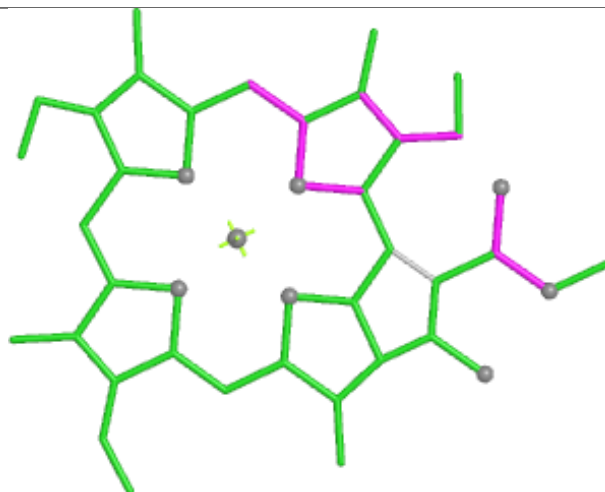
Rings



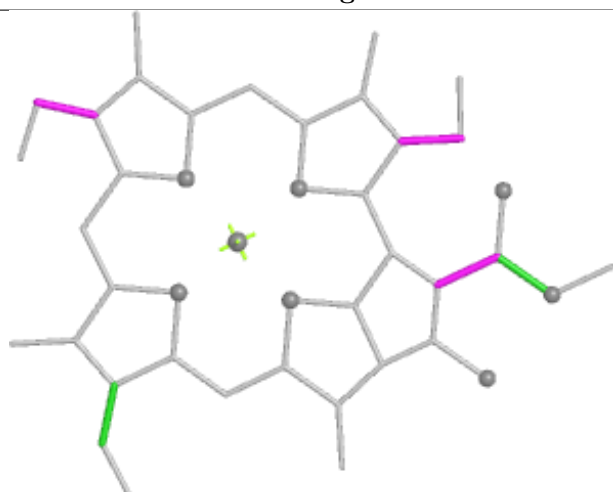
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Bond lengths



Bond angles

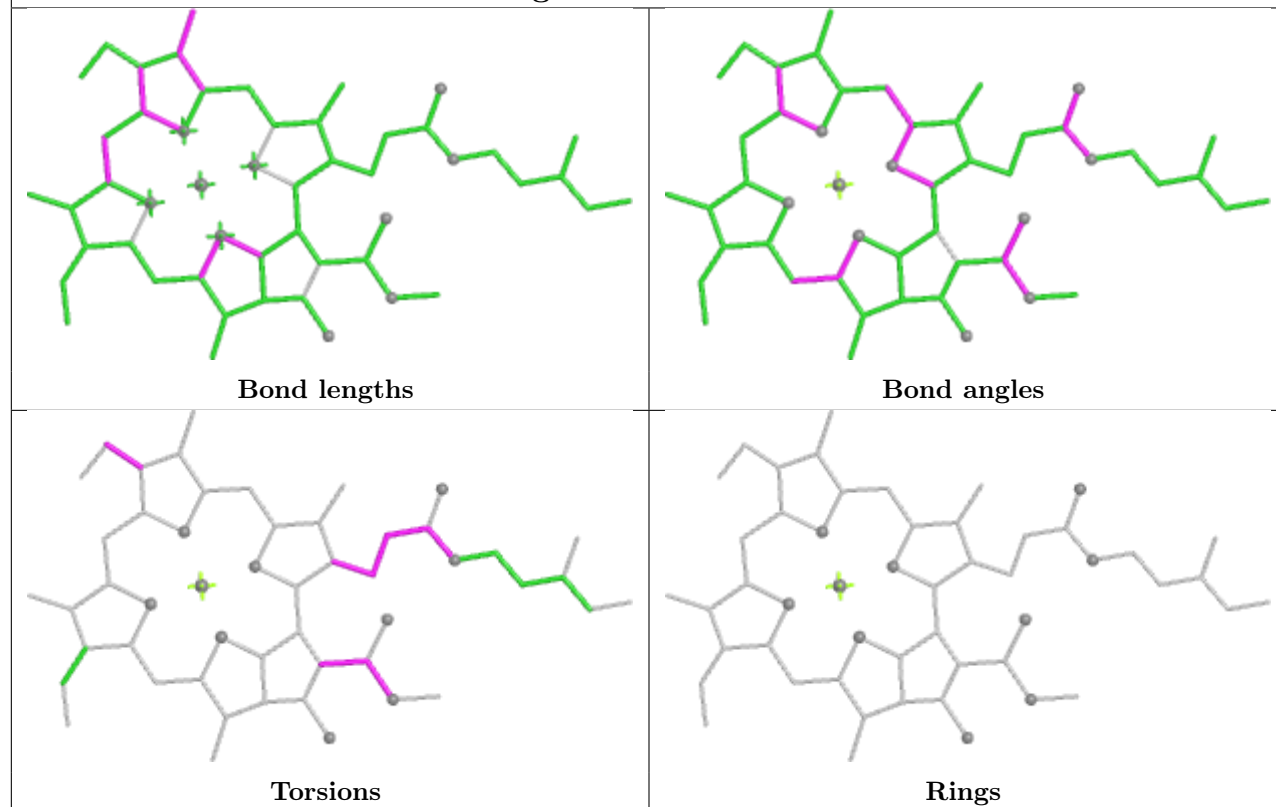


Torsions

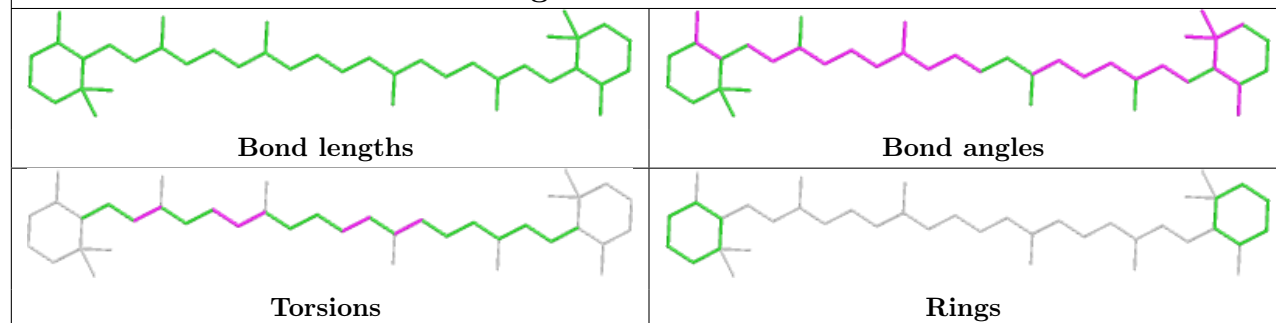


Rings

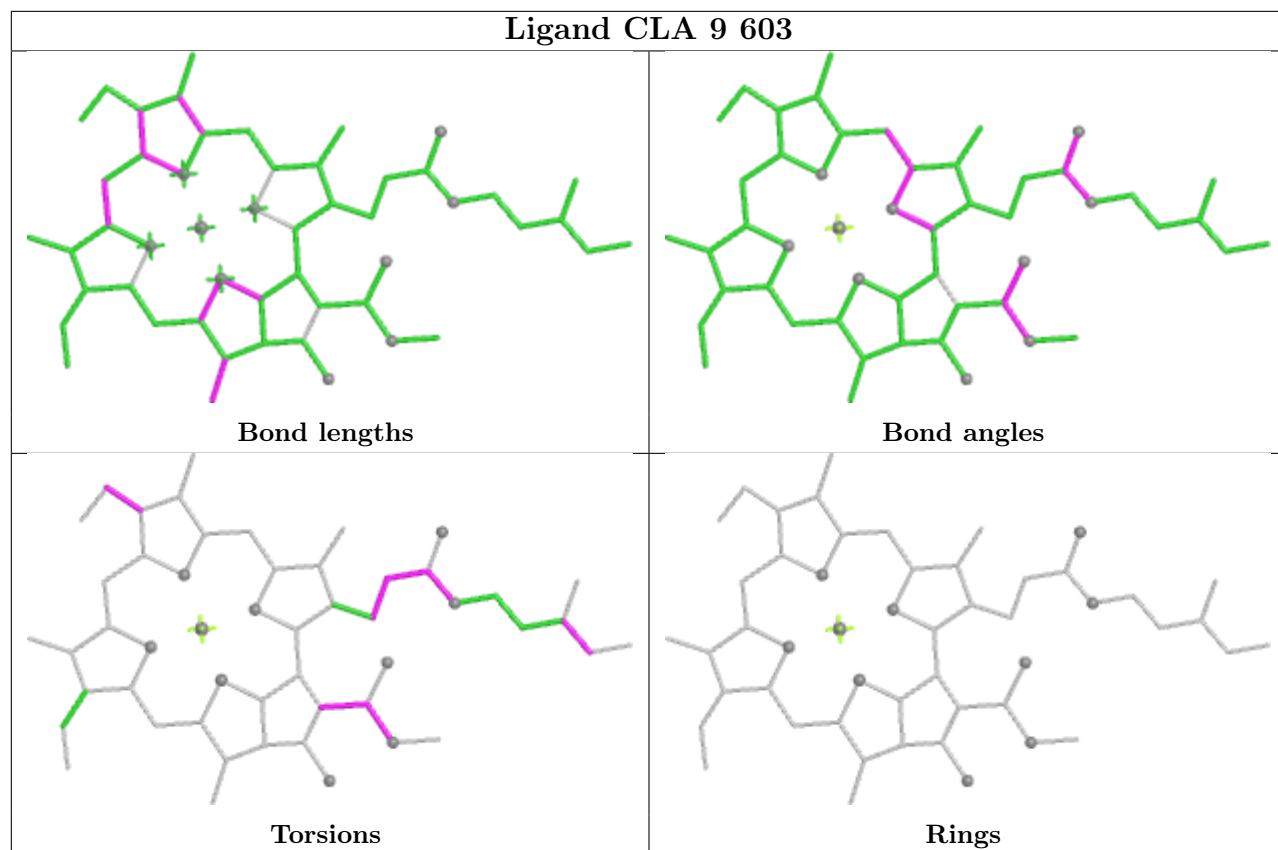
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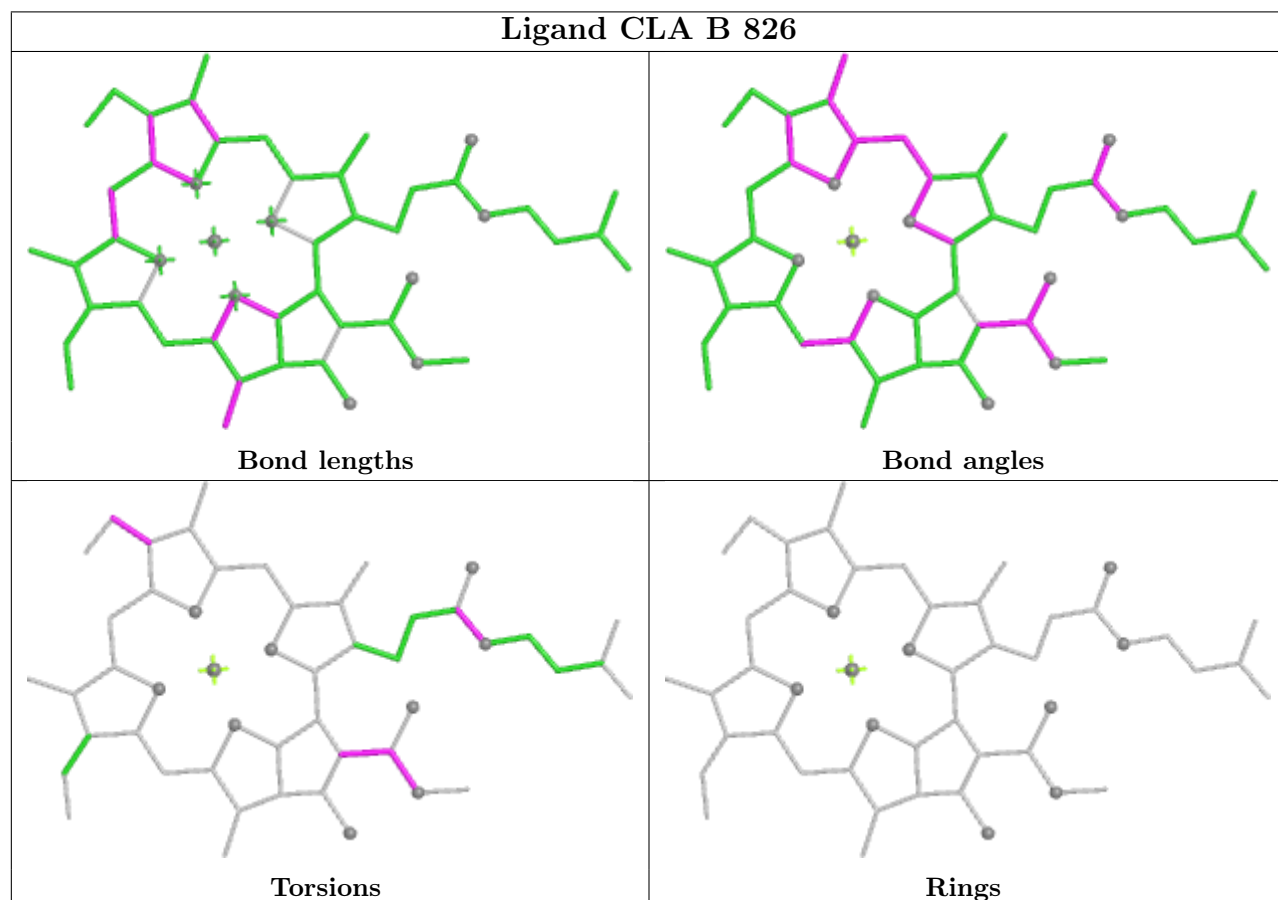
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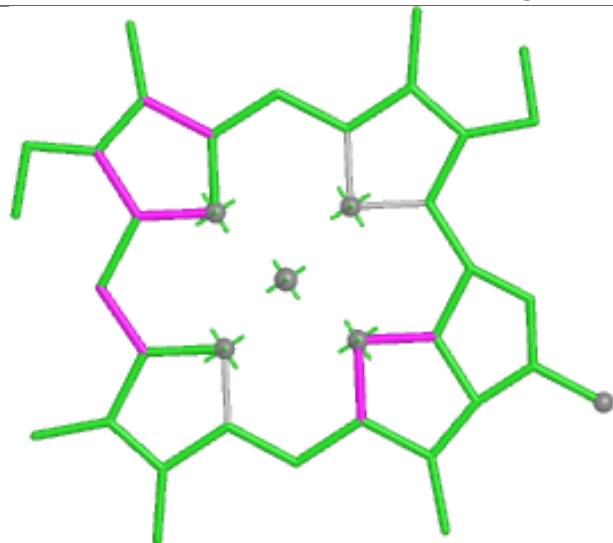
Ligand CLA 9 603



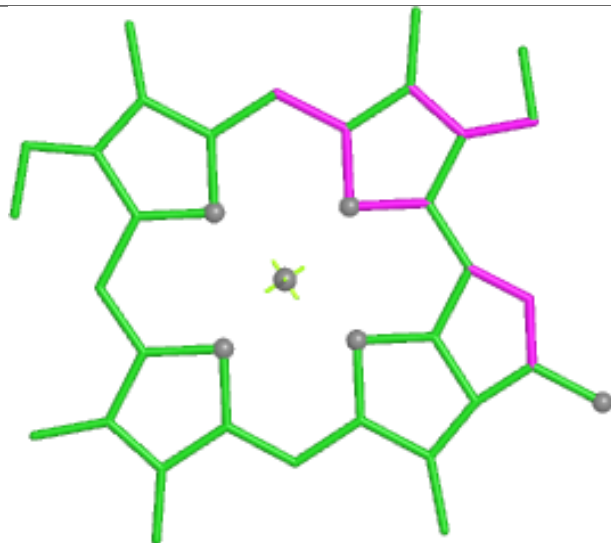
Ligand CLA B 826



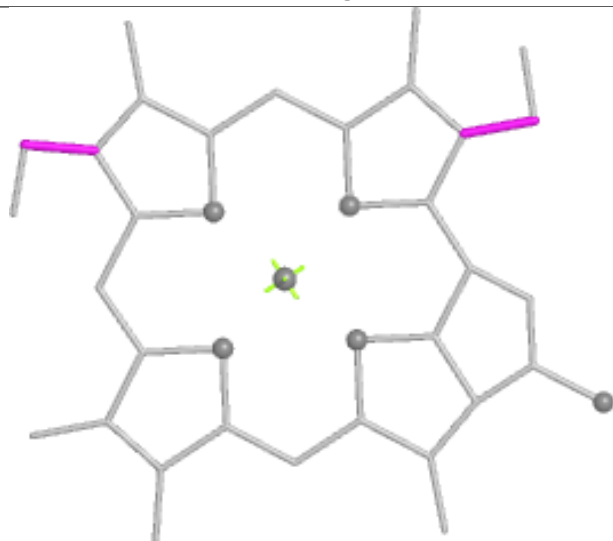
Ligand CLA 2 604



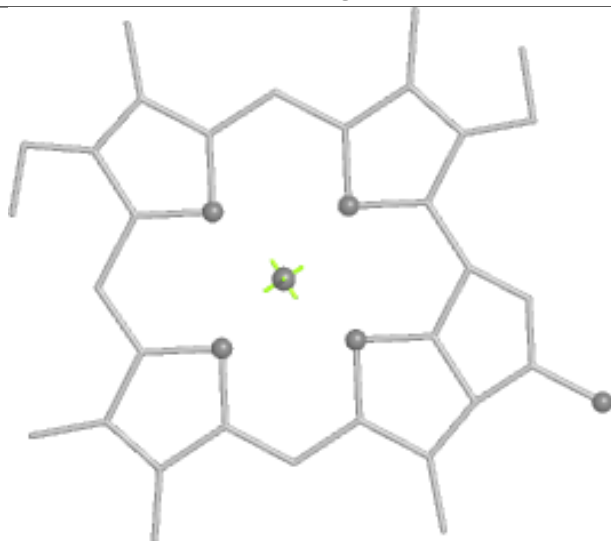
Bond lengths



Bond angles

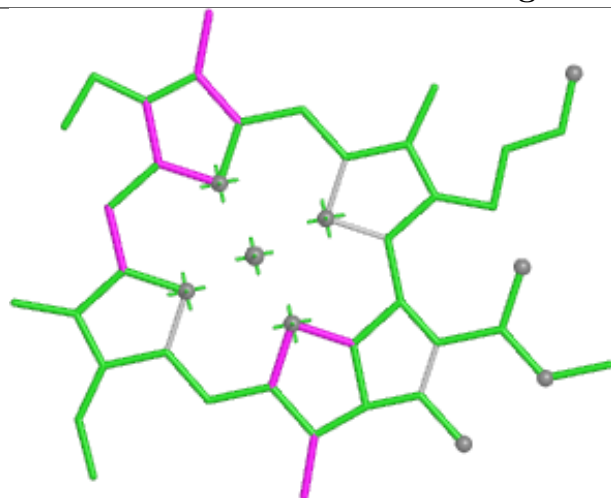


Torsions

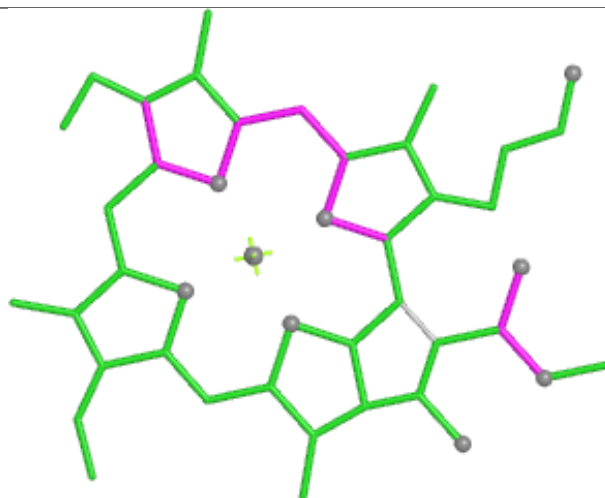


Rings

Ligand CLA 9 604



Bond lengths



Bond angles

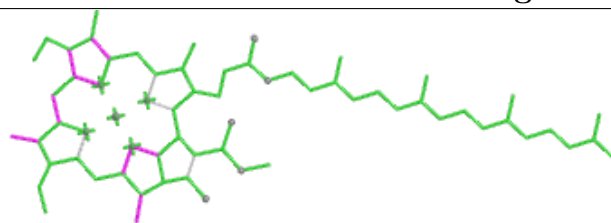


Torsions

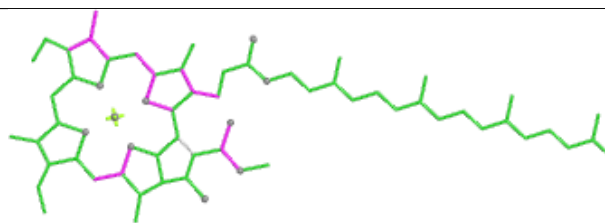


Rings

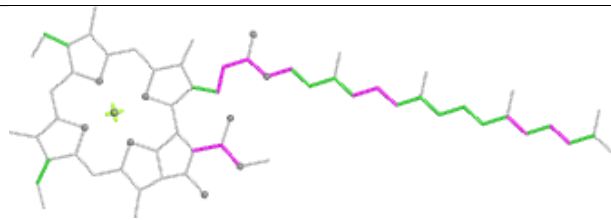
Ligand CLA B 807



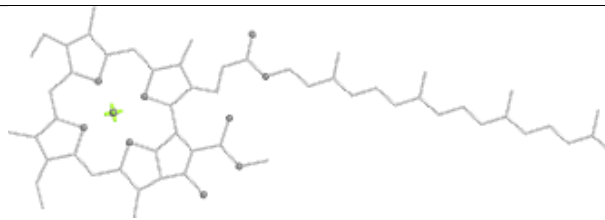
Bond lengths



Bond angles

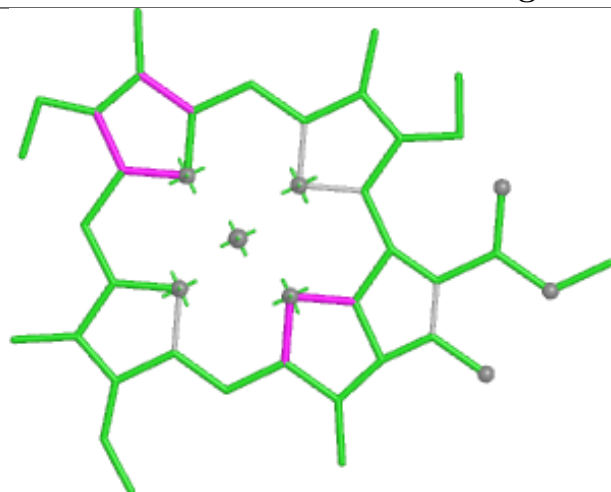


Torsions

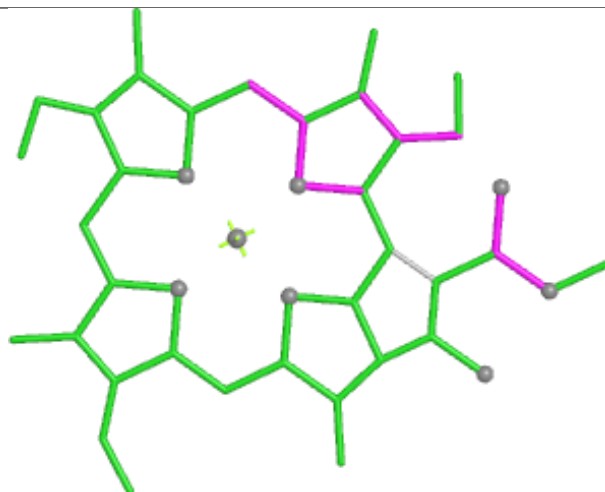


Rings

Ligand CLA 9 610



Bond lengths



Bond angles

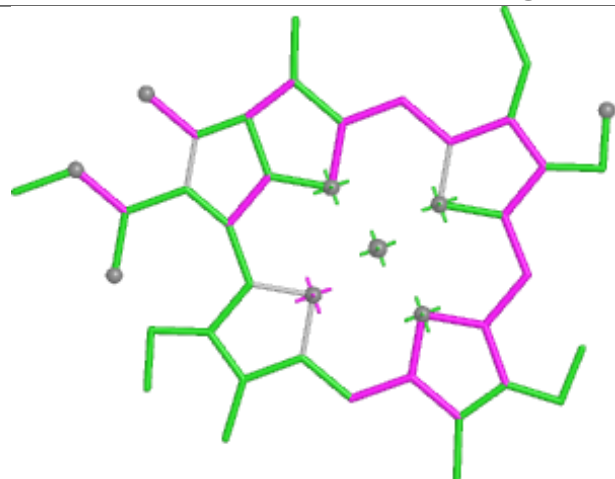


Torsions

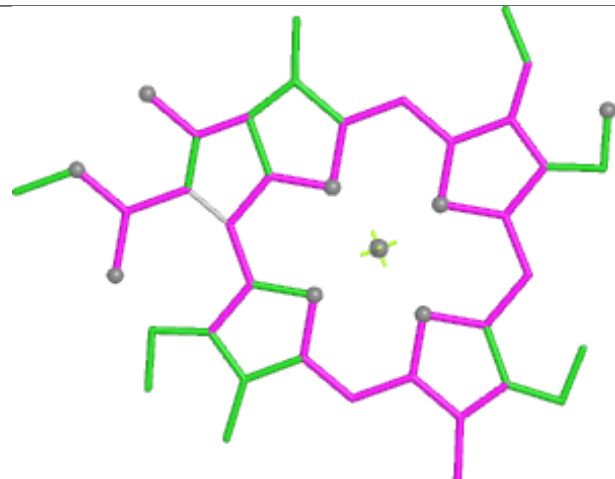


Rings

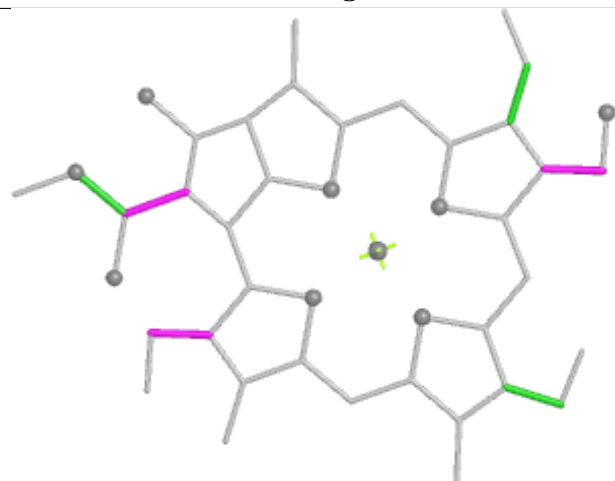
Ligand CHL 9 601



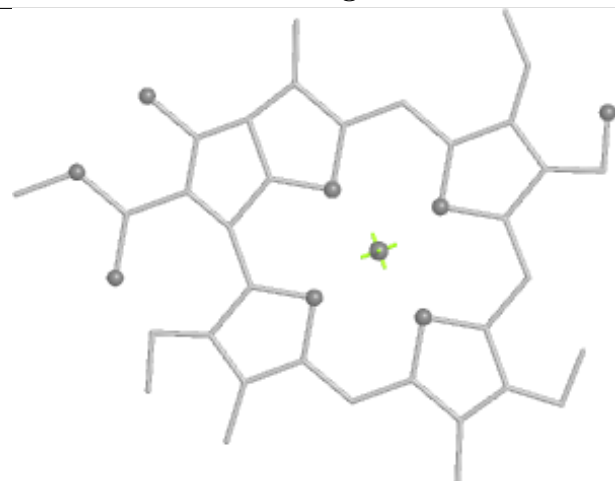
Bond lengths



Bond angles

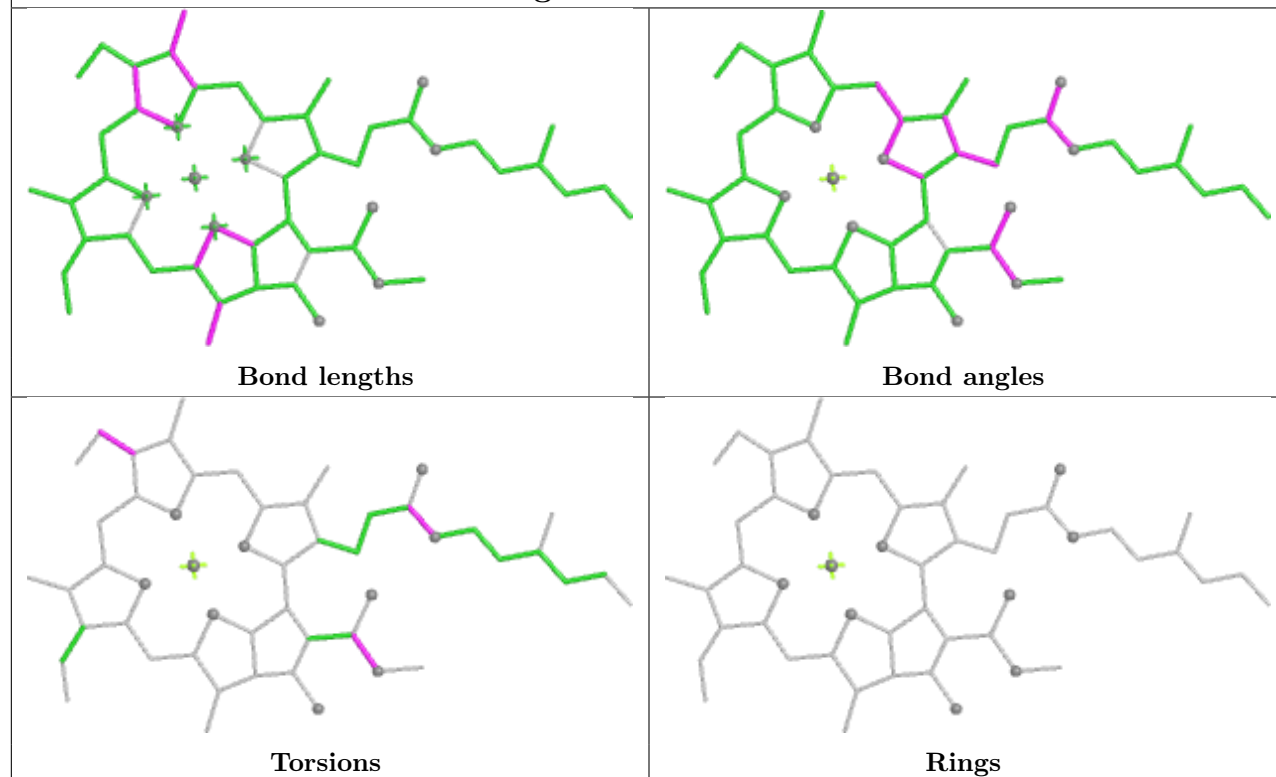


Torsions

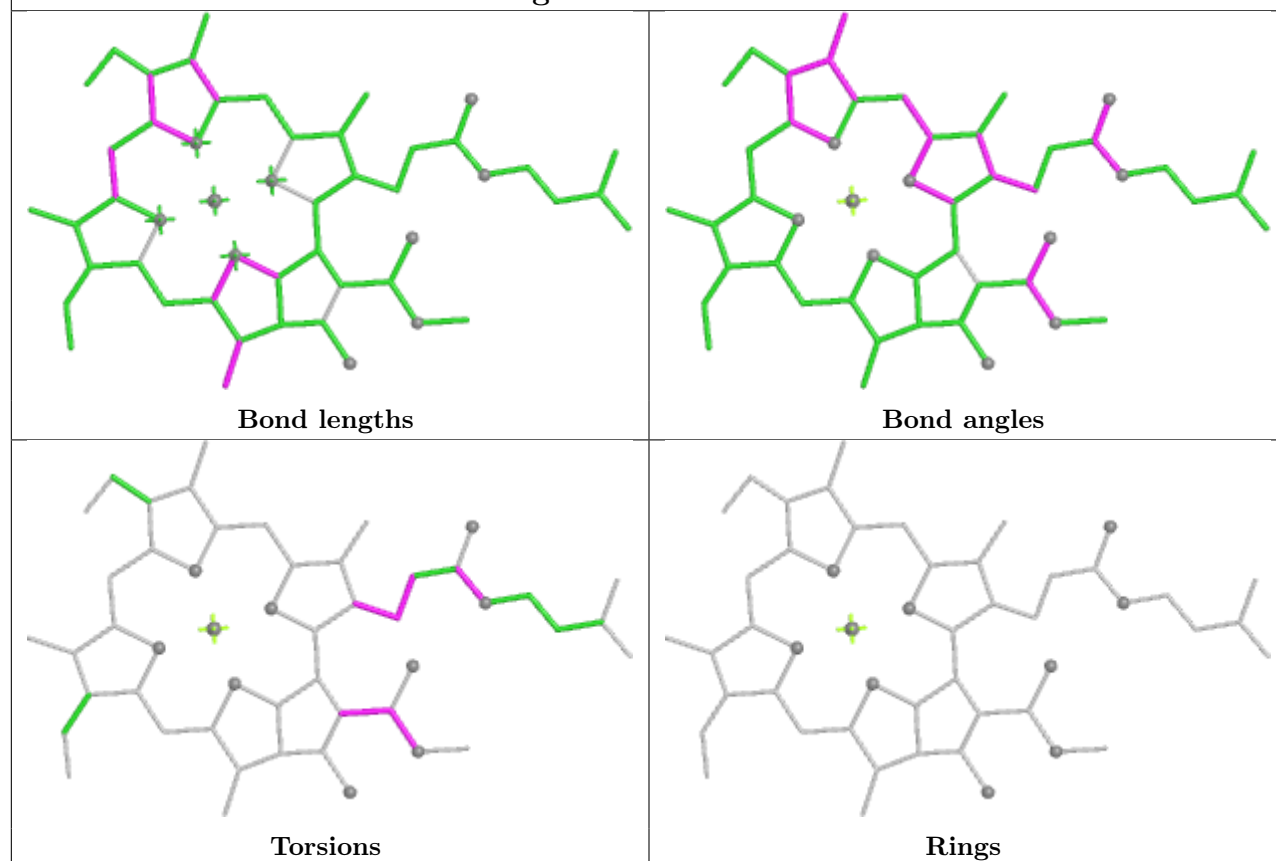


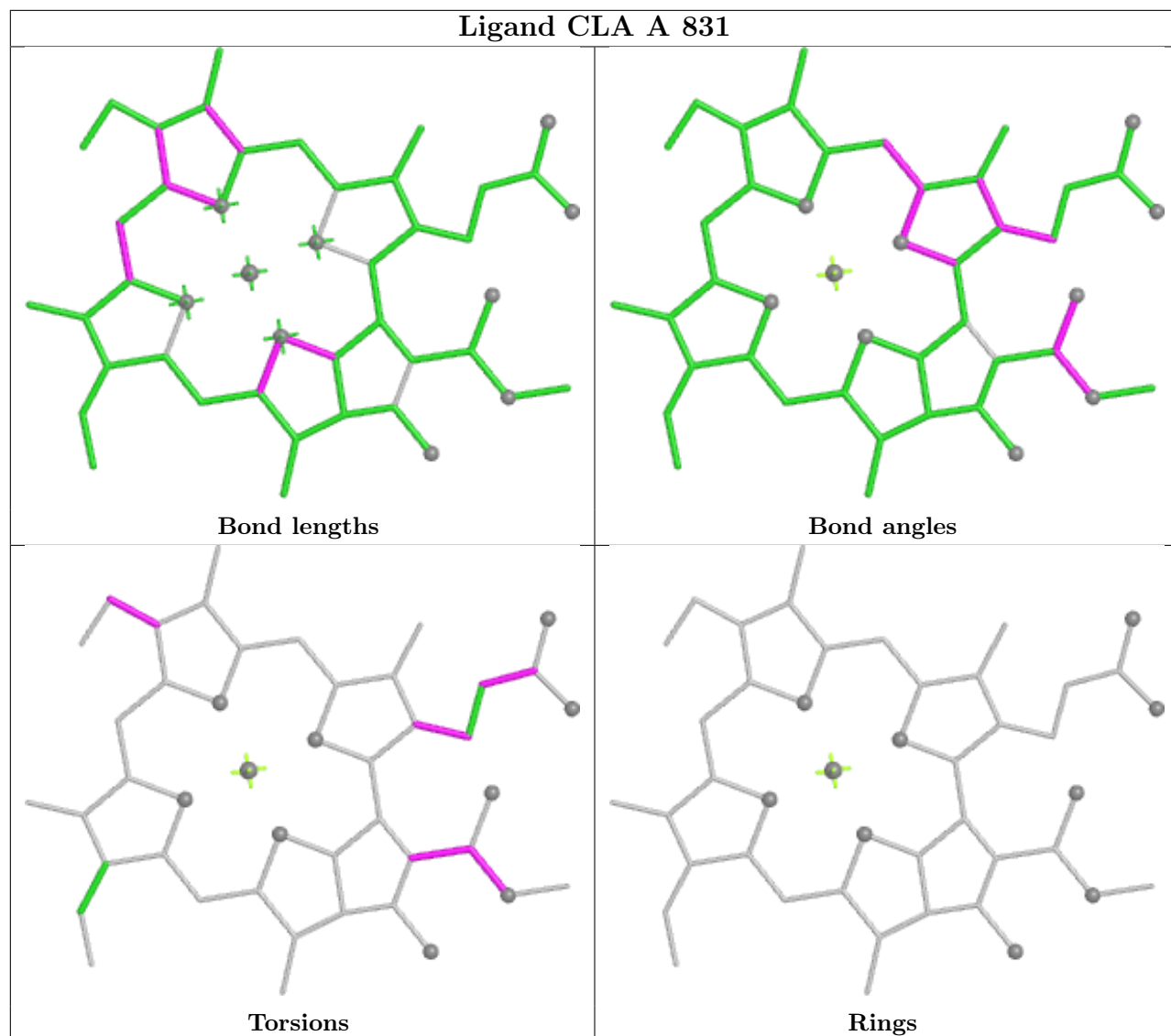
Rings

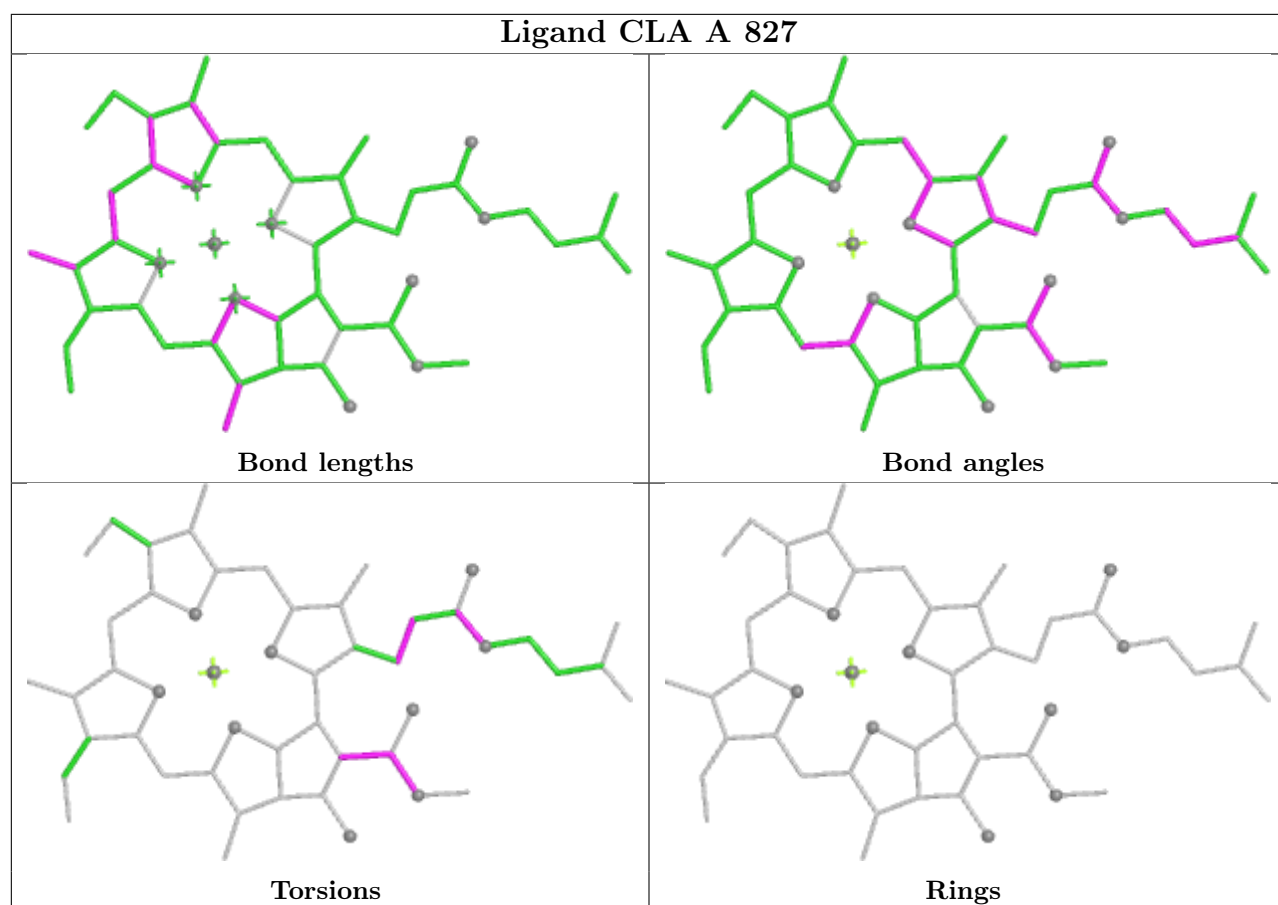
Ligand CLA F 802



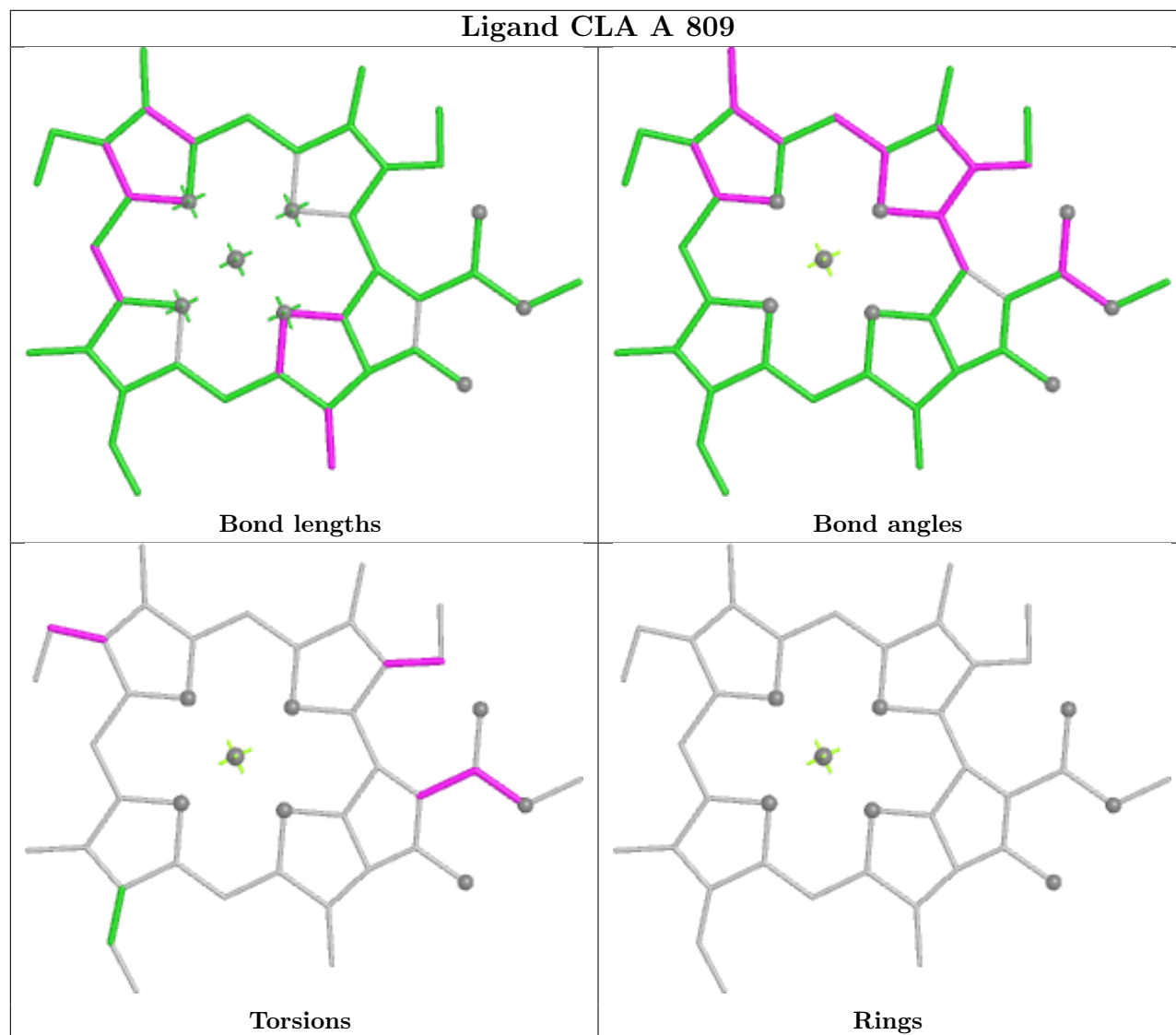
Ligand CLA B 836



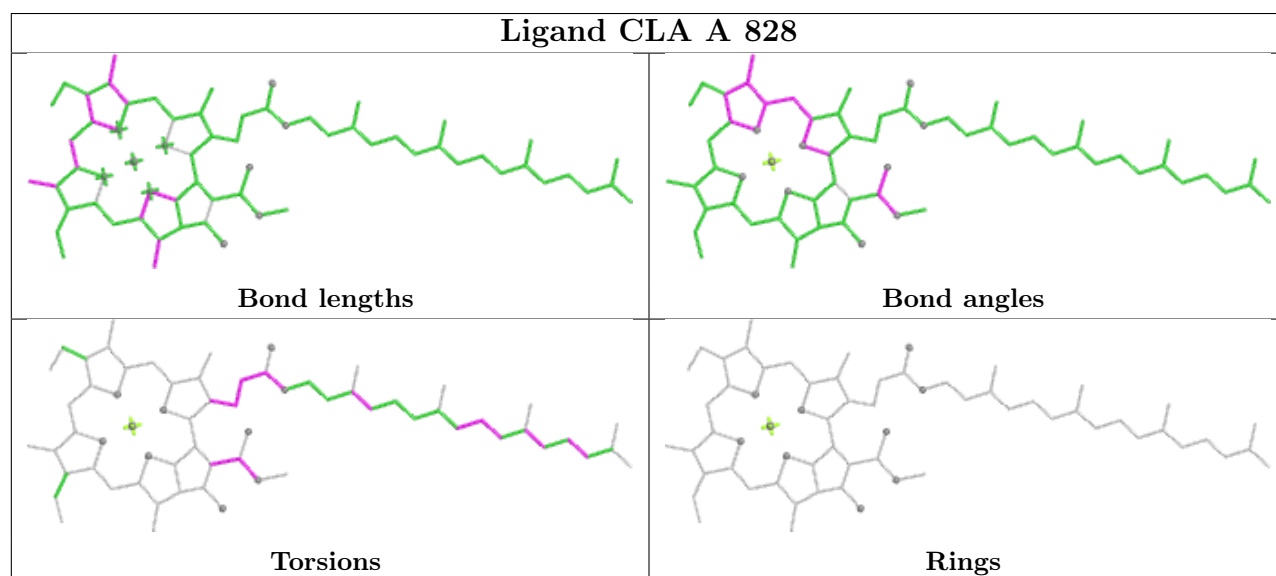


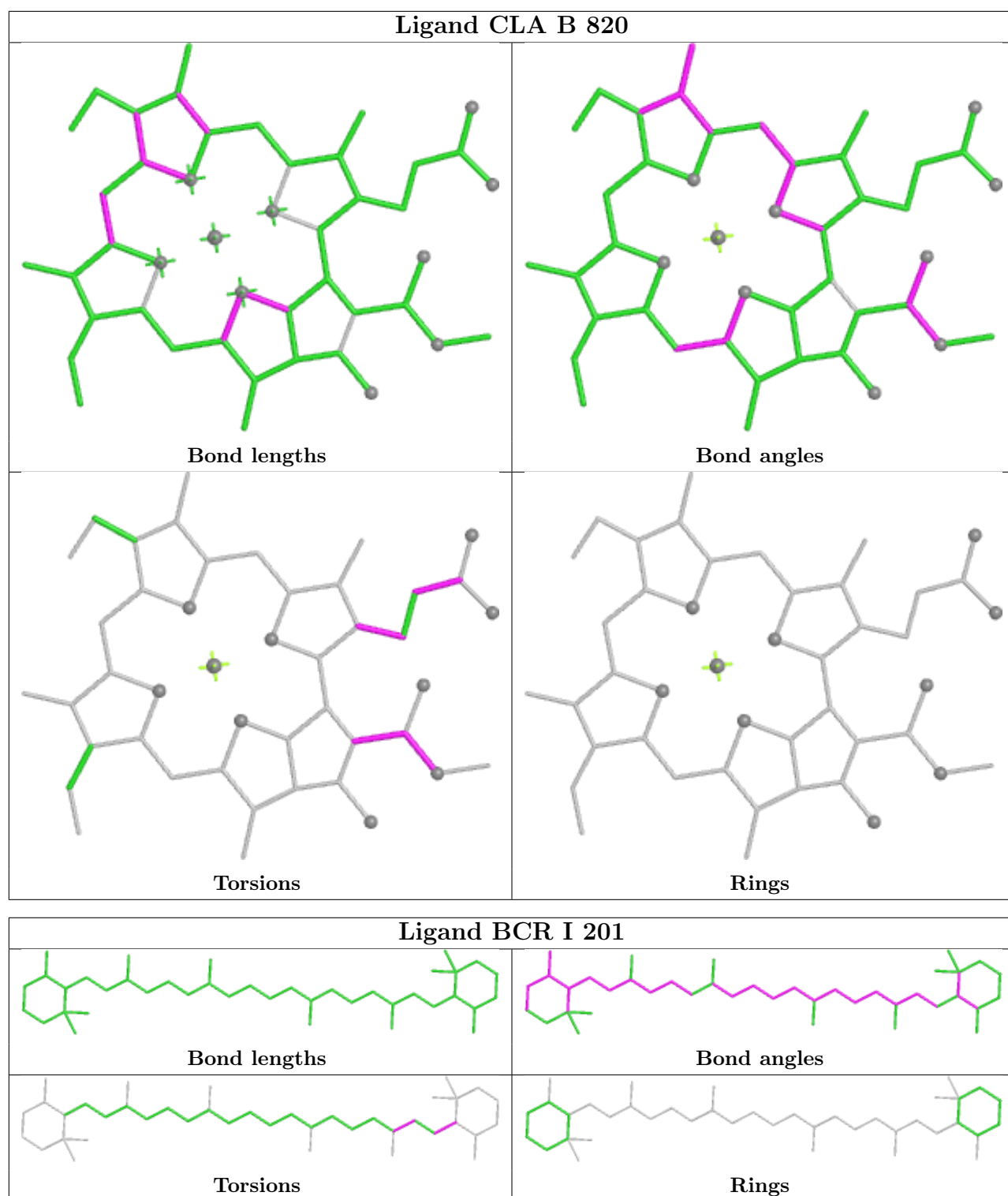


Ligand CLA A 809

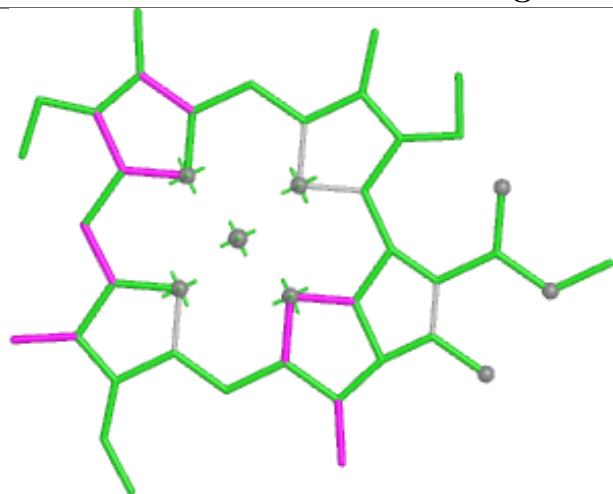


Ligand CLA A 828

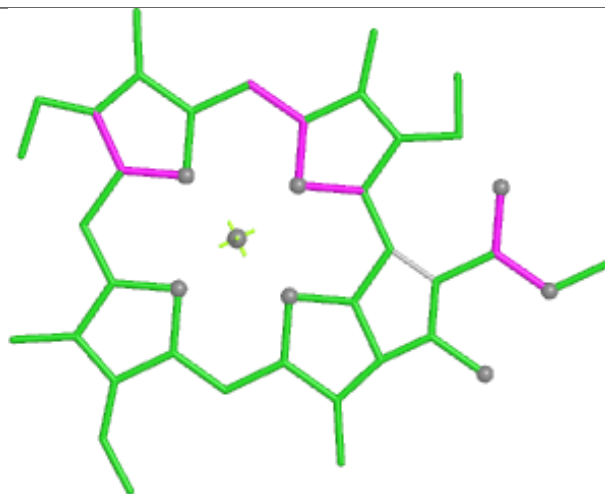




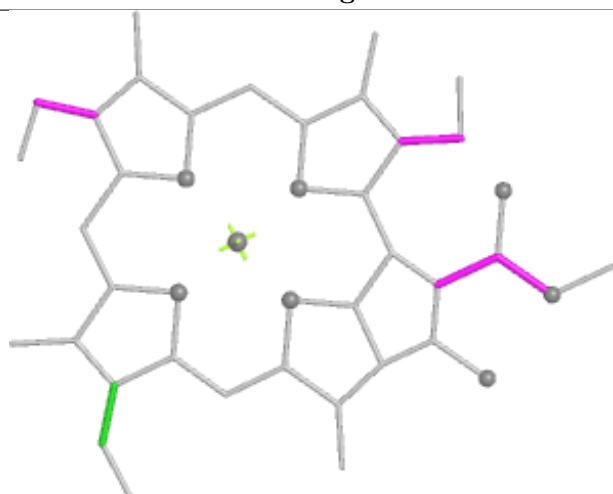
Ligand CLA A 852



Bond lengths



Bond angles

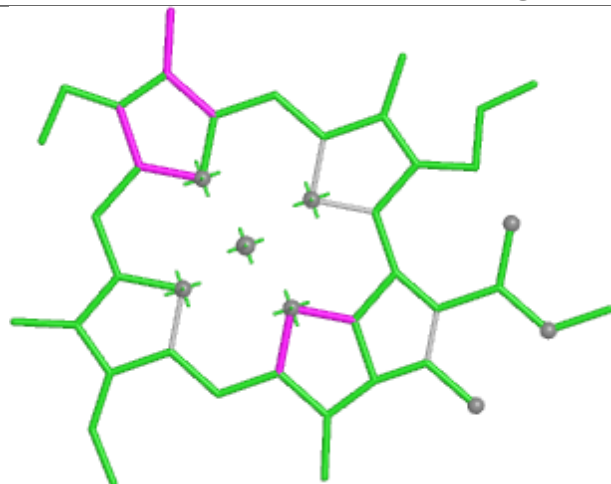


Torsions

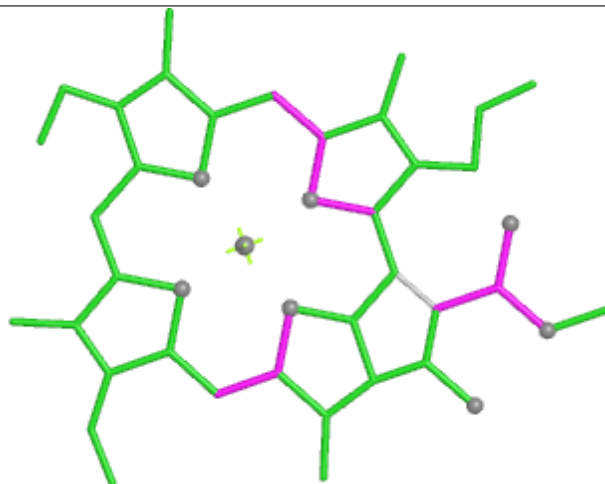


Rings

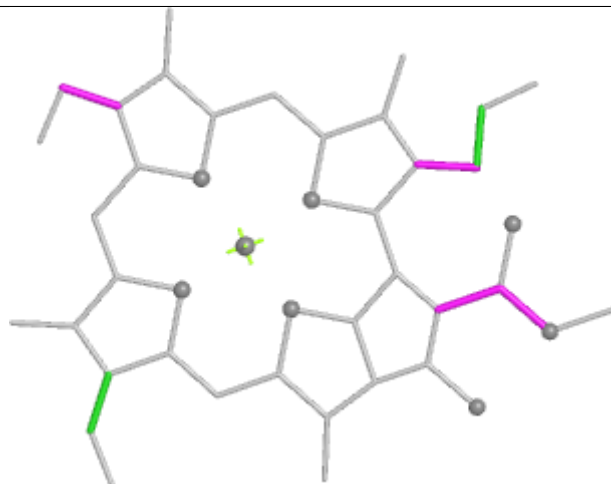
Ligand CLA B 831



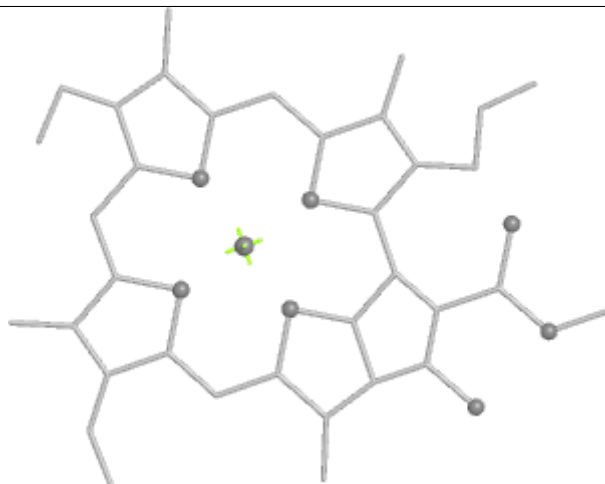
Bond lengths



Bond angles

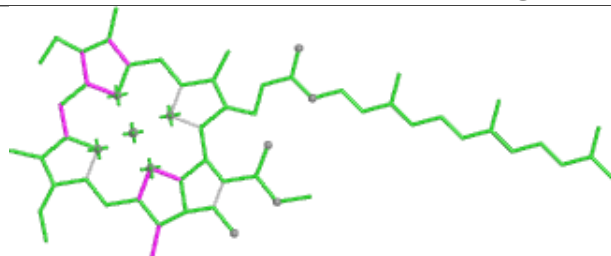


Torsions

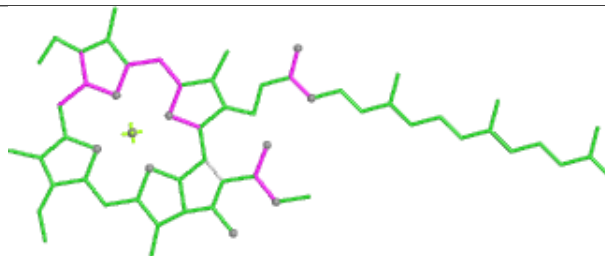


Rings

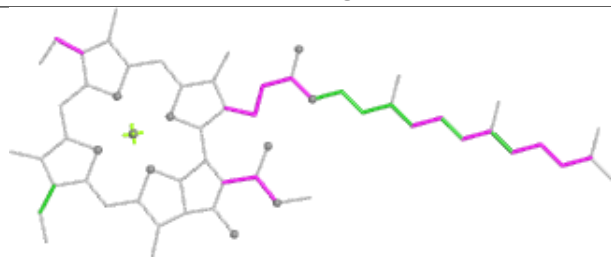
Ligand CLA B 828



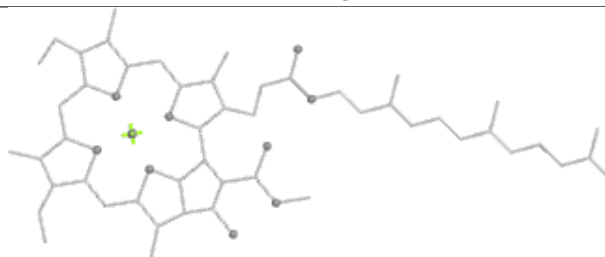
Bond lengths



Bond angles

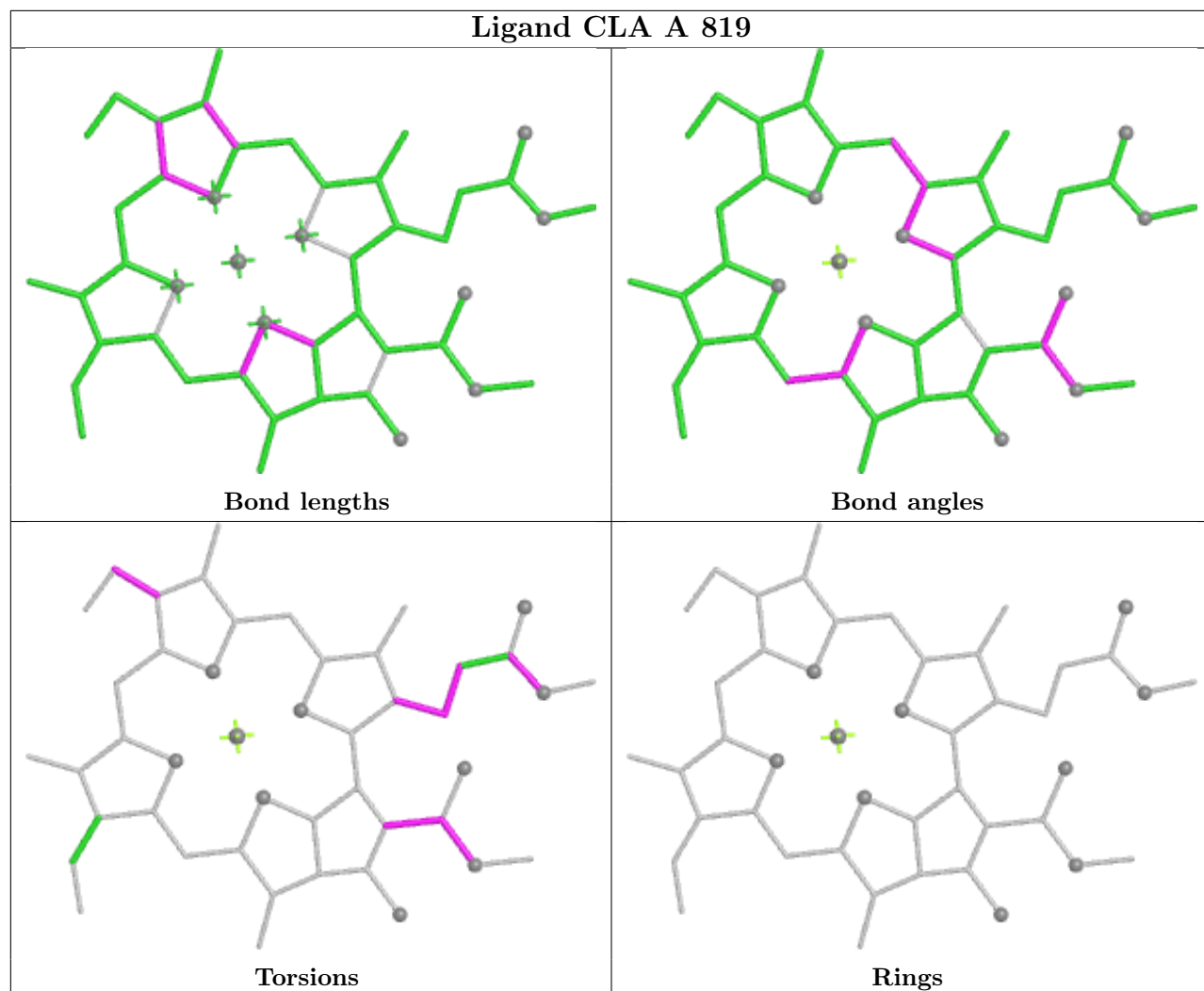


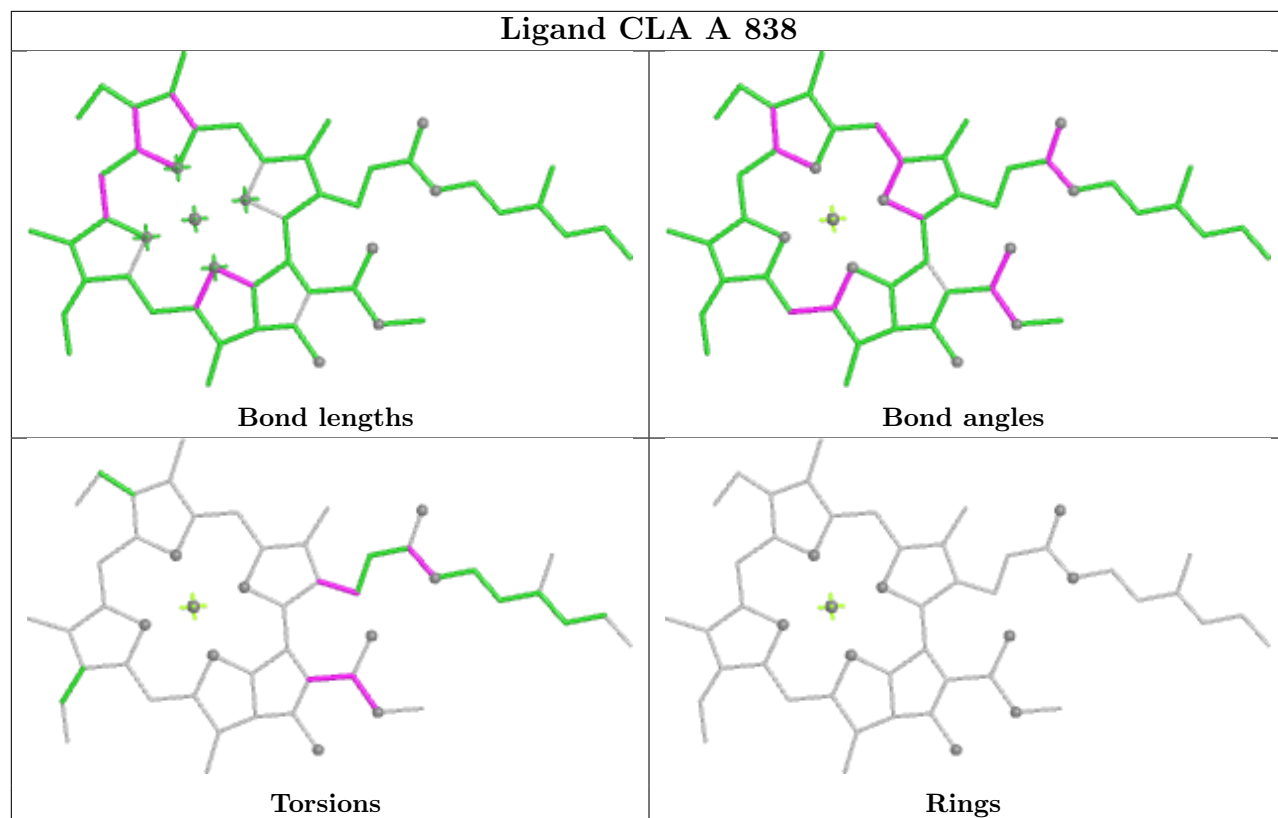
Torsions



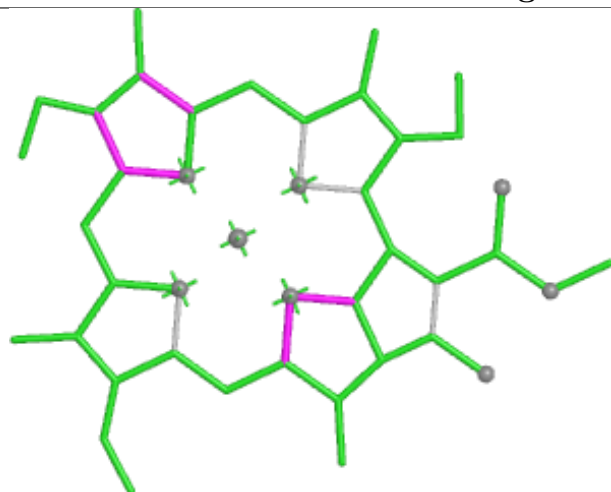
Rings

Ligand CLA A 819

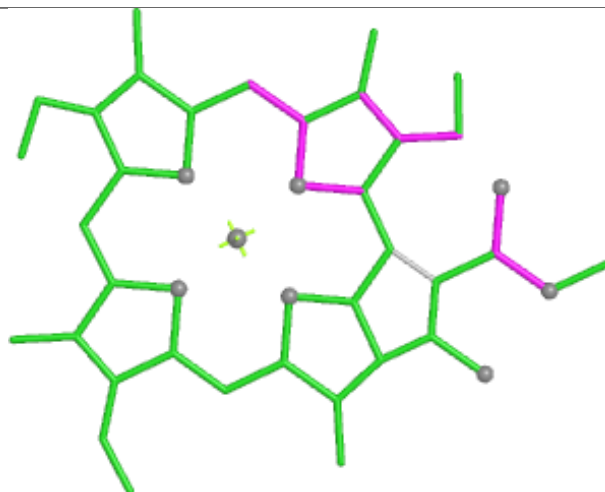




Ligand CLA J 102



Bond lengths



Bond angles

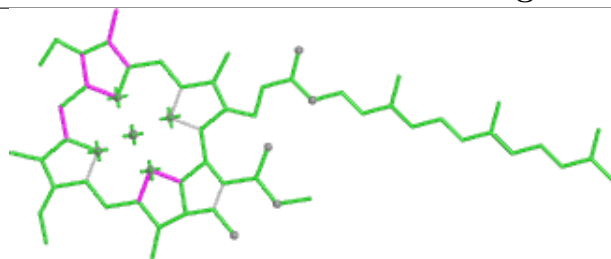


Torsions

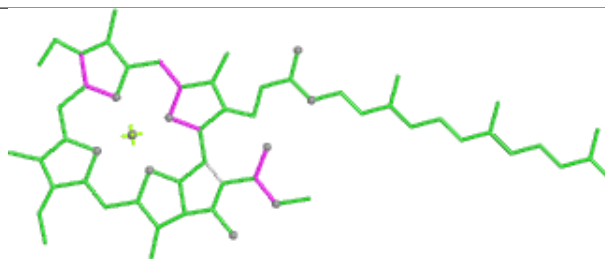


Rings

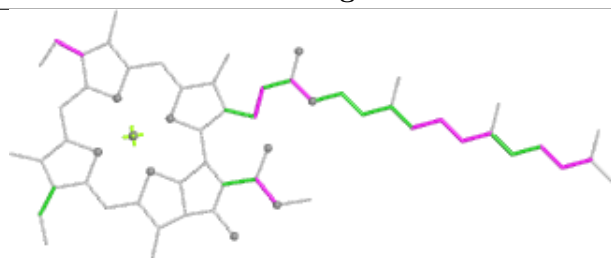
Ligand CLA L 303



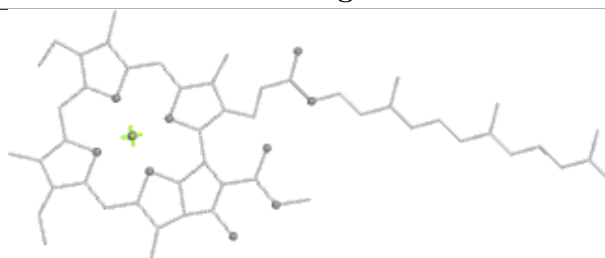
Bond lengths



Bond angles

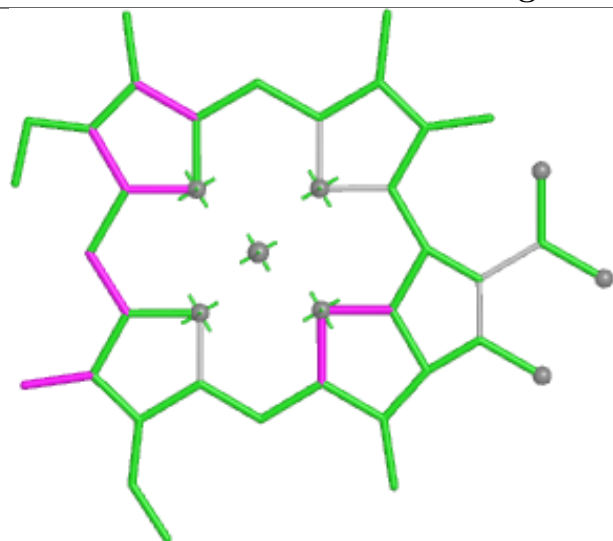


Torsions

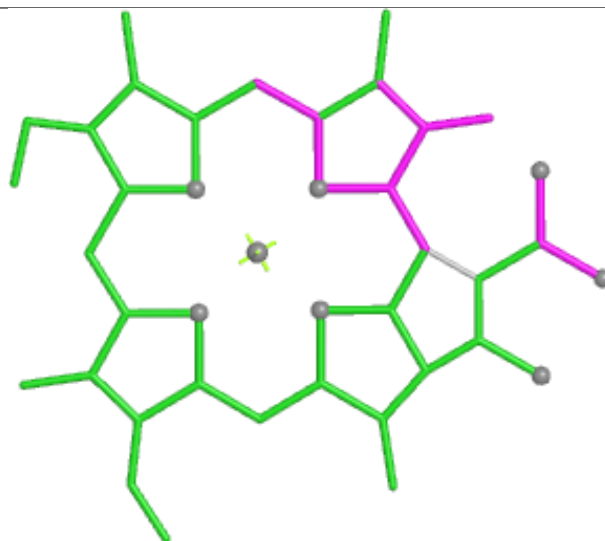


Rings

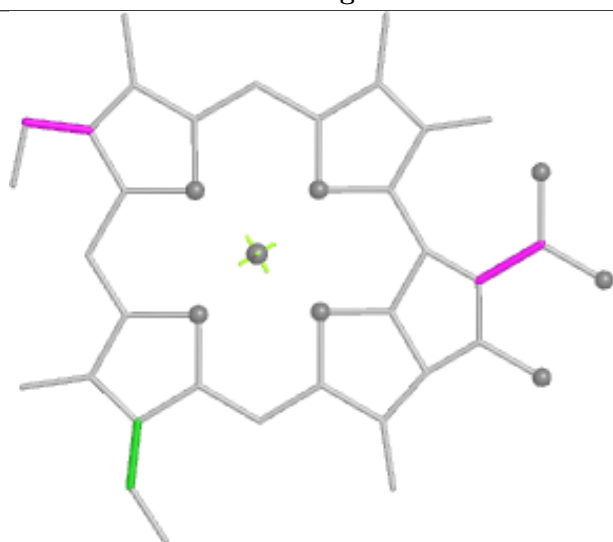
Ligand CLA 2 603



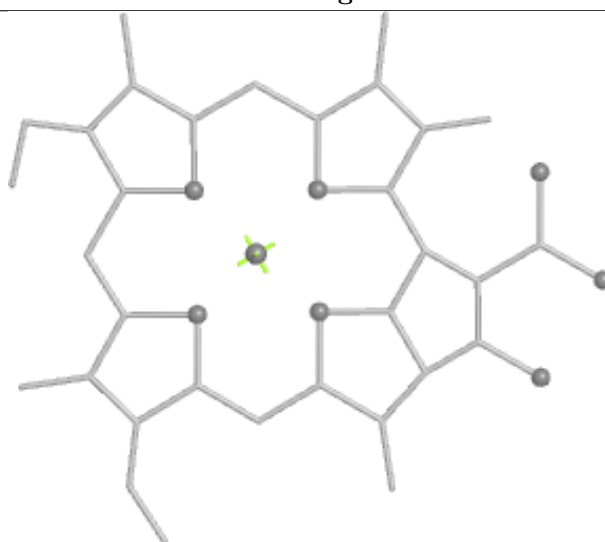
Bond lengths



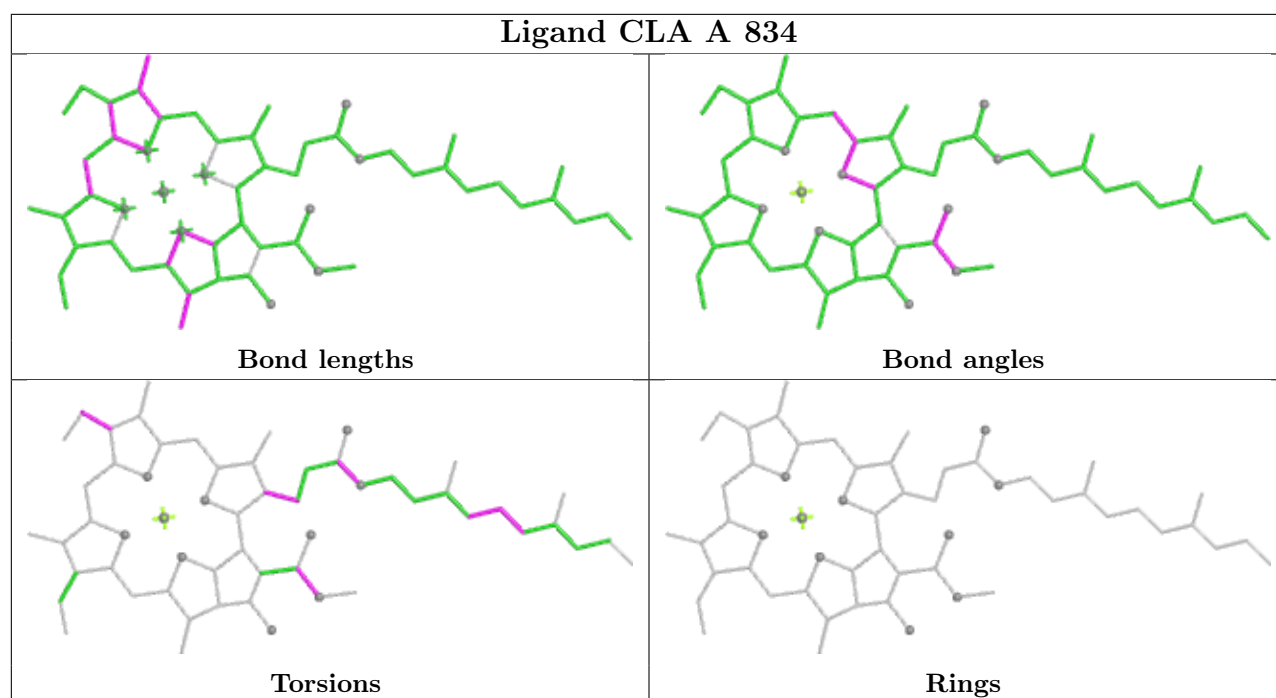
Bond angles



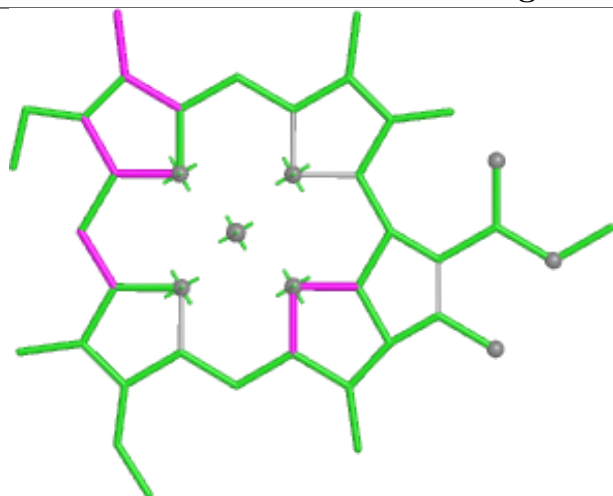
Torsions



Rings



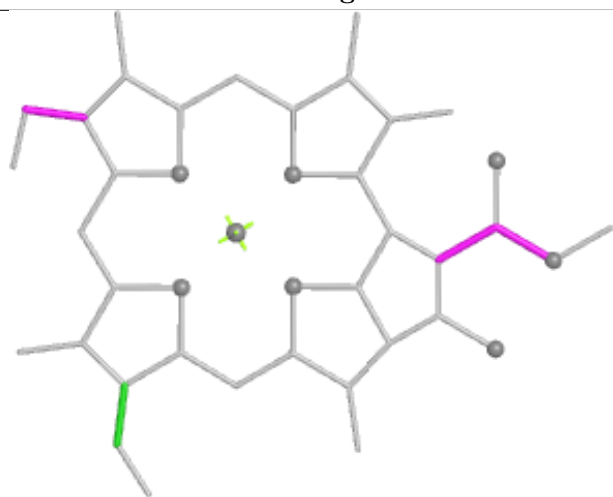
Ligand CLA 2 608



Bond lengths



Bond angles

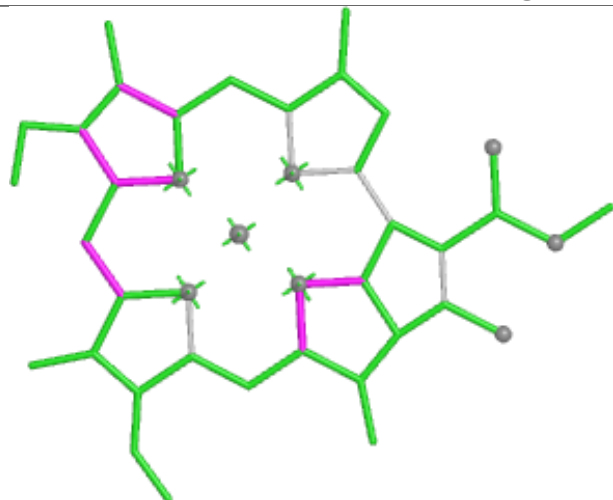


Torsions

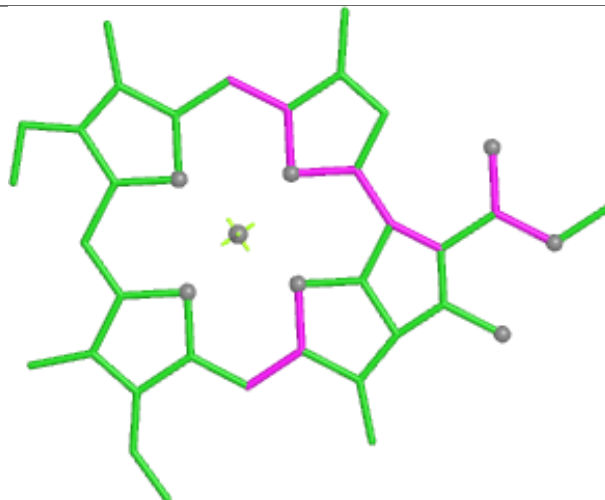


Rings

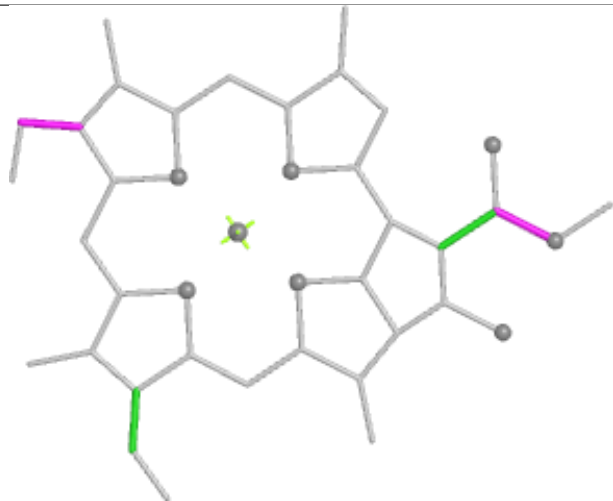
Ligand CLA 9 608



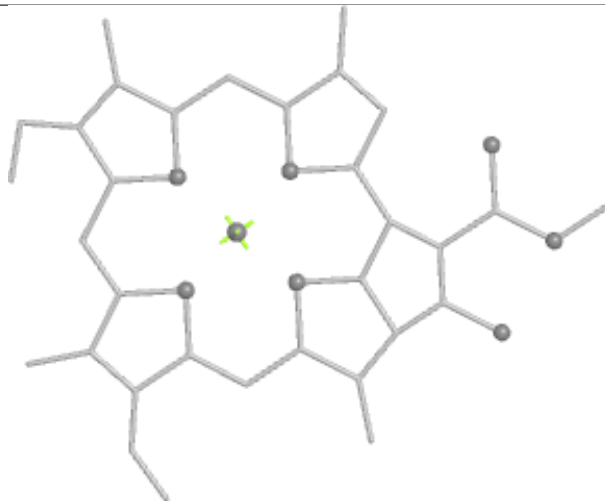
Bond lengths



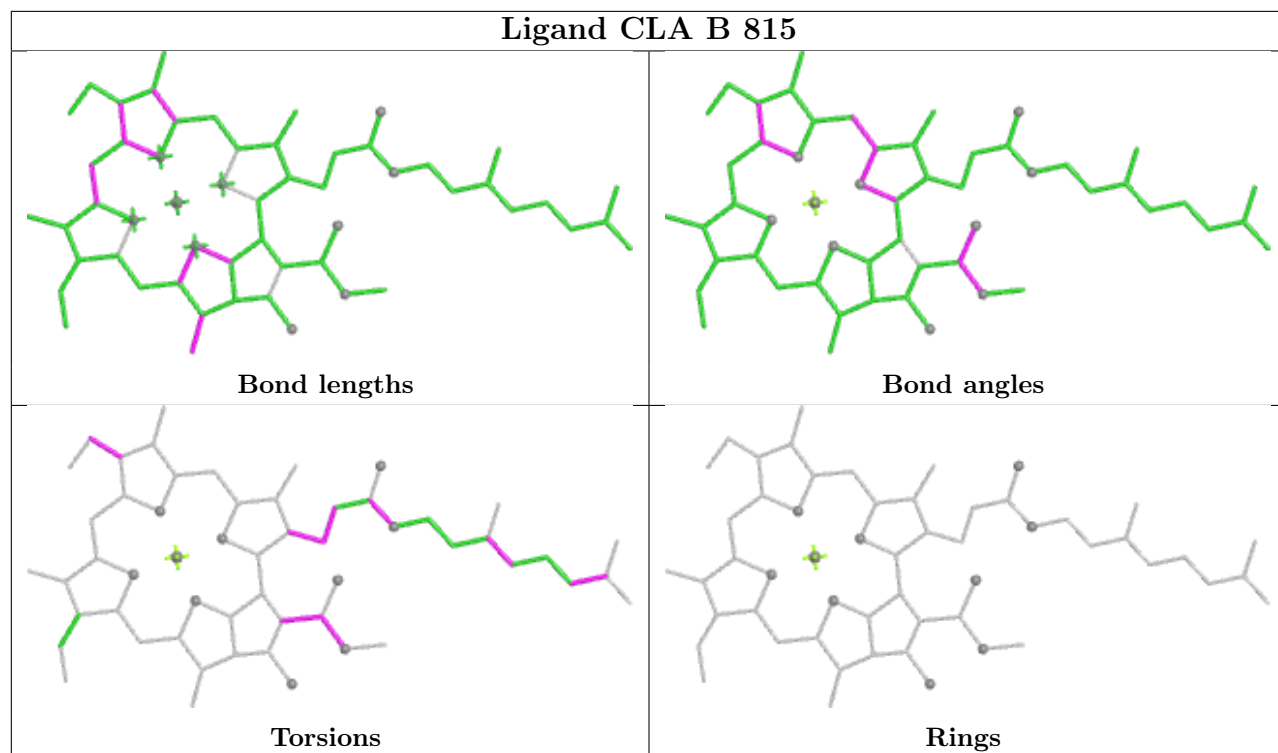
Bond angles

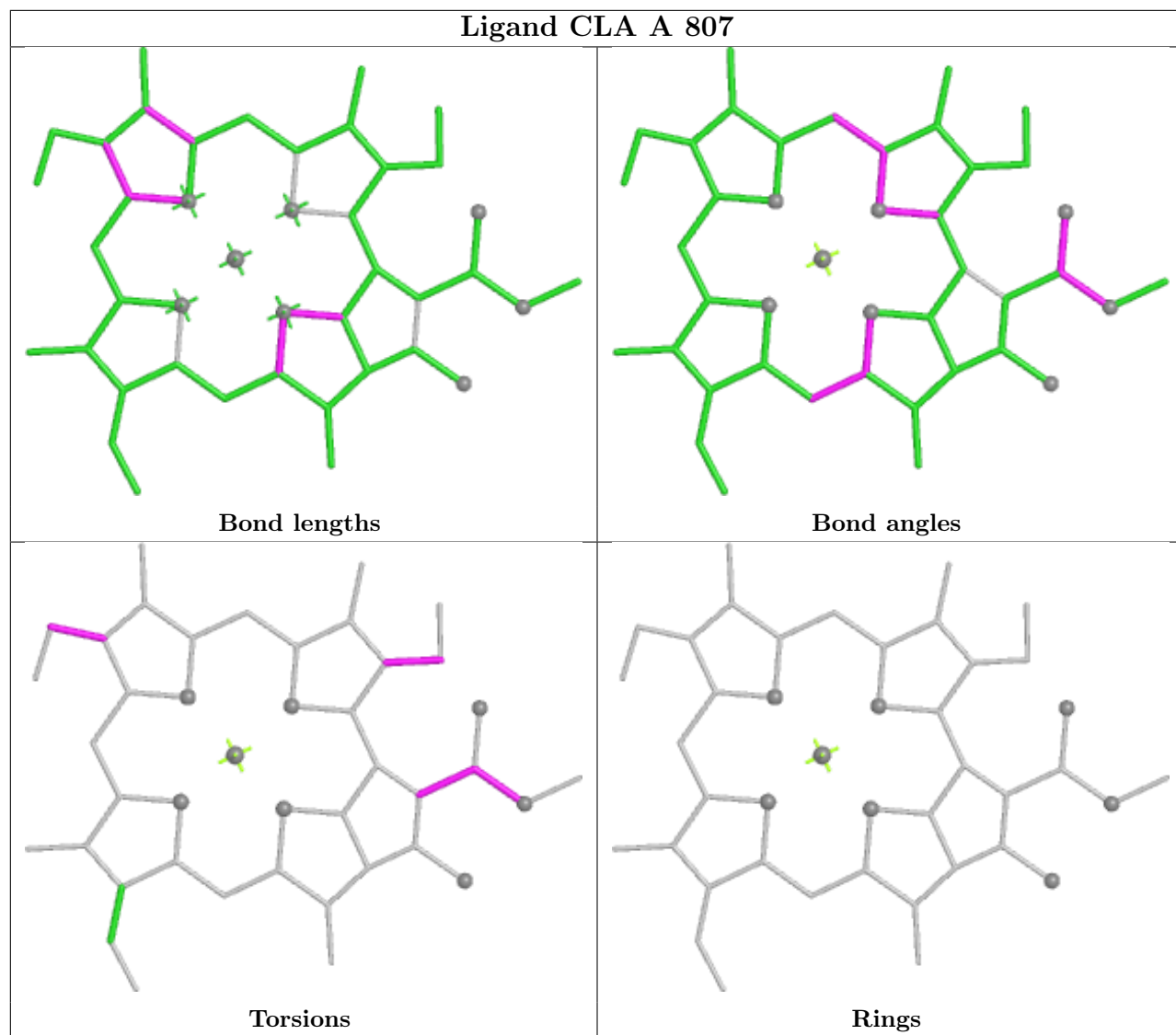


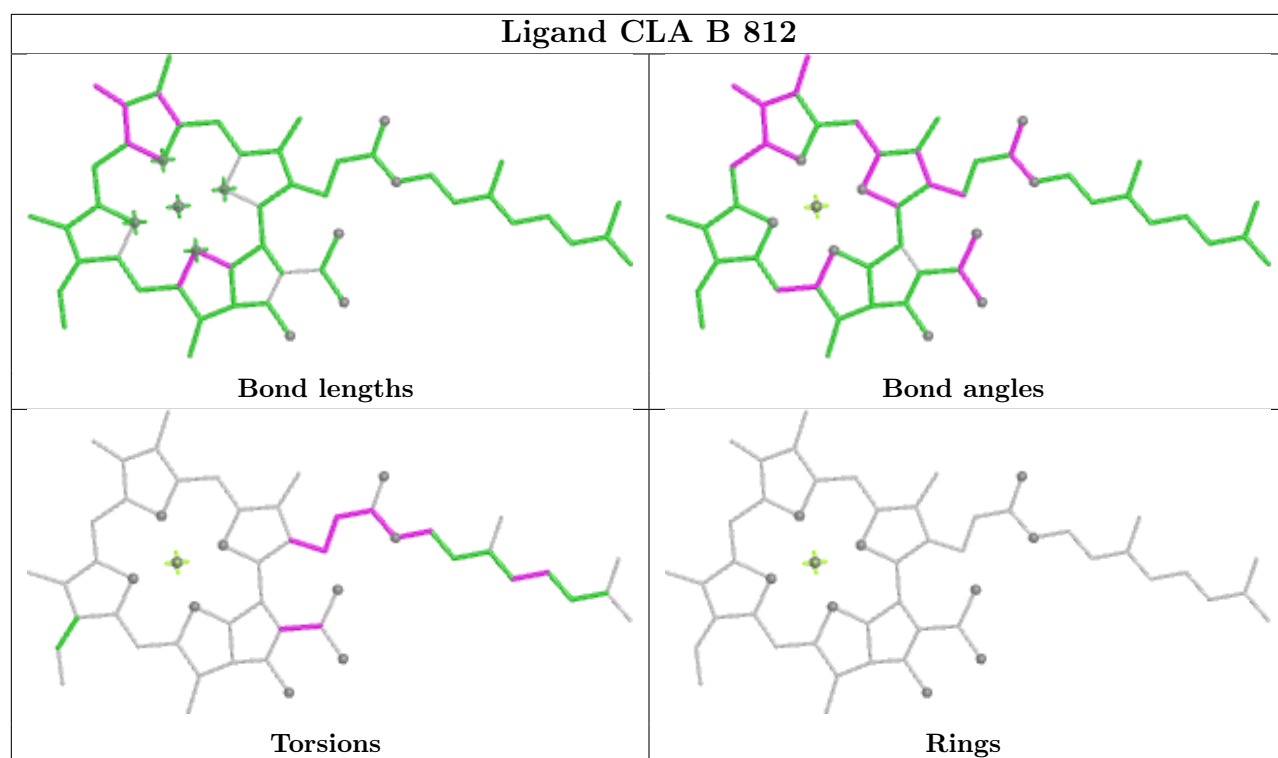
Torsions

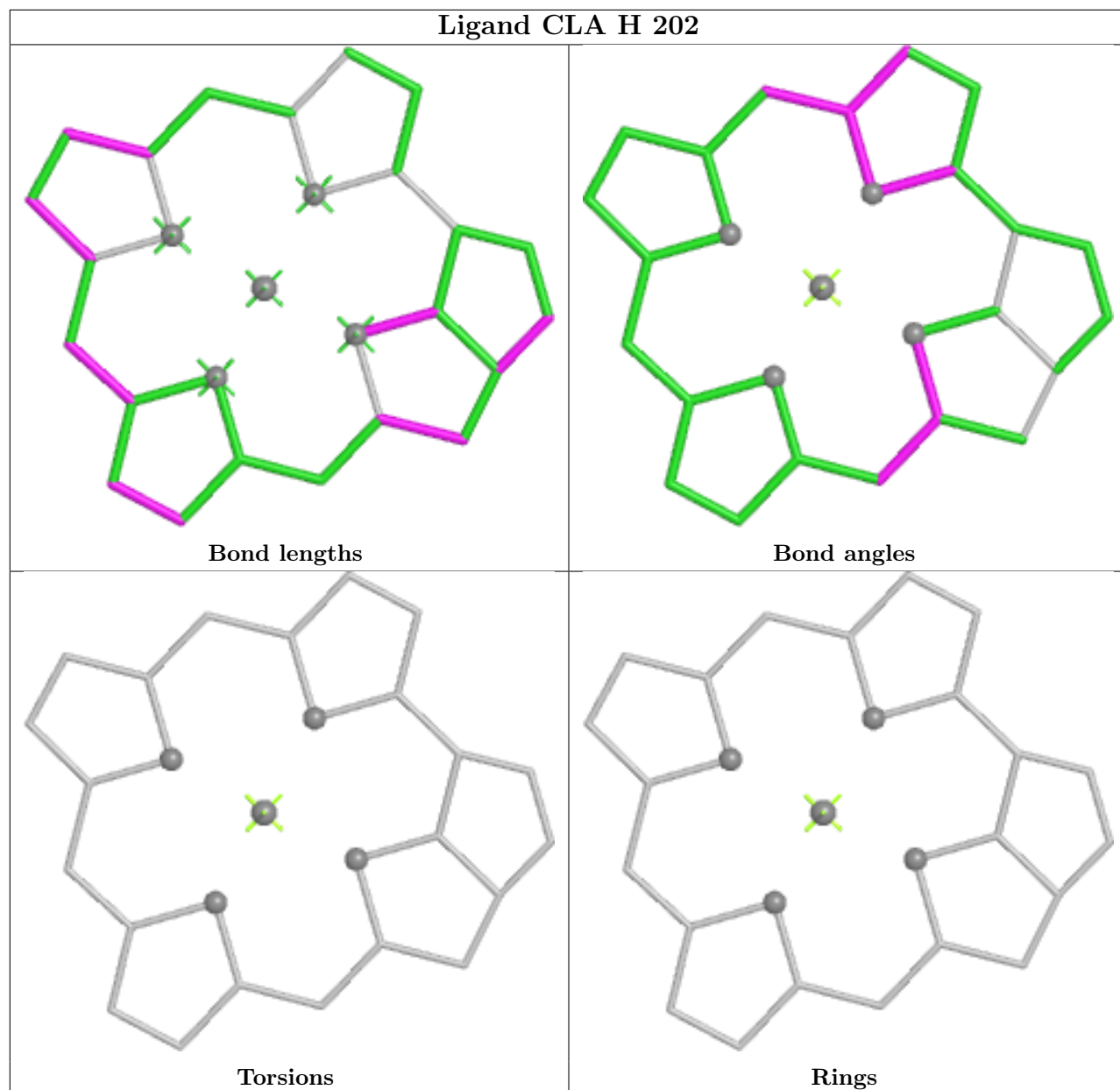


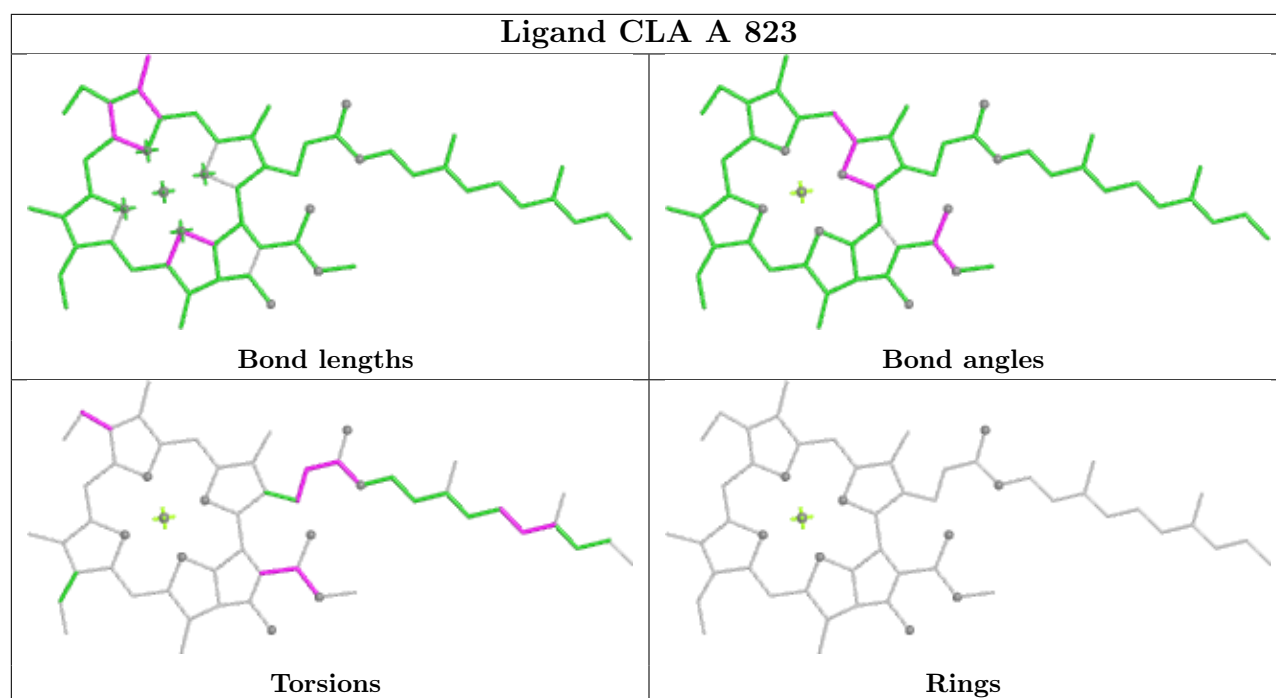
Rings



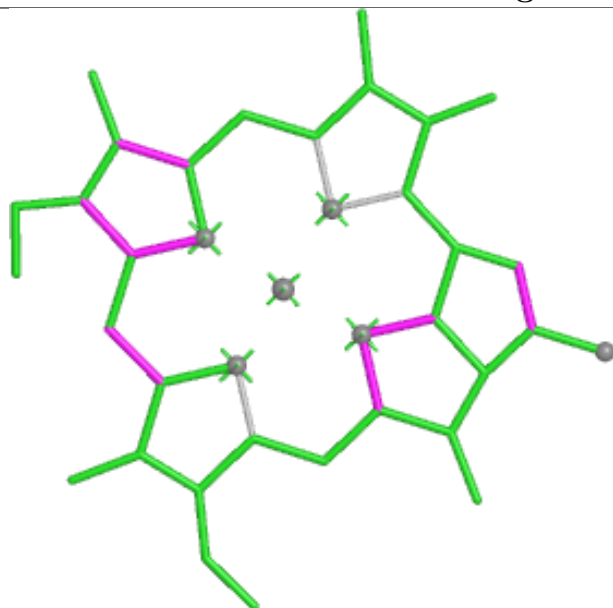




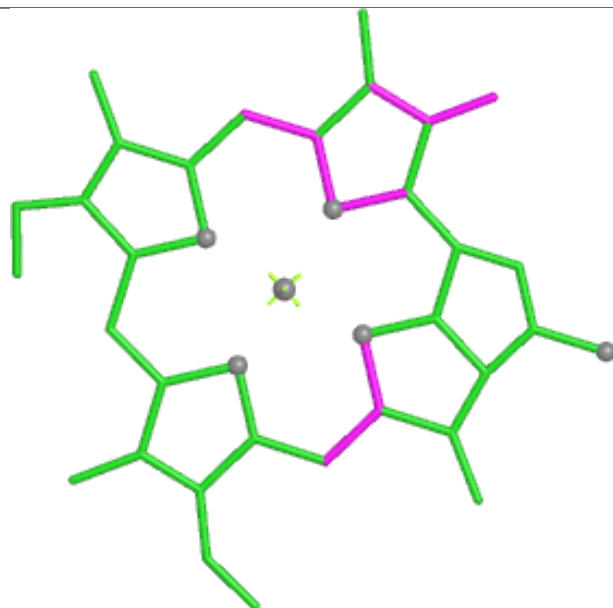




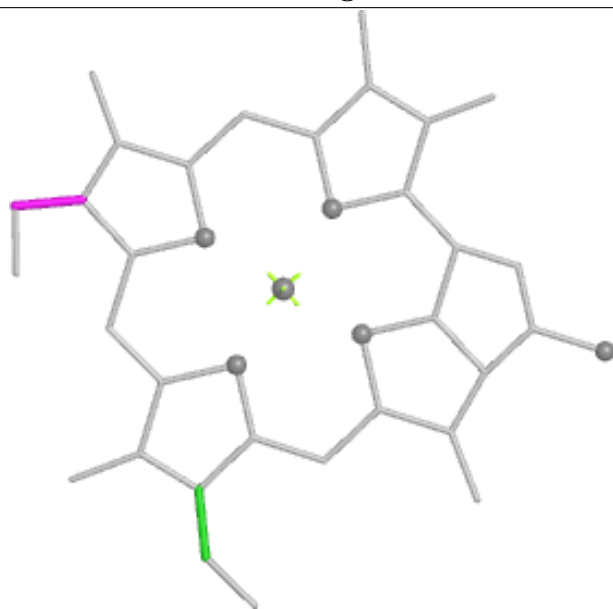
Ligand CLA L 304



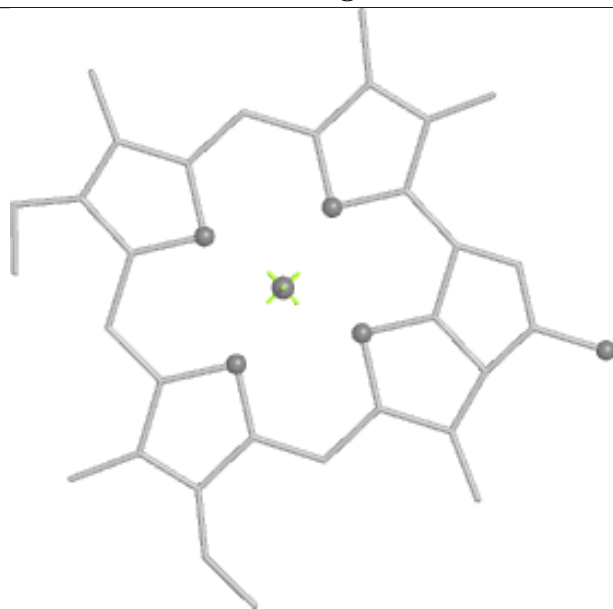
Bond lengths



Bond angles

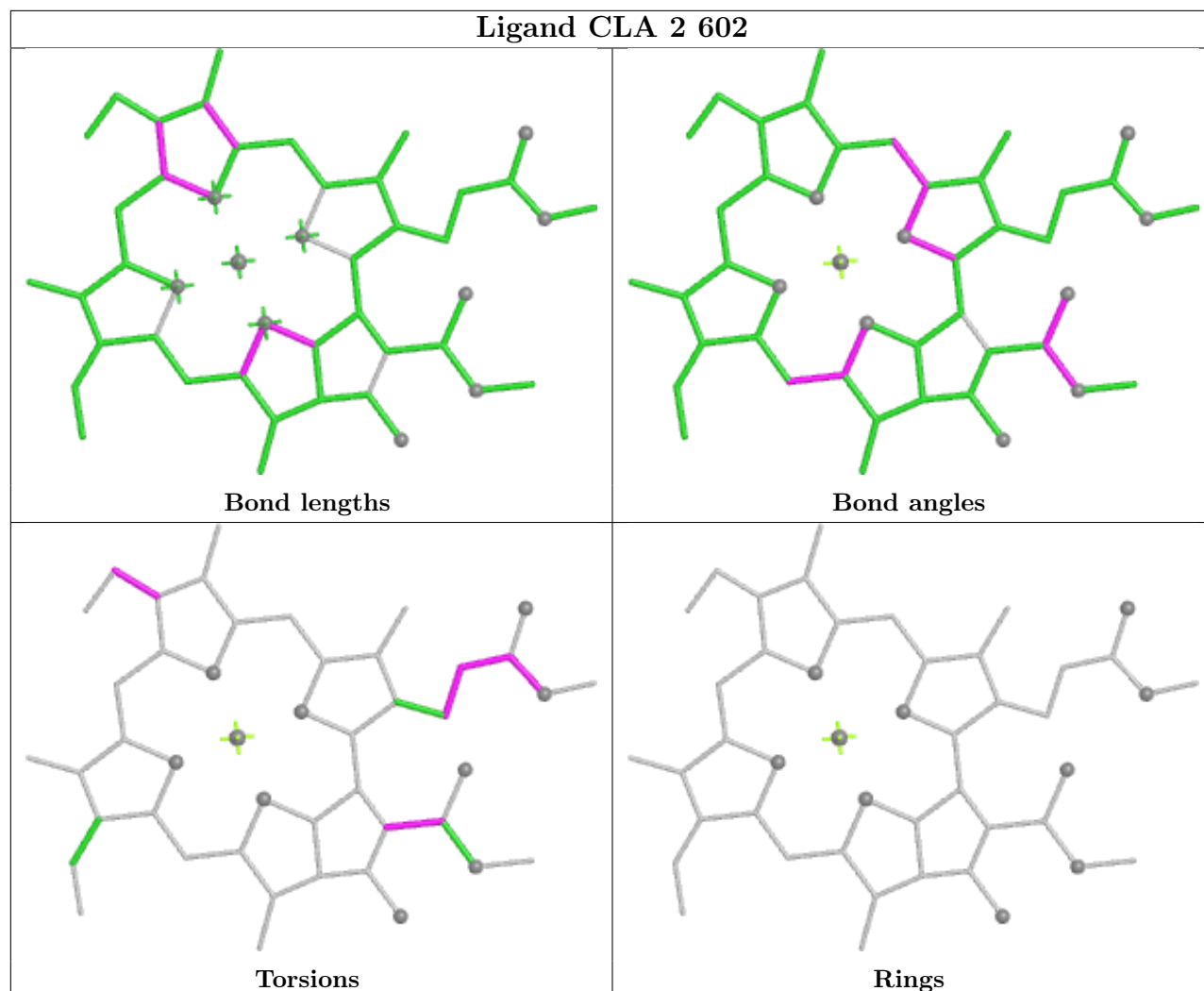


Torsions

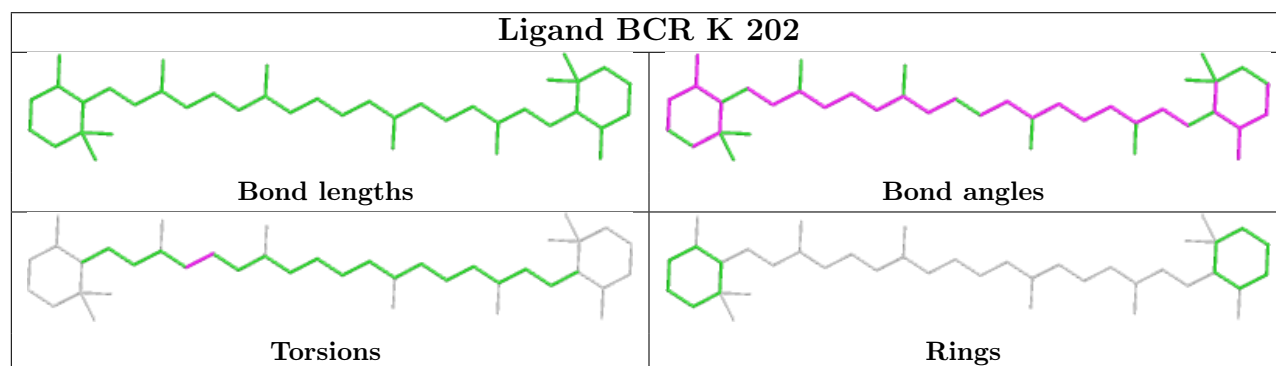


Rings

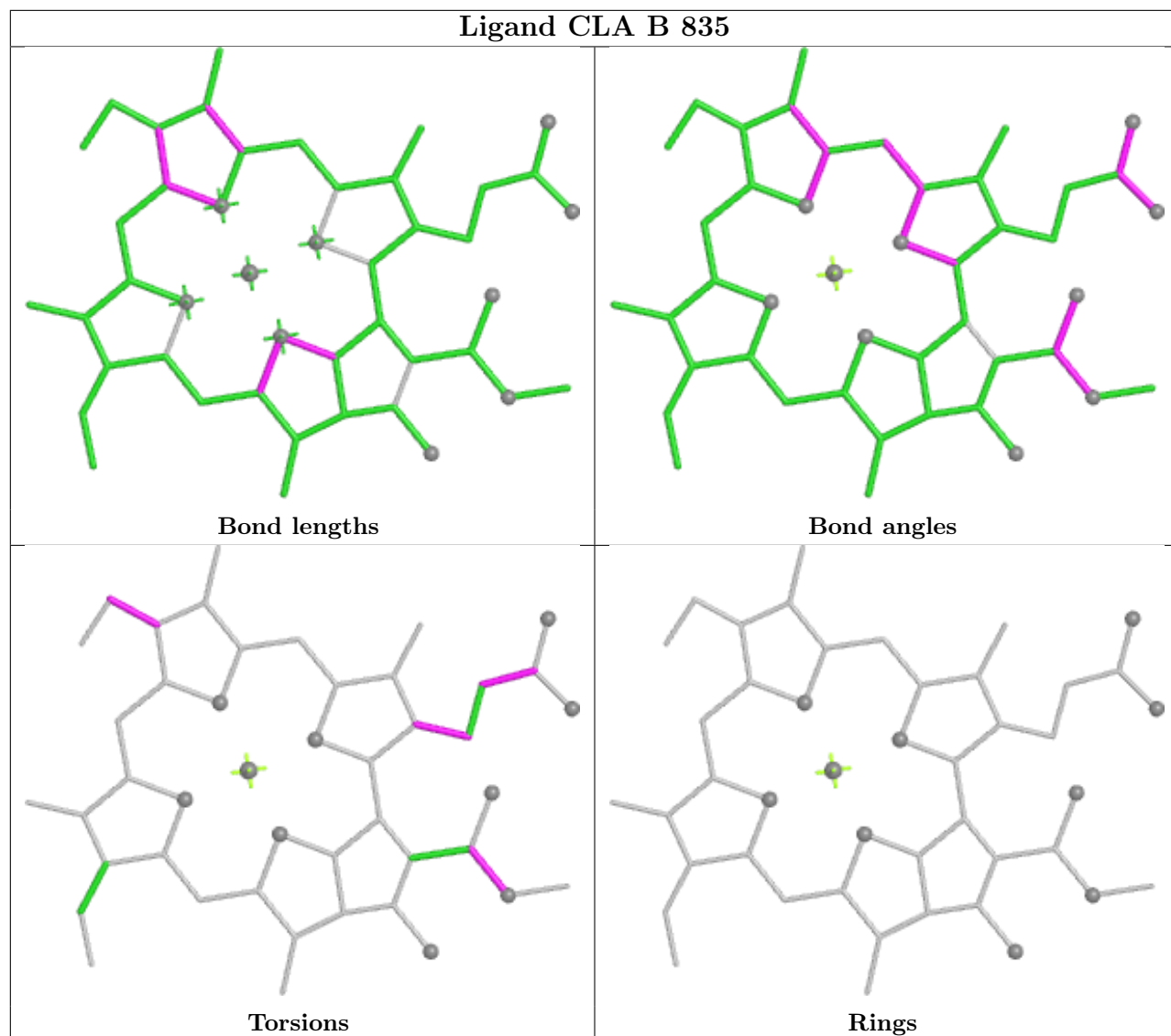
Ligand CLA 2 602



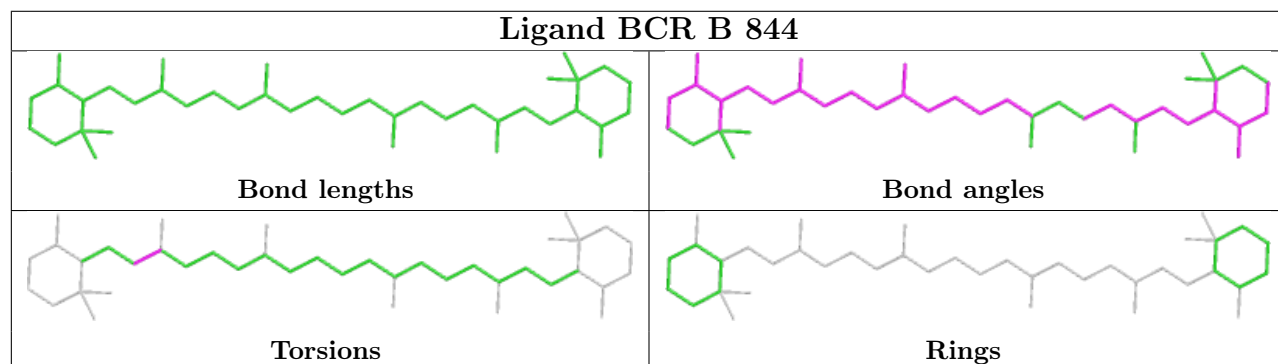
Ligand BCR K 202

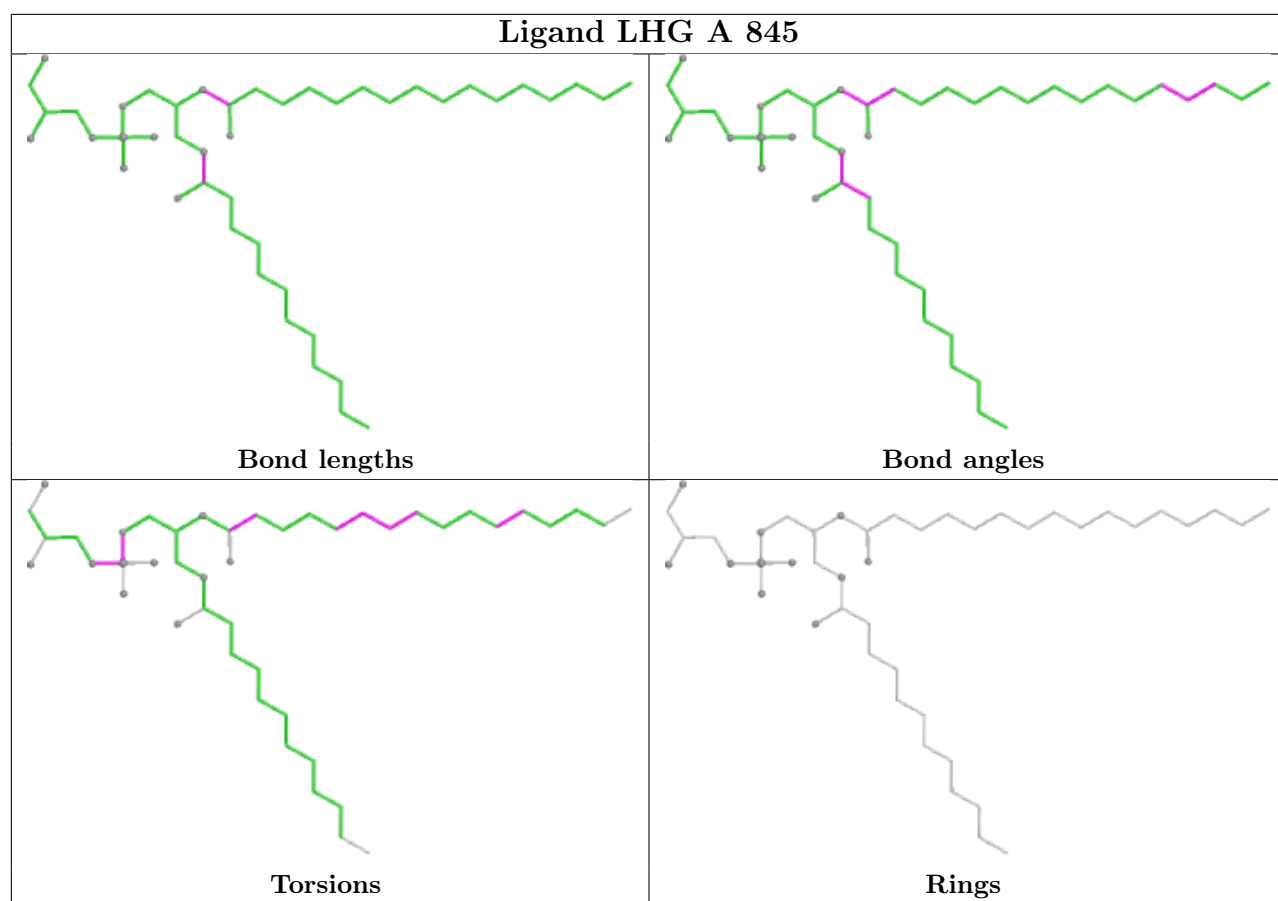


Ligand CLA B 835

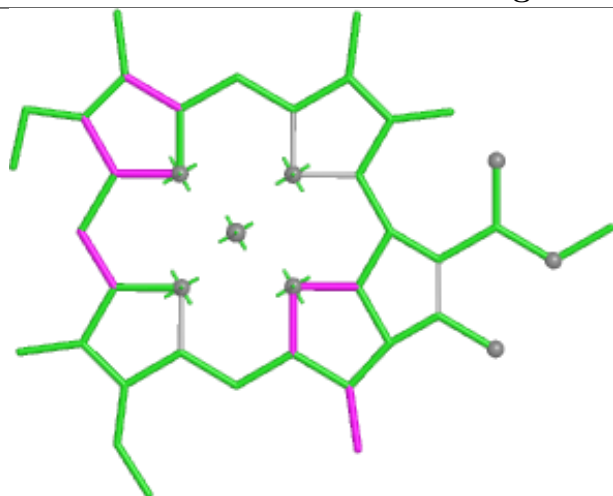


Ligand BCR B 844





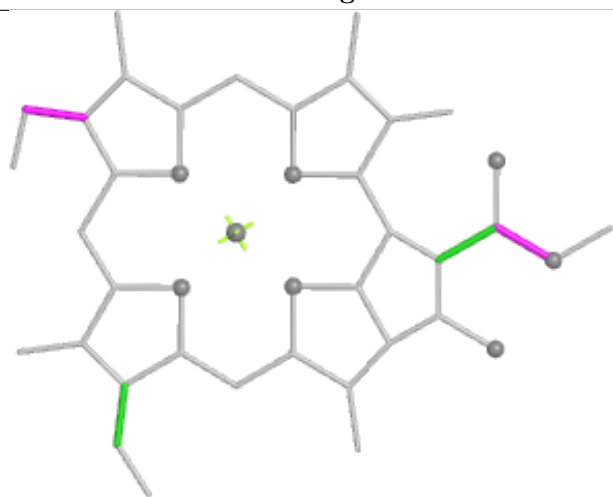
Ligand CLA K 201



Bond lengths



Bond angles

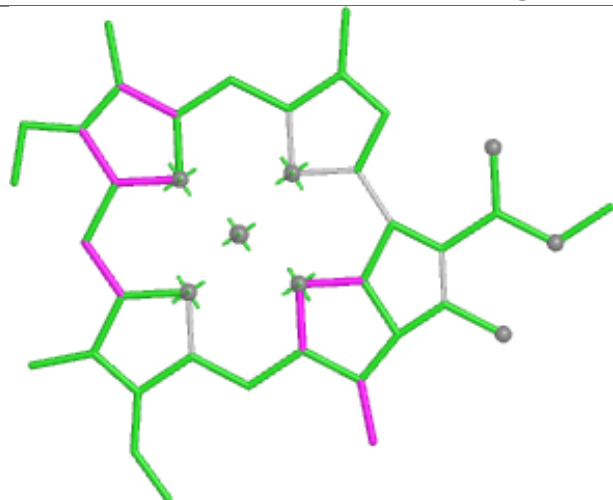


Torsions

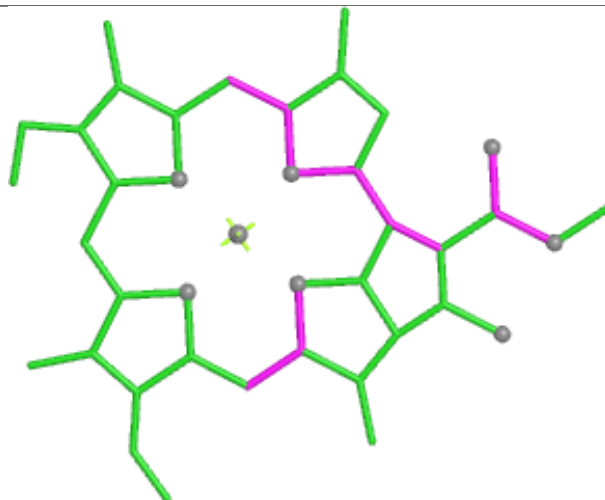


Rings

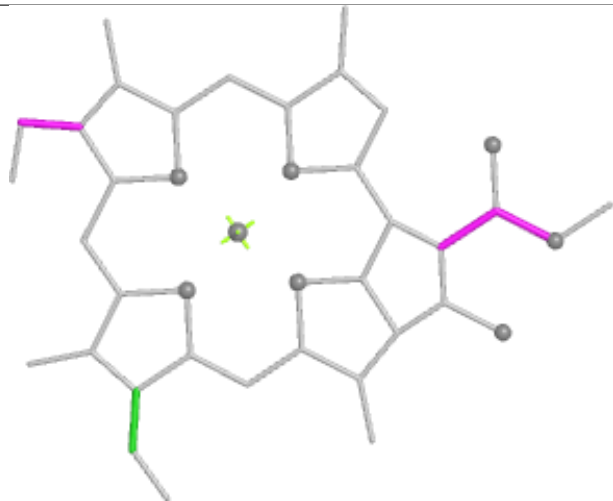
Ligand CLA A 814



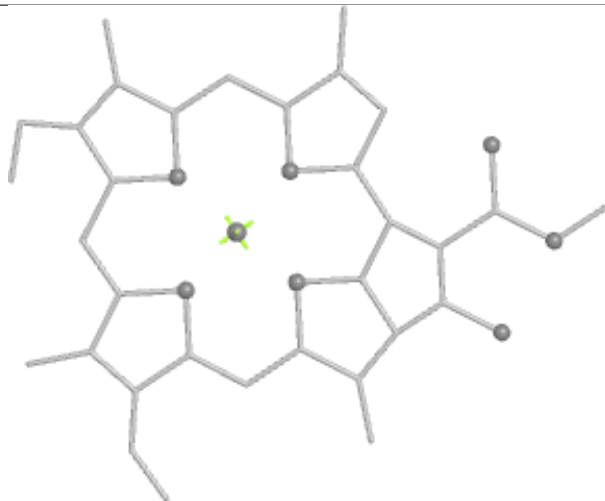
Bond lengths



Bond angles

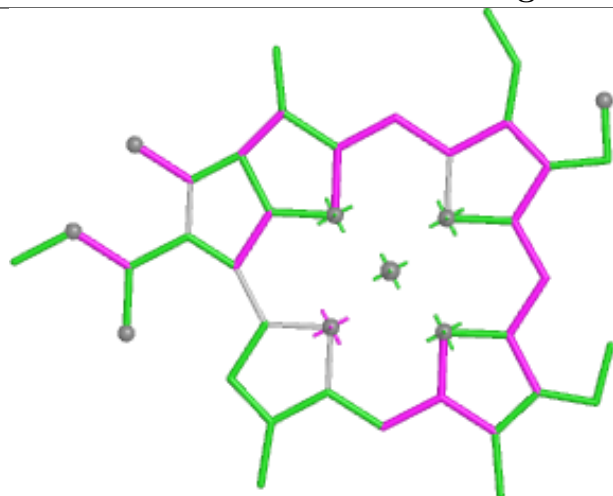


Torsions

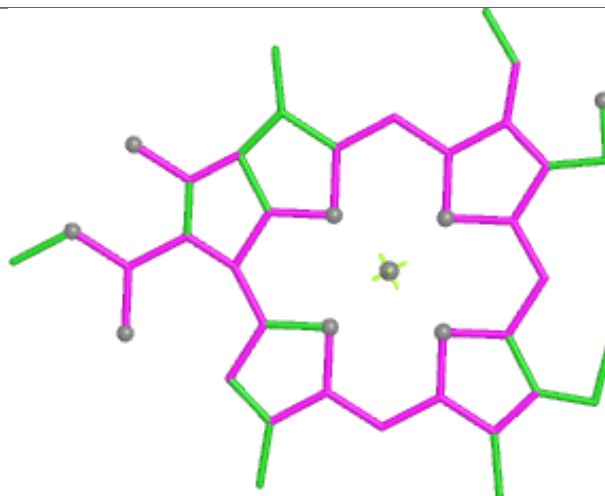


Rings

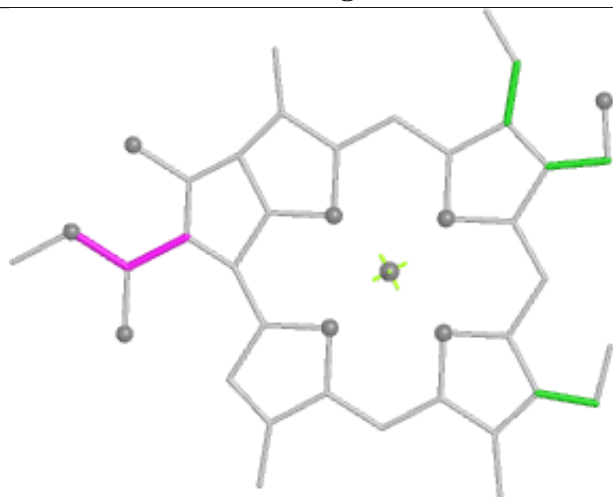
Ligand CHL 9 605



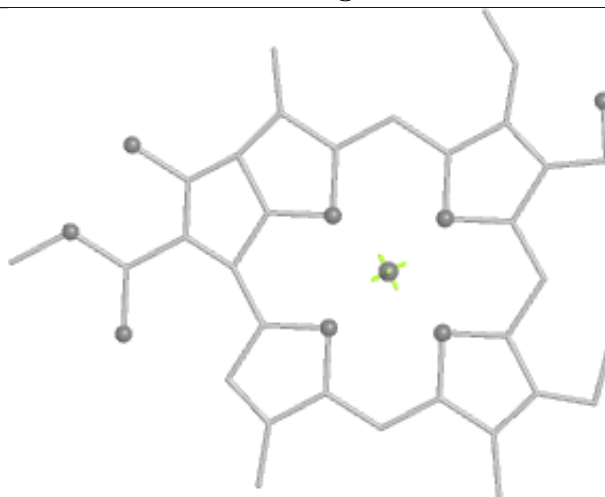
Bond lengths



Bond angles

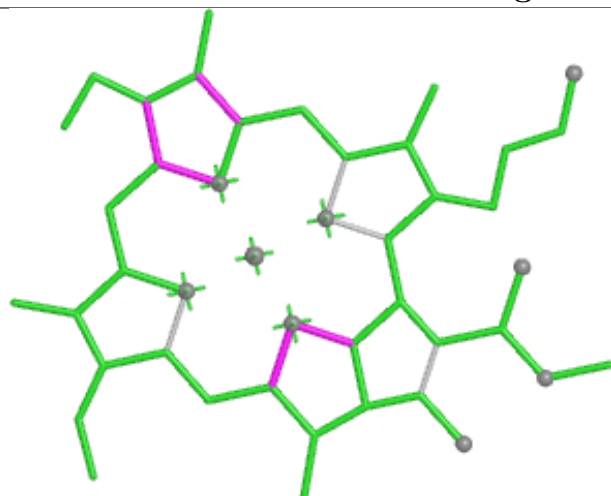


Torsions

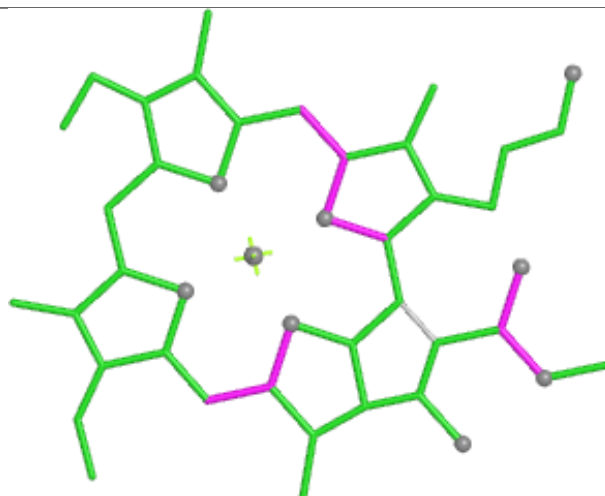


Rings

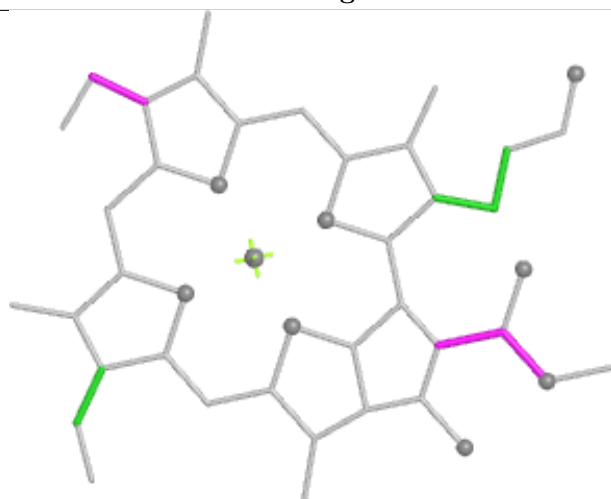
Ligand CLA B 823



Bond lengths



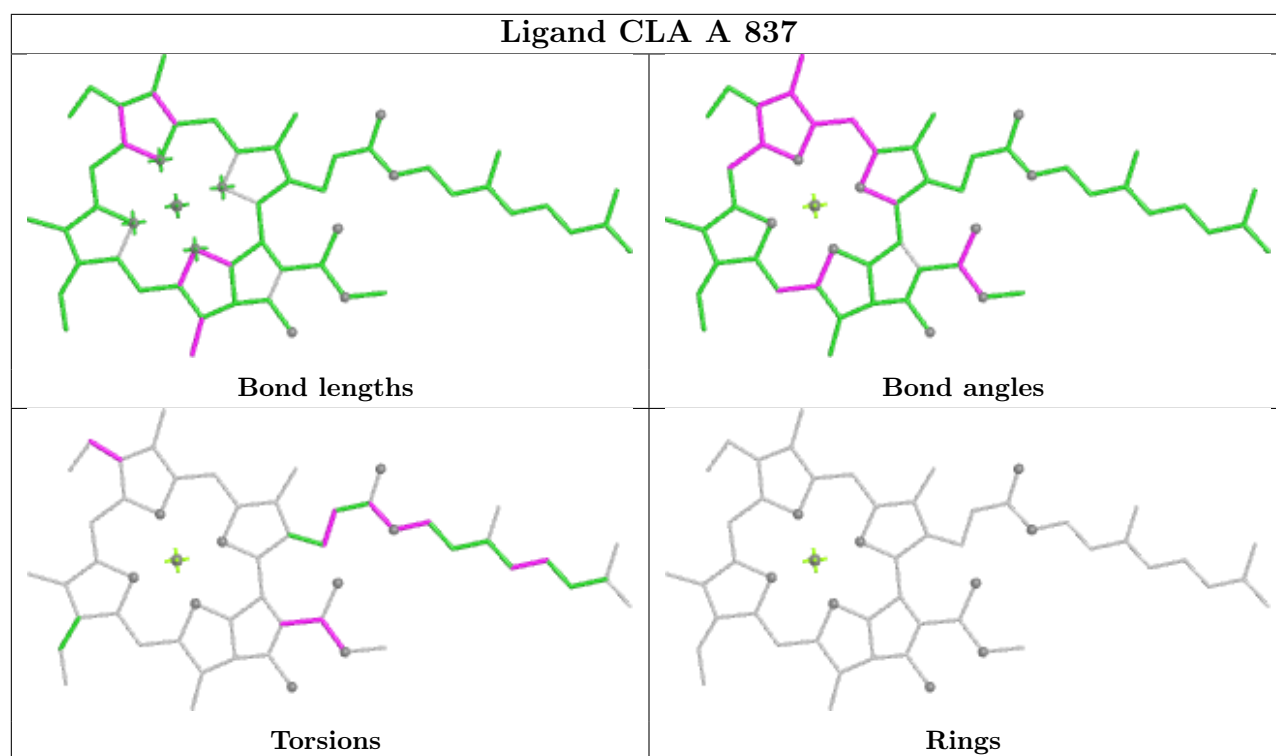
Bond angles



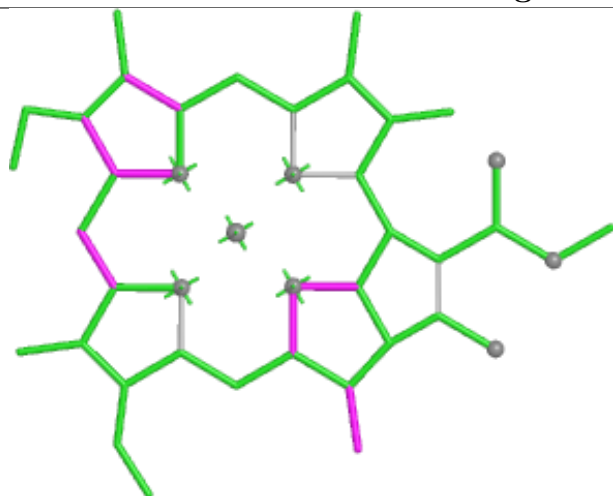
Torsions



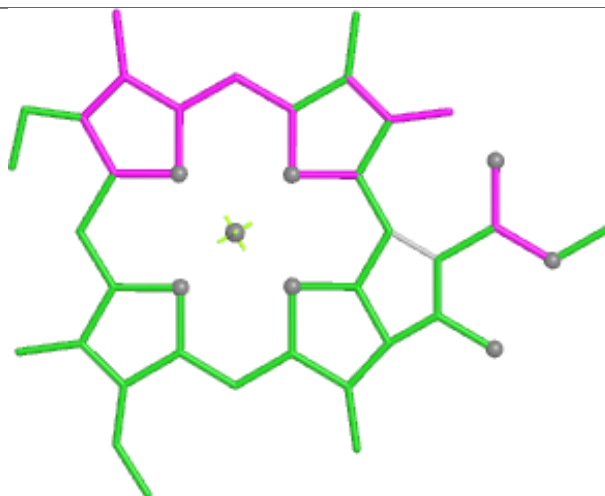
Rings



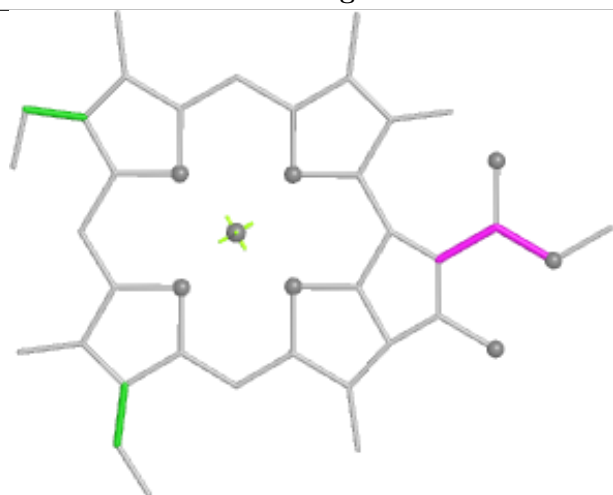
Ligand CLA B 805



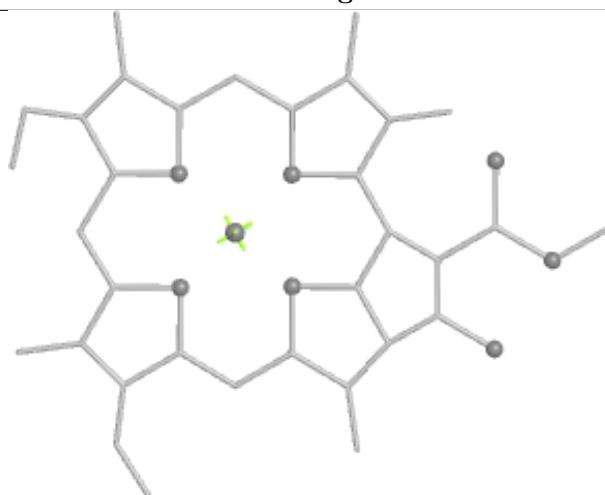
Bond lengths



Bond angles

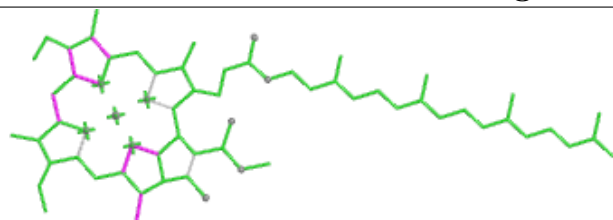


Torsions

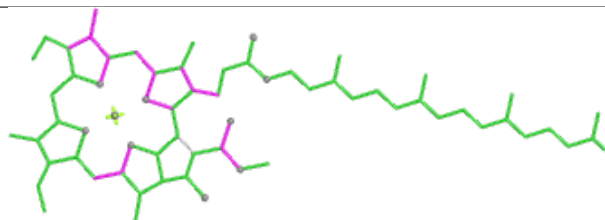


Rings

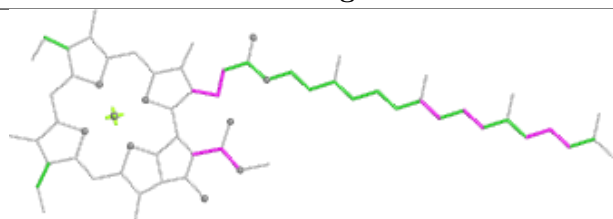
Ligand CLA A 802



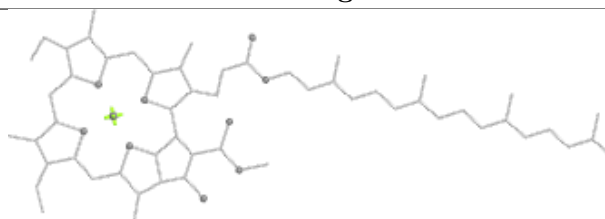
Bond lengths



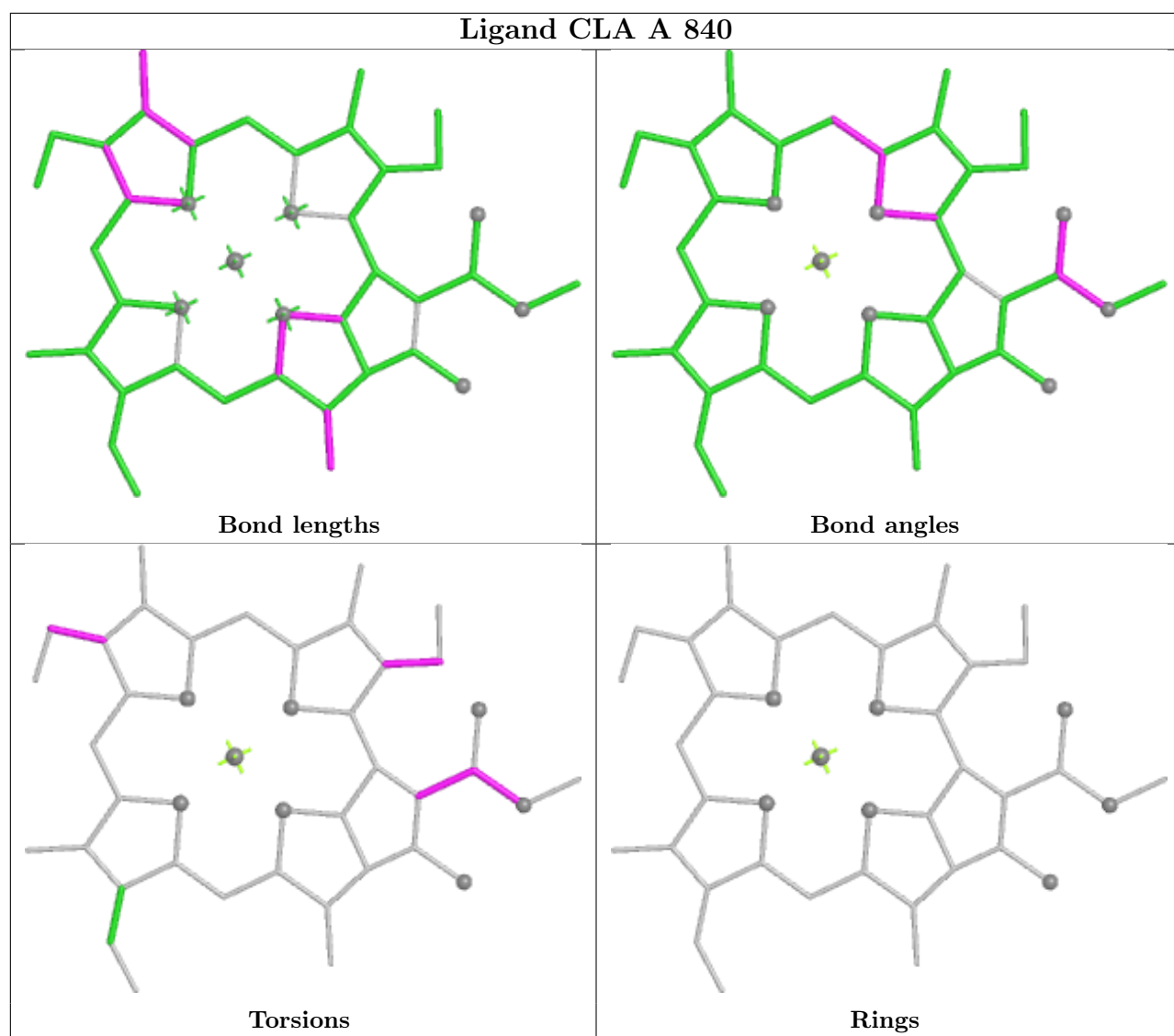
Bond angles



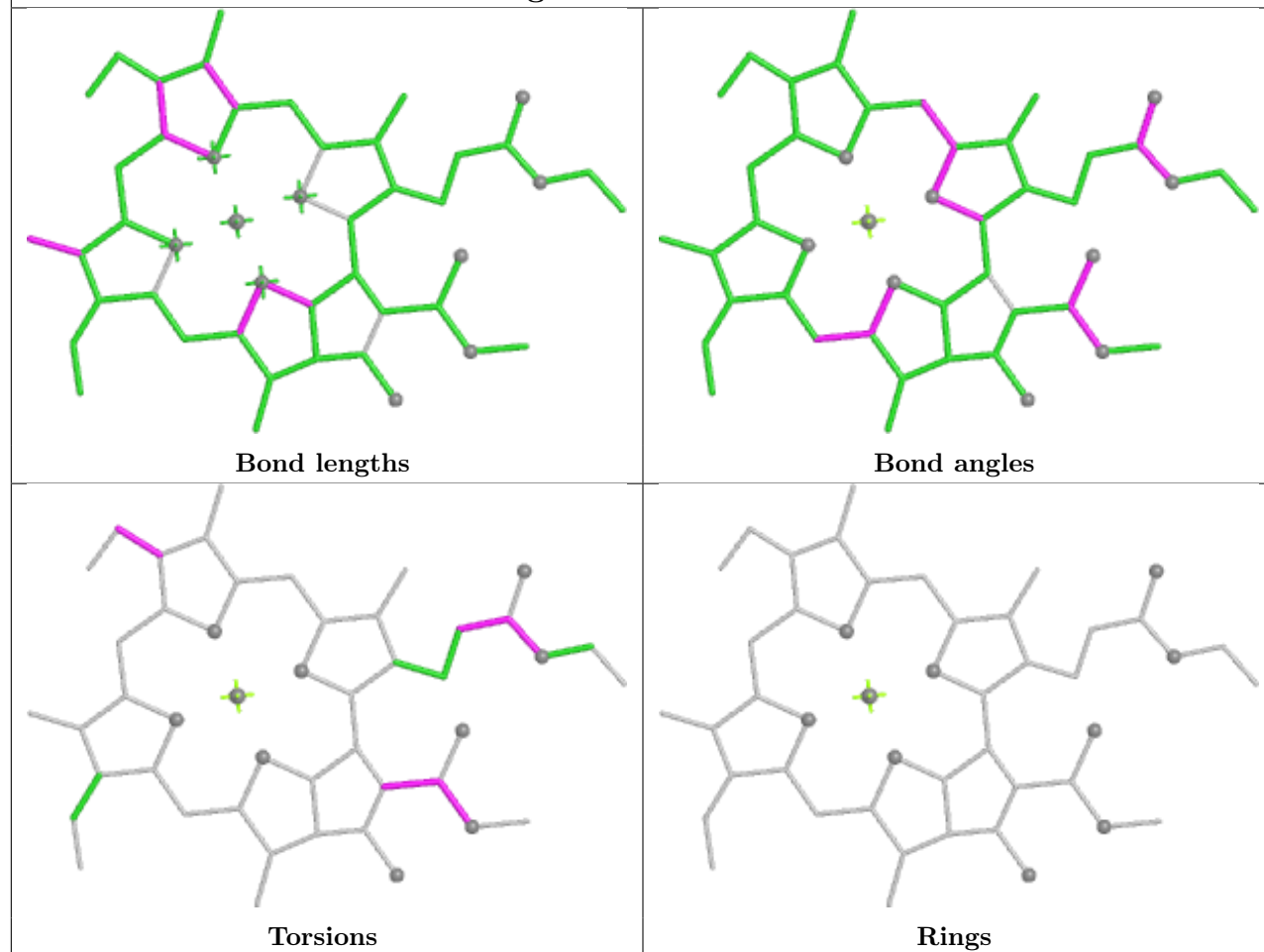
Torsions



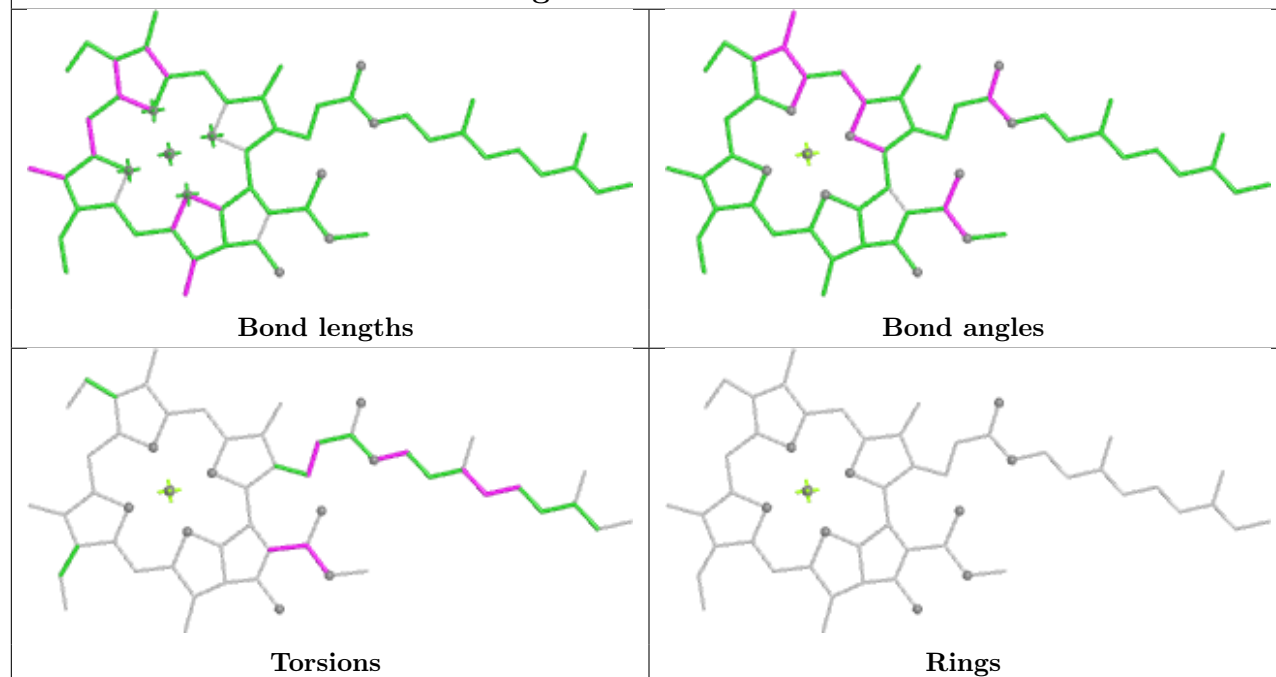
Rings

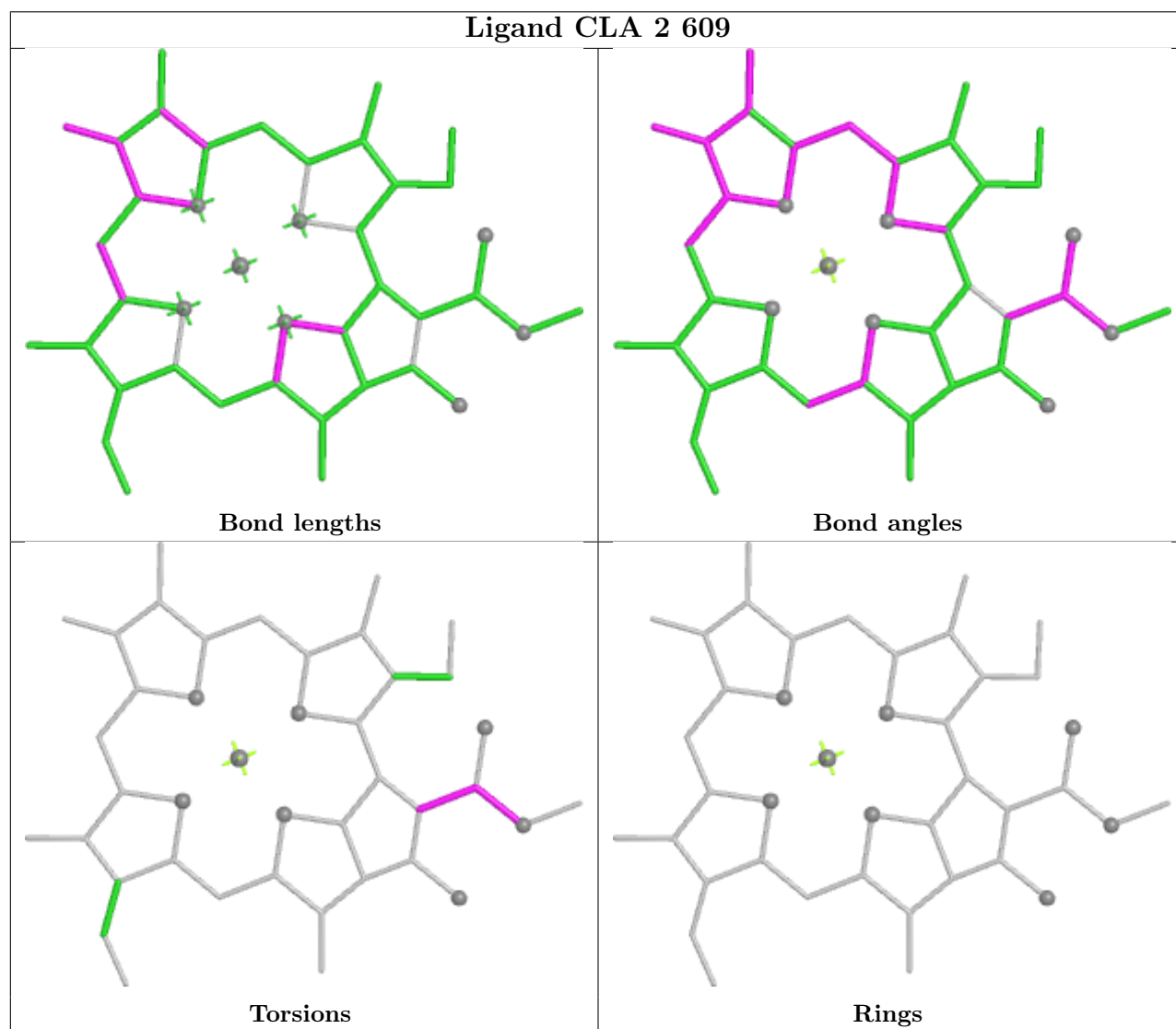
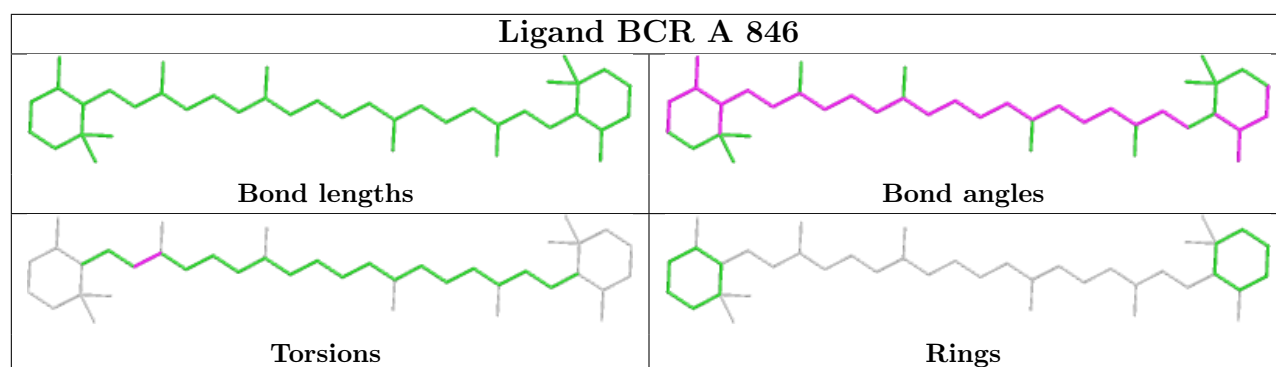


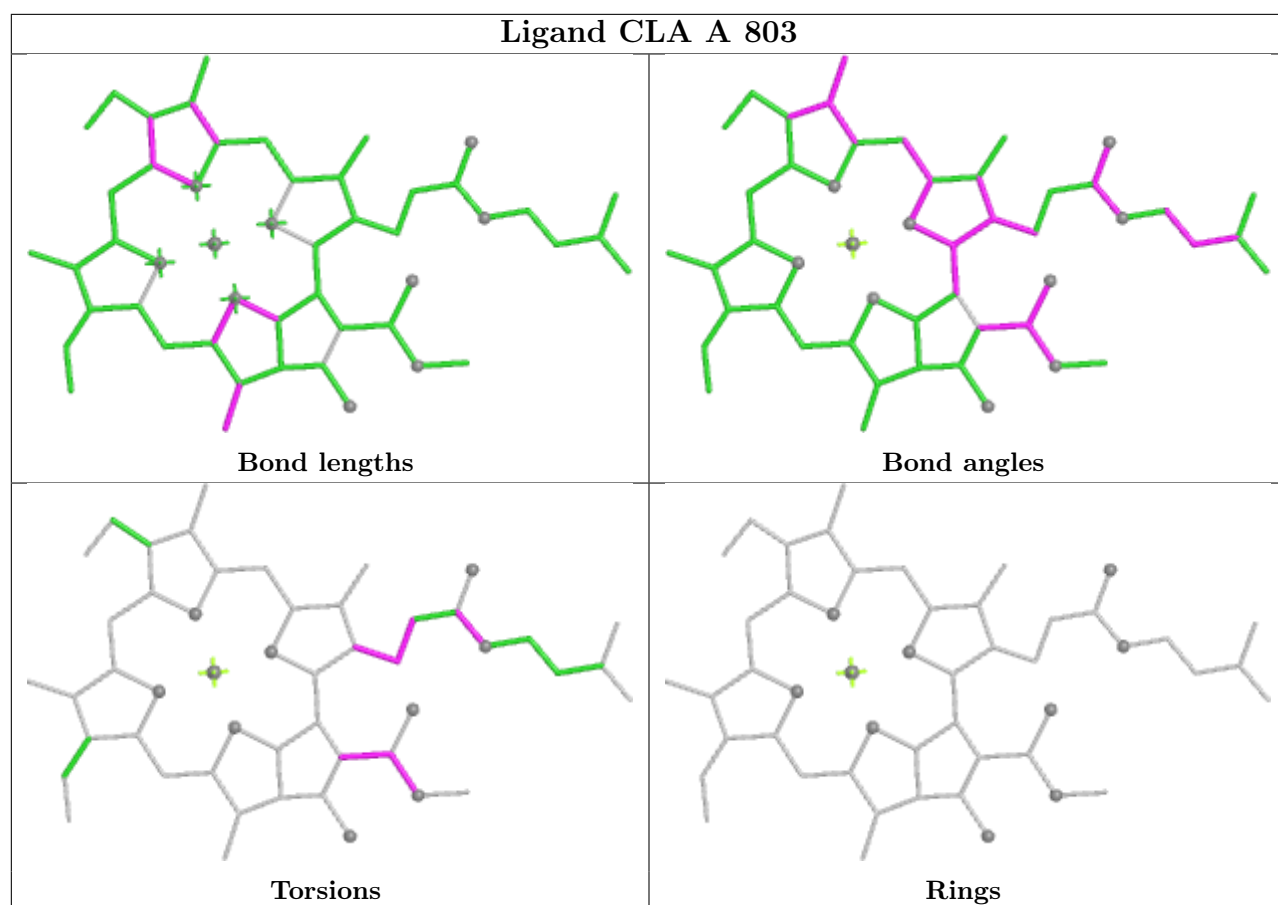
Ligand CLA B 833



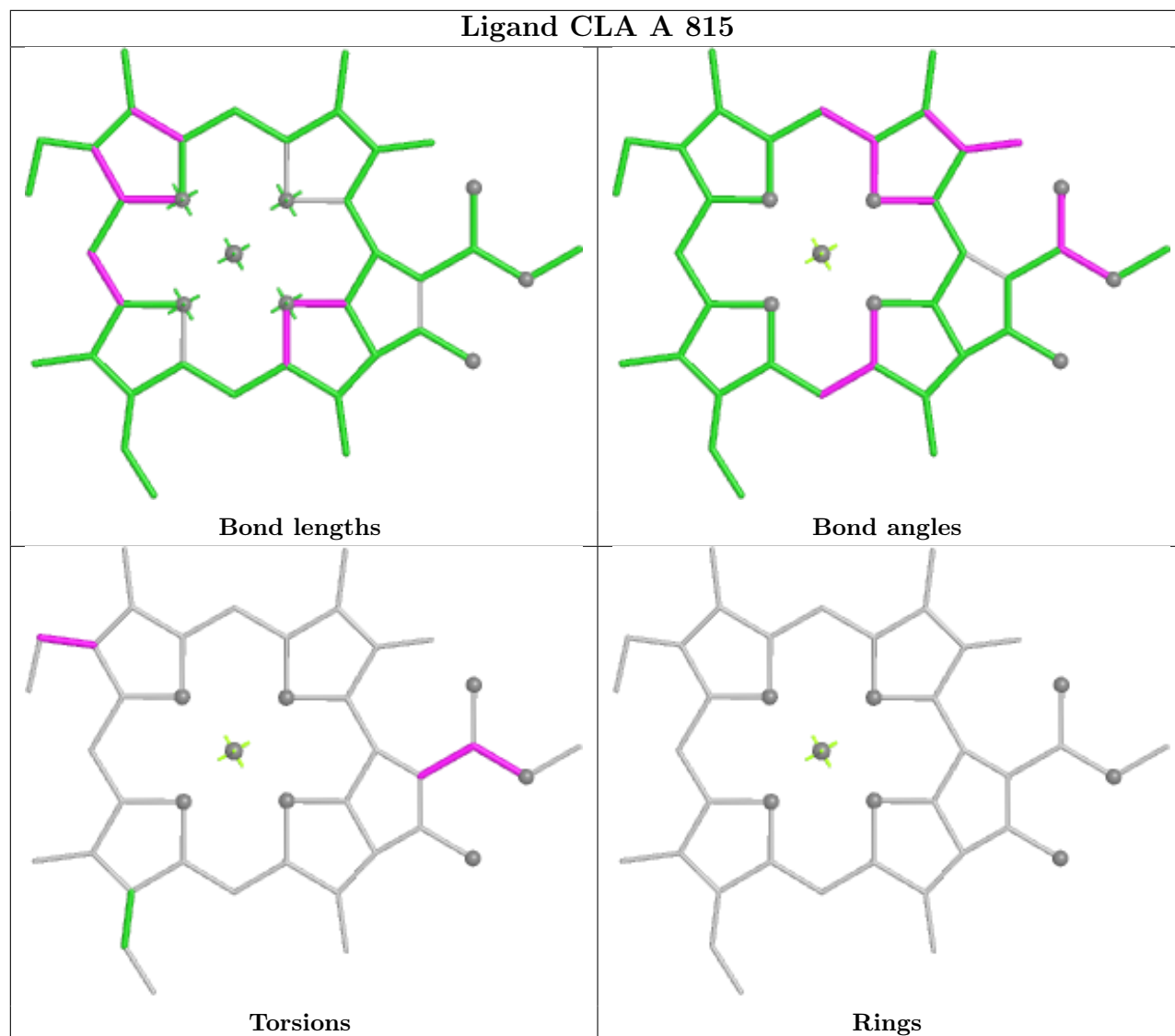
Ligand CLA B 802



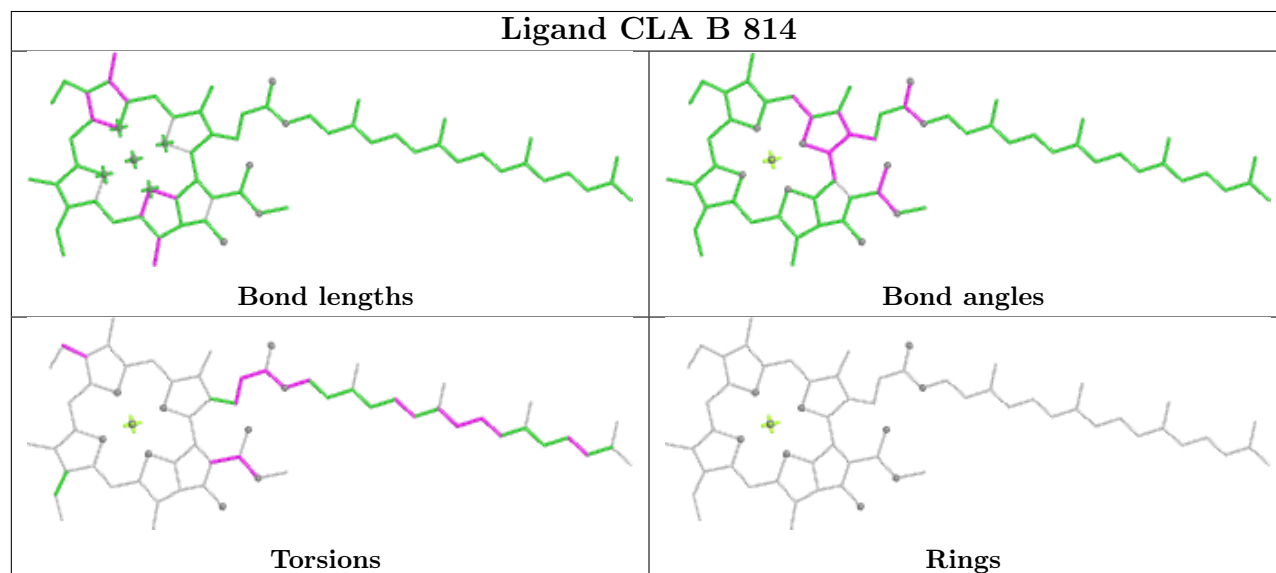


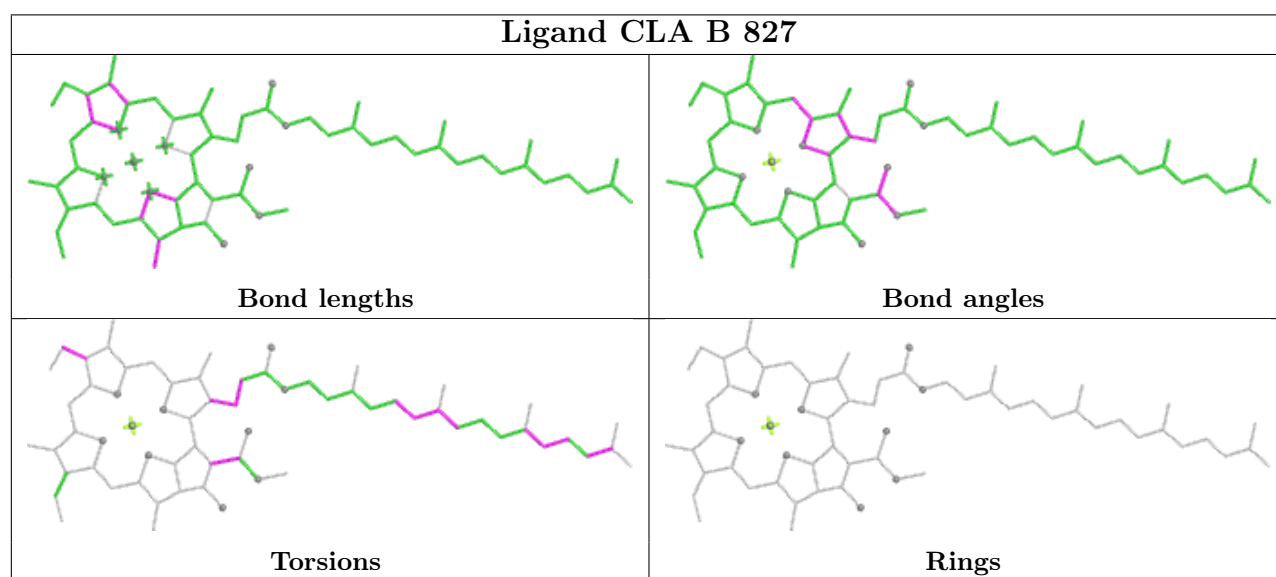
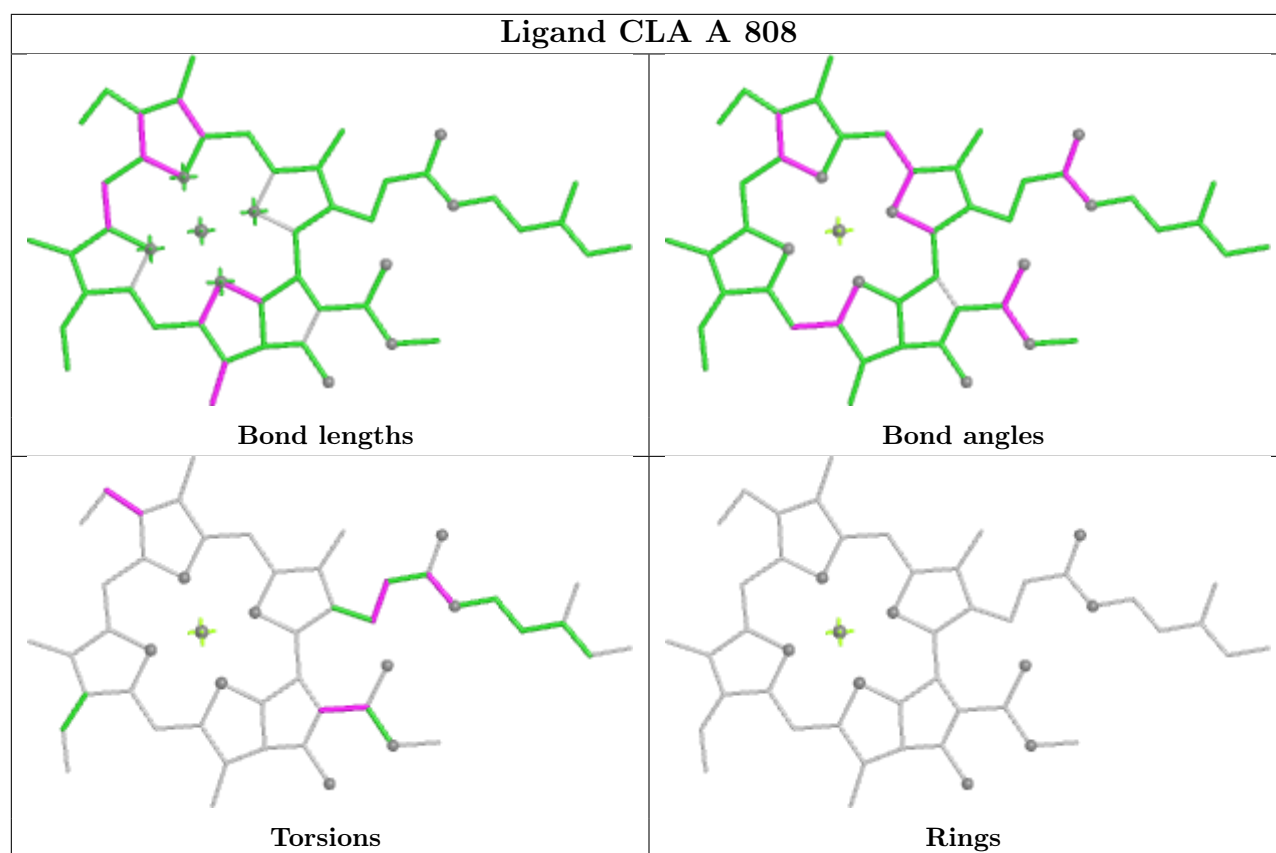


Ligand CLA A 815

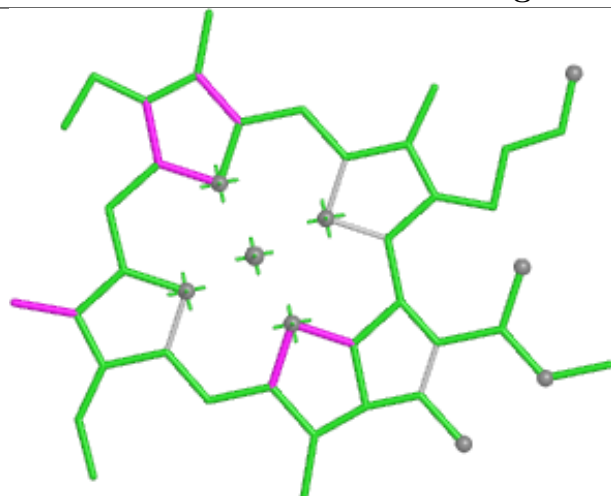


Ligand CLA B 814

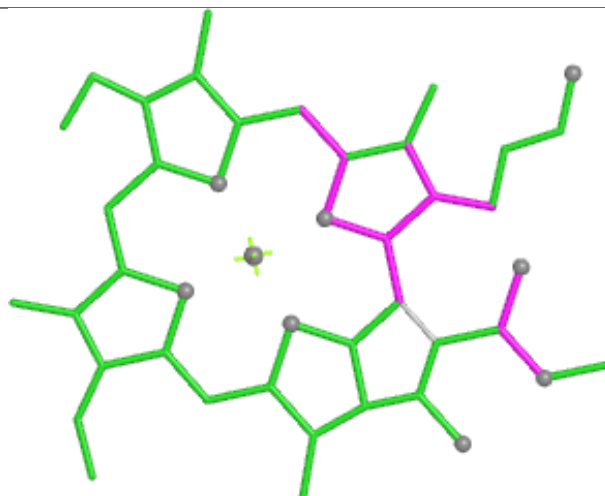




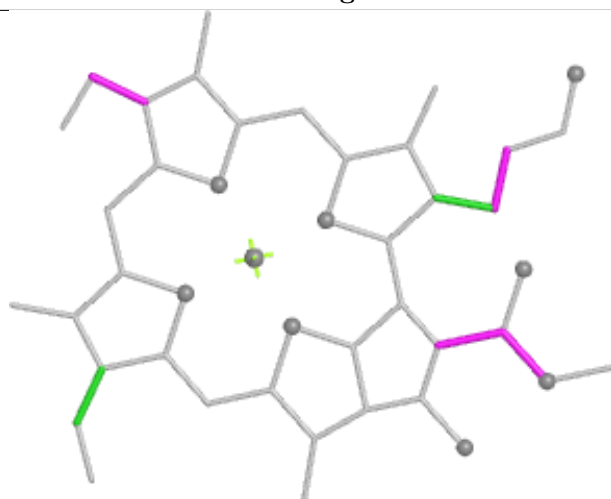
Ligand CLA A 813



Bond lengths



Bond angles

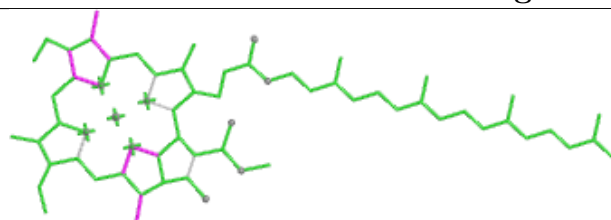


Torsions

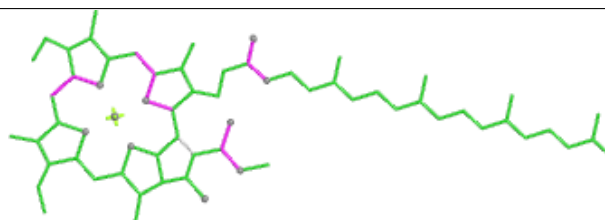


Rings

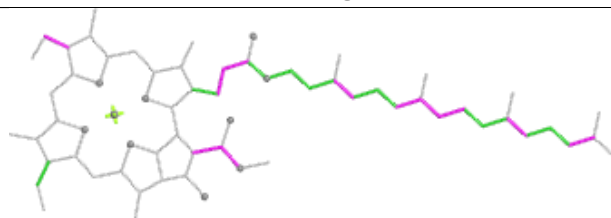
Ligand CLA B 803



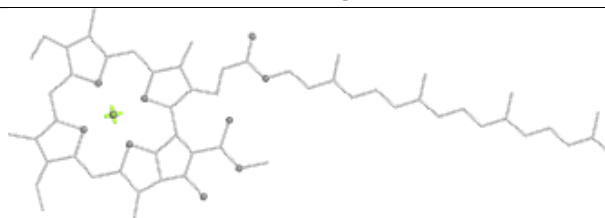
Bond lengths



Bond angles

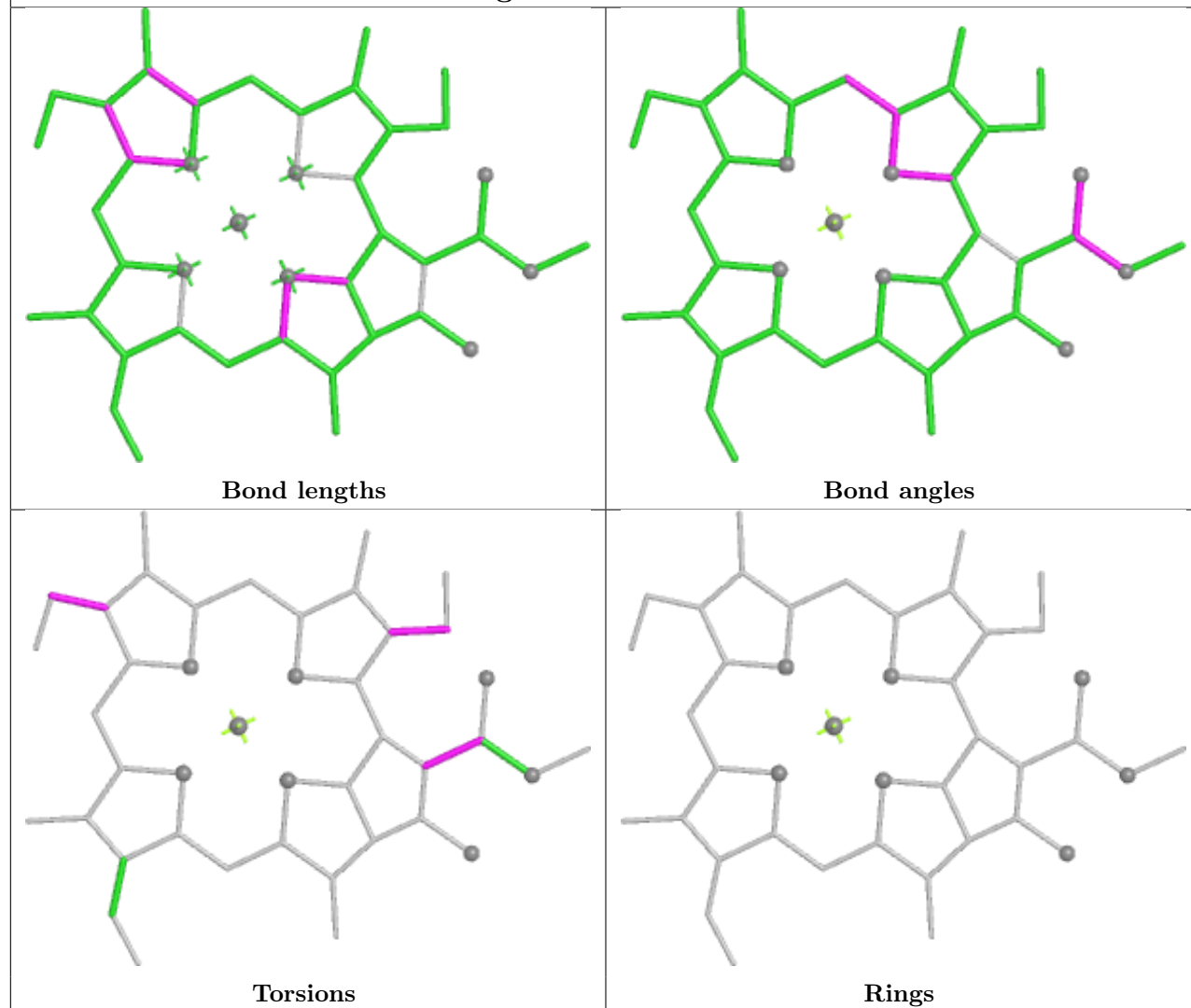


Torsions

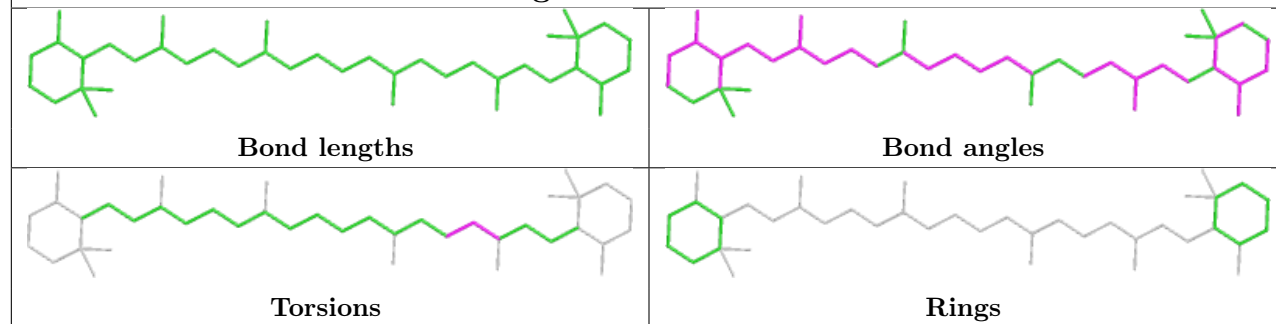


Rings

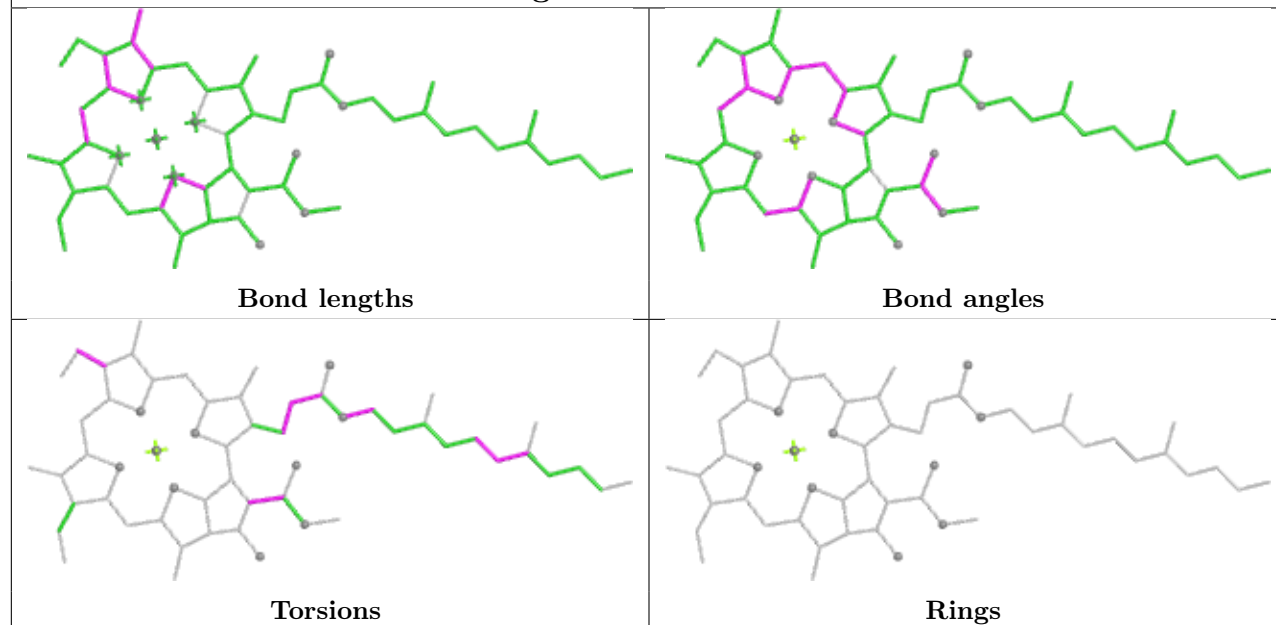
Ligand CLA A 821



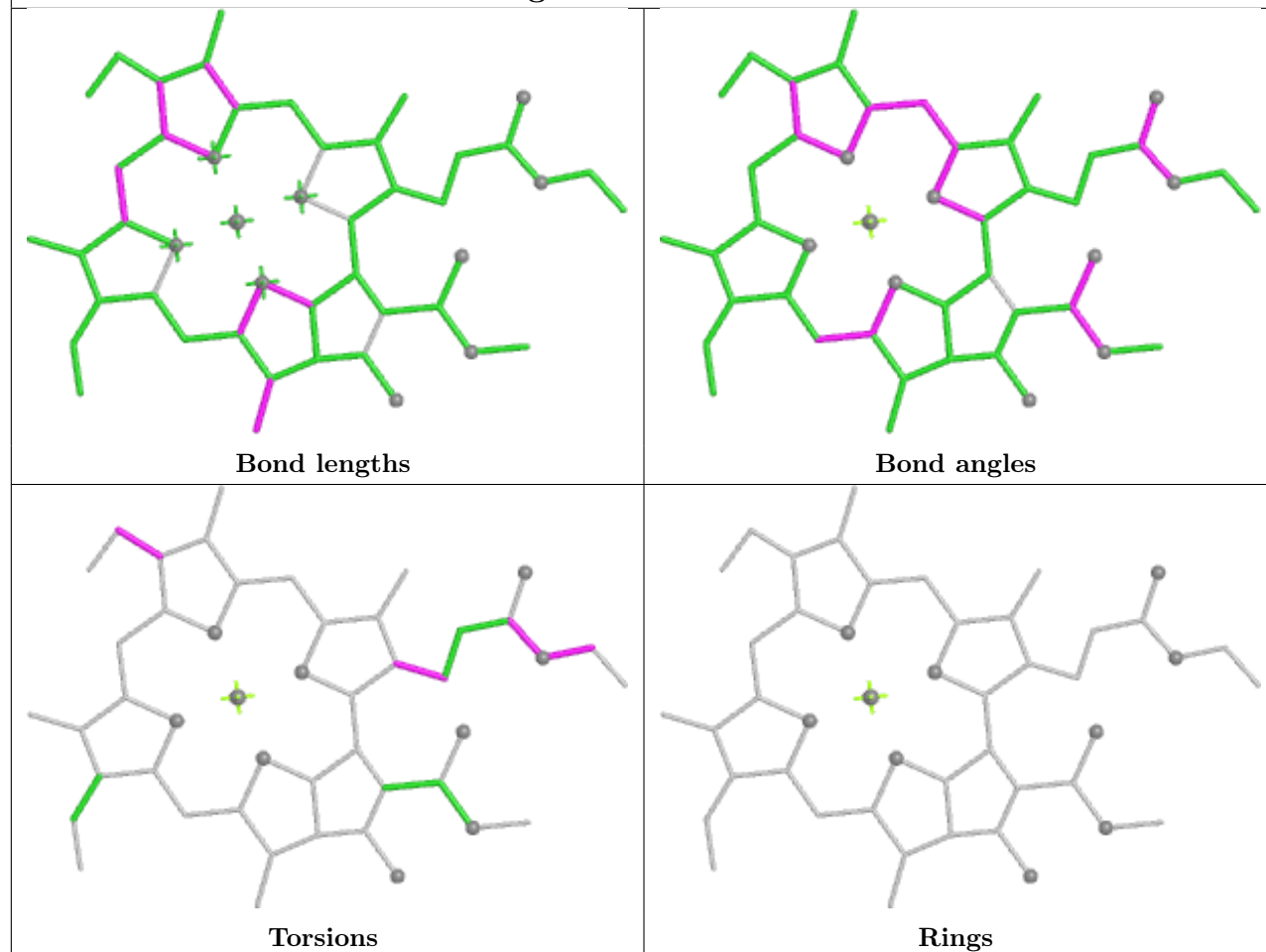
Ligand BCR L 301

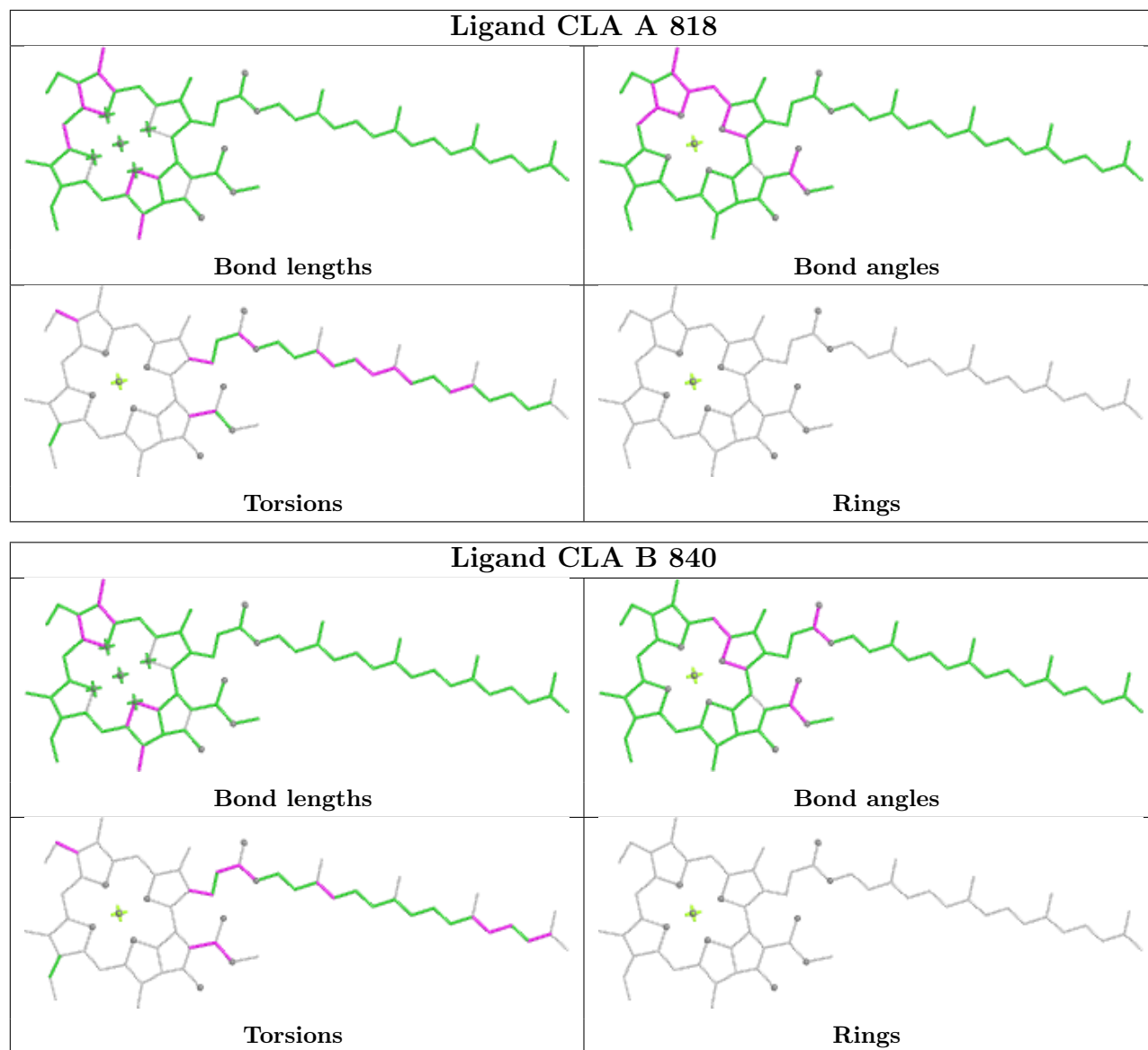


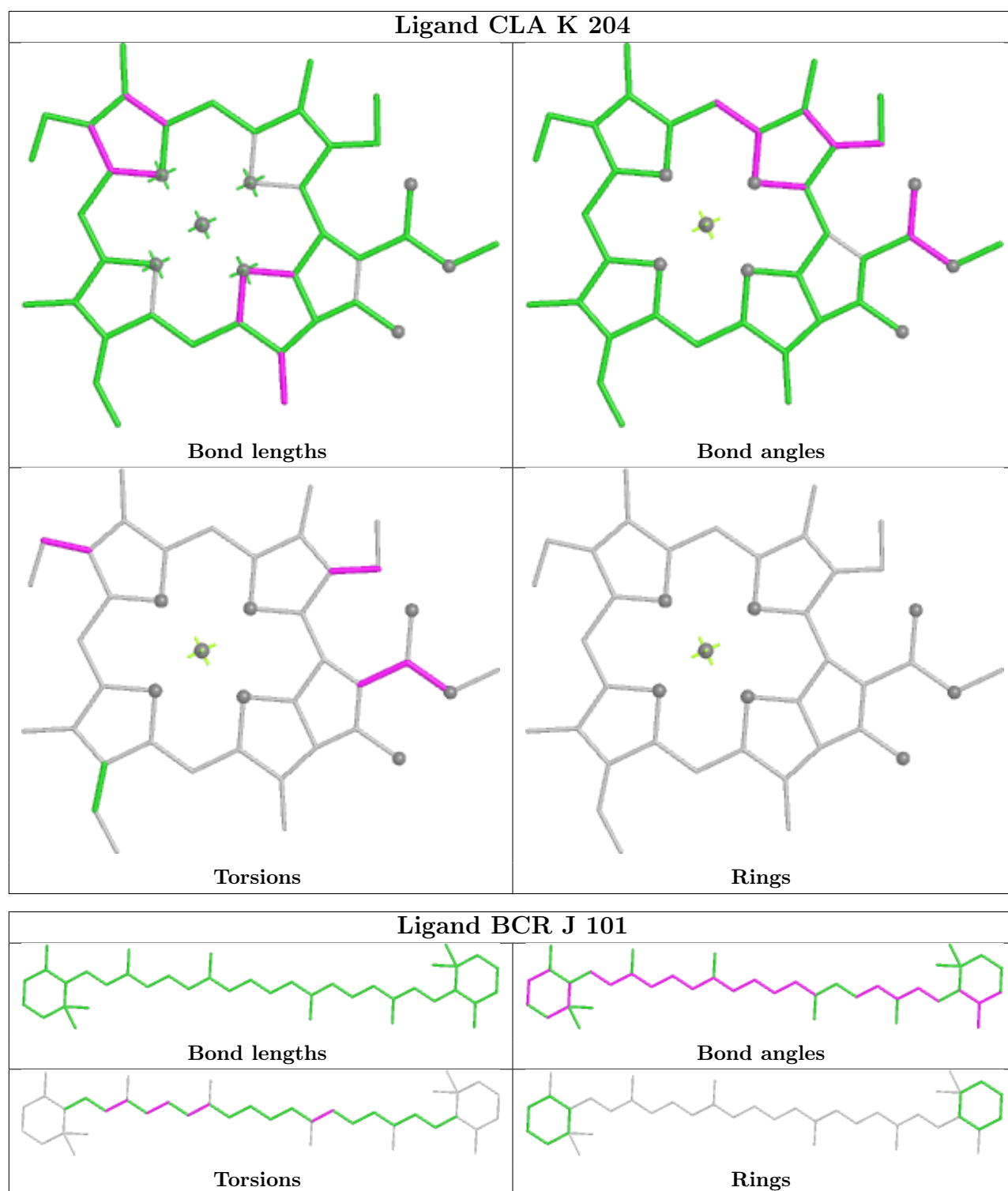
Ligand CLA B 837



Ligand CLA B 838







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.

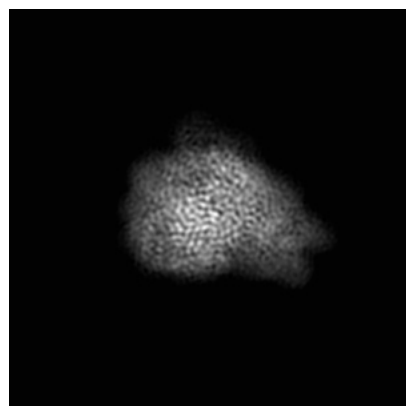
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-81136. These allow visual inspection of the internal detail of the map and identification of artifacts.

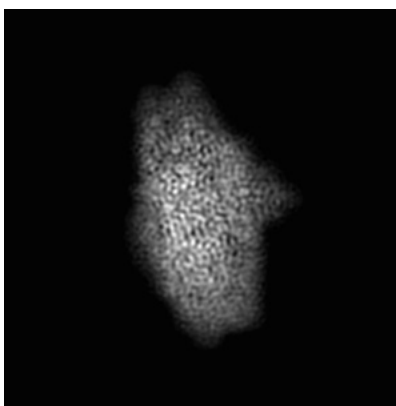
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

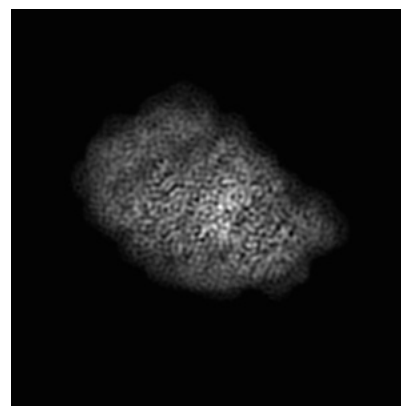
6.1.1 Primary map



X

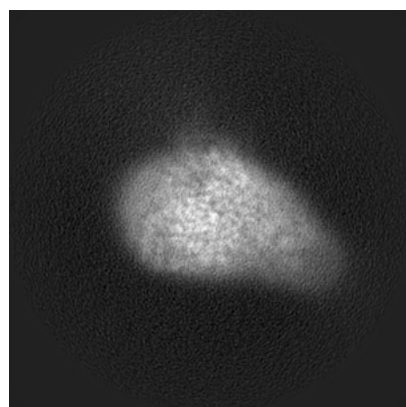


Y

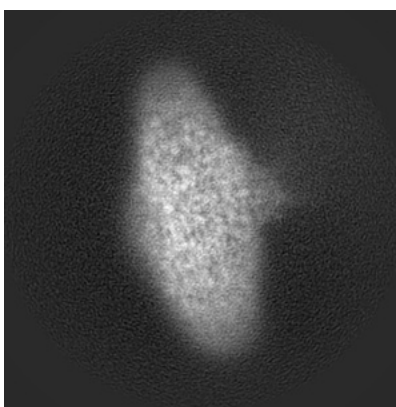


Z

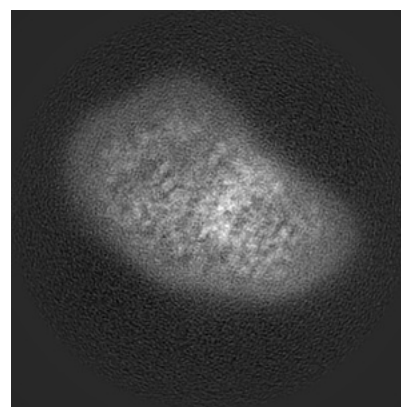
6.1.2 Raw map



X



Y

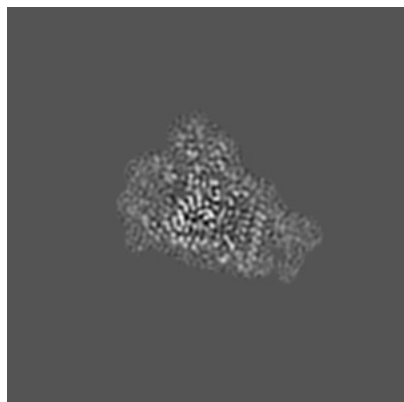


Z

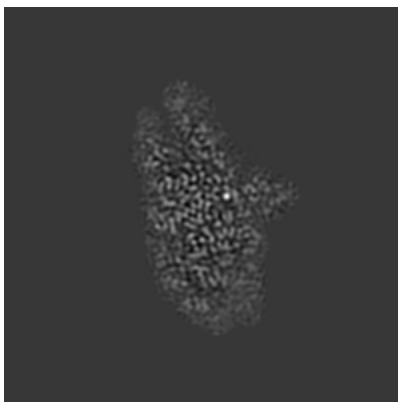
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

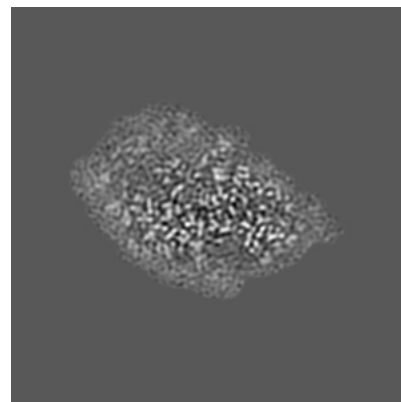
6.2.1 Primary map



X Index: 128

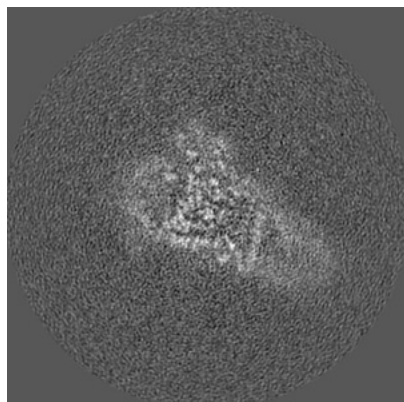


Y Index: 128

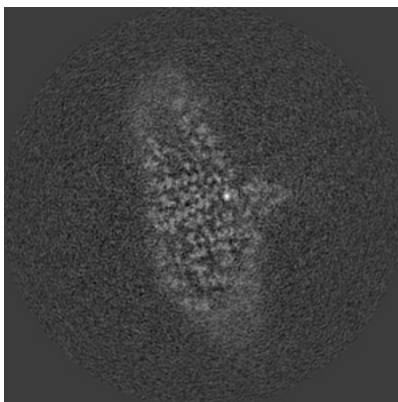


Z Index: 128

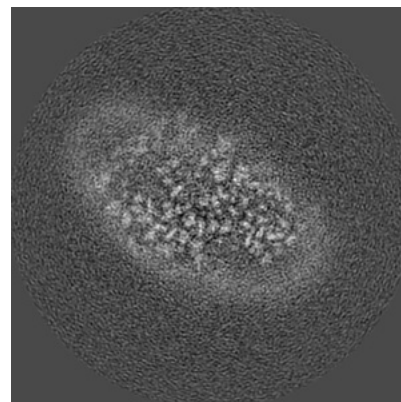
6.2.2 Raw map



X Index: 128



Y Index: 128

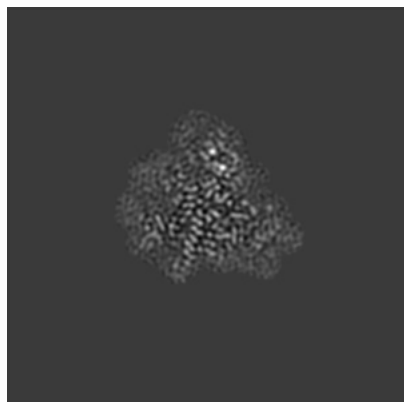


Z Index: 128

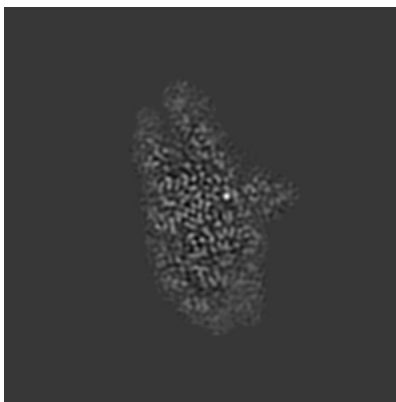
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

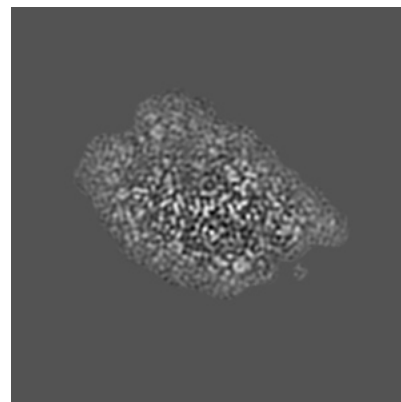
6.3.1 Primary map



X Index: 139

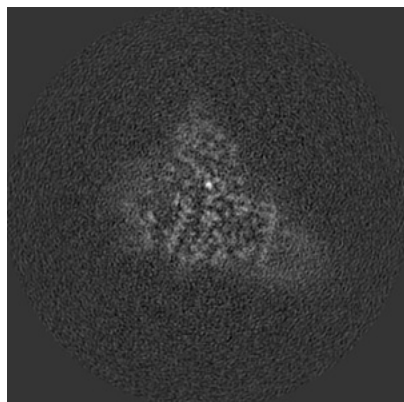


Y Index: 128

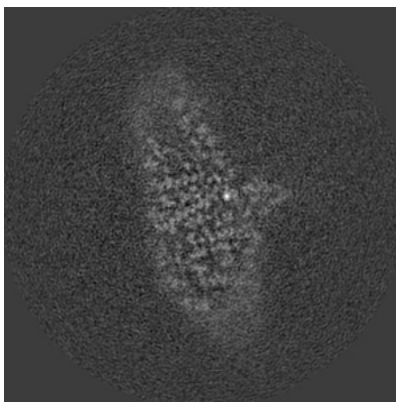


Z Index: 121

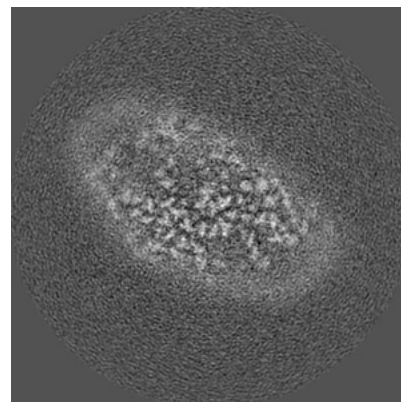
6.3.2 Raw map



X Index: 135



Y Index: 128

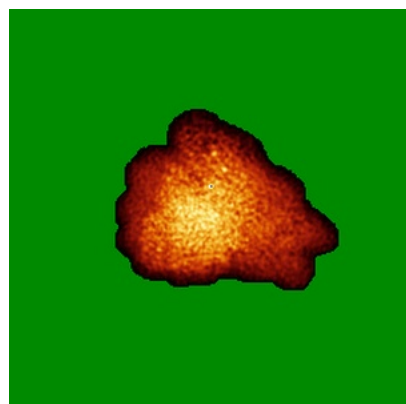


Z Index: 124

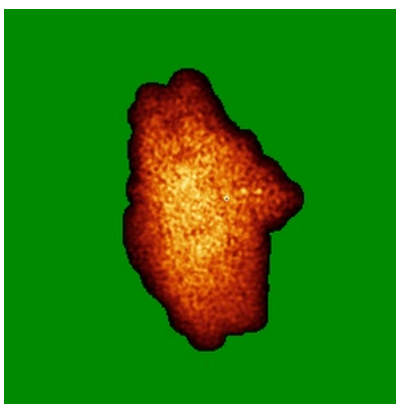
The images above show the largest variance slices of the map in three orthogonal directions.

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

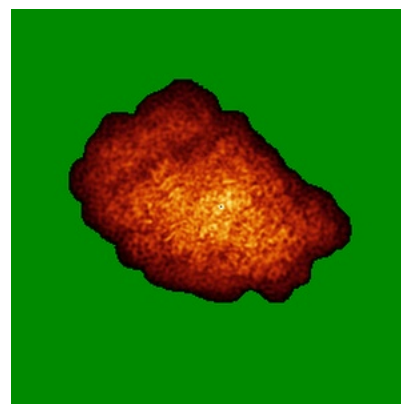
6.4.1 Primary map



X

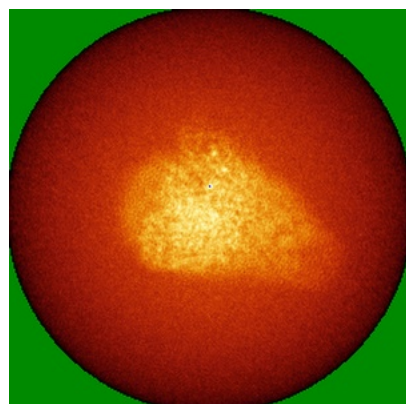


Y

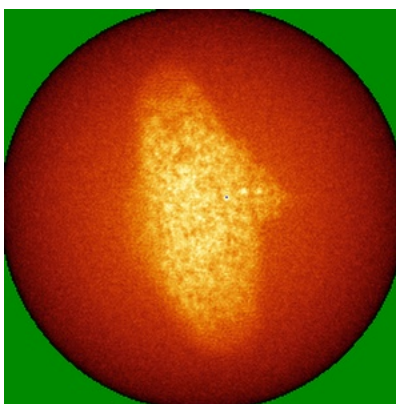


Z

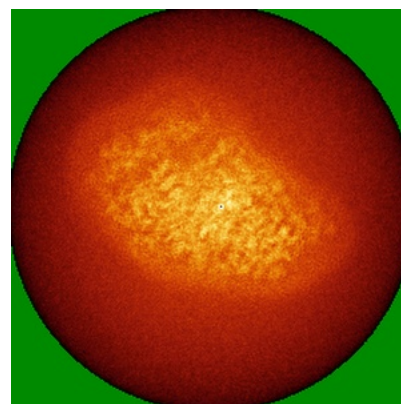
6.4.2 Raw map



X



Y

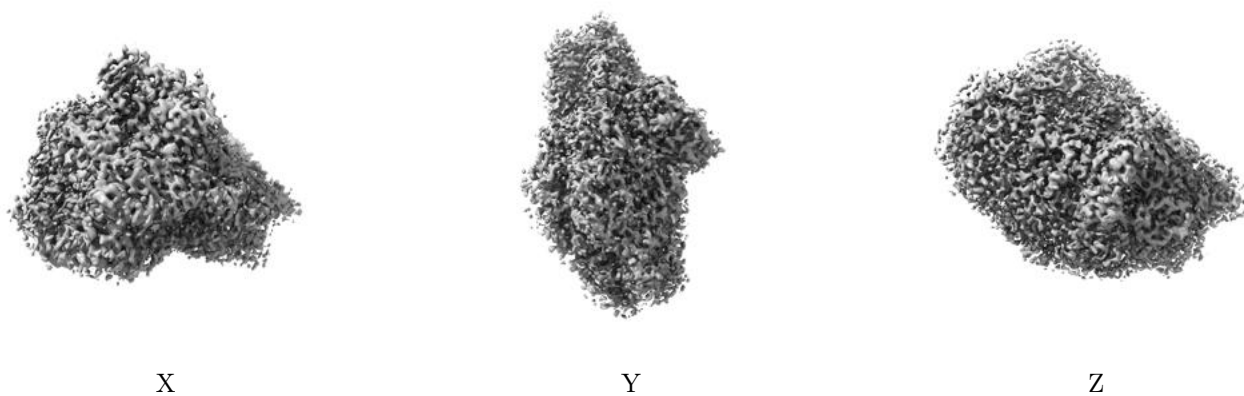


Z

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.

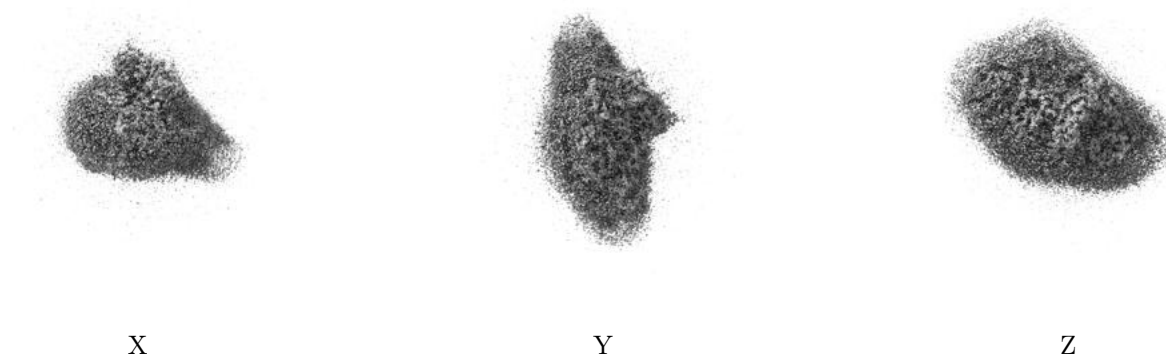
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

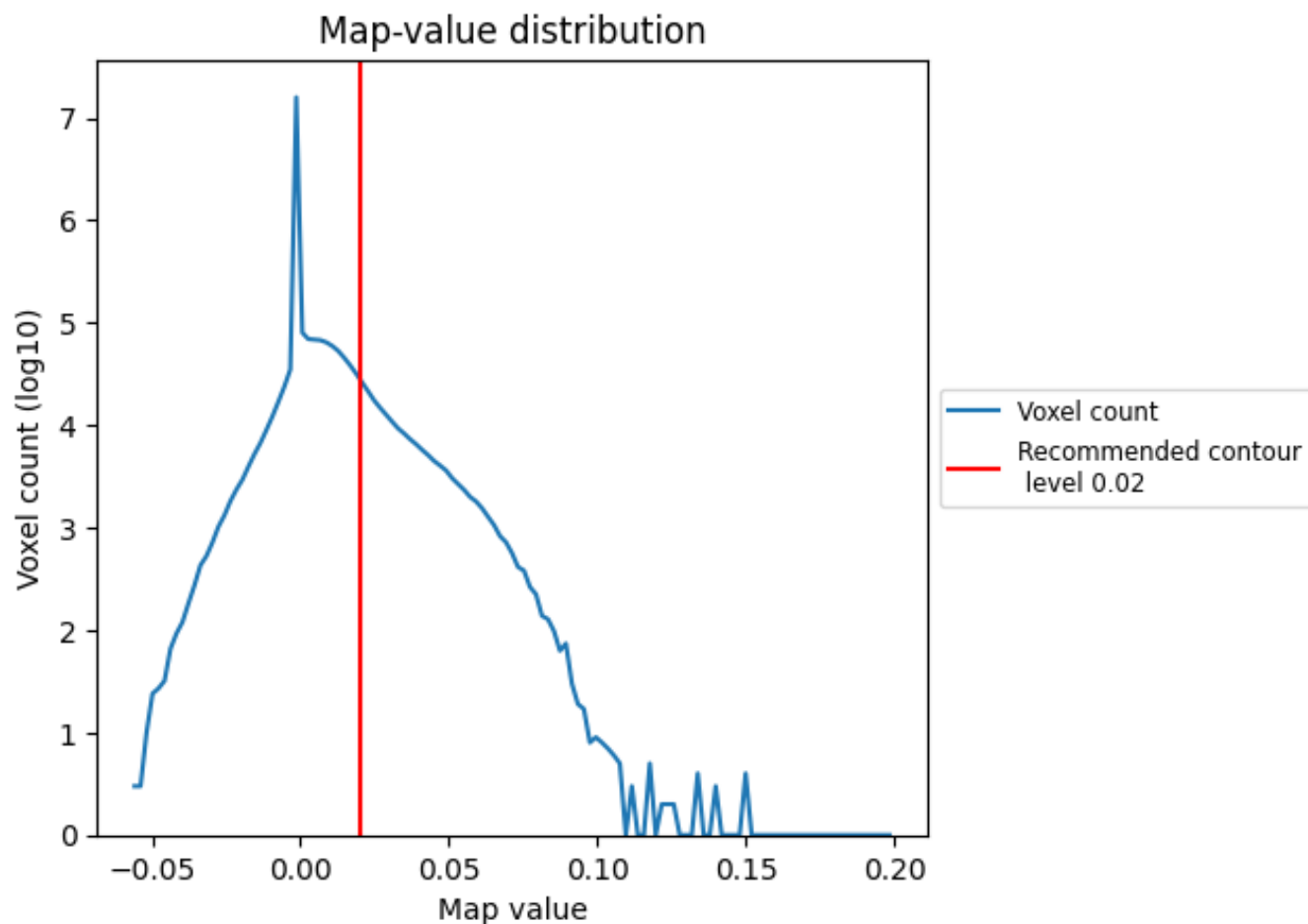
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

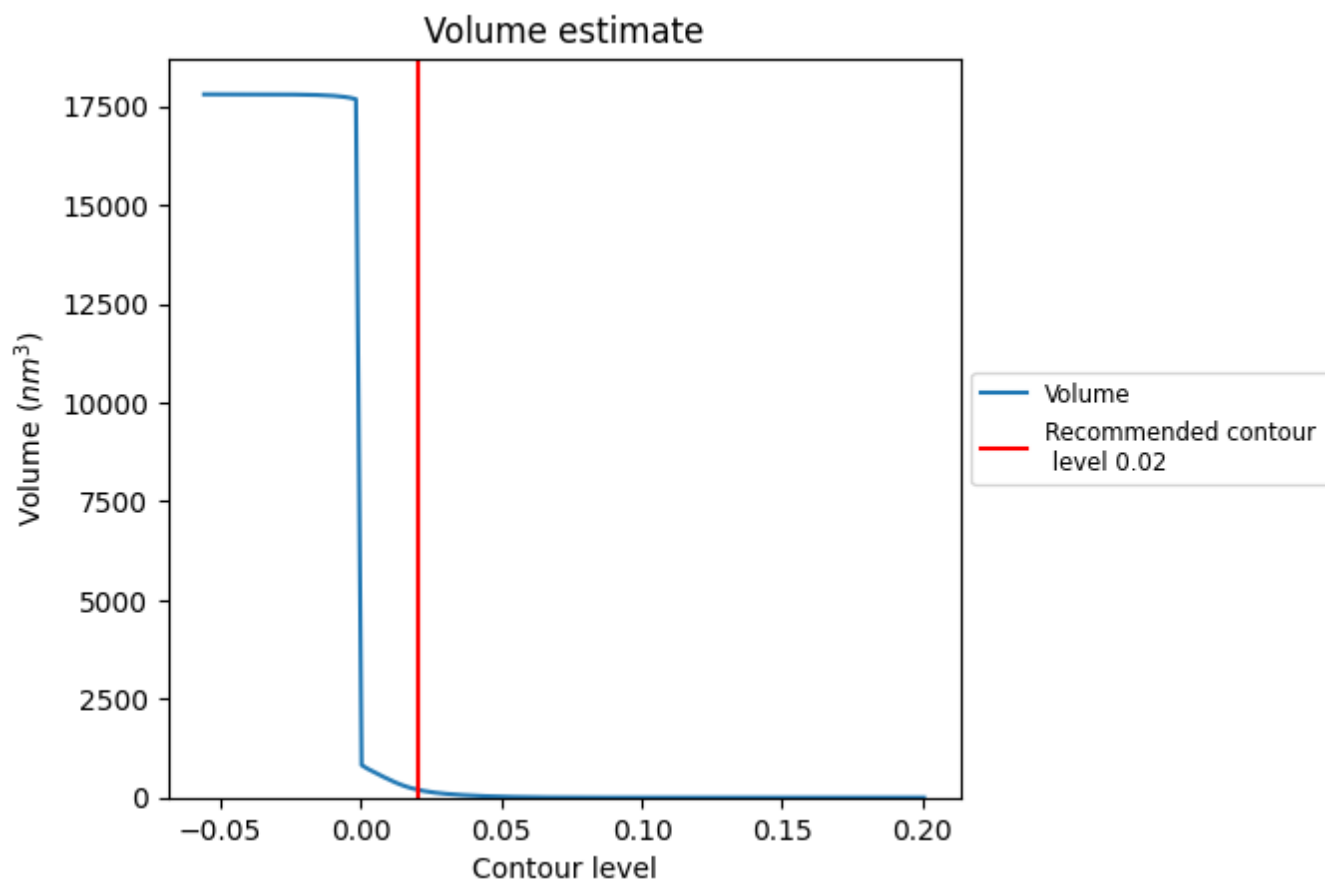
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

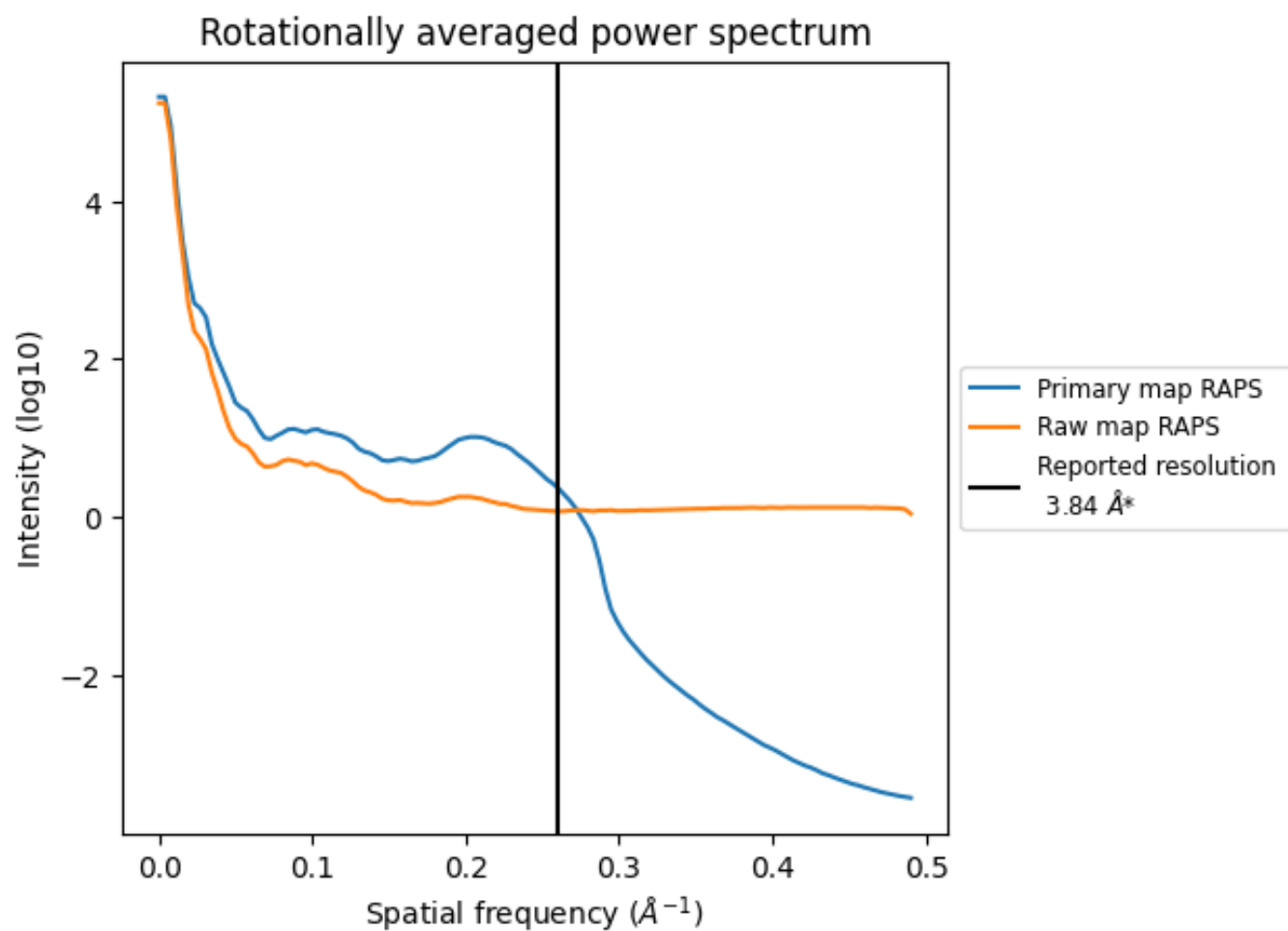
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 202 nm^3 ; this corresponds to an approximate mass of 183 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 ⓘ

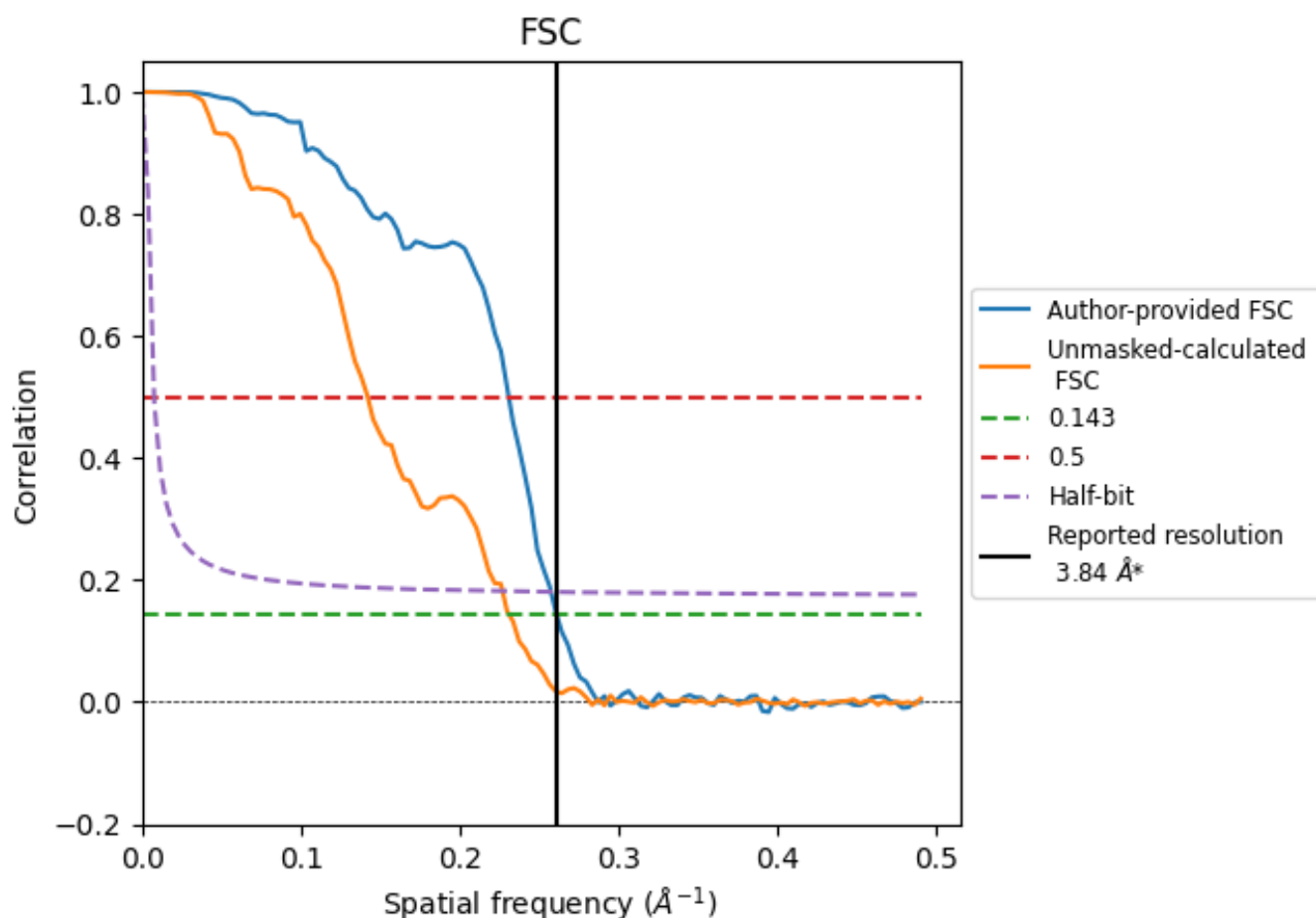


*Reported resolution corresponds to spatial frequency of 0.260 $\text{\AA}^{-1}$

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 0.260 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

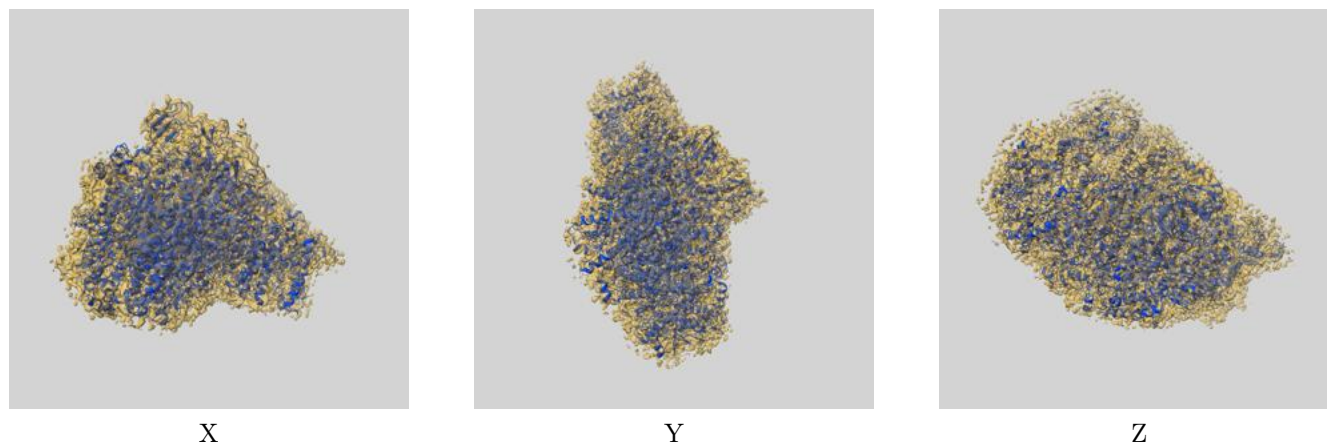
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.84	-	-
Author-provided FSC curve	3.83	4.33	3.88
Unmasked-calculated*	4.33	7.04	4.41

*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 4.33 differs from the reported value 3.84 by more than 10 %

9 Map-model fit [i](#)

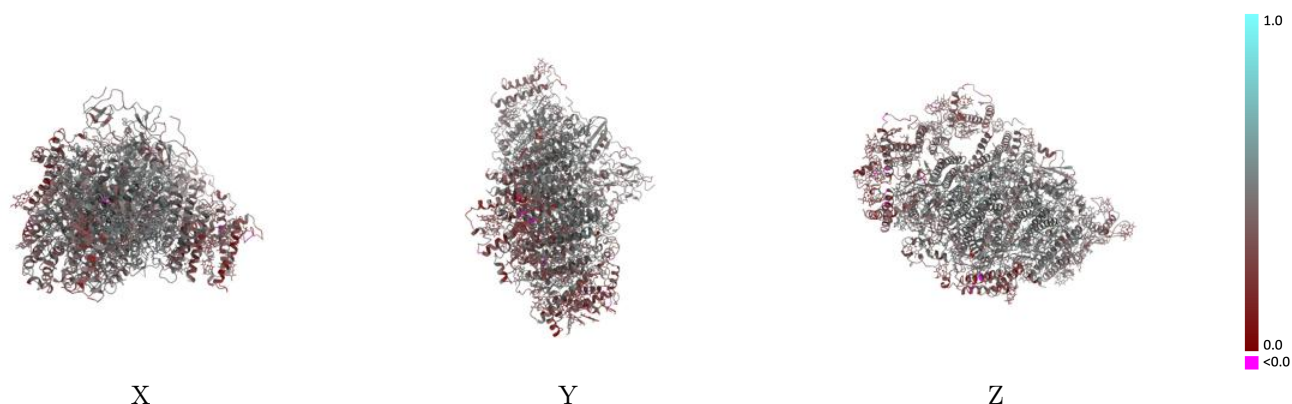
This section contains information regarding the fit between EMDB map EMD-81136 and PDB model 27GG. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



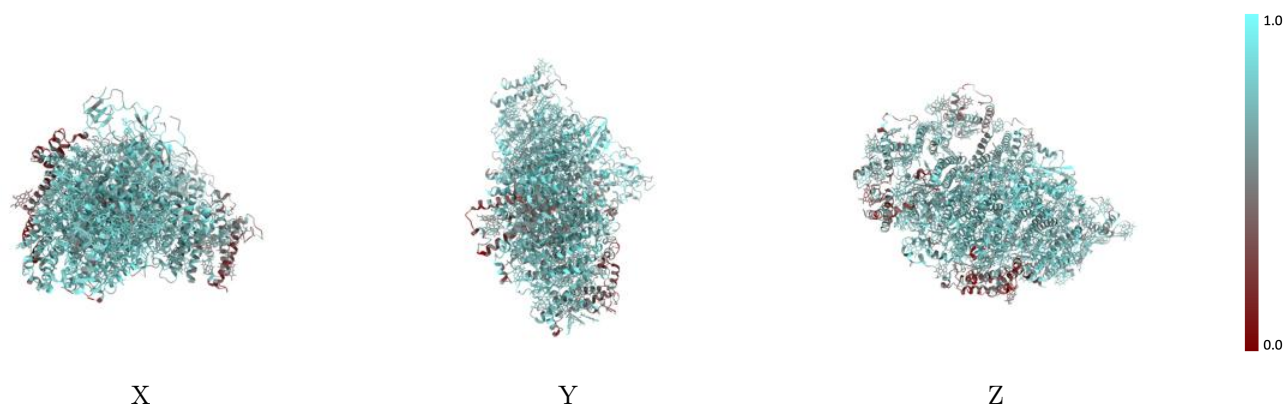
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



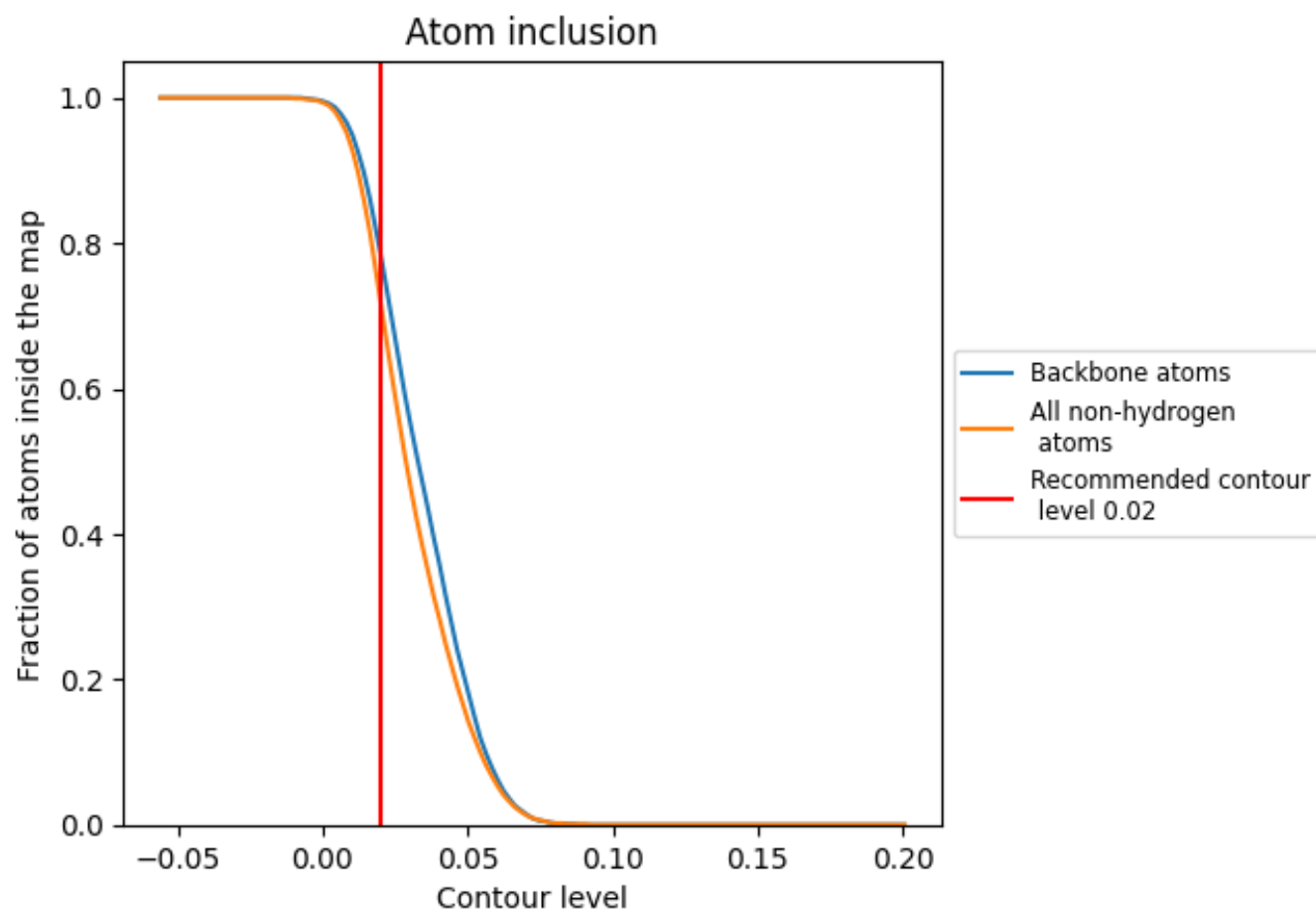
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7190	0.4170
2	0.5590	0.3110
9	0.6600	0.3320
A	0.8020	0.4630
B	0.8030	0.4640
C	0.7880	0.4390
D	0.7500	0.4460
E	0.7440	0.4290
F	0.3190	0.2940
G	0.3660	0.2700
H	0.6380	0.3720
I	0.7180	0.4170
J	0.4020	0.2880
K	0.6350	0.3520
L	0.7260	0.3980
M	0.6960	0.4040

1.0

0.0

<0.0