



Full wwPDB EM Validation Report ⓘ

Sep 8, 2026 – 12:51 PM EDT

PDB ID : 10KF / pdb_000010kf
EMDB ID : EMD-75232
Title : Cryo-EM structure of a chemically treated Cyanobacterial Photosystem I core with bound platinum nanoparticles
Authors : Emerson, M.D.; Gisriel, C.J.
Deposited on : 2026-01-23
Resolution : 3.57 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

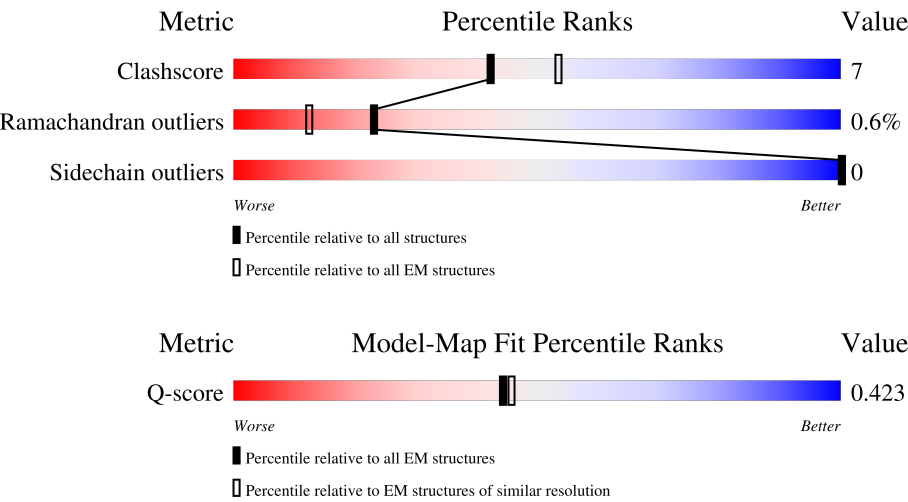
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.57 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	12682 (3.07 - 4.07)

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

Mol	Chain	Length	Quality of chain
1	A	763	
2	B	734	
3	F	159	
4	I	38	

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Mol	Chain	Length	Quality of chain
5	J	44	36% 89% 5% 7%
6	K	80	40% 90% 10%
7	M	29	86% 14%

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 18035 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	737	Total	C	N	O	S	0	0
			5739	3763	982	977	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5789	3811	970	994	14		

- Molecule 3 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	72	Total	C	N	O	0	0
			353	209	72	72		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	32	Total	C	N	O	S	0	0
			235	163	32	39	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	J	41	Total	C	N	O	0	0
			204	121	41	42		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	MET	-	insertion	UNP Q5N5C7
J	2	LEU	-	insertion	UNP Q5N5C7
J	3	ALA	-	insertion	UNP Q5N5C7

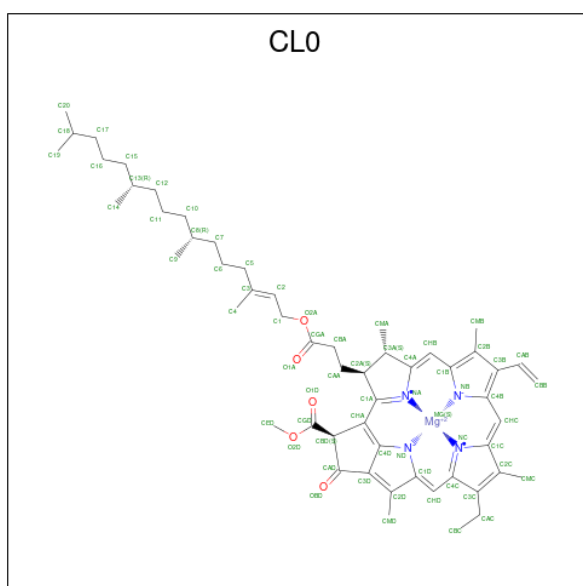
- Molecule 6 is a protein called Photosystem I reaction center subunit Psak.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	K	72	Total	C	N	O	0	0
			351	206	72	73		

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

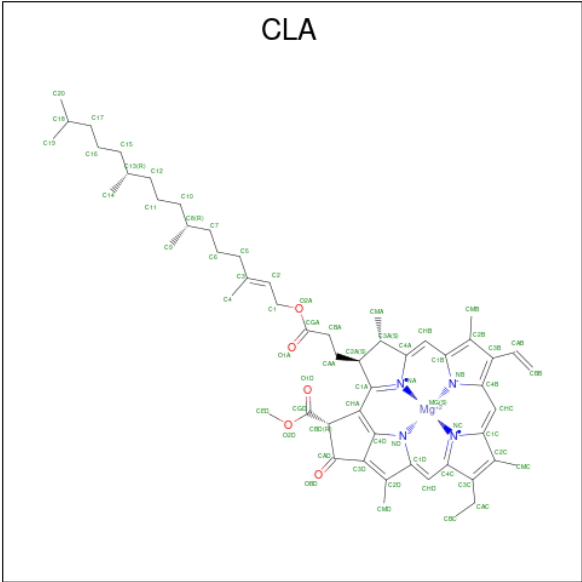
Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	29	Total	C	N	O	S	0	0
			228	151	36	40	1		

- Molecule 8 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

- Molecule 9 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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

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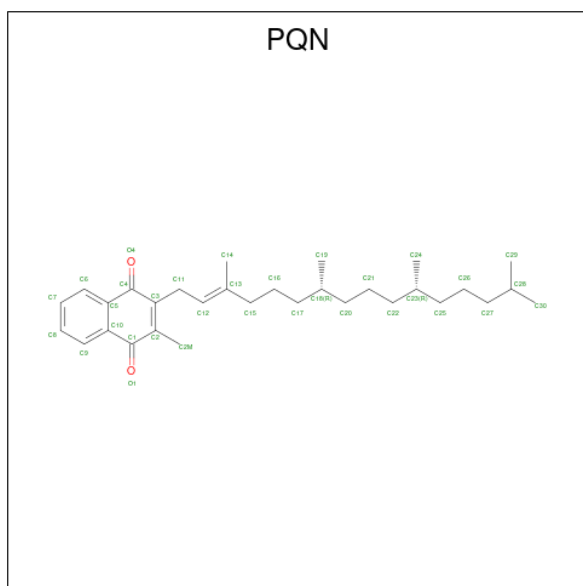
Mol	Chain	Residues	Atoms					AltConf
9	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			45	35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

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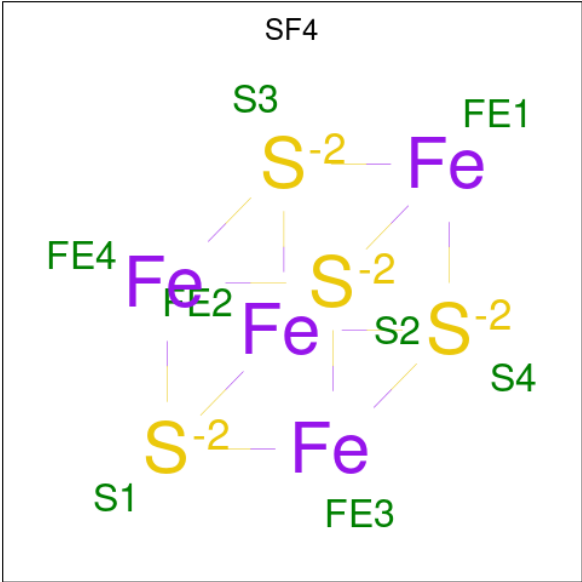
Mol	Chain	Residues	Atoms					AltConf
9	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

- Molecule 10 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



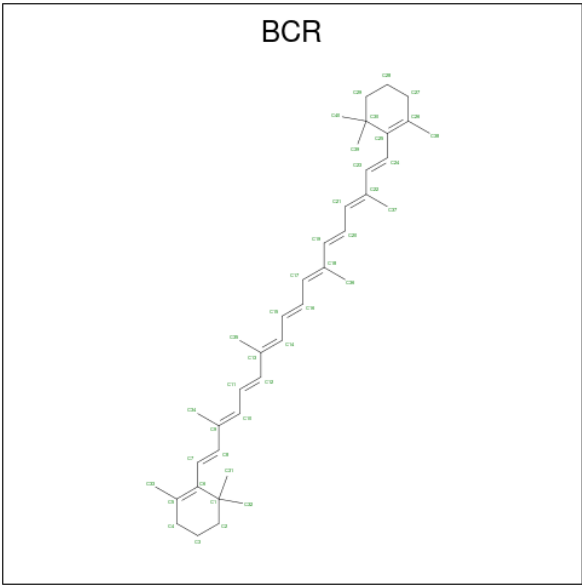
Mol	Chain	Residues	Atoms			AltConf
10	A	1	Total	C	O	0
			33	31	2	
10	B	1	Total	C	O	0
			33	31	2	

- Molecule 11 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 12 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



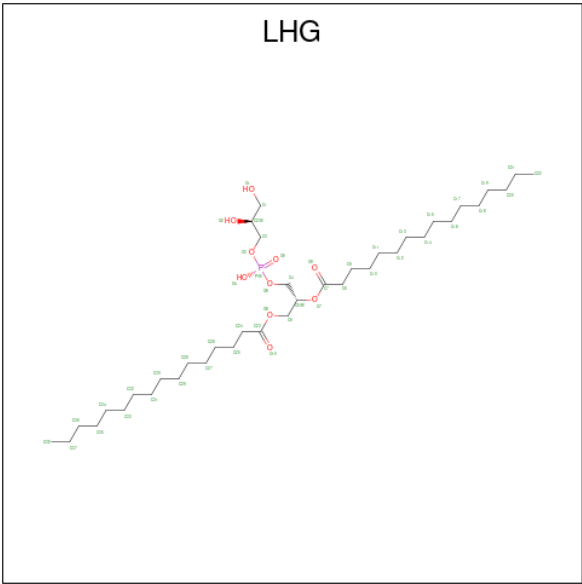
Mol	Chain	Residues	Atoms		AltConf
12	A	1	Total	C	0
			40	40	
12	A	1	Total	C	0
			40	40	
12	A	1	Total	C	0
			40	40	

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

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



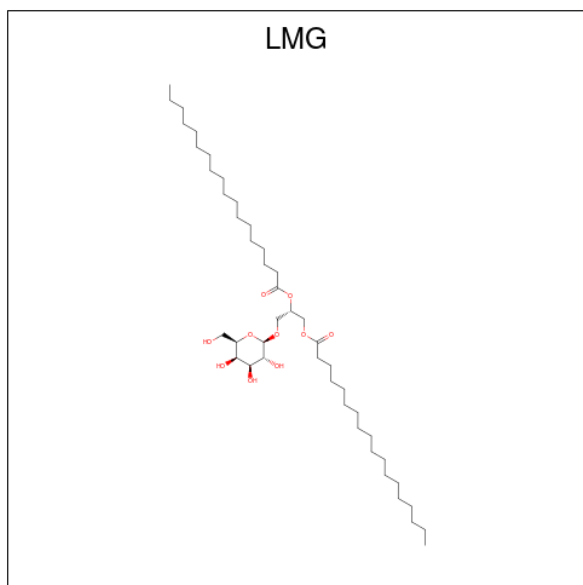
Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
13	A	1	27	16	10	1	0

- Molecule 14 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).

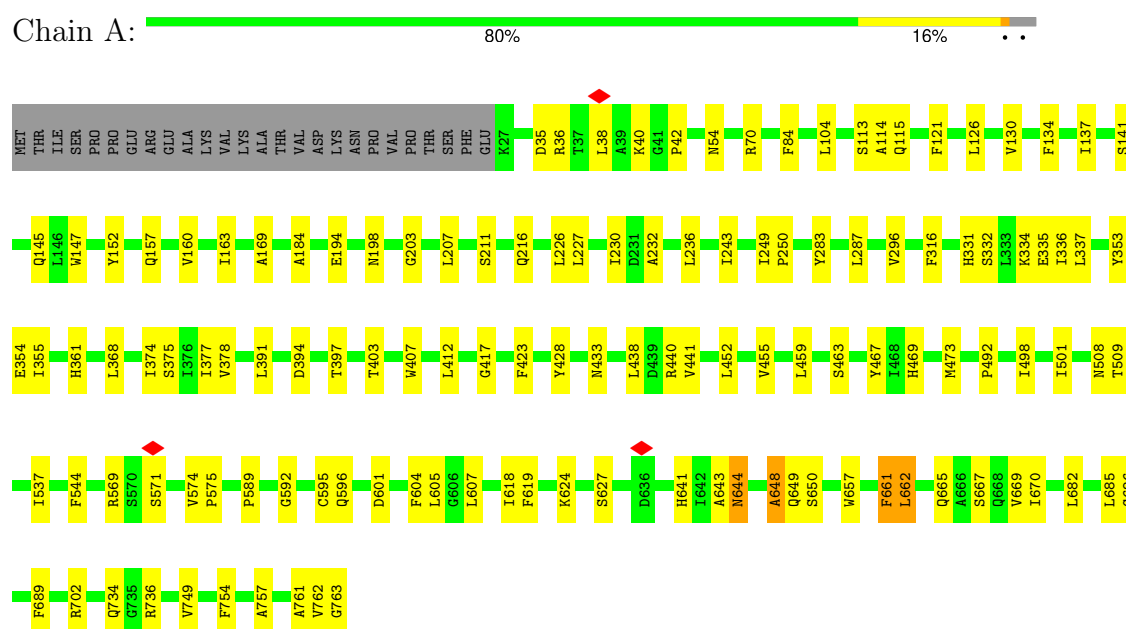


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O		
14	B	1	49	39	10		0

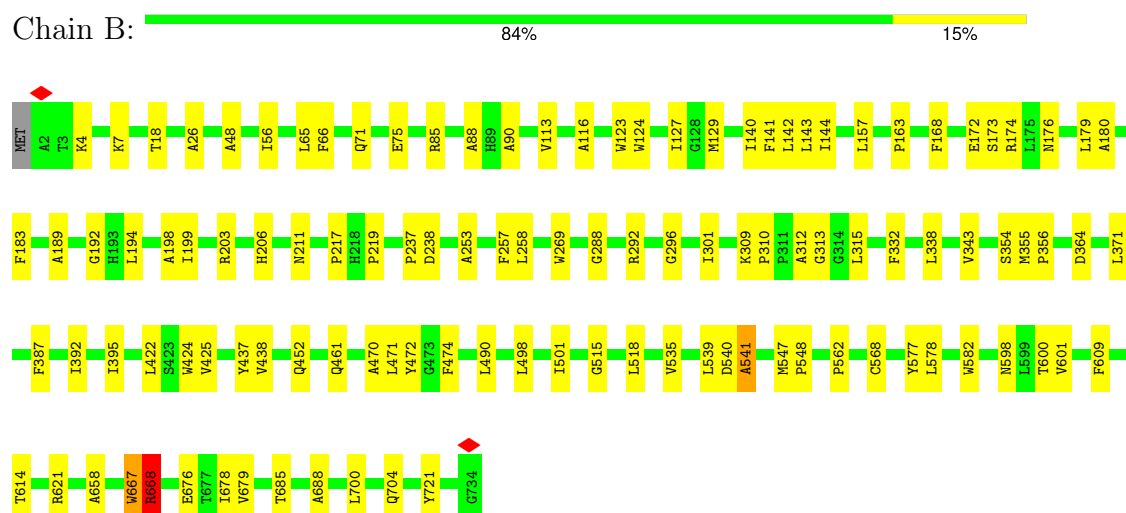
3 Residue-property plots

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

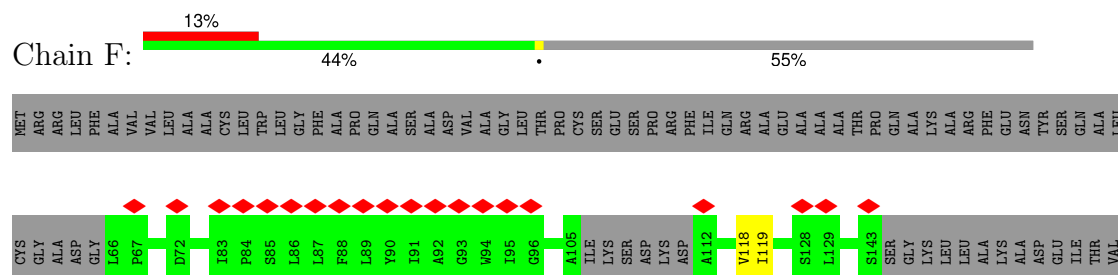
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



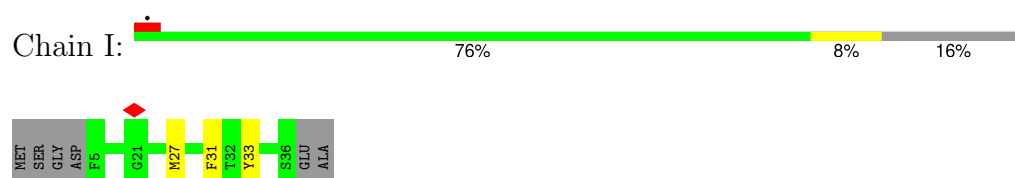
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



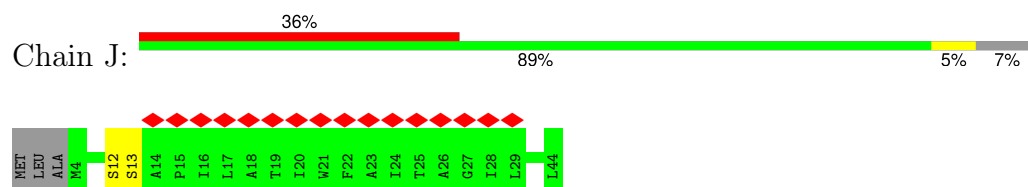
- Molecule 3: Photosystem I reaction center subunit III



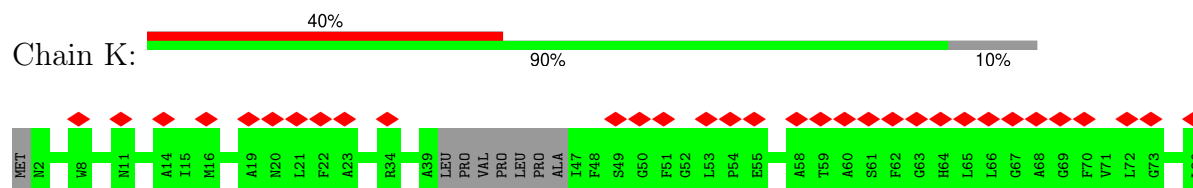
- Molecule 4: Photosystem I reaction center subunit VIII



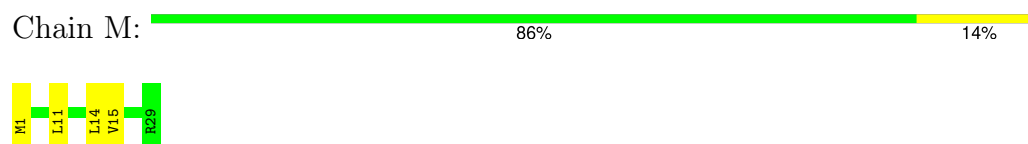
- Molecule 5: Photosystem I reaction center subunit IX



- Molecule 6: Photosystem I reaction center subunit PsaK



- Molecule 7: 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	53098	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.612	Depositor
Minimum map value	-0.201	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.164	Depositor
Map size (Å)	272.384, 272.384, 272.384	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.064, 1.064, 1.064	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.32	0/5932	0.75	6/8094 (0.1%)
2	B	0.33	0/5999	0.78	10/8199 (0.1%)
3	F	0.14	0/351	0.43	0/484
4	I	0.42	0/241	1.03	0/331
5	J	0.16	0/203	0.52	0/280
6	K	0.19	0/349	0.59	0/478
7	M	0.63	1/231 (0.4%)	1.03	0/314
All	All	0.33	1/13306 (0.0%)	0.76	16/18180 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	4
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	15	VAL	C-N	7.14	1.42	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	PRO	CA-N-CD	-9.94	98.09	112.00
2	B	217	PRO	CA-C-N	5.84	132.34	122.65
2	B	217	PRO	C-N-CA	5.84	132.34	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	219	PRO	CA-N-CD	-5.83	103.84	112.00
2	B	309	LYS	CA-CB-CG	5.77	125.63	114.10
1	A	121	PHE	CB-CA-C	-5.74	109.42	117.23
2	B	667	TRP	CA-C-N	5.67	132.37	121.54
2	B	667	TRP	C-N-CA	5.67	132.37	121.54
1	A	643	ALA	CA-C-N	5.50	132.04	121.54
1	A	643	ALA	C-N-CA	5.50	132.04	121.54
2	B	18	THR	CA-C-N	5.34	129.23	120.63
2	B	18	THR	C-N-CA	5.34	129.23	120.63
1	A	575	PRO	CA-N-CD	-5.30	104.58	112.00
1	A	492	PRO	CA-N-CD	-5.26	104.64	112.00
2	B	474	PHE	CA-C-N	5.06	131.21	121.54
2	B	474	PHE	C-N-CA	5.06	131.21	121.54

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	648	ALA	Peptide
1	A	661	PHE	Peptide
2	B	183	PHE	Peptide
2	B	312	ALA	Peptide
2	B	313	GLY	Peptide
2	B	668	ARG	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5739	0	5601	79	0
2	B	5789	0	5575	80	0
3	F	353	0	172	2	0
4	I	235	0	249	2	0
5	J	204	0	92	2	0
6	K	351	0	188	0	0
7	M	228	0	246	3	0
8	A	60	0	59	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	2200	0	1880	32	0
9	B	2071	0	1799	52	0
9	I	45	0	32	1	0
9	K	41	0	28	0	0
10	A	33	0	46	3	0
10	B	33	0	46	4	0
11	A	8	0	0	0	0
12	A	200	0	245	14	0
12	B	240	0	293	15	0
12	F	40	0	48	2	0
12	M	40	0	49	4	0
13	A	76	0	98	3	0
14	B	49	0	71	6	0
All	All	18035	0	16817	235	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (235) 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)
2:B:301:ILE:HG21	9:B:824:CLA:HAC1	1.69	0.75
2:B:56:ILE:HD11	12:M:101:BCR:HC7	1.71	0.72
2:B:189:ALA:HA	9:B:815:CLA:HBB2	1.74	0.68
10:B:841:PQN:H301	14:B:848:LMG:H192	1.73	0.68
2:B:387:PHE:HZ	9:B:825:CLA:HAB	1.61	0.65
1:A:115:GLN:HB3	1:A:137:ILE:HB	1.82	0.62
7:M:11:LEU:HA	7:M:14:LEU:HD23	1.82	0.61
1:A:661:PHE:HD1	1:A:662:LEU:HD12	1.65	0.60
2:B:371:LEU:HD11	9:B:828:CLA:HED3	1.84	0.60
1:A:589:PRO:HD3	2:B:562:PRO:HD2	1.84	0.59
9:A:806:CLA:HED1	9:A:830:CLA:H2	1.85	0.59
1:A:104:LEU:HD11	1:A:227:LEU:HD11	1.85	0.58
1:A:749:VAL:HG22	12:A:851:BCR:HC21	1.87	0.57
9:A:821:CLA:H18	12:A:849:BCR:HC41	1.87	0.56
1:A:702:ARG:H	2:B:568:CYS:HB2	1.71	0.56
2:B:168:PHE:O	2:B:174:ARG:NH2	2.39	0.56
9:B:834:CLA:HBB2	9:B:836:CLA:HBA1	1.88	0.56
2:B:515:GLY:HA2	2:B:518:LEU:HD12	1.87	0.55
1:A:368:LEU:HD11	1:A:412:LEU:HD22	1.87	0.55
2:B:437:TYR:HD2	9:B:803:CLA:H203	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:452:GLN:NE2	2:B:614:THR:OG1	2.39	0.55
2:B:461:GLN:O	2:B:472:TYR:OH	2.24	0.55
1:A:35:ASP:OD1	1:A:54:ASN:ND2	2.40	0.55
1:A:334:LYS:NZ	1:A:354:GLU:OE2	2.40	0.55
1:A:592:GLY:HA3	2:B:668:ARG:HH21	1.72	0.55
1:A:669:VAL:HG22	1:A:757:ALA:HB3	1.89	0.54
2:B:498:LEU:HA	2:B:501:ILE:HG22	1.88	0.54
9:B:806:CLA:HAA2	9:B:806:CLA:H2	1.89	0.54
1:A:377:ILE:HD13	9:A:826:CLA:HED3	1.88	0.54
9:A:802:CLA:H172	12:B:847:BCR:H321	1.89	0.54
9:A:841:CLA:HAB	10:A:845:PQN:H162	1.90	0.54
2:B:85:ARG:NH2	2:B:364:ASP:OD1	2.41	0.54
1:A:194:GLU:O	1:A:198:ASN:ND2	2.42	0.53
9:A:807:CLA:HBA1	9:A:809:CLA:HAA1	1.91	0.53
2:B:422:LEU:HD22	9:B:838:CLA:HBB1	1.90	0.53
1:A:216:GLN:NE2	9:A:819:CLA:O1D	2.42	0.53
2:B:180:ALA:HB2	2:B:288:GLY:HA3	1.90	0.53
1:A:332:SER:OG	1:A:335:GLU:OE1	2.26	0.53
2:B:310:PRO:HG3	2:B:315:LEU:HB2	1.90	0.53
2:B:424:TRP:CE2	9:B:831:CLA:HAB	2.44	0.53
1:A:126:LEU:HB3	1:A:137:ILE:HD11	1.90	0.53
2:B:292:ARG:NH1	2:B:296:GLY:O	2.42	0.52
1:A:141:SER:HB3	9:A:828:CLA:HAA2	1.91	0.52
2:B:704:GLN:HG3	14:B:848:LMG:H131	1.91	0.52
2:B:203:ARG:NH2	2:B:253:ALA:O	2.41	0.52
4:I:27:MET:O	4:I:31:PHE:HB2	2.10	0.52
9:B:819:CLA:H41	9:B:826:CLA:H121	1.90	0.52
2:B:598:ASN:HA	2:B:601:VAL:HG12	1.90	0.52
9:A:805:CLA:H192	9:A:813:CLA:H51	1.91	0.52
9:B:830:CLA:HBC2	12:B:845:BCR:H282	1.91	0.52
7:M:11:LEU:HD21	12:M:101:BCR:H292	1.92	0.52
2:B:48:ALA:HB2	2:B:157:LEU:HD21	1.92	0.51
1:A:375:SER:HA	1:A:378:VAL:HG22	1.91	0.51
2:B:338:LEU:HD21	9:B:829:CLA:HAB	1.93	0.51
2:B:142:LEU:HD11	12:B:844:BCR:H24C	1.90	0.51
9:B:809:CLA:HAB	9:B:810:CLA:HBA1	1.92	0.51
2:B:354:SER:OG	2:B:355:MET:N	2.42	0.51
2:B:600:THR:HG21	2:B:609:PHE:HB2	1.92	0.51
1:A:407:TRP:HE1	1:A:618:ILE:HD13	1.76	0.51
1:A:459:LEU:O	1:A:463:SER:HB3	2.11	0.51
1:A:595:CYS:HB2	2:B:668:ARG:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:TRP:HB3	8:A:801:CL0:H45	1.92	0.50
1:A:670:ILE:HG22	2:B:621:ARG:HD3	1.92	0.50
1:A:682:LEU:HD23	9:B:802:CLA:H62	1.93	0.50
9:B:815:CLA:HAB	12:B:842:BCR:H333	1.94	0.50
1:A:230:ILE:HD11	1:A:243:ILE:HG22	1.94	0.50
2:B:179:LEU:HD23	2:B:288:GLY:HA2	1.94	0.50
2:B:90:ALA:HA	2:B:113:VAL:HA	1.94	0.50
2:B:422:LEU:HA	2:B:425:VAL:HG12	1.93	0.50
2:B:582:TRP:CH2	9:B:802:CLA:HAB	2.46	0.50
2:B:578:LEU:HD23	9:B:801:CLA:HMD3	1.92	0.49
1:A:665:GLN:HG3	1:A:754:PHE:HZ	1.78	0.49
10:B:841:PQN:H142	12:B:847:BCR:H271	1.94	0.49
2:B:257:PHE:HB3	9:B:816:CLA:HED3	1.95	0.49
1:A:734:GLN:HE21	13:A:852:LHG:HC91	1.78	0.49
2:B:387:PHE:CZ	9:B:825:CLA:HAB	2.45	0.48
2:B:173:SER:HA	2:B:176:ASN:HB2	1.94	0.48
1:A:428:TYR:HE1	1:A:433:ASN:HD22	1.59	0.48
2:B:7:LYS:NZ	4:I:33:TYR:OH	2.43	0.48
2:B:685:THR:HG23	2:B:688:ALA:HB3	1.95	0.48
1:A:440:ARG:NH2	9:A:831:CLA:O1D	2.45	0.48
1:A:417:GLY:HA2	12:A:850:BCR:HC41	1.95	0.47
1:A:761:ALA:O	1:A:763:GLY:N	2.47	0.47
12:A:851:BCR:H372	2:B:438:VAL:HG11	1.95	0.47
2:B:163:PRO:HG2	2:B:168:PHE:HE2	1.79	0.47
1:A:403:THR:HG23	1:A:618:ILE:HG21	1.96	0.47
1:A:36:ARG:O	1:A:40:LYS:NZ	2.48	0.47
9:B:810:CLA:HMA2	9:I:101:CLA:HBB1	1.97	0.47
9:B:832:CLA:HBB1	12:F:201:BCR:HC8	1.97	0.47
13:A:852:LHG:H121	13:A:852:LHG:H152	1.65	0.47
2:B:75:GLU:OE1	2:B:75:GLU:N	2.48	0.47
14:B:848:LMG:H211	14:B:848:LMG:H241	1.75	0.47
9:A:807:CLA:H3A	9:A:807:CLA:HBA2	1.53	0.47
2:B:438:VAL:HG23	9:B:802:CLA:H52	1.97	0.46
1:A:147:TRP:HB3	1:A:152:TYR:HD1	1.79	0.46
1:A:604:PHE:HD2	1:A:605:LEU:HD12	1.79	0.46
9:A:830:CLA:H42	13:A:852:LHG:H252	1.98	0.46
9:B:813:CLA:H203	12:B:843:BCR:H271	1.97	0.46
1:A:438:LEU:HA	1:A:441:VAL:HG22	1.97	0.46
2:B:577:TYR:HD2	2:B:578:LEU:HD12	1.81	0.46
2:B:676:GLU:O	2:B:679:VAL:HB	2.16	0.46
9:B:830:CLA:H3A	9:B:830:CLA:HBA2	1.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:828:CLA:H3A	9:B:828:CLA:HBA2	1.61	0.46
12:A:848:BCR:H351	12:A:848:BCR:H15C	1.69	0.46
2:B:206:HIS:O	2:B:211:ASN:ND2	2.44	0.46
2:B:238:ASP:HB2	2:B:269:TRP:HZ3	1.80	0.46
2:B:678:ILE:HG22	9:B:839:CLA:HAC2	1.96	0.46
9:B:818:CLA:H3A	9:B:818:CLA:HBA2	1.71	0.46
1:A:469:HIS:O	1:A:473:MET:HB2	2.17	0.45
9:A:828:CLA:H41	9:A:828:CLA:H62	1.64	0.45
2:B:355:MET:HA	2:B:356:PRO:HD2	1.92	0.45
1:A:355:ILE:HG12	1:A:423:PHE:HZ	1.82	0.45
1:A:452:LEU:HA	1:A:455:VAL:HG12	1.98	0.45
9:A:828:CLA:H141	9:A:828:CLA:H162	1.83	0.45
1:A:337:LEU:HD23	1:A:353:TYR:HB2	1.98	0.45
9:B:817:CLA:H3A	9:B:817:CLA:HBA2	1.55	0.45
1:A:283:TYR:HB3	1:A:287:LEU:HD12	1.97	0.45
12:A:848:BCR:H371	12:A:848:BCR:H24C	1.72	0.45
3:F:119:ILE:N	5:J:12:SER:O	2.47	0.45
2:B:658:ALA:C	9:B:804:CLA:HAB	2.42	0.45
12:B:845:BCR:H351	12:B:845:BCR:H15C	1.67	0.45
12:A:849:BCR:H24C	12:A:849:BCR:H371	1.71	0.45
2:B:172:GLU:OE1	2:B:172:GLU:N	2.50	0.45
1:A:361:HIS:CD2	9:A:805:CLA:HBC1	2.53	0.44
1:A:394:ASP:OD2	1:A:397:THR:OG1	2.30	0.44
1:A:428:TYR:HD2	1:A:569:ARG:HE	1.65	0.44
1:A:685:LEU:HB2	9:B:802:CLA:H43	1.99	0.44
12:B:847:BCR:H351	12:B:847:BCR:H15C	1.75	0.44
9:A:835:CLA:HBA2	9:A:835:CLA:H3A	1.61	0.44
1:A:508:ASN:OD1	1:A:509:THR:N	2.51	0.44
2:B:470:ALA:O	2:B:472:TYR:N	2.51	0.44
9:B:813:CLA:H143	9:B:813:CLA:H112	1.80	0.44
1:A:160:VAL:HA	1:A:163:ILE:HG12	2.00	0.44
9:A:829:CLA:H91	9:A:829:CLA:H111	1.83	0.44
2:B:26:ALA:HB1	14:B:848:LMG:H292	2.00	0.44
12:B:844:BCR:H351	12:B:844:BCR:H15C	1.78	0.44
12:A:851:BCR:H371	12:A:851:BCR:H24C	1.73	0.44
9:B:808:CLA:HHB	9:B:809:CLA:HMB3	2.00	0.44
1:A:207:LEU:HD22	12:A:847:BCR:H361	2.00	0.44
9:A:818:CLA:H3A	9:A:818:CLA:HBA2	1.60	0.44
12:A:847:BCR:H24C	12:A:847:BCR:H371	1.71	0.44
1:A:669:VAL:HG21	1:A:754:PHE:HD1	1.83	0.44
2:B:192:GLY:HA3	9:B:815:CLA:HBB1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:535:VAL:O	2:B:539:LEU:CB	2.66	0.44
2:B:547:MET:HA	2:B:548:PRO:HD3	1.78	0.44
2:B:315:LEU:HG	9:B:830:CLA:HMD3	2.00	0.44
2:B:343:VAL:HG13	9:B:825:CLA:HED1	2.00	0.44
9:B:827:CLA:H3A	9:B:827:CLA:HBA2	1.66	0.44
9:B:840:CLA:HED2	14:B:848:LMG:H171	1.99	0.44
9:B:803:CLA:H71	9:B:803:CLA:H111	1.52	0.43
9:A:826:CLA:H72	9:A:835:CLA:HAB	1.99	0.43
1:A:467:TYR:HE2	8:A:801:CL0:H52	1.83	0.43
1:A:203:GLY:HA2	9:A:820:CLA:HBC1	2.00	0.43
1:A:226:LEU:HA	1:A:236:LEU:HD21	1.99	0.43
8:A:801:CL0:H46	8:A:801:CL0:H35	2.01	0.43
1:A:601:ASP:OD1	1:A:736:ARG:NH1	2.50	0.43
2:B:88:ALA:HB2	2:B:116:ALA:HB2	2.00	0.43
12:B:843:BCR:H15C	12:B:843:BCR:H351	1.66	0.43
12:M:101:BCR:H371	12:M:101:BCR:H24C	1.71	0.43
1:A:84:PHE:HB3	1:A:169:ALA:HB2	2.01	0.43
2:B:721:TYR:HB2	9:B:803:CLA:HED3	2.00	0.43
9:A:825:CLA:H112	9:A:825:CLA:H152	1.77	0.43
2:B:140:ILE:O	2:B:144:ILE:HG12	2.19	0.43
9:B:836:CLA:H41	9:B:836:CLA:H61	1.59	0.43
3:F:118:VAL:HA	5:J:13:SER:HA	2.00	0.42
1:A:537:ILE:HG23	1:A:624:LYS:HE2	2.01	0.42
1:A:627:SER:O	1:A:641:HIS:ND1	2.52	0.42
2:B:71:GLN:OE1	2:B:90:ALA:N	2.43	0.42
2:B:141:PHE:HD1	2:B:142:LEU:HD12	1.84	0.42
2:B:700:LEU:HD12	2:B:704:GLN:HG2	2.01	0.42
2:B:194:LEU:HA	2:B:198:ALA:HB3	2.01	0.42
2:B:211:ASN:OD1	2:B:211:ASN:N	2.53	0.42
9:B:807:CLA:H143	9:B:828:CLA:HBB2	2.02	0.42
12:B:847:BCR:H24C	12:B:847:BCR:H371	1.70	0.42
10:A:845:PQN:H161	10:A:845:PQN:H141	1.76	0.42
2:B:123:TRP:O	2:B:127:ILE:HG12	2.20	0.42
2:B:143:LEU:HD23	2:B:143:LEU:HA	1.88	0.42
12:M:101:BCR:H15C	12:M:101:BCR:H351	1.73	0.42
12:A:850:BCR:H351	12:A:850:BCR:H15C	1.70	0.42
1:A:544:PHE:HA	9:A:838:CLA:HED1	2.02	0.42
2:B:237:PRO:HB3	2:B:258:LEU:HD11	2.01	0.42
12:F:201:BCR:H371	12:F:201:BCR:H24C	1.69	0.42
1:A:596:GLN:OE1	2:B:667:TRP:N	2.48	0.42
2:B:540:ASP:OD1	2:B:541:ALA:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:GLN:HG2	1:A:391:LEU:HB2	2.01	0.42
2:B:66:PHE:HE2	7:M:1:MET:HE1	1.84	0.42
1:A:441:VAL:HG21	9:A:821:CLA:H192	2.01	0.42
8:A:801:CL0:H72	8:A:801:CL0:H9	1.54	0.42
9:B:803:CLA:H41	9:B:803:CLA:H62	1.77	0.42
1:A:211:SER:HB3	9:A:814:CLA:HAB	2.02	0.42
2:B:332:PHE:HE1	12:B:846:BCR:H401	1.84	0.42
1:A:232:ALA:HB2	1:A:296:VAL:HG21	2.02	0.41
9:A:828:CLA:HBA2	9:A:828:CLA:H3A	1.78	0.41
1:A:35:ASP:HB3	1:A:38:LEU:HB2	2.02	0.41
9:A:808:CLA:HBA2	9:A:808:CLA:H3A	1.65	0.41
2:B:124:TRP:HB3	2:B:129:MET:HG3	2.02	0.41
9:A:819:CLA:H72	9:A:819:CLA:H111	1.88	0.41
9:B:801:CLA:H92	9:B:801:CLA:H62	1.89	0.41
1:A:374:ILE:HD11	9:A:827:CLA:H52	2.03	0.41
9:B:828:CLA:H52	12:B:844:BCR:H391	2.02	0.41
1:A:316:PHE:HE1	9:A:821:CLA:HAB	1.85	0.41
1:A:619:PHE:HE2	8:A:801:CL0:H37	1.85	0.41
1:A:459:LEU:HD21	9:A:838:CLA:CAB	2.50	0.41
1:A:648:ALA:O	1:A:650:SER:N	2.54	0.41
12:A:847:BCR:H15C	12:A:847:BCR:H351	1.82	0.41
12:A:850:BCR:H371	12:A:850:BCR:H24C	1.73	0.41
2:B:65:LEU:HD11	12:B:844:BCR:H271	2.03	0.41
2:B:174:ARG:HB2	9:B:813:CLA:HBC2	2.03	0.41
10:B:841:PQN:H141	10:B:841:PQN:H161	1.85	0.41
1:A:641:HIS:HB2	1:A:644:ASN:HA	2.01	0.41
2:B:310:PRO:HB3	2:B:315:LEU:HD22	2.02	0.41
12:B:842:BCR:H351	12:B:842:BCR:H15C	1.68	0.41
1:A:157:GLN:HA	1:A:160:VAL:HG12	2.03	0.41
1:A:114:ALA:HA	1:A:134:PHE:HE2	1.86	0.41
1:A:686:GLY:O	1:A:689:PHE:HB3	2.20	0.41
2:B:199:ILE:HG22	2:B:203:ARG:HE	1.85	0.41
1:A:249:ILE:HD12	1:A:250:PRO:HD2	2.03	0.41
1:A:571:SER:OG	1:A:574:VAL:O	2.31	0.41
14:B:848:LMG:H232	14:B:848:LMG:H262	1.86	0.41
1:A:70:ARG:HH11	1:A:184:ALA:HB3	1.85	0.40
1:A:113:SER:HB3	1:A:130:VAL:HG21	2.03	0.40
9:A:825:CLA:H151	9:A:825:CLA:H18	1.81	0.40
9:B:839:CLA:HBB2	10:B:841:PQN:H141	2.03	0.40
1:A:498:ILE:HA	1:A:501:ILE:HG22	2.03	0.40
1:A:607:LEU:HD23	1:A:607:LEU:HA	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:802:CLA:H61	9:B:802:CLA:H41	1.78	0.40
1:A:331:HIS:HD2	1:A:336:ILE:HD11	1.87	0.40
2:B:392:ILE:HA	2:B:395:ILE:HG22	2.03	0.40
9:B:807:CLA:H72	9:B:807:CLA:H111	1.90	0.40
9:B:818:CLA:H41	9:B:818:CLA:H62	1.78	0.40
9:B:828:CLA:HBB1	9:B:828:CLA:HHC	2.04	0.40
12:A:851:BCR:H351	12:A:851:BCR:H15C	1.73	0.40
9:A:840:CLA:HAC1	10:A:845:PQN:H221	2.03	0.40
9:B:807:CLA:HBA1	9:B:807:CLA:H3A	1.86	0.40
9:B:809:CLA:H2	9:B:809:CLA:H13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	735/763 (96%)	685 (93%)	45 (6%)	5 (1%)	18	51
2	B	731/734 (100%)	667 (91%)	59 (8%)	5 (1%)	18	51
3	F	68/159 (43%)	60 (88%)	8 (12%)	0	100	100
4	I	30/38 (79%)	29 (97%)	1 (3%)	0	100	100
5	J	39/44 (89%)	37 (95%)	2 (5%)	0	100	100
6	K	68/80 (85%)	60 (88%)	8 (12%)	0	100	100
7	M	27/29 (93%)	27 (100%)	0	0	100	100
All	All	1698/1847 (92%)	1565 (92%)	123 (7%)	10 (1%)	23	54

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	644	ASN

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Mol	Chain	Res	Type
1	A	667	SER
1	A	762	VAL
2	B	471	LEU
2	B	668	ARG
1	A	662	LEU
1	A	649	GLN
2	B	490	LEU
2	B	541	ALA
2	B	4	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	583/611 (95%)	583 (100%)	0	100	100
2	B	583/584 (100%)	583 (100%)	0	100	100
4	I	25/30 (83%)	25 (100%)	0	100	100
7	M	24/24 (100%)	24 (100%)	0	100	100
All	All	1215/1249 (97%)	1215 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	79	HIS
1	A	198	ASN
1	A	199	HIS
1	A	216	GLN
1	A	331	HIS
1	A	367	ASN
1	A	453	ASN
1	A	470	ASN

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Mol	Chain	Res	Type
1	A	499	GLN
1	A	547	HIS
2	B	193	HIS
2	B	327	ASN
2	B	389	HIS
2	B	414	HIS
2	B	452	GLN
2	B	464	GLN
2	B	496	ASN
2	B	528	HIS
7	M	5	GLN

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](#)

105 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	$\# Z > 2$
9	CLA	A	844	13	49,53,73	2.58	22 (44%)	58,89,113	2.79	22 (37%)
9	CLA	A	835	-	49,53,73	2.56	22 (44%)	58,89,113	2.78	23 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	CLA	A	807	1	49,53,73	2.54	22 (44%)	58,89,113	2.83	23 (39%)
9	CLA	B	836	-	59,63,73	2.44	23 (38%)	70,101,113	2.60	28 (40%)
9	CLA	B	806	-	64,68,73	2.34	24 (37%)	76,107,113	2.61	29 (38%)
12	BCR	A	849	-	41,41,41	2.61	6 (14%)	56,56,56	6.72	26 (46%)
9	CLA	B	810	-	49,53,73	2.56	21 (42%)	58,89,113	2.76	22 (37%)
12	BCR	A	847	-	41,41,41	2.60	6 (14%)	56,56,56	6.62	25 (44%)
8	CL0	A	801	-	64,68,73	2.35	23 (35%)	76,107,113	2.47	32 (42%)
13	LHG	A	853	9	26,26,48	1.26	2 (7%)	29,32,54	1.31	3 (10%)
12	BCR	B	846	-	41,41,41	2.65	6 (14%)	56,56,56	6.79	28 (50%)
9	CLA	A	813	1	64,68,73	2.29	23 (35%)	76,107,113	2.57	30 (39%)
9	CLA	B	803	-	69,73,73	2.20	20 (28%)	82,113,113	2.40	26 (31%)
9	CLA	B	818	2	64,68,73	2.33	24 (37%)	76,107,113	2.54	26 (34%)
9	CLA	B	827	2	59,63,73	2.40	21 (35%)	70,101,113	2.57	26 (37%)
9	CLA	B	809	2	69,73,73	2.25	22 (31%)	82,113,113	2.55	27 (32%)
9	CLA	A	825	-	69,73,73	2.25	23 (33%)	82,113,113	2.62	30 (36%)
9	CLA	B	823	2	49,53,73	2.58	25 (51%)	58,89,113	2.79	24 (41%)
9	CLA	B	831	-	49,53,73	2.56	22 (44%)	58,89,113	2.71	23 (39%)
12	BCR	B	845	-	41,41,41	2.66	6 (14%)	56,56,56	6.79	25 (44%)
9	CLA	B	807	-	69,73,73	2.25	23 (33%)	82,113,113	2.45	26 (31%)
12	BCR	M	101	-	41,41,41	2.58	6 (14%)	56,56,56	6.76	20 (35%)
9	CLA	A	838	-	49,53,73	2.54	22 (44%)	58,89,113	2.82	26 (44%)
9	CLA	A	836	-	49,53,73	2.58	22 (44%)	58,89,113	2.80	23 (39%)
9	CLA	A	803	1	49,53,73	2.55	22 (44%)	58,89,113	2.83	24 (41%)
9	CLA	B	813	-	69,73,73	2.24	23 (33%)	82,113,113	2.59	27 (32%)
12	BCR	B	842	-	41,41,41	2.64	6 (14%)	56,56,56	6.57	25 (44%)
9	CLA	A	822	-	49,53,73	2.56	23 (46%)	58,89,113	2.80	25 (43%)
9	CLA	B	811	-	49,53,73	2.55	22 (44%)	58,89,113	2.77	23 (39%)
9	CLA	B	825	-	49,53,73	2.57	22 (44%)	58,89,113	2.77	25 (43%)
9	CLA	B	805	-	49,53,73	2.55	23 (46%)	58,89,113	2.82	23 (39%)
9	CLA	B	837	-	64,68,73	2.33	23 (35%)	76,107,113	2.54	27 (35%)
9	CLA	A	815	1	49,53,73	2.56	22 (44%)	58,89,113	2.80	24 (41%)
9	CLA	A	828	1	69,73,73	2.25	23 (33%)	82,113,113	2.51	27 (32%)
9	CLA	A	837	-	49,53,73	2.55	22 (44%)	58,89,113	2.83	23 (39%)
9	CLA	B	838	-	49,53,73	2.56	21 (42%)	58,89,113	2.81	24 (41%)
12	BCR	B	847	-	41,41,41	2.60	6 (14%)	56,56,56	6.62	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	BCR	F	201	-	41,41,41	2.56	6 (14%)	56,56,56	6.65	27 (48%)
9	CLA	B	816	-	49,53,73	2.56	22 (44%)	58,89,113	2.80	24 (41%)
9	CLA	B	835	-	49,53,73	2.56	23 (46%)	58,89,113	2.77	23 (39%)
9	CLA	A	819	1	69,73,73	2.25	23 (33%)	82,113,113	2.52	28 (34%)
9	CLA	A	843	-	49,53,73	2.55	23 (46%)	58,89,113	2.80	24 (41%)
9	CLA	B	814	-	59,63,73	2.41	21 (35%)	70,101,113	2.73	30 (42%)
9	CLA	A	802	-	69,73,73	2.26	22 (31%)	82,113,113	2.44	31 (37%)
11	SF4	A	846	2,1	0,12,12	-	-	-		
12	BCR	A	851	-	41,41,41	2.63	6 (14%)	56,56,56	6.90	25 (44%)
9	CLA	A	817	-	54,58,73	2.54	22 (40%)	64,95,113	2.78	26 (40%)
9	CLA	A	809	-	54,58,73	2.53	23 (42%)	64,95,113	2.75	26 (40%)
9	CLA	B	830	-	49,53,73	2.58	23 (46%)	58,89,113	2.76	27 (46%)
9	CLA	A	826	-	64,68,73	2.33	24 (37%)	76,107,113	2.59	26 (34%)
9	CLA	A	821	-	69,73,73	2.27	22 (31%)	82,113,113	2.39	29 (35%)
9	CLA	A	841	-	49,53,73	2.54	23 (46%)	58,89,113	2.80	24 (41%)
9	CLA	B	808	2	49,53,73	2.54	21 (42%)	58,89,113	2.94	25 (43%)
9	CLA	A	806	1	69,73,73	2.25	21 (30%)	82,113,113	2.47	24 (29%)
9	CLA	B	817	-	59,63,73	2.44	22 (37%)	70,101,113	2.64	31 (44%)
9	CLA	B	833	2	49,53,73	2.56	23 (46%)	58,89,113	2.75	23 (39%)
9	CLA	A	812	-	49,53,73	2.57	23 (46%)	58,89,113	2.80	23 (39%)
9	CLA	B	819	-	59,63,73	2.44	24 (40%)	70,101,113	2.64	25 (35%)
9	CLA	B	821	-	49,53,73	2.56	22 (44%)	58,89,113	2.81	24 (41%)
12	BCR	A	850	-	41,41,41	2.68	6 (14%)	56,56,56	6.49	23 (41%)
9	CLA	B	802	-	69,73,73	2.25	22 (31%)	82,113,113	2.46	24 (29%)
9	CLA	A	829	-	69,73,73	2.25	22 (31%)	82,113,113	2.37	26 (31%)
9	CLA	A	834	1	49,53,73	2.56	22 (44%)	58,89,113	2.87	25 (43%)
9	CLA	B	839	-	49,53,73	2.53	22 (44%)	58,89,113	2.89	23 (39%)
12	BCR	A	848	-	41,41,41	2.62	6 (14%)	56,56,56	6.56	22 (39%)
13	LHG	A	852	-	48,48,48	0.94	2 (4%)	51,54,54	1.01	3 (5%)
14	LMG	B	848	-	49,49,55	1.40	6 (12%)	57,57,63	1.15	4 (7%)
9	CLA	B	824	-	49,53,73	2.51	22 (44%)	58,89,113	2.91	25 (43%)
12	BCR	B	843	-	41,41,41	2.65	6 (14%)	56,56,56	6.64	26 (46%)
9	CLA	B	834	-	49,53,73	2.55	23 (46%)	58,89,113	2.80	23 (39%)
9	CLA	A	808	1	49,53,73	2.53	21 (42%)	58,89,113	2.81	25 (43%)
9	CLA	B	815	2	49,53,73	2.53	22 (44%)	58,89,113	2.83	24 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	BCR	B	844	-	41,41,41	2.58	6 (14%)	56,56,56	6.70	21 (37%)
10	PQN	B	841	-	34,34,34	1.62	2 (5%)	43,45,45	1.01	2 (4%)
10	PQN	A	845	-	34,34,34	1.62	2 (5%)	43,45,45	1.09	3 (6%)
9	CLA	A	831	-	49,53,73	2.56	23 (46%)	58,89,113	2.74	24 (41%)
9	CLA	A	842	1	54,58,73	2.55	23 (42%)	64,95,113	2.83	26 (40%)
9	CLA	B	804	-	69,73,73	2.22	22 (31%)	82,113,113	2.29	26 (31%)
9	CLA	A	804	9	49,53,73	2.56	23 (46%)	58,89,113	2.84	25 (43%)
9	CLA	B	822	-	49,53,73	2.55	23 (46%)	58,89,113	2.76	23 (39%)
9	CLA	B	840	-	49,53,73	2.52	22 (44%)	58,89,113	2.88	25 (43%)
9	CLA	A	816	-	49,53,73	2.54	22 (44%)	58,89,113	2.79	23 (39%)
9	CLA	A	814	1	49,53,73	2.56	23 (46%)	58,89,113	2.82	25 (43%)
9	CLA	I	101	-	49,53,73	2.54	22 (44%)	58,89,113	2.81	25 (43%)
9	CLA	A	830	1	69,73,73	2.23	24 (34%)	82,113,113	2.49	26 (31%)
9	CLA	B	812	-	49,53,73	2.56	22 (44%)	58,89,113	2.76	25 (43%)
9	CLA	A	827	-	69,73,73	2.24	22 (31%)	82,113,113	2.54	29 (35%)
9	CLA	B	828	-	69,73,73	2.26	22 (31%)	82,113,113	2.36	27 (32%)
9	CLA	A	840	-	54,58,73	2.54	24 (44%)	64,95,113	2.76	27 (42%)
9	CLA	B	801	-	64,68,73	2.30	22 (34%)	76,107,113	2.51	27 (35%)
9	CLA	B	829	-	49,53,73	2.55	22 (44%)	58,89,113	2.82	25 (43%)
9	CLA	A	823	-	49,53,73	2.56	23 (46%)	58,89,113	2.81	23 (39%)
9	CLA	A	811	9	49,53,73	2.56	23 (46%)	58,89,113	2.84	23 (39%)
9	CLA	B	826	-	69,73,73	2.26	23 (33%)	82,113,113	2.49	28 (34%)
9	CLA	A	818	1	54,58,73	2.55	23 (42%)	64,95,113	2.74	28 (43%)
9	CLA	A	810	-	49,53,73	2.55	22 (44%)	58,89,113	2.80	22 (37%)
9	CLA	B	832	2	49,53,73	2.56	22 (44%)	58,89,113	2.79	23 (39%)
9	CLA	A	824	-	49,53,73	2.56	23 (46%)	58,89,113	2.80	26 (44%)
9	CLA	B	820	2	49,53,73	2.55	22 (44%)	58,89,113	2.80	24 (41%)
9	CLA	A	805	-	69,73,73	2.21	21 (30%)	82,113,113	2.51	28 (34%)
9	CLA	A	832	-	49,53,73	2.56	23 (46%)	58,89,113	2.80	24 (41%)
9	CLA	A	820	-	59,63,73	2.40	21 (35%)	70,101,113	2.74	30 (42%)
9	CLA	A	839	-	49,53,73	2.55	22 (44%)	58,89,113	2.79	24 (41%)
9	CLA	K	101	-	45,49,73	2.50	21 (46%)	54,83,113	2.79	20 (37%)
9	CLA	A	833	1	49,53,73	2.56	22 (44%)	58,89,113	2.76	25 (43%)

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
9	CLA	A	844	13	-	11/15/91/115	-
9	CLA	A	835	-	-	9/15/91/115	-
9	CLA	A	807	1	-	8/15/91/115	-
9	CLA	B	836	-	-	11/27/103/115	-
9	CLA	B	806	-	-	12/33/109/115	-
12	BCR	A	849	-	-	9/29/63/63	0/2/2/2
9	CLA	B	810	-	-	8/15/91/115	-
12	BCR	A	847	-	-	6/29/63/63	0/2/2/2
8	CL0	A	801	-	-	15/33/109/115	-
13	LHG	A	853	9	-	16/31/31/53	-
12	BCR	B	846	-	-	11/29/63/63	0/2/2/2
9	CLA	A	813	1	-	17/33/109/115	-
9	CLA	B	803	-	-	17/39/115/115	-
9	CLA	B	818	2	-	15/33/109/115	-
9	CLA	B	827	2	-	13/27/103/115	-
9	CLA	B	809	2	-	15/39/115/115	-
9	CLA	A	825	-	-	16/39/115/115	-
9	CLA	B	823	2	-	2/15/91/115	-
9	CLA	B	831	-	-	5/15/91/115	-
12	BCR	B	845	-	-	6/29/63/63	0/2/2/2
9	CLA	B	807	-	-	15/39/115/115	-
12	BCR	M	101	-	-	9/29/63/63	0/2/2/2
9	CLA	A	838	-	-	3/15/91/115	-
9	CLA	A	836	-	-	7/15/91/115	-
9	CLA	A	803	1	-	10/15/91/115	-
9	CLA	B	813	-	-	23/39/115/115	-
12	BCR	B	842	-	-	11/29/63/63	0/2/2/2
9	CLA	A	822	-	-	7/15/91/115	-
9	CLA	B	811	-	-	5/15/91/115	-
9	CLA	B	825	-	-	4/15/91/115	-
9	CLA	B	805	-	-	5/15/91/115	-
9	CLA	B	837	-	-	13/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLA	A	815	1	-	7/15/91/115	-
9	CLA	A	828	1	-	17/39/115/115	-
9	CLA	A	837	-	-	8/15/91/115	-
9	CLA	B	838	-	-	5/15/91/115	-
12	BCR	B	847	-	-	7/29/63/63	0/2/2/2
12	BCR	F	201	-	-	5/29/63/63	0/2/2/2
9	CLA	B	816	-	-	7/15/91/115	-
9	CLA	B	835	-	-	5/15/91/115	-
9	CLA	A	819	1	-	15/39/115/115	-
9	CLA	A	843	-	-	8/15/91/115	-
9	CLA	B	814	-	-	12/27/103/115	-
9	CLA	A	802	-	-	17/39/115/115	-
11	SF4	A	846	2,1	-	-	0/6/5/5
12	BCR	A	851	-	-	9/29/63/63	0/2/2/2
9	CLA	A	817	-	-	7/21/97/115	-
9	CLA	A	809	-	-	6/21/97/115	-
9	CLA	B	830	-	-	11/15/91/115	-
9	CLA	A	826	-	-	9/33/109/115	-
9	CLA	A	821	-	-	14/39/115/115	-
9	CLA	A	841	-	-	7/15/91/115	-
9	CLA	B	808	2	-	7/15/91/115	-
9	CLA	A	806	1	-	12/39/115/115	-
9	CLA	B	817	-	-	8/27/103/115	-
9	CLA	B	833	2	-	6/15/91/115	-
9	CLA	A	812	-	-	6/15/91/115	-
9	CLA	B	819	-	-	5/27/103/115	-
9	CLA	B	821	-	-	7/15/91/115	-
12	BCR	A	850	-	-	9/29/63/63	0/2/2/2
9	CLA	B	802	-	-	16/39/115/115	-
9	CLA	A	829	-	-	15/39/115/115	-
9	CLA	A	834	1	-	7/15/91/115	-
9	CLA	B	839	-	-	7/15/91/115	-
12	BCR	A	848	-	-	10/29/63/63	0/2/2/2
13	LHG	A	852	-	-	34/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	LMG	B	848	-	-	23/44/64/70	0/1/1/1
9	CLA	B	824	-	-	9/15/91/115	-
12	BCR	B	843	-	-	9/29/63/63	0/2/2/2
9	CLA	B	834	-	-	6/15/91/115	-
9	CLA	A	808	1	-	9/15/91/115	-
9	CLA	B	815	2	-	9/15/91/115	-
12	BCR	B	844	-	-	9/29/63/63	0/2/2/2
10	PQN	B	841	-	-	9/23/43/43	0/2/2/2
10	PQN	A	845	-	-	4/23/43/43	0/2/2/2
9	CLA	A	831	-	-	7/15/91/115	-
9	CLA	A	842	1	-	8/21/97/115	-
9	CLA	B	804	-	-	12/39/115/115	-
9	CLA	A	804	9	-	8/15/91/115	-
9	CLA	B	822	-	-	8/15/91/115	-
9	CLA	B	840	-	-	7/15/91/115	-
9	CLA	A	816	-	-	7/15/91/115	-
9	CLA	A	814	1	-	4/15/91/115	-
9	CLA	I	101	-	-	8/15/91/115	-
9	CLA	A	830	1	-	14/39/115/115	-
9	CLA	B	812	-	-	5/15/91/115	-
9	CLA	A	827	-	-	12/39/115/115	-
9	CLA	B	828	-	-	14/39/115/115	-
9	CLA	A	840	-	-	6/21/97/115	-
9	CLA	B	801	-	-	10/33/109/115	-
9	CLA	B	829	-	-	5/15/91/115	-
9	CLA	A	823	-	-	8/15/91/115	-
9	CLA	A	811	9	-	7/15/91/115	-
9	CLA	B	826	-	-	17/39/115/115	-
9	CLA	A	818	1	-	10/21/97/115	-
9	CLA	A	810	-	-	5/15/91/115	-
9	CLA	B	832	2	-	3/15/91/115	-
9	CLA	A	824	-	-	8/15/91/115	-
9	CLA	B	820	2	-	8/15/91/115	-
9	CLA	A	805	-	-	22/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLA	A	832	-	-	5/15/91/115	-
9	CLA	A	820	-	-	10/27/103/115	-
9	CLA	A	839	-	-	7/15/91/115	-
9	CLA	K	101	-	-	4/9/81/115	-
9	CLA	A	833	1	-	6/15/91/115	-

All (2017) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	842	BCR	C8-C9	-8.41	1.28	1.46
12	A	848	BCR	C8-C9	-8.34	1.28	1.46
12	B	845	BCR	C11-C10	-8.33	1.17	1.43
12	B	846	BCR	C11-C10	-8.30	1.17	1.43
12	B	843	BCR	C8-C9	-8.27	1.28	1.46
12	A	850	BCR	C11-C10	-8.24	1.17	1.43
12	A	851	BCR	C8-C9	-8.21	1.28	1.46
12	A	850	BCR	C8-C9	-8.19	1.28	1.46
12	A	849	BCR	C8-C9	-8.12	1.28	1.46
12	M	101	BCR	C8-C9	-8.12	1.28	1.46
12	B	845	BCR	C8-C9	-8.10	1.28	1.46
12	A	847	BCR	C8-C9	-8.05	1.28	1.46
12	B	842	BCR	C11-C10	-8.03	1.18	1.43
12	B	844	BCR	C8-C9	-8.00	1.28	1.46
12	B	843	BCR	C11-C10	-8.00	1.18	1.43
12	A	851	BCR	C11-C10	-7.99	1.18	1.43
12	B	847	BCR	C8-C9	-7.97	1.28	1.46
12	A	847	BCR	C11-C10	-7.97	1.18	1.43
12	A	848	BCR	C11-C10	-7.96	1.18	1.43
12	A	849	BCR	C11-C10	-7.95	1.18	1.43
12	B	844	BCR	C11-C10	-7.92	1.18	1.43
12	B	847	BCR	C11-C10	-7.92	1.18	1.43
12	M	101	BCR	C11-C10	-7.90	1.18	1.43
12	F	201	BCR	C11-C10	-7.86	1.18	1.43
12	B	846	BCR	C8-C9	-7.77	1.29	1.46
9	A	825	CLA	MG-NA	7.74	2.24	2.06
9	B	817	CLA	MG-NA	7.72	2.24	2.06
10	B	841	PQN	C3-C2	7.72	1.49	1.35
10	A	845	PQN	C3-C2	7.68	1.49	1.35
9	A	831	CLA	MG-NA	7.68	2.24	2.06
9	B	830	CLA	MG-NA	7.67	2.24	2.06
12	F	201	BCR	C8-C9	-7.67	1.29	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	836	CLA	MG-NA	7.66	2.24	2.06
9	A	822	CLA	MG-NA	7.64	2.24	2.06
9	B	816	CLA	MG-NA	7.63	2.24	2.06
9	A	838	CLA	MG-NA	7.63	2.24	2.06
9	A	836	CLA	MG-NA	7.62	2.24	2.06
9	K	101	CLA	MG-NA	7.61	2.24	2.06
9	B	814	CLA	MG-NA	7.61	2.24	2.06
9	B	828	CLA	MG-NA	7.61	2.24	2.06
9	A	803	CLA	MG-NA	7.61	2.24	2.06
9	A	810	CLA	MG-NA	7.61	2.24	2.06
9	B	806	CLA	MG-NA	7.61	2.24	2.06
9	A	815	CLA	MG-NA	7.61	2.24	2.06
9	B	820	CLA	MG-NA	7.60	2.24	2.06
9	B	838	CLA	MG-NA	7.60	2.24	2.06
9	B	835	CLA	MG-NA	7.59	2.24	2.06
9	B	802	CLA	MG-NA	7.59	2.24	2.06
9	B	822	CLA	MG-NA	7.59	2.24	2.06
9	A	829	CLA	MG-NA	7.59	2.24	2.06
9	A	811	CLA	MG-NA	7.59	2.24	2.06
9	A	828	CLA	MG-NA	7.58	2.24	2.06
9	A	817	CLA	MG-NA	7.58	2.24	2.06
9	B	819	CLA	MG-NA	7.58	2.24	2.06
9	A	833	CLA	MG-NA	7.58	2.24	2.06
9	A	834	CLA	MG-NA	7.57	2.24	2.06
9	A	839	CLA	MG-NA	7.57	2.24	2.06
9	A	808	CLA	MG-NA	7.57	2.24	2.06
9	B	808	CLA	MG-NA	7.57	2.24	2.06
9	A	823	CLA	MG-NA	7.56	2.24	2.06
9	A	821	CLA	MG-NA	7.56	2.24	2.06
9	A	804	CLA	MG-NA	7.56	2.24	2.06
9	B	815	CLA	MG-NA	7.56	2.24	2.06
9	A	844	CLA	MG-NA	7.56	2.24	2.06
9	A	827	CLA	MG-NA	7.56	2.24	2.06
9	A	843	CLA	MG-NA	7.56	2.24	2.06
9	B	823	CLA	MG-NA	7.56	2.24	2.06
9	B	807	CLA	MG-NA	7.55	2.24	2.06
9	A	837	CLA	MG-NA	7.55	2.24	2.06
9	A	812	CLA	MG-NA	7.55	2.24	2.06
9	A	807	CLA	MG-NA	7.54	2.24	2.06
9	B	832	CLA	MG-NA	7.54	2.24	2.06
9	B	821	CLA	MG-NA	7.54	2.24	2.06
9	B	810	CLA	MG-NA	7.54	2.24	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	101	CLA	MG-NA	7.54	2.24	2.06
9	B	826	CLA	MG-NA	7.53	2.24	2.06
9	B	833	CLA	MG-NA	7.53	2.24	2.06
9	B	837	CLA	MG-NA	7.53	2.24	2.06
9	B	840	CLA	MG-NA	7.53	2.24	2.06
12	B	846	BCR	C20-C21	-7.53	1.19	1.43
9	A	824	CLA	MG-NA	7.52	2.24	2.06
9	B	831	CLA	MG-NA	7.52	2.24	2.06
9	A	835	CLA	MG-NA	7.51	2.24	2.06
9	B	818	CLA	MG-NA	7.51	2.24	2.06
9	B	813	CLA	MG-NA	7.50	2.24	2.06
9	B	812	CLA	MG-NA	7.50	2.24	2.06
9	A	842	CLA	MG-NA	7.49	2.24	2.06
9	A	818	CLA	MG-NA	7.49	2.24	2.06
9	A	819	CLA	MG-NA	7.48	2.24	2.06
9	A	816	CLA	MG-NA	7.48	2.24	2.06
9	A	840	CLA	MG-NA	7.48	2.24	2.06
9	A	841	CLA	MG-NA	7.48	2.24	2.06
9	A	802	CLA	MG-NA	7.47	2.24	2.06
9	B	811	CLA	MG-NA	7.46	2.24	2.06
9	A	813	CLA	MG-NA	7.46	2.24	2.06
9	A	806	CLA	MG-NA	7.46	2.24	2.06
9	B	825	CLA	MG-NA	7.45	2.24	2.06
9	B	805	CLA	MG-NA	7.45	2.24	2.06
9	A	832	CLA	MG-NA	7.44	2.24	2.06
9	A	814	CLA	MG-NA	7.44	2.23	2.06
12	B	843	BCR	C20-C21	-7.44	1.20	1.43
9	A	809	CLA	MG-NA	7.43	2.23	2.06
9	A	820	CLA	MG-NA	7.41	2.23	2.06
9	B	809	CLA	MG-NA	7.40	2.23	2.06
12	A	851	BCR	C20-C21	-7.40	1.20	1.43
9	B	804	CLA	MG-NA	7.39	2.23	2.06
12	A	850	BCR	C20-C21	-7.39	1.20	1.43
9	B	827	CLA	MG-NA	7.38	2.23	2.06
8	A	801	CL0	MG-NA	7.37	2.23	2.06
12	B	845	BCR	C20-C21	-7.35	1.20	1.43
9	B	834	CLA	MG-NA	7.35	2.23	2.06
12	B	843	BCR	C16-C17	-7.35	1.20	1.43
12	A	850	BCR	C16-C17	-7.35	1.20	1.43
9	A	805	CLA	MG-NA	7.34	2.23	2.06
9	A	826	CLA	MG-NA	7.34	2.23	2.06
12	B	842	BCR	C20-C21	-7.33	1.20	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	824	CLA	MG-NA	7.33	2.23	2.06
12	B	846	BCR	C16-C17	-7.31	1.20	1.43
9	A	830	CLA	MG-NA	7.31	2.23	2.06
12	B	847	BCR	C20-C21	-7.31	1.20	1.43
12	A	849	BCR	C20-C21	-7.28	1.20	1.43
12	B	845	BCR	C16-C17	-7.28	1.20	1.43
9	B	839	CLA	MG-NA	7.27	2.23	2.06
12	A	848	BCR	C20-C21	-7.27	1.20	1.43
9	B	829	CLA	MG-NA	7.25	2.23	2.06
12	A	847	BCR	C20-C21	-7.25	1.20	1.43
12	B	842	BCR	C16-C17	-7.24	1.20	1.43
9	B	803	CLA	MG-NA	7.23	2.23	2.06
12	A	851	BCR	C16-C17	-7.23	1.20	1.43
12	B	844	BCR	C20-C21	-7.23	1.20	1.43
12	A	847	BCR	C16-C17	-7.21	1.20	1.43
12	A	849	BCR	C16-C17	-7.21	1.20	1.43
12	B	847	BCR	C16-C17	-7.20	1.20	1.43
12	M	101	BCR	C20-C21	-7.19	1.20	1.43
12	A	848	BCR	C16-C17	-7.19	1.20	1.43
12	F	201	BCR	C20-C21	-7.17	1.20	1.43
12	M	101	BCR	C16-C17	-7.15	1.21	1.43
12	B	844	BCR	C16-C17	-7.12	1.21	1.43
12	F	201	BCR	C16-C17	-7.11	1.21	1.43
9	B	801	CLA	MG-NA	7.08	2.23	2.06
9	B	802	CLA	O2A-C1	5.73	1.61	1.46
9	B	809	CLA	O2A-C1	5.68	1.61	1.46
9	A	842	CLA	O2A-C1	5.56	1.61	1.46
9	A	802	CLA	O2A-C1	5.49	1.60	1.46
8	A	801	CL0	O2A-C1	5.47	1.60	1.46
9	A	821	CLA	O2A-C1	5.44	1.60	1.46
9	A	806	CLA	O2A-C1	5.44	1.60	1.46
9	A	813	CLA	O2A-C1	5.43	1.60	1.46
9	B	828	CLA	O2A-C1	5.43	1.60	1.46
9	B	804	CLA	O2A-C1	5.42	1.60	1.46
9	B	801	CLA	O2A-C1	5.41	1.60	1.46
9	B	826	CLA	O2A-C1	5.39	1.60	1.46
9	B	803	CLA	O2A-C1	5.39	1.60	1.46
9	A	819	CLA	O2A-C1	5.37	1.60	1.46
9	B	817	CLA	O2A-C1	5.37	1.60	1.46
9	A	809	CLA	O2A-C1	5.37	1.60	1.46
9	A	827	CLA	O2A-C1	5.37	1.60	1.46
9	A	820	CLA	O2A-C1	5.37	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	830	CLA	O2A-C1	5.35	1.60	1.46
9	B	827	CLA	O2A-C1	5.33	1.60	1.46
9	A	818	CLA	O2A-C1	5.33	1.60	1.46
9	B	818	CLA	O2A-C1	5.33	1.60	1.46
9	A	825	CLA	O2A-C1	5.32	1.60	1.46
9	A	840	CLA	O2A-C1	5.31	1.60	1.46
9	A	826	CLA	O2A-C1	5.30	1.60	1.46
9	B	806	CLA	O2A-C1	5.30	1.60	1.46
9	A	817	CLA	O2A-C1	5.30	1.60	1.46
9	B	828	CLA	O2D-CGD	5.29	1.46	1.33
9	B	836	CLA	O2A-C1	5.27	1.60	1.46
9	B	813	CLA	O2A-C1	5.27	1.60	1.46
9	A	828	CLA	O2A-C1	5.26	1.60	1.46
9	A	805	CLA	O2A-C1	5.26	1.60	1.46
9	B	837	CLA	O2A-C1	5.26	1.60	1.46
9	B	807	CLA	O2A-C1	5.26	1.60	1.46
9	A	829	CLA	O2A-C1	5.22	1.60	1.46
9	B	819	CLA	O2A-C1	5.20	1.60	1.46
9	B	816	CLA	O2D-CGD	5.19	1.46	1.33
9	B	814	CLA	O2A-C1	5.18	1.60	1.46
9	B	839	CLA	O2D-CGD	5.18	1.46	1.33
9	B	831	CLA	O2D-CGD	5.16	1.45	1.33
8	A	801	CL0	O2D-CGD	5.15	1.45	1.33
9	A	821	CLA	O2D-CGD	5.15	1.45	1.33
9	B	835	CLA	O2D-CGD	5.14	1.45	1.33
9	A	836	CLA	O2D-CGD	5.13	1.45	1.33
9	B	811	CLA	O2D-CGD	5.13	1.45	1.33
9	A	817	CLA	O2D-CGD	5.13	1.45	1.33
9	A	820	CLA	O2D-CGD	5.13	1.45	1.33
9	A	830	CLA	O2D-CGD	5.12	1.45	1.33
9	B	812	CLA	O2D-CGD	5.12	1.45	1.33
9	A	803	CLA	O2D-CGD	5.12	1.45	1.33
9	A	841	CLA	O2D-CGD	5.12	1.45	1.33
9	A	842	CLA	O2D-CGD	5.11	1.45	1.33
9	B	833	CLA	O2D-CGD	5.11	1.45	1.33
9	A	829	CLA	O2D-CGD	5.11	1.45	1.33
9	A	824	CLA	O2D-CGD	5.11	1.45	1.33
9	A	840	CLA	O2D-CGD	5.11	1.45	1.33
9	A	811	CLA	O2D-CGD	5.11	1.45	1.33
9	B	827	CLA	O2D-CGD	5.11	1.45	1.33
9	B	807	CLA	O2D-CGD	5.11	1.45	1.33
9	B	837	CLA	O2D-CGD	5.11	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	812	CLA	O2D-CGD	5.10	1.45	1.33
9	A	835	CLA	O2D-CGD	5.10	1.45	1.33
9	I	101	CLA	O2D-CGD	5.10	1.45	1.33
9	A	832	CLA	O2D-CGD	5.10	1.45	1.33
9	A	823	CLA	O2D-CGD	5.10	1.45	1.33
9	A	844	CLA	O2D-CGD	5.10	1.45	1.33
9	A	815	CLA	O2D-CGD	5.09	1.45	1.33
9	A	819	CLA	O2D-CGD	5.09	1.45	1.33
9	B	813	CLA	O2D-CGD	5.09	1.45	1.33
9	A	827	CLA	CHC-C1C	5.09	1.48	1.38
9	A	828	CLA	O2D-CGD	5.09	1.45	1.33
9	B	808	CLA	O2D-CGD	5.08	1.45	1.33
9	B	830	CLA	O2D-CGD	5.08	1.45	1.33
9	B	814	CLA	O2D-CGD	5.08	1.45	1.33
9	A	822	CLA	O2D-CGD	5.08	1.45	1.33
9	B	817	CLA	O2D-CGD	5.08	1.45	1.33
9	B	801	CLA	CHC-C1C	5.08	1.48	1.38
9	B	821	CLA	O2D-CGD	5.07	1.45	1.33
9	B	802	CLA	O2D-CGD	5.07	1.45	1.33
9	B	803	CLA	O2D-CGD	5.07	1.45	1.33
9	A	843	CLA	O2D-CGD	5.07	1.45	1.33
9	B	810	CLA	O2D-CGD	5.07	1.45	1.33
9	A	839	CLA	O2D-CGD	5.06	1.45	1.33
9	B	823	CLA	O2D-CGD	5.06	1.45	1.33
9	A	810	CLA	O2D-CGD	5.06	1.45	1.33
9	A	833	CLA	O2D-CGD	5.06	1.45	1.33
9	A	807	CLA	O2D-CGD	5.06	1.45	1.33
9	A	802	CLA	O2D-CGD	5.05	1.45	1.33
9	B	819	CLA	O2D-CGD	5.05	1.45	1.33
9	A	834	CLA	O2D-CGD	5.05	1.45	1.33
9	B	801	CLA	O2D-CGD	5.04	1.45	1.33
9	B	825	CLA	O2D-CGD	5.04	1.45	1.33
9	B	822	CLA	O2D-CGD	5.04	1.45	1.33
9	B	826	CLA	O2D-CGD	5.04	1.45	1.33
9	A	808	CLA	O2D-CGD	5.04	1.45	1.33
9	B	840	CLA	O2D-CGD	5.04	1.45	1.33
9	B	805	CLA	O2D-CGD	5.03	1.45	1.33
9	A	826	CLA	O2D-CGD	5.02	1.45	1.33
9	B	820	CLA	O2D-CGD	5.02	1.45	1.33
9	A	818	CLA	O2D-CGD	5.00	1.45	1.33
9	A	816	CLA	O2D-CGD	5.00	1.45	1.33
9	A	809	CLA	O2D-CGD	5.00	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	831	CLA	O2D-CGD	4.99	1.45	1.33
9	B	809	CLA	O2D-CGD	4.99	1.45	1.33
9	B	838	CLA	O2D-CGD	4.98	1.45	1.33
9	B	824	CLA	O2D-CGD	4.98	1.45	1.33
9	A	837	CLA	O2D-CGD	4.98	1.45	1.33
9	B	829	CLA	O2D-CGD	4.97	1.45	1.33
9	A	804	CLA	O2D-CGD	4.97	1.45	1.33
9	A	814	CLA	O2D-CGD	4.96	1.45	1.33
9	B	804	CLA	O2D-CGD	4.95	1.45	1.33
9	A	827	CLA	O2D-CGD	4.95	1.45	1.33
9	A	806	CLA	O2D-CGD	4.95	1.45	1.33
9	A	805	CLA	O2D-CGD	4.94	1.45	1.33
9	B	832	CLA	O2D-CGD	4.94	1.45	1.33
9	A	825	CLA	O2D-CGD	4.94	1.45	1.33
10	A	845	PQN	C10-C5	4.93	1.48	1.40
9	B	804	CLA	CHC-C1C	4.93	1.48	1.38
9	A	821	CLA	CHC-C1C	4.92	1.48	1.38
9	B	806	CLA	O2D-CGD	4.91	1.45	1.33
9	B	818	CLA	O2D-CGD	4.91	1.45	1.33
9	A	838	CLA	O2D-CGD	4.90	1.45	1.33
9	B	834	CLA	O2D-CGD	4.90	1.45	1.33
9	B	836	CLA	O2D-CGD	4.90	1.45	1.33
9	B	815	CLA	O2D-CGD	4.87	1.45	1.33
9	B	823	CLA	CHC-C1C	4.85	1.48	1.38
12	A	850	BCR	C10-C9	-4.83	1.24	1.35
9	A	802	CLA	CHC-C1C	4.82	1.48	1.38
9	A	844	CLA	C3C-C2C	4.79	1.47	1.36
10	B	841	PQN	C10-C5	4.77	1.48	1.40
12	B	845	BCR	C10-C9	-4.77	1.24	1.35
9	B	824	CLA	CHC-C1C	4.76	1.48	1.38
9	A	804	CLA	CHC-C1C	4.76	1.48	1.38
9	B	810	CLA	CHC-C1C	4.75	1.48	1.38
9	A	831	CLA	CHC-C1C	4.75	1.48	1.38
9	B	839	CLA	CHC-C1C	4.74	1.48	1.38
9	A	813	CLA	O2D-CGD	4.73	1.44	1.33
9	B	819	CLA	CHC-C1C	4.72	1.47	1.38
9	A	821	CLA	CHD-C1D	4.72	1.47	1.38
9	A	818	CLA	CHC-C1C	4.71	1.47	1.38
9	B	805	CLA	CHC-C1C	4.71	1.47	1.38
9	B	825	CLA	CHC-C1C	4.70	1.47	1.38
9	B	829	CLA	CHD-C1D	4.70	1.47	1.38
9	B	808	CLA	CHC-C1C	4.70	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	826	CLA	CHC-C1C	4.70	1.47	1.38
9	B	817	CLA	CHD-C1D	4.69	1.47	1.38
9	B	835	CLA	CHC-C1C	4.69	1.47	1.38
9	B	833	CLA	CHC-C1C	4.69	1.47	1.38
9	B	830	CLA	CHD-C1D	4.69	1.47	1.38
9	A	824	CLA	CHC-C1C	4.69	1.47	1.38
9	K	101	CLA	CHC-C1C	4.68	1.47	1.38
9	A	822	CLA	CHC-C1C	4.68	1.47	1.38
9	A	824	CLA	CHD-C1D	4.68	1.47	1.38
8	A	801	CL0	CHC-C1C	4.68	1.47	1.38
9	A	814	CLA	CHC-C1C	4.67	1.47	1.38
9	A	840	CLA	CHD-C1D	4.67	1.47	1.38
9	A	806	CLA	CHC-C1C	4.67	1.47	1.38
9	K	101	CLA	CHD-C1D	4.67	1.47	1.38
9	A	844	CLA	CHC-C1C	4.67	1.47	1.38
9	A	841	CLA	CHD-C1D	4.67	1.47	1.38
9	B	831	CLA	CHC-C1C	4.66	1.47	1.38
9	A	835	CLA	CHD-C1D	4.66	1.47	1.38
9	B	834	CLA	CHC-C1C	4.65	1.47	1.38
9	B	822	CLA	CHC-C1C	4.65	1.47	1.38
9	A	811	CLA	CHC-C1C	4.65	1.47	1.38
9	A	836	CLA	CHC-C1C	4.65	1.47	1.38
9	B	815	CLA	CHC-C1C	4.64	1.47	1.38
9	B	809	CLA	CHC-C1C	4.64	1.47	1.38
9	B	826	CLA	CHC-C1C	4.64	1.47	1.38
9	B	832	CLA	CHC-C1C	4.63	1.47	1.38
9	A	816	CLA	CHC-C1C	4.63	1.47	1.38
9	B	817	CLA	CHC-C1C	4.63	1.47	1.38
9	A	815	CLA	CHC-C1C	4.63	1.47	1.38
9	A	837	CLA	CHC-C1C	4.62	1.47	1.38
9	A	803	CLA	CHC-C1C	4.62	1.47	1.38
9	A	831	CLA	CHD-C1D	4.61	1.47	1.38
9	A	842	CLA	CHC-C1C	4.61	1.47	1.38
9	A	812	CLA	CHD-C1D	4.61	1.47	1.38
9	A	814	CLA	CHD-C1D	4.61	1.47	1.38
9	A	819	CLA	CHC-C1C	4.61	1.47	1.38
9	A	802	CLA	CHD-C1D	4.61	1.47	1.38
9	B	813	CLA	CHC-C1C	4.61	1.47	1.38
9	A	807	CLA	CHC-C1C	4.61	1.47	1.38
9	B	838	CLA	CHC-C1C	4.61	1.47	1.38
9	A	832	CLA	CHC-C1C	4.61	1.47	1.38
9	A	834	CLA	CHD-C1D	4.61	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	834	CLA	CHD-C1D	4.61	1.47	1.38
9	B	806	CLA	CHD-C1D	4.60	1.47	1.38
9	A	816	CLA	CHD-C1D	4.60	1.47	1.38
9	B	823	CLA	CHD-C1D	4.60	1.47	1.38
12	F	201	BCR	C10-C9	-4.60	1.25	1.35
9	B	812	CLA	CHD-C1D	4.60	1.47	1.38
9	A	835	CLA	CHC-C1C	4.60	1.47	1.38
9	A	818	CLA	CHD-C1D	4.60	1.47	1.38
9	A	832	CLA	CHD-C1D	4.59	1.47	1.38
9	B	807	CLA	CHD-C1D	4.59	1.47	1.38
9	A	808	CLA	CHC-C1C	4.59	1.47	1.38
9	A	810	CLA	CHC-C1C	4.59	1.47	1.38
9	A	836	CLA	CHD-C1D	4.59	1.47	1.38
9	A	833	CLA	CHD-C1D	4.59	1.47	1.38
9	B	816	CLA	CHC-C1C	4.59	1.47	1.38
9	A	840	CLA	CHC-C1C	4.59	1.47	1.38
9	A	812	CLA	CHC-C1C	4.59	1.47	1.38
9	A	809	CLA	CHD-C1D	4.59	1.47	1.38
9	B	820	CLA	CHC-C1C	4.58	1.47	1.38
9	B	816	CLA	CHD-C1D	4.58	1.47	1.38
9	A	813	CLA	CHC-C1C	4.58	1.47	1.38
9	A	804	CLA	CHD-C1D	4.58	1.47	1.38
9	A	833	CLA	CHC-C1C	4.58	1.47	1.38
9	A	838	CLA	CHC-C1C	4.58	1.47	1.38
9	B	821	CLA	CHD-C1D	4.58	1.47	1.38
9	A	830	CLA	CHC-C1C	4.58	1.47	1.38
9	A	817	CLA	CHC-C1C	4.57	1.47	1.38
9	B	827	CLA	CHC-C1C	4.57	1.47	1.38
9	A	803	CLA	CHD-C1D	4.57	1.47	1.38
9	B	836	CLA	C3C-C2C	4.57	1.46	1.36
9	B	824	CLA	C3C-C2C	4.57	1.46	1.36
9	B	829	CLA	C3C-C2C	4.57	1.46	1.36
9	A	843	CLA	CHC-C1C	4.57	1.47	1.38
9	A	819	CLA	CHD-C1D	4.56	1.47	1.38
9	B	833	CLA	CHD-C1D	4.56	1.47	1.38
9	A	811	CLA	CHD-C1D	4.56	1.47	1.38
9	A	823	CLA	CHD-C1D	4.56	1.47	1.38
9	B	807	CLA	CHC-C1C	4.56	1.47	1.38
9	B	836	CLA	CHD-C1D	4.55	1.47	1.38
9	A	805	CLA	CHD-C1D	4.55	1.47	1.38
9	A	823	CLA	CHC-C1C	4.55	1.47	1.38
9	B	811	CLA	CHD-C1D	4.55	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	835	CLA	CHD-C1D	4.55	1.47	1.38
9	B	836	CLA	CHC-C1C	4.55	1.47	1.38
8	A	801	CL0	CHD-C1D	4.54	1.47	1.38
9	B	832	CLA	CHD-C1D	4.54	1.47	1.38
9	B	818	CLA	CHC-C1C	4.54	1.47	1.38
9	B	831	CLA	CHD-C1D	4.54	1.47	1.38
9	B	820	CLA	CHD-C1D	4.54	1.47	1.38
9	B	830	CLA	CHC-C1C	4.54	1.47	1.38
9	B	837	CLA	CHC-C1C	4.53	1.47	1.38
9	A	839	CLA	CHD-C1D	4.53	1.47	1.38
9	A	842	CLA	CHD-C1D	4.53	1.47	1.38
9	B	812	CLA	CHC-C1C	4.53	1.47	1.38
9	A	821	CLA	C3C-C2C	4.53	1.46	1.36
9	B	805	CLA	CHD-C1D	4.53	1.47	1.38
9	A	829	CLA	CHC-C1C	4.52	1.47	1.38
9	I	101	CLA	CHD-C1D	4.52	1.47	1.38
9	B	837	CLA	CHD-C1D	4.52	1.47	1.38
9	B	811	CLA	C3C-C2C	4.52	1.46	1.36
9	B	811	CLA	CHC-C1C	4.51	1.47	1.38
9	B	819	CLA	C3C-C2C	4.51	1.46	1.36
9	B	838	CLA	CHD-C1D	4.51	1.47	1.38
9	B	807	CLA	C3C-C2C	4.51	1.46	1.36
9	B	817	CLA	C3C-C2C	4.51	1.46	1.36
9	A	818	CLA	C3C-C2C	4.51	1.46	1.36
9	B	814	CLA	CHC-C1C	4.50	1.47	1.38
9	A	837	CLA	CHD-C1D	4.50	1.47	1.38
9	B	840	CLA	CHD-C1D	4.49	1.47	1.38
9	A	826	CLA	C3C-C2C	4.49	1.46	1.36
9	A	839	CLA	CHC-C1C	4.49	1.47	1.38
9	A	834	CLA	CHC-C1C	4.49	1.47	1.38
9	B	830	CLA	C3C-C2C	4.48	1.46	1.36
9	B	809	CLA	CHD-C1D	4.48	1.47	1.38
9	A	820	CLA	CHC-C1C	4.48	1.47	1.38
9	A	834	CLA	C3C-C2C	4.48	1.46	1.36
9	A	804	CLA	C3C-C2C	4.47	1.46	1.36
9	B	826	CLA	C3C-C2C	4.47	1.46	1.36
9	A	817	CLA	CHD-C1D	4.47	1.47	1.38
9	A	844	CLA	CHD-C1D	4.47	1.47	1.38
9	A	802	CLA	C3C-C2C	4.47	1.46	1.36
9	A	806	CLA	CHD-C1D	4.47	1.47	1.38
9	A	810	CLA	CHD-C1D	4.47	1.47	1.38
9	B	813	CLA	CHD-C1D	4.47	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	839	CLA	C3C-C2C	4.47	1.46	1.36
9	A	823	CLA	C3C-C2C	4.47	1.46	1.36
9	A	815	CLA	CHD-C1D	4.47	1.47	1.38
9	A	809	CLA	CHC-C1C	4.47	1.47	1.38
9	B	825	CLA	C3C-C2C	4.47	1.46	1.36
9	A	830	CLA	CHD-C1D	4.47	1.47	1.38
9	A	832	CLA	C3C-C2C	4.47	1.46	1.36
9	A	825	CLA	CHC-C1C	4.47	1.47	1.38
9	A	826	CLA	CHD-C1D	4.46	1.47	1.38
9	A	824	CLA	C3C-C2C	4.46	1.46	1.36
9	B	822	CLA	CHD-C1D	4.46	1.47	1.38
9	B	806	CLA	CHC-C1C	4.46	1.47	1.38
9	A	841	CLA	CHC-C1C	4.46	1.47	1.38
9	B	803	CLA	CHC-C1C	4.46	1.47	1.38
9	A	843	CLA	CHD-C1D	4.45	1.47	1.38
9	B	802	CLA	CHC-C1C	4.45	1.47	1.38
9	B	821	CLA	CHC-C1C	4.45	1.47	1.38
9	B	822	CLA	C3C-C2C	4.45	1.46	1.36
9	A	828	CLA	CHD-C1D	4.45	1.47	1.38
9	K	101	CLA	C3C-C2C	4.45	1.46	1.36
9	B	825	CLA	CHD-C1D	4.45	1.47	1.38
9	A	803	CLA	C3C-C2C	4.45	1.46	1.36
9	A	814	CLA	C3C-C2C	4.45	1.46	1.36
9	A	805	CLA	CHC-C1C	4.45	1.47	1.38
9	B	830	CLA	C3D-C4D	-4.44	1.34	1.44
9	A	817	CLA	C3C-C2C	4.44	1.46	1.36
9	A	830	CLA	C3C-C2C	4.44	1.46	1.36
9	A	807	CLA	CHD-C1D	4.44	1.47	1.38
9	A	822	CLA	CHD-C1D	4.44	1.47	1.38
9	A	843	CLA	C3C-C2C	4.44	1.46	1.36
9	A	838	CLA	CHD-C1D	4.44	1.47	1.38
9	B	839	CLA	CHD-C1D	4.43	1.47	1.38
9	A	813	CLA	C3D-C4D	-4.43	1.34	1.44
9	A	840	CLA	C3C-C2C	4.43	1.46	1.36
9	A	815	CLA	C3C-C2C	4.43	1.46	1.36
9	B	810	CLA	CHD-C1D	4.43	1.47	1.38
9	B	835	CLA	C3C-C2C	4.43	1.46	1.36
9	B	834	CLA	C3C-C2C	4.43	1.46	1.36
9	B	837	CLA	C3C-C2C	4.43	1.46	1.36
9	A	835	CLA	C3C-C2C	4.42	1.46	1.36
9	B	816	CLA	C3C-C2C	4.42	1.46	1.36
9	A	831	CLA	C3D-C4D	-4.42	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	809	CLA	C3C-C2C	4.42	1.46	1.36
9	B	831	CLA	C3C-C2C	4.42	1.46	1.36
9	A	833	CLA	C3C-C2C	4.42	1.46	1.36
9	B	808	CLA	C3C-C2C	4.42	1.46	1.36
9	B	828	CLA	C3C-C2C	4.42	1.46	1.36
9	A	816	CLA	C3C-C2C	4.42	1.46	1.36
9	B	838	CLA	C3C-C2C	4.42	1.46	1.36
9	A	806	CLA	C3C-C2C	4.42	1.46	1.36
9	B	802	CLA	C3C-C2C	4.42	1.46	1.36
9	B	826	CLA	CHD-C1D	4.41	1.47	1.38
9	A	837	CLA	C3C-C2C	4.41	1.46	1.36
9	A	808	CLA	CHD-C1D	4.40	1.47	1.38
9	B	829	CLA	C3D-C4D	-4.40	1.34	1.44
9	A	811	CLA	C3C-C2C	4.40	1.46	1.36
9	A	842	CLA	C3C-C2C	4.40	1.46	1.36
9	B	812	CLA	C3C-C2C	4.40	1.46	1.36
9	B	818	CLA	CHD-C1D	4.40	1.47	1.38
9	A	810	CLA	C3C-C2C	4.40	1.46	1.36
9	B	832	CLA	C3C-C2C	4.40	1.46	1.36
9	B	840	CLA	C3C-C2C	4.39	1.46	1.36
9	B	826	CLA	C3D-C4D	-4.39	1.34	1.44
9	B	828	CLA	CHD-C1D	4.39	1.47	1.38
9	B	817	CLA	C3D-C4D	-4.39	1.34	1.44
9	B	814	CLA	CHD-C1D	4.39	1.47	1.38
9	B	809	CLA	C3C-C2C	4.38	1.46	1.36
9	A	836	CLA	C3C-C2C	4.38	1.46	1.36
9	B	823	CLA	C3C-C2C	4.38	1.46	1.36
9	A	812	CLA	C3C-C2C	4.38	1.46	1.36
9	I	101	CLA	CHC-C1C	4.38	1.47	1.38
9	A	820	CLA	CHD-C1D	4.38	1.47	1.38
9	A	829	CLA	CHD-C1D	4.37	1.47	1.38
9	A	820	CLA	C3D-C4D	-4.37	1.34	1.44
9	B	810	CLA	C3C-C2C	4.37	1.46	1.36
9	A	822	CLA	C3C-C2C	4.37	1.46	1.36
9	B	820	CLA	C3C-C2C	4.37	1.46	1.36
9	B	813	CLA	C3D-C4D	-4.37	1.34	1.44
8	A	801	CL0	C3D-C4D	-4.37	1.34	1.44
9	A	825	CLA	CHD-C1D	4.36	1.46	1.38
9	B	820	CLA	C3D-C4D	-4.36	1.34	1.44
9	A	841	CLA	C3C-C2C	4.36	1.46	1.36
9	B	819	CLA	CHD-C1D	4.36	1.46	1.38
9	B	814	CLA	C3C-C2C	4.36	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	839	CLA	C3D-C4D	-4.36	1.34	1.44
9	I	101	CLA	C3C-C2C	4.36	1.46	1.36
9	A	827	CLA	C3D-C4D	-4.36	1.34	1.44
9	B	829	CLA	CHC-C1C	4.35	1.47	1.38
9	A	829	CLA	C3C-C2C	4.35	1.46	1.36
9	B	809	CLA	C3D-C4D	-4.35	1.34	1.44
9	A	807	CLA	C3C-C2C	4.35	1.46	1.36
9	A	819	CLA	C3C-C2C	4.35	1.46	1.36
9	B	815	CLA	CHD-C1D	4.35	1.46	1.38
9	A	839	CLA	C3C-C2C	4.34	1.46	1.36
9	B	806	CLA	C3C-C2C	4.34	1.46	1.36
9	B	808	CLA	C3D-C4D	-4.34	1.34	1.44
9	A	802	CLA	C3D-C4D	-4.34	1.34	1.44
12	A	847	BCR	C10-C9	-4.34	1.25	1.35
9	A	839	CLA	C3D-C4D	-4.34	1.34	1.44
9	A	820	CLA	C3C-C2C	4.34	1.46	1.36
12	A	849	BCR	C10-C9	-4.34	1.25	1.35
12	B	843	BCR	C10-C9	-4.33	1.25	1.35
9	B	828	CLA	CHC-C1C	4.33	1.47	1.38
9	A	811	CLA	C3D-C4D	-4.33	1.34	1.44
9	B	814	CLA	C3D-C4D	-4.33	1.34	1.44
9	A	808	CLA	C3C-C2C	4.33	1.46	1.36
9	A	821	CLA	C3D-C4D	-4.33	1.34	1.44
9	A	838	CLA	C3C-C2C	4.33	1.46	1.36
9	B	838	CLA	C3D-C4D	-4.33	1.34	1.44
13	A	853	LHG	O8-C23	4.33	1.46	1.33
9	A	813	CLA	CHD-C1D	4.32	1.46	1.38
9	A	828	CLA	CHC-C1C	4.32	1.47	1.38
9	B	821	CLA	C3C-C2C	4.32	1.46	1.36
9	A	831	CLA	C3C-C2C	4.31	1.46	1.36
9	B	831	CLA	C3D-C4D	-4.31	1.34	1.44
9	B	803	CLA	C3D-C4D	-4.31	1.34	1.44
12	A	851	BCR	C10-C9	-4.31	1.25	1.35
9	B	805	CLA	C3C-C2C	4.31	1.46	1.36
9	B	825	CLA	C3D-C4D	-4.30	1.34	1.44
12	B	842	BCR	C10-C9	-4.30	1.25	1.35
8	A	801	CL0	C3C-C2C	4.30	1.46	1.36
9	B	833	CLA	C3C-C2C	4.30	1.46	1.36
9	A	808	CLA	C3D-C4D	-4.30	1.34	1.44
9	A	832	CLA	C3D-C4D	-4.30	1.34	1.44
9	A	830	CLA	C3D-C4D	-4.29	1.34	1.44
9	A	824	CLA	C3D-C4D	-4.29	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	815	CLA	C3C-C2C	4.28	1.46	1.36
9	B	818	CLA	C3C-C2C	4.28	1.46	1.36
9	A	805	CLA	C3D-C4D	-4.28	1.34	1.44
9	B	821	CLA	C3D-C4D	-4.28	1.34	1.44
9	A	805	CLA	C3C-C2C	4.28	1.46	1.36
9	A	818	CLA	C3D-C4D	-4.28	1.34	1.44
9	A	825	CLA	C3D-C4D	-4.28	1.34	1.44
9	B	840	CLA	C3D-C4D	-4.28	1.34	1.44
9	B	807	CLA	C3D-C4D	-4.27	1.34	1.44
9	A	806	CLA	C3D-C4D	-4.27	1.34	1.44
9	B	811	CLA	C3D-C4D	-4.27	1.34	1.44
9	B	837	CLA	C3D-C4D	-4.27	1.34	1.44
9	B	827	CLA	C3C-C2C	4.27	1.46	1.36
9	A	825	CLA	C3C-C2C	4.27	1.46	1.36
9	B	810	CLA	C3D-C4D	-4.27	1.34	1.44
9	A	835	CLA	C3D-C4D	-4.27	1.34	1.44
9	B	812	CLA	C3D-C4D	-4.27	1.34	1.44
9	A	816	CLA	C3D-C4D	-4.27	1.34	1.44
9	B	832	CLA	C3D-C4D	-4.26	1.34	1.44
9	A	828	CLA	C3C-C2C	4.26	1.46	1.36
9	A	843	CLA	C3D-C4D	-4.26	1.34	1.44
9	A	819	CLA	C3D-C4D	-4.26	1.34	1.44
9	A	817	CLA	C3D-C4D	-4.25	1.34	1.44
12	B	847	BCR	C10-C9	-4.25	1.26	1.35
9	A	828	CLA	C3D-C4D	-4.25	1.34	1.44
9	A	833	CLA	C3D-C4D	-4.25	1.34	1.44
12	A	848	BCR	C10-C9	-4.25	1.26	1.35
9	B	828	CLA	C3D-C4D	-4.25	1.34	1.44
9	B	835	CLA	C3D-C4D	-4.24	1.34	1.44
9	B	806	CLA	C3D-C4D	-4.24	1.34	1.44
9	B	804	CLA	C3D-C4D	-4.24	1.34	1.44
9	A	844	CLA	C3D-C4D	-4.24	1.34	1.44
9	B	833	CLA	C3D-C4D	-4.24	1.34	1.44
9	A	823	CLA	C3D-C4D	-4.24	1.34	1.44
9	A	834	CLA	C3D-C4D	-4.24	1.34	1.44
9	A	815	CLA	C3D-C4D	-4.23	1.34	1.44
9	A	826	CLA	C3D-C4D	-4.23	1.34	1.44
9	A	837	CLA	C3D-C4D	-4.23	1.34	1.44
9	B	836	CLA	C3D-C4D	-4.23	1.34	1.44
9	B	834	CLA	C3D-C4D	-4.23	1.34	1.44
9	A	840	CLA	C3D-C4D	-4.23	1.34	1.44
9	A	803	CLA	C3D-C4D	-4.23	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	101	CLA	C3D-C4D	-4.22	1.34	1.44
9	A	836	CLA	C3D-C4D	-4.22	1.34	1.44
9	A	814	CLA	C3D-C4D	-4.22	1.34	1.44
9	B	823	CLA	C3D-C4D	-4.22	1.34	1.44
9	A	807	CLA	C3D-C4D	-4.22	1.34	1.44
9	I	101	CLA	C3D-C4D	-4.22	1.34	1.44
9	B	827	CLA	C3D-C4D	-4.22	1.34	1.44
9	B	840	CLA	CHC-C1C	4.20	1.46	1.38
9	B	827	CLA	CHD-C1D	4.20	1.46	1.38
12	B	844	BCR	C10-C9	-4.20	1.26	1.35
12	M	101	BCR	C10-C9	-4.20	1.26	1.35
9	A	838	CLA	C3D-C4D	-4.20	1.34	1.44
9	A	809	CLA	C3D-C4D	-4.20	1.34	1.44
13	A	852	LHG	O8-C23	4.19	1.45	1.33
9	B	805	CLA	C3D-C4D	-4.19	1.34	1.44
9	B	813	CLA	C3C-C2C	4.19	1.45	1.36
9	A	810	CLA	C3D-C4D	-4.18	1.34	1.44
9	B	822	CLA	C3D-C4D	-4.18	1.34	1.44
9	A	841	CLA	C3D-C4D	-4.18	1.34	1.44
9	B	816	CLA	C3D-C4D	-4.18	1.34	1.44
9	B	824	CLA	C3D-C4D	-4.17	1.34	1.44
9	A	827	CLA	CHC-C4B	4.17	1.48	1.39
9	A	827	CLA	C3C-C2C	4.17	1.45	1.36
9	A	822	CLA	C3D-C4D	-4.17	1.34	1.44
9	B	804	CLA	CHC-C4B	4.16	1.48	1.39
9	A	842	CLA	C3D-C4D	-4.16	1.34	1.44
14	B	848	LMG	O7-C10	4.15	1.46	1.34
9	B	818	CLA	C3D-C4D	-4.14	1.34	1.44
14	B	848	LMG	O8-C28	4.13	1.45	1.33
9	B	819	CLA	C3D-C4D	-4.13	1.34	1.44
9	B	801	CLA	C3D-C4D	-4.12	1.34	1.44
9	B	815	CLA	C3D-C4D	-4.12	1.34	1.44
9	A	829	CLA	C3D-C4D	-4.12	1.34	1.44
9	B	802	CLA	C3D-C4D	-4.11	1.34	1.44
13	A	852	LHG	O7-C7	4.10	1.45	1.34
9	A	812	CLA	C3D-C4D	-4.10	1.35	1.44
9	A	804	CLA	C3D-C4D	-4.09	1.35	1.44
9	A	821	CLA	CHD-C4C	4.07	1.48	1.39
9	B	829	CLA	CHD-C4C	4.05	1.48	1.39
9	B	817	CLA	CHD-C4C	4.05	1.48	1.39
9	K	101	CLA	CHD-C4C	4.05	1.48	1.39
9	B	821	CLA	CHD-C4C	4.04	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	853	LHG	O7-C7	4.04	1.45	1.34
9	B	803	CLA	CHD-C1D	4.04	1.46	1.38
9	B	823	CLA	CHD-C4C	4.03	1.48	1.39
9	B	803	CLA	C3C-C2C	4.03	1.45	1.36
9	B	802	CLA	CHD-C1D	4.02	1.46	1.38
9	A	802	CLA	CHD-C4C	4.02	1.48	1.39
9	A	833	CLA	CHD-C4C	4.02	1.48	1.39
12	B	846	BCR	C10-C9	-4.02	1.26	1.35
9	B	834	CLA	CHD-C4C	4.01	1.48	1.39
9	A	813	CLA	C3C-C2C	4.01	1.45	1.36
9	B	825	CLA	CHD-C4C	4.00	1.48	1.39
9	B	801	CLA	CHC-C4B	4.00	1.48	1.39
9	A	814	CLA	CHD-C4C	4.00	1.48	1.39
9	A	836	CLA	CHD-C4C	3.99	1.48	1.39
9	A	809	CLA	CHD-C4C	3.99	1.48	1.39
9	B	835	CLA	CHD-C4C	3.99	1.48	1.39
9	B	804	CLA	C1D-ND	-3.99	1.32	1.37
9	A	832	CLA	CHD-C4C	3.99	1.48	1.39
9	A	838	CLA	CHC-C4B	3.99	1.48	1.39
9	A	841	CLA	CHD-C4C	3.99	1.48	1.39
9	B	832	CLA	CHD-C4C	3.99	1.48	1.39
9	A	824	CLA	CHD-C4C	3.99	1.48	1.39
9	A	834	CLA	CHD-C4C	3.99	1.48	1.39
9	B	809	CLA	CHD-C4C	3.99	1.48	1.39
9	A	840	CLA	CHD-C4C	3.98	1.48	1.39
9	A	816	CLA	CHD-C4C	3.98	1.48	1.39
9	A	835	CLA	CHD-C4C	3.97	1.48	1.39
9	A	818	CLA	CHD-C4C	3.97	1.48	1.39
9	A	811	CLA	CHD-C4C	3.97	1.48	1.39
9	A	804	CLA	CHD-C4C	3.97	1.48	1.39
9	B	838	CLA	CHD-C4C	3.97	1.48	1.39
9	B	806	CLA	CHD-C4C	3.97	1.48	1.39
9	B	831	CLA	CHD-C4C	3.96	1.48	1.39
9	B	839	CLA	CHD-C4C	3.96	1.48	1.39
9	B	816	CLA	CHD-C4C	3.96	1.48	1.39
9	A	827	CLA	CHD-C1D	3.96	1.46	1.38
9	A	812	CLA	CHD-C4C	3.96	1.48	1.39
9	B	802	CLA	CHB-C1B	3.96	1.48	1.39
9	A	842	CLA	CHD-C4C	3.95	1.48	1.39
9	B	812	CLA	CHD-C4C	3.94	1.48	1.39
9	A	806	CLA	CHD-C4C	3.94	1.48	1.39
9	B	805	CLA	CHD-C4C	3.94	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	820	CLA	CHD-C4C	3.94	1.48	1.39
9	B	807	CLA	CHD-C4C	3.94	1.48	1.39
9	B	830	CLA	CHD-C4C	3.94	1.48	1.39
9	A	807	CLA	CHD-C4C	3.94	1.48	1.39
9	A	843	CLA	CHD-C4C	3.93	1.48	1.39
9	A	803	CLA	CHD-C4C	3.93	1.48	1.39
9	B	822	CLA	CHD-C4C	3.93	1.48	1.39
9	B	826	CLA	CHD-C4C	3.92	1.48	1.39
9	A	844	CLA	CHD-C4C	3.91	1.48	1.39
9	A	821	CLA	CHC-C4B	3.91	1.48	1.39
9	B	837	CLA	CHD-C4C	3.91	1.48	1.39
9	A	810	CLA	CHD-C4C	3.91	1.48	1.39
9	A	826	CLA	CHD-C4C	3.91	1.48	1.39
9	B	824	CLA	CHC-C4B	3.91	1.48	1.39
9	A	831	CLA	CHD-C4C	3.91	1.48	1.39
9	A	823	CLA	CHD-C4C	3.91	1.48	1.39
9	B	808	CLA	CHB-C1B	3.90	1.48	1.39
9	B	811	CLA	CHD-C4C	3.90	1.48	1.39
9	A	837	CLA	CHD-C4C	3.90	1.48	1.39
9	A	819	CLA	CHD-C4C	3.90	1.48	1.39
9	A	839	CLA	CHD-C4C	3.90	1.48	1.39
9	B	824	CLA	CHB-C1B	3.89	1.48	1.39
9	A	817	CLA	CHD-C4C	3.89	1.48	1.39
9	B	819	CLA	CHD-C4C	3.89	1.48	1.39
9	A	820	CLA	CHD-C4C	3.88	1.48	1.39
9	B	801	CLA	C3C-C2C	3.88	1.45	1.36
9	B	833	CLA	CHD-C4C	3.88	1.48	1.39
9	B	836	CLA	CHD-C4C	3.88	1.48	1.39
9	B	823	CLA	CHC-C4B	3.88	1.48	1.39
9	I	101	CLA	CHD-C4C	3.88	1.48	1.39
9	A	805	CLA	CHD-C4C	3.88	1.48	1.39
9	B	812	CLA	CHC-C4B	3.88	1.48	1.39
9	A	831	CLA	CHC-C4B	3.87	1.48	1.39
8	A	801	CL0	CHD-C4C	3.87	1.48	1.39
9	B	828	CLA	CHC-C4B	3.87	1.48	1.39
9	A	839	CLA	CHC-C4B	3.87	1.48	1.39
9	A	818	CLA	CHC-C4B	3.87	1.48	1.39
9	B	840	CLA	CHB-C1B	3.86	1.48	1.39
9	B	811	CLA	CHB-C1B	3.86	1.48	1.39
9	A	822	CLA	CHD-C4C	3.86	1.48	1.39
9	B	840	CLA	CHD-C4C	3.86	1.48	1.39
9	A	815	CLA	CHD-C4C	3.86	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	810	CLA	CHD-C4C	3.85	1.48	1.39
9	B	815	CLA	CHD-C4C	3.85	1.48	1.39
9	B	810	CLA	CHC-C4B	3.85	1.48	1.39
9	B	813	CLA	CHD-C4C	3.85	1.48	1.39
9	B	801	CLA	CHD-C1D	3.85	1.45	1.38
9	B	818	CLA	CHD-C4C	3.84	1.48	1.39
9	B	839	CLA	CHC-C4B	3.84	1.48	1.39
9	A	825	CLA	CHD-C4C	3.84	1.47	1.39
9	A	830	CLA	CHD-C4C	3.84	1.47	1.39
9	B	819	CLA	CHC-C4B	3.83	1.48	1.39
9	B	815	CLA	CHC-C4B	3.83	1.48	1.39
9	A	825	CLA	CHB-C1B	3.82	1.48	1.39
9	B	824	CLA	CHD-C1D	3.82	1.45	1.38
9	A	826	CLA	CHC-C4B	3.82	1.48	1.39
9	A	838	CLA	CHD-C4C	3.82	1.47	1.39
9	B	825	CLA	CHC-C4B	3.81	1.48	1.39
9	B	835	CLA	CHC-C4B	3.80	1.47	1.39
9	K	101	CLA	CHC-C4B	3.80	1.47	1.39
9	A	843	CLA	CHC-C4B	3.80	1.47	1.39
9	B	808	CLA	CHC-C4B	3.79	1.47	1.39
9	B	814	CLA	CHD-C4C	3.79	1.47	1.39
9	B	805	CLA	CHC-C4B	3.79	1.47	1.39
9	A	804	CLA	CHC-C4B	3.79	1.47	1.39
9	A	817	CLA	CHC-C4B	3.78	1.47	1.39
9	B	822	CLA	CHC-C4B	3.78	1.47	1.39
9	B	826	CLA	CHC-C4B	3.78	1.47	1.39
9	A	828	CLA	CHD-C4C	3.78	1.47	1.39
9	B	808	CLA	CHD-C4C	3.78	1.47	1.39
9	B	803	CLA	CHB-C1B	3.77	1.47	1.39
9	B	814	CLA	CHB-C1B	3.77	1.47	1.39
9	A	816	CLA	OBD-CAD	3.77	1.29	1.22
9	A	808	CLA	CHD-C4C	3.77	1.47	1.39
9	A	823	CLA	OBD-CAD	3.76	1.29	1.22
9	B	804	CLA	C3C-C2C	3.76	1.44	1.36
9	B	838	CLA	CHC-C4B	3.76	1.47	1.39
9	A	822	CLA	OBD-CAD	3.75	1.28	1.22
9	A	844	CLA	CHC-C4B	3.75	1.47	1.39
9	A	836	CLA	OBD-CAD	3.74	1.28	1.22
9	B	819	CLA	OBD-CAD	3.74	1.28	1.22
9	B	831	CLA	CHC-C4B	3.74	1.47	1.39
9	A	843	CLA	OBD-CAD	3.74	1.28	1.22
9	B	832	CLA	CHC-C4B	3.74	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	808	CLA	CHC-C4B	3.74	1.47	1.39
9	A	811	CLA	CHC-C4B	3.74	1.47	1.39
9	A	844	CLA	OBD-CAD	3.74	1.28	1.22
9	A	822	CLA	CHC-C4B	3.74	1.47	1.39
9	B	833	CLA	CHC-C4B	3.74	1.47	1.39
9	B	830	CLA	CHC-C4B	3.74	1.47	1.39
9	A	815	CLA	CHC-C4B	3.74	1.47	1.39
9	A	823	CLA	CHC-C4B	3.74	1.47	1.39
9	A	815	CLA	OBD-CAD	3.73	1.28	1.22
9	A	820	CLA	CHB-C1B	3.73	1.47	1.39
8	A	801	CL0	CHC-C4B	3.73	1.47	1.39
9	B	833	CLA	OBD-CAD	3.73	1.28	1.22
9	B	834	CLA	CHC-C4B	3.73	1.47	1.39
9	B	805	CLA	OBD-CAD	3.73	1.28	1.22
9	A	830	CLA	CHC-C4B	3.73	1.47	1.39
9	B	816	CLA	CHC-C4B	3.73	1.47	1.39
9	B	818	CLA	OBD-CAD	3.73	1.28	1.22
9	A	824	CLA	CHC-C4B	3.72	1.47	1.39
9	I	101	CLA	CHB-C1B	3.72	1.47	1.39
9	A	832	CLA	OBD-CAD	3.72	1.28	1.22
9	A	816	CLA	CHC-C4B	3.72	1.47	1.39
9	A	806	CLA	CHC-C4B	3.72	1.47	1.39
9	A	831	CLA	OBD-CAD	3.72	1.28	1.22
9	B	806	CLA	CHC-C4B	3.72	1.47	1.39
9	B	836	CLA	CHC-C4B	3.72	1.47	1.39
9	I	101	CLA	OBD-CAD	3.72	1.28	1.22
9	B	802	CLA	CHC-C4B	3.72	1.47	1.39
9	B	812	CLA	OBD-CAD	3.71	1.28	1.22
9	A	815	CLA	CHB-C1B	3.71	1.47	1.39
9	A	825	CLA	OBD-CAD	3.71	1.28	1.22
9	A	841	CLA	CHC-C4B	3.71	1.47	1.39
9	B	827	CLA	CHD-C4C	3.71	1.47	1.39
9	B	815	CLA	OBD-CAD	3.71	1.28	1.22
9	A	803	CLA	CHC-C4B	3.71	1.47	1.39
14	B	848	LMG	C22-C21	-3.71	1.33	1.51
9	A	841	CLA	OBD-CAD	3.71	1.28	1.22
9	B	809	CLA	CHC-C4B	3.71	1.47	1.39
9	A	810	CLA	CHC-C4B	3.71	1.47	1.39
9	A	814	CLA	CHC-C4B	3.71	1.47	1.39
9	B	822	CLA	OBD-CAD	3.71	1.28	1.22
9	B	832	CLA	OBD-CAD	3.71	1.28	1.22
9	B	820	CLA	CHC-C4B	3.70	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	829	CLA	OBD-CAD	3.70	1.28	1.22
9	A	829	CLA	CHD-C4C	3.70	1.47	1.39
14	B	848	LMG	C19-C18	-3.70	1.33	1.51
9	A	820	CLA	CHC-C4B	3.70	1.47	1.39
9	A	834	CLA	OBD-CAD	3.70	1.28	1.22
9	A	842	CLA	OBD-CAD	3.70	1.28	1.22
9	B	816	CLA	OBD-CAD	3.70	1.28	1.22
9	B	823	CLA	OBD-CAD	3.70	1.28	1.22
9	A	830	CLA	CHB-C1B	3.70	1.47	1.39
9	A	840	CLA	CHC-C4B	3.70	1.47	1.39
9	B	834	CLA	OBD-CAD	3.70	1.28	1.22
9	B	809	CLA	OBD-CAD	3.70	1.28	1.22
9	B	821	CLA	OBD-CAD	3.70	1.28	1.22
9	B	825	CLA	OBD-CAD	3.70	1.28	1.22
9	A	803	CLA	CHB-C1B	3.70	1.47	1.39
9	A	837	CLA	CHC-C4B	3.70	1.47	1.39
9	B	803	CLA	CHC-C4B	3.70	1.47	1.39
9	B	810	CLA	CHB-C1B	3.70	1.47	1.39
9	A	810	CLA	OBD-CAD	3.70	1.28	1.22
9	A	824	CLA	OBD-CAD	3.70	1.28	1.22
9	A	819	CLA	CHC-C4B	3.70	1.47	1.39
9	A	842	CLA	CHC-C4B	3.69	1.47	1.39
9	B	835	CLA	OBD-CAD	3.69	1.28	1.22
9	A	803	CLA	OBD-CAD	3.69	1.28	1.22
12	B	846	BCR	C11-C12	-3.69	1.25	1.34
9	B	827	CLA	OBD-CAD	3.69	1.28	1.22
9	A	844	CLA	CHB-C1B	3.69	1.47	1.39
9	B	811	CLA	CHC-C4B	3.69	1.47	1.39
9	B	820	CLA	OBD-CAD	3.69	1.28	1.22
9	B	830	CLA	OBD-CAD	3.69	1.28	1.22
9	A	839	CLA	OBD-CAD	3.69	1.28	1.22
9	B	807	CLA	CHC-C4B	3.68	1.47	1.39
9	A	832	CLA	CHC-C4B	3.68	1.47	1.39
9	A	833	CLA	CHC-C4B	3.68	1.47	1.39
9	B	828	CLA	CHD-C4C	3.68	1.47	1.39
9	B	801	CLA	OBD-CAD	3.68	1.28	1.22
9	B	821	CLA	CHB-C1B	3.68	1.47	1.39
9	A	812	CLA	OBD-CAD	3.68	1.28	1.22
9	A	837	CLA	OBD-CAD	3.68	1.28	1.22
9	A	832	CLA	CHB-C1B	3.68	1.47	1.39
9	A	836	CLA	CHC-C4B	3.68	1.47	1.39
9	A	825	CLA	CHC-C4B	3.67	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	818	CLA	CHB-C1B	3.67	1.47	1.39
9	A	837	CLA	CHB-C1B	3.67	1.47	1.39
9	A	826	CLA	OBD-CAD	3.67	1.28	1.22
9	A	805	CLA	OBD-CAD	3.67	1.28	1.22
9	B	839	CLA	OBD-CAD	3.67	1.28	1.22
9	B	808	CLA	CHD-C1D	3.67	1.45	1.38
9	A	829	CLA	CHB-C1B	3.67	1.47	1.39
9	A	840	CLA	OBD-CAD	3.67	1.28	1.22
9	B	837	CLA	CHC-C4B	3.67	1.47	1.39
9	A	828	CLA	CHB-C1B	3.66	1.47	1.39
9	A	823	CLA	CHB-C1B	3.66	1.47	1.39
9	B	835	CLA	CHB-C1B	3.66	1.47	1.39
9	B	811	CLA	OBD-CAD	3.66	1.28	1.22
9	A	828	CLA	OBD-CAD	3.66	1.28	1.22
9	B	804	CLA	OBD-CAD	3.66	1.28	1.22
9	A	843	CLA	CHB-C1B	3.66	1.47	1.39
9	A	807	CLA	CHB-C1B	3.66	1.47	1.39
9	A	809	CLA	OBD-CAD	3.66	1.28	1.22
9	A	835	CLA	CHC-C4B	3.66	1.47	1.39
9	A	804	CLA	OBD-CAD	3.66	1.28	1.22
9	A	807	CLA	CHC-C4B	3.66	1.47	1.39
9	A	813	CLA	CHC-C4B	3.65	1.47	1.39
9	A	808	CLA	CHB-C1B	3.65	1.47	1.39
9	B	817	CLA	CHC-C4B	3.65	1.47	1.39
9	A	807	CLA	OBD-CAD	3.65	1.28	1.22
9	A	819	CLA	OBD-CAD	3.65	1.28	1.22
9	B	828	CLA	OBD-CAD	3.65	1.28	1.22
9	A	813	CLA	CHD-C4C	3.65	1.47	1.39
9	B	810	CLA	OBD-CAD	3.65	1.28	1.22
9	A	817	CLA	OBD-CAD	3.65	1.28	1.22
9	A	810	CLA	CHB-C1B	3.65	1.47	1.39
9	A	812	CLA	CHC-C4B	3.65	1.47	1.39
9	B	813	CLA	CHC-C4B	3.65	1.47	1.39
9	A	833	CLA	OBD-CAD	3.65	1.28	1.22
9	A	806	CLA	OBD-CAD	3.64	1.28	1.22
9	B	818	CLA	CHC-C4B	3.64	1.47	1.39
9	B	838	CLA	CHB-C1B	3.64	1.47	1.39
9	B	814	CLA	CHC-C4B	3.64	1.47	1.39
9	B	837	CLA	OBD-CAD	3.64	1.28	1.22
9	A	802	CLA	CHC-C4B	3.63	1.47	1.39
9	B	804	CLA	CHD-C1D	3.63	1.45	1.38
9	A	812	CLA	CHB-C1B	3.63	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	834	CLA	CHC-C4B	3.63	1.47	1.39
9	A	827	CLA	CHD-C4C	3.63	1.47	1.39
9	A	818	CLA	OBD-CAD	3.62	1.28	1.22
9	A	814	CLA	OBD-CAD	3.62	1.28	1.22
14	B	848	LMG	C25-C24	-3.62	1.33	1.51
9	A	829	CLA	OBD-CAD	3.62	1.28	1.22
12	A	850	BCR	C11-C12	-3.62	1.25	1.34
14	B	848	LMG	C37-C36	-3.62	1.33	1.51
9	A	841	CLA	CHB-C1B	3.62	1.47	1.39
9	A	817	CLA	CHB-C1B	3.61	1.47	1.39
9	K	101	CLA	CHB-C1B	3.61	1.47	1.39
9	B	826	CLA	CHB-C1B	3.61	1.47	1.39
9	A	835	CLA	OBD-CAD	3.61	1.28	1.22
9	A	805	CLA	CHB-C1B	3.61	1.47	1.39
9	A	819	CLA	CHB-C1B	3.61	1.47	1.39
9	A	842	CLA	CHB-C1B	3.61	1.47	1.39
9	A	836	CLA	CHB-C1B	3.61	1.47	1.39
9	B	806	CLA	OBD-CAD	3.61	1.28	1.22
9	A	811	CLA	OBD-CAD	3.61	1.28	1.22
9	B	824	CLA	OBD-CAD	3.60	1.28	1.22
9	A	811	CLA	CHB-C1B	3.60	1.47	1.39
9	A	834	CLA	CHB-C1B	3.60	1.47	1.39
9	B	831	CLA	OBD-CAD	3.60	1.28	1.22
9	A	829	CLA	CHC-C4B	3.60	1.47	1.39
9	A	839	CLA	CHB-C1B	3.60	1.47	1.39
9	B	807	CLA	CHB-C1B	3.60	1.47	1.39
9	B	828	CLA	CHB-C1B	3.59	1.47	1.39
8	A	801	CL0	C1B-NB	-3.59	1.33	1.37
9	B	804	CLA	CHB-C1B	3.59	1.47	1.39
9	B	808	CLA	OBD-CAD	3.59	1.28	1.22
9	A	830	CLA	OBD-CAD	3.59	1.28	1.22
9	B	829	CLA	CHB-C1B	3.58	1.47	1.39
9	B	837	CLA	CHB-C1B	3.58	1.47	1.39
9	B	807	CLA	OBD-CAD	3.58	1.28	1.22
9	B	820	CLA	CHB-C1B	3.58	1.47	1.39
9	A	833	CLA	CHB-C1B	3.57	1.47	1.39
9	B	839	CLA	CHB-C1B	3.57	1.47	1.39
9	B	827	CLA	CHC-C4B	3.57	1.47	1.39
9	A	831	CLA	CHB-C1B	3.57	1.47	1.39
9	B	801	CLA	C1D-ND	-3.57	1.33	1.37
9	A	806	CLA	CHB-C1B	3.56	1.47	1.39
9	A	802	CLA	OBD-CAD	3.56	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	840	CLA	OBD-CAD	3.56	1.28	1.22
9	A	816	CLA	CHB-C1B	3.56	1.47	1.39
9	B	836	CLA	OBD-CAD	3.56	1.28	1.22
9	A	838	CLA	OBD-CAD	3.56	1.28	1.22
9	A	809	CLA	CHC-C4B	3.56	1.47	1.39
9	A	805	CLA	CHC-C4B	3.55	1.47	1.39
9	B	821	CLA	CHC-C4B	3.55	1.47	1.39
9	I	101	CLA	CHC-C4B	3.55	1.47	1.39
9	B	805	CLA	CHB-C1B	3.55	1.47	1.39
9	B	809	CLA	CHB-C1B	3.54	1.47	1.39
9	A	838	CLA	CHB-C1B	3.54	1.47	1.39
9	B	833	CLA	CHB-C1B	3.54	1.47	1.39
9	B	812	CLA	CHB-C1B	3.54	1.47	1.39
9	B	814	CLA	OBD-CAD	3.54	1.28	1.22
9	B	838	CLA	OBD-CAD	3.53	1.28	1.22
9	A	822	CLA	CHB-C1B	3.52	1.47	1.39
9	A	828	CLA	CHC-C4B	3.52	1.47	1.39
9	B	822	CLA	CHB-C1B	3.52	1.47	1.39
9	B	832	CLA	CHB-C1B	3.52	1.47	1.39
9	A	827	CLA	CHB-C1B	3.52	1.47	1.39
9	A	820	CLA	OBD-CAD	3.51	1.28	1.22
9	B	816	CLA	CHB-C1B	3.51	1.47	1.39
9	B	829	CLA	CHC-C4B	3.51	1.47	1.39
9	A	809	CLA	CHB-C1B	3.50	1.47	1.39
9	A	824	CLA	CHB-C1B	3.49	1.47	1.39
9	B	831	CLA	CHB-C1B	3.49	1.47	1.39
9	A	840	CLA	CHB-C1B	3.49	1.47	1.39
12	B	845	BCR	C11-C12	-3.49	1.25	1.34
9	B	830	CLA	CHB-C1B	3.49	1.47	1.39
9	B	836	CLA	CHB-C1B	3.49	1.47	1.39
9	B	803	CLA	CHD-C4C	3.48	1.47	1.39
9	B	801	CLA	CHD-C4C	3.48	1.47	1.39
9	A	813	CLA	CHB-C1B	3.47	1.47	1.39
9	A	821	CLA	OBD-CAD	3.47	1.28	1.22
9	A	808	CLA	OBD-CAD	3.47	1.28	1.22
9	B	819	CLA	CHB-C1B	3.46	1.47	1.39
9	B	802	CLA	CHD-C4C	3.46	1.47	1.39
9	B	840	CLA	CHC-C4B	3.45	1.47	1.39
9	B	827	CLA	CHB-C1B	3.45	1.47	1.39
9	B	813	CLA	CHB-C1B	3.42	1.47	1.39
12	B	843	BCR	C11-C12	-3.42	1.25	1.34
9	B	806	CLA	CHB-C1B	3.42	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	802	CLA	C1D-ND	-3.41	1.33	1.37
9	B	801	CLA	C1B-NB	-3.41	1.33	1.37
9	B	824	CLA	CHD-C4C	3.41	1.47	1.39
9	A	826	CLA	CHB-C1B	3.41	1.47	1.39
9	B	804	CLA	MG-ND	-3.41	1.99	2.05
9	B	826	CLA	OBD-CAD	3.40	1.28	1.22
9	B	825	CLA	CHB-C1B	3.40	1.47	1.39
9	B	813	CLA	OBD-CAD	3.40	1.28	1.22
12	A	847	BCR	C11-C12	-3.39	1.25	1.34
9	B	815	CLA	CHB-C1B	3.39	1.47	1.39
9	A	835	CLA	CHB-C1B	3.39	1.47	1.39
9	B	808	CLA	C1D-ND	-3.39	1.33	1.37
12	A	851	BCR	C11-C12	-3.38	1.25	1.34
9	A	802	CLA	CHB-C1B	3.38	1.47	1.39
9	B	834	CLA	CHB-C1B	3.36	1.47	1.39
12	B	842	BCR	C11-C12	-3.36	1.25	1.34
9	B	827	CLA	C1D-ND	-3.36	1.33	1.37
9	B	803	CLA	C1D-ND	-3.35	1.33	1.37
9	A	814	CLA	CHB-C1B	3.35	1.46	1.39
9	B	823	CLA	CHB-C1B	3.35	1.46	1.39
12	A	849	BCR	C11-C12	-3.32	1.26	1.34
9	A	804	CLA	CHB-C1B	3.32	1.46	1.39
12	F	201	BCR	C11-C12	-3.32	1.26	1.34
9	A	818	CLA	CHB-C1B	3.31	1.46	1.39
12	A	848	BCR	C11-C12	-3.31	1.26	1.34
9	B	803	CLA	OBD-CAD	3.30	1.28	1.22
9	B	817	CLA	CHB-C1B	3.30	1.46	1.39
12	B	844	BCR	C11-C12	-3.29	1.26	1.34
12	B	847	BCR	C11-C12	-3.29	1.26	1.34
8	A	801	CL0	OBD-CAD	3.29	1.28	1.22
9	B	802	CLA	MG-NC	3.29	2.14	2.06
12	M	101	BCR	C11-C12	-3.29	1.26	1.34
9	A	825	CLA	MG-NC	3.28	2.14	2.06
9	B	802	CLA	OBD-CAD	3.27	1.28	1.22
9	A	829	CLA	C1D-ND	-3.26	1.33	1.37
9	B	824	CLA	C1D-ND	-3.23	1.33	1.37
8	A	801	CL0	C1D-ND	-3.23	1.33	1.37
9	A	827	CLA	OBD-CAD	3.21	1.28	1.22
9	B	804	CLA	C1B-NB	-3.21	1.33	1.37
9	B	804	CLA	CHD-C4C	3.21	1.46	1.39
9	A	828	CLA	MG-NC	3.21	2.13	2.06
9	B	828	CLA	C1D-ND	-3.20	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	801	CL0	MG-ND	-3.20	1.99	2.05
9	A	832	CLA	MG-NC	3.19	2.13	2.06
9	B	830	CLA	MG-NC	3.18	2.13	2.06
9	A	831	CLA	MG-NC	3.17	2.13	2.06
9	A	815	CLA	MG-NC	3.17	2.13	2.06
9	A	844	CLA	MG-NC	3.17	2.13	2.06
9	B	802	CLA	C3D-C2D	3.17	1.47	1.39
9	A	822	CLA	MG-NC	3.16	2.13	2.06
9	A	813	CLA	OBD-CAD	3.16	1.27	1.22
9	A	834	CLA	MG-NC	3.16	2.13	2.06
9	B	808	CLA	MG-NC	3.15	2.13	2.06
9	A	811	CLA	MG-NC	3.15	2.13	2.06
9	A	808	CLA	MG-NC	3.15	2.13	2.06
9	K	101	CLA	MG-NC	3.15	2.13	2.06
9	A	817	CLA	MG-NC	3.14	2.13	2.06
9	A	812	CLA	MG-NC	3.14	2.13	2.06
9	A	821	CLA	C1B-NB	-3.14	1.33	1.37
9	B	820	CLA	MG-NC	3.14	2.13	2.06
9	A	823	CLA	MG-NC	3.14	2.13	2.06
9	B	826	CLA	MG-NC	3.13	2.13	2.06
9	B	822	CLA	MG-NC	3.13	2.13	2.06
9	B	801	CLA	CHB-C1B	3.13	1.46	1.39
8	A	801	CL0	CHB-C1B	3.12	1.46	1.39
9	B	806	CLA	MG-NC	3.12	2.13	2.06
9	B	817	CLA	C1B-NB	-3.12	1.33	1.37
9	B	802	CLA	C1B-C2B	3.12	1.50	1.43
9	B	816	CLA	MG-NC	3.12	2.13	2.06
9	A	810	CLA	MG-NC	3.12	2.13	2.06
9	I	101	CLA	MG-NC	3.12	2.13	2.06
9	B	810	CLA	C3D-C2D	3.11	1.47	1.39
9	A	829	CLA	MG-NC	3.11	2.13	2.06
9	B	835	CLA	MG-NC	3.11	2.13	2.06
9	B	832	CLA	MG-NC	3.11	2.13	2.06
9	A	829	CLA	C1B-NB	-3.11	1.33	1.37
9	B	828	CLA	MG-NC	3.11	2.13	2.06
9	B	840	CLA	C1B-C2B	3.11	1.50	1.43
9	B	818	CLA	C1D-ND	-3.10	1.33	1.37
9	B	810	CLA	MG-NC	3.10	2.13	2.06
9	A	814	CLA	C4D-CHA	3.10	1.49	1.38
9	B	825	CLA	C1D-ND	-3.10	1.33	1.37
9	B	814	CLA	MG-NC	3.10	2.13	2.06
9	A	836	CLA	MG-NC	3.09	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	812	CLA	C3D-C2D	3.09	1.47	1.39
9	A	842	CLA	MG-NC	3.09	2.13	2.06
9	A	843	CLA	MG-NC	3.09	2.13	2.06
9	A	818	CLA	C1B-NB	-3.09	1.33	1.37
9	B	830	CLA	C1B-NB	-3.08	1.33	1.37
9	B	821	CLA	MG-NC	3.08	2.13	2.06
9	B	823	CLA	C1B-NB	-3.08	1.33	1.37
9	A	814	CLA	MG-NC	3.08	2.13	2.06
9	A	802	CLA	MG-NC	3.08	2.13	2.06
9	A	827	CLA	MG-NC	3.08	2.13	2.06
9	B	818	CLA	MG-NC	3.08	2.13	2.06
9	B	819	CLA	MG-NC	3.08	2.13	2.06
9	A	804	CLA	C4D-CHA	3.08	1.48	1.38
9	B	830	CLA	C1D-ND	-3.07	1.33	1.37
9	B	838	CLA	MG-NC	3.07	2.13	2.06
9	B	812	CLA	MG-NC	3.07	2.13	2.06
9	B	837	CLA	MG-NC	3.07	2.13	2.06
9	B	828	CLA	C1B-NB	-3.07	1.33	1.37
9	A	824	CLA	MG-NC	3.06	2.13	2.06
9	A	833	CLA	MG-NC	3.06	2.13	2.06
9	B	840	CLA	MG-NC	3.06	2.13	2.06
9	B	802	CLA	MG-ND	-3.06	1.99	2.05
9	B	803	CLA	MG-ND	-3.06	1.99	2.05
9	B	825	CLA	MG-NC	3.06	2.13	2.06
9	B	803	CLA	C3D-C2D	3.05	1.47	1.39
9	B	817	CLA	C3D-C2D	3.05	1.47	1.39
9	B	815	CLA	MG-NC	3.05	2.13	2.06
9	A	807	CLA	MG-NC	3.05	2.13	2.06
9	A	813	CLA	C4D-CHA	3.05	1.48	1.38
9	A	803	CLA	MG-NC	3.05	2.13	2.06
9	A	804	CLA	MG-NC	3.04	2.13	2.06
9	A	837	CLA	MG-NC	3.04	2.13	2.06
9	A	834	CLA	C4D-CHA	3.04	1.48	1.38
9	B	836	CLA	MG-NC	3.04	2.13	2.06
9	B	831	CLA	MG-NC	3.04	2.13	2.06
9	A	830	CLA	C3D-C2D	3.04	1.47	1.39
9	A	829	CLA	C3D-C2D	3.04	1.47	1.39
9	A	802	CLA	C3D-C2D	3.04	1.47	1.39
9	A	822	CLA	C3D-C2D	3.04	1.47	1.39
9	A	828	CLA	C1D-ND	-3.04	1.33	1.37
9	B	811	CLA	MG-NC	3.03	2.13	2.06
9	B	825	CLA	C3D-C2D	3.03	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	817	CLA	OBD-CAD	3.03	1.27	1.22
9	B	829	CLA	C1B-NB	-3.03	1.33	1.37
9	A	839	CLA	MG-NC	3.03	2.13	2.06
9	B	807	CLA	MG-NC	3.03	2.13	2.06
9	A	840	CLA	MG-NC	3.03	2.13	2.06
9	A	821	CLA	CHB-C1B	3.03	1.46	1.39
9	A	844	CLA	C3D-C2D	3.02	1.47	1.39
9	A	835	CLA	MG-NC	3.02	2.13	2.06
9	A	826	CLA	C1D-ND	-3.02	1.33	1.37
9	B	813	CLA	MG-NC	3.02	2.13	2.06
9	I	101	CLA	C3D-C2D	3.02	1.47	1.39
9	A	827	CLA	C1D-ND	-3.02	1.33	1.37
9	B	837	CLA	C3D-C2D	3.02	1.47	1.39
9	A	809	CLA	C3D-C2D	3.02	1.47	1.39
9	B	814	CLA	C1B-C2B	3.02	1.50	1.43
9	A	831	CLA	C1B-NB	-3.02	1.33	1.37
9	A	821	CLA	MG-NC	3.02	2.13	2.06
9	B	833	CLA	C3D-C2D	3.01	1.47	1.39
9	A	838	CLA	MG-NC	3.01	2.13	2.06
9	B	818	CLA	C3D-C2D	3.01	1.47	1.39
9	B	812	CLA	C4D-CHA	3.01	1.48	1.38
9	A	818	CLA	MG-NC	3.01	2.13	2.06
9	A	819	CLA	MG-NC	3.01	2.13	2.06
9	B	805	CLA	MG-NC	3.01	2.13	2.06
9	A	815	CLA	C3D-C2D	3.01	1.47	1.39
9	A	832	CLA	C3D-C2D	3.01	1.47	1.39
9	B	815	CLA	C4D-CHA	3.01	1.48	1.38
9	B	836	CLA	C4D-CHA	3.01	1.48	1.38
9	B	820	CLA	C4D-CHA	3.01	1.48	1.38
9	A	841	CLA	C3D-C2D	3.00	1.47	1.39
9	B	822	CLA	C4D-CHA	3.00	1.48	1.38
9	B	823	CLA	C4D-CHA	3.00	1.48	1.38
9	A	840	CLA	C4D-CHA	3.00	1.48	1.38
9	A	803	CLA	C3D-C2D	3.00	1.47	1.39
9	B	831	CLA	C3D-C2D	3.00	1.47	1.39
9	B	827	CLA	C3D-C2D	3.00	1.47	1.39
9	A	841	CLA	MG-NC	3.00	2.13	2.06
9	B	817	CLA	MG-NC	3.00	2.13	2.06
9	A	816	CLA	C3D-C2D	2.99	1.47	1.39
9	A	842	CLA	C3D-C2D	2.99	1.47	1.39
9	B	813	CLA	C4D-CHA	2.99	1.48	1.38
9	B	834	CLA	C1B-NB	-2.99	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	822	CLA	C4D-CHA	2.99	1.48	1.38
9	B	823	CLA	MG-NC	2.99	2.13	2.06
9	A	844	CLA	C4D-CHA	2.99	1.48	1.38
9	A	824	CLA	C3D-C2D	2.99	1.47	1.39
9	B	830	CLA	MG-ND	-2.99	1.99	2.05
9	A	808	CLA	C4D-CHA	2.99	1.48	1.38
9	A	817	CLA	C1D-ND	-2.99	1.33	1.37
9	A	834	CLA	C3D-C2D	2.99	1.47	1.39
9	A	804	CLA	C3D-C2D	2.98	1.47	1.39
9	B	802	CLA	C4D-CHA	2.98	1.48	1.38
9	B	816	CLA	C3D-C2D	2.98	1.47	1.39
9	B	832	CLA	C3D-C2D	2.98	1.47	1.39
9	B	840	CLA	C4D-CHA	2.98	1.48	1.38
9	A	836	CLA	C4D-CHA	2.98	1.48	1.38
9	A	809	CLA	C4D-CHA	2.98	1.48	1.38
9	B	805	CLA	C3D-C2D	2.98	1.47	1.39
9	B	804	CLA	MG-NC	2.98	2.13	2.06
9	B	816	CLA	C4D-CHA	2.98	1.48	1.38
9	A	821	CLA	C4D-CHA	2.98	1.48	1.38
9	A	826	CLA	C3D-C2D	2.98	1.47	1.39
9	B	819	CLA	C1B-NB	-2.98	1.33	1.37
9	B	806	CLA	C4D-CHA	2.98	1.48	1.38
9	B	836	CLA	C3D-C2D	2.98	1.47	1.39
9	B	838	CLA	C3D-C2D	2.98	1.47	1.39
9	B	808	CLA	C1B-C2B	2.98	1.50	1.43
9	B	834	CLA	C4D-CHA	2.98	1.48	1.38
9	B	819	CLA	C4D-CHA	2.98	1.48	1.38
9	A	813	CLA	MG-NC	2.97	2.13	2.06
9	B	823	CLA	C3D-C2D	2.97	1.47	1.39
9	B	809	CLA	MG-NC	2.97	2.13	2.06
9	B	833	CLA	MG-NC	2.97	2.13	2.06
9	A	836	CLA	C1B-NB	-2.97	1.34	1.37
9	B	827	CLA	MG-ND	-2.97	1.99	2.05
9	A	836	CLA	C3D-C2D	2.97	1.47	1.39
9	B	811	CLA	C3D-C2D	2.97	1.47	1.39
9	A	816	CLA	MG-NC	2.97	2.13	2.06
8	A	801	CL0	C4D-CHA	2.97	1.48	1.38
9	B	821	CLA	C3D-C2D	2.97	1.47	1.39
9	A	817	CLA	C3D-C2D	2.97	1.47	1.39
9	A	831	CLA	MG-ND	-2.97	1.99	2.05
9	A	842	CLA	C4D-CHA	2.97	1.48	1.38
9	A	841	CLA	C4D-CHA	2.97	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	821	CLA	C3D-C2D	2.97	1.47	1.39
9	A	802	CLA	C1D-ND	-2.97	1.34	1.37
9	A	830	CLA	C1D-ND	-2.97	1.34	1.37
9	B	812	CLA	C3D-C2D	2.96	1.47	1.39
9	A	809	CLA	MG-NC	2.96	2.13	2.06
9	B	840	CLA	C3D-C2D	2.96	1.47	1.39
9	A	831	CLA	C1D-ND	-2.96	1.34	1.37
9	A	829	CLA	MG-ND	-2.96	1.99	2.05
9	A	823	CLA	C4D-CHA	2.96	1.48	1.38
9	B	824	CLA	C1B-C2B	2.96	1.50	1.43
9	A	806	CLA	MG-NC	2.96	2.13	2.06
9	A	833	CLA	C3D-C2D	2.96	1.47	1.39
9	A	812	CLA	C4D-CHA	2.96	1.48	1.38
9	B	818	CLA	C4D-CHA	2.96	1.48	1.38
9	A	833	CLA	C4D-CHA	2.96	1.48	1.38
9	A	839	CLA	C3D-C2D	2.96	1.47	1.39
9	A	838	CLA	C4D-CHA	2.96	1.48	1.38
8	A	801	CL0	C3D-C2D	2.96	1.47	1.39
9	A	828	CLA	C3D-C2D	2.95	1.47	1.39
9	A	840	CLA	C3D-C2D	2.95	1.47	1.39
9	I	101	CLA	C4D-CHA	2.95	1.48	1.38
9	B	834	CLA	MG-NC	2.95	2.13	2.06
9	A	810	CLA	C4D-CHA	2.95	1.48	1.38
9	A	826	CLA	MG-NC	2.95	2.13	2.06
9	I	101	CLA	C1B-C2B	2.95	1.50	1.43
9	A	828	CLA	C4D-CHA	2.95	1.48	1.38
9	A	810	CLA	C3D-C2D	2.95	1.47	1.39
9	A	829	CLA	C4D-CHA	2.95	1.48	1.38
9	A	835	CLA	C3D-C2D	2.95	1.47	1.39
9	A	843	CLA	C3D-C2D	2.95	1.47	1.39
9	B	822	CLA	C3D-C2D	2.95	1.47	1.39
9	B	821	CLA	C4D-CHA	2.95	1.48	1.38
9	A	819	CLA	C3D-C2D	2.95	1.47	1.39
9	B	801	CLA	MG-ND	-2.95	1.99	2.05
9	B	828	CLA	MG-ND	-2.95	1.99	2.05
9	A	805	CLA	C3D-C2D	2.95	1.47	1.39
9	B	810	CLA	C1D-ND	-2.95	1.34	1.37
9	A	837	CLA	C1B-NB	-2.94	1.34	1.37
9	A	828	CLA	MG-ND	-2.94	2.00	2.05
9	B	807	CLA	C3D-C2D	2.94	1.47	1.39
9	B	807	CLA	C4D-CHA	2.94	1.48	1.38
9	B	828	CLA	C4D-CHA	2.94	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	805	CLA	C4D-CHA	2.94	1.48	1.38
9	A	820	CLA	C1D-ND	-2.94	1.34	1.37
9	B	821	CLA	C1D-ND	-2.94	1.34	1.37
9	B	835	CLA	C3D-C2D	2.94	1.47	1.39
9	B	801	CLA	C4D-CHA	2.94	1.48	1.38
9	A	825	CLA	C1B-NB	-2.94	1.34	1.37
9	A	814	CLA	C1D-ND	-2.94	1.34	1.37
9	B	809	CLA	C3D-C2D	2.94	1.47	1.39
9	A	818	CLA	C1D-ND	-2.94	1.34	1.37
9	B	826	CLA	C4D-CHA	2.94	1.48	1.38
9	B	801	CLA	C3D-C2D	2.94	1.47	1.39
9	B	806	CLA	C3D-C2D	2.94	1.47	1.39
9	B	814	CLA	C3D-C2D	2.94	1.47	1.39
9	B	830	CLA	C4D-CHA	2.93	1.48	1.38
9	B	814	CLA	C1D-ND	-2.93	1.34	1.37
9	A	814	CLA	C3D-C2D	2.93	1.47	1.39
9	A	822	CLA	C1D-ND	-2.93	1.34	1.37
9	A	838	CLA	C3D-C2D	2.93	1.47	1.39
9	A	815	CLA	C1D-ND	-2.93	1.34	1.37
9	B	806	CLA	C1B-NB	-2.93	1.34	1.37
9	A	837	CLA	C4D-CHA	2.93	1.48	1.38
9	A	827	CLA	C1B-NB	-2.93	1.34	1.37
9	B	831	CLA	C1D-ND	-2.92	1.34	1.37
9	A	803	CLA	C4D-CHA	2.92	1.48	1.38
9	A	805	CLA	C4D-CHA	2.92	1.48	1.38
9	A	814	CLA	C1B-NB	-2.92	1.34	1.37
9	A	828	CLA	C1B-C2B	2.92	1.50	1.43
9	A	818	CLA	C4D-CHA	2.92	1.48	1.38
9	A	813	CLA	C1B-NB	-2.92	1.34	1.37
9	B	817	CLA	C4D-CHA	2.92	1.48	1.38
9	A	806	CLA	C3D-C2D	2.92	1.46	1.39
9	A	837	CLA	C3D-C2D	2.92	1.46	1.39
9	A	825	CLA	C1D-ND	-2.92	1.34	1.37
9	B	837	CLA	C1D-ND	-2.92	1.34	1.37
9	A	808	CLA	C1D-ND	-2.92	1.34	1.37
9	A	843	CLA	C4D-CHA	2.91	1.48	1.38
9	A	820	CLA	MG-NC	2.91	2.13	2.06
9	A	833	CLA	C1D-ND	-2.91	1.34	1.37
9	B	818	CLA	C1B-NB	-2.91	1.34	1.37
9	B	833	CLA	C4D-CHA	2.91	1.48	1.38
9	A	827	CLA	C4D-CHA	2.91	1.48	1.38
9	A	807	CLA	C3D-C2D	2.91	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	802	CLA	MG-ND	-2.91	2.00	2.05
9	A	818	CLA	C3D-C2D	2.91	1.46	1.39
9	B	829	CLA	C4D-CHA	2.91	1.48	1.38
9	B	832	CLA	C1D-ND	-2.91	1.34	1.37
9	A	805	CLA	C1B-C2B	2.91	1.49	1.43
9	B	809	CLA	C1D-ND	-2.91	1.34	1.37
9	B	811	CLA	C1B-C2B	2.90	1.49	1.43
9	B	820	CLA	C1D-ND	-2.90	1.34	1.37
9	A	843	CLA	C1D-ND	-2.90	1.34	1.37
9	B	833	CLA	C1D-ND	-2.90	1.34	1.37
9	A	832	CLA	C4D-CHA	2.90	1.48	1.38
9	B	826	CLA	MG-ND	-2.90	2.00	2.05
9	A	811	CLA	C4D-CHA	2.90	1.48	1.38
9	A	826	CLA	C4D-CHA	2.90	1.48	1.38
9	A	831	CLA	C4D-CHA	2.90	1.48	1.38
9	A	806	CLA	C4D-CHA	2.90	1.48	1.38
9	B	827	CLA	MG-NC	2.90	2.13	2.06
9	A	823	CLA	C3D-C2D	2.90	1.46	1.39
9	B	821	CLA	C1B-C2B	2.90	1.49	1.43
9	B	831	CLA	C4D-CHA	2.90	1.48	1.38
9	A	824	CLA	C4D-CHA	2.90	1.48	1.38
9	A	807	CLA	C1D-ND	-2.90	1.34	1.37
9	B	834	CLA	C3D-C2D	2.90	1.46	1.39
9	B	825	CLA	C4D-CHA	2.89	1.48	1.38
9	B	835	CLA	C4D-CHA	2.89	1.48	1.38
9	B	815	CLA	C1D-ND	-2.89	1.34	1.37
9	B	815	CLA	C3D-C2D	2.89	1.46	1.39
9	A	825	CLA	C1B-C2B	2.89	1.49	1.43
9	A	839	CLA	C1D-ND	-2.89	1.34	1.37
9	B	839	CLA	C1D-ND	-2.89	1.34	1.37
9	B	832	CLA	C4D-CHA	2.89	1.48	1.38
9	A	808	CLA	MG-ND	-2.89	2.00	2.05
9	A	835	CLA	C4D-CHA	2.89	1.48	1.38
9	A	811	CLA	C3D-C2D	2.89	1.46	1.39
9	A	802	CLA	C4D-CHA	2.89	1.48	1.38
9	B	810	CLA	C4D-CHA	2.89	1.48	1.38
9	A	804	CLA	C1B-NB	-2.89	1.34	1.37
9	B	811	CLA	C4D-CHA	2.89	1.48	1.38
9	A	812	CLA	C1B-NB	-2.88	1.34	1.37
9	A	825	CLA	C4D-CHA	2.88	1.48	1.38
9	B	836	CLA	C1B-NB	-2.88	1.34	1.37
9	A	820	CLA	C3D-C2D	2.88	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	101	CLA	C3D-C2D	2.88	1.46	1.39
9	B	838	CLA	C1D-ND	-2.88	1.34	1.37
9	A	812	CLA	C1D-ND	-2.88	1.34	1.37
9	B	809	CLA	C4D-CHA	2.88	1.48	1.38
9	A	819	CLA	C4D-CHA	2.88	1.48	1.38
9	A	803	CLA	C1B-C2B	2.88	1.49	1.43
9	B	812	CLA	C1B-NB	-2.88	1.34	1.37
9	A	813	CLA	MG-ND	-2.87	2.00	2.05
9	B	824	CLA	C3D-C2D	2.87	1.46	1.39
9	A	815	CLA	C4D-CHA	2.87	1.48	1.38
9	K	101	CLA	OBD-CAD	2.87	1.28	1.23
9	A	821	CLA	MG-ND	-2.87	2.00	2.05
9	B	806	CLA	C1D-ND	-2.87	1.34	1.37
9	A	813	CLA	C1D-ND	-2.87	1.34	1.37
9	B	805	CLA	C1B-NB	-2.87	1.34	1.37
9	B	817	CLA	MG-ND	-2.87	2.00	2.05
9	B	803	CLA	C1B-C2B	2.87	1.49	1.43
9	B	819	CLA	C3D-C2D	2.87	1.46	1.39
9	A	830	CLA	MG-NC	2.86	2.13	2.06
9	B	818	CLA	C1B-C2B	2.86	1.49	1.43
9	A	820	CLA	C4D-CHA	2.86	1.48	1.38
9	A	818	CLA	MG-ND	-2.86	2.00	2.05
9	B	837	CLA	C4D-CHA	2.86	1.48	1.38
9	A	837	CLA	C1D-ND	-2.86	1.34	1.37
9	B	812	CLA	C1D-ND	-2.86	1.34	1.37
9	B	827	CLA	C1B-NB	-2.86	1.34	1.37
9	B	804	CLA	C4D-CHA	2.86	1.48	1.38
9	B	803	CLA	C1B-NB	-2.86	1.34	1.37
9	A	827	CLA	MG-ND	-2.86	2.00	2.05
9	A	817	CLA	C4D-CHA	2.86	1.48	1.38
9	B	819	CLA	C1D-ND	-2.86	1.34	1.37
9	A	814	CLA	MG-ND	-2.86	2.00	2.05
9	A	807	CLA	C4D-CHA	2.85	1.48	1.38
9	A	821	CLA	C1D-ND	-2.85	1.34	1.37
8	A	801	CL0	MG-NC	2.85	2.13	2.06
9	B	828	CLA	C3D-C2D	2.85	1.46	1.39
9	A	807	CLA	C1B-C2B	2.85	1.49	1.43
9	A	810	CLA	C1B-C2B	2.85	1.49	1.43
9	B	814	CLA	MG-ND	-2.85	2.00	2.05
9	B	827	CLA	C4D-CHA	2.84	1.48	1.38
9	B	825	CLA	MG-ND	-2.84	2.00	2.05
9	A	805	CLA	C1B-NB	-2.84	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	830	CLA	C4D-CHA	2.84	1.48	1.38
9	A	806	CLA	C1D-ND	-2.84	1.34	1.37
9	A	834	CLA	C1D-ND	-2.84	1.34	1.37
9	B	829	CLA	C1D-ND	-2.84	1.34	1.37
9	I	101	CLA	MG-ND	-2.84	2.00	2.05
9	A	822	CLA	C1B-NB	-2.84	1.34	1.37
9	B	839	CLA	MG-NC	2.84	2.13	2.06
9	B	825	CLA	C1B-NB	-2.84	1.34	1.37
9	A	816	CLA	C4D-CHA	2.83	1.48	1.38
9	A	832	CLA	C1D-ND	-2.83	1.34	1.37
9	B	831	CLA	MG-ND	-2.83	2.00	2.05
9	A	808	CLA	C3D-C2D	2.83	1.46	1.39
9	B	839	CLA	C3D-C2D	2.83	1.46	1.39
9	A	817	CLA	MG-ND	-2.83	2.00	2.05
9	B	824	CLA	MG-NC	2.83	2.13	2.06
9	A	832	CLA	C1B-C2B	2.83	1.49	1.43
9	A	825	CLA	MG-ND	-2.83	2.00	2.05
9	B	814	CLA	C4D-CHA	2.82	1.48	1.38
9	B	803	CLA	MG-NC	2.82	2.13	2.06
9	B	813	CLA	MG-ND	-2.82	2.00	2.05
9	B	829	CLA	MG-NC	2.82	2.13	2.06
9	A	841	CLA	C1B-C2B	2.82	1.49	1.43
9	B	836	CLA	MG-ND	-2.82	2.00	2.05
9	A	833	CLA	C1B-NB	-2.82	1.34	1.37
9	B	803	CLA	C4D-CHA	2.82	1.48	1.38
9	B	838	CLA	C4D-CHA	2.82	1.48	1.38
9	A	823	CLA	C1B-C2B	2.81	1.49	1.43
9	A	820	CLA	C1B-C2B	2.81	1.49	1.43
9	B	820	CLA	MG-ND	-2.81	2.00	2.05
9	A	819	CLA	C1B-C2B	2.81	1.49	1.43
9	B	811	CLA	C1D-ND	-2.81	1.34	1.37
9	B	822	CLA	C1D-ND	-2.81	1.34	1.37
9	B	836	CLA	C1B-C2B	2.81	1.49	1.43
9	A	819	CLA	C1D-ND	-2.81	1.34	1.37
9	A	810	CLA	C1D-ND	-2.81	1.34	1.37
9	A	824	CLA	C1D-ND	-2.81	1.34	1.37
9	A	844	CLA	C1B-C2B	2.81	1.49	1.43
9	B	810	CLA	C1B-C2B	2.80	1.49	1.43
9	B	813	CLA	C1B-NB	-2.80	1.34	1.37
9	A	834	CLA	C1B-C2B	2.80	1.49	1.43
9	B	808	CLA	MG-ND	-2.80	2.00	2.05
9	B	805	CLA	C1D-ND	-2.80	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	836	CLA	C1D-ND	-2.80	1.34	1.37
9	K	101	CLA	C1B-C2B	2.80	1.49	1.43
9	A	844	CLA	C1D-ND	-2.80	1.34	1.37
9	B	826	CLA	C3D-C2D	2.80	1.46	1.39
9	A	842	CLA	C1B-C2B	2.80	1.49	1.43
9	A	842	CLA	C1D-ND	-2.80	1.34	1.37
9	B	809	CLA	MG-ND	-2.80	2.00	2.05
9	B	817	CLA	C1D-ND	-2.80	1.34	1.37
9	B	834	CLA	C1D-ND	-2.80	1.34	1.37
9	A	832	CLA	MG-ND	-2.79	2.00	2.05
9	B	822	CLA	C1B-NB	-2.79	1.34	1.37
9	A	812	CLA	C1B-C2B	2.79	1.49	1.43
9	B	829	CLA	MG-ND	-2.79	2.00	2.05
9	A	838	CLA	C1D-ND	-2.79	1.34	1.37
9	B	826	CLA	C1B-NB	-2.79	1.34	1.37
9	B	826	CLA	C1B-C2B	2.79	1.49	1.43
9	B	837	CLA	MG-ND	-2.79	2.00	2.05
9	A	823	CLA	C1D-ND	-2.79	1.34	1.37
9	A	834	CLA	MG-ND	-2.79	2.00	2.05
9	B	815	CLA	MG-ND	-2.79	2.00	2.05
9	B	824	CLA	C4D-CHA	2.78	1.47	1.38
9	B	826	CLA	C1D-ND	-2.78	1.34	1.37
9	A	826	CLA	C1B-NB	-2.78	1.34	1.37
9	B	809	CLA	C1B-C2B	2.78	1.49	1.43
9	A	815	CLA	MG-ND	-2.78	2.00	2.05
9	A	811	CLA	C1D-ND	-2.78	1.34	1.37
9	A	835	CLA	C1D-ND	-2.78	1.34	1.37
9	I	101	CLA	C1D-ND	-2.78	1.34	1.37
9	A	815	CLA	C1B-C2B	2.78	1.49	1.43
9	A	804	CLA	C1D-ND	-2.78	1.34	1.37
9	B	813	CLA	C3D-C2D	2.78	1.46	1.39
9	B	837	CLA	C1B-NB	-2.78	1.34	1.37
9	B	824	CLA	C1B-NB	-2.78	1.34	1.37
9	B	819	CLA	MG-ND	-2.78	2.00	2.05
9	B	829	CLA	C3D-C2D	2.78	1.46	1.39
9	A	839	CLA	C4D-CHA	2.78	1.47	1.38
9	A	810	CLA	C1B-NB	-2.78	1.34	1.37
9	A	827	CLA	C3D-C2D	2.78	1.46	1.39
9	B	833	CLA	MG-ND	-2.78	2.00	2.05
9	B	839	CLA	C4D-CHA	2.77	1.47	1.38
9	A	806	CLA	C1B-NB	-2.77	1.34	1.37
9	B	833	CLA	C1B-NB	-2.77	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	823	CLA	C1D-ND	-2.77	1.34	1.37
9	A	838	CLA	C1B-NB	-2.77	1.34	1.37
9	B	829	CLA	C1C-NC	-2.77	1.33	1.37
9	A	806	CLA	C1B-C2B	2.77	1.49	1.43
9	A	838	CLA	C3B-C4B	2.77	1.50	1.42
9	B	807	CLA	C1D-ND	-2.77	1.34	1.37
9	B	830	CLA	C3D-C2D	2.77	1.46	1.39
9	A	811	CLA	C1B-C2B	2.77	1.49	1.43
9	A	840	CLA	C1B-C2B	2.77	1.49	1.43
9	A	811	CLA	MG-ND	-2.76	2.00	2.05
9	B	810	CLA	MG-ND	-2.76	2.00	2.05
9	B	807	CLA	C1B-C2B	2.76	1.49	1.43
9	A	816	CLA	C1D-ND	-2.76	1.34	1.37
9	A	808	CLA	C1B-C2B	2.76	1.49	1.43
9	A	830	CLA	MG-ND	-2.75	2.00	2.05
9	B	806	CLA	MG-ND	-2.75	2.00	2.05
9	B	838	CLA	MG-ND	-2.75	2.00	2.05
9	A	813	CLA	C3D-C2D	2.75	1.46	1.39
9	A	828	CLA	C4B-NB	-2.75	1.34	1.37
9	B	801	CLA	MG-NC	2.75	2.12	2.06
9	A	809	CLA	MG-ND	-2.75	2.00	2.05
9	B	813	CLA	C1B-C2B	2.75	1.49	1.43
9	A	822	CLA	MG-ND	-2.75	2.00	2.05
9	A	843	CLA	C1B-C2B	2.75	1.49	1.43
9	B	813	CLA	C1D-ND	-2.75	1.34	1.37
9	A	829	CLA	C1B-C2B	2.75	1.49	1.43
9	B	835	CLA	C1B-C2B	2.74	1.49	1.43
9	B	838	CLA	C1B-C2B	2.74	1.49	1.43
9	A	820	CLA	MG-ND	-2.74	2.00	2.05
9	B	840	CLA	C1D-ND	-2.74	1.34	1.37
9	B	816	CLA	MG-ND	-2.74	2.00	2.05
9	A	836	CLA	C1B-C2B	2.74	1.49	1.43
9	B	835	CLA	C1D-ND	-2.74	1.34	1.37
9	A	835	CLA	MG-ND	-2.74	2.00	2.05
9	A	817	CLA	C1B-NB	-2.74	1.34	1.37
9	B	820	CLA	C1B-NB	-2.74	1.34	1.37
9	A	805	CLA	MG-NC	2.74	2.12	2.06
9	A	805	CLA	C1D-ND	-2.73	1.34	1.37
9	A	816	CLA	C1B-NB	-2.73	1.34	1.37
9	B	820	CLA	C1B-C2B	2.73	1.49	1.43
9	B	821	CLA	C1B-NB	-2.73	1.34	1.37
9	A	809	CLA	C1B-C2B	2.73	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	806	CLA	MG-ND	-2.73	2.00	2.05
9	A	835	CLA	C1B-NB	-2.73	1.34	1.37
9	A	844	CLA	MG-ND	-2.73	2.00	2.05
9	B	805	CLA	C1B-C2B	2.73	1.49	1.43
9	A	809	CLA	C1D-ND	-2.73	1.34	1.37
9	B	816	CLA	C1B-C2B	2.73	1.49	1.43
9	A	822	CLA	C1B-C2B	2.73	1.49	1.43
9	A	807	CLA	MG-ND	-2.73	2.00	2.05
9	B	832	CLA	C1B-C2B	2.73	1.49	1.43
9	B	807	CLA	C1B-NB	-2.72	1.34	1.37
9	A	840	CLA	C1B-NB	-2.72	1.34	1.37
9	A	835	CLA	C1B-C2B	2.72	1.49	1.43
9	B	837	CLA	C1B-C2B	2.72	1.49	1.43
9	B	821	CLA	MG-ND	-2.72	2.00	2.05
9	B	824	CLA	MG-ND	-2.72	2.00	2.05
9	B	836	CLA	C1C-NC	-2.72	1.33	1.37
9	B	828	CLA	C1C-NC	-2.72	1.33	1.37
9	B	840	CLA	MG-ND	-2.72	2.00	2.05
9	B	810	CLA	C1B-NB	-2.72	1.34	1.37
9	B	834	CLA	MG-ND	-2.71	2.00	2.05
9	B	818	CLA	MG-ND	-2.71	2.00	2.05
9	A	817	CLA	C1B-C2B	2.71	1.49	1.43
9	A	826	CLA	MG-ND	-2.71	2.00	2.05
9	A	841	CLA	C1B-NB	-2.71	1.34	1.37
9	A	808	CLA	C1B-NB	-2.71	1.34	1.37
9	A	813	CLA	C1B-C2B	2.71	1.49	1.43
9	B	832	CLA	MG-ND	-2.71	2.00	2.05
9	A	815	CLA	C1B-NB	-2.71	1.34	1.37
9	A	840	CLA	C1D-ND	-2.71	1.34	1.37
9	B	807	CLA	MG-ND	-2.71	2.00	2.05
9	A	837	CLA	C1B-C2B	2.71	1.49	1.43
9	A	802	CLA	C1B-NB	-2.70	1.34	1.37
9	B	838	CLA	C1B-NB	-2.70	1.34	1.37
9	A	837	CLA	MG-ND	-2.70	2.00	2.05
9	A	828	CLA	C1B-NB	-2.70	1.34	1.37
9	B	831	CLA	C1B-NB	-2.70	1.34	1.37
9	A	823	CLA	MG-ND	-2.70	2.00	2.05
9	A	843	CLA	MG-ND	-2.70	2.00	2.05
9	A	816	CLA	C1B-C2B	2.70	1.49	1.43
9	B	816	CLA	C1D-ND	-2.70	1.34	1.37
9	A	803	CLA	C1D-ND	-2.70	1.34	1.37
9	B	813	CLA	C4B-NB	-2.69	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	833	CLA	MG-ND	-2.69	2.00	2.05
9	A	839	CLA	MG-ND	-2.69	2.00	2.05
9	A	810	CLA	MG-ND	-2.69	2.00	2.05
9	A	804	CLA	MG-ND	-2.69	2.00	2.05
9	B	822	CLA	C1B-C2B	2.69	1.49	1.43
9	A	831	CLA	C3D-C2D	2.69	1.46	1.39
9	B	836	CLA	C4B-NB	-2.69	1.34	1.37
9	A	809	CLA	C1B-NB	-2.69	1.34	1.37
9	B	808	CLA	C3D-C2D	2.69	1.46	1.39
9	B	833	CLA	C1B-C2B	2.68	1.49	1.43
9	A	840	CLA	MG-ND	-2.68	2.00	2.05
9	B	816	CLA	C1B-NB	-2.68	1.34	1.37
9	A	830	CLA	C1B-NB	-2.68	1.34	1.37
9	A	819	CLA	MG-ND	-2.68	2.00	2.05
9	A	824	CLA	C1B-C2B	2.68	1.49	1.43
9	A	836	CLA	MG-ND	-2.68	2.00	2.05
9	B	835	CLA	MG-ND	-2.68	2.00	2.05
9	B	823	CLA	MG-ND	-2.68	2.00	2.05
9	B	828	CLA	C3B-C4B	2.67	1.50	1.42
9	K	101	CLA	C1D-ND	-2.67	1.34	1.37
9	A	812	CLA	MG-ND	-2.67	2.00	2.05
9	B	836	CLA	C1D-ND	-2.67	1.34	1.37
9	A	819	CLA	C1B-NB	-2.67	1.34	1.37
9	B	822	CLA	MG-ND	-2.66	2.00	2.05
9	B	808	CLA	C4D-CHA	2.66	1.47	1.38
9	A	824	CLA	MG-ND	-2.66	2.00	2.05
9	A	807	CLA	C1B-NB	-2.66	1.34	1.37
9	B	832	CLA	C1B-NB	-2.66	1.34	1.37
9	A	842	CLA	C1B-NB	-2.66	1.34	1.37
9	A	830	CLA	C1B-C2B	2.66	1.49	1.43
9	A	820	CLA	C1B-NB	-2.66	1.34	1.37
9	A	803	CLA	MG-ND	-2.66	2.00	2.05
9	I	101	CLA	C1B-NB	-2.66	1.34	1.37
9	B	815	CLA	C1B-C2B	2.66	1.49	1.43
9	A	833	CLA	C1B-C2B	2.66	1.49	1.43
9	A	824	CLA	C1B-NB	-2.66	1.34	1.37
9	B	833	CLA	C1C-NC	-2.65	1.33	1.37
9	A	839	CLA	C1B-C2B	2.65	1.49	1.43
9	B	820	CLA	C3D-C2D	2.65	1.46	1.39
9	B	814	CLA	C1B-NB	-2.64	1.34	1.37
9	B	839	CLA	C1B-C2B	2.64	1.49	1.43
9	B	812	CLA	MG-ND	-2.64	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	804	CLA	C3D-C2D	2.64	1.46	1.39
9	B	811	CLA	MG-ND	-2.63	2.00	2.05
9	B	829	CLA	C1B-C2B	2.63	1.49	1.43
9	B	815	CLA	C1B-NB	-2.63	1.34	1.37
9	B	839	CLA	C1B-NB	-2.63	1.34	1.37
9	A	842	CLA	MG-ND	-2.63	2.00	2.05
9	B	803	CLA	C1C-NC	-2.63	1.33	1.37
9	A	825	CLA	C3D-C2D	2.63	1.46	1.39
9	B	805	CLA	MG-ND	-2.63	2.00	2.05
9	A	803	CLA	C1B-NB	-2.63	1.34	1.37
9	A	834	CLA	C1B-NB	-2.63	1.34	1.37
9	B	834	CLA	C1B-C2B	2.62	1.49	1.43
9	A	816	CLA	MG-ND	-2.62	2.00	2.05
9	A	841	CLA	C1D-ND	-2.62	1.34	1.37
9	B	827	CLA	C1C-NC	-2.61	1.33	1.37
9	A	804	CLA	C1B-C2B	2.61	1.49	1.43
9	A	832	CLA	C1B-NB	-2.61	1.34	1.37
9	B	825	CLA	C1B-C2B	2.60	1.49	1.43
9	B	840	CLA	C1C-NC	-2.60	1.33	1.37
9	A	823	CLA	C1B-NB	-2.60	1.34	1.37
9	B	839	CLA	MG-ND	-2.59	2.00	2.05
9	A	809	CLA	C1C-NC	-2.59	1.33	1.37
9	A	826	CLA	C1B-C2B	2.59	1.49	1.43
9	B	806	CLA	C1B-C2B	2.59	1.49	1.43
9	B	835	CLA	C1B-NB	-2.59	1.34	1.37
9	I	101	CLA	C4B-NB	-2.59	1.34	1.37
9	A	813	CLA	C1C-NC	-2.59	1.33	1.37
9	A	838	CLA	MG-ND	-2.59	2.00	2.05
9	A	839	CLA	C1B-NB	-2.58	1.34	1.37
9	B	808	CLA	C4C-C3C	2.58	1.49	1.45
9	B	812	CLA	C1B-C2B	2.58	1.49	1.43
9	B	825	CLA	C4B-NB	-2.58	1.34	1.37
9	B	831	CLA	C1B-C2B	2.58	1.49	1.43
9	B	826	CLA	C1C-NC	-2.57	1.33	1.37
9	A	811	CLA	C1B-NB	-2.57	1.34	1.37
9	A	841	CLA	MG-ND	-2.56	2.00	2.05
9	A	843	CLA	C1B-NB	-2.56	1.34	1.37
9	A	805	CLA	MG-ND	-2.56	2.00	2.05
9	K	101	CLA	MG-ND	-2.56	2.00	2.05
9	A	837	CLA	C4B-NB	-2.56	1.34	1.37
9	A	830	CLA	C1C-NC	-2.56	1.33	1.37
9	A	838	CLA	C1C-NC	-2.56	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	814	CLA	C1B-C2B	2.56	1.49	1.43
9	A	844	CLA	C1B-NB	-2.56	1.34	1.37
9	K	101	CLA	C1D-C2D	2.56	1.50	1.45
9	B	813	CLA	C1C-NC	-2.56	1.33	1.37
9	B	804	CLA	C1B-C2B	2.56	1.49	1.43
9	K	101	CLA	C1B-NB	-2.55	1.34	1.37
9	A	827	CLA	C1B-C2B	2.55	1.49	1.43
9	A	809	CLA	C4B-NB	-2.54	1.34	1.37
9	B	821	CLA	C4B-NB	-2.54	1.34	1.37
9	A	835	CLA	C4B-NB	-2.54	1.34	1.37
9	B	819	CLA	C1B-C2B	2.53	1.49	1.43
9	B	811	CLA	C1B-NB	-2.53	1.34	1.37
9	A	829	CLA	C1C-NC	-2.52	1.33	1.37
9	A	812	CLA	C4B-NB	-2.52	1.34	1.37
9	B	838	CLA	C4B-NB	-2.52	1.34	1.37
9	B	812	CLA	C3B-C4B	2.51	1.50	1.42
9	B	811	CLA	C1C-NC	-2.51	1.33	1.37
9	B	832	CLA	C4B-NB	-2.51	1.34	1.37
9	A	841	CLA	C1D-C2D	2.51	1.50	1.45
9	B	803	CLA	C4B-NB	-2.51	1.34	1.37
9	B	831	CLA	C4B-NB	-2.51	1.34	1.37
9	B	834	CLA	C4B-NB	-2.50	1.34	1.37
9	B	823	CLA	C1B-C2B	2.50	1.49	1.43
9	A	816	CLA	C1D-C2D	2.50	1.50	1.45
9	B	812	CLA	C1C-NC	-2.50	1.34	1.37
9	B	802	CLA	C1B-NB	-2.50	1.34	1.37
9	B	818	CLA	C4B-NB	-2.50	1.34	1.37
9	A	823	CLA	C1D-C2D	2.50	1.50	1.45
9	B	808	CLA	C1C-NC	-2.49	1.34	1.37
9	B	825	CLA	C1C-NC	-2.49	1.34	1.37
9	B	827	CLA	C1B-C2B	2.49	1.49	1.43
9	A	814	CLA	C4B-NB	-2.49	1.34	1.37
9	A	824	CLA	C1D-C2D	2.49	1.50	1.45
8	A	801	CL0	C4B-NB	-2.49	1.34	1.37
9	A	813	CLA	C4B-NB	-2.48	1.34	1.37
9	A	829	CLA	C4B-NB	-2.48	1.34	1.37
9	B	809	CLA	C1B-NB	-2.48	1.34	1.37
9	B	817	CLA	C4B-NB	-2.48	1.34	1.37
9	B	840	CLA	C1B-NB	-2.48	1.34	1.37
9	A	840	CLA	C1D-C2D	2.47	1.50	1.45
9	A	838	CLA	C1B-C2B	2.47	1.48	1.43
9	A	806	CLA	C4B-NB	-2.47	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	839	CLA	C1C-NC	-2.47	1.34	1.37
9	B	829	CLA	C4B-NB	-2.47	1.34	1.37
9	B	808	CLA	C1B-NB	-2.47	1.34	1.37
9	B	839	CLA	C1D-C2D	2.46	1.50	1.45
9	A	836	CLA	C4B-NB	-2.45	1.34	1.37
9	A	828	CLA	C1C-NC	-2.45	1.34	1.37
9	B	826	CLA	C4B-NB	-2.45	1.34	1.37
9	I	101	CLA	C1C-NC	-2.45	1.34	1.37
9	A	805	CLA	C1C-NC	-2.45	1.34	1.37
9	A	835	CLA	C1D-C2D	2.45	1.50	1.45
9	A	831	CLA	C1B-C2B	2.45	1.48	1.43
9	A	802	CLA	C1B-C2B	2.45	1.48	1.43
9	A	811	CLA	C1D-C2D	2.44	1.50	1.45
9	A	826	CLA	C1D-C2D	2.44	1.50	1.45
9	B	836	CLA	C4C-C3C	2.43	1.49	1.45
9	A	842	CLA	C1C-NC	-2.43	1.34	1.37
9	B	809	CLA	C1C-NC	-2.43	1.34	1.37
9	A	811	CLA	C1C-NC	-2.43	1.34	1.37
9	A	802	CLA	C4B-NB	-2.43	1.34	1.37
9	B	826	CLA	C4C-C3C	2.43	1.49	1.45
9	A	835	CLA	C1C-NC	-2.43	1.34	1.37
9	A	836	CLA	C1D-C2D	2.43	1.50	1.45
9	A	825	CLA	C4B-NB	-2.42	1.34	1.37
8	A	801	CL0	C1C-NC	-2.42	1.34	1.37
9	B	804	CLA	C1C-NC	-2.42	1.34	1.37
9	B	823	CLA	C1D-C2D	2.42	1.50	1.45
9	B	814	CLA	C4B-NB	-2.42	1.34	1.37
9	B	815	CLA	C4B-NB	-2.42	1.34	1.37
9	B	816	CLA	C4B-NB	-2.42	1.34	1.37
9	A	819	CLA	C4B-NB	-2.41	1.34	1.37
9	A	809	CLA	C1D-C2D	2.41	1.50	1.45
9	B	829	CLA	C4C-C3C	2.41	1.49	1.45
9	A	802	CLA	C1C-NC	-2.41	1.34	1.37
9	B	802	CLA	C4B-NB	-2.41	1.34	1.37
9	A	803	CLA	C1D-C2D	2.41	1.50	1.45
9	B	807	CLA	C4B-NB	-2.41	1.34	1.37
9	B	814	CLA	C1C-NC	-2.41	1.34	1.37
9	B	818	CLA	C1C-NC	-2.41	1.34	1.37
9	A	844	CLA	C1D-C2D	2.41	1.50	1.45
9	B	821	CLA	C4C-C3C	2.41	1.49	1.45
9	A	834	CLA	C1C-NC	-2.41	1.34	1.37
9	A	832	CLA	C1D-C2D	2.41	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	827	CLA	C1C-C2C	2.40	1.49	1.44
9	A	808	CLA	C1C-NC	-2.40	1.34	1.37
9	B	828	CLA	C1B-C2B	2.40	1.48	1.43
9	B	817	CLA	C1D-C2D	2.40	1.50	1.45
9	A	840	CLA	C4B-NB	-2.40	1.34	1.37
9	A	806	CLA	C1D-C2D	2.40	1.50	1.45
9	A	826	CLA	C4B-NB	-2.40	1.34	1.37
9	B	807	CLA	C1C-NC	-2.40	1.34	1.37
9	A	802	CLA	C1D-C2D	2.40	1.50	1.45
9	B	831	CLA	C1D-C2D	2.40	1.50	1.45
9	A	805	CLA	C4B-NB	-2.39	1.34	1.37
9	A	824	CLA	C4B-NB	-2.39	1.34	1.37
9	B	834	CLA	C1C-NC	-2.39	1.34	1.37
9	B	832	CLA	C1D-C2D	2.39	1.50	1.45
9	A	837	CLA	C1D-C2D	2.39	1.50	1.45
9	B	835	CLA	C1D-C2D	2.39	1.50	1.45
9	B	837	CLA	C4B-NB	-2.39	1.34	1.37
9	A	807	CLA	C1D-C2D	2.39	1.50	1.45
9	B	812	CLA	C4C-C3C	2.39	1.49	1.45
9	A	804	CLA	C1D-C2D	2.39	1.50	1.45
9	A	833	CLA	C1D-C2D	2.39	1.50	1.45
9	A	814	CLA	C1C-NC	-2.39	1.34	1.37
9	B	830	CLA	C1D-C2D	2.38	1.50	1.45
9	A	809	CLA	C4C-C3C	2.38	1.49	1.45
9	A	821	CLA	C1D-C2D	2.38	1.50	1.45
9	B	831	CLA	C1C-NC	-2.38	1.34	1.37
9	B	823	CLA	C4B-NB	-2.38	1.34	1.37
9	B	821	CLA	C1C-NC	-2.38	1.34	1.37
9	A	826	CLA	C1C-NC	-2.38	1.34	1.37
9	A	844	CLA	C1C-NC	-2.38	1.34	1.37
9	B	827	CLA	C4B-NB	-2.38	1.34	1.37
9	A	834	CLA	C1D-C2D	2.38	1.50	1.45
9	A	841	CLA	C1C-NC	-2.38	1.34	1.37
9	A	815	CLA	C4B-NB	-2.38	1.34	1.37
9	A	823	CLA	C1C-NC	-2.37	1.34	1.37
9	B	837	CLA	C1C-NC	-2.37	1.34	1.37
9	A	819	CLA	C1C-NC	-2.37	1.34	1.37
9	A	812	CLA	C1D-C2D	2.37	1.50	1.45
9	A	837	CLA	C1C-NC	-2.37	1.34	1.37
9	B	837	CLA	C1D-C2D	2.37	1.50	1.45
9	B	807	CLA	C1D-C2D	2.36	1.50	1.45
9	B	824	CLA	C1C-NC	-2.36	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	807	CLA	C1C-NC	-2.36	1.34	1.37
9	B	808	CLA	C4B-NB	-2.36	1.34	1.37
9	A	839	CLA	C1D-C2D	2.36	1.50	1.45
9	A	842	CLA	C1D-C2D	2.36	1.50	1.45
9	B	838	CLA	C1D-C2D	2.36	1.50	1.45
9	A	807	CLA	C4B-NB	-2.36	1.34	1.37
9	B	834	CLA	C1D-C2D	2.36	1.50	1.45
9	B	819	CLA	C4B-NB	-2.35	1.34	1.37
9	B	819	CLA	C1C-NC	-2.35	1.34	1.37
9	A	835	CLA	C4C-C3C	2.35	1.49	1.45
9	A	810	CLA	C1D-C2D	2.35	1.50	1.45
9	B	816	CLA	C1D-C2D	2.35	1.50	1.45
9	A	802	CLA	C4C-C3C	2.35	1.49	1.45
9	B	811	CLA	C1D-C2D	2.35	1.50	1.45
9	B	806	CLA	C1C-NC	-2.35	1.34	1.37
9	B	830	CLA	C4C-C3C	2.35	1.49	1.45
9	B	824	CLA	C4B-NB	-2.35	1.34	1.37
9	B	805	CLA	C4B-NB	-2.35	1.34	1.37
9	A	843	CLA	C1C-NC	-2.35	1.34	1.37
9	B	820	CLA	C1C-NC	-2.35	1.34	1.37
9	B	829	CLA	C1D-C2D	2.35	1.50	1.45
9	A	812	CLA	C4C-C3C	2.35	1.49	1.45
9	B	809	CLA	C4B-NB	-2.35	1.34	1.37
9	A	808	CLA	C4B-NB	-2.35	1.34	1.37
9	A	812	CLA	C1C-NC	-2.34	1.34	1.37
9	B	806	CLA	C1D-C2D	2.34	1.50	1.45
9	K	101	CLA	C4C-C3C	2.34	1.49	1.45
9	B	832	CLA	C1C-NC	-2.34	1.34	1.37
9	A	821	CLA	C4C-C3C	2.34	1.49	1.45
9	A	836	CLA	C4C-C3C	2.34	1.49	1.45
9	B	840	CLA	C1D-C2D	2.34	1.50	1.45
9	A	818	CLA	C1C-NC	-2.34	1.34	1.37
9	A	843	CLA	C1D-C2D	2.34	1.50	1.45
9	A	817	CLA	C1D-C2D	2.34	1.50	1.45
9	B	817	CLA	C1C-NC	-2.34	1.34	1.37
9	A	820	CLA	C1C-NC	-2.34	1.34	1.37
9	I	101	CLA	C4C-C3C	2.34	1.49	1.45
9	B	816	CLA	C1C-NC	-2.34	1.34	1.37
9	A	834	CLA	C4C-C3C	2.33	1.49	1.45
9	A	806	CLA	C1C-NC	-2.33	1.34	1.37
9	B	805	CLA	C1D-C2D	2.33	1.50	1.45
9	A	822	CLA	C4B-NB	-2.33	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	840	CLA	C4B-NB	-2.33	1.34	1.37
9	A	810	CLA	C4B-NB	-2.33	1.34	1.37
9	A	816	CLA	C1C-NC	-2.33	1.34	1.37
9	A	817	CLA	C4B-NB	-2.33	1.34	1.37
9	B	810	CLA	C4B-NB	-2.33	1.34	1.37
9	A	811	CLA	C4C-C3C	2.33	1.49	1.45
9	A	822	CLA	C1C-NC	-2.32	1.34	1.37
9	A	824	CLA	C4C-C3C	2.32	1.49	1.45
9	B	838	CLA	C1C-NC	-2.32	1.34	1.37
9	A	819	CLA	C1D-C2D	2.32	1.49	1.45
9	B	802	CLA	C1C-NC	-2.32	1.34	1.37
9	A	833	CLA	C4B-NB	-2.32	1.34	1.37
9	A	824	CLA	C1C-NC	-2.31	1.34	1.37
9	B	801	CLA	C1C-NC	-2.31	1.34	1.37
9	B	835	CLA	C4C-C3C	2.31	1.49	1.45
9	B	821	CLA	C1D-C2D	2.31	1.49	1.45
9	A	817	CLA	C1C-NC	-2.31	1.34	1.37
9	A	820	CLA	C1D-C2D	2.31	1.49	1.45
9	B	822	CLA	C1D-C2D	2.31	1.49	1.45
9	A	804	CLA	C1C-NC	-2.31	1.34	1.37
9	A	811	CLA	C4B-NB	-2.31	1.34	1.37
9	B	815	CLA	C1C-NC	-2.31	1.34	1.37
9	B	806	CLA	C4C-C3C	2.31	1.49	1.45
9	A	820	CLA	C4B-NB	-2.31	1.34	1.37
9	A	815	CLA	C1C-NC	-2.31	1.34	1.37
9	B	817	CLA	C4C-C3C	2.31	1.49	1.45
9	A	832	CLA	C1C-NC	-2.31	1.34	1.37
9	B	801	CLA	C3B-C4B	2.31	1.49	1.42
9	B	835	CLA	C1C-NC	-2.30	1.34	1.37
9	A	844	CLA	C4B-NB	-2.30	1.34	1.37
9	A	818	CLA	C1D-C2D	2.30	1.49	1.45
9	B	839	CLA	C1C-NC	-2.30	1.34	1.37
9	A	814	CLA	C4C-C3C	2.30	1.48	1.45
9	A	804	CLA	C4B-NB	-2.30	1.34	1.37
9	B	806	CLA	C3B-C4B	2.30	1.49	1.42
9	B	805	CLA	C1C-NC	-2.30	1.34	1.37
9	B	833	CLA	C4B-NB	-2.30	1.34	1.37
9	A	839	CLA	C4C-C3C	2.30	1.48	1.45
9	B	813	CLA	C1D-C2D	2.30	1.49	1.45
9	A	833	CLA	C1C-NC	-2.29	1.34	1.37
9	I	101	CLA	C1D-C2D	2.29	1.49	1.45
9	A	814	CLA	C1D-C2D	2.29	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	801	CLA	C4B-NB	-2.29	1.34	1.37
9	A	805	CLA	C1D-C2D	2.29	1.49	1.45
9	A	821	CLA	C1C-NC	-2.29	1.34	1.37
9	B	833	CLA	C1D-C2D	2.29	1.49	1.45
9	A	810	CLA	C1C-NC	-2.29	1.34	1.37
9	B	832	CLA	C4C-C3C	2.29	1.48	1.45
9	A	827	CLA	C3B-C4B	2.28	1.49	1.42
9	B	817	CLA	C1B-C2B	2.28	1.48	1.43
9	B	825	CLA	C4C-C3C	2.28	1.48	1.45
9	A	830	CLA	C1D-C2D	2.28	1.49	1.45
9	B	830	CLA	C1B-C2B	2.28	1.48	1.43
9	B	839	CLA	C4B-NB	-2.28	1.34	1.37
9	A	843	CLA	C4B-NB	-2.28	1.34	1.37
9	A	803	CLA	C1C-NC	-2.28	1.34	1.37
9	A	832	CLA	C4C-C3C	2.27	1.48	1.45
9	B	826	CLA	C1D-C2D	2.27	1.49	1.45
9	B	802	CLA	C1C-C2C	2.27	1.49	1.44
9	A	836	CLA	C1C-NC	-2.27	1.34	1.37
9	A	818	CLA	C4B-NB	-2.27	1.34	1.37
9	B	816	CLA	C4C-C3C	2.27	1.48	1.45
9	A	821	CLA	C3B-C4B	2.27	1.49	1.42
9	A	827	CLA	C4B-NB	-2.27	1.34	1.37
9	B	823	CLA	C4C-C3C	2.27	1.48	1.45
9	B	820	CLA	C4B-NB	-2.27	1.34	1.37
9	A	815	CLA	C1D-C2D	2.27	1.49	1.45
9	A	839	CLA	C3B-C4B	2.26	1.49	1.42
9	B	815	CLA	C1D-C2D	2.26	1.49	1.45
9	B	815	CLA	C1A-CHA	2.26	1.52	1.43
9	A	843	CLA	C4C-C3C	2.26	1.48	1.45
9	A	840	CLA	C1C-NC	-2.26	1.34	1.37
9	B	831	CLA	C4C-C3C	2.26	1.48	1.45
9	A	823	CLA	C4C-C3C	2.26	1.48	1.45
9	A	825	CLA	C1C-NC	-2.26	1.34	1.37
9	B	810	CLA	C1C-NC	-2.26	1.34	1.37
9	K	101	CLA	C1C-NC	-2.26	1.34	1.37
9	A	825	CLA	C4C-C3C	2.26	1.48	1.45
9	A	840	CLA	C4C-C3C	2.26	1.48	1.45
9	A	804	CLA	C4C-C3C	2.26	1.48	1.45
9	B	823	CLA	C3B-C4B	2.26	1.49	1.42
9	A	842	CLA	C4B-NB	-2.25	1.34	1.37
9	A	803	CLA	C4B-NB	-2.25	1.34	1.37
9	B	834	CLA	C4C-C3C	2.25	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	833	CLA	C4C-C3C	2.25	1.48	1.45
9	B	822	CLA	C1C-NC	-2.25	1.34	1.37
9	A	828	CLA	C4C-C3C	2.25	1.48	1.45
9	A	844	CLA	C4C-C3C	2.24	1.48	1.45
9	A	832	CLA	C4B-NB	-2.24	1.34	1.37
9	A	804	CLA	C1A-CHA	2.24	1.52	1.43
9	B	823	CLA	C1C-NC	-2.24	1.34	1.37
9	B	810	CLA	C1D-C2D	2.24	1.49	1.45
9	B	812	CLA	C1D-C2D	2.24	1.49	1.45
9	A	816	CLA	C4B-NB	-2.24	1.34	1.37
9	A	841	CLA	C4C-C3C	2.24	1.48	1.45
9	B	819	CLA	C1D-C2D	2.24	1.49	1.45
9	A	823	CLA	C4B-NB	-2.24	1.34	1.37
9	B	809	CLA	C1D-C2D	2.23	1.49	1.45
9	B	825	CLA	C1D-C2D	2.23	1.49	1.45
9	B	822	CLA	C4B-NB	-2.23	1.34	1.37
9	A	825	CLA	C1A-CHA	2.23	1.52	1.43
9	B	836	CLA	C1D-C2D	2.23	1.49	1.45
9	A	838	CLA	C4C-C3C	2.23	1.48	1.45
9	A	818	CLA	C4C-C3C	2.23	1.48	1.45
9	A	831	CLA	C1C-NC	-2.23	1.34	1.37
9	B	838	CLA	C4C-C3C	2.22	1.48	1.45
9	B	819	CLA	C4C-C3C	2.22	1.48	1.45
9	A	804	CLA	C3B-C4B	2.22	1.49	1.42
9	A	822	CLA	C1A-CHA	2.22	1.52	1.43
9	B	814	CLA	C1D-C2D	2.22	1.49	1.45
9	A	830	CLA	C4B-NB	-2.22	1.34	1.37
9	A	818	CLA	C1B-C2B	2.22	1.48	1.43
9	B	830	CLA	C1C-NC	-2.22	1.34	1.37
9	A	803	CLA	C4C-C3C	2.22	1.48	1.45
9	A	829	CLA	C4C-C3C	2.21	1.48	1.45
9	B	801	CLA	C1A-CHA	2.21	1.52	1.43
9	A	831	CLA	C4C-C3C	2.21	1.48	1.45
9	A	815	CLA	C4C-C3C	2.21	1.48	1.45
9	B	840	CLA	C4C-C3C	2.21	1.48	1.45
9	A	807	CLA	C4C-C3C	2.21	1.48	1.45
9	B	811	CLA	C4C-C3C	2.20	1.48	1.45
9	A	834	CLA	C4B-NB	-2.20	1.35	1.37
9	B	828	CLA	C1A-CHA	2.20	1.52	1.43
9	B	820	CLA	C4C-C3C	2.20	1.48	1.45
9	K	101	CLA	C4B-NB	-2.19	1.35	1.37
9	B	828	CLA	C4C-C3C	2.19	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	819	CLA	C4C-C3C	2.19	1.48	1.45
9	A	839	CLA	C4B-NB	-2.19	1.35	1.37
9	A	821	CLA	C4B-NB	-2.19	1.35	1.37
9	A	822	CLA	C4C-C3C	2.19	1.48	1.45
9	A	838	CLA	C1D-C2D	2.18	1.49	1.45
9	B	811	CLA	C4B-NB	-2.18	1.35	1.37
9	A	834	CLA	C1A-CHA	2.18	1.52	1.43
9	A	814	CLA	C1A-CHA	2.18	1.52	1.43
9	B	837	CLA	C4C-C3C	2.17	1.48	1.45
9	B	824	CLA	C1C-C2C	2.17	1.48	1.44
9	A	810	CLA	C1A-CHA	2.17	1.52	1.43
9	A	842	CLA	C1A-CHA	2.16	1.52	1.43
9	B	807	CLA	C4C-C3C	2.16	1.48	1.45
9	B	820	CLA	C1A-CHA	2.16	1.52	1.43
9	A	813	CLA	C1D-C2D	2.16	1.49	1.45
9	A	827	CLA	C1C-NC	-2.16	1.34	1.37
9	B	822	CLA	C1A-CHA	2.16	1.52	1.43
9	B	809	CLA	C4C-C3C	2.16	1.48	1.45
9	B	833	CLA	C4C-C3C	2.16	1.48	1.45
9	A	828	CLA	C1A-CHA	2.15	1.52	1.43
9	A	829	CLA	C1A-CHA	2.15	1.52	1.43
9	B	801	CLA	C1B-C2B	2.15	1.48	1.43
9	A	822	CLA	C1D-C2D	2.15	1.49	1.45
9	B	806	CLA	C1A-CHA	2.15	1.51	1.43
9	B	813	CLA	C4C-C3C	2.15	1.48	1.45
9	A	842	CLA	C4C-C3C	2.14	1.48	1.45
9	B	805	CLA	C1A-CHA	2.14	1.51	1.43
9	A	813	CLA	C4C-C3C	2.14	1.48	1.45
9	B	822	CLA	C4C-C3C	2.14	1.48	1.45
9	A	812	CLA	C1A-CHA	2.14	1.51	1.43
9	A	841	CLA	C4B-NB	-2.14	1.35	1.37
9	B	806	CLA	C4B-NB	-2.14	1.35	1.37
9	A	836	CLA	C1A-CHA	2.14	1.51	1.43
9	B	830	CLA	C4B-NB	-2.14	1.35	1.37
9	A	814	CLA	C3B-C4B	2.14	1.49	1.42
9	A	808	CLA	C1A-CHA	2.13	1.51	1.43
9	B	819	CLA	C1A-CHA	2.13	1.51	1.43
9	A	818	CLA	C3B-C4B	2.13	1.49	1.42
9	B	840	CLA	C1A-CHA	2.13	1.51	1.43
9	A	841	CLA	C3B-C4B	2.13	1.48	1.42
9	A	840	CLA	C1A-CHA	2.13	1.51	1.43
9	B	835	CLA	C4B-NB	-2.12	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	816	CLA	C4C-C3C	2.12	1.48	1.45
9	A	841	CLA	C1A-CHA	2.12	1.51	1.43
9	B	818	CLA	C4C-C3C	2.12	1.48	1.45
9	A	810	CLA	C4C-C3C	2.12	1.48	1.45
9	A	825	CLA	C1D-C2D	2.12	1.49	1.45
9	B	823	CLA	C1A-CHA	2.11	1.51	1.43
9	A	826	CLA	C4C-C3C	2.11	1.48	1.45
9	B	816	CLA	C1A-CHA	2.11	1.51	1.43
9	A	831	CLA	C4B-NB	-2.11	1.35	1.37
9	B	834	CLA	C1A-CHA	2.11	1.51	1.43
9	B	818	CLA	C1A-CHA	2.10	1.51	1.43
9	A	813	CLA	C1A-CHA	2.10	1.51	1.43
9	B	804	CLA	C3B-C4B	2.10	1.48	1.42
9	B	835	CLA	C3B-C4B	2.10	1.48	1.42
9	B	818	CLA	C1D-C2D	2.10	1.49	1.45
9	A	844	CLA	C1A-CHA	2.09	1.51	1.43
9	B	802	CLA	C1A-CHA	2.09	1.51	1.43
9	B	820	CLA	C1D-C2D	2.09	1.49	1.45
9	A	828	CLA	C1D-C2D	2.09	1.49	1.45
9	B	836	CLA	C1A-CHA	2.09	1.51	1.43
9	A	826	CLA	C3B-C4B	2.09	1.48	1.42
9	B	830	CLA	C3B-C4B	2.09	1.48	1.42
9	B	833	CLA	C1A-CHA	2.08	1.51	1.43
8	A	801	CL0	C3B-C4B	2.08	1.48	1.42
9	B	807	CLA	C1A-CHA	2.08	1.51	1.43
9	A	819	CLA	C1A-CHA	2.08	1.51	1.43
9	A	830	CLA	C4C-C3C	2.08	1.48	1.45
9	B	804	CLA	C4B-NB	-2.08	1.35	1.37
9	B	839	CLA	C3B-C4B	2.08	1.48	1.42
9	B	824	CLA	C3B-C4B	2.08	1.48	1.42
9	B	808	CLA	C1D-C2D	2.08	1.49	1.45
9	B	812	CLA	C1A-CHA	2.07	1.51	1.43
9	A	838	CLA	C1A-CHA	2.07	1.51	1.43
8	A	801	CL0	C1B-C2B	2.07	1.48	1.43
9	A	843	CLA	C1A-CHA	2.07	1.51	1.43
9	A	807	CLA	C1A-CHA	2.07	1.51	1.43
9	B	821	CLA	C1A-CHA	2.07	1.51	1.43
9	B	827	CLA	C1A-CHA	2.07	1.51	1.43
9	A	843	CLA	C3B-C4B	2.06	1.48	1.42
9	B	804	CLA	C1A-CHA	2.06	1.51	1.43
9	A	822	CLA	C3B-C4B	2.06	1.48	1.42
9	A	817	CLA	C4C-C3C	2.06	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	809	CLA	C1A-CHA	2.06	1.51	1.43
9	B	824	CLA	C1A-CHA	2.06	1.51	1.43
9	A	833	CLA	C1A-CHA	2.06	1.51	1.43
9	B	819	CLA	C3B-C4B	2.06	1.48	1.42
9	B	818	CLA	C3B-C4B	2.06	1.48	1.42
9	B	805	CLA	C3B-C4B	2.05	1.48	1.42
9	K	101	CLA	C1A-CHA	2.05	1.51	1.43
9	A	837	CLA	C4C-C3C	2.05	1.48	1.45
9	B	830	CLA	C1A-CHA	2.05	1.51	1.43
9	A	835	CLA	C1A-CHA	2.05	1.51	1.43
9	K	101	CLA	C3B-C4B	2.05	1.48	1.42
9	B	810	CLA	C3B-C4B	2.05	1.48	1.42
9	A	824	CLA	C1A-CHA	2.05	1.51	1.43
9	B	832	CLA	C1A-CHA	2.04	1.51	1.43
8	A	801	CL0	C1D-C2D	2.04	1.49	1.45
9	A	812	CLA	C3B-C4B	2.04	1.48	1.42
9	A	811	CLA	C1A-CHA	2.04	1.51	1.43
9	B	813	CLA	C1A-CHA	2.04	1.51	1.43
9	B	822	CLA	C3B-C4B	2.04	1.48	1.42
9	I	101	CLA	C1A-CHA	2.04	1.51	1.43
9	B	833	CLA	C3B-C4B	2.04	1.48	1.42
9	A	840	CLA	C3B-C4B	2.03	1.48	1.42
9	A	823	CLA	C3B-C4B	2.03	1.48	1.42
9	B	829	CLA	C1A-CHA	2.03	1.51	1.43
9	A	831	CLA	C1A-CHA	2.03	1.51	1.43
9	A	831	CLA	C1D-C2D	2.03	1.49	1.45
9	A	823	CLA	C1A-CHA	2.03	1.51	1.43
9	A	831	CLA	C3B-C4B	2.03	1.48	1.42
9	B	815	CLA	C4C-C3C	2.03	1.48	1.45
8	A	801	CL0	C4C-C3C	2.03	1.48	1.45
9	A	815	CLA	C1A-CHA	2.03	1.51	1.43
9	B	823	CLA	C1C-C2C	2.02	1.48	1.44
9	A	824	CLA	C3B-C4B	2.02	1.48	1.42
9	B	835	CLA	C1A-CHA	2.02	1.51	1.43
9	B	825	CLA	C3B-C4B	2.02	1.48	1.42
9	B	831	CLA	C3B-C4B	2.02	1.48	1.42
9	A	826	CLA	C1A-CHA	2.02	1.51	1.43
9	A	832	CLA	C1A-CHA	2.02	1.51	1.43
9	B	826	CLA	C1A-CHA	2.02	1.51	1.43
9	B	834	CLA	C3B-C4B	2.02	1.48	1.42
9	B	811	CLA	C1A-CHA	2.02	1.51	1.43
9	A	808	CLA	C3B-C4B	2.02	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	832	CLA	C3B-C4B	2.01	1.48	1.42
9	A	803	CLA	C1A-CHA	2.01	1.51	1.43
9	B	839	CLA	C1A-CHA	2.01	1.51	1.43
9	A	811	CLA	C3B-C4B	2.01	1.48	1.42
9	A	816	CLA	C3B-C4B	2.01	1.48	1.42
9	A	830	CLA	C3B-C4B	2.01	1.48	1.42
9	A	837	CLA	C1A-CHA	2.01	1.51	1.43
9	B	837	CLA	C1A-CHA	2.01	1.51	1.43
9	B	823	CLA	C3B-C2B	2.01	1.47	1.41
9	B	805	CLA	C4C-C3C	2.00	1.48	1.45
9	A	830	CLA	C1A-CHA	2.00	1.51	1.43

All (2509) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	847	BCR	C15-C16-C17	22.88	170.33	123.52
12	A	851	BCR	C20-C21-C22	22.83	159.29	127.28
12	B	844	BCR	C20-C21-C22	22.51	158.84	127.28
12	B	845	BCR	C20-C21-C22	22.29	158.54	127.28
12	B	845	BCR	C16-C17-C18	21.77	157.80	127.28
12	A	849	BCR	C20-C21-C22	21.59	157.56	127.28
12	B	846	BCR	C16-C17-C18	21.52	157.46	127.28
12	A	851	BCR	C16-C17-C18	21.51	157.44	127.28
12	M	101	BCR	C20-C21-C22	21.48	157.41	127.28
12	F	201	BCR	C16-C17-C18	21.42	157.32	127.28
12	B	847	BCR	C15-C16-C17	21.02	166.53	123.52
12	M	101	BCR	C16-C17-C18	20.85	156.52	127.28
12	B	847	BCR	C20-C21-C22	20.85	156.51	127.28
12	B	842	BCR	C16-C17-C18	20.83	156.48	127.28
12	F	201	BCR	C20-C21-C22	20.79	156.43	127.28
12	B	846	BCR	C20-C21-C22	20.75	156.38	127.28
12	M	101	BCR	C15-C16-C17	20.70	165.88	123.52
12	A	847	BCR	C20-C21-C22	20.69	156.29	127.28
12	A	849	BCR	C16-C17-C18	20.68	156.28	127.28
12	B	843	BCR	C16-C17-C18	20.64	156.22	127.28
12	B	844	BCR	C15-C16-C17	20.61	165.68	123.52
12	A	850	BCR	C20-C21-C22	20.59	156.16	127.28
12	A	848	BCR	C15-C16-C17	20.57	165.60	123.52
12	A	849	BCR	C15-C16-C17	20.54	165.55	123.52
12	A	850	BCR	C15-C16-C17	20.41	165.29	123.52
12	B	847	BCR	C16-C17-C18	20.27	155.70	127.28
12	A	848	BCR	C20-C21-C22	19.74	154.96	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	848	BCR	C16-C17-C18	19.65	154.84	127.28
12	B	843	BCR	C20-C21-C22	19.62	154.80	127.28
12	B	843	BCR	C15-C16-C17	19.55	163.52	123.52
12	A	851	BCR	C15-C16-C17	19.52	163.46	123.52
12	B	842	BCR	C20-C21-C22	19.52	154.65	127.28
12	B	842	BCR	C15-C16-C17	19.47	163.36	123.52
12	B	844	BCR	C16-C17-C18	19.28	154.32	127.28
12	B	845	BCR	C10-C11-C12	19.25	178.96	123.20
12	F	201	BCR	C15-C16-C17	19.17	162.74	123.52
12	A	850	BCR	C16-C17-C18	18.97	153.88	127.28
12	B	845	BCR	C15-C16-C17	18.94	162.26	123.52
12	B	847	BCR	C10-C11-C12	18.85	177.82	123.20
12	B	843	BCR	C10-C11-C12	18.84	177.78	123.20
12	A	847	BCR	C10-C11-C12	18.78	177.60	123.20
12	M	101	BCR	C10-C11-C12	18.76	177.57	123.20
12	A	848	BCR	C10-C11-C12	18.74	177.51	123.20
12	A	849	BCR	C10-C11-C12	18.72	177.45	123.20
12	B	846	BCR	C10-C11-C12	18.71	177.42	123.20
12	B	846	BCR	C15-C16-C17	18.62	161.62	123.52
12	A	847	BCR	C16-C17-C18	18.33	152.98	127.28
12	B	842	BCR	C10-C11-C12	18.16	175.81	123.20
12	B	844	BCR	C10-C11-C12	17.87	174.97	123.20
12	A	850	BCR	C10-C11-C12	17.60	174.19	123.20
12	A	851	BCR	C10-C11-C12	17.54	174.03	123.20
12	F	201	BCR	C10-C11-C12	17.43	173.72	123.20
12	F	201	BCR	C16-C15-C14	15.29	154.81	123.52
12	A	851	BCR	C11-C10-C9	15.24	148.65	127.28
12	B	844	BCR	C11-C10-C9	14.77	147.99	127.28
12	A	848	BCR	C21-C20-C19	14.72	165.85	123.20
12	A	850	BCR	C21-C20-C19	14.23	164.44	123.20
12	B	842	BCR	C21-C20-C19	14.16	164.24	123.20
12	B	843	BCR	C21-C20-C19	14.16	164.22	123.20
12	B	847	BCR	C21-C20-C19	14.11	164.10	123.20
12	A	847	BCR	C21-C20-C19	14.09	164.03	123.20
12	B	846	BCR	C11-C10-C9	13.83	146.67	127.28
12	B	844	BCR	C21-C20-C19	13.75	163.05	123.20
12	B	846	BCR	C21-C20-C19	13.73	162.98	123.20
12	B	846	BCR	C16-C15-C14	13.73	151.61	123.52
12	F	201	BCR	C21-C20-C19	13.70	162.91	123.20
12	B	845	BCR	C16-C15-C14	13.64	151.44	123.52
12	M	101	BCR	C21-C20-C19	13.63	162.69	123.20
12	A	849	BCR	C21-C20-C19	13.60	162.61	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	842	BCR	C16-C15-C14	13.39	150.92	123.52
12	A	848	BCR	C11-C10-C9	13.20	145.79	127.28
12	A	849	BCR	C11-C10-C9	13.18	145.76	127.28
12	A	851	BCR	C21-C20-C19	13.13	161.25	123.20
12	M	101	BCR	C11-C10-C9	13.09	145.63	127.28
12	B	843	BCR	C16-C15-C14	13.07	150.26	123.52
12	A	850	BCR	C11-C10-C9	12.89	145.35	127.28
12	B	845	BCR	C11-C10-C9	12.86	145.31	127.28
12	B	845	BCR	C21-C20-C19	12.79	160.26	123.20
12	A	851	BCR	C16-C15-C14	12.75	149.61	123.52
12	B	843	BCR	C11-C10-C9	12.70	145.09	127.28
12	M	101	BCR	C16-C15-C14	12.70	149.50	123.52
12	B	847	BCR	C11-C10-C9	12.67	145.04	127.28
12	B	842	BCR	C11-C10-C9	12.65	145.02	127.28
12	A	848	BCR	C16-C15-C14	12.62	149.35	123.52
12	A	849	BCR	C16-C15-C14	12.53	149.15	123.52
12	A	847	BCR	C11-C10-C9	12.40	144.66	127.28
12	A	850	BCR	C16-C15-C14	12.26	148.61	123.52
12	B	844	BCR	C16-C15-C14	12.25	148.58	123.52
12	A	851	BCR	C11-C12-C13	12.03	159.35	126.36
12	B	847	BCR	C16-C15-C14	12.01	148.09	123.52
12	B	844	BCR	C11-C12-C13	11.85	158.86	126.36
12	F	201	BCR	C11-C10-C9	11.74	143.74	127.28
12	B	845	BCR	C11-C12-C13	11.55	158.02	126.36
12	A	847	BCR	C11-C12-C13	11.21	157.10	126.36
12	B	846	BCR	C11-C12-C13	11.17	157.00	126.36
12	M	101	BCR	C11-C12-C13	11.00	156.51	126.36
12	B	842	BCR	C11-C12-C13	10.99	156.50	126.36
12	A	847	BCR	C16-C15-C14	10.94	145.91	123.52
12	A	850	BCR	C11-C12-C13	10.92	156.29	126.36
12	B	843	BCR	C11-C12-C13	10.84	156.08	126.36
12	B	847	BCR	C11-C12-C13	10.67	155.62	126.36
12	F	201	BCR	C11-C12-C13	10.49	155.11	126.36
12	A	848	BCR	C11-C12-C13	10.46	155.04	126.36
12	A	849	BCR	C11-C12-C13	10.39	154.85	126.36
9	B	830	CLA	CMD-C2D-C1D	8.75	140.14	124.73
9	B	839	CLA	CMD-C2D-C1D	8.74	140.12	124.73
9	A	825	CLA	CMD-C2D-C1D	8.74	140.11	124.73
9	A	811	CLA	CMD-C2D-C1D	8.67	139.99	124.73
9	B	813	CLA	CMD-C2D-C1D	8.67	139.99	124.73
9	A	813	CLA	CMD-C2D-C1D	8.62	139.91	124.73
9	K	101	CLA	CMD-C2D-C1D	8.61	139.90	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	826	CLA	CMD-C2D-C1D	8.61	139.89	124.73
9	B	820	CLA	CMD-C2D-C1D	8.59	139.86	124.73
9	A	823	CLA	CMD-C2D-C1D	8.49	139.68	124.73
9	B	808	CLA	CMD-C2D-C1D	8.46	139.62	124.73
9	B	829	CLA	CMD-C2D-C1D	8.44	139.60	124.73
9	B	834	CLA	CMD-C2D-C1D	8.36	139.45	124.73
12	B	845	BCR	C20-C19-C18	8.32	149.18	126.36
9	B	835	CLA	CMD-C2D-C1D	8.31	139.37	124.73
9	B	806	CLA	CMD-C2D-C1D	8.31	139.36	124.73
9	A	831	CLA	CMD-C2D-C1D	8.30	139.35	124.73
9	A	840	CLA	CMD-C2D-C1D	8.28	139.31	124.73
9	B	819	CLA	CMD-C2D-C1D	8.27	139.30	124.73
9	B	815	CLA	CMD-C2D-C1D	8.27	139.29	124.73
9	B	807	CLA	CMD-C2D-C1D	8.27	139.29	124.73
9	A	806	CLA	CMD-C2D-C1D	8.26	139.27	124.73
9	A	835	CLA	CMD-C2D-C1D	8.26	139.27	124.73
9	A	807	CLA	CMD-C2D-C1D	8.25	139.26	124.73
9	A	826	CLA	CMD-C2D-C1D	8.25	139.25	124.73
9	A	816	CLA	CMD-C2D-C1D	8.24	139.24	124.73
9	A	827	CLA	CMD-C2D-C1D	8.24	139.24	124.73
9	A	818	CLA	CMD-C2D-C1D	8.24	139.24	124.73
9	B	832	CLA	CMD-C2D-C1D	8.24	139.24	124.73
9	B	822	CLA	CMD-C2D-C1D	8.24	139.23	124.73
9	A	820	CLA	CMD-C2D-C1D	8.23	139.23	124.73
9	A	804	CLA	CMD-C2D-C1D	8.22	139.21	124.73
9	A	836	CLA	CMD-C2D-C1D	8.22	139.21	124.73
9	A	841	CLA	CMD-C2D-C1D	8.22	139.21	124.73
9	A	843	CLA	CMD-C2D-C1D	8.22	139.21	124.73
9	B	838	CLA	CMD-C2D-C1D	8.22	139.21	124.73
9	A	810	CLA	CMD-C2D-C1D	8.22	139.20	124.73
9	B	816	CLA	CMD-C2D-C1D	8.21	139.19	124.73
9	B	823	CLA	CMD-C2D-C1D	8.21	139.19	124.73
9	B	817	CLA	CMD-C2D-C1D	8.21	139.19	124.73
9	A	824	CLA	CMD-C2D-C1D	8.21	139.19	124.73
9	A	837	CLA	CMD-C2D-C1D	8.20	139.17	124.73
9	B	811	CLA	CMD-C2D-C1D	8.20	139.16	124.73
9	B	840	CLA	CMD-C2D-C1D	8.18	139.13	124.73
9	A	821	CLA	CMD-C2D-C1D	8.17	139.11	124.73
9	A	805	CLA	CMD-C2D-C1D	8.16	139.10	124.73
9	B	805	CLA	CMD-C2D-C1D	8.15	139.08	124.73
9	A	832	CLA	CMD-C2D-C1D	8.15	139.08	124.73
9	A	834	CLA	CMD-C2D-C1D	8.14	139.07	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	814	CLA	CMD-C2D-C1D	8.14	139.06	124.73
9	A	809	CLA	CMD-C2D-C1D	8.14	139.06	124.73
9	B	831	CLA	CMD-C2D-C1D	8.13	139.05	124.73
9	A	833	CLA	CMD-C2D-C1D	8.13	139.05	124.73
9	A	803	CLA	CMD-C2D-C1D	8.13	139.04	124.73
9	A	839	CLA	CMD-C2D-C1D	8.12	139.02	124.73
9	B	821	CLA	CMD-C2D-C1D	8.11	139.00	124.73
9	A	842	CLA	CMD-C2D-C1D	8.10	138.99	124.73
9	A	844	CLA	CMD-C2D-C1D	8.09	138.97	124.73
9	A	819	CLA	CMD-C2D-C1D	8.07	138.94	124.73
9	B	809	CLA	CMD-C2D-C1D	8.07	138.94	124.73
9	B	836	CLA	CMD-C2D-C1D	8.06	138.93	124.73
9	A	802	CLA	CMD-C2D-C1D	8.02	138.85	124.73
9	A	838	CLA	CMD-C2D-C1D	8.01	138.83	124.73
9	A	817	CLA	CMD-C2D-C1D	8.00	138.81	124.73
12	A	851	BCR	C20-C19-C18	7.99	148.28	126.36
9	B	812	CLA	CMD-C2D-C1D	7.94	138.72	124.73
9	A	808	CLA	CMD-C2D-C1D	7.93	138.69	124.73
9	B	837	CLA	CMD-C2D-C1D	7.92	138.68	124.73
9	B	833	CLA	CMD-C2D-C1D	7.92	138.68	124.73
9	A	815	CLA	CMD-C2D-C1D	7.90	138.64	124.73
9	A	812	CLA	CMD-C2D-C1D	7.90	138.63	124.73
12	F	201	BCR	C20-C19-C18	7.88	147.98	126.36
9	I	101	CLA	CMD-C2D-C1D	7.88	138.60	124.73
9	B	825	CLA	CMD-C2D-C1D	7.83	138.52	124.73
9	B	814	CLA	CMD-C2D-C1D	7.83	138.51	124.73
9	A	830	CLA	CMD-C2D-C1D	7.81	138.48	124.73
9	B	810	CLA	CMD-C2D-C1D	7.64	138.18	124.73
9	A	828	CLA	CMD-C2D-C1D	7.63	138.16	124.73
9	A	822	CLA	CMD-C2D-C1D	7.62	138.16	124.73
12	A	849	BCR	C20-C19-C18	7.61	147.24	126.36
8	A	801	CL0	CMD-C2D-C1D	7.60	138.11	124.73
12	M	101	BCR	C20-C19-C18	7.50	146.92	126.36
9	B	818	CLA	CMD-C2D-C1D	7.40	137.76	124.73
12	B	846	BCR	C20-C19-C18	7.28	146.33	126.36
12	B	842	BCR	C20-C19-C18	7.16	146.01	126.36
9	B	827	CLA	CMD-C2D-C1D	7.16	137.33	124.73
12	B	844	BCR	C20-C19-C18	7.15	145.97	126.36
12	B	846	BCR	C24-C23-C22	-7.14	115.67	126.23
9	B	828	CLA	CMD-C2D-C1D	7.05	137.15	124.73
12	B	847	BCR	C20-C19-C18	7.04	145.67	126.36
12	B	843	BCR	C20-C19-C18	7.03	145.65	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	824	CLA	CMD-C2D-C1D	6.96	136.99	124.73
12	A	847	BCR	C20-C19-C18	6.91	145.32	126.36
9	B	840	CLA	C2C-C1C-NC	6.73	117.05	109.98
9	A	834	CLA	O2D-CGD-CBD	6.71	122.97	111.23
9	A	829	CLA	CMD-C2D-C1D	6.70	136.53	124.73
9	B	813	CLA	O2D-CGD-CBD	6.69	122.92	111.23
9	B	803	CLA	CMD-C2D-C1D	6.68	136.49	124.73
12	A	850	BCR	C20-C19-C18	6.66	144.63	126.36
9	B	801	CLA	CMD-C2D-C1D	6.63	136.40	124.73
12	A	848	BCR	C20-C19-C18	6.62	144.53	126.36
9	B	829	CLA	O2D-CGD-CBD	6.55	122.68	111.23
9	A	828	CLA	C2C-C1C-NC	6.48	116.79	109.98
9	B	806	CLA	C2C-C1C-NC	6.44	116.75	109.98
9	A	825	CLA	C2C-C1C-NC	6.43	116.73	109.98
9	I	101	CLA	C2C-C1C-NC	6.41	116.71	109.98
9	B	824	CLA	C4A-NA-C1A	6.40	109.60	106.68
9	B	828	CLA	C2C-C1C-NC	6.39	116.69	109.98
9	A	830	CLA	O2D-CGD-CBD	6.36	122.35	111.23
9	A	841	CLA	C2C-C1C-NC	6.33	116.63	109.98
9	B	829	CLA	C2C-C1C-NC	6.29	116.59	109.98
9	B	821	CLA	C2C-C1C-NC	6.28	116.57	109.98
9	B	802	CLA	C2C-C1C-NC	6.26	116.55	109.98
9	B	812	CLA	C2C-C1C-NC	6.19	116.49	109.98
9	B	830	CLA	C2C-C1C-NC	6.19	116.49	109.98
9	A	834	CLA	C2C-C1C-NC	6.19	116.48	109.98
9	A	823	CLA	C2C-C1C-NC	6.19	116.48	109.98
9	A	829	CLA	C2C-C1C-NC	6.18	116.47	109.98
9	B	807	CLA	C2C-C1C-NC	6.16	116.45	109.98
9	A	812	CLA	C2C-C1C-NC	6.16	116.45	109.98
9	A	844	CLA	C2C-C1C-NC	6.16	116.45	109.98
9	B	818	CLA	C2C-C1C-NC	6.16	116.45	109.98
9	B	814	CLA	C2C-C1C-NC	6.14	116.43	109.98
9	A	832	CLA	C2C-C1C-NC	6.14	116.43	109.98
12	M	101	BCR	C7-C8-C9	-6.14	117.16	126.23
9	A	810	CLA	C2C-C1C-NC	6.14	116.43	109.98
9	B	837	CLA	C2C-C1C-NC	6.13	116.42	109.98
9	A	837	CLA	C2C-C1C-NC	6.13	116.42	109.98
9	A	809	CLA	C2C-C1C-NC	6.12	116.41	109.98
9	B	840	CLA	C4A-NA-C1A	6.12	109.47	106.68
9	B	820	CLA	C2C-C1C-NC	6.11	116.39	109.98
9	A	815	CLA	C2C-C1C-NC	6.09	116.38	109.98
9	B	809	CLA	C4A-NA-C1A	6.09	109.46	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	803	CLA	C2C-C1C-NC	6.08	116.37	109.98
9	B	836	CLA	C2C-C1C-NC	6.08	116.37	109.98
9	A	814	CLA	C2C-C1C-NC	6.06	116.35	109.98
9	B	814	CLA	C4A-NA-C1A	6.06	109.44	106.68
9	B	816	CLA	C2C-C1C-NC	6.06	116.34	109.98
9	A	842	CLA	C2C-C1C-NC	6.05	116.34	109.98
9	A	820	CLA	C2C-C1C-NC	6.05	116.34	109.98
9	B	811	CLA	C2C-C1C-NC	6.05	116.33	109.98
9	A	836	CLA	C2C-C1C-NC	6.05	116.33	109.98
9	A	828	CLA	C4A-NA-C1A	6.05	109.44	106.68
9	A	805	CLA	C2C-C1C-NC	6.04	116.33	109.98
9	A	838	CLA	C2C-C1C-NC	6.03	116.31	109.98
9	A	839	CLA	C2C-C1C-NC	6.02	116.31	109.98
9	A	808	CLA	O2D-CGD-CBD	6.02	121.76	111.23
9	B	808	CLA	C2D-C1D-ND	6.02	116.08	110.13
9	A	824	CLA	C2C-C1C-NC	6.01	116.30	109.98
9	A	831	CLA	O2D-CGD-CBD	6.01	121.74	111.23
9	B	817	CLA	C2C-C1C-NC	6.01	116.29	109.98
9	A	808	CLA	C2C-C1C-NC	6.01	116.29	109.98
9	A	822	CLA	C2C-C1C-NC	6.00	116.28	109.98
12	B	843	BCR	C24-C23-C22	-5.99	117.37	126.23
9	A	833	CLA	C2C-C1C-NC	5.98	116.27	109.98
9	B	824	CLA	C2D-C1D-ND	5.98	116.05	110.13
9	A	838	CLA	O2D-CGD-CBD	5.98	121.68	111.23
9	A	840	CLA	C2C-C1C-NC	5.97	116.25	109.98
9	A	843	CLA	C2C-C1C-NC	5.97	116.25	109.98
9	B	838	CLA	C2C-C1C-NC	5.96	116.24	109.98
9	B	832	CLA	C2C-C1C-NC	5.96	116.24	109.98
9	A	817	CLA	C2C-C1C-NC	5.93	116.21	109.98
9	B	835	CLA	C2C-C1C-NC	5.93	116.21	109.98
9	K	101	CLA	C2C-C1C-NC	5.93	116.21	109.98
9	B	802	CLA	CMD-C2D-C1D	5.92	135.16	124.73
9	A	816	CLA	C2C-C1C-NC	5.92	116.20	109.98
9	A	835	CLA	C2C-C1C-NC	5.92	116.20	109.98
9	A	819	CLA	C2C-C1C-NC	5.92	116.20	109.98
9	A	806	CLA	C2C-C1C-NC	5.92	116.19	109.98
9	A	817	CLA	O2D-CGD-CBD	5.90	121.55	111.23
9	A	825	CLA	O2D-CGD-CBD	5.90	121.55	111.23
9	A	807	CLA	C2C-C1C-NC	5.90	116.17	109.98
9	B	826	CLA	C2C-C1C-NC	5.89	116.17	109.98
9	B	824	CLA	O2D-CGD-CBD	5.87	121.49	111.23
9	A	825	CLA	C4A-NA-C1A	5.87	109.36	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	808	CLA	C2C-C1C-NC	5.87	116.14	109.98
9	A	811	CLA	C2C-C1C-NC	5.86	116.14	109.98
9	A	818	CLA	C2C-C1C-NC	5.86	116.14	109.98
9	B	822	CLA	C2C-C1C-NC	5.86	116.14	109.98
9	B	827	CLA	C2C-C1C-NC	5.85	116.13	109.98
9	B	840	CLA	C1C-C2C-C3C	-5.85	100.83	106.98
9	B	806	CLA	O2A-CGA-O1A	-5.84	109.03	123.63
9	B	813	CLA	C2C-C1C-NC	5.83	116.10	109.98
9	B	831	CLA	C2C-C1C-NC	5.82	116.10	109.98
9	A	827	CLA	C3D-C2D-C1D	-5.82	97.88	105.83
9	B	834	CLA	C2C-C1C-NC	5.82	116.10	109.98
9	B	825	CLA	C3B-C2B-C1B	-5.81	100.32	107.17
9	B	801	CLA	C2D-C1D-ND	5.81	115.88	110.13
9	B	805	CLA	C2C-C1C-NC	5.81	116.08	109.98
9	A	831	CLA	C2C-C1C-NC	5.80	116.08	109.98
9	B	808	CLA	C3D-C2D-C1D	-5.79	97.93	105.83
9	B	819	CLA	C2C-C1C-NC	5.78	116.05	109.98
9	A	804	CLA	C2C-C1C-NC	5.78	116.05	109.98
9	A	816	CLA	O2D-CGD-CBD	5.78	121.33	111.23
9	B	815	CLA	C3B-C2B-C1B	-5.77	100.36	107.17
9	B	809	CLA	C2C-C1C-NC	5.77	116.04	109.98
9	A	820	CLA	C1C-C2C-C3C	-5.77	100.92	106.98
9	B	824	CLA	C1C-C2C-C3C	-5.76	100.92	106.98
9	A	827	CLA	C2D-C1D-ND	5.74	115.81	110.13
9	B	810	CLA	C2C-C1C-NC	5.74	116.01	109.98
9	B	802	CLA	C4A-NA-C1A	5.74	109.30	106.68
9	A	841	CLA	C1C-C2C-C3C	-5.74	100.95	106.98
9	A	830	CLA	C2C-C1C-NC	5.72	115.98	109.98
9	A	826	CLA	C2C-C1C-NC	5.71	115.98	109.98
9	B	824	CLA	C2C-C1C-NC	5.71	115.98	109.98
9	I	101	CLA	O2D-CGD-CBD	5.70	121.19	111.23
9	B	803	CLA	C4A-NA-C1A	5.70	109.28	106.68
9	A	802	CLA	C2C-C1C-NC	5.69	115.96	109.98
9	B	808	CLA	C4A-NA-C1A	5.69	109.28	106.68
9	A	814	CLA	C3B-C2B-C1B	-5.68	100.48	107.17
9	B	804	CLA	C4A-NA-C1A	5.64	109.25	106.68
9	B	815	CLA	C2C-C1C-NC	5.63	115.90	109.98
9	A	805	CLA	C1C-C2C-C3C	-5.63	101.06	106.98
9	B	833	CLA	C2C-C1C-NC	5.63	115.90	109.98
9	B	834	CLA	C3B-C2B-C1B	-5.62	100.55	107.17
9	B	821	CLA	C1C-C2C-C3C	-5.62	101.07	106.98
9	B	838	CLA	O2D-CGD-CBD	5.61	121.05	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	802	CLA	C1C-C2C-C3C	-5.61	101.08	106.98
9	A	806	CLA	C1C-C2C-C3C	-5.61	101.08	106.98
9	B	806	CLA	C1C-C2C-C3C	-5.61	101.08	106.98
9	B	807	CLA	C1C-C2C-C3C	-5.60	101.09	106.98
9	A	837	CLA	C1C-C2C-C3C	-5.59	101.10	106.98
9	B	801	CLA	C3B-C2B-C1B	-5.59	100.58	107.17
9	B	825	CLA	C2C-C1C-NC	5.59	115.86	109.98
9	B	825	CLA	O2D-CGD-CBD	5.59	121.00	111.23
9	A	804	CLA	C3B-C2B-C1B	-5.58	100.59	107.17
9	A	804	CLA	O2D-CGD-CBD	5.58	120.98	111.23
9	A	828	CLA	C1C-C2C-C3C	-5.58	101.11	106.98
9	A	829	CLA	C4A-NA-C1A	5.58	109.22	106.68
9	B	818	CLA	C4A-NA-C1A	5.58	109.22	106.68
9	A	822	CLA	C4A-NA-C1A	5.57	109.22	106.68
9	A	826	CLA	C3B-C2B-C1B	-5.56	100.61	107.17
9	B	809	CLA	O2D-CGD-CBD	5.56	120.96	111.23
9	A	803	CLA	O2D-CGD-CBD	5.56	120.95	111.23
9	B	823	CLA	C2C-C1C-NC	5.56	115.82	109.98
9	A	813	CLA	C3D-C2D-C1D	-5.56	98.24	105.83
9	A	828	CLA	C3B-C2B-C1B	-5.56	100.62	107.17
9	B	823	CLA	C3B-C2B-C1B	-5.56	100.62	107.17
9	A	842	CLA	O2D-CGD-CBD	5.56	120.94	111.23
9	B	813	CLA	C3B-C2B-C1B	-5.55	100.62	107.17
9	A	812	CLA	C4A-NA-C1A	5.55	109.21	106.68
9	B	836	CLA	C3B-C2B-C1B	-5.55	100.62	107.17
9	A	805	CLA	C4A-NA-C1A	5.55	109.21	106.68
9	B	808	CLA	C1D-ND-C4D	-5.55	102.42	106.31
9	A	814	CLA	C4A-NA-C1A	5.54	109.21	106.68
9	A	827	CLA	C3B-C2B-C1B	-5.54	100.64	107.17
9	B	804	CLA	CMD-C2D-C1D	5.53	134.47	124.73
9	A	807	CLA	O2D-CGD-CBD	5.53	120.89	111.23
9	B	832	CLA	C3B-C2B-C1B	-5.53	100.65	107.17
9	B	814	CLA	C1C-C2C-C3C	-5.52	101.17	106.98
9	A	837	CLA	O2D-CGD-CBD	5.52	120.88	111.23
9	B	802	CLA	C2D-C1D-ND	5.52	115.59	110.13
9	B	824	CLA	C3D-C2D-C1D	-5.52	98.30	105.83
9	A	803	CLA	C1C-C2C-C3C	-5.51	101.18	106.98
9	B	801	CLA	C4A-NA-C1A	5.51	109.19	106.68
9	A	810	CLA	C1C-C2C-C3C	-5.51	101.19	106.98
9	A	821	CLA	C2C-C1C-NC	5.51	115.77	109.98
9	A	809	CLA	C3B-C2B-C1B	-5.51	100.68	107.17
12	B	842	BCR	C24-C23-C22	-5.51	118.09	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	820	CLA	C1C-C2C-C3C	-5.51	101.19	106.98
9	B	839	CLA	C2C-C1C-NC	5.50	115.76	109.98
9	A	810	CLA	C4A-NA-C1A	5.50	109.19	106.68
9	I	101	CLA	C1C-C2C-C3C	-5.49	101.20	106.98
9	A	835	CLA	C3B-C2B-C1B	-5.49	100.70	107.17
9	A	822	CLA	O2D-CGD-CBD	5.49	120.83	111.23
9	B	803	CLA	C2C-C1C-NC	5.49	115.75	109.98
12	A	850	BCR	C24-C23-C22	-5.49	118.11	126.23
9	B	817	CLA	C1C-C2C-C3C	-5.49	101.21	106.98
9	A	813	CLA	C2C-C1C-NC	5.48	115.74	109.98
9	B	818	CLA	C1C-C2C-C3C	-5.48	101.22	106.98
9	B	809	CLA	C3B-C2B-C1B	-5.48	100.71	107.17
9	B	826	CLA	C3B-C2B-C1B	-5.48	100.71	107.17
9	B	817	CLA	O2D-CGD-CBD	5.48	120.81	111.23
9	B	816	CLA	C3B-C2B-C1B	-5.47	100.72	107.17
9	A	842	CLA	C1C-C2C-C3C	-5.47	101.23	106.98
9	B	834	CLA	O2D-CGD-CBD	5.47	120.79	111.23
9	B	839	CLA	O2D-CGD-CBD	5.47	120.79	111.23
9	A	844	CLA	C1C-C2C-C3C	-5.47	101.23	106.98
9	A	820	CLA	O2A-CGA-O1A	-5.47	109.95	123.63
12	B	843	BCR	C3-C4-C5	-5.46	104.31	114.06
9	A	825	CLA	C1C-C2C-C3C	-5.46	101.23	106.98
8	A	801	CL0	C2C-C1C-NC	5.46	115.72	109.98
9	A	840	CLA	C3B-C2B-C1B	-5.46	100.73	107.17
9	B	805	CLA	C3B-C2B-C1B	-5.46	100.73	107.17
9	B	837	CLA	C1C-C2C-C3C	-5.46	101.24	106.98
9	B	805	CLA	O2D-CGD-CBD	5.46	120.77	111.23
9	A	813	CLA	C3B-C2B-C1B	-5.46	100.74	107.17
9	B	805	CLA	C1C-C2C-C3C	-5.45	101.24	106.98
9	B	839	CLA	C3B-C2B-C1B	-5.45	100.75	107.17
9	A	823	CLA	C1C-C2C-C3C	-5.45	101.25	106.98
9	A	840	CLA	C1C-C2C-C3C	-5.44	101.25	106.98
9	A	819	CLA	O2D-CGD-CBD	5.44	120.74	111.23
9	B	828	CLA	C1C-C2C-C3C	-5.44	101.26	106.98
9	B	834	CLA	C4A-NA-C1A	5.44	109.16	106.68
9	B	830	CLA	O2D-CGD-CBD	5.44	120.73	111.23
9	A	812	CLA	C3B-C2B-C1B	-5.43	100.76	107.17
9	A	816	CLA	C1C-C2C-C3C	-5.43	101.27	106.98
9	B	831	CLA	C3B-C2B-C1B	-5.43	100.77	107.17
9	B	824	CLA	C1D-ND-C4D	-5.42	102.51	106.31
9	A	804	CLA	C4A-NA-C1A	5.42	109.15	106.68
9	A	806	CLA	C3B-C2B-C1B	-5.42	100.78	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	201	BCR	C24-C23-C22	-5.41	118.23	126.23
9	A	840	CLA	C4A-NA-C1A	5.41	109.15	106.68
9	B	838	CLA	C3B-C2B-C1B	-5.41	100.79	107.17
9	B	816	CLA	C1C-C2C-C3C	-5.41	101.29	106.98
9	A	830	CLA	C4A-NA-C1A	5.41	109.14	106.68
9	B	830	CLA	C1C-C2C-C3C	-5.40	101.30	106.98
9	A	815	CLA	C1C-C2C-C3C	-5.40	101.30	106.98
9	A	807	CLA	C3B-C2B-C1B	-5.40	100.81	107.17
9	A	819	CLA	C3B-C2B-C1B	-5.40	100.81	107.17
9	A	824	CLA	C3B-C2B-C1B	-5.39	100.81	107.17
9	A	817	CLA	C1C-C2C-C3C	-5.39	101.31	106.98
9	B	815	CLA	C3D-C2D-C1D	-5.39	98.48	105.83
9	A	832	CLA	C1C-C2C-C3C	-5.39	101.31	106.98
9	A	833	CLA	C1C-C2C-C3C	-5.39	101.31	106.98
9	A	839	CLA	O2D-CGD-CBD	5.39	120.65	111.23
9	B	833	CLA	C3B-C2B-C1B	-5.39	100.82	107.17
9	B	803	CLA	C2D-C1D-ND	5.38	115.45	110.13
9	A	808	CLA	C1C-C2C-C3C	-5.38	101.32	106.98
9	A	824	CLA	C1C-C2C-C3C	-5.38	101.32	106.98
9	A	824	CLA	O2D-CGD-CBD	5.38	120.63	111.23
9	A	826	CLA	C1C-C2C-C3C	-5.37	101.33	106.98
9	A	833	CLA	C3B-C2B-C1B	-5.37	100.84	107.17
9	B	821	CLA	C3B-C2B-C1B	-5.37	100.84	107.17
9	A	818	CLA	C1C-C2C-C3C	-5.36	101.34	106.98
9	A	836	CLA	C1C-C2C-C3C	-5.36	101.34	106.98
9	A	814	CLA	C1C-C2C-C3C	-5.36	101.34	106.98
9	B	819	CLA	C3B-C2B-C1B	-5.36	100.85	107.17
9	A	834	CLA	C4A-NA-C1A	5.36	109.12	106.68
9	B	839	CLA	C4A-NA-C1A	5.36	109.12	106.68
9	A	822	CLA	C1C-C2C-C3C	-5.36	101.35	106.98
9	B	812	CLA	C1C-C2C-C3C	-5.36	101.35	106.98
9	B	812	CLA	O2D-CGD-CBD	5.35	120.59	111.23
9	B	819	CLA	C3D-C2D-C1D	-5.35	98.53	105.83
9	B	839	CLA	C1C-C2C-C3C	-5.35	101.35	106.98
9	B	804	CLA	C3B-C2B-C1B	-5.35	100.87	107.17
9	A	822	CLA	C3B-C2B-C1B	-5.35	100.87	107.17
9	A	836	CLA	C3B-C2B-C1B	-5.35	100.87	107.17
9	A	834	CLA	C1C-C2C-C3C	-5.34	101.36	106.98
9	K	101	CLA	C1C-C2C-C3C	-5.34	101.36	106.98
9	A	835	CLA	C1C-C2C-C3C	-5.33	101.37	106.98
9	B	818	CLA	C3B-C2B-C1B	-5.33	100.88	107.17
9	K	101	CLA	C3B-C2B-C1B	-5.33	100.89	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	832	CLA	C3B-C2B-C1B	-5.32	100.90	107.17
9	A	844	CLA	C3B-C2B-C1B	-5.32	100.90	107.17
9	B	820	CLA	C3B-C2B-C1B	-5.32	100.90	107.17
9	A	842	CLA	C4A-NA-C1A	5.32	109.10	106.68
9	A	820	CLA	O2D-CGD-CBD	5.31	120.52	111.23
9	B	810	CLA	C3B-C2B-C1B	-5.31	100.91	107.17
8	A	801	CL0	O2A-CGA-O1A	-5.31	110.35	123.63
9	B	834	CLA	C1C-C2C-C3C	-5.31	101.40	106.98
9	B	818	CLA	O2D-CGD-CBD	5.31	120.51	111.23
9	A	817	CLA	C3B-C2B-C1B	-5.31	100.92	107.17
9	B	809	CLA	O2A-CGA-O1A	-5.30	110.37	123.63
9	B	811	CLA	C1C-C2C-C3C	-5.30	101.40	106.98
9	B	838	CLA	C1C-C2C-C3C	-5.30	101.41	106.98
9	A	839	CLA	C1C-C2C-C3C	-5.29	101.41	106.98
9	B	829	CLA	C4A-NA-C1A	5.29	109.09	106.68
9	B	832	CLA	C1C-C2C-C3C	-5.29	101.42	106.98
12	A	848	BCR	C24-C23-C22	-5.29	118.41	126.23
9	A	843	CLA	C1C-C2C-C3C	-5.29	101.42	106.98
9	A	807	CLA	C4A-NA-C1A	5.29	109.09	106.68
9	A	818	CLA	O2D-CGD-CBD	5.29	120.47	111.23
9	B	837	CLA	C3B-C2B-C1B	-5.29	100.94	107.17
9	B	807	CLA	C3B-C2B-C1B	-5.29	100.94	107.17
9	A	807	CLA	C3D-C2D-C1D	-5.28	98.62	105.83
9	A	807	CLA	C1C-C2C-C3C	-5.28	101.42	106.98
9	A	819	CLA	C4A-NA-C1A	5.28	109.09	106.68
9	B	840	CLA	C3D-C2D-C1D	-5.28	98.62	105.83
9	A	815	CLA	C3B-C2B-C1B	-5.28	100.94	107.17
9	B	806	CLA	O2D-CGD-CBD	5.28	120.46	111.23
9	B	829	CLA	C1C-C2C-C3C	-5.28	101.42	106.98
9	B	817	CLA	C3B-C2B-C1B	-5.28	100.95	107.17
9	B	817	CLA	C3D-C2D-C1D	-5.28	98.63	105.83
12	B	846	BCR	C38-C26-C25	-5.27	118.73	124.48
9	B	822	CLA	C3B-C2B-C1B	-5.27	100.96	107.17
9	A	812	CLA	C1C-C2C-C3C	-5.27	101.44	106.98
9	B	822	CLA	C1C-C2C-C3C	-5.27	101.44	106.98
9	A	810	CLA	C3D-C2D-C1D	-5.27	98.64	105.83
9	A	808	CLA	C3B-C2B-C1B	-5.27	100.96	107.17
9	B	804	CLA	C2D-C1D-ND	5.27	115.34	110.13
9	B	826	CLA	C3D-C2D-C1D	-5.27	98.65	105.83
9	A	811	CLA	C3B-C2B-C1B	-5.27	100.96	107.17
9	A	804	CLA	C1C-C2C-C3C	-5.26	101.45	106.98
9	B	822	CLA	C3D-C2D-C1D	-5.26	98.65	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	816	CLA	O2D-CGD-CBD	5.26	120.42	111.23
9	B	805	CLA	C3D-C2D-C1D	-5.26	98.66	105.83
9	B	821	CLA	O2D-CGD-CBD	5.26	120.42	111.23
9	B	810	CLA	C1C-C2C-C3C	-5.25	101.45	106.98
9	A	834	CLA	C3B-C2B-C1B	-5.25	100.98	107.17
9	A	826	CLA	O2D-CGD-CBD	5.25	120.41	111.23
9	A	838	CLA	C1C-C2C-C3C	-5.25	101.46	106.98
9	B	824	CLA	C3B-C2B-C1B	-5.25	100.98	107.17
9	B	814	CLA	C3B-C2B-C1B	-5.25	100.98	107.17
9	A	831	CLA	C1C-C2C-C3C	-5.25	101.46	106.98
9	A	837	CLA	C3B-C2B-C1B	-5.25	100.99	107.17
9	B	807	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
9	A	803	CLA	C3B-C2B-C1B	-5.24	100.99	107.17
9	I	101	CLA	C3B-C2B-C1B	-5.24	100.99	107.17
9	B	805	CLA	C4A-NA-C1A	5.24	109.07	106.68
9	B	835	CLA	C1C-C2C-C3C	-5.24	101.47	106.98
9	A	806	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
9	A	838	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
9	A	809	CLA	C4A-NA-C1A	5.24	109.07	106.68
9	A	814	CLA	O2D-CGD-CBD	5.23	120.38	111.23
9	A	804	CLA	C3D-C2D-C1D	-5.23	98.70	105.83
9	A	820	CLA	C3D-C2D-C1D	-5.23	98.70	105.83
9	A	819	CLA	C1C-C2C-C3C	-5.23	101.48	106.98
9	B	816	CLA	C4A-NA-C1A	5.22	109.06	106.68
9	A	826	CLA	C3D-C2D-C1D	-5.22	98.70	105.83
9	B	803	CLA	C3D-C2D-C1D	-5.22	98.71	105.83
9	B	814	CLA	O2D-CGD-CBD	5.22	120.36	111.23
9	B	821	CLA	C4A-NA-C1A	5.22	109.06	106.68
9	B	813	CLA	C3D-C2D-C1D	-5.22	98.71	105.83
9	A	802	CLA	C3B-C2B-C1B	-5.22	101.02	107.17
9	A	842	CLA	C3B-C2B-C1B	-5.22	101.02	107.17
9	B	823	CLA	C1C-C2C-C3C	-5.21	101.50	106.98
9	A	844	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
9	A	814	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
9	B	801	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
9	B	832	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
12	M	101	BCR	C24-C23-C22	-5.21	118.53	126.23
9	B	819	CLA	C4A-NA-C1A	5.21	109.05	106.68
9	A	836	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
9	A	816	CLA	C3B-C2B-C1B	-5.20	101.04	107.17
9	A	808	CLA	C4A-NA-C1A	5.20	109.05	106.68
9	A	844	CLA	C4A-NA-C1A	5.20	109.05	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	815	CLA	C4A-NA-C1A	5.20	109.05	106.68
9	B	836	CLA	C3D-C2D-C1D	-5.20	98.74	105.83
9	B	808	CLA	C3B-C2B-C1B	-5.20	101.05	107.17
9	B	827	CLA	C2D-C1D-ND	5.20	115.27	110.13
9	A	837	CLA	C3D-C2D-C1D	-5.20	98.74	105.83
9	A	815	CLA	C4A-NA-C1A	5.19	109.05	106.68
9	A	805	CLA	C3B-C2B-C1B	-5.19	101.05	107.17
9	A	825	CLA	C3B-C2B-C1B	-5.19	101.05	107.17
9	B	838	CLA	C3D-C2D-C1D	-5.19	98.74	105.83
9	A	815	CLA	O2D-CGD-CBD	5.19	120.31	111.23
9	I	101	CLA	C4A-NA-C1A	5.19	109.05	106.68
9	A	817	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
9	A	803	CLA	C3D-C2D-C1D	-5.19	98.76	105.83
9	A	822	CLA	C3D-C2D-C1D	-5.19	98.76	105.83
9	A	811	CLA	C1C-C2C-C3C	-5.18	101.53	106.98
9	A	837	CLA	C4A-NA-C1A	5.18	109.04	106.68
9	A	816	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
9	B	818	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
9	A	813	CLA	C4A-NA-C1A	5.18	109.04	106.68
9	B	820	CLA	O2D-CGD-CBD	5.18	120.29	111.23
9	A	809	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
9	A	810	CLA	C3B-C2B-C1B	-5.18	101.07	107.17
9	A	829	CLA	C1C-C2C-C3C	-5.18	101.54	106.98
12	B	847	BCR	C24-C23-C22	-5.17	118.58	126.23
9	B	833	CLA	O2D-CGD-CBD	5.17	120.27	111.23
9	A	836	CLA	O2D-CGD-CBD	5.17	120.27	111.23
9	B	810	CLA	C3D-C2D-C1D	-5.17	98.78	105.83
9	A	843	CLA	O2D-CGD-CBD	5.17	120.26	111.23
9	B	806	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
9	A	833	CLA	O2D-CGD-CBD	5.16	120.25	111.23
9	A	843	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
9	A	823	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
9	B	827	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
9	B	811	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
9	B	819	CLA	C2D-C1D-ND	5.15	115.23	110.13
9	B	816	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
9	A	827	CLA	O2D-CGD-CBD	5.15	120.24	111.23
9	A	843	CLA	C3B-C2B-C1B	-5.15	101.10	107.17
9	A	819	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
9	B	837	CLA	C4A-NA-C1A	5.15	109.03	106.68
9	A	820	CLA	C3B-C2B-C1B	-5.15	101.10	107.17
9	A	821	CLA	C1C-C2C-C3C	-5.15	101.56	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	832	CLA	O2D-CGD-CBD	5.15	120.23	111.23
9	A	842	CLA	C3D-C2D-C1D	-5.15	98.81	105.83
9	B	813	CLA	O2A-CGA-O1A	-5.15	110.75	123.63
9	A	823	CLA	C3B-C2B-C1B	-5.15	101.10	107.17
9	A	832	CLA	C3D-C2D-C1D	-5.15	98.81	105.83
9	A	817	CLA	C4A-NA-C1A	5.14	109.03	106.68
9	B	831	CLA	C1C-C2C-C3C	-5.14	101.57	106.98
9	A	833	CLA	C3D-C2D-C1D	-5.14	98.81	105.83
9	A	806	CLA	O2A-CGA-O1A	-5.14	110.77	123.63
9	A	815	CLA	C3D-C2D-C1D	-5.14	98.82	105.83
9	A	830	CLA	C3D-C2D-C1D	-5.14	98.82	105.83
9	B	803	CLA	C3B-C2B-C1B	-5.14	101.12	107.17
9	A	805	CLA	C3D-C2D-C1D	-5.14	98.82	105.83
9	A	841	CLA	C3D-C2D-C1D	-5.13	98.82	105.83
9	B	815	CLA	C2D-C1D-ND	5.13	115.21	110.13
9	B	806	CLA	C4A-NA-C1A	5.13	109.02	106.68
9	B	822	CLA	C4A-NA-C1A	5.13	109.02	106.68
9	B	815	CLA	C1C-C2C-C3C	-5.13	101.59	106.98
9	B	837	CLA	O2D-CGD-CBD	5.12	120.19	111.23
9	A	823	CLA	C4A-NA-C1A	5.12	109.02	106.68
9	B	833	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
9	B	809	CLA	C1C-C2C-C3C	-5.12	101.59	106.98
9	A	812	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
9	A	835	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
9	B	825	CLA	C3D-C2D-C1D	-5.12	98.85	105.83
9	A	838	CLA	C2D-C1D-ND	5.11	115.19	110.13
9	B	808	CLA	O2D-CGD-CBD	5.11	120.17	111.23
9	A	803	CLA	C4A-NA-C1A	5.11	109.01	106.68
9	B	813	CLA	C1C-C2C-C3C	-5.11	101.61	106.98
9	B	827	CLA	C4A-NA-C1A	5.11	109.01	106.68
9	A	839	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
9	B	809	CLA	O2A-CGA-CBA	5.11	127.41	111.83
9	B	828	CLA	C4A-NA-C1A	5.11	109.01	106.68
9	B	827	CLA	O2A-CGA-O1A	-5.11	110.86	123.63
9	A	841	CLA	C3B-C2B-C1B	-5.10	101.16	107.17
9	A	809	CLA	C1C-C2C-C3C	-5.10	101.61	106.98
9	B	819	CLA	C1C-C2C-C3C	-5.10	101.61	106.98
9	A	811	CLA	C3D-C2D-C1D	-5.10	98.88	105.83
9	A	836	CLA	C4A-NA-C1A	5.10	109.00	106.68
9	A	828	CLA	C3D-C2D-C1D	-5.09	98.88	105.83
9	A	823	CLA	O2D-CGD-CBD	5.09	120.13	111.23
9	B	823	CLA	C3D-C2D-C1D	-5.09	98.88	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	808	CLA	C3D-C2D-C1D	-5.09	98.88	105.83
9	B	838	CLA	C4A-NA-C1A	5.09	109.00	106.68
9	B	802	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
9	A	821	CLA	C3B-C2B-C1B	-5.09	101.17	107.17
9	B	818	CLA	C2D-C1D-ND	5.09	115.16	110.13
9	B	811	CLA	C4A-NA-C1A	5.09	109.00	106.68
9	A	828	CLA	O2D-CGD-CBD	5.09	120.12	111.23
9	B	839	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
9	I	101	CLA	C3D-C2D-C1D	-5.08	98.89	105.83
9	A	830	CLA	C1C-C2C-C3C	-5.08	101.63	106.98
9	A	818	CLA	O2A-CGA-O1A	-5.08	110.92	123.63
9	B	835	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
9	B	831	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
9	B	802	CLA	C3B-C2B-C1B	-5.08	101.18	107.17
9	K	101	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
9	B	820	CLA	C4A-NA-C1A	5.08	109.00	106.68
8	A	801	CL0	C3B-C2B-C1B	-5.07	101.19	107.17
9	B	834	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
9	B	802	CLA	O2A-C1-C2	5.07	127.62	108.11
9	B	805	CLA	C2D-C1D-ND	5.07	115.14	110.13
9	A	811	CLA	C4A-NA-C1A	5.07	108.99	106.68
9	A	834	CLA	C3D-C2D-C1D	-5.07	98.92	105.83
9	A	802	CLA	O2D-CGD-CBD	5.07	120.09	111.23
9	B	814	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
9	A	807	CLA	C2D-C1D-ND	5.06	115.13	110.13
9	A	824	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
9	B	819	CLA	O2A-CGA-O1A	-5.05	110.99	123.63
9	A	832	CLA	C4A-NA-C1A	5.05	108.98	106.68
9	B	802	CLA	O2A-CGA-O1A	-5.05	111.00	123.63
9	A	805	CLA	O2D-CGD-CBD	5.05	120.05	111.23
9	B	809	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
9	A	835	CLA	O2D-CGD-CBD	5.04	120.05	111.23
9	A	840	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
12	B	845	BCR	C24-C23-C22	-5.04	118.78	126.23
9	B	835	CLA	C3B-C2B-C1B	-5.04	101.23	107.17
9	A	813	CLA	O2A-CGA-O1A	-5.03	111.03	123.63
9	A	818	CLA	C3B-C2B-C1B	-5.03	101.24	107.17
9	B	806	CLA	C3B-C2B-C1B	-5.03	101.24	107.17
9	A	826	CLA	O2A-CGA-O1A	-5.03	111.05	123.63
9	A	840	CLA	O2D-CGD-CBD	5.03	120.02	111.23
9	B	840	CLA	O2D-CGD-CBD	5.02	120.01	111.23
9	B	837	CLA	C3D-C2D-C1D	-5.02	98.98	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	802	CLA	O2D-CGD-CBD	5.02	120.01	111.23
9	A	810	CLA	C2D-C1D-ND	5.02	115.09	110.13
9	B	812	CLA	C4A-NA-C1A	5.02	108.97	106.68
9	A	822	CLA	C2D-C1D-ND	5.01	115.08	110.13
9	B	801	CLA	O2A-CGA-O1A	-5.01	111.10	123.63
9	A	830	CLA	C2D-C1D-ND	5.01	115.08	110.13
9	A	843	CLA	C4A-NA-C1A	5.01	108.96	106.68
9	B	810	CLA	C2D-C1D-ND	5.00	115.08	110.13
9	A	820	CLA	C4A-NA-C1A	5.00	108.96	106.68
9	A	829	CLA	O2A-CGA-O1A	-5.00	111.11	123.63
9	A	802	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
9	B	825	CLA	C1C-C2C-C3C	-4.99	101.73	106.98
9	B	810	CLA	O2D-CGD-CBD	4.99	119.95	111.23
9	B	803	CLA	C1C-C2C-C3C	-4.99	101.74	106.98
8	A	801	CL0	C1C-C2C-C3C	-4.98	101.74	106.98
9	A	829	CLA	C3B-C2B-C1B	-4.98	101.30	107.17
9	A	839	CLA	C3B-C2B-C1B	-4.98	101.30	107.17
9	A	828	CLA	O2A-C1-C2	4.98	127.26	108.11
9	A	812	CLA	O2D-CGD-CBD	4.97	119.93	111.23
9	B	836	CLA	O2D-CGD-CBD	4.97	119.92	111.23
9	B	826	CLA	C4A-NA-C1A	4.97	108.95	106.68
9	A	818	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
9	A	821	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
9	B	822	CLA	C2D-C1D-ND	4.97	115.04	110.13
9	B	815	CLA	O2D-CGD-CBD	4.96	119.91	111.23
9	A	813	CLA	C2D-C1D-ND	4.96	115.04	110.13
9	B	812	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
9	B	807	CLA	O2D-CGD-CBD	4.96	119.90	111.23
9	B	839	CLA	C1D-ND-C4D	-4.95	102.84	106.31
9	B	806	CLA	O2A-CGA-CBA	4.94	126.91	111.83
9	A	820	CLA	O2A-CGA-CBA	4.94	126.90	111.83
9	B	827	CLA	C3B-C2B-C1B	-4.94	101.35	107.17
9	A	820	CLA	C2D-C1D-ND	4.94	115.01	110.13
9	B	821	CLA	C3D-C2D-C1D	-4.94	99.10	105.83
9	A	817	CLA	C2D-C1D-ND	4.93	115.01	110.13
9	B	811	CLA	O2D-CGD-CBD	4.93	119.84	111.23
9	B	823	CLA	O2D-CGD-CBD	4.93	119.84	111.23
9	A	842	CLA	C2D-C1D-ND	4.92	115.00	110.13
9	B	832	CLA	C2D-C1D-ND	4.92	114.99	110.13
9	B	801	CLA	C1D-ND-C4D	-4.92	102.86	106.31
9	A	813	CLA	O2D-CGD-CBD	4.92	119.82	111.23
9	B	811	CLA	C2D-C1D-ND	4.91	114.99	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	826	CLA	C2D-C1D-ND	4.91	114.99	110.13
9	A	805	CLA	C2D-C1D-ND	4.91	114.99	110.13
9	A	842	CLA	O2A-CGA-O1A	-4.91	111.34	123.63
9	A	806	CLA	C2D-C1D-ND	4.91	114.98	110.13
9	A	819	CLA	C2D-C1D-ND	4.91	114.98	110.13
9	B	804	CLA	O2A-CGA-O1A	-4.91	111.35	123.63
12	B	842	BCR	C7-C8-C9	-4.91	118.98	126.23
9	A	803	CLA	C2D-C1D-ND	4.89	114.97	110.13
9	A	825	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
9	A	825	CLA	CAA-CBA-CGA	-4.89	99.33	113.21
9	A	806	CLA	O2D-CGD-CBD	4.89	119.77	111.23
9	A	837	CLA	C2D-C1D-ND	4.89	114.96	110.13
9	A	815	CLA	C2D-C1D-ND	4.89	114.96	110.13
9	B	801	CLA	C2B-C1B-NB	4.88	115.39	110.33
9	B	839	CLA	C2D-C1D-ND	4.88	114.96	110.13
9	A	827	CLA	C2C-C1C-NC	4.88	115.11	109.98
9	A	831	CLA	C3B-C2B-C1B	-4.88	101.42	107.17
9	B	829	CLA	C3B-C2B-C1B	-4.87	101.42	107.17
9	B	814	CLA	O2A-C1-C2	4.87	126.85	108.11
9	A	843	CLA	C2D-C1D-ND	4.87	114.95	110.13
9	B	811	CLA	C3B-C2B-C1B	-4.87	101.43	107.17
9	B	814	CLA	C2D-C1D-ND	4.87	114.94	110.13
9	A	827	CLA	C1D-ND-C4D	-4.87	102.90	106.31
9	B	834	CLA	O2A-CGA-O1A	-4.86	110.82	123.33
9	A	839	CLA	C2D-C1D-ND	4.86	114.94	110.13
9	B	837	CLA	O2A-CGA-O1A	-4.86	111.47	123.63
9	A	838	CLA	C4A-NA-C1A	4.86	108.90	106.68
9	B	840	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
9	B	805	CLA	O2A-CGA-O1A	-4.86	110.84	123.33
9	A	811	CLA	O2A-CGA-O1A	-4.85	110.86	123.33
9	B	825	CLA	C2D-C1D-ND	4.85	114.92	110.13
9	A	828	CLA	C2D-C1D-ND	4.85	114.92	110.13
9	K	101	CLA	O2A-CGA-O1A	-4.84	110.87	123.33
9	B	820	CLA	O2A-CGA-O1A	-4.84	110.88	123.33
9	B	810	CLA	C4A-NA-C1A	4.84	108.89	106.68
9	B	807	CLA	C2D-C1D-ND	4.84	114.92	110.13
9	A	812	CLA	C2D-C1D-ND	4.84	114.91	110.13
9	B	840	CLA	C2D-C1D-ND	4.84	114.91	110.13
9	B	808	CLA	C1C-C2C-C3C	-4.83	101.90	106.98
9	A	817	CLA	O2A-CGA-O1A	-4.83	111.54	123.63
9	A	841	CLA	O2D-CGD-CBD	4.83	119.68	111.23
9	K	101	CLA	C4A-NA-C1A	4.83	108.88	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	830	CLA	C3B-C2B-C1B	-4.83	101.48	107.17
9	B	817	CLA	O2A-CGA-O1A	-4.83	111.55	123.63
9	A	804	CLA	C2D-C1D-ND	4.83	114.90	110.13
9	B	833	CLA	C1C-C2C-C3C	-4.82	101.91	106.98
9	B	831	CLA	O2A-CGA-O1A	-4.82	110.93	123.33
9	A	829	CLA	C2D-C1D-ND	4.82	114.89	110.13
9	A	808	CLA	C2D-C1D-ND	4.81	114.89	110.13
9	A	809	CLA	O2A-CGA-O1A	-4.81	111.59	123.63
9	A	821	CLA	O2A-CGA-O1A	-4.81	111.59	123.63
9	B	833	CLA	C2D-C1D-ND	4.81	114.89	110.13
9	B	816	CLA	O2A-CGA-O1A	-4.80	110.97	123.33
9	A	833	CLA	O2A-CGA-O1A	-4.80	110.98	123.33
9	B	838	CLA	C2D-C1D-ND	4.80	114.88	110.13
9	B	816	CLA	C2D-C1D-ND	4.80	114.88	110.13
9	B	823	CLA	O2A-CGA-O1A	-4.80	111.00	123.33
9	A	802	CLA	C1C-C2C-C3C	-4.79	101.94	106.98
9	B	810	CLA	O2A-CGA-O1A	-4.79	111.01	123.33
9	A	836	CLA	C2D-C1D-ND	4.79	114.87	110.13
9	A	844	CLA	C2D-C1D-ND	4.79	114.86	110.13
12	A	851	BCR	C24-C23-C22	-4.78	119.16	126.23
9	A	808	CLA	O2A-CGA-O1A	-4.78	111.03	123.33
9	A	803	CLA	O2A-CGA-O1A	-4.78	111.03	123.33
9	B	833	CLA	O2A-CGA-O1A	-4.78	111.04	123.33
9	B	836	CLA	C2D-C1D-ND	4.78	114.86	110.13
9	B	830	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
9	A	830	CLA	O2A-CGA-O1A	-4.78	111.68	123.63
9	B	829	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
9	A	838	CLA	O2A-CGA-O1A	-4.78	111.05	123.33
9	B	808	CLA	O2A-CGA-O1A	-4.77	111.06	123.33
9	A	835	CLA	C4A-NA-C1A	4.77	108.85	106.68
9	B	832	CLA	O2A-CGA-O1A	-4.77	111.07	123.33
9	A	829	CLA	C3D-C2D-C1D	-4.77	99.33	105.83
9	B	809	CLA	C2D-C1D-ND	4.77	114.84	110.13
9	B	825	CLA	O2A-CGA-O1A	-4.77	111.08	123.33
9	B	839	CLA	O2A-CGA-O1A	-4.77	111.08	123.33
9	A	839	CLA	O2A-CGA-O1A	-4.76	111.08	123.33
9	A	810	CLA	O2D-CGD-CBD	4.76	119.56	111.23
9	B	835	CLA	C2D-C1D-ND	4.76	114.84	110.13
9	B	830	CLA	O2A-CGA-O1A	-4.76	111.09	123.33
9	B	807	CLA	O2A-CGA-O1A	-4.76	111.72	123.63
9	B	835	CLA	C4A-NA-C1A	4.76	108.85	106.68
9	B	815	CLA	O2A-CGA-O1A	-4.76	111.10	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	839	CLA	C4A-NA-C1A	4.76	108.85	106.68
9	B	832	CLA	O2D-CGD-CBD	4.76	119.54	111.23
9	A	816	CLA	C2D-C1D-ND	4.75	114.83	110.13
9	A	814	CLA	C2D-C1D-ND	4.75	114.83	110.13
9	B	836	CLA	C4A-NA-C1A	4.75	108.85	106.68
9	B	806	CLA	C2D-C1D-ND	4.75	114.82	110.13
9	B	811	CLA	O2A-CGA-O1A	-4.74	111.13	123.33
9	A	841	CLA	C4A-NA-C1A	4.74	108.84	106.68
9	B	826	CLA	O2D-CGD-CBD	4.74	119.52	111.23
9	A	834	CLA	O2A-CGA-O1A	-4.74	111.14	123.33
8	A	801	CL0	O2A-CGA-CBA	4.74	126.29	111.83
9	A	816	CLA	O2A-CGA-O1A	-4.74	111.14	123.33
9	B	801	CLA	O2D-CGD-CBD	4.74	119.52	111.23
9	A	809	CLA	C2D-C1D-ND	4.74	114.82	110.13
9	A	823	CLA	C2D-C1D-ND	4.74	114.82	110.13
9	A	844	CLA	O2A-CGA-O1A	-4.74	111.15	123.33
9	B	821	CLA	O2A-CGA-O1A	-4.74	111.15	123.33
9	A	841	CLA	C2D-C1D-ND	4.74	114.81	110.13
12	A	849	BCR	C24-C23-C22	-4.74	119.23	126.23
9	B	826	CLA	O2A-CGA-O1A	-4.74	111.78	123.63
9	A	843	CLA	O2A-CGA-O1A	-4.74	111.15	123.33
9	A	814	CLA	O2A-CGA-O1A	-4.74	111.15	123.33
9	A	832	CLA	C2D-C1D-ND	4.74	114.81	110.13
9	B	812	CLA	C2D-C1D-ND	4.73	114.81	110.13
9	B	834	CLA	C2D-C1D-ND	4.73	114.81	110.13
9	A	841	CLA	O2A-CGA-O1A	-4.73	111.17	123.33
9	A	815	CLA	O2A-CGA-O1A	-4.73	111.17	123.33
9	A	809	CLA	O2D-CGD-CBD	4.73	119.49	111.23
9	B	840	CLA	O2A-CGA-O1A	-4.73	111.18	123.33
9	B	827	CLA	C1C-C2C-C3C	-4.72	102.01	106.98
9	B	823	CLA	C2D-C1D-ND	4.72	114.80	110.13
9	I	101	CLA	O2A-CGA-O1A	-4.72	111.20	123.33
9	A	835	CLA	O2A-CGA-O1A	-4.71	111.21	123.33
9	A	835	CLA	C2D-C1D-ND	4.71	114.79	110.13
9	A	837	CLA	O2A-CGA-O1A	-4.71	111.21	123.33
9	B	826	CLA	C1C-C2C-C3C	-4.71	102.03	106.98
9	A	810	CLA	O2A-CGA-O1A	-4.71	111.22	123.33
9	A	836	CLA	O2A-CGA-O1A	-4.71	111.22	123.33
9	A	814	CLA	C2B-C1B-NB	4.71	115.21	110.33
9	B	826	CLA	C2D-C1D-ND	4.71	114.78	110.13
9	B	804	CLA	C2C-C1C-NC	4.71	114.93	109.98
9	A	824	CLA	O2A-CGA-O1A	-4.70	111.24	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	812	CLA	C3B-C2B-C1B	-4.70	101.63	107.17
8	A	801	CL0	C3D-C2D-C1D	-4.70	99.41	105.83
9	A	827	CLA	C1C-C2C-C3C	-4.70	102.04	106.98
9	A	804	CLA	O2A-CGA-O1A	-4.70	111.24	123.33
9	B	803	CLA	O2A-CGA-O1A	-4.70	111.87	123.63
9	A	833	CLA	C2D-C1D-ND	4.70	114.78	110.13
9	B	837	CLA	C2D-C1D-ND	4.70	114.78	110.13
9	B	833	CLA	C4A-NA-C1A	4.70	108.82	106.68
9	A	822	CLA	O2A-CGA-O1A	-4.70	111.25	123.33
9	A	832	CLA	O2A-CGA-O1A	-4.70	111.26	123.33
9	B	836	CLA	C1C-C2C-C3C	-4.69	102.04	106.98
9	A	807	CLA	O2A-CGA-O1A	-4.69	111.27	123.33
9	A	823	CLA	O2A-CGA-O1A	-4.69	111.27	123.33
9	B	824	CLA	O2A-CGA-O1A	-4.69	111.27	123.33
12	A	847	BCR	C24-C23-C22	-4.69	119.30	126.23
9	A	812	CLA	O2A-CGA-O1A	-4.69	111.27	123.33
9	A	840	CLA	O2A-CGA-O1A	-4.69	111.90	123.63
9	A	830	CLA	C1D-ND-C4D	-4.69	103.02	106.31
9	I	101	CLA	C2D-C1D-ND	4.69	114.77	110.13
9	B	823	CLA	C2B-C1B-NB	4.69	115.19	110.33
9	B	812	CLA	O2A-CGA-O1A	-4.68	111.29	123.33
9	B	835	CLA	O2A-CGA-O1A	-4.68	111.29	123.33
9	A	831	CLA	O2A-CGA-O1A	-4.68	111.30	123.33
9	B	835	CLA	O2D-CGD-CBD	4.68	119.41	111.23
9	B	830	CLA	C3B-C2B-C1B	-4.68	101.66	107.17
9	B	813	CLA	C2D-C1D-ND	4.68	114.75	110.13
9	A	816	CLA	C4A-NA-C1A	4.68	108.81	106.68
9	A	824	CLA	C4A-NA-C1A	4.68	108.81	106.68
9	A	827	CLA	C4A-NA-C1A	4.67	108.81	106.68
9	A	839	CLA	C1D-ND-C4D	-4.67	103.04	106.31
9	B	822	CLA	O2A-CGA-O1A	-4.67	111.33	123.33
9	B	838	CLA	O2A-CGA-O1A	-4.66	111.33	123.33
9	B	807	CLA	C4A-NA-C1A	4.66	108.81	106.68
9	B	813	CLA	C4A-NA-C1A	4.66	108.81	106.68
9	A	844	CLA	O2D-CGD-CBD	4.66	119.37	111.23
9	K	101	CLA	C2D-C1D-ND	4.65	114.73	110.13
9	B	831	CLA	C2D-C1D-ND	4.65	114.72	110.13
9	A	825	CLA	C2D-C1D-ND	4.65	114.72	110.13
9	B	820	CLA	C3D-C2D-C1D	-4.64	99.49	105.83
9	B	828	CLA	O2A-CGA-O1A	-4.64	112.02	123.63
12	A	851	BCR	C7-C8-C9	-4.64	119.38	126.23
9	A	804	CLA	C2B-C1B-NB	4.63	115.12	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	824	CLA	C2D-C1D-ND	4.62	114.70	110.13
8	A	801	CL0	O2D-CGD-CBD	4.62	119.31	111.23
9	A	806	CLA	O2A-CGA-CBA	4.62	125.92	111.83
9	A	826	CLA	C4A-NA-C1A	4.62	108.79	106.68
9	B	832	CLA	C4A-NA-C1A	4.62	108.79	106.68
9	B	831	CLA	O2D-CGD-CBD	4.62	119.30	111.23
9	B	814	CLA	C1D-ND-C4D	-4.61	103.08	106.31
9	A	805	CLA	C1D-ND-C4D	-4.61	103.08	106.31
9	B	836	CLA	O2A-CGA-O1A	-4.61	112.10	123.63
9	A	840	CLA	C2D-C1D-ND	4.60	114.68	110.13
9	B	817	CLA	C2D-C1D-ND	4.60	114.68	110.13
9	A	807	CLA	C1D-ND-C4D	-4.60	103.08	106.31
9	A	820	CLA	C1D-ND-C4D	-4.59	103.09	106.31
9	A	838	CLA	C1D-ND-C4D	-4.59	103.09	106.31
9	B	811	CLA	C1D-ND-C4D	-4.58	103.10	106.31
9	A	842	CLA	O2A-CGA-CBA	4.58	125.80	111.83
9	A	834	CLA	C2D-C1D-ND	4.58	114.65	110.13
9	B	828	CLA	C2D-C1D-ND	4.57	114.65	110.13
9	B	827	CLA	O2D-CGD-CBD	4.57	119.21	111.23
9	A	819	CLA	C1D-ND-C4D	-4.56	103.11	106.31
9	B	805	CLA	C1D-ND-C4D	-4.56	103.12	106.31
9	A	818	CLA	C2D-C1D-ND	4.55	114.63	110.13
9	B	821	CLA	C2D-C1D-ND	4.55	114.63	110.13
9	A	811	CLA	C2D-C1D-ND	4.55	114.63	110.13
9	B	804	CLA	C1D-ND-C4D	-4.54	103.13	106.31
9	A	821	CLA	O2D-CGD-CBD	4.53	119.14	111.23
9	B	829	CLA	O2A-CGA-O1A	-4.52	111.72	123.33
9	B	803	CLA	O2D-CGD-CBD	4.51	119.12	111.23
9	B	810	CLA	C1D-ND-C4D	-4.51	103.15	106.31
9	A	803	CLA	C1D-ND-C4D	-4.50	103.15	106.31
9	A	806	CLA	C1D-ND-C4D	-4.50	103.15	106.31
9	A	811	CLA	O2D-CGD-CBD	4.49	119.09	111.23
14	B	848	LMG	O7-C10-C11	4.49	121.20	111.48
9	B	803	CLA	C1D-ND-C4D	-4.49	103.16	106.31
9	B	832	CLA	C1D-ND-C4D	-4.49	103.16	106.31
9	A	833	CLA	C4A-NA-C1A	4.48	108.72	106.68
9	B	804	CLA	O2A-CGA-CBA	4.48	125.50	111.83
9	B	828	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
9	B	802	CLA	O2A-CGA-CBA	4.47	125.47	111.83
9	A	831	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
12	B	842	BCR	C3-C4-C5	-4.46	106.09	114.06
9	A	802	CLA	C2D-C1D-ND	4.46	114.55	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	851	BCR	C30-C25-C24	4.46	127.75	115.65
9	B	834	CLA	C2B-C1B-NB	4.46	114.95	110.33
9	A	802	CLA	O2A-CGA-O1A	-4.46	112.47	123.63
9	B	819	CLA	C1D-ND-C4D	-4.46	103.19	106.31
9	A	810	CLA	C1D-ND-C4D	-4.45	103.19	106.31
9	A	817	CLA	C1D-ND-C4D	-4.45	103.19	106.31
9	B	835	CLA	C1D-ND-C4D	-4.45	103.19	106.31
9	A	828	CLA	O2A-CGA-O1A	-4.45	112.50	123.63
9	A	842	CLA	C1D-ND-C4D	-4.45	103.19	106.31
9	A	813	CLA	C1C-C2C-C3C	-4.45	102.30	106.98
9	K	101	CLA	C1D-ND-C4D	-4.44	103.20	106.31
9	A	827	CLA	CMC-C2C-C1C	4.43	131.96	125.03
9	A	837	CLA	C1D-ND-C4D	-4.43	103.20	106.31
9	B	804	CLA	O2A-C1-C2	4.43	125.16	108.11
9	B	818	CLA	O2A-CGA-O1A	-4.43	112.55	123.63
9	A	825	CLA	O2A-CGA-O1A	-4.43	112.56	123.63
9	A	838	CLA	C3B-C2B-C1B	-4.42	101.95	107.17
9	A	819	CLA	O2A-CGA-O1A	-4.42	112.56	123.63
9	B	809	CLA	C1D-ND-C4D	-4.42	103.21	106.31
9	B	819	CLA	O2A-C1-C2	4.41	125.10	108.11
9	A	821	CLA	C2D-C1D-ND	4.41	114.50	110.13
9	A	825	CLA	C1D-ND-C4D	-4.41	103.22	106.31
9	A	843	CLA	C1D-ND-C4D	-4.41	103.22	106.31
9	B	818	CLA	O2A-CGA-CBA	4.40	125.25	111.83
9	B	825	CLA	C2B-C1B-NB	4.40	114.89	110.33
12	M	101	BCR	C33-C5-C6	-4.39	119.69	124.48
9	B	822	CLA	O2D-CGD-CBD	4.39	118.90	111.23
9	A	819	CLA	O2A-C1-C2	4.38	124.98	108.11
9	A	826	CLA	C1D-ND-C4D	-4.38	103.24	106.31
9	B	838	CLA	C1D-ND-C4D	-4.38	103.24	106.31
9	A	841	CLA	C1D-ND-C4D	-4.37	103.25	106.31
9	A	816	CLA	C1D-ND-C4D	-4.36	103.25	106.31
9	A	823	CLA	C1D-ND-C4D	-4.36	103.26	106.31
9	B	812	CLA	C1D-ND-C4D	-4.35	103.26	106.31
9	B	801	CLA	O2A-CGA-CBA	4.34	125.08	111.83
9	B	827	CLA	C1D-ND-C4D	-4.34	103.27	106.31
9	B	804	CLA	C3D-C2D-C1D	-4.34	99.91	105.83
9	B	814	CLA	O2A-CGA-O1A	-4.34	112.78	123.63
9	A	815	CLA	C1D-ND-C4D	-4.34	103.27	106.31
9	B	802	CLA	C1D-ND-C4D	-4.33	103.27	106.31
9	A	806	CLA	C4A-NA-C1A	4.33	108.66	106.68
9	A	835	CLA	C1D-ND-C4D	-4.33	103.27	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	809	CLA	O2A-C1-C2	4.33	124.76	108.11
9	B	822	CLA	C1D-ND-C4D	-4.32	103.28	106.31
9	A	821	CLA	C2B-C1B-NB	4.30	114.79	110.33
9	A	832	CLA	C1D-ND-C4D	-4.30	103.29	106.31
12	B	846	BCR	C7-C8-C9	-4.30	119.88	126.23
9	B	837	CLA	C1D-ND-C4D	-4.30	103.30	106.31
9	B	818	CLA	C1D-ND-C4D	-4.29	103.30	106.31
9	B	831	CLA	C4A-NA-C1A	4.29	108.63	106.68
9	B	815	CLA	C1D-ND-C4D	-4.28	103.31	106.31
9	B	807	CLA	C1D-ND-C4D	-4.28	103.31	106.31
9	B	833	CLA	C1D-ND-C4D	-4.27	103.32	106.31
9	B	829	CLA	C2D-C1D-ND	4.27	114.35	110.13
9	A	818	CLA	O2A-CGA-CBA	4.27	124.85	111.83
9	B	834	CLA	C1D-ND-C4D	-4.26	103.32	106.31
9	A	824	CLA	C1D-ND-C4D	-4.26	103.32	106.31
9	B	823	CLA	C1D-ND-C4D	-4.25	103.33	106.31
9	B	813	CLA	O2A-CGA-CBA	4.25	124.79	111.83
8	A	801	CL0	C2B-C1B-NB	4.24	114.72	110.33
9	B	816	CLA	C1D-ND-C4D	-4.24	103.34	106.31
9	A	842	CLA	O2A-C1-C2	4.23	124.40	108.11
13	A	852	LHG	O7-C7-C8	4.23	120.63	111.48
9	A	822	CLA	C1D-ND-C4D	-4.23	103.34	106.31
9	B	825	CLA	C1D-ND-C4D	-4.23	103.34	106.31
9	B	823	CLA	C4A-NA-C1A	4.23	108.61	106.68
9	A	812	CLA	C2B-C1B-NB	4.23	114.71	110.33
8	A	801	CL0	C2D-C1D-ND	4.21	114.30	110.13
9	B	840	CLA	C1D-ND-C4D	-4.21	103.36	106.31
9	A	827	CLA	C2B-C1B-NB	4.20	114.69	110.33
9	B	827	CLA	O2A-CGA-CBA	4.20	124.65	111.83
9	A	836	CLA	C1D-ND-C4D	-4.20	103.37	106.31
9	A	805	CLA	O2A-CGA-O1A	-4.20	113.13	123.63
9	A	840	CLA	C1D-ND-C4D	-4.19	103.37	106.31
9	B	802	CLA	CMB-C2B-C1B	4.19	131.79	125.42
9	B	805	CLA	C2B-C1B-NB	4.19	114.67	110.33
9	A	829	CLA	O2D-CGD-CBD	4.19	118.55	111.23
9	B	801	CLA	C2C-C1C-NC	4.18	114.37	109.98
9	A	826	CLA	C2B-C1B-NB	4.17	114.65	110.33
9	B	820	CLA	C2D-C1D-ND	4.17	114.25	110.13
9	B	831	CLA	C1D-ND-C4D	-4.16	103.39	106.31
9	A	844	CLA	C1D-ND-C4D	-4.16	103.39	106.31
9	B	813	CLA	C1D-ND-C4D	-4.16	103.40	106.31
9	B	828	CLA	C1D-ND-C4D	-4.16	103.40	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	848	BCR	C7-C8-C9	-4.16	120.09	126.23
9	A	813	CLA	O2A-CGA-CBA	4.15	124.49	111.83
9	A	827	CLA	O2A-CGA-O1A	-4.15	113.25	123.63
9	B	819	CLA	C2B-C1B-NB	4.14	114.62	110.33
9	B	830	CLA	C4A-NA-C1A	4.14	108.57	106.68
9	A	811	CLA	C1D-ND-C4D	-4.13	103.41	106.31
9	B	826	CLA	C1D-ND-C4D	-4.13	103.41	106.31
9	A	809	CLA	C1D-ND-C4D	-4.12	103.42	106.31
12	A	849	BCR	C7-C8-C9	-4.12	120.14	126.23
9	A	818	CLA	C4A-NA-C1A	4.12	108.56	106.68
9	A	836	CLA	C2B-C1B-NB	4.12	114.60	110.33
9	B	829	CLA	C1D-ND-C4D	-4.11	103.43	106.31
9	B	806	CLA	C2B-C1B-NB	4.11	114.59	110.33
9	A	812	CLA	C1D-ND-C4D	-4.11	103.43	106.31
9	A	828	CLA	C1D-ND-C4D	-4.11	103.43	106.31
9	B	833	CLA	C2B-C1B-NB	4.11	114.58	110.33
9	B	830	CLA	C2D-C1D-ND	4.10	114.19	110.13
9	A	808	CLA	C1D-ND-C4D	-4.10	103.44	106.31
9	A	840	CLA	C2B-C1B-NB	4.09	114.57	110.33
9	B	836	CLA	C1D-ND-C4D	-4.09	103.44	106.31
9	A	802	CLA	C4A-NA-C1A	4.09	108.54	106.68
9	B	806	CLA	C1D-ND-C4D	-4.08	103.45	106.31
9	B	821	CLA	C1D-ND-C4D	-4.08	103.45	106.31
9	B	817	CLA	O2A-CGA-CBA	4.08	124.27	111.83
9	A	809	CLA	O2A-CGA-CBA	4.08	124.27	111.83
9	B	840	CLA	CMB-C2B-C1B	4.08	131.63	125.42
9	A	833	CLA	C1D-ND-C4D	-4.07	103.45	106.31
9	B	818	CLA	C2B-C1B-NB	4.07	114.55	110.33
9	B	815	CLA	C2B-C1B-NB	4.07	114.55	110.33
9	B	817	CLA	C2B-C1B-NB	4.07	114.55	110.33
9	A	831	CLA	C2D-C1D-ND	4.07	114.15	110.13
9	B	801	CLA	C1C-C2C-C3C	-4.07	102.70	106.98
9	A	805	CLA	CAA-C2A-C3A	-4.07	102.01	113.00
9	A	818	CLA	C1D-ND-C4D	-4.06	103.46	106.31
9	I	101	CLA	C1D-ND-C4D	-4.06	103.46	106.31
9	B	817	CLA	C4A-NA-C1A	4.06	108.53	106.68
9	A	821	CLA	O2A-C1-C2	4.05	123.69	108.11
9	A	831	CLA	C4A-NA-C1A	4.05	108.53	106.68
9	A	826	CLA	O2A-CGA-CBA	4.05	124.17	111.83
12	B	843	BCR	C27-C26-C25	-4.04	117.25	122.70
9	A	809	CLA	C2B-C1B-NB	4.03	114.51	110.33
9	B	836	CLA	C2B-C1B-NB	4.03	114.50	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	822	CLA	C2B-C1B-NB	4.03	114.50	110.33
9	B	825	CLA	C4A-NA-C1A	4.02	108.52	106.68
9	B	819	CLA	O2A-CGA-CBA	4.01	124.08	111.83
9	A	826	CLA	CHD-C1D-ND	-4.01	119.16	124.80
9	A	813	CLA	C1D-ND-C4D	-4.00	103.50	106.31
9	B	826	CLA	O2A-CGA-CBA	3.98	123.97	111.83
9	A	813	CLA	C2B-C1B-NB	3.98	114.45	110.33
9	A	818	CLA	C2B-C1B-NB	3.98	114.45	110.33
9	A	804	CLA	C1D-ND-C4D	-3.97	103.53	106.31
12	B	845	BCR	C15-C14-C13	-3.97	121.71	127.28
13	A	853	LHG	O7-C7-C8	3.97	120.06	111.48
9	B	803	CLA	O2A-C1-C2	3.97	123.37	108.11
9	B	813	CLA	C2B-C1B-NB	3.96	114.44	110.33
9	B	839	CLA	C2B-C1B-NB	3.96	114.43	110.33
9	B	828	CLA	C3B-C2B-C1B	-3.95	102.51	107.17
9	A	829	CLA	C1D-ND-C4D	-3.95	103.54	106.31
9	A	802	CLA	C1D-ND-C4D	-3.94	103.55	106.31
12	B	847	BCR	C33-C5-C6	-3.93	120.20	124.48
9	A	835	CLA	C2B-C1B-NB	3.92	114.39	110.33
9	A	831	CLA	C1D-ND-C4D	-3.92	103.56	106.31
9	A	829	CLA	O2A-CGA-CBA	3.92	123.79	111.83
9	A	833	CLA	C2B-C1B-NB	3.92	114.39	110.33
9	B	831	CLA	C2B-C1B-NB	3.91	114.38	110.33
9	A	811	CLA	OBD-CAD-C3D	-3.90	119.30	128.42
9	B	839	CLA	CHD-C1D-ND	-3.90	119.31	124.80
9	A	821	CLA	C1D-ND-C4D	-3.90	103.58	106.31
9	B	801	CLA	O2A-C1-C2	3.90	123.10	108.11
9	A	834	CLA	C1D-ND-C4D	-3.89	103.58	106.31
9	A	824	CLA	C2B-C1B-NB	3.89	114.36	110.33
9	B	828	CLA	O2D-CGD-CBD	3.88	118.01	111.23
9	B	812	CLA	C2B-C1B-NB	3.88	114.35	110.33
9	B	816	CLA	C2B-C1B-NB	3.88	114.34	110.33
9	B	817	CLA	C1D-ND-C4D	-3.88	103.59	106.31
12	B	844	BCR	C33-C5-C6	-3.87	120.26	124.48
9	B	807	CLA	O2A-CGA-CBA	3.86	123.62	111.83
9	B	820	CLA	C1D-ND-C4D	-3.86	103.60	106.31
9	A	814	CLA	C1D-ND-C4D	-3.86	103.60	106.31
9	B	832	CLA	C2B-C1B-NB	3.86	114.33	110.33
9	B	808	CLA	CAC-C3C-C4C	3.85	129.80	124.79
9	A	802	CLA	O2A-CGA-CBA	3.85	123.56	111.83
9	A	806	CLA	C2B-C1B-NB	3.85	114.31	110.33
8	A	801	CL0	C4A-NA-C1A	3.84	108.43	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	851	BCR	C3-C4-C5	-3.84	107.20	114.06
9	A	832	CLA	C2B-C1B-NB	3.84	114.31	110.33
12	A	850	BCR	C38-C26-C25	-3.84	120.29	124.48
9	B	838	CLA	C2B-C1B-NB	3.83	114.30	110.33
9	A	830	CLA	O2A-C1-C2	3.83	122.85	108.11
9	B	828	CLA	O2A-CGA-CBA	3.83	123.52	111.83
9	B	822	CLA	C2B-C1B-NB	3.83	114.30	110.33
9	B	836	CLA	O2A-C1-C2	3.83	122.84	108.11
9	A	838	CLA	C2B-C1B-NB	3.82	114.29	110.33
9	B	826	CLA	C2B-C1B-NB	3.82	114.29	110.33
9	A	816	CLA	C2B-C1B-NB	3.81	114.28	110.33
9	A	817	CLA	O2A-CGA-CBA	3.81	123.46	111.83
9	A	825	CLA	C4D-C3D-CAD	3.81	112.25	108.11
9	B	809	CLA	C2B-C1B-NB	3.81	114.27	110.33
9	B	803	CLA	O2A-CGA-CBA	3.81	123.44	111.83
9	A	841	CLA	C2B-C1B-NB	3.80	114.27	110.33
12	B	846	BCR	C39-C30-C25	-3.80	104.28	110.24
9	A	819	CLA	C2B-C1B-NB	3.80	114.26	110.33
9	B	820	CLA	C2B-C1B-NB	3.79	114.26	110.33
9	A	825	CLA	CMA-C3A-C4A	3.79	121.97	111.77
9	K	101	CLA	C2B-C1B-NB	3.79	114.26	110.33
9	A	834	CLA	C2B-C1B-NB	3.79	114.25	110.33
9	A	806	CLA	CAA-C2A-C3A	-3.79	102.76	113.00
9	A	810	CLA	C2B-C1B-NB	3.78	114.24	110.33
9	A	807	CLA	C2B-C1B-NB	3.77	114.23	110.33
12	B	847	BCR	C38-C26-C25	-3.77	120.37	124.48
9	B	808	CLA	CHD-C1D-ND	-3.77	119.50	124.80
9	A	827	CLA	O2A-C1-C2	3.77	122.60	108.11
9	A	827	CLA	O2A-CGA-CBA	3.76	123.31	111.83
9	A	837	CLA	C2B-C1B-NB	3.76	114.23	110.33
9	A	821	CLA	C4A-NA-C1A	3.76	108.40	106.68
9	B	837	CLA	O2A-CGA-CBA	3.76	123.30	111.83
9	A	802	CLA	O2A-C1-C2	3.76	122.57	108.11
9	B	807	CLA	C2B-C1B-NB	3.76	114.22	110.33
9	A	826	CLA	CAA-C2A-C3A	-3.75	102.86	113.00
9	B	821	CLA	C2B-C1B-NB	3.75	114.22	110.33
12	A	851	BCR	C38-C26-C25	-3.75	120.39	124.48
9	A	809	CLA	O2A-C1-C2	3.75	122.54	108.11
9	B	813	CLA	CAA-C2A-C3A	-3.74	102.88	113.00
9	A	805	CLA	O2A-C1-C2	3.74	122.50	108.11
9	A	819	CLA	C1-C2-C3	-3.74	120.07	126.20
9	B	829	CLA	C2B-C1B-NB	3.73	114.19	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	804	CLA	C2B-C1B-NB	3.73	114.19	110.33
9	B	819	CLA	C1-C2-C3	-3.72	120.10	126.20
9	B	830	CLA	C1D-ND-C4D	-3.72	103.70	106.31
9	B	837	CLA	C2B-C1B-NB	3.72	114.18	110.33
9	A	840	CLA	O2A-CGA-CBA	3.71	123.16	111.83
9	B	807	CLA	O2A-C1-C2	3.71	122.37	108.11
9	B	802	CLA	CMA-C3A-C4A	3.71	121.73	111.77
9	A	830	CLA	O2A-CGA-CBA	3.70	123.13	111.83
9	A	805	CLA	C2B-C1B-NB	3.70	114.16	110.33
12	A	849	BCR	C38-C26-C25	-3.70	120.45	124.48
9	A	802	CLA	C2B-C1B-NB	3.69	114.16	110.33
9	B	810	CLA	C2B-C1B-NB	3.69	114.16	110.33
9	B	824	CLA	C2B-C1B-NB	3.69	114.15	110.33
12	F	201	BCR	C3-C4-C5	-3.68	107.48	114.06
9	A	828	CLA	O2A-CGA-CBA	3.68	123.06	111.83
9	B	826	CLA	O2A-C1-C2	3.68	122.27	108.11
9	A	805	CLA	C1-C2-C3	-3.68	120.17	126.20
9	B	830	CLA	C2B-C1B-NB	3.68	114.14	110.33
9	A	839	CLA	C2B-C1B-NB	3.67	114.14	110.33
9	A	842	CLA	C2B-C1B-NB	3.67	114.14	110.33
9	A	825	CLA	C2B-C1B-NB	3.67	114.13	110.33
9	A	821	CLA	O2A-CGA-CBA	3.66	123.01	111.83
9	A	820	CLA	O2A-C1-C2	3.66	122.20	108.11
12	B	844	BCR	C34-C9-C10	-3.66	116.89	122.82
9	A	811	CLA	C2B-C1B-NB	3.66	114.12	110.33
9	B	804	CLA	O2D-CGD-CBD	3.65	117.62	111.23
9	A	815	CLA	C2B-C1B-NB	3.65	114.11	110.33
9	A	844	CLA	C2B-C1B-NB	3.65	114.11	110.33
12	A	851	BCR	C33-C5-C6	-3.65	120.50	124.48
9	B	817	CLA	O2A-C1-C2	3.65	122.17	108.11
12	A	847	BCR	C3-C4-C5	-3.65	107.55	114.06
9	B	804	CLA	C1C-C2C-C3C	-3.65	103.15	106.98
9	B	813	CLA	O2A-C1-C2	3.65	122.14	108.11
9	B	801	CLA	CMC-C2C-C1C	3.64	130.73	125.03
9	B	832	CLA	CHD-C1D-ND	-3.64	119.68	124.80
9	A	803	CLA	C2B-C1B-NB	3.64	114.10	110.33
9	A	817	CLA	C2B-C1B-NB	3.63	114.09	110.33
9	A	818	CLA	O2A-C1-C2	3.63	122.08	108.11
9	A	843	CLA	C2B-C1B-NB	3.63	114.09	110.33
9	A	829	CLA	C2B-C1B-NB	3.63	114.09	110.33
9	A	820	CLA	CHD-C1D-ND	-3.63	119.70	124.80
9	A	824	CLA	CHD-C1D-ND	-3.62	119.71	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	827	CLA	C2B-C1B-NB	3.62	114.08	110.33
9	B	817	CLA	CHD-C1D-ND	-3.61	119.72	124.80
9	K	101	CLA	CHD-C1D-ND	-3.61	119.72	124.80
9	A	830	CLA	CHD-C1D-ND	-3.61	119.73	124.80
9	B	828	CLA	O2A-C1-C2	3.60	121.97	108.11
9	B	830	CLA	CHD-C1D-ND	-3.59	119.75	124.80
9	B	819	CLA	O2D-CGD-CBD	3.59	117.51	111.23
9	A	808	CLA	C2B-C1B-NB	3.59	114.05	110.33
9	A	829	CLA	O2A-C1-C2	3.58	121.90	108.11
9	A	823	CLA	C2B-C1B-NB	3.58	114.04	110.33
9	A	802	CLA	CHD-C1D-ND	-3.58	119.76	124.80
9	A	823	CLA	CHD-C1D-ND	-3.58	119.77	124.80
9	A	811	CLA	C4D-C3D-CAD	3.58	111.99	108.11
9	A	816	CLA	CHD-C1D-ND	-3.57	119.77	124.80
9	A	811	CLA	CHD-C1D-ND	-3.57	119.78	124.80
9	B	804	CLA	CAC-C3C-C4C	3.57	129.44	124.79
9	A	806	CLA	CHD-C1D-ND	-3.57	119.78	124.80
9	B	822	CLA	CHD-C1D-ND	-3.55	119.81	124.80
9	A	813	CLA	CAC-C3C-C4C	3.54	129.40	124.79
9	A	802	CLA	CMB-C2B-C1B	3.54	130.81	125.42
12	B	846	BCR	C3-C4-C5	-3.54	107.74	114.06
9	A	828	CLA	C2B-C1B-NB	3.54	113.99	110.33
9	A	826	CLA	O2A-C1-C2	3.53	121.71	108.11
9	A	820	CLA	C2B-C1B-NB	3.53	113.99	110.33
9	A	839	CLA	CHD-C1D-ND	-3.53	119.83	124.80
9	A	814	CLA	CHD-C1D-ND	-3.53	119.84	124.80
9	B	835	CLA	CHD-C1D-ND	-3.53	119.84	124.80
9	A	837	CLA	CHD-C1D-ND	-3.53	119.84	124.80
9	A	818	CLA	C1-C2-C3	-3.52	121.06	126.76
9	B	835	CLA	C2B-C1B-NB	3.52	113.98	110.33
9	A	807	CLA	CHD-C1D-ND	-3.52	119.85	124.80
9	A	818	CLA	CHD-C1D-ND	-3.52	119.85	124.80
9	A	832	CLA	CHD-C1D-ND	-3.52	119.85	124.80
8	A	801	CL0	O2A-C1-C2	3.52	121.65	108.11
9	A	825	CLA	O2A-C1-C2	3.52	121.65	108.11
9	B	823	CLA	CHD-C1D-ND	-3.52	119.85	124.80
9	B	838	CLA	CHD-C1D-ND	-3.52	119.85	124.80
9	B	831	CLA	CHD-C1D-ND	-3.52	119.85	124.80
9	A	806	CLA	O2A-C1-C2	3.51	121.63	108.11
9	A	803	CLA	CHD-C1D-ND	-3.51	119.86	124.80
8	A	801	CL0	C4-C3-C5	3.51	121.32	115.23
12	A	849	BCR	C33-C5-C6	-3.51	120.66	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	201	BCR	C28-C27-C26	-3.51	107.80	114.06
9	A	843	CLA	CHD-C1D-ND	-3.51	119.87	124.80
12	B	843	BCR	C7-C8-C9	-3.50	121.05	126.23
9	B	807	CLA	CHD-C1D-ND	-3.50	119.87	124.80
9	A	805	CLA	CHD-C1D-ND	-3.50	119.88	124.80
12	M	101	BCR	C28-C27-C26	-3.50	107.82	114.06
9	B	834	CLA	CHD-C1D-ND	-3.49	119.89	124.80
9	A	833	CLA	CHD-C1D-ND	-3.49	119.89	124.80
9	A	831	CLA	C2B-C1B-NB	3.49	113.95	110.33
9	A	842	CLA	CHD-C1D-ND	-3.48	119.90	124.80
9	A	844	CLA	CHD-C1D-ND	-3.48	119.91	124.80
9	B	821	CLA	CHD-C1D-ND	-3.48	119.91	124.80
9	B	802	CLA	C3C-C4C-NC	3.48	114.89	110.43
9	A	821	CLA	CHD-C1D-ND	-3.48	119.91	124.80
9	B	839	CLA	CAA-C2A-C3A	-3.48	103.60	113.00
9	A	819	CLA	O2A-CGA-CBA	3.48	122.44	111.83
9	B	811	CLA	CHD-C1D-ND	-3.47	119.91	124.80
12	A	851	BCR	C34-C9-C10	-3.47	117.19	122.82
12	A	851	BCR	C24-C25-C26	-3.46	113.57	121.56
9	B	825	CLA	CAA-C2A-C3A	-3.46	103.65	113.00
9	A	827	CLA	CHD-C1D-ND	-3.46	119.93	124.80
12	B	845	BCR	C33-C5-C6	-3.46	120.71	124.48
9	B	836	CLA	O2A-CGA-CBA	3.45	122.36	111.83
9	A	819	CLA	CHD-C1D-ND	-3.45	119.95	124.80
9	B	805	CLA	CHD-C1D-ND	-3.45	119.95	124.80
9	B	825	CLA	CHD-C1D-ND	-3.45	119.95	124.80
9	B	819	CLA	CHD-C1D-ND	-3.44	119.96	124.80
9	A	841	CLA	CHD-C1D-ND	-3.44	119.96	124.80
9	B	815	CLA	CHD-C1D-ND	-3.44	119.96	124.80
9	A	810	CLA	CHD-C1D-ND	-3.44	119.96	124.80
9	A	811	CLA	O2A-CGA-CBA	3.44	124.86	114.00
12	B	846	BCR	C15-C14-C13	-3.43	122.46	127.28
9	B	816	CLA	CHD-C1D-ND	-3.43	119.97	124.80
9	A	842	CLA	CMA-C3A-C4A	3.43	120.99	111.77
9	A	844	CLA	CMA-C3A-C4A	3.43	120.99	111.77
9	A	835	CLA	CHD-C1D-ND	-3.42	119.99	124.80
9	A	840	CLA	CHD-C1D-ND	-3.42	119.99	124.80
9	B	813	CLA	CMC-C2C-C1C	3.42	130.38	125.03
9	B	828	CLA	C2B-C1B-NB	3.42	113.87	110.33
9	B	828	CLA	CED-O2D-CGD	3.41	123.66	115.92
8	A	801	CL0	C1D-ND-C4D	-3.41	103.92	106.31
9	A	817	CLA	CHD-C1D-ND	-3.41	120.01	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	803	CLA	C2B-C1B-NB	3.40	113.86	110.33
9	B	818	CLA	C4-C3-C5	3.40	121.13	115.23
9	B	820	CLA	C4D-C3D-CAD	3.40	111.80	108.11
9	B	827	CLA	O2A-C1-C2	3.40	121.17	108.11
9	B	806	CLA	CHD-C1D-ND	-3.39	120.03	124.80
9	A	809	CLA	CHD-C1D-ND	-3.39	120.03	124.80
9	B	837	CLA	CHD-C1D-ND	-3.39	120.03	124.80
9	A	830	CLA	CAA-C2A-C3A	-3.38	103.85	113.00
12	A	847	BCR	C19-C18-C17	3.38	124.33	119.01
9	A	836	CLA	CHD-C1D-ND	-3.38	120.05	124.80
12	B	846	BCR	C33-C5-C6	-3.37	120.80	124.48
9	B	810	CLA	CHD-C1D-ND	-3.37	120.06	124.80
12	B	843	BCR	C4-C5-C6	-3.37	118.16	122.70
9	A	804	CLA	CHD-C1D-ND	-3.36	120.07	124.80
9	B	840	CLA	CHD-C1D-ND	-3.36	120.07	124.80
9	A	812	CLA	CHD-C1D-ND	-3.36	120.08	124.80
9	B	809	CLA	CHD-C1D-ND	-3.36	120.08	124.80
9	A	808	CLA	O2A-CGA-CBA	3.36	124.60	114.00
12	B	845	BCR	C3-C4-C5	-3.35	108.08	114.06
9	A	815	CLA	CHD-C1D-ND	-3.35	120.09	124.80
9	B	836	CLA	C4-C3-C5	3.34	121.03	115.23
9	B	826	CLA	CHD-C1D-ND	-3.34	120.11	124.80
12	A	850	BCR	C7-C8-C9	-3.33	121.31	126.23
9	A	805	CLA	O2A-CGA-CBA	3.33	122.00	111.83
9	B	820	CLA	O2A-CGA-CBA	3.33	124.53	114.00
9	B	813	CLA	CHD-C1D-ND	-3.32	120.12	124.80
9	A	819	CLA	CMA-C3A-C4A	3.32	120.70	111.77
9	A	834	CLA	CHD-C1D-ND	-3.32	120.14	124.80
12	F	201	BCR	C7-C8-C9	-3.31	121.33	126.23
12	B	843	BCR	C37-C22-C21	-3.31	117.46	122.82
9	B	829	CLA	CHD-C1D-ND	-3.31	120.15	124.80
9	A	830	CLA	C2B-C1B-NB	3.30	113.75	110.33
9	I	101	CLA	C2B-C1B-NB	3.30	113.75	110.33
9	B	833	CLA	CHD-C1D-ND	-3.29	120.17	124.80
10	B	841	PQN	C14-C13-C15	3.29	120.95	115.23
9	A	813	CLA	CHD-C1D-ND	-3.29	120.17	124.80
9	B	833	CLA	O2A-CGA-CBA	3.29	124.40	114.00
9	A	838	CLA	CHD-C1D-ND	-3.28	120.18	124.80
9	B	829	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
9	B	804	CLA	C3C-C4C-NC	3.28	114.63	110.43
9	A	841	CLA	O2A-CGA-CBA	3.27	124.35	114.00
9	B	829	CLA	O2A-CGA-CBA	3.27	124.35	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	201	BCR	C34-C9-C10	-3.27	117.51	122.82
9	B	825	CLA	O2A-CGA-CBA	3.27	124.34	114.00
9	A	816	CLA	O2A-CGA-CBA	3.27	124.33	114.00
9	A	839	CLA	O2A-CGA-CBA	3.27	124.33	114.00
9	A	813	CLA	O2A-C1-C2	3.27	120.68	108.11
9	B	814	CLA	C2B-C1B-NB	3.27	113.71	110.33
9	A	815	CLA	O2A-CGA-CBA	3.27	124.32	114.00
9	B	810	CLA	O2A-CGA-CBA	3.26	124.31	114.00
9	A	844	CLA	O2A-CGA-CBA	3.26	124.30	114.00
9	B	803	CLA	CAA-C2A-C3A	-3.26	104.19	113.00
9	B	830	CLA	O2A-CGA-CBA	3.26	124.29	114.00
12	B	844	BCR	C24-C23-C22	-3.26	121.42	126.23
9	A	803	CLA	O2A-CGA-CBA	3.25	124.28	114.00
9	A	834	CLA	O2A-CGA-CBA	3.25	124.28	114.00
9	B	840	CLA	O2A-CGA-CBA	3.25	124.28	114.00
9	A	817	CLA	O2A-C1-C2	3.25	120.61	108.11
9	B	821	CLA	O2A-CGA-CBA	3.24	124.25	114.00
9	B	839	CLA	O2A-CGA-CBA	3.24	124.25	114.00
10	A	845	PQN	C14-C13-C15	3.24	120.85	115.23
9	B	828	CLA	C4D-C3D-CAD	3.23	111.62	108.11
12	B	844	BCR	C7-C8-C9	-3.23	121.46	126.23
9	B	811	CLA	C2B-C1B-NB	3.23	113.67	110.33
9	B	837	CLA	CMA-C3A-C4A	3.23	120.45	111.77
9	B	808	CLA	C4D-C3D-CAD	3.23	111.61	108.11
9	B	818	CLA	O2A-C1-C2	3.23	120.53	108.11
9	B	838	CLA	O2A-CGA-CBA	3.22	124.19	114.00
9	B	814	CLA	CAA-C2A-C3A	-3.22	104.29	113.00
9	B	824	CLA	C3C-C4C-NC	3.22	114.56	110.43
9	B	814	CLA	CHD-C1D-ND	-3.22	120.27	124.80
12	A	847	BCR	C38-C26-C25	-3.22	120.97	124.48
12	A	847	BCR	C36-C18-C17	-3.22	117.60	122.82
9	B	839	CLA	CMA-C3A-C4A	3.22	120.42	111.77
9	A	835	CLA	O2A-CGA-CBA	3.22	124.16	114.00
9	B	824	CLA	O2A-CGA-CBA	3.22	124.16	114.00
9	A	831	CLA	O2A-CGA-CBA	3.21	124.15	114.00
9	B	832	CLA	O2A-CGA-CBA	3.21	124.14	114.00
9	I	101	CLA	O2A-CGA-CBA	3.21	124.14	114.00
9	A	843	CLA	O2A-CGA-CBA	3.20	124.12	114.00
9	A	828	CLA	CMA-C3A-C4A	3.20	120.38	111.77
9	B	815	CLA	O2A-CGA-CBA	3.20	124.12	114.00
9	B	811	CLA	CMB-C2B-C1B	3.20	130.29	125.42
12	A	847	BCR	C7-C8-C9	-3.20	121.51	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	822	CLA	O2A-CGA-CBA	3.19	124.09	114.00
9	B	824	CLA	CHD-C1D-ND	-3.19	120.31	124.80
9	B	823	CLA	O2A-CGA-CBA	3.19	124.08	114.00
9	B	811	CLA	O2A-CGA-CBA	3.19	124.08	114.00
12	A	850	BCR	C34-C9-C10	-3.19	117.66	122.82
9	A	803	CLA	CMA-C3A-C4A	3.18	120.33	111.77
9	A	810	CLA	O2A-CGA-CBA	3.18	124.06	114.00
9	A	838	CLA	O2A-CGA-CBA	3.18	124.06	114.00
9	A	829	CLA	CMA-C3A-C4A	3.18	120.33	111.77
9	A	824	CLA	O2A-CGA-CBA	3.18	124.05	114.00
9	A	804	CLA	O2A-CGA-CBA	3.18	124.05	114.00
9	B	814	CLA	CMB-C2B-C1B	3.18	130.26	125.42
12	B	842	BCR	C37-C22-C21	-3.18	117.66	122.82
9	K	101	CLA	CMA-C3A-C4A	3.18	120.32	111.77
9	A	832	CLA	O2A-CGA-CBA	3.18	124.05	114.00
9	A	834	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
9	A	827	CLA	CAA-C2A-C3A	-3.18	104.42	113.00
9	A	823	CLA	CMA-C3A-C4A	3.17	120.31	111.77
9	B	834	CLA	O2A-CGA-CBA	3.17	124.02	114.00
9	B	812	CLA	CHD-C1D-ND	-3.17	120.34	124.80
9	B	816	CLA	O2A-CGA-CBA	3.17	124.01	114.00
9	B	818	CLA	CHD-C1D-ND	-3.17	120.34	124.80
9	A	807	CLA	O2A-CGA-CBA	3.17	124.00	114.00
12	B	847	BCR	C7-C8-C9	-3.16	121.55	126.23
9	A	833	CLA	O2A-CGA-CBA	3.16	124.00	114.00
9	A	823	CLA	O2A-CGA-CBA	3.16	123.99	114.00
9	B	823	CLA	CMB-C2B-C3B	3.16	133.99	126.55
9	B	815	CLA	CMC-C2C-C1C	3.16	129.97	125.03
9	B	805	CLA	O2A-CGA-CBA	3.16	123.97	114.00
9	A	804	CLA	C4D-C3D-CAD	3.16	111.53	108.11
9	A	829	CLA	C1-C2-C3	-3.15	121.03	126.20
9	A	836	CLA	O2A-CGA-CBA	3.15	123.95	114.00
9	B	835	CLA	O2A-CGA-CBA	3.15	123.95	114.00
9	K	101	CLA	O2A-CGA-CBA	3.15	123.95	114.00
9	B	823	CLA	CMC-C2C-C1C	3.15	129.95	125.03
9	A	825	CLA	CHD-C1D-ND	-3.15	120.38	124.80
9	A	825	CLA	O2A-CGA-CBA	3.15	121.43	111.83
9	A	837	CLA	O2A-CGA-CBA	3.14	123.93	114.00
9	B	827	CLA	CHD-C1D-ND	-3.14	120.38	124.80
9	B	812	CLA	O2A-CGA-CBA	3.14	123.93	114.00
9	B	801	CLA	CMB-C2B-C3B	3.13	133.91	126.55
9	B	835	CLA	CMA-C3A-C4A	3.13	120.19	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	805	CLA	CMC-C2C-C1C	3.13	129.93	125.03
9	A	822	CLA	CHD-C1D-ND	-3.13	120.40	124.80
9	B	818	CLA	CMA-C3A-C4A	3.13	120.18	111.77
9	A	812	CLA	O2A-CGA-CBA	3.13	123.88	114.00
9	B	808	CLA	C2B-C1B-NB	3.13	113.57	110.33
9	B	822	CLA	O2A-CGA-CBA	3.13	123.88	114.00
9	B	820	CLA	CMA-C3A-C4A	3.13	120.17	111.77
9	A	837	CLA	CMA-C3A-C4A	3.12	120.16	111.77
9	A	835	CLA	C4D-C3D-CAD	3.12	111.49	108.11
9	A	836	CLA	CMA-C3A-C4A	3.12	120.16	111.77
9	A	827	CLA	CMA-C3A-C4A	3.12	120.15	111.77
9	I	101	CLA	CHD-C1D-ND	-3.12	120.42	124.80
9	B	830	CLA	CMD-C2D-C3D	-3.11	120.55	127.69
12	A	848	BCR	C19-C18-C17	3.11	123.90	119.01
9	A	814	CLA	O2A-CGA-CBA	3.11	123.83	114.00
12	A	849	BCR	C3-C4-C5	-3.11	108.51	114.06
9	B	821	CLA	CMA-C3A-C4A	3.11	120.13	111.77
9	B	813	CLA	O1D-CGD-CBD	-3.11	118.39	124.52
9	B	806	CLA	C4D-C3D-CAD	3.11	111.48	108.11
9	B	831	CLA	O2A-CGA-CBA	3.11	123.82	114.00
9	B	808	CLA	O2A-CGA-CBA	3.11	123.81	114.00
9	B	811	CLA	CAA-C2A-C3A	-3.11	104.61	113.00
9	B	808	CLA	CMA-C3A-C4A	3.10	120.11	111.77
9	A	831	CLA	C4D-C3D-CAD	3.10	111.48	108.11
9	B	822	CLA	CMA-C3A-C4A	3.10	120.10	111.77
9	B	829	CLA	C4D-C3D-CAD	3.10	111.47	108.11
9	A	834	CLA	CMA-C3A-C4A	3.10	120.09	111.77
9	A	824	CLA	CMA-C3A-C4A	3.09	120.09	111.77
9	A	812	CLA	CMA-C3A-C4A	3.09	120.07	111.77
12	B	844	BCR	C19-C18-C17	3.09	123.86	119.01
9	A	843	CLA	CMA-C3A-C4A	3.08	120.06	111.77
9	B	802	CLA	CMC-C2C-C1C	3.07	129.84	125.03
9	A	822	CLA	CMA-C3A-C4A	3.07	120.03	111.77
9	B	836	CLA	CHD-C1D-ND	-3.07	120.48	124.80
9	B	820	CLA	CMD-C2D-C3D	-3.07	120.65	127.69
9	B	815	CLA	CMB-C2B-C1B	3.07	130.09	125.42
9	A	805	CLA	CBC-CAC-C3C	-3.07	104.10	112.42
9	A	815	CLA	CMA-C3A-C4A	3.07	120.02	111.77
9	A	809	CLA	CMA-C3A-C4A	3.06	120.00	111.77
9	A	827	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
9	B	840	CLA	CMA-C3A-C4A	3.06	120.00	111.77
9	A	838	CLA	CMA-C3A-C4A	3.06	120.00	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	826	CLA	CMA-C3A-C4A	3.06	120.00	111.77
9	B	806	CLA	O2A-C1-C2	3.06	119.88	108.11
13	A	853	LHG	O8-C23-C24	3.06	120.42	111.15
9	A	828	CLA	CMC-C2C-C1C	3.06	129.81	125.03
9	A	831	CLA	CMC-C2C-C1C	3.05	129.80	125.03
12	B	847	BCR	C19-C18-C17	3.05	123.81	119.01
9	A	811	CLA	CMA-C3A-C4A	3.05	119.97	111.77
9	A	828	CLA	CHD-C1D-ND	-3.05	120.51	124.80
9	B	803	CLA	CMC-C2C-C1C	3.04	129.79	125.03
12	A	848	BCR	C28-C27-C26	-3.04	108.64	114.06
9	B	839	CLA	C4D-C3D-CAD	3.04	111.41	108.11
9	A	840	CLA	O2A-C1-C2	3.04	119.80	108.11
9	B	804	CLA	C4D-C3D-CAD	3.04	111.41	108.11
8	A	801	CL0	CHD-C1D-ND	-3.04	120.53	124.80
9	A	825	CLA	CMD-C2D-C3D	-3.03	120.73	127.69
9	A	808	CLA	CHD-C1D-ND	-3.03	120.53	124.80
12	B	845	BCR	C34-C9-C10	-3.03	117.90	122.82
9	A	817	CLA	O1D-CGD-CBD	-3.03	118.54	124.52
9	A	824	CLA	CAA-C2A-C3A	-3.02	104.83	113.00
12	B	845	BCR	C38-C26-C25	-3.02	121.19	124.48
9	B	814	CLA	O2A-CGA-CBA	3.02	121.04	111.83
9	B	824	CLA	CMC-C2C-C1C	3.02	129.75	125.03
9	A	831	CLA	CHD-C1D-ND	-3.02	120.56	124.80
9	B	814	CLA	C1-C2-C3	-3.01	121.26	126.20
9	B	801	CLA	CHD-C1D-ND	-3.01	120.56	124.80
9	A	827	CLA	C3C-C4C-NC	3.01	114.29	110.43
12	B	846	BCR	C34-C9-C8	3.01	122.69	118.09
9	B	809	CLA	CMA-C3A-C4A	3.01	119.85	111.77
9	A	830	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
9	A	842	CLA	C1-C2-C3	-3.00	121.91	126.76
12	F	201	BCR	C33-C5-C6	-3.00	121.21	124.48
9	B	820	CLA	CHD-C1D-ND	-3.00	120.58	124.80
9	B	828	CLA	CMA-C3A-C4A	3.00	119.83	111.77
9	A	809	CLA	C1-C2-C3	-3.00	121.91	126.76
9	B	840	CLA	C2B-C1B-NB	3.00	113.43	110.33
9	B	830	CLA	CMA-C3A-C4A	2.99	119.82	111.77
9	B	810	CLA	CMC-C2C-C1C	2.99	129.71	125.03
12	F	201	BCR	C37-C22-C21	-2.99	117.97	122.82
9	B	830	CLA	C4D-C3D-CAD	2.99	111.35	108.11
9	A	817	CLA	CMA-C3A-C4A	2.99	119.80	111.77
12	A	848	BCR	C37-C22-C21	-2.98	117.99	122.82
9	A	831	CLA	CMA-C3A-C4A	2.98	119.78	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	813	CLA	CAC-C3C-C4C	2.98	128.66	124.79
9	A	802	CLA	C1-O2A-CGA	2.98	123.86	116.65
12	B	844	BCR	C36-C18-C17	-2.97	118.00	122.82
9	A	841	CLA	CAA-C2A-C3A	-2.97	104.97	113.00
12	A	849	BCR	C38-C26-C27	2.97	119.93	113.60
9	B	824	CLA	CMA-C3A-C4A	2.97	119.75	111.77
12	A	848	BCR	C36-C18-C17	-2.97	118.01	122.82
9	B	813	CLA	CMA-C3A-C4A	2.96	119.74	111.77
9	A	818	CLA	CMA-C3A-C4A	2.96	119.74	111.77
9	B	819	CLA	CMA-C3A-C4A	2.96	119.74	111.77
9	B	835	CLA	CAA-C2A-C3A	-2.96	104.99	113.00
12	A	850	BCR	C19-C18-C17	2.96	123.67	119.01
9	B	827	CLA	CMA-C3A-C4A	2.96	119.72	111.77
9	B	802	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
9	A	831	CLA	CMD-C2D-C3D	-2.95	120.92	127.69
9	B	803	CLA	CHD-C1D-ND	-2.95	120.65	124.80
9	B	810	CLA	CAA-C2A-C3A	-2.94	105.04	113.00
9	A	808	CLA	CMB-C2B-C1B	2.94	129.90	125.42
12	B	843	BCR	C30-C25-C26	-2.94	118.61	122.64
9	A	822	CLA	CMC-C2C-C1C	2.94	129.63	125.03
9	B	801	CLA	C4-C3-C5	2.94	120.33	115.23
9	A	832	CLA	CMA-C3A-C4A	2.94	119.67	111.77
14	B	848	LMG	C8-O7-C10	-2.94	110.76	117.80
12	A	850	BCR	C36-C18-C17	-2.94	118.05	122.82
9	B	814	CLA	CMA-C3A-C4A	2.94	119.67	111.77
12	A	850	BCR	C33-C5-C6	-2.94	121.28	124.48
9	A	802	CLA	OBD-CAD-C3D	-2.94	121.55	128.42
9	B	811	CLA	CMA-C3A-C4A	2.94	119.66	111.77
9	A	844	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
12	A	851	BCR	C30-C25-C26	-2.93	118.63	122.64
9	A	838	CLA	C4D-C3D-CAD	2.93	111.29	108.11
9	A	807	CLA	CMC-C2C-C1C	2.93	129.61	125.03
9	B	809	CLA	CMB-C2B-C1B	2.93	129.88	125.42
9	B	835	CLA	C4D-C3D-CAD	2.93	111.29	108.11
9	B	804	CLA	CMC-C2C-C1C	2.93	129.61	125.03
9	B	819	CLA	C4D-C3D-CAD	2.92	111.28	108.11
9	B	828	CLA	C4-C3-C5	2.92	120.30	115.23
9	B	810	CLA	CMA-C3A-C4A	2.92	119.63	111.77
9	B	839	CLA	CMD-C2D-C3D	-2.92	120.99	127.69
12	B	843	BCR	C33-C5-C4	2.92	119.82	113.60
9	A	817	CLA	C1-C2-C3	-2.92	122.04	126.76
9	B	803	CLA	C4-C3-C5	2.92	120.29	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	802	CLA	CAA-C2A-C3A	-2.92	105.11	113.00
9	A	810	CLA	CMA-C3A-C4A	2.91	119.61	111.77
9	A	803	CLA	CAA-C2A-C3A	-2.91	105.12	113.00
9	B	824	CLA	CHD-C4C-C3C	-2.91	120.53	124.77
9	A	830	CLA	CMA-C3A-C4A	2.90	119.58	111.77
9	A	808	CLA	CMA-C3A-C4A	2.90	119.58	111.77
9	B	809	CLA	CAA-C2A-C3A	-2.90	105.15	113.00
9	B	812	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
9	B	837	CLA	C4D-C3D-CAD	2.89	111.25	108.11
9	B	826	CLA	C4D-C3D-CAD	2.89	111.25	108.11
12	A	849	BCR	C31-C1-C6	-2.89	105.71	110.24
12	A	848	BCR	C38-C26-C25	-2.89	121.33	124.48
9	A	825	CLA	CMC-C2C-C1C	2.89	129.55	125.03
12	A	851	BCR	C38-C26-C27	2.89	119.75	113.60
9	A	802	CLA	CMA-C3A-C4A	2.88	119.53	111.77
9	B	820	CLA	CMC-C2C-C1C	2.88	129.54	125.03
9	A	841	CLA	C4D-C3D-CAD	2.88	111.24	108.11
9	B	816	CLA	CMA-C3A-C4A	2.88	119.52	111.77
9	B	829	CLA	CMD-C2D-C3D	-2.88	121.09	127.69
9	B	823	CLA	CAA-C2A-C3A	-2.88	105.22	113.00
9	A	825	CLA	CBA-CAA-C2A	2.88	122.35	113.79
9	B	813	CLA	C4D-C3D-CAD	2.87	111.23	108.11
9	B	808	CLA	CMC-C2C-C1C	2.87	129.52	125.03
9	A	823	CLA	CMB-C2B-C1B	2.87	129.79	125.42
9	B	839	CLA	C3D-C4D-ND	2.87	114.65	109.99
9	B	827	CLA	C1-C2-C3	-2.87	121.49	126.20
12	B	842	BCR	C28-C27-C26	-2.87	108.94	114.06
9	A	814	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
8	A	801	CL0	CMB-C2B-C3B	2.87	133.29	126.55
9	A	838	CLA	CMC-C2C-C1C	2.86	129.51	125.03
12	B	842	BCR	C23-C22-C21	2.86	123.51	119.01
12	B	846	BCR	C34-C9-C10	-2.86	118.18	122.82
12	B	842	BCR	C34-C9-C10	-2.86	118.18	122.82
9	A	811	CLA	CMD-C2D-C3D	-2.86	121.13	127.69
9	A	831	CLA	CAA-C2A-C3A	-2.86	105.28	113.00
9	B	831	CLA	C4D-C3D-CAD	2.86	111.21	108.11
9	A	837	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
9	B	840	CLA	C4D-C3D-CAD	2.86	111.21	108.11
9	B	835	CLA	CMB-C2B-C1B	2.85	129.76	125.42
9	B	826	CLA	CAA-C2A-C3A	-2.85	105.29	113.00
9	A	828	CLA	C4D-C3D-CAD	2.85	111.20	108.11
12	A	847	BCR	C38-C26-C27	2.85	119.67	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	807	CLA	CMA-C3A-C4A	2.85	119.43	111.77
9	B	802	CLA	CAA-C2A-C3A	-2.85	105.30	113.00
9	A	813	CLA	CMC-C2C-C1C	2.85	129.48	125.03
12	B	846	BCR	C33-C5-C4	2.85	119.67	113.60
12	B	843	BCR	C23-C22-C21	2.85	123.49	119.01
9	B	809	CLA	C4D-C3D-CAD	2.85	111.20	108.11
9	B	834	CLA	C4D-C3D-CAD	2.85	111.20	108.11
12	A	848	BCR	C3-C4-C5	-2.84	108.98	114.06
9	A	838	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
9	B	826	CLA	C4-C3-C5	2.84	120.16	115.23
9	A	840	CLA	CMA-C3A-C4A	2.84	119.41	111.77
9	B	815	CLA	CMA-C3A-C4A	2.84	119.41	111.77
9	A	810	CLA	C4D-C3D-CAD	2.84	111.19	108.11
9	A	820	CLA	CMC-C2C-C1C	2.84	129.47	125.03
9	A	814	CLA	CMB-C2B-C3B	2.84	133.23	126.55
12	A	847	BCR	C33-C5-C6	-2.84	121.39	124.48
9	K	101	CLA	C4D-C3D-CAD	2.84	111.24	107.69
9	B	829	CLA	CAA-C2A-C3A	-2.84	105.34	113.00
9	A	825	CLA	CAC-C3C-C4C	2.83	128.48	124.79
9	A	831	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
9	A	832	CLA	CAA-C2A-C3A	-2.83	105.34	113.00
9	B	808	CLA	C3C-C4C-NC	2.83	114.06	110.43
9	K	101	CLA	CMD-C2D-C3D	-2.83	121.20	127.69
9	A	808	CLA	C4D-C3D-CAD	2.83	111.18	108.11
9	A	843	CLA	C4D-C3D-CAD	2.83	111.18	108.11
12	B	845	BCR	C33-C5-C4	2.83	119.62	113.60
9	A	844	CLA	C3C-C4C-NC	2.83	114.05	110.43
12	B	843	BCR	C15-C14-C13	-2.83	123.31	127.28
9	B	805	CLA	C4D-C3D-CAD	2.82	111.17	108.11
9	A	842	CLA	CMB-C2B-C1B	2.82	129.72	125.42
9	A	804	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
9	A	809	CLA	CAA-C2A-C3A	-2.82	105.38	113.00
9	A	830	CLA	CMB-C2B-C1B	2.82	129.71	125.42
9	A	813	CLA	CAA-C2A-C3A	-2.82	105.38	113.00
9	A	815	CLA	CMC-C2C-C1C	2.82	129.43	125.03
9	A	839	CLA	CMA-C3A-C4A	2.81	119.34	111.77
9	A	834	CLA	CMB-C2B-C1B	2.81	129.70	125.42
9	B	826	CLA	CAC-C3C-C4C	2.81	128.45	124.79
9	A	812	CLA	C4D-C3D-CAD	2.81	111.16	108.11
9	A	808	CLA	CMC-C2C-C1C	2.81	129.43	125.03
9	A	837	CLA	C4D-C3D-CAD	2.81	111.16	108.11
12	M	101	BCR	C38-C26-C25	-2.81	121.42	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	842	CLA	CMC-C2C-C1C	2.81	129.42	125.03
9	A	829	CLA	C3C-C4C-NC	2.80	114.02	110.43
12	A	850	BCR	C38-C26-C27	2.80	119.56	113.60
9	A	810	CLA	CMC-C2C-C1C	2.79	129.40	125.03
9	B	832	CLA	CMA-C3A-C4A	2.79	119.28	111.77
9	A	834	CLA	CAA-C2A-C3A	-2.79	105.45	113.00
9	B	821	CLA	CAA-C2A-C3A	-2.79	105.45	113.00
9	B	818	CLA	CMC-C2C-C1C	2.79	129.40	125.03
9	A	817	CLA	CMC-C2C-C1C	2.79	129.39	125.03
9	B	813	CLA	CMD-C2D-C3D	-2.79	121.30	127.69
9	A	806	CLA	CMC-C2C-C1C	2.79	129.39	125.03
9	B	837	CLA	O2A-C1-C2	2.79	118.83	108.11
12	F	201	BCR	C15-C14-C13	-2.79	123.37	127.28
9	B	807	CLA	C1-C2-C3	-2.78	121.64	126.20
9	A	839	CLA	C3D-C4D-ND	2.78	114.51	109.99
9	A	818	CLA	C4D-C3D-CAD	2.78	111.13	108.11
9	B	803	CLA	C3C-C4C-NC	2.78	113.99	110.43
12	B	844	BCR	C33-C5-C4	2.78	119.52	113.60
9	A	821	CLA	C4D-C3D-CAD	2.78	111.12	108.11
9	A	840	CLA	CMC-C2C-C1C	2.78	129.38	125.03
9	A	840	CLA	C4D-C3D-CAD	2.78	111.12	108.11
9	B	811	CLA	C4D-C3D-CAD	2.78	111.12	108.11
9	B	827	CLA	C3C-C4C-NC	2.78	113.99	110.43
9	A	811	CLA	CMC-C2C-C1C	2.78	129.37	125.03
9	A	840	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
9	A	830	CLA	C3D-C4D-ND	2.78	114.50	109.99
9	I	101	CLA	CMA-C3A-C4A	2.77	119.23	111.77
9	B	838	CLA	CMC-C2C-C1C	2.77	129.37	125.03
12	B	843	BCR	C32-C1-C6	-2.77	105.90	110.24
9	B	823	CLA	C4D-C3D-CAD	2.77	111.11	108.11
9	B	809	CLA	C1-C2-C3	-2.77	121.66	126.20
9	B	836	CLA	C3C-C4C-NC	2.77	113.97	110.43
9	B	828	CLA	C3C-C4C-NC	2.77	113.97	110.43
9	A	816	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
9	A	835	CLA	CMB-C2B-C1B	2.76	129.62	125.42
9	B	812	CLA	C4D-C3D-CAD	2.76	111.10	108.11
9	B	808	CLA	OBD-CAD-C3D	-2.76	121.97	128.42
9	A	839	CLA	CMC-C2C-C1C	2.75	129.34	125.03
9	A	830	CLA	C1-C2-C3	-2.75	121.69	126.20
9	A	802	CLA	C4D-C3D-CAD	2.75	111.09	108.11
9	B	835	CLA	CMC-C2C-C1C	2.75	129.33	125.03
9	A	843	CLA	CMC-C2C-C1C	2.75	129.32	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	832	CLA	CMC-C2C-C1C	2.74	129.32	125.03
9	B	824	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
12	B	844	BCR	C1-C6-C5	-2.74	118.89	122.64
9	A	836	CLA	CMC-C2C-C1C	2.74	129.32	125.03
9	A	822	CLA	C4D-C3D-CAD	2.73	111.08	108.11
9	B	814	CLA	C3D-C4D-ND	2.73	114.43	109.99
12	B	845	BCR	C34-C9-C8	2.73	122.26	118.09
9	A	804	CLA	CMC-C2C-C1C	2.73	129.30	125.03
9	A	812	CLA	CAC-C3C-C4C	2.73	128.34	124.79
9	B	826	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
9	A	825	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
9	B	821	CLA	C4D-C3D-CAD	2.73	111.07	108.11
9	A	844	CLA	CAA-C2A-C3A	-2.72	105.64	113.00
12	B	847	BCR	C36-C18-C17	-2.72	118.41	122.82
9	B	815	CLA	C4D-C3D-CAD	2.72	111.06	108.11
9	A	832	CLA	CMC-C2C-C1C	2.72	129.29	125.03
9	A	808	CLA	C3C-C4C-NC	2.72	113.92	110.43
9	B	822	CLA	C4D-C3D-CAD	2.72	111.06	108.11
9	A	833	CLA	C4D-C3D-CAD	2.72	111.06	108.11
9	B	833	CLA	CAA-C2A-C3A	-2.72	105.65	113.00
9	A	821	CLA	CMC-C2C-C1C	2.72	129.28	125.03
9	A	803	CLA	CMC-C2C-C1C	2.72	129.28	125.03
12	M	101	BCR	C36-C18-C17	-2.71	118.42	122.82
9	I	101	CLA	CAA-C2A-C3A	-2.71	105.67	113.00
9	B	826	CLA	CMD-C2D-C3D	-2.71	121.47	127.69
9	B	820	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
9	A	814	CLA	C4D-C3D-CAD	2.71	111.05	108.11
9	B	803	CLA	OBD-CAD-C3D	-2.71	122.09	128.42
8	A	801	CL0	CMC-C2C-C1C	2.71	129.26	125.03
9	A	836	CLA	CMB-C2B-C3B	2.70	132.91	126.55
10	A	845	PQN	C2M-C2-C3	-2.70	120.00	124.45
9	A	839	CLA	C4D-C3D-CAD	2.70	111.04	108.11
9	A	825	CLA	C3C-C4C-NC	2.70	113.89	110.43
9	A	827	CLA	CMB-C2B-C3B	2.70	132.90	126.55
9	A	808	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
12	F	201	BCR	C36-C18-C17	-2.70	118.44	122.82
9	B	821	CLA	CMC-C2C-C1C	2.70	129.25	125.03
9	B	810	CLA	C3D-C4D-ND	2.70	114.37	109.99
9	A	819	CLA	CMC-C2C-C1C	2.70	129.25	125.03
9	B	803	CLA	C4D-C3D-CAD	2.70	111.04	108.11
8	A	801	CL0	C1-O2A-CGA	2.70	123.18	116.65
9	A	843	CLA	CAA-C2A-C3A	-2.70	105.71	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	833	CLA	CAC-C3C-C4C	2.70	128.30	124.79
9	A	807	CLA	C4D-C3D-CAD	2.69	111.03	108.11
9	K	101	CLA	CMC-C2C-C1C	2.69	129.24	125.03
9	B	814	CLA	CMC-C2C-C1C	2.69	129.24	125.03
9	A	837	CLA	CMC-C2C-C1C	2.69	129.24	125.03
9	A	823	CLA	CMD-C2D-C3D	-2.69	121.52	127.69
9	B	812	CLA	CMA-C3A-C4A	2.68	118.99	111.77
9	B	833	CLA	C4D-C3D-CAD	2.68	111.02	108.11
9	A	820	CLA	CMB-C2B-C1B	2.68	129.50	125.42
9	A	816	CLA	CMC-C2C-C1C	2.68	129.22	125.03
9	A	820	CLA	CAA-C2A-C3A	-2.67	105.77	113.00
9	A	834	CLA	C4D-C3D-CAD	2.67	111.01	108.11
12	B	847	BCR	C37-C22-C21	-2.67	118.49	122.82
9	B	808	CLA	C3D-C4D-ND	2.67	114.33	109.99
12	A	847	BCR	C34-C9-C8	2.67	122.17	118.09
9	A	809	CLA	CAC-C3C-C4C	2.67	128.26	124.79
9	I	101	CLA	CMB-C2B-C1B	2.67	129.48	125.42
9	B	819	CLA	C3C-C4C-NC	2.67	113.85	110.43
12	A	849	BCR	C30-C25-C24	2.67	122.88	115.65
9	B	816	CLA	C4D-C3D-CAD	2.67	111.00	108.11
9	B	839	CLA	CMC-C2C-C1C	2.66	129.20	125.03
9	B	837	CLA	C3D-C4D-ND	2.66	114.32	109.99
9	B	824	CLA	C3D-C4D-ND	2.66	114.32	109.99
9	B	827	CLA	C4D-C3D-CAD	2.66	111.00	108.11
9	B	801	CLA	C3C-C4C-NC	2.66	113.84	110.43
9	A	835	CLA	CMC-C2C-C1C	2.66	129.19	125.03
12	B	842	BCR	C15-C14-C13	-2.66	123.55	127.28
12	A	847	BCR	C34-C9-C10	-2.66	118.50	122.82
9	B	838	CLA	C3D-C4D-ND	2.66	114.31	109.99
9	A	823	CLA	C4D-C3D-CAD	2.66	111.00	108.11
9	B	819	CLA	CMC-C2C-C1C	2.66	129.19	125.03
9	B	822	CLA	CMC-C2C-C1C	2.66	129.19	125.03
9	B	812	CLA	CAC-C3C-C4C	2.66	128.25	124.79
9	A	842	CLA	C4D-C3D-CAD	2.66	110.99	108.11
9	A	833	CLA	CMC-C2C-C1C	2.66	129.18	125.03
9	A	813	CLA	CMA-C3A-C4A	2.65	118.91	111.77
9	B	816	CLA	CMC-C2C-C1C	2.65	129.18	125.03
9	I	101	CLA	CAC-C3C-C4C	2.65	128.24	124.79
9	B	813	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
9	B	820	CLA	CMB-C2B-C1B	2.65	129.46	125.42
9	B	834	CLA	CMC-C2C-C1C	2.65	129.18	125.03
9	I	101	CLA	CMC-C2C-C1C	2.65	129.18	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	840	CLA	CAA-C2A-C3A	-2.65	105.83	113.00
9	A	812	CLA	CMB-C2B-C3B	2.65	132.79	126.55
9	B	810	CLA	C4D-C3D-CAD	2.65	110.99	108.11
9	K	101	CLA	CMB-C2B-C1B	2.65	129.46	125.42
9	B	810	CLA	C3C-C4C-NC	2.65	113.82	110.43
9	A	837	CLA	CAA-C2A-C3A	-2.65	105.84	113.00
9	A	827	CLA	C1-C2-C3	-2.65	121.86	126.20
9	A	828	CLA	C3C-C4C-NC	2.65	113.82	110.43
9	B	806	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
9	B	832	CLA	C3D-C4D-ND	2.64	114.28	109.99
9	B	811	CLA	C3D-C4D-ND	2.64	114.28	109.99
9	A	827	CLA	CHD-C4C-C3C	-2.64	120.92	124.77
9	B	826	CLA	C3C-C4C-NC	2.64	113.81	110.43
9	B	813	CLA	C1-C2-C3	-2.64	121.87	126.20
9	B	802	CLA	C2B-C1B-NB	2.64	113.06	110.33
12	B	847	BCR	C34-C9-C10	-2.64	118.54	122.82
12	F	201	BCR	C19-C18-C17	2.64	123.16	119.01
9	B	831	CLA	CMC-C2C-C1C	2.64	129.16	125.03
9	B	834	CLA	CMD-C2D-C3D	-2.64	121.64	127.69
12	B	845	BCR	C28-C27-C26	-2.64	109.36	114.06
9	A	829	CLA	CHD-C1D-ND	-2.64	121.09	124.80
9	B	822	CLA	C3C-C4C-NC	2.63	113.81	110.43
9	A	817	CLA	C3C-C4C-NC	2.63	113.80	110.43
9	A	820	CLA	C1-O2A-CGA	2.63	123.02	116.65
9	A	840	CLA	C1-C2-C3	-2.63	122.50	126.76
9	A	813	CLA	C3C-C4C-NC	2.63	113.80	110.43
9	A	832	CLA	C3D-C4D-ND	2.63	114.27	109.99
9	A	811	CLA	CMB-C2B-C1B	2.63	129.42	125.42
9	B	812	CLA	CMC-C2C-C1C	2.63	129.14	125.03
9	A	819	CLA	C3D-C4D-ND	2.63	114.26	109.99
9	A	816	CLA	C3D-C4D-ND	2.63	114.26	109.99
9	A	826	CLA	C1-C2-C3	-2.63	121.89	126.20
9	A	820	CLA	C4D-C3D-CAD	2.63	110.96	108.11
9	B	801	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
9	I	101	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
9	A	840	CLA	C1-O2A-CGA	2.62	122.99	116.65
9	A	817	CLA	C3D-C4D-ND	2.62	114.25	109.99
9	K	101	CLA	C3D-C4D-ND	2.62	114.25	109.99
9	B	825	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
9	B	809	CLA	C3D-C4D-ND	2.62	114.24	109.99
9	A	821	CLA	C1-O2A-CGA	2.62	122.99	116.65
9	B	835	CLA	C3D-C4D-ND	2.62	114.24	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	824	CLA	C3D-C4D-ND	2.61	114.23	109.99
9	A	826	CLA	C3D-C4D-ND	2.61	114.23	109.99
12	A	851	BCR	C8-C9-C10	2.61	123.12	119.01
9	B	836	CLA	C4D-C3D-CAD	2.61	110.94	108.11
9	A	803	CLA	C4D-C3D-CAD	2.61	110.94	108.11
9	A	834	CLA	O1D-CGD-CBD	-2.61	119.37	124.52
9	B	821	CLA	CAC-C3C-C4C	2.61	128.19	124.79
9	A	815	CLA	CAA-C2A-C3A	-2.61	105.94	113.00
9	B	814	CLA	C1-O2A-CGA	2.61	122.97	116.65
9	A	803	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
9	A	820	CLA	C3D-C4D-ND	2.61	114.23	109.99
9	A	842	CLA	C1-O2A-CGA	2.61	122.97	116.65
9	A	833	CLA	CAA-C2A-C3A	-2.61	105.95	113.00
9	A	841	CLA	CMB-C2B-C1B	2.61	129.39	125.42
9	A	843	CLA	CMB-C2B-C1B	2.61	129.39	125.42
9	B	827	CLA	CAC-C3C-C4C	2.61	128.18	124.79
9	B	807	CLA	C4D-C3D-CAD	2.60	110.93	108.11
9	A	818	CLA	CMD-C2D-C3D	-2.60	121.72	127.69
9	B	836	CLA	C1-C2-C3	-2.60	121.93	126.20
9	A	802	CLA	C3D-C4D-ND	2.60	114.22	109.99
9	A	828	CLA	CAC-C3C-C4C	2.60	128.18	124.79
9	B	838	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
9	A	815	CLA	C4D-C3D-CAD	2.60	110.93	108.11
9	A	805	CLA	C3D-C4D-ND	2.60	114.21	109.99
9	A	805	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
9	A	822	CLA	C3C-C4C-NC	2.60	113.76	110.43
9	B	835	CLA	CMD-C2D-C3D	-2.60	121.73	127.69
9	B	830	CLA	CMC-C2C-C1C	2.60	129.09	125.03
9	A	841	CLA	C3D-C4D-ND	2.60	114.20	109.99
9	A	840	CLA	CMD-C2D-C3D	-2.59	121.74	127.69
9	B	838	CLA	CAA-C2A-C3A	-2.59	105.99	113.00
9	A	826	CLA	CMC-C2C-C1C	2.59	129.08	125.03
9	A	806	CLA	C3D-C4D-ND	2.59	114.20	109.99
8	A	801	CL0	C4D-C3D-CAD	2.59	110.92	108.11
9	B	833	CLA	C3D-C4D-ND	2.59	114.20	109.99
9	B	801	CLA	CHD-C4C-C3C	-2.59	121.00	124.77
9	A	807	CLA	CMB-C2B-C1B	2.59	129.36	125.42
9	A	838	CLA	C3C-C4C-NC	2.59	113.75	110.43
9	B	831	CLA	C3D-C4D-ND	2.59	114.19	109.99
12	M	101	BCR	C19-C18-C17	2.59	123.08	119.01
9	A	819	CLA	C4D-C3D-CAD	2.59	110.92	108.11
9	A	805	CLA	C4D-C3D-CAD	2.59	110.92	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	807	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
9	A	803	CLA	C3D-C4D-ND	2.58	114.19	109.99
9	B	806	CLA	CMB-C2B-C1B	2.58	129.35	125.42
9	A	823	CLA	CMC-C2C-C1C	2.58	129.07	125.03
9	A	835	CLA	C3D-C4D-ND	2.58	114.18	109.99
9	B	828	CLA	CMB-C2B-C1B	2.58	129.35	125.42
9	A	816	CLA	C4D-C3D-CAD	2.58	110.91	108.11
9	B	837	CLA	CMC-C2C-C1C	2.58	129.06	125.03
9	A	842	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
9	A	843	CLA	C3D-C4D-ND	2.58	114.18	109.99
9	A	814	CLA	CMC-C2C-C1C	2.58	129.06	125.03
9	A	802	CLA	C3C-C4C-NC	2.58	113.73	110.43
9	A	833	CLA	CMA-C3A-C4A	2.57	118.69	111.77
9	A	836	CLA	C4D-C3D-CAD	2.57	110.90	108.11
9	B	825	CLA	C3D-C4D-ND	2.57	114.17	109.99
9	A	815	CLA	C3C-C4C-NC	2.57	113.73	110.43
9	A	815	CLA	C3D-C4D-ND	2.57	114.17	109.99
9	A	811	CLA	CAC-C3C-C4C	2.57	128.13	124.79
9	A	832	CLA	C4D-C3D-CAD	2.57	110.90	108.11
9	B	804	CLA	C4C-C3C-C2C	-2.57	103.15	106.89
9	A	818	CLA	CMC-C2C-C1C	2.57	129.05	125.03
9	B	833	CLA	CMA-C3A-C4A	2.57	118.67	111.77
9	A	807	CLA	C3D-C4D-ND	2.57	114.16	109.99
9	A	842	CLA	C3D-C4D-ND	2.57	114.16	109.99
9	B	815	CLA	C3C-C4C-NC	2.57	113.72	110.43
9	B	840	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
9	B	825	CLA	CAC-C3C-C4C	2.56	128.12	124.79
9	B	804	CLA	CAA-C2A-C3A	-2.56	106.08	113.00
9	A	823	CLA	C3D-C4D-ND	2.56	114.15	109.99
9	A	817	CLA	C1-O2A-CGA	2.56	122.85	116.65
9	B	830	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
9	A	831	CLA	CAC-C3C-C4C	2.56	128.12	124.79
9	A	839	CLA	CAC-C3C-C4C	2.56	128.12	124.79
8	A	801	CL0	CBA-CAA-C2A	2.56	121.41	113.79
9	A	812	CLA	CMC-C2C-C1C	2.56	129.03	125.03
9	B	824	CLA	C4D-C3D-CAD	2.55	110.88	108.11
9	B	834	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
9	A	803	CLA	CMB-C2B-C1B	2.55	129.31	125.42
12	B	844	BCR	C34-C9-C8	2.55	121.98	118.09
9	A	821	CLA	CMD-C2D-C3D	-2.55	121.84	127.69
9	B	812	CLA	C3D-C4D-ND	2.55	114.13	109.99
9	A	837	CLA	C3D-C4D-ND	2.55	114.13	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	813	CLA	CMD-C2D-C3D	-2.55	121.85	127.69
9	A	810	CLA	C3C-C4C-NC	2.55	113.69	110.43
9	B	821	CLA	C3D-C4D-ND	2.55	114.12	109.99
9	B	806	CLA	CMD-C2D-C3D	-2.54	121.86	127.69
9	A	807	CLA	CAC-C3C-C4C	2.54	128.10	124.79
9	A	829	CLA	CAC-C3C-C4C	2.54	128.09	124.79
9	B	819	CLA	CMB-C2B-C3B	2.54	132.52	126.55
9	A	822	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
9	B	809	CLA	CMC-C2C-C1C	2.54	129.00	125.03
13	A	852	LHG	O8-C23-C24	2.54	119.58	111.83
9	B	829	CLA	C3D-C4D-ND	2.54	114.11	109.99
9	A	806	CLA	C4D-C3D-CAD	2.54	110.86	108.11
14	B	848	LMG	O8-C28-C29	2.54	119.57	111.83
9	A	839	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
9	A	823	CLA	C3C-C4C-NC	2.54	113.68	110.43
9	I	101	CLA	C4D-C3D-CAD	2.54	110.86	108.11
9	A	814	CLA	CAC-C3C-C4C	2.53	128.09	124.79
9	B	835	CLA	CAC-C3C-C4C	2.53	128.09	124.79
12	A	850	BCR	C35-C13-C12	2.53	121.96	118.09
9	A	824	CLA	CMD-C2D-C3D	-2.53	121.88	127.69
9	A	835	CLA	CMD-C2D-C3D	-2.53	121.89	127.69
9	A	836	CLA	CAC-C3C-C4C	2.53	128.08	124.79
9	A	813	CLA	C4D-C3D-CAD	2.53	110.85	108.11
9	A	839	CLA	CMB-C2B-C1B	2.53	129.27	125.42
9	B	832	CLA	CAA-C2A-C3A	-2.53	106.17	113.00
9	B	814	CLA	C4D-C3D-CAD	2.52	110.85	108.11
9	A	835	CLA	CAC-C3C-C4C	2.52	128.07	124.79
9	B	821	CLA	CMD-C2D-C3D	-2.52	121.90	127.69
9	A	841	CLA	CMC-C2C-C1C	2.52	128.98	125.03
9	A	829	CLA	C4D-C3D-CAD	2.52	110.84	108.11
9	A	825	CLA	C1-O2A-CGA	2.52	122.75	116.65
9	A	832	CLA	C3C-C4C-NC	2.52	113.66	110.43
12	A	849	BCR	C36-C18-C17	-2.52	118.73	122.82
12	A	850	BCR	C37-C22-C21	-2.52	118.73	122.82
12	B	847	BCR	C34-C9-C8	2.52	121.94	118.09
8	A	801	CL0	CAA-C2A-C3A	-2.52	106.19	113.00
12	B	843	BCR	C2-C1-C6	2.52	114.10	110.44
9	A	819	CLA	CBA-CAA-C2A	2.52	121.28	113.79
9	B	832	CLA	C4D-C3D-CAD	2.52	110.84	108.11
9	B	834	CLA	CMB-C2B-C3B	2.51	132.46	126.55
9	A	840	CLA	CAC-C3C-C4C	2.51	128.06	124.79
9	B	809	CLA	O2D-CGD-O1D	-2.51	118.95	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	824	CLA	CMC-C2C-C1C	2.51	128.96	125.03
9	A	817	CLA	C4D-C3D-CAD	2.51	110.83	108.11
9	B	823	CLA	CMD-C2D-C3D	-2.51	121.93	127.69
9	B	805	CLA	C3D-C4D-ND	2.51	114.07	109.99
9	B	823	CLA	CAC-C3C-C4C	2.51	128.06	124.79
9	A	818	CLA	C3D-C4D-ND	2.51	114.07	109.99
9	A	836	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
9	A	830	CLA	CMC-C2C-C1C	2.51	128.96	125.03
9	B	808	CLA	CMB-C2B-C1B	2.51	129.24	125.42
9	A	834	CLA	C3C-C4C-NC	2.51	113.64	110.43
9	B	830	CLA	C3C-C4C-NC	2.51	113.64	110.43
12	A	851	BCR	C33-C5-C4	2.51	118.94	113.60
9	A	806	CLA	C4-C3-C5	2.51	119.58	115.23
9	B	818	CLA	CBA-CAA-C2A	2.51	121.25	113.79
9	B	802	CLA	CHD-C1D-ND	-2.51	121.28	124.80
9	B	831	CLA	CAC-C3C-C4C	2.50	128.05	124.79
9	B	826	CLA	C1-C2-C3	-2.50	122.09	126.20
9	B	823	CLA	C3D-C4D-ND	2.50	114.06	109.99
9	A	839	CLA	CAA-C2A-C3A	-2.50	106.23	113.00
9	A	824	CLA	O2D-CGD-O1D	-2.50	118.97	123.85
12	A	851	BCR	C1-C6-C7	2.50	122.44	115.65
9	B	832	CLA	CAC-C3C-C4C	2.50	128.05	124.79
9	A	828	CLA	CMB-C2B-C1B	2.50	129.23	125.42
9	A	825	CLA	C4-C3-C5	2.50	119.57	115.23
9	A	821	CLA	C1-C2-C3	-2.50	122.10	126.20
9	A	822	CLA	CAC-C3C-C4C	2.50	128.04	124.79
9	B	827	CLA	C3D-C4D-ND	2.50	114.05	109.99
9	A	812	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
9	A	824	CLA	CMB-C2B-C1B	2.50	129.22	125.42
12	A	850	BCR	C34-C9-C8	2.50	121.90	118.09
9	A	826	CLA	CMA-C3A-C4A	2.50	118.48	111.77
9	A	840	CLA	C3D-C4D-ND	2.50	114.05	109.99
9	A	841	CLA	CMD-C2D-C3D	-2.50	121.96	127.69
9	I	101	CLA	C3C-C4C-NC	2.50	113.63	110.43
9	A	811	CLA	C3D-C4D-ND	2.50	114.04	109.99
9	A	821	CLA	CAC-C3C-C4C	2.50	128.04	124.79
9	B	838	CLA	CAC-C3C-C4C	2.49	128.03	124.79
9	B	812	CLA	C3C-C4C-NC	2.49	113.62	110.43
9	B	814	CLA	C3C-C4C-NC	2.49	113.62	110.43
9	A	821	CLA	CHB-C1B-C2B	-2.49	120.20	127.43
9	B	818	CLA	C3C-C4C-NC	2.49	113.62	110.43
9	A	824	CLA	C4D-C3D-CAD	2.49	110.81	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	846	BCR	C38-C26-C27	2.49	118.90	113.60
9	B	814	CLA	CBA-CAA-C2A	2.49	121.19	113.79
9	A	843	CLA	C3C-C4C-NC	2.48	113.61	110.43
9	A	819	CLA	CAC-C3C-C4C	2.48	128.02	124.79
9	B	838	CLA	C4D-C3D-CAD	2.48	110.80	108.11
9	A	816	CLA	CAA-C2A-C3A	-2.48	106.30	113.00
9	A	809	CLA	C4D-C3D-CAD	2.48	110.80	108.11
9	A	816	CLA	CMD-C2D-C3D	-2.48	122.00	127.69
9	A	838	CLA	CMB-C2B-C1B	2.48	129.19	125.42
12	A	847	BCR	C27-C26-C25	-2.48	119.35	122.70
9	A	844	CLA	C4D-C3D-CAD	2.48	110.80	108.11
9	A	843	CLA	CMD-C2D-C3D	-2.48	122.00	127.69
9	B	816	CLA	CMD-C2D-C3D	-2.48	122.01	127.69
12	F	201	BCR	C38-C26-C25	-2.48	121.78	124.48
9	B	804	CLA	C4-C3-C5	2.48	119.53	115.23
9	B	828	CLA	C3D-C4D-ND	2.48	114.01	109.99
12	A	847	BCR	C37-C22-C21	-2.48	118.81	122.82
9	B	817	CLA	O1D-CGD-CBD	-2.48	119.64	124.52
9	A	834	CLA	CMD-C2D-C3D	-2.48	122.01	127.69
9	B	818	CLA	C3D-C4D-ND	2.48	114.01	109.99
9	B	825	CLA	C4D-C3D-CAD	2.47	110.79	108.11
9	A	825	CLA	C3D-C4D-ND	2.47	114.01	109.99
9	B	805	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
9	A	811	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
9	A	838	CLA	CAC-C3C-C4C	2.47	128.01	124.79
9	B	811	CLA	C3C-C4C-NC	2.47	113.60	110.43
9	A	826	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
12	M	101	BCR	C34-C9-C10	-2.47	118.81	122.82
9	A	808	CLA	O1D-CGD-CBD	-2.47	119.64	124.52
9	A	830	CLA	O1D-CGD-CBD	-2.47	119.65	124.52
9	B	803	CLA	C3D-C4D-ND	2.47	114.00	109.99
9	A	812	CLA	C3C-C4C-NC	2.47	113.59	110.43
9	A	821	CLA	C3D-C4D-ND	2.47	114.00	109.99
9	B	812	CLA	CAA-C2A-C3A	-2.47	106.33	113.00
9	A	812	CLA	C3D-C4D-ND	2.47	114.00	109.99
9	A	802	CLA	C4-C3-C5	2.47	119.51	115.23
12	M	101	BCR	C37-C22-C21	-2.47	118.82	122.82
9	A	810	CLA	C3D-C4D-ND	2.47	113.99	109.99
9	B	808	CLA	O2D-CGD-O1D	-2.46	119.05	123.85
9	B	807	CLA	CMD-C2D-C3D	-2.46	122.04	127.69
9	B	811	CLA	CMD-C2D-C3D	-2.46	122.04	127.69
9	B	837	CLA	C1-O2A-CGA	2.46	122.61	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	832	CLA	CMD-C2D-C3D	-2.46	122.04	127.69
9	B	807	CLA	CMC-C2C-C1C	2.46	128.88	125.03
9	A	826	CLA	CMD-C2D-C3D	-2.46	122.04	127.69
9	A	844	CLA	C3D-C4D-ND	2.46	113.99	109.99
9	A	809	CLA	C3D-C4D-ND	2.46	113.99	109.99
9	A	838	CLA	C3D-C4D-ND	2.46	113.99	109.99
9	A	807	CLA	C3C-C4C-NC	2.46	113.58	110.43
9	B	835	CLA	C3C-C4C-NC	2.46	113.58	110.43
9	A	830	CLA	CAC-C3C-C4C	2.46	127.99	124.79
9	B	803	CLA	C1-C2-C3	-2.46	122.17	126.20
9	A	806	CLA	CMD-C2D-C3D	-2.46	122.05	127.69
9	B	831	CLA	CMD-C2D-C3D	-2.46	122.05	127.69
9	B	838	CLA	CMD-C2D-C3D	-2.46	122.05	127.69
9	A	833	CLA	C3D-C4D-ND	2.46	113.98	109.99
9	B	817	CLA	C1-C2-C3	-2.46	122.17	126.20
9	B	837	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
9	B	813	CLA	C3C-C4C-NC	2.46	113.58	110.43
9	B	816	CLA	C3C-C4C-NC	2.46	113.58	110.43
9	A	831	CLA	C3D-C4D-ND	2.46	113.98	109.99
9	B	833	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
9	B	823	CLA	O2D-CGD-O1D	-2.46	119.07	123.85
9	B	838	CLA	C3C-C4C-NC	2.46	113.58	110.43
9	B	837	CLA	C3C-C4C-NC	2.46	113.58	110.43
9	A	836	CLA	CMD-C2D-C3D	-2.45	122.06	127.69
9	B	830	CLA	C3D-C4D-ND	2.45	113.98	109.99
9	B	816	CLA	C3D-C4D-ND	2.45	113.97	109.99
12	F	201	BCR	C33-C5-C4	2.45	118.83	113.60
9	A	820	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
9	B	838	CLA	CMA-C3A-C4A	2.45	118.36	111.77
9	I	101	CLA	C3D-C4D-ND	2.45	113.97	109.99
9	B	820	CLA	C3C-C4C-NC	2.45	113.57	110.43
9	A	805	CLA	CMD-C2D-C3D	-2.45	122.07	127.69
9	A	820	CLA	CMD-C2D-C3D	-2.45	122.07	127.69
9	A	831	CLA	C3C-C4C-NC	2.45	113.56	110.43
9	B	801	CLA	C3D-C4D-ND	2.45	113.96	109.99
9	B	817	CLA	CMC-C2C-C1C	2.45	128.85	125.03
9	A	827	CLA	C4-C3-C5	2.44	119.47	115.23
9	A	819	CLA	C7-C6-C5	-2.44	106.75	113.26
9	B	822	CLA	CMB-C2B-C1B	2.44	129.14	125.42
9	K	101	CLA	CAC-C3C-C4C	2.44	127.97	124.79
9	A	836	CLA	C3D-C4D-ND	2.44	113.96	109.99
9	A	837	CLA	CMD-C2D-C3D	-2.44	122.09	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	819	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
9	B	829	CLA	CAC-C3C-C4C	2.44	127.97	124.79
9	A	804	CLA	CMD-C2D-C3D	-2.44	122.09	127.69
9	B	825	CLA	CMC-C2C-C1C	2.44	128.85	125.03
9	B	803	CLA	C1-O2A-CGA	2.44	122.56	116.65
9	B	818	CLA	CMB-C2B-C3B	2.44	132.29	126.55
9	A	814	CLA	C3C-C4C-NC	2.43	113.55	110.43
9	B	809	CLA	CMD-C2D-C3D	-2.43	122.11	127.69
9	B	817	CLA	C3D-C4D-ND	2.43	113.94	109.99
9	B	822	CLA	CMD-C2D-C3D	-2.43	122.11	127.69
9	B	825	CLA	CMB-C2B-C3B	2.43	132.27	126.55
9	A	830	CLA	C4D-C3D-CAD	2.43	110.75	108.11
9	B	823	CLA	CMA-C3A-C4A	2.43	118.31	111.77
9	A	807	CLA	CMD-C2D-C3D	-2.43	122.11	127.69
9	A	832	CLA	CMD-C2D-C3D	-2.43	122.11	127.69
9	A	839	CLA	CMD-C2D-C3D	-2.43	122.12	127.69
9	B	801	CLA	C1-O2A-CGA	2.43	122.53	116.65
9	B	826	CLA	OB-D-CAD-C3D	-2.43	122.74	128.42
9	B	824	CLA	CAA-C2A-C3A	-2.43	106.44	113.00
9	B	807	CLA	C3D-C4D-ND	2.43	113.93	109.99
9	A	833	CLA	C3C-C4C-NC	2.43	113.54	110.43
9	B	834	CLA	C3D-C4D-ND	2.43	113.93	109.99
9	B	837	CLA	C4-C3-C5	2.42	119.44	115.23
9	A	842	CLA	C3C-C4C-NC	2.42	113.54	110.43
9	A	815	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
9	A	836	CLA	C3C-C4C-NC	2.42	113.53	110.43
9	A	833	CLA	CMD-C2D-C3D	-2.42	122.13	127.69
9	A	813	CLA	C4-C3-C5	2.42	119.43	115.23
9	A	802	CLA	CMD-C2D-C3D	-2.42	122.14	127.69
9	B	825	CLA	CMA-C3A-C4A	2.42	118.27	111.77
9	A	839	CLA	C3C-C4C-NC	2.42	113.53	110.43
9	B	829	CLA	CHC-C1C-C2C	-2.42	120.08	126.95
12	A	849	BCR	C30-C25-C26	-2.42	119.33	122.64
12	B	846	BCR	C1-C6-C5	-2.42	119.33	122.64
9	A	819	CLA	C3C-C4C-NC	2.42	113.53	110.43
9	A	828	CLA	C4-C3-C5	2.42	119.42	115.23
9	B	806	CLA	C4-C3-C5	2.42	119.42	115.23
9	B	831	CLA	C3C-C4C-NC	2.41	113.52	110.43
9	B	822	CLA	C3D-C4D-ND	2.41	113.91	109.99
9	B	817	CLA	C4-C3-C5	2.41	119.41	115.23
9	A	810	CLA	CMD-C2D-C3D	-2.41	122.16	127.69
9	A	820	CLA	C1-C2-C3	-2.41	122.25	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	836	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
9	B	810	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
9	B	840	CLA	C3D-C4D-ND	2.41	113.90	109.99
9	A	820	CLA	C4-C3-C5	2.41	119.40	115.23
12	B	845	BCR	C1-C6-C5	-2.40	119.35	122.64
9	A	809	CLA	CMD-C2D-C3D	-2.40	122.18	127.69
9	B	819	CLA	CMD-C2D-C3D	-2.40	122.18	127.69
9	B	807	CLA	CMB-C2B-C1B	2.40	129.08	125.42
9	B	817	CLA	CMD-C2D-C3D	-2.40	122.18	127.69
9	B	801	CLA	CHB-C4A-NA	2.40	127.87	124.40
9	B	833	CLA	CMC-C2C-C1C	2.40	128.79	125.03
9	A	821	CLA	CMA-C3A-C4A	2.40	118.23	111.77
9	B	817	CLA	C4D-C3D-CAD	2.40	110.71	108.11
9	A	835	CLA	OBD-CAD-C3D	-2.40	122.81	128.42
9	B	815	CLA	CAC-C3C-C4C	2.40	127.91	124.79
12	A	847	BCR	C30-C25-C26	-2.40	119.36	122.64
9	B	806	CLA	C3C-C4C-NC	2.40	113.50	110.43
9	A	832	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
9	A	805	CLA	CMC-C2C-C1C	2.40	128.78	125.03
12	B	845	BCR	C7-C8-C9	-2.40	122.69	126.23
9	A	837	CLA	C3C-C4C-NC	2.40	113.50	110.43
8	A	801	CL0	C3C-C4C-NC	2.40	113.50	110.43
9	B	836	CLA	CAC-C3C-C4C	2.40	127.91	124.79
9	A	805	CLA	CMA-C3A-C4A	2.39	118.21	111.77
9	B	833	CLA	C3C-C4C-NC	2.39	113.50	110.43
9	B	834	CLA	CAC-C3C-C4C	2.39	127.91	124.79
9	A	829	CLA	C3D-C4D-ND	2.39	113.88	109.99
9	B	802	CLA	C4D-C3D-CAD	2.39	110.71	108.11
9	B	832	CLA	C3C-C4C-NC	2.39	113.50	110.43
9	A	822	CLA	C3D-C4D-ND	2.39	113.88	109.99
9	A	842	CLA	CMD-C2D-C3D	-2.39	122.20	127.69
9	A	803	CLA	CMD-C2D-C3D	-2.39	122.20	127.69
9	A	843	CLA	CAC-C3C-C4C	2.39	127.90	124.79
9	B	836	CLA	C4C-C3C-C2C	-2.39	103.41	106.89
9	A	834	CLA	CMC-C2C-C1C	2.39	128.77	125.03
9	B	809	CLA	C3C-C4C-NC	2.39	113.49	110.43
9	B	816	CLA	O1D-CGD-CBD	-2.39	119.81	124.52
9	A	829	CLA	CMC-C2C-C1C	2.39	128.76	125.03
9	B	806	CLA	CAC-C3C-C4C	2.39	127.90	124.79
9	A	841	CLA	CMA-C3A-C4A	2.39	118.19	111.77
9	A	814	CLA	CMD-C2D-C3D	-2.39	122.22	127.69
12	B	846	BCR	C37-C22-C21	-2.39	118.95	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	826	CLA	C4D-C3D-CAD	2.39	110.70	108.11
9	A	804	CLA	C3C-C4C-NC	2.39	113.49	110.43
9	B	825	CLA	C3C-C4C-NC	2.39	113.49	110.43
9	A	824	CLA	CED-O2D-CGD	2.38	121.32	115.92
9	B	839	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
9	B	812	CLA	CMD-C2D-C3D	-2.38	122.22	127.69
12	B	842	BCR	C33-C5-C6	-2.38	121.89	124.48
9	B	814	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
9	B	815	CLA	CMD-C2D-C3D	-2.38	122.23	127.69
9	A	820	CLA	CAA-CBA-CGA	-2.38	106.45	113.21
9	A	828	CLA	C3D-C4D-ND	2.38	113.85	109.99
9	B	819	CLA	C3D-C4D-ND	2.38	113.85	109.99
12	A	847	BCR	C30-C25-C24	2.38	122.09	115.65
9	A	827	CLA	C4D-C3D-CAD	2.38	110.69	108.11
9	B	840	CLA	CMD-C2D-C3D	-2.37	122.25	127.69
9	B	828	CLA	CHD-C1D-ND	-2.37	121.46	124.80
9	A	818	CLA	C3C-C4C-NC	2.37	113.47	110.43
9	A	820	CLA	CMA-C3A-C4A	2.37	118.15	111.77
9	B	820	CLA	CAC-C3C-C4C	2.37	127.87	124.79
9	B	821	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
9	A	819	CLA	CMD-C2D-C3D	-2.37	122.26	127.69
12	A	851	BCR	C35-C13-C12	2.37	121.71	118.09
12	A	849	BCR	C34-C9-C10	-2.37	118.98	122.82
9	A	811	CLA	C3C-C4C-NC	2.37	113.46	110.43
9	B	806	CLA	C3D-C4D-ND	2.37	113.83	109.99
9	A	833	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
12	B	843	BCR	C34-C9-C10	-2.37	118.98	122.82
9	B	805	CLA	CMD-C2D-C3D	-2.37	122.26	127.69
9	B	813	CLA	CMB-C2B-C1B	2.37	129.02	125.42
9	A	826	CLA	C4-C3-C5	2.37	119.33	115.23
12	A	849	BCR	C37-C22-C21	-2.36	118.99	122.82
9	B	829	CLA	O1D-CGD-CBD	-2.36	119.86	124.52
9	A	826	CLA	C3C-C4C-NC	2.36	113.46	110.43
9	A	829	CLA	CED-O2D-CGD	2.36	121.27	115.92
9	B	807	CLA	C3C-C4C-NC	2.36	113.45	110.43
9	B	806	CLA	CBA-CAA-C2A	2.36	120.81	113.79
9	B	807	CLA	O2D-CGD-O1D	-2.36	119.26	123.85
9	B	834	CLA	CHB-C4A-NA	2.36	127.80	124.40
9	B	840	CLA	CHC-C1C-C2C	-2.36	120.25	126.95
9	A	834	CLA	C3D-C4D-ND	2.36	113.81	109.99
9	A	815	CLA	CAC-C3C-C4C	2.35	127.85	124.79
9	B	805	CLA	C3C-C4C-NC	2.35	113.44	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	846	BCR	C4-C5-C6	-2.35	119.53	122.70
9	A	823	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
12	A	848	BCR	C15-C14-C13	-2.35	123.98	127.28
9	A	830	CLA	C3C-C4C-NC	2.35	113.44	110.43
9	B	812	CLA	CMB-C2B-C1B	2.35	129.00	125.42
9	A	844	CLA	CMD-C2D-C3D	-2.34	122.31	127.69
9	A	806	CLA	C3C-C4C-NC	2.34	113.43	110.43
9	A	838	CLA	CAA-C2A-C3A	-2.34	106.67	113.00
9	B	836	CLA	C3D-C4D-ND	2.34	113.79	109.99
9	B	817	CLA	CHA-C1A-NA	-2.34	121.09	126.39
12	M	101	BCR	C33-C5-C4	2.34	118.58	113.60
9	A	824	CLA	C3C-C4C-NC	2.34	113.43	110.43
9	B	840	CLA	C3C-C4C-NC	2.34	113.43	110.43
9	A	828	CLA	O1D-CGD-CBD	-2.34	119.91	124.52
9	B	828	CLA	CAC-C3C-C4C	2.34	127.83	124.79
9	B	820	CLA	C3D-C4D-ND	2.34	113.79	109.99
13	A	853	LHG	C5-O7-C7	-2.34	112.20	117.80
9	B	806	CLA	CMC-C2C-C1C	2.34	128.69	125.03
9	A	825	CLA	O1D-CGD-CBD	-2.34	119.91	124.52
9	A	809	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
9	B	818	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
12	A	847	BCR	C31-C1-C6	-2.34	106.58	110.24
9	A	804	CLA	CHB-C4A-NA	2.34	127.77	124.40
9	A	827	CLA	C1-O2A-CGA	2.33	122.30	116.65
9	B	836	CLA	CMD-C2D-C3D	-2.33	122.34	127.69
9	A	835	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
12	B	842	BCR	C36-C18-C17	-2.33	119.03	122.82
9	B	837	CLA	CMD-C2D-C3D	-2.33	122.34	127.69
9	B	814	CLA	CAA-C2A-C1A	2.33	119.62	111.97
9	A	818	CLA	CBA-CAA-C2A	2.33	120.73	113.79
9	B	815	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
9	A	803	CLA	C3C-C4C-NC	2.33	113.42	110.43
9	B	801	CLA	CAC-C3C-C4C	2.33	127.82	124.79
9	A	802	CLA	CAC-C3C-C4C	2.33	127.82	124.79
12	A	849	BCR	C19-C18-C17	2.33	122.67	119.01
9	A	818	CLA	O1D-CGD-CBD	-2.33	119.93	124.52
9	B	819	CLA	CAA-C2A-C3A	-2.33	106.71	113.00
9	A	831	CLA	O1D-CGD-CBD	-2.33	119.93	124.52
9	A	821	CLA	O2D-CGD-O1D	-2.33	119.32	123.85
9	A	805	CLA	C1-O2A-CGA	2.33	122.28	116.65
9	A	805	CLA	CMB-C2B-C1B	2.32	128.96	125.42
9	A	805	CLA	C4-C3-C5	2.32	119.26	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	828	CLA	CMC-C2C-C1C	2.32	128.66	125.03
9	B	827	CLA	CMB-C2B-C1B	2.32	128.96	125.42
9	B	827	CLA	CBA-CAA-C2A	2.32	120.70	113.79
9	B	826	CLA	C3D-C4D-ND	2.32	113.76	109.99
9	B	808	CLA	CAA-C2A-C3A	-2.32	106.73	113.00
9	A	816	CLA	CMA-C3A-C4A	2.32	118.01	111.77
9	B	813	CLA	C3D-C4D-ND	2.32	113.76	109.99
9	A	813	CLA	CMB-C2B-C1B	2.32	128.95	125.42
12	M	101	BCR	C38-C26-C27	2.32	118.54	113.60
9	B	829	CLA	CMA-C3A-C4A	2.32	118.00	111.77
9	B	817	CLA	OBD-CAD-C3D	-2.32	123.00	128.42
9	A	824	CLA	CAC-C3C-C4C	2.32	127.80	124.79
9	B	802	CLA	CHD-C4C-C3C	-2.32	121.40	124.77
9	A	816	CLA	C3C-C4C-NC	2.32	113.40	110.43
12	B	846	BCR	C30-C25-C24	2.31	121.92	115.65
9	A	828	CLA	CAA-CBA-CGA	-2.31	106.64	113.21
9	A	820	CLA	CBC-CAC-C3C	-2.31	106.15	112.42
9	A	843	CLA	O1D-CGD-CBD	-2.31	119.96	124.52
12	A	849	BCR	C15-C14-C13	-2.31	124.04	127.28
9	B	824	CLA	CMB-C2B-C3B	2.31	131.97	126.55
9	B	804	CLA	C3D-C4D-ND	2.31	113.73	109.99
8	A	801	CL0	C3D-C4D-ND	2.31	113.73	109.99
9	B	811	CLA	O2D-CGD-O1D	-2.31	119.36	123.85
9	B	836	CLA	CMB-C2B-C3B	2.30	131.97	126.55
9	B	806	CLA	CHA-C1A-NA	-2.30	121.18	126.39
12	B	843	BCR	C36-C18-C17	-2.30	119.09	122.82
9	A	813	CLA	O2D-CGD-O1D	-2.30	119.38	123.85
9	B	828	CLA	C1-C2-C3	-2.30	122.43	126.20
9	A	829	CLA	CMB-C2B-C3B	2.30	131.95	126.55
9	B	802	CLA	C3D-C4D-ND	2.30	113.72	109.99
9	A	844	CLA	CMB-C2B-C1B	2.29	128.91	125.42
9	A	808	CLA	CMD-C2D-C3D	-2.29	122.43	127.69
9	B	839	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
9	A	817	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
9	B	824	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
9	A	838	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
9	B	836	CLA	CMA-C3A-C4A	2.29	117.92	111.77
9	B	808	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
9	A	821	CLA	CAA-C2A-C3A	-2.29	106.82	113.00
9	A	809	CLA	C3C-C4C-NC	2.29	113.36	110.43
9	B	818	CLA	C4D-C3D-CAD	2.29	110.59	108.11
9	A	802	CLA	C1-C2-C3	-2.29	122.45	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	844	BCR	C35-C13-C12	2.29	121.58	118.09
9	B	818	CLA	CAC-C3C-C4C	2.29	127.76	124.79
8	A	801	CL0	CHB-C1B-C2B	-2.28	120.79	127.43
12	A	849	BCR	C27-C26-C25	-2.28	119.62	122.70
13	A	852	LHG	C5-O7-C7	-2.28	112.34	117.80
9	A	809	CLA	CMB-C2B-C1B	2.28	128.89	125.42
8	A	801	CL0	CED-O2D-CGD	2.28	121.08	115.92
10	B	841	PQN	C2M-C2-C3	-2.28	120.71	124.45
9	A	806	CLA	O2D-CGD-O1D	-2.27	119.42	123.85
8	A	801	CL0	CMD-C2D-C3D	-2.27	122.48	127.69
9	B	801	CLA	CAA-C2A-C3A	-2.27	106.86	113.00
9	A	840	CLA	CAA-C2A-C3A	-2.27	106.86	113.00
9	A	829	CLA	C4-C3-C5	2.27	119.17	115.23
9	B	833	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
9	A	838	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
9	A	841	CLA	CAC-C3C-C4C	2.27	127.74	124.79
9	B	830	CLA	CAC-C3C-C4C	2.27	127.74	124.79
9	B	815	CLA	C3D-C4D-ND	2.26	113.67	109.99
9	A	834	CLA	CAC-C3C-C4C	2.26	127.74	124.79
9	A	821	CLA	C4-C3-C5	2.26	119.16	115.23
9	A	841	CLA	O2D-CGD-O1D	-2.26	119.44	123.85
9	I	101	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
9	I	101	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
12	B	843	BCR	C33-C5-C6	-2.26	122.02	124.48
9	B	807	CLA	C4-C3-C5	2.26	119.14	115.23
8	A	801	CL0	CAC-C3C-C4C	2.26	127.72	124.79
9	A	809	CLA	CHC-C1C-C2C	-2.26	120.54	126.95
9	B	809	CLA	CBA-CAA-C2A	2.25	120.50	113.79
9	A	812	CLA	CMD-C2D-C3D	-2.25	122.52	127.69
12	B	845	BCR	C4-C5-C6	-2.25	119.66	122.70
9	B	805	CLA	CMA-C3A-C4A	2.25	117.82	111.77
9	B	831	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
9	B	835	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
9	A	804	CLA	C3D-C4D-ND	2.25	113.64	109.99
9	B	806	CLA	OBD-CAD-C3D	-2.25	123.17	128.42
9	B	809	CLA	O1D-CGD-CBD	-2.25	120.09	124.52
9	B	806	CLA	CHC-C1C-C2C	-2.25	120.57	126.95
12	B	842	BCR	C29-C28-C27	-2.25	106.34	111.28
9	A	815	CLA	CMD-C2D-C3D	-2.25	122.54	127.69
9	B	824	CLA	CAC-C3C-C2C	2.24	131.68	127.56
9	A	804	CLA	CAC-C3C-C4C	2.24	127.70	124.79
9	A	827	CLA	CAC-C3C-C4C	2.24	127.70	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	101	CLA	C3C-C4C-NC	2.24	113.30	110.43
9	B	814	CLA	CMD-C2D-C3D	-2.24	122.56	127.69
9	B	839	CLA	CMB-C2B-C1B	2.24	128.82	125.42
9	B	801	CLA	CHB-C1B-C2B	-2.23	120.94	127.43
9	A	827	CLA	C3D-C4D-ND	2.23	113.62	109.99
9	A	835	CLA	C3C-C4C-NC	2.23	113.29	110.43
9	B	801	CLA	C4D-C3D-CAD	2.23	110.53	108.11
9	A	823	CLA	CAC-C3C-C4C	2.23	127.69	124.79
12	A	848	BCR	C38-C26-C27	2.23	118.35	113.60
9	B	823	CLA	CHB-C1B-C2B	-2.23	120.96	127.43
9	A	808	CLA	CBA-CAA-C2A	2.23	120.42	113.79
9	B	823	CLA	C3C-C4C-NC	2.23	113.28	110.43
14	B	848	LMG	O7-C10-O9	-2.23	118.50	123.70
9	B	834	CLA	C3C-C4C-NC	2.23	113.28	110.43
12	F	201	BCR	C1-C6-C5	-2.22	119.60	122.64
9	B	828	CLA	C1-O2A-CGA	2.22	122.03	116.65
9	A	802	CLA	O2D-CGD-O1D	-2.22	119.52	123.85
9	A	808	CLA	C3D-C4D-ND	2.22	113.60	109.99
9	A	840	CLA	C3C-C4C-NC	2.22	113.27	110.43
9	A	832	CLA	CAC-C3C-C4C	2.22	127.67	124.79
9	B	809	CLA	CAC-C3C-C4C	2.21	127.67	124.79
12	F	201	BCR	C23-C22-C21	2.21	122.49	119.01
12	A	848	BCR	C30-C25-C26	-2.21	119.61	122.64
9	A	804	CLA	CHA-C1A-NA	-2.21	121.39	126.39
12	A	849	BCR	C34-C9-C8	2.21	121.47	118.09
12	A	847	BCR	C35-C13-C12	2.21	121.46	118.09
9	B	815	CLA	CBB-CAB-C3B	-2.21	116.49	127.53
9	A	814	CLA	C3D-C4D-ND	2.21	113.58	109.99
9	A	819	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
9	B	817	CLA	CMA-C3A-C4A	2.21	117.71	111.77
9	A	817	CLA	CMB-C2B-C1B	2.21	128.78	125.42
9	B	825	CLA	CMD-C2D-C3D	-2.21	122.63	127.69
12	A	848	BCR	C23-C22-C21	2.20	122.48	119.01
9	A	810	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
9	A	820	CLA	C3C-C4C-NC	2.20	113.25	110.43
9	B	839	CLA	C3C-C4C-NC	2.20	113.25	110.43
9	B	817	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
9	B	838	CLA	O1D-CGD-CBD	-2.20	120.17	124.52
9	A	802	CLA	CMC-C2C-C1C	2.20	128.48	125.03
9	A	838	CLA	C4B-CHC-C1C	2.20	131.42	126.25
9	B	832	CLA	CMB-C2B-C1B	2.20	128.77	125.42
9	B	818	CLA	O1D-CGD-CBD	-2.20	120.18	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	808	CLA	C4C-C3C-C2C	-2.20	103.69	106.89
9	B	803	CLA	CMA-C3A-C4A	2.20	117.68	111.77
9	B	816	CLA	CED-O2D-CGD	2.20	120.90	115.92
9	B	831	CLA	CED-O2D-CGD	2.20	120.90	115.92
9	B	826	CLA	C4C-C3C-C2C	-2.19	103.70	106.89
9	A	804	CLA	CMB-C2B-C3B	2.19	131.71	126.55
9	B	805	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
9	A	818	CLA	O2D-CGD-O1D	-2.19	119.58	123.85
9	A	842	CLA	CAC-C3C-C4C	2.19	127.64	124.79
9	A	829	CLA	O2D-CGD-O1D	-2.19	119.59	123.85
9	B	832	CLA	O2D-CGD-O1D	-2.19	119.59	123.85
9	B	806	CLA	CHB-C4A-NA	2.19	127.56	124.40
9	A	816	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
8	A	801	CL0	C4-C3-C2	-2.19	118.02	123.63
9	A	832	CLA	CMB-C2B-C1B	2.18	128.75	125.42
9	B	838	CLA	CMB-C2B-C3B	2.18	131.69	126.55
9	A	819	CLA	C1-O2A-CGA	2.18	121.94	116.65
12	A	849	BCR	C33-C5-C4	2.18	118.25	113.60
9	A	841	CLA	CHC-C1C-C2C	-2.18	120.75	126.95
12	B	842	BCR	C29-C30-C25	2.18	113.60	110.44
9	B	837	CLA	CAC-C3C-C4C	2.18	127.62	124.79
12	F	201	BCR	C34-C9-C8	2.18	121.41	118.09
9	A	842	CLA	O1D-CGD-CBD	-2.18	120.23	124.52
9	A	830	CLA	CMD-C2D-C3D	-2.18	122.70	127.69
9	B	817	CLA	C3C-C4C-NC	2.17	113.22	110.43
12	B	843	BCR	C34-C9-C8	2.17	121.41	118.09
9	A	818	CLA	CHB-C1B-C2B	-2.17	121.12	127.43
8	A	801	CL0	O2D-CGD-O1D	-2.17	119.62	123.85
9	A	813	CLA	C6-C5-C3	-2.17	108.18	113.47
9	B	807	CLA	CAA-C2A-C3A	-2.17	107.14	113.00
9	B	825	CLA	O1D-CGD-CBD	-2.16	120.25	124.52
9	A	833	CLA	CAC-C3C-C4C	2.16	127.60	124.79
9	A	821	CLA	C3C-C4C-NC	2.16	113.20	110.43
9	B	836	CLA	CHC-C1C-C2C	-2.16	120.82	126.95
12	B	846	BCR	C28-C27-C26	-2.16	110.21	114.06
9	A	822	CLA	O1D-CGD-CBD	-2.16	120.27	124.52
9	B	816	CLA	CMB-C2B-C1B	2.15	128.70	125.42
9	B	821	CLA	CHC-C1C-C2C	-2.15	120.84	126.95
12	A	851	BCR	C31-C1-C6	-2.15	106.87	110.24
9	A	828	CLA	C5-C3-C2	-2.15	116.34	121.17
9	A	803	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
9	A	825	CLA	C1-C2-C3	-2.15	122.67	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	814	CLA	CHB-C1B-C2B	-2.15	121.19	127.43
9	B	816	CLA	CAC-C3C-C4C	2.15	127.58	124.79
9	A	833	CLA	CMB-C2B-C1B	2.15	128.69	125.42
9	B	830	CLA	CHA-C1A-NA	-2.15	121.53	126.39
9	A	807	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
9	B	805	CLA	CMB-C2B-C3B	2.15	131.60	126.55
9	B	804	CLA	CMA-C3A-C4A	2.15	117.54	111.77
9	A	805	CLA	CHC-C1C-C2C	-2.14	120.85	126.95
9	B	840	CLA	CMC-C2C-C1C	2.14	128.38	125.03
9	B	811	CLA	CMC-C2C-C1C	2.14	128.38	125.03
9	B	827	CLA	C4C-C3C-C2C	-2.14	103.78	106.89
9	B	827	CLA	CHC-C1C-C2C	-2.14	120.87	126.95
9	B	831	CLA	CAA-C2A-C3A	-2.14	107.22	113.00
12	B	842	BCR	C31-C1-C6	-2.14	106.89	110.24
9	B	817	CLA	CHB-C1B-C2B	-2.14	121.22	127.43
9	A	802	CLA	CHA-C1A-NA	-2.14	121.55	126.39
9	B	837	CLA	CMB-C2B-C1B	2.14	128.67	125.42
9	B	814	CLA	CHA-C1A-NA	-2.13	121.56	126.39
9	A	806	CLA	C1-C2-C3	-2.13	122.70	126.20
9	A	825	CLA	CMB-C2B-C3B	2.13	131.56	126.55
9	A	804	CLA	CMA-C3A-C2A	2.13	122.21	113.98
9	B	831	CLA	CMA-C3A-C4A	2.13	117.49	111.77
9	A	813	CLA	C4C-C3C-C2C	-2.13	103.80	106.89
9	B	834	CLA	O1D-CGD-CBD	-2.13	120.33	124.52
9	B	817	CLA	CAC-C3C-C4C	2.13	127.56	124.79
9	B	821	CLA	C3C-C4C-NC	2.12	113.15	110.43
9	A	813	CLA	CHA-C4D-ND	2.12	136.93	132.55
12	B	842	BCR	C39-C30-C25	-2.12	106.92	110.24
9	A	840	CLA	C5-C3-C4	2.12	119.47	114.59
9	B	826	CLA	CMB-C2B-C1B	2.12	128.65	125.42
9	B	804	CLA	C1-C2-C3	-2.12	122.73	126.20
9	B	821	CLA	O1D-CGD-CBD	-2.12	120.34	124.52
12	B	842	BCR	C19-C18-C17	2.12	122.34	119.01
8	A	801	CL0	CHA-C1A-NA	-2.11	121.60	126.39
9	B	829	CLA	C3C-C4C-NC	2.11	113.14	110.43
9	A	814	CLA	CHB-C4A-NA	2.11	127.44	124.40
9	A	841	CLA	C3C-C4C-NC	2.11	113.13	110.43
12	A	851	BCR	C27-C26-C25	-2.11	119.85	122.70
9	B	830	CLA	CHB-C1B-C2B	-2.11	121.30	127.43
12	B	843	BCR	C24-C25-C26	2.11	126.41	121.56
9	A	814	CLA	CMA-C3A-C4A	2.11	117.44	111.77
9	B	829	CLA	CMB-C2B-C3B	2.11	131.50	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	845	BCR	C8-C7-C6	-2.11	121.37	127.00
9	B	812	CLA	CED-O2D-CGD	2.11	120.69	115.92
9	B	813	CLA	CAA-CBA-CGA	-2.10	107.23	113.21
9	B	819	CLA	CAC-C3C-C4C	2.10	127.53	124.79
9	I	101	CLA	CHC-C1C-C2C	-2.10	120.97	126.95
12	B	846	BCR	C8-C7-C6	-2.10	121.39	127.00
9	A	827	CLA	CMD-C2D-C3D	-2.10	122.88	127.69
9	B	816	CLA	O2D-CGD-O1D	-2.10	119.76	123.85
9	B	828	CLA	CHC-C1C-C2C	-2.10	120.98	126.95
9	B	822	CLA	O2D-CGD-O1D	-2.10	119.77	123.85
9	B	827	CLA	C4-C3-C5	2.10	118.87	115.23
10	A	845	PQN	C11-C12-C13	-2.10	123.22	126.83
9	B	815	CLA	CHA-C1A-NA	-2.10	121.65	126.39
9	B	837	CLA	C6-C5-C3	-2.09	108.37	113.47
9	B	828	CLA	C4B-CHC-C1C	2.09	131.17	126.25
9	A	802	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
9	B	833	CLA	CMB-C2B-C3B	2.09	131.47	126.55
9	A	827	CLA	CHB-C1B-C2B	-2.09	121.35	127.43
9	A	837	CLA	CMB-C2B-C3B	2.09	131.47	126.55
9	A	843	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
9	A	824	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
9	A	822	CLA	CMB-C2B-C3B	2.09	131.46	126.55
9	B	830	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
9	B	836	CLA	CHA-C1A-NA	-2.09	121.67	126.39
12	B	845	BCR	C37-C22-C21	-2.09	119.44	122.82
9	A	820	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
9	A	818	CLA	CMB-C2B-C3B	2.08	131.45	126.55
8	A	801	CL0	CHB-C4A-NA	2.08	127.40	124.40
9	B	805	CLA	CAC-C3C-C4C	2.08	127.50	124.79
9	A	810	CLA	CHA-C1A-NA	-2.08	121.69	126.39
9	A	822	CLA	CBA-CAA-C2A	2.08	119.97	113.79
9	B	840	CLA	OBD-CAD-C3D	-2.08	123.56	128.42
9	A	812	CLA	CHC-C1C-C2C	-2.08	121.05	126.95
12	A	850	BCR	C29-C28-C27	2.08	115.84	111.28
9	B	840	CLA	CAC-C3C-C4C	2.07	127.49	124.79
9	B	814	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
9	A	829	CLA	CHC-C1C-C2C	-2.07	121.07	126.95
9	A	839	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
9	A	813	CLA	CHA-C1A-NA	-2.07	121.71	126.39
9	A	825	CLA	CHC-C1C-C2C	-2.07	121.07	126.95
9	A	821	CLA	CHA-C1A-NA	-2.07	121.71	126.39
9	B	803	CLA	CHD-C4C-C3C	-2.07	121.76	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	817	CLA	CMB-C2B-C3B	2.07	131.41	126.55
12	F	201	BCR	C29-C28-C27	-2.06	106.74	111.28
9	A	819	CLA	CMB-C2B-C1B	2.06	128.56	125.42
9	A	828	CLA	CMD-C2D-C3D	-2.06	122.95	127.69
9	B	806	CLA	C1-C2-C3	-2.06	122.82	126.20
12	B	842	BCR	C2-C1-C6	2.06	113.43	110.44
9	B	817	CLA	CBA-CAA-C2A	2.06	119.92	113.79
9	B	827	CLA	CMC-C2C-C1C	2.06	128.25	125.03
12	A	850	BCR	C15-C14-C13	-2.06	124.39	127.28
9	B	822	CLA	CAC-C3C-C4C	2.06	127.47	124.79
9	A	815	CLA	CMB-C2B-C1B	2.06	128.55	125.42
9	A	821	CLA	CED-O2D-CGD	2.06	120.58	115.92
9	B	804	CLA	O2D-CGD-O1D	-2.05	119.85	123.85
9	A	834	CLA	CHC-C1C-C2C	-2.05	121.12	126.95
9	B	817	CLA	CHC-C1C-C2C	-2.05	121.12	126.95
9	B	810	CLA	CMB-C2B-C1B	2.05	128.54	125.42
9	A	844	CLA	CMC-C2C-C1C	2.05	128.24	125.03
9	B	811	CLA	CHC-C1C-C2C	-2.05	121.12	126.95
9	B	826	CLA	CHC-C1C-C2C	-2.05	121.12	126.95
9	A	802	CLA	C4C-C3C-C2C	-2.05	103.91	106.89
9	B	804	CLA	CHB-C4A-NA	2.05	127.35	124.40
9	A	806	CLA	CHA-C1A-NA	-2.05	121.76	126.39
12	F	201	BCR	C39-C30-C25	-2.05	107.04	110.24
9	B	829	CLA	CMC-C2C-C3C	2.04	131.68	126.15
9	A	817	CLA	C5-C3-C4	2.04	119.29	114.59
12	B	847	BCR	C33-C5-C4	2.04	117.95	113.60
9	B	803	CLA	O2D-CGD-O1D	-2.04	119.87	123.85
12	F	201	BCR	C4-C5-C6	-2.04	119.94	122.70
9	A	803	CLA	CAC-C3C-C4C	2.04	127.45	124.79
9	A	813	CLA	C1-C2-C3	-2.04	122.86	126.20
9	B	830	CLA	CHC-C1C-C2C	-2.04	121.16	126.95
12	B	845	BCR	C36-C18-C17	-2.04	119.52	122.82
9	A	805	CLA	C3C-C4C-NC	2.04	113.04	110.43
9	A	838	CLA	CHB-C1B-C2B	-2.04	121.51	127.43
9	A	823	CLA	CHC-C1C-C2C	-2.04	121.16	126.95
9	B	822	CLA	CHA-C1A-NA	-2.04	121.78	126.39
12	A	850	BCR	C3-C4-C5	-2.04	110.43	114.06
9	B	820	CLA	CHA-C4D-ND	2.04	136.75	132.55
12	B	846	BCR	C1-C6-C7	2.03	121.17	115.65
9	A	833	CLA	O1D-CGD-CBD	-2.03	120.50	124.52
9	A	831	CLA	CHA-C4D-ND	2.03	136.74	132.55
9	A	816	CLA	CMB-C2B-C1B	2.03	128.51	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	835	CLA	CHB-C4A-NA	2.03	127.33	124.40
9	A	810	CLA	CMB-C2B-C3B	2.03	131.33	126.55
9	B	836	CLA	CAA-C2A-C3A	-2.03	107.51	113.00
9	B	837	CLA	CHC-C1C-C2C	-2.03	121.18	126.95
8	A	801	CL0	CHA-C4D-ND	2.03	136.74	132.55
9	B	830	CLA	CBA-CAA-C2A	2.03	119.82	113.79
9	A	840	CLA	CHC-C1C-C2C	-2.03	121.19	126.95
9	B	819	CLA	CHB-C1B-C2B	-2.03	121.55	127.43
9	A	809	CLA	C5-C3-C4	2.03	119.25	114.59
9	B	810	CLA	CMD-C2D-C3D	-2.03	123.05	127.69
9	B	814	CLA	CHC-C1C-C2C	-2.02	121.19	126.95
9	A	813	CLA	C3D-C4D-ND	2.02	113.28	109.99
9	A	822	CLA	CHA-C1A-NA	-2.02	121.81	126.39
9	A	817	CLA	O2D-CGD-O1D	-2.02	119.91	123.85
12	B	844	BCR	C38-C26-C25	-2.02	122.28	124.48
9	B	807	CLA	CHA-C1A-NA	-2.02	121.81	126.39
9	A	818	CLA	CAA-C2A-C3A	-2.02	107.54	113.00
9	B	830	CLA	CMB-C2B-C3B	2.02	131.29	126.55
9	A	808	CLA	CAC-C3C-C4C	2.02	127.41	124.79
9	A	826	CLA	CMB-C2B-C1B	2.02	128.49	125.42
9	B	818	CLA	CHC-C1C-C2C	-2.02	121.22	126.95
9	A	804	CLA	OBD-CAD-C3D	-2.02	123.71	128.42
9	B	824	CLA	CHC-C1C-NC	-2.02	121.28	124.31
12	B	846	BCR	C30-C25-C26	-2.02	119.88	122.64
9	A	836	CLA	CHC-C1C-C2C	-2.01	121.22	126.95
9	A	837	CLA	CHC-C1C-C2C	-2.01	121.22	126.95
9	A	814	CLA	CHC-C1C-C2C	-2.01	121.23	126.95
9	A	833	CLA	CHA-C1A-NA	-2.01	121.83	126.39
9	B	802	CLA	OBD-CAD-C3D	-2.01	123.71	128.42
9	A	820	CLA	CHC-C1C-C2C	-2.01	121.23	126.95
12	A	848	BCR	C33-C5-C6	-2.01	122.29	124.48
9	A	826	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
9	A	832	CLA	CHC-C1C-C2C	-2.01	121.23	126.95
12	B	844	BCR	C28-C27-C26	-2.01	110.47	114.06
9	A	818	CLA	CHA-C1A-NA	-2.01	121.84	126.39
9	A	824	CLA	CHC-C1C-C2C	-2.01	121.24	126.95
9	B	825	CLA	CHB-C1B-C2B	-2.01	121.60	127.43
9	B	804	CLA	CMB-C2B-C3B	2.01	131.27	126.55
9	A	808	CLA	CHA-C1A-NA	-2.01	121.85	126.39
12	B	845	BCR	C30-C25-C26	-2.01	119.89	122.64
9	A	822	CLA	CMD-C2D-C3D	-2.01	123.09	127.69
9	A	815	CLA	O1D-CGD-CBD	-2.01	120.56	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	828	CLA	CHC-C1C-C2C	-2.00	121.25	126.95
9	B	812	CLA	CHC-C1C-C2C	-2.00	121.25	126.95
9	B	807	CLA	CHC-C1C-C2C	-2.00	121.26	126.95
9	B	820	CLA	CHC-C1C-C2C	-2.00	121.26	126.95

There are no chirality outliers.

All (1001) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	801	CL0	C1A-C2A-CAA-CBA
8	A	801	CL0	C3A-C2A-CAA-CBA
8	A	801	CL0	C4-C3-C5-C6
9	A	802	CLA	C4B-C3B-CAB-CBB
9	A	803	CLA	CHA-CBD-CGD-O1D
9	A	803	CLA	CHA-CBD-CGD-O2D
9	A	804	CLA	C1A-C2A-CAA-CBA
9	A	804	CLA	C3A-C2A-CAA-CBA
9	A	805	CLA	C2-C1-O2A-CGA
9	A	805	CLA	CAD-CBD-CGD-O2D
9	A	805	CLA	CBD-CGD-O2D-CED
9	A	807	CLA	C3A-C2A-CAA-CBA
9	A	807	CLA	CBD-CGD-O2D-CED
9	A	808	CLA	C3A-C2A-CAA-CBA
9	A	808	CLA	C2B-C3B-CAB-CBB
9	A	808	CLA	C4B-C3B-CAB-CBB
9	A	808	CLA	CHA-CBD-CGD-O1D
9	A	808	CLA	CHA-CBD-CGD-O2D
9	A	810	CLA	C1A-C2A-CAA-CBA
9	A	810	CLA	C3A-C2A-CAA-CBA
9	A	811	CLA	C2B-C3B-CAB-CBB
9	A	811	CLA	C4B-C3B-CAB-CBB
9	A	812	CLA	C1A-C2A-CAA-CBA
9	A	814	CLA	CAD-CBD-CGD-O1D
9	A	814	CLA	CAD-CBD-CGD-O2D
9	A	815	CLA	CBD-CGD-O2D-CED
9	A	816	CLA	CBD-CGD-O2D-CED
9	A	818	CLA	C1A-C2A-CAA-CBA
9	A	818	CLA	C3A-C2A-CAA-CBA
9	A	818	CLA	C2B-C3B-CAB-CBB
9	A	818	CLA	C4B-C3B-CAB-CBB
9	A	819	CLA	C1A-C2A-CAA-CBA
9	A	819	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
9	A	820	CLA	CBA-CGA-O2A-C1
9	A	820	CLA	C2B-C3B-CAB-CBB
9	A	820	CLA	C4B-C3B-CAB-CBB
9	A	820	CLA	CHA-CBD-CGD-O1D
9	A	820	CLA	CHA-CBD-CGD-O2D
9	A	822	CLA	C1A-C2A-CAA-CBA
9	A	822	CLA	C3A-C2A-CAA-CBA
9	A	822	CLA	CBD-CGD-O2D-CED
9	A	823	CLA	C2B-C3B-CAB-CBB
9	A	823	CLA	C4B-C3B-CAB-CBB
9	A	824	CLA	C2B-C3B-CAB-CBB
9	A	824	CLA	C4B-C3B-CAB-CBB
9	A	825	CLA	C3A-C2A-CAA-CBA
9	A	825	CLA	CHA-CBD-CGD-O1D
9	A	825	CLA	CHA-CBD-CGD-O2D
9	A	827	CLA	CAD-CBD-CGD-O1D
9	A	827	CLA	CAD-CBD-CGD-O2D
9	A	828	CLA	O2A-C1-C2-C3
9	A	828	CLA	C4-C3-C5-C6
9	A	830	CLA	C2B-C3B-CAB-CBB
9	A	830	CLA	C4B-C3B-CAB-CBB
9	A	830	CLA	CHA-CBD-CGD-O1D
9	A	830	CLA	CHA-CBD-CGD-O2D
9	A	831	CLA	C2B-C3B-CAB-CBB
9	A	831	CLA	C4B-C3B-CAB-CBB
9	A	831	CLA	CHA-CBD-CGD-O1D
9	A	831	CLA	CHA-CBD-CGD-O2D
9	A	834	CLA	C2B-C3B-CAB-CBB
9	A	834	CLA	C4B-C3B-CAB-CBB
9	A	834	CLA	CHA-CBD-CGD-O1D
9	A	834	CLA	CHA-CBD-CGD-O2D
9	A	835	CLA	C1A-C2A-CAA-CBA
9	A	835	CLA	C3A-C2A-CAA-CBA
9	A	835	CLA	C4B-C3B-CAB-CBB
9	A	835	CLA	CBD-CGD-O2D-CED
9	A	836	CLA	C1A-C2A-CAA-CBA
9	A	836	CLA	C3A-C2A-CAA-CBA
9	A	840	CLA	CBD-CGD-O2D-CED
9	A	841	CLA	C4B-C3B-CAB-CBB
9	A	842	CLA	C2B-C3B-CAB-CBB
9	A	842	CLA	C4B-C3B-CAB-CBB
9	A	843	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
9	A	843	CLA	C4B-C3B-CAB-CBB
9	A	844	CLA	CAD-CBD-CGD-O1D
9	A	844	CLA	CAD-CBD-CGD-O2D
9	A	844	CLA	CBD-CGD-O2D-CED
9	B	801	CLA	CBA-CGA-O2A-C1
9	B	801	CLA	O1A-CGA-O2A-C1
9	B	802	CLA	CAD-CBD-CGD-O1D
9	B	802	CLA	CAD-CBD-CGD-O2D
9	B	803	CLA	CBD-CGD-O2D-CED
9	B	804	CLA	CBD-CGD-O2D-CED
9	B	804	CLA	O1D-CGD-O2D-CED
9	B	805	CLA	CBD-CGD-O2D-CED
9	B	806	CLA	C3A-C2A-CAA-CBA
9	B	809	CLA	C2B-C3B-CAB-CBB
9	B	809	CLA	C4B-C3B-CAB-CBB
9	B	809	CLA	CHA-CBD-CGD-O1D
9	B	809	CLA	CHA-CBD-CGD-O2D
9	B	810	CLA	C1A-C2A-CAA-CBA
9	B	810	CLA	C3A-C2A-CAA-CBA
9	B	810	CLA	CBD-CGD-O2D-CED
9	B	811	CLA	C2B-C3B-CAB-CBB
9	B	811	CLA	C4B-C3B-CAB-CBB
9	B	813	CLA	C1A-C2A-CAA-CBA
9	B	813	CLA	CHA-CBD-CGD-O2D
9	B	814	CLA	C1A-C2A-CAA-CBA
9	B	814	CLA	CHA-CBD-CGD-O1D
9	B	814	CLA	CHA-CBD-CGD-O2D
9	B	815	CLA	C1A-C2A-CAA-CBA
9	B	815	CLA	C3A-C2A-CAA-CBA
9	B	815	CLA	C2B-C3B-CAB-CBB
9	B	815	CLA	C4B-C3B-CAB-CBB
9	B	817	CLA	C3A-C2A-CAA-CBA
9	B	817	CLA	C4B-C3B-CAB-CBB
9	B	817	CLA	CBD-CGD-O2D-CED
9	B	818	CLA	C1A-C2A-CAA-CBA
9	B	818	CLA	C3A-C2A-CAA-CBA
9	B	818	CLA	CBD-CGD-O2D-CED
9	B	818	CLA	C2-C3-C5-C6
9	B	818	CLA	C4-C3-C5-C6
9	B	820	CLA	C1A-C2A-CAA-CBA
9	B	820	CLA	C3A-C2A-CAA-CBA
9	B	820	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
9	B	820	CLA	C4B-C3B-CAB-CBB
9	B	820	CLA	CAD-CBD-CGD-O1D
9	B	820	CLA	CAD-CBD-CGD-O2D
9	B	821	CLA	CBD-CGD-O2D-CED
9	B	822	CLA	C1A-C2A-CAA-CBA
9	B	822	CLA	C3A-C2A-CAA-CBA
9	B	822	CLA	C2B-C3B-CAB-CBB
9	B	822	CLA	C4B-C3B-CAB-CBB
9	B	822	CLA	CBD-CGD-O2D-CED
9	B	823	CLA	CBD-CGD-O2D-CED
9	B	824	CLA	CHA-CBD-CGD-O1D
9	B	824	CLA	CHA-CBD-CGD-O2D
9	B	825	CLA	CHA-CBD-CGD-O1D
9	B	825	CLA	CHA-CBD-CGD-O2D
9	B	826	CLA	CAD-CBD-CGD-O1D
9	B	826	CLA	CAD-CBD-CGD-O2D
9	B	826	CLA	CBD-CGD-O2D-CED
9	B	827	CLA	C3A-C2A-CAA-CBA
9	B	827	CLA	C2B-C3B-CAB-CBB
9	B	827	CLA	C4B-C3B-CAB-CBB
9	B	828	CLA	C1A-C2A-CAA-CBA
9	B	828	CLA	C3A-C2A-CAA-CBA
9	B	829	CLA	CHA-CBD-CGD-O1D
9	B	829	CLA	CHA-CBD-CGD-O2D
9	B	830	CLA	C3A-C2A-CAA-CBA
9	B	830	CLA	C2B-C3B-CAB-CBB
9	B	830	CLA	C4B-C3B-CAB-CBB
9	B	830	CLA	CHA-CBD-CGD-O1D
9	B	830	CLA	CHA-CBD-CGD-O2D
9	B	830	CLA	CBD-CGD-O2D-CED
9	B	831	CLA	CBD-CGD-O2D-CED
9	B	833	CLA	CHA-CBD-CGD-O1D
9	B	833	CLA	CHA-CBD-CGD-O2D
9	B	833	CLA	CBD-CGD-O2D-CED
9	B	834	CLA	CBD-CGD-O2D-CED
9	B	835	CLA	C2B-C3B-CAB-CBB
9	B	835	CLA	C4B-C3B-CAB-CBB
9	B	836	CLA	CBD-CGD-O2D-CED
9	B	839	CLA	CBD-CGD-O2D-CED
9	B	840	CLA	C2B-C3B-CAB-CBB
9	B	840	CLA	C4B-C3B-CAB-CBB
9	B	840	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
9	I	101	CLA	CHA-CBD-CGD-O1D
9	I	101	CLA	CHA-CBD-CGD-O2D
9	K	101	CLA	C1A-C2A-CAA-CBA
9	K	101	CLA	C2B-C3B-CAB-CBB
9	K	101	CLA	C4B-C3B-CAB-CBB
10	A	845	PQN	C14-C13-C15-C16
12	A	847	BCR	C11-C10-C9-C8
12	A	847	BCR	C11-C10-C9-C34
12	A	847	BCR	C23-C24-C25-C26
12	A	848	BCR	C7-C8-C9-C10
12	A	848	BCR	C7-C8-C9-C34
12	A	848	BCR	C11-C10-C9-C8
12	A	848	BCR	C11-C10-C9-C34
12	A	848	BCR	C10-C11-C12-C13
12	A	848	BCR	C17-C18-C19-C20
12	A	849	BCR	C11-C10-C9-C8
12	A	849	BCR	C11-C10-C9-C34
12	A	849	BCR	C10-C11-C12-C13
12	A	849	BCR	C23-C24-C25-C26
12	A	849	BCR	C23-C24-C25-C30
12	A	850	BCR	C7-C8-C9-C10
12	A	850	BCR	C7-C8-C9-C34
12	A	850	BCR	C11-C10-C9-C8
12	A	850	BCR	C11-C10-C9-C34
12	A	850	BCR	C9-C10-C11-C12
12	A	851	BCR	C7-C8-C9-C10
12	A	851	BCR	C7-C8-C9-C34
12	A	851	BCR	C11-C10-C9-C8
12	A	851	BCR	C11-C10-C9-C34
12	A	851	BCR	C17-C18-C19-C20
12	B	842	BCR	C7-C8-C9-C10
12	B	842	BCR	C7-C8-C9-C34
12	B	842	BCR	C11-C10-C9-C8
12	B	842	BCR	C11-C10-C9-C34
12	B	842	BCR	C21-C22-C23-C24
12	B	843	BCR	C7-C8-C9-C10
12	B	843	BCR	C11-C10-C9-C8
12	B	843	BCR	C11-C10-C9-C34
12	B	844	BCR	C21-C22-C23-C24
12	B	845	BCR	C11-C10-C9-C8
12	B	845	BCR	C11-C10-C9-C34
12	B	845	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
12	B	846	BCR	C7-C8-C9-C10
12	B	846	BCR	C11-C10-C9-C8
12	B	846	BCR	C11-C10-C9-C34
12	B	846	BCR	C17-C18-C19-C20
12	B	846	BCR	C21-C22-C23-C24
12	B	847	BCR	C11-C10-C9-C8
12	B	847	BCR	C11-C10-C9-C34
12	B	847	BCR	C10-C11-C12-C13
12	F	201	BCR	C11-C10-C9-C8
12	F	201	BCR	C11-C10-C9-C34
12	M	101	BCR	C11-C10-C9-C8
12	M	101	BCR	C11-C10-C9-C34
13	A	852	LHG	O1-C1-C2-O2
13	A	852	LHG	O1-C1-C2-C3
13	A	852	LHG	C1-C2-C3-O3
13	A	852	LHG	C3-O3-P-O4
13	A	852	LHG	C3-O3-P-O6
13	A	852	LHG	C4-O6-P-O3
13	A	852	LHG	C4-O6-P-O4
13	A	852	LHG	C4-O6-P-O5
13	A	853	LHG	C4-O6-P-O3
13	A	853	LHG	C4-O6-P-O4
9	A	809	CLA	O1D-CGD-O2D-CED
9	A	810	CLA	O1D-CGD-O2D-CED
9	B	823	CLA	O1D-CGD-O2D-CED
9	B	835	CLA	O1D-CGD-O2D-CED
9	A	806	CLA	O1D-CGD-O2D-CED
9	A	811	CLA	O1D-CGD-O2D-CED
9	A	821	CLA	O1D-CGD-O2D-CED
9	A	824	CLA	O1D-CGD-O2D-CED
9	A	828	CLA	O1D-CGD-O2D-CED
9	A	841	CLA	O1D-CGD-O2D-CED
9	B	803	CLA	O1D-CGD-O2D-CED
9	B	822	CLA	O1D-CGD-O2D-CED
8	A	801	CL0	CBD-CGD-O2D-CED
9	A	802	CLA	CBD-CGD-O2D-CED
9	A	803	CLA	CBD-CGD-O2D-CED
9	A	806	CLA	CBD-CGD-O2D-CED
9	A	808	CLA	CBD-CGD-O2D-CED
9	A	809	CLA	CBD-CGD-O2D-CED
9	A	810	CLA	CBD-CGD-O2D-CED
9	A	811	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
9	A	812	CLA	CBD-CGD-O2D-CED
9	A	813	CLA	CBD-CGD-O2D-CED
9	A	817	CLA	CBD-CGD-O2D-CED
9	A	818	CLA	CBD-CGD-O2D-CED
9	A	819	CLA	CBD-CGD-O2D-CED
9	A	820	CLA	CBD-CGD-O2D-CED
9	A	821	CLA	CBD-CGD-O2D-CED
9	A	823	CLA	CBD-CGD-O2D-CED
9	A	824	CLA	CBD-CGD-O2D-CED
9	A	828	CLA	CBD-CGD-O2D-CED
9	A	830	CLA	CBD-CGD-O2D-CED
9	A	832	CLA	CBD-CGD-O2D-CED
9	A	833	CLA	CBD-CGD-O2D-CED
9	A	836	CLA	CBD-CGD-O2D-CED
9	A	837	CLA	CBD-CGD-O2D-CED
9	A	841	CLA	CBD-CGD-O2D-CED
9	A	843	CLA	CBD-CGD-O2D-CED
9	B	806	CLA	CBD-CGD-O2D-CED
9	B	807	CLA	CBD-CGD-O2D-CED
9	B	809	CLA	CBD-CGD-O2D-CED
9	B	811	CLA	CBD-CGD-O2D-CED
9	B	812	CLA	CBD-CGD-O2D-CED
9	B	813	CLA	CBD-CGD-O2D-CED
9	B	814	CLA	CBD-CGD-O2D-CED
9	B	815	CLA	CBD-CGD-O2D-CED
9	B	816	CLA	CBD-CGD-O2D-CED
9	B	820	CLA	CBD-CGD-O2D-CED
9	B	825	CLA	CBD-CGD-O2D-CED
9	B	827	CLA	CBD-CGD-O2D-CED
9	B	835	CLA	CBD-CGD-O2D-CED
9	B	837	CLA	CBD-CGD-O2D-CED
8	A	801	CL0	O1A-CGA-O2A-C1
9	A	820	CLA	O1A-CGA-O2A-C1
9	B	819	CLA	O1A-CGA-O2A-C1
9	A	812	CLA	O1D-CGD-O2D-CED
9	A	813	CLA	O1D-CGD-O2D-CED
9	A	818	CLA	O1D-CGD-O2D-CED
9	A	823	CLA	O1D-CGD-O2D-CED
9	A	843	CLA	O1D-CGD-O2D-CED
9	B	807	CLA	O1D-CGD-O2D-CED
9	B	811	CLA	O1D-CGD-O2D-CED
9	B	816	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
9	B	827	CLA	O1D-CGD-O2D-CED
8	A	801	CL0	CBA-CGA-O2A-C1
9	B	819	CLA	CBA-CGA-O2A-C1
9	A	834	CLA	CBD-CGD-O2D-CED
9	I	101	CLA	CBD-CGD-O2D-CED
9	A	819	CLA	O1A-CGA-O2A-C1
14	B	848	LMG	O10-C28-O8-C9
9	A	802	CLA	O1D-CGD-O2D-CED
9	A	832	CLA	O1D-CGD-O2D-CED
9	A	833	CLA	O1D-CGD-O2D-CED
9	A	844	CLA	O1D-CGD-O2D-CED
9	B	810	CLA	O1D-CGD-O2D-CED
9	B	815	CLA	O1D-CGD-O2D-CED
9	B	818	CLA	O1D-CGD-O2D-CED
9	B	831	CLA	O1D-CGD-O2D-CED
9	B	840	CLA	O1D-CGD-O2D-CED
9	A	815	CLA	O1D-CGD-O2D-CED
9	A	816	CLA	O1D-CGD-O2D-CED
9	A	835	CLA	O1D-CGD-O2D-CED
9	A	840	CLA	O1D-CGD-O2D-CED
9	B	805	CLA	O1D-CGD-O2D-CED
9	B	817	CLA	O1D-CGD-O2D-CED
9	B	821	CLA	O1D-CGD-O2D-CED
9	B	833	CLA	O1D-CGD-O2D-CED
9	B	834	CLA	O1D-CGD-O2D-CED
9	B	836	CLA	O1D-CGD-O2D-CED
8	A	801	CL0	C3-C5-C6-C7
9	A	806	CLA	C3-C5-C6-C7
9	A	825	CLA	C3-C5-C6-C7
9	B	801	CLA	C3-C5-C6-C7
9	B	807	CLA	C3-C5-C6-C7
9	B	813	CLA	C3-C5-C6-C7
9	B	836	CLA	C3-C5-C6-C7
10	A	845	PQN	C13-C15-C16-C17
9	B	818	CLA	CBA-CGA-O2A-C1
9	B	836	CLA	CBA-CGA-O2A-C1
14	B	848	LMG	C29-C28-O8-C9
9	A	804	CLA	CBD-CGD-O2D-CED
9	A	826	CLA	CBD-CGD-O2D-CED
9	A	831	CLA	CBD-CGD-O2D-CED
9	A	842	CLA	CBD-CGD-O2D-CED
9	B	801	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
9	B	808	CLA	CBD-CGD-O2D-CED
9	B	829	CLA	CBD-CGD-O2D-CED
9	B	838	CLA	CBD-CGD-O2D-CED
9	A	805	CLA	O1D-CGD-O2D-CED
9	A	807	CLA	O1D-CGD-O2D-CED
9	A	822	CLA	O1D-CGD-O2D-CED
9	B	826	CLA	O1D-CGD-O2D-CED
9	B	839	CLA	O1D-CGD-O2D-CED
9	B	830	CLA	O1D-CGD-O2D-CED
8	A	801	CL0	C2-C3-C5-C6
9	A	828	CLA	C2-C3-C5-C6
10	A	845	PQN	C12-C13-C15-C16
9	A	817	CLA	O1D-CGD-O2D-CED
9	A	819	CLA	O1D-CGD-O2D-CED
9	B	814	CLA	O1D-CGD-O2D-CED
9	B	820	CLA	O1D-CGD-O2D-CED
9	B	837	CLA	O1D-CGD-O2D-CED
9	A	829	CLA	C2A-CAA-CBA-CGA
9	A	805	CLA	C3-C5-C6-C7
9	A	827	CLA	C3-C5-C6-C7
9	B	803	CLA	C3-C5-C6-C7
9	B	809	CLA	C3-C5-C6-C7
9	B	818	CLA	C3-C5-C6-C7
9	B	826	CLA	C3-C5-C6-C7
10	B	841	PQN	C13-C15-C16-C17
9	A	819	CLA	CBA-CGA-O2A-C1
9	B	806	CLA	CBA-CGA-O2A-C1
14	B	848	LMG	C23-C24-C25-C26
14	B	848	LMG	C35-C36-C37-C38
12	B	846	BCR	C9-C10-C11-C12
12	F	201	BCR	C15-C16-C17-C18
9	A	836	CLA	O1D-CGD-O2D-CED
9	A	837	CLA	O1D-CGD-O2D-CED
9	B	806	CLA	O1D-CGD-O2D-CED
9	A	802	CLA	C3-C5-C6-C7
13	A	852	LHG	O2-C2-C3-O3
9	A	803	CLA	O1D-CGD-O2D-CED
9	A	830	CLA	O1D-CGD-O2D-CED
9	B	809	CLA	O1D-CGD-O2D-CED
9	A	830	CLA	CBA-CGA-O2A-C1
9	B	806	CLA	O1A-CGA-O2A-C1
9	B	818	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
9	B	836	CLA	O1A-CGA-O2A-C1
9	A	820	CLA	O1D-CGD-O2D-CED
9	A	814	CLA	CBD-CGD-O2D-CED
8	A	801	CL0	O1D-CGD-O2D-CED
9	A	808	CLA	O1D-CGD-O2D-CED
9	B	825	CLA	O1D-CGD-O2D-CED
9	A	830	CLA	O1A-CGA-O2A-C1
9	B	812	CLA	O1D-CGD-O2D-CED
9	I	101	CLA	O1D-CGD-O2D-CED
9	B	813	CLA	O1D-CGD-O2D-CED
9	A	834	CLA	O1D-CGD-O2D-CED
9	A	805	CLA	CBA-CGA-O2A-C1
9	A	826	CLA	CBA-CGA-O2A-C1
9	B	801	CLA	O1D-CGD-O2D-CED
9	B	808	CLA	O1D-CGD-O2D-CED
9	B	803	CLA	C4-C3-C5-C6
9	B	836	CLA	C4-C3-C5-C6
9	B	836	CLA	C2-C3-C5-C6
10	B	841	PQN	C12-C13-C15-C16
9	A	828	CLA	C3-C5-C6-C7
9	A	805	CLA	C6-C7-C8-C9
9	B	803	CLA	C6-C7-C8-C9
9	B	818	CLA	C6-C7-C8-C9
9	A	831	CLA	O1D-CGD-O2D-CED
9	B	838	CLA	O1D-CGD-O2D-CED
12	A	848	BCR	C36-C18-C19-C20
12	A	849	BCR	C7-C8-C9-C34
12	A	851	BCR	C36-C18-C19-C20
12	B	842	BCR	C37-C22-C23-C24
12	B	843	BCR	C7-C8-C9-C34
12	B	843	BCR	C37-C22-C23-C24
12	B	844	BCR	C37-C22-C23-C24
12	B	845	BCR	C11-C12-C13-C35
12	B	846	BCR	C7-C8-C9-C34
12	B	846	BCR	C36-C18-C19-C20
12	B	846	BCR	C37-C22-C23-C24
12	M	101	BCR	C7-C8-C9-C34
12	B	843	BCR	C21-C22-C23-C24
12	M	101	BCR	C7-C8-C9-C10
9	B	830	CLA	C2A-CAA-CBA-CGA
9	A	805	CLA	O1A-CGA-O2A-C1
13	A	852	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
9	A	829	CLA	C5-C6-C7-C8
9	B	803	CLA	C2-C1-O2A-CGA
9	B	807	CLA	C2-C1-O2A-CGA
9	A	842	CLA	O1D-CGD-O2D-CED
9	B	829	CLA	O1D-CGD-O2D-CED
9	A	828	CLA	C8-C10-C11-C12
13	A	853	LHG	O1-C1-C2-O2
9	A	813	CLA	C3-C5-C6-C7
9	A	830	CLA	C10-C11-C12-C13
9	B	803	CLA	C11-C10-C8-C7
9	A	828	CLA	CBA-CGA-O2A-C1
10	B	841	PQN	C14-C13-C15-C16
13	A	852	LHG	C23-C24-C25-C26
9	B	813	CLA	C10-C11-C12-C13
9	A	826	CLA	O1A-CGA-O2A-C1
9	A	826	CLA	O1D-CGD-O2D-CED
9	A	805	CLA	C15-C16-C17-C18
9	B	818	CLA	C5-C6-C7-C8
9	B	818	CLA	C8-C10-C11-C12
9	B	826	CLA	C8-C10-C11-C12
9	B	801	CLA	C2A-CAA-CBA-CGA
9	B	810	CLA	C2A-CAA-CBA-CGA
9	B	815	CLA	C2A-CAA-CBA-CGA
9	B	817	CLA	C2A-CAA-CBA-CGA
12	A	847	BCR	C10-C11-C12-C13
9	A	806	CLA	C5-C6-C7-C8
9	A	827	CLA	C10-C11-C12-C13
9	B	807	CLA	C10-C11-C12-C13
14	B	848	LMG	C10-C11-C12-C13
14	B	848	LMG	O6-C1-O1-C7
9	A	804	CLA	O1D-CGD-O2D-CED
9	B	837	CLA	C10-C11-C12-C13
10	B	841	PQN	C18-C20-C21-C22
9	A	805	CLA	C13-C15-C16-C17
9	B	804	CLA	C10-C11-C12-C13
9	B	807	CLA	C13-C15-C16-C17
9	A	814	CLA	O1D-CGD-O2D-CED
9	B	824	CLA	CBD-CGD-O2D-CED
9	A	829	CLA	C15-C16-C17-C18
9	B	809	CLA	C13-C15-C16-C17
9	B	828	CLA	C8-C10-C11-C12
10	B	841	PQN	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
9	A	821	CLA	CBA-CGA-O2A-C1
9	A	825	CLA	CBA-CGA-O2A-C1
12	A	848	BCR	C9-C10-C11-C12
12	B	847	BCR	C9-C10-C11-C12
9	A	807	CLA	C2A-CAA-CBA-CGA
9	A	843	CLA	C2A-CAA-CBA-CGA
9	B	839	CLA	C2A-CAA-CBA-CGA
9	B	801	CLA	C8-C10-C11-C12
9	A	819	CLA	C15-C16-C17-C18
9	A	826	CLA	C5-C6-C7-C8
9	A	829	CLA	C8-C10-C11-C12
9	B	804	CLA	C8-C10-C11-C12
9	B	807	CLA	C5-C6-C7-C8
9	B	827	CLA	CBA-CGA-O2A-C1
9	B	826	CLA	C4-C3-C5-C6
14	B	848	LMG	C2-C1-O1-C7
9	B	813	CLA	CBA-CGA-O2A-C1
9	B	801	CLA	C10-C11-C12-C13
12	A	850	BCR	C36-C18-C19-C20
9	B	816	CLA	C2A-CAA-CBA-CGA
9	B	819	CLA	C2A-CAA-CBA-CGA
9	B	831	CLA	C2A-CAA-CBA-CGA
13	A	853	LHG	O1-C1-C2-C3
13	A	852	LHG	C7-C8-C9-C10
9	A	829	CLA	CBD-CGD-O2D-CED
9	B	804	CLA	CBA-CGA-O2A-C1
9	A	828	CLA	O1A-CGA-O2A-C1
9	A	827	CLA	C15-C16-C17-C18
13	A	853	LHG	C7-C8-C9-C10
9	A	821	CLA	C2-C1-O2A-CGA
9	A	825	CLA	C2-C1-O2A-CGA
9	A	826	CLA	C2-C1-O2A-CGA
9	A	842	CLA	C2-C1-O2A-CGA
9	B	804	CLA	C2-C1-O2A-CGA
9	B	814	CLA	C2-C1-O2A-CGA
9	A	819	CLA	C16-C17-C18-C20
9	B	807	CLA	C16-C17-C18-C19
9	B	828	CLA	C13-C15-C16-C17
9	B	803	CLA	C10-C11-C12-C13
9	B	809	CLA	C10-C11-C12-C13
9	A	817	CLA	C4B-C3B-CAB-CBB
9	A	821	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
9	A	833	CLA	C4B-C3B-CAB-CBB
9	B	839	CLA	C4B-C3B-CAB-CBB
9	I	101	CLA	C4B-C3B-CAB-CBB
9	A	819	CLA	C16-C17-C18-C19
9	B	807	CLA	C16-C17-C18-C20
9	A	802	CLA	C2A-CAA-CBA-CGA
9	B	804	CLA	C2A-CAA-CBA-CGA
9	A	825	CLA	C8-C10-C11-C12
9	B	804	CLA	C13-C15-C16-C17
9	A	821	CLA	O1A-CGA-O2A-C1
9	A	803	CLA	C3A-C2A-CAA-CBA
9	A	805	CLA	C3A-C2A-CAA-CBA
9	A	806	CLA	C3A-C2A-CAA-CBA
9	A	827	CLA	C3A-C2A-CAA-CBA
9	A	837	CLA	C3A-C2A-CAA-CBA
9	B	813	CLA	C3A-C2A-CAA-CBA
9	B	814	CLA	C3A-C2A-CAA-CBA
9	B	824	CLA	C3A-C2A-CAA-CBA
9	B	826	CLA	C3A-C2A-CAA-CBA
9	K	101	CLA	C3A-C2A-CAA-CBA
12	A	851	BCR	C19-C20-C21-C22
12	B	844	BCR	C19-C20-C21-C22
9	A	825	CLA	O1A-CGA-O2A-C1
9	A	813	CLA	CBA-CGA-O2A-C1
9	B	814	CLA	C3-C5-C6-C7
9	B	828	CLA	C15-C16-C17-C18
9	A	802	CLA	C16-C17-C18-C19
9	B	827	CLA	O1A-CGA-O2A-C1
9	A	802	CLA	C2B-C3B-CAB-CBB
9	A	835	CLA	C2B-C3B-CAB-CBB
9	A	841	CLA	C2B-C3B-CAB-CBB
9	B	817	CLA	C2B-C3B-CAB-CBB
12	A	847	BCR	C23-C24-C25-C30
12	A	848	BCR	C1-C6-C7-C8
12	A	848	BCR	C5-C6-C7-C8
12	A	850	BCR	C1-C6-C7-C8
12	A	850	BCR	C5-C6-C7-C8
12	B	844	BCR	C23-C24-C25-C26
12	B	844	BCR	C23-C24-C25-C30
9	A	813	CLA	C2A-CAA-CBA-CGA
9	A	816	CLA	C2A-CAA-CBA-CGA
9	B	802	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
9	B	813	CLA	C2A-CAA-CBA-CGA
9	A	813	CLA	O1A-CGA-O2A-C1
9	B	804	CLA	O1A-CGA-O2A-C1
9	B	813	CLA	O1A-CGA-O2A-C1
12	B	842	BCR	C10-C11-C12-C13
12	B	843	BCR	C10-C11-C12-C13
12	M	101	BCR	C10-C11-C12-C13
9	B	803	CLA	C2-C3-C5-C6
9	B	826	CLA	C2-C3-C5-C6
9	B	803	CLA	CBA-CGA-O2A-C1
9	A	806	CLA	C15-C16-C17-C18
12	A	849	BCR	C9-C10-C11-C12
13	A	852	LHG	C29-C30-C31-C32
12	B	845	BCR	C11-C12-C13-C14
9	A	811	CLA	C2A-CAA-CBA-CGA
9	A	802	CLA	C16-C17-C18-C20
13	A	852	LHG	C34-C35-C36-C37
14	B	848	LMG	C11-C10-O7-C8
10	A	845	PQN	C15-C16-C17-C18
14	B	848	LMG	C22-C23-C24-C25
9	A	825	CLA	C5-C6-C7-C8
14	B	848	LMG	O6-C5-C6-O5
13	A	853	LHG	O7-C5-C6-O8
14	B	848	LMG	C12-C13-C14-C15
9	A	830	CLA	C13-C15-C16-C17
9	B	805	CLA	C2A-CAA-CBA-CGA
9	B	827	CLA	C2A-CAA-CBA-CGA
9	B	828	CLA	CBD-CGD-O2D-CED
9	B	803	CLA	C8-C10-C11-C12
9	A	803	CLA	C1A-C2A-CAA-CBA
9	A	805	CLA	C1A-C2A-CAA-CBA
9	A	806	CLA	C1A-C2A-CAA-CBA
9	A	807	CLA	C1A-C2A-CAA-CBA
9	A	808	CLA	C1A-C2A-CAA-CBA
9	A	815	CLA	C1A-C2A-CAA-CBA
9	A	816	CLA	C1A-C2A-CAA-CBA
9	A	824	CLA	C1A-C2A-CAA-CBA
9	A	825	CLA	C1A-C2A-CAA-CBA
9	A	827	CLA	C1A-C2A-CAA-CBA
9	A	830	CLA	C1A-C2A-CAA-CBA
9	A	831	CLA	C1A-C2A-CAA-CBA
9	A	832	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
9	A	834	CLA	C1A-C2A-CAA-CBA
9	A	837	CLA	C1A-C2A-CAA-CBA
9	A	844	CLA	C1A-C2A-CAA-CBA
9	B	806	CLA	C1A-C2A-CAA-CBA
9	B	811	CLA	C1A-C2A-CAA-CBA
9	B	817	CLA	C1A-C2A-CAA-CBA
9	B	821	CLA	C1A-C2A-CAA-CBA
9	B	824	CLA	C1A-C2A-CAA-CBA
9	B	826	CLA	C1A-C2A-CAA-CBA
9	B	827	CLA	C1A-C2A-CAA-CBA
9	B	829	CLA	C1A-C2A-CAA-CBA
9	B	830	CLA	C1A-C2A-CAA-CBA
9	B	832	CLA	C1A-C2A-CAA-CBA
9	B	835	CLA	C1A-C2A-CAA-CBA
9	B	838	CLA	C1A-C2A-CAA-CBA
9	B	839	CLA	C1A-C2A-CAA-CBA
9	B	840	CLA	C1A-C2A-CAA-CBA
9	A	839	CLA	CBD-CGD-O2D-CED
13	A	852	LHG	C11-C12-C13-C14
13	A	852	LHG	C30-C31-C32-C33
9	A	805	CLA	C6-C7-C8-C10
9	A	806	CLA	C11-C12-C13-C15
9	A	819	CLA	C11-C12-C13-C15
9	A	819	CLA	C12-C13-C15-C16
9	B	802	CLA	C12-C13-C15-C16
13	A	852	LHG	C12-C13-C14-C15
8	A	801	CL0	C8-C10-C11-C12
9	B	803	CLA	O1A-CGA-O2A-C1
9	B	813	CLA	C2-C3-C5-C6
9	A	810	CLA	C2A-CAA-CBA-CGA
9	A	806	CLA	C11-C12-C13-C14
9	A	813	CLA	C11-C10-C8-C9
9	A	819	CLA	C11-C12-C13-C14
9	A	819	CLA	C14-C13-C15-C16
9	B	803	CLA	C11-C12-C13-C14
9	B	807	CLA	CBA-CGA-O2A-C1
9	A	821	CLA	C10-C11-C12-C13
13	A	852	LHG	C4-C5-C6-O8
9	A	805	CLA	C8-C10-C11-C12
9	A	806	CLA	C10-C11-C12-C13
9	A	830	CLA	C5-C6-C7-C8
9	A	829	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
9	A	829	CLA	O1D-CGD-O2D-CED
9	B	813	CLA	C13-C15-C16-C17
12	A	849	BCR	C7-C8-C9-C10
9	B	807	CLA	O1A-CGA-O2A-C1
13	A	853	LHG	C24-C23-O8-C6
9	B	802	CLA	O2A-C1-C2-C3
13	A	852	LHG	C33-C34-C35-C36
12	B	846	BCR	C10-C11-C12-C13
12	B	842	BCR	C19-C20-C21-C22
9	B	824	CLA	O1D-CGD-O2D-CED
9	B	828	CLA	C16-C17-C18-C19
14	B	848	LMG	C24-C25-C26-C27
9	B	818	CLA	C2-C1-O2A-CGA
8	A	801	CL0	C11-C12-C13-C14
9	B	827	CLA	C4-C3-C5-C6
9	B	814	CLA	CBA-CGA-O2A-C1
9	A	825	CLA	C14-C13-C15-C16
9	A	829	CLA	C11-C12-C13-C14
9	B	802	CLA	C14-C13-C15-C16
9	B	813	CLA	C14-C13-C15-C16
9	B	828	CLA	C14-C13-C15-C16
9	B	826	CLA	C5-C6-C7-C8
9	A	803	CLA	C4B-C3B-CAB-CBB
9	A	807	CLA	C4B-C3B-CAB-CBB
9	A	809	CLA	C4B-C3B-CAB-CBB
9	A	813	CLA	C4B-C3B-CAB-CBB
9	A	815	CLA	C4B-C3B-CAB-CBB
9	A	816	CLA	C4B-C3B-CAB-CBB
9	A	819	CLA	C4B-C3B-CAB-CBB
9	A	826	CLA	C4B-C3B-CAB-CBB
9	A	828	CLA	C4B-C3B-CAB-CBB
9	A	832	CLA	C4B-C3B-CAB-CBB
9	A	839	CLA	C4B-C3B-CAB-CBB
9	A	844	CLA	C4B-C3B-CAB-CBB
9	B	802	CLA	C4B-C3B-CAB-CBB
9	B	804	CLA	C4B-C3B-CAB-CBB
9	B	807	CLA	C4B-C3B-CAB-CBB
9	B	808	CLA	C4B-C3B-CAB-CBB
9	B	810	CLA	C4B-C3B-CAB-CBB
9	B	813	CLA	C4B-C3B-CAB-CBB
9	B	814	CLA	C4B-C3B-CAB-CBB
9	B	816	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
9	B	831	CLA	C4B-C3B-CAB-CBB
9	B	837	CLA	C4B-C3B-CAB-CBB
14	B	848	LMG	C31-C32-C33-C34
8	A	801	CL0	C2A-CAA-CBA-CGA
13	A	852	LHG	O6-C4-C5-C6
9	A	805	CLA	C11-C10-C8-C7
9	A	813	CLA	C11-C10-C8-C7
9	A	821	CLA	C11-C10-C8-C7
9	A	825	CLA	C12-C13-C15-C16
9	A	828	CLA	C11-C12-C13-C15
9	A	829	CLA	C11-C12-C13-C15
9	B	802	CLA	C11-C10-C8-C7
9	B	803	CLA	C11-C12-C13-C15
9	B	813	CLA	C12-C13-C15-C16
9	B	828	CLA	C12-C13-C15-C16
13	A	852	LHG	C10-C11-C12-C13
8	A	801	CL0	C11-C12-C13-C15
9	A	829	CLA	O1A-CGA-O2A-C1
9	A	812	CLA	C3A-C2A-CAA-CBA
9	A	823	CLA	C3A-C2A-CAA-CBA
9	B	809	CLA	C3A-C2A-CAA-CBA
9	B	813	CLA	C4-C3-C5-C6
9	B	819	CLA	C2-C3-C5-C6
9	A	818	CLA	CBA-CGA-O2A-C1
12	A	850	BCR	C17-C18-C19-C20
13	A	852	LHG	C35-C36-C37-C38
13	A	853	LHG	C4-C5-C6-O8
9	A	821	CLA	C4-C3-C5-C6
9	B	802	CLA	C4-C3-C5-C6
9	B	819	CLA	C4-C3-C5-C6
9	B	827	CLA	C2-C3-C5-C6
14	B	848	LMG	O9-C10-O7-C8
9	B	802	CLA	C13-C15-C16-C17
13	A	852	LHG	O6-C4-C5-O7
12	B	847	BCR	C23-C24-C25-C30
9	B	828	CLA	C16-C17-C18-C20
13	A	853	LHG	O10-C23-O8-C6
9	A	805	CLA	C11-C10-C8-C9
9	A	828	CLA	C11-C12-C13-C14
9	B	803	CLA	C11-C10-C8-C9
9	A	839	CLA	O1D-CGD-O2D-CED
9	B	828	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
9	A	825	CLA	C13-C15-C16-C17
9	B	806	CLA	C3-C5-C6-C7
13	A	853	LHG	C8-C7-O7-C5
14	B	848	LMG	C34-C35-C36-C37
9	A	805	CLA	C11-C12-C13-C15
9	B	837	CLA	C11-C10-C8-C7
14	B	848	LMG	C11-C12-C13-C14
9	A	808	CLA	C2A-CAA-CBA-CGA
9	B	812	CLA	C2A-CAA-CBA-CGA
9	A	825	CLA	C4-C3-C5-C6
9	B	837	CLA	C4-C3-C5-C6
9	B	814	CLA	O1A-CGA-O2A-C1
12	B	843	BCR	C19-C20-C21-C22
12	B	845	BCR	C19-C20-C21-C22
9	A	818	CLA	O1A-CGA-O2A-C1
13	A	852	LHG	C26-C27-C28-C29
9	A	829	CLA	CAA-CBA-CGA-O2A
9	A	821	CLA	C2-C3-C5-C6
9	B	837	CLA	C5-C6-C7-C8
9	A	805	CLA	C11-C12-C13-C14
9	B	802	CLA	C11-C10-C8-C9
9	A	842	CLA	CAA-CBA-CGA-O2A
9	A	828	CLA	C13-C15-C16-C17
9	B	809	CLA	C15-C16-C17-C18
10	B	841	PQN	C23-C25-C26-C27
9	A	823	CLA	C1A-C2A-CAA-CBA
9	A	839	CLA	C1A-C2A-CAA-CBA
9	A	843	CLA	C1A-C2A-CAA-CBA
9	B	806	CLA	C4B-C3B-CAB-CBB
9	B	809	CLA	C4-C3-C5-C6
9	A	830	CLA	C11-C10-C8-C7
9	B	803	CLA	C6-C7-C8-C10
9	A	842	CLA	C3A-C2A-CAA-CBA
9	B	837	CLA	C2-C3-C5-C6
13	A	853	LHG	O9-C7-O7-C5
9	A	821	CLA	C11-C10-C8-C9
9	A	825	CLA	C2-C3-C5-C6
9	A	804	CLA	CAD-CBD-CGD-O2D
9	A	837	CLA	CAD-CBD-CGD-O2D
9	B	834	CLA	CAD-CBD-CGD-O2D
9	B	836	CLA	CAD-CBD-CGD-O2D
9	A	828	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
9	A	804	CLA	CAD-CBD-CGD-O1D
9	A	805	CLA	CAD-CBD-CGD-O1D
9	A	837	CLA	CAD-CBD-CGD-O1D
9	B	813	CLA	CHA-CBD-CGD-O1D
9	B	821	CLA	CHA-CBD-CGD-O1D
9	B	834	CLA	CAD-CBD-CGD-O1D
9	B	836	CLA	CAD-CBD-CGD-O1D
13	A	853	LHG	C4-O6-P-O5
9	A	813	CLA	C8-C10-C11-C12
9	B	828	CLA	C4-C3-C5-C6
9	A	817	CLA	C2B-C3B-CAB-CBB
9	A	821	CLA	C2B-C3B-CAB-CBB
9	A	833	CLA	C2B-C3B-CAB-CBB
9	A	839	CLA	C2B-C3B-CAB-CBB
9	B	806	CLA	C2B-C3B-CAB-CBB
9	B	814	CLA	C2B-C3B-CAB-CBB
9	B	839	CLA	C2B-C3B-CAB-CBB
9	I	101	CLA	C2B-C3B-CAB-CBB
9	B	802	CLA	C2-C3-C5-C6
9	B	813	CLA	C8-C10-C11-C12
9	A	828	CLA	C5-C6-C7-C8
9	A	805	CLA	C5-C6-C7-C8
10	B	841	PQN	C25-C26-C27-C28
9	A	844	CLA	C2C-C3C-CAC-CBC
13	A	852	LHG	C13-C14-C15-C16
9	B	809	CLA	C16-C17-C18-C19
14	B	848	LMG	O7-C8-C9-O8
9	B	836	CLA	C2A-CAA-CBA-CGA
9	A	802	CLA	C2-C1-O2A-CGA
9	B	806	CLA	C2-C1-O2A-CGA
9	B	826	CLA	C2-C1-O2A-CGA
9	B	827	CLA	CAA-CBA-CGA-O2A
9	A	824	CLA	C2A-CAA-CBA-CGA
9	A	827	CLA	C2A-CAA-CBA-CGA
9	A	841	CLA	C2A-CAA-CBA-CGA
12	M	101	BCR	C15-C16-C17-C18
9	B	801	CLA	C4-C3-C5-C6
9	A	821	CLA	C16-C17-C18-C19
9	A	844	CLA	CAA-CBA-CGA-O2A
9	A	830	CLA	C11-C10-C8-C9
9	B	832	CLA	C4B-C3B-CAB-CBB
9	A	804	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
13	A	852	LHG	C19-C20-C21-C22
9	A	802	CLA	C4-C3-C5-C6
9	A	802	CLA	C6-C7-C8-C10
9	A	825	CLA	C11-C12-C13-C15
9	A	827	CLA	O1D-CGD-O2D-CED
9	B	827	CLA	C3-C5-C6-C7
9	B	837	CLA	C3A-C2A-CAA-CBA
9	A	833	CLA	CAA-CBA-CGA-O2A
9	B	812	CLA	CAA-CBA-CGA-O1A
12	A	851	BCR	C16-C17-C18-C36
12	B	844	BCR	C11-C10-C9-C34
12	B	844	BCR	C20-C21-C22-C37
9	A	844	CLA	C4C-C3C-CAC-CBC
9	B	838	CLA	CAA-CBA-CGA-O2A
12	B	842	BCR	C9-C10-C11-C12
12	M	101	BCR	C19-C20-C21-C22
9	A	844	CLA	CAA-CBA-CGA-O1A
9	B	821	CLA	CAA-CBA-CGA-O2A
14	B	848	LMG	C21-C22-C23-C24
9	B	821	CLA	CAA-CBA-CGA-O1A
9	B	809	CLA	C2-C3-C5-C6
12	F	201	BCR	C14-C15-C16-C17
9	A	804	CLA	CAA-CBA-CGA-O1A
9	A	812	CLA	CAA-CBA-CGA-O1A
9	A	833	CLA	CAA-CBA-CGA-O1A
9	B	822	CLA	CAA-CBA-CGA-O1A
9	A	802	CLA	C6-C7-C8-C9
9	A	813	CLA	C6-C7-C8-C9
9	B	802	CLA	C6-C7-C8-C9
9	B	813	CLA	C11-C12-C13-C14
9	A	803	CLA	CAA-CBA-CGA-O1A
9	B	815	CLA	CAA-CBA-CGA-O1A
9	B	824	CLA	CAA-CBA-CGA-O1A
9	B	838	CLA	CAA-CBA-CGA-O1A
13	A	852	LHG	O9-C7-O7-C5
9	A	827	CLA	CBD-CGD-O2D-CED
9	A	836	CLA	CAA-CBA-CGA-O1A
9	A	802	CLA	C2-C3-C5-C6
14	B	848	LMG	C29-C30-C31-C32
9	A	809	CLA	C1A-C2A-CAA-CBA
9	A	820	CLA	C1A-C2A-CAA-CBA
12	A	851	BCR	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
12	B	844	BCR	C11-C10-C9-C8
9	A	803	CLA	CAA-CBA-CGA-O2A
9	A	812	CLA	CAA-CBA-CGA-O2A
9	A	803	CLA	C2B-C3B-CAB-CBB
9	A	807	CLA	C2B-C3B-CAB-CBB
9	A	809	CLA	C2B-C3B-CAB-CBB
9	A	813	CLA	C2B-C3B-CAB-CBB
9	A	819	CLA	C2B-C3B-CAB-CBB
9	A	826	CLA	C2B-C3B-CAB-CBB
9	A	840	CLA	C2B-C3B-CAB-CBB
9	A	844	CLA	C2B-C3B-CAB-CBB
9	B	802	CLA	C2B-C3B-CAB-CBB
9	B	804	CLA	C2B-C3B-CAB-CBB
9	B	807	CLA	C2B-C3B-CAB-CBB
9	B	808	CLA	C2B-C3B-CAB-CBB
9	B	813	CLA	C2B-C3B-CAB-CBB
9	B	832	CLA	C2B-C3B-CAB-CBB
9	B	837	CLA	C2B-C3B-CAB-CBB
12	B	842	BCR	C23-C24-C25-C30
12	B	847	BCR	C23-C24-C25-C26
12	M	101	BCR	C1-C6-C7-C8
12	M	101	BCR	C5-C6-C7-C8
13	A	853	LHG	O8-C23-C24-C25
9	B	822	CLA	CAA-CBA-CGA-O2A
9	A	838	CLA	CAA-CBA-CGA-O2A
9	A	802	CLA	C11-C12-C13-C15
9	A	806	CLA	C12-C13-C15-C16
9	A	822	CLA	C2A-CAA-CBA-CGA
9	B	812	CLA	CAA-CBA-CGA-O2A
9	A	823	CLA	CAA-CBA-CGA-O2A
9	A	836	CLA	CAA-CBA-CGA-O2A
9	A	838	CLA	CAA-CBA-CGA-O1A
9	A	827	CLA	C4-C3-C5-C6
9	B	826	CLA	C15-C16-C17-C18
9	A	823	CLA	CAA-CBA-CGA-O1A
13	A	852	LHG	C8-C7-O7-C5
9	A	843	CLA	CAA-CBA-CGA-O2A
9	B	805	CLA	CAA-CBA-CGA-O2A
9	B	815	CLA	CAA-CBA-CGA-O2A
9	A	813	CLA	C4-C3-C5-C6
9	A	820	CLA	C4-C3-C5-C6
9	B	801	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
9	B	809	CLA	C16-C17-C18-C20
9	A	839	CLA	CAA-CBA-CGA-O2A
12	B	847	BCR	C15-C16-C17-C18
9	B	808	CLA	CAA-CBA-CGA-O2A
9	B	816	CLA	CAA-CBA-CGA-O2A
9	A	805	CLA	C4B-C3B-CAB-CBB
9	A	840	CLA	C4B-C3B-CAB-CBB
9	B	826	CLA	C4B-C3B-CAB-CBB
9	B	824	CLA	CAA-CBA-CGA-O2A
9	B	830	CLA	CAA-CBA-CGA-O2A
14	B	848	LMG	C28-C29-C30-C31
9	A	826	CLA	C8-C10-C11-C12
9	A	813	CLA	C2-C3-C5-C6
9	B	818	CLA	C6-C7-C8-C10
9	A	843	CLA	CAA-CBA-CGA-O1A
9	B	805	CLA	CAA-CBA-CGA-O1A
9	I	101	CLA	CAA-CBA-CGA-O2A
9	A	802	CLA	C13-C15-C16-C17
13	A	853	LHG	C11-C10-C9-C8
9	B	830	CLA	CAA-CBA-CGA-O1A
9	B	833	CLA	CAA-CBA-CGA-O2A
9	B	834	CLA	CAA-CBA-CGA-O2A
9	A	829	CLA	C14-C13-C15-C16
9	B	807	CLA	C11-C12-C13-C14
13	A	853	LHG	O10-C23-C24-C25
14	B	848	LMG	C16-C17-C18-C19
13	A	852	LHG	C28-C29-C30-C31
9	B	816	CLA	CAA-CBA-CGA-O1A
9	A	817	CLA	C2-C1-O2A-CGA
9	A	802	CLA	C3A-C2A-CAA-CBA
9	A	813	CLA	C3A-C2A-CAA-CBA
9	A	828	CLA	C3A-C2A-CAA-CBA
9	A	829	CLA	C3A-C2A-CAA-CBA
9	B	828	CLA	C2-C3-C5-C6
9	B	808	CLA	CAA-CBA-CGA-O1A
9	B	834	CLA	CAA-CBA-CGA-O1A
9	B	840	CLA	CAA-CBA-CGA-O2A
12	B	844	BCR	C20-C21-C22-C23
9	A	841	CLA	CAA-CBA-CGA-O2A
9	B	833	CLA	CAA-CBA-CGA-O1A
9	A	839	CLA	CAA-CBA-CGA-O1A
13	A	852	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
9	I	101	CLA	CAA-CBA-CGA-O1A
9	B	837	CLA	C11-C10-C8-C9
10	B	841	PQN	C19-C18-C20-C21
9	A	817	CLA	CAA-CBA-CGA-O2A
9	A	840	CLA	CAA-CBA-CGA-O2A
9	B	837	CLA	CAA-CBA-CGA-O2A
9	B	824	CLA	C2A-CAA-CBA-CGA
9	A	829	CLA	C12-C13-C15-C16
9	B	807	CLA	C11-C12-C13-C15
9	B	826	CLA	C11-C10-C8-C7
13	A	852	LHG	C15-C16-C17-C18
9	B	840	CLA	CAA-CBA-CGA-O1A
9	A	815	CLA	C2B-C3B-CAB-CBB
9	A	816	CLA	C2B-C3B-CAB-CBB
9	A	828	CLA	C2B-C3B-CAB-CBB
9	A	832	CLA	C2B-C3B-CAB-CBB
9	A	836	CLA	C2B-C3B-CAB-CBB
9	B	810	CLA	C2B-C3B-CAB-CBB
9	B	816	CLA	C2B-C3B-CAB-CBB
9	B	826	CLA	C2B-C3B-CAB-CBB
9	B	831	CLA	C2B-C3B-CAB-CBB
12	B	842	BCR	C23-C24-C25-C26
12	B	846	BCR	C23-C24-C25-C26
9	A	813	CLA	C2-C1-O2A-CGA
12	A	847	BCR	C9-C10-C11-C12
13	A	852	LHG	O8-C23-C24-C25
9	A	821	CLA	C16-C17-C18-C20
9	A	835	CLA	C2A-CAA-CBA-CGA
9	A	841	CLA	CAA-CBA-CGA-O1A
9	B	813	CLA	C15-C16-C17-C18
9	A	835	CLA	CAA-CBA-CGA-O2A
9	A	837	CLA	CAA-CBA-CGA-O2A
9	B	806	CLA	CAA-CBA-CGA-O2A
9	B	817	CLA	C3-C5-C6-C7
9	A	811	CLA	CAA-CBA-CGA-O2A
9	A	815	CLA	CAA-CBA-CGA-O2A
9	A	806	CLA	C14-C13-C15-C16
9	B	818	CLA	C11-C10-C8-C9
14	B	848	LMG	C7-C8-C9-O8
9	A	802	CLA	C1A-C2A-CAA-CBA
9	A	813	CLA	C1A-C2A-CAA-CBA
8	A	801	CL0	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
9	A	805	CLA	CAA-CBA-CGA-O2A
9	A	822	CLA	CAA-CBA-CGA-O2A
9	A	835	CLA	CAA-CBA-CGA-O1A
12	B	843	BCR	C9-C10-C11-C12
12	F	201	BCR	C9-C10-C11-C12
9	B	813	CLA	CAA-CBA-CGA-O2A
9	A	838	CLA	C2A-CAA-CBA-CGA
9	B	836	CLA	C6-C7-C8-C10
9	A	842	CLA	CAA-CBA-CGA-O1A
9	A	829	CLA	CAA-CBA-CGA-O1A
9	A	818	CLA	C2-C1-O2A-CGA
10	B	841	PQN	C21-C22-C23-C25
9	B	828	CLA	C2A-CAA-CBA-CGA
9	A	824	CLA	CAA-CBA-CGA-O2A
9	B	802	CLA	C3A-C2A-CAA-CBA
9	B	803	CLA	C3A-C2A-CAA-CBA
13	A	852	LHG	C31-C32-C33-C34
9	A	837	CLA	CAA-CBA-CGA-O1A
9	A	840	CLA	CAA-CBA-CGA-O1A
13	A	852	LHG	O10-C23-C24-C25
14	B	848	LMG	C33-C34-C35-C36
9	A	822	CLA	CAA-CBA-CGA-O1A
9	A	811	CLA	CAA-CBA-CGA-O1A
9	A	815	CLA	CAA-CBA-CGA-O1A
9	A	816	CLA	CAA-CBA-CGA-O2A
12	A	849	BCR	C11-C12-C13-C14
8	A	801	CL0	CAA-CBA-CGA-O1A
9	A	817	CLA	CAA-CBA-CGA-O1A
9	B	837	CLA	CAA-CBA-CGA-O1A
9	B	808	CLA	C2A-CAA-CBA-CGA
9	A	807	CLA	CAA-CBA-CGA-O2A
9	B	802	CLA	C10-C11-C12-C13
9	B	804	CLA	C5-C6-C7-C8
9	B	821	CLA	CAD-CBD-CGD-O2D
9	A	818	CLA	C2A-CAA-CBA-CGA
9	A	824	CLA	CAA-CBA-CGA-O1A
9	B	810	CLA	CAA-CBA-CGA-O2A
9	A	809	CLA	CAA-CBA-CGA-O2A
9	B	826	CLA	CAA-CBA-CGA-O2A
9	A	827	CLA	C13-C15-C16-C17
9	B	806	CLA	CAA-CBA-CGA-O1A
9	B	813	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
13	A	853	LHG	C9-C10-C11-C12
9	B	839	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

71 monomers are involved in 126 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	835	CLA	2	0
9	A	807	CLA	2	0
9	B	836	CLA	2	0
9	B	806	CLA	1	0
12	A	849	BCR	2	0
9	B	810	CLA	2	0
12	A	847	BCR	3	0
8	A	801	CL0	5	0
12	B	846	BCR	1	0
9	A	813	CLA	1	0
9	B	803	CLA	4	0
9	B	818	CLA	2	0
9	B	827	CLA	1	0
9	B	809	CLA	3	0
9	A	825	CLA	2	0
9	B	831	CLA	1	0
12	B	845	BCR	2	0
9	B	807	CLA	3	0
12	M	101	BCR	4	0
9	A	838	CLA	2	0
9	B	813	CLA	3	0
12	B	842	BCR	2	0
9	B	825	CLA	3	0
9	A	828	CLA	4	0
9	B	838	CLA	1	0
12	B	847	BCR	4	0
12	F	201	BCR	2	0
9	B	816	CLA	1	0
9	A	819	CLA	2	0
9	A	802	CLA	1	0
12	A	851	BCR	4	0
9	A	809	CLA	1	0
9	B	830	CLA	3	0
9	A	826	CLA	2	0
9	A	821	CLA	3	0

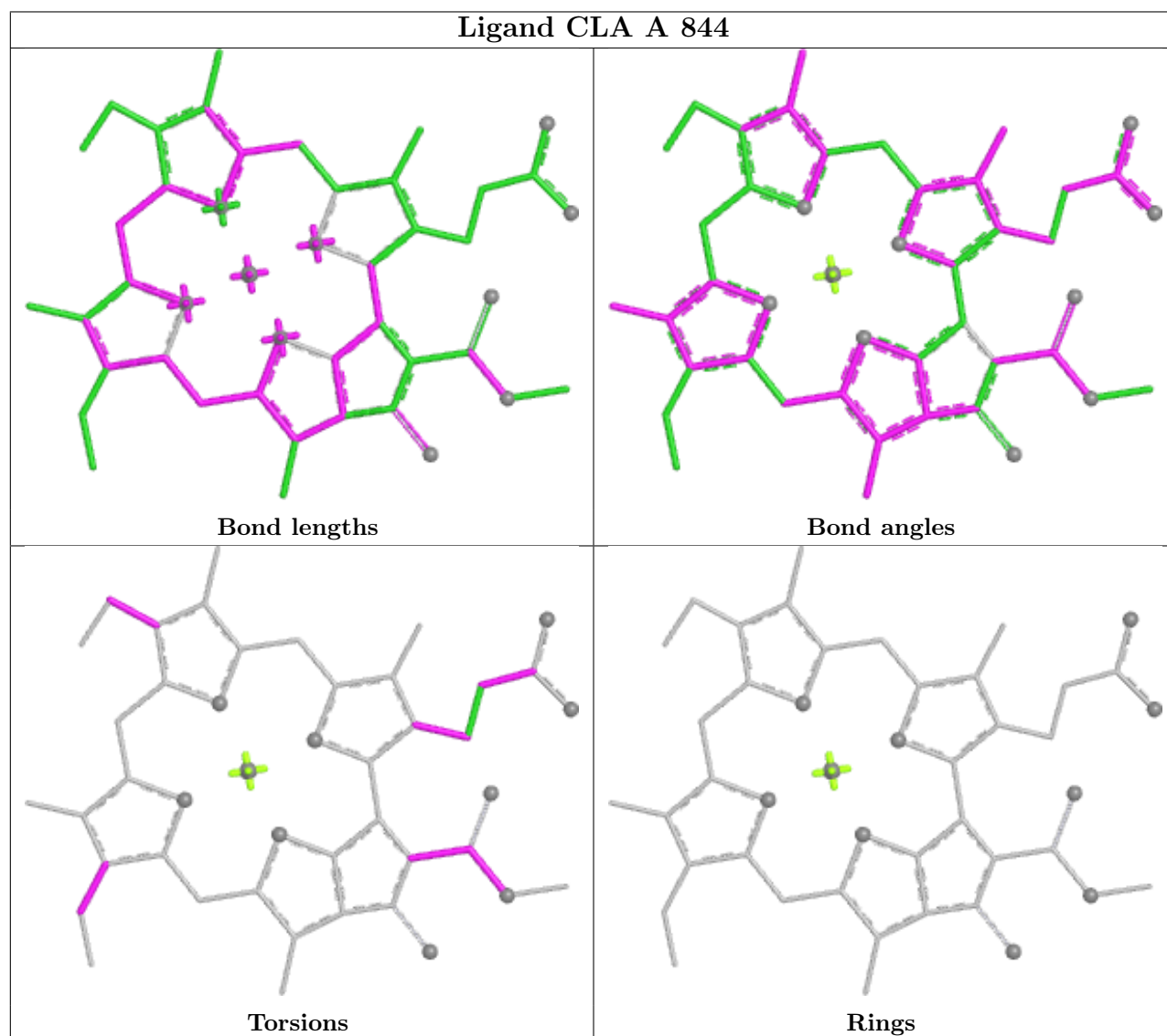
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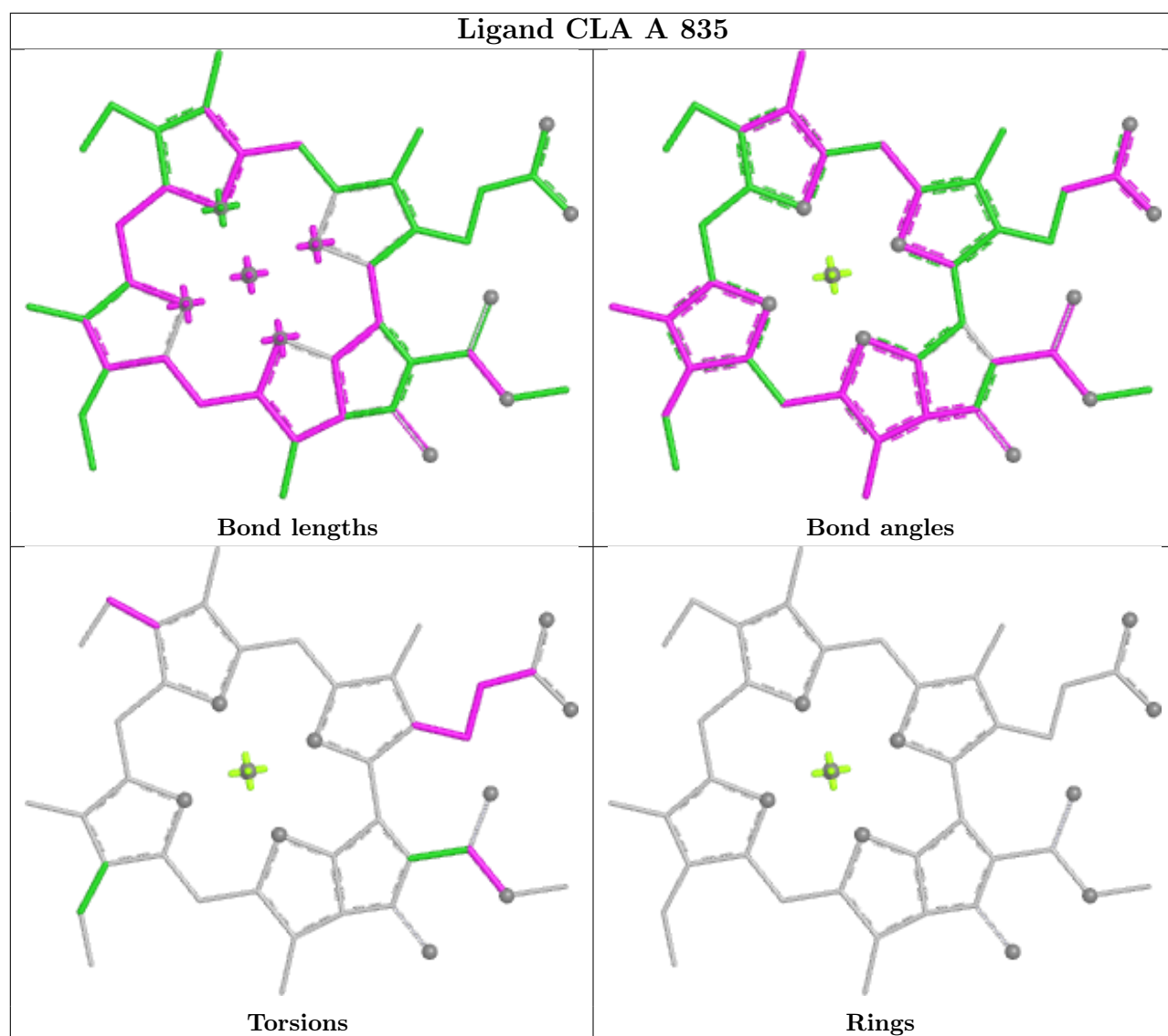
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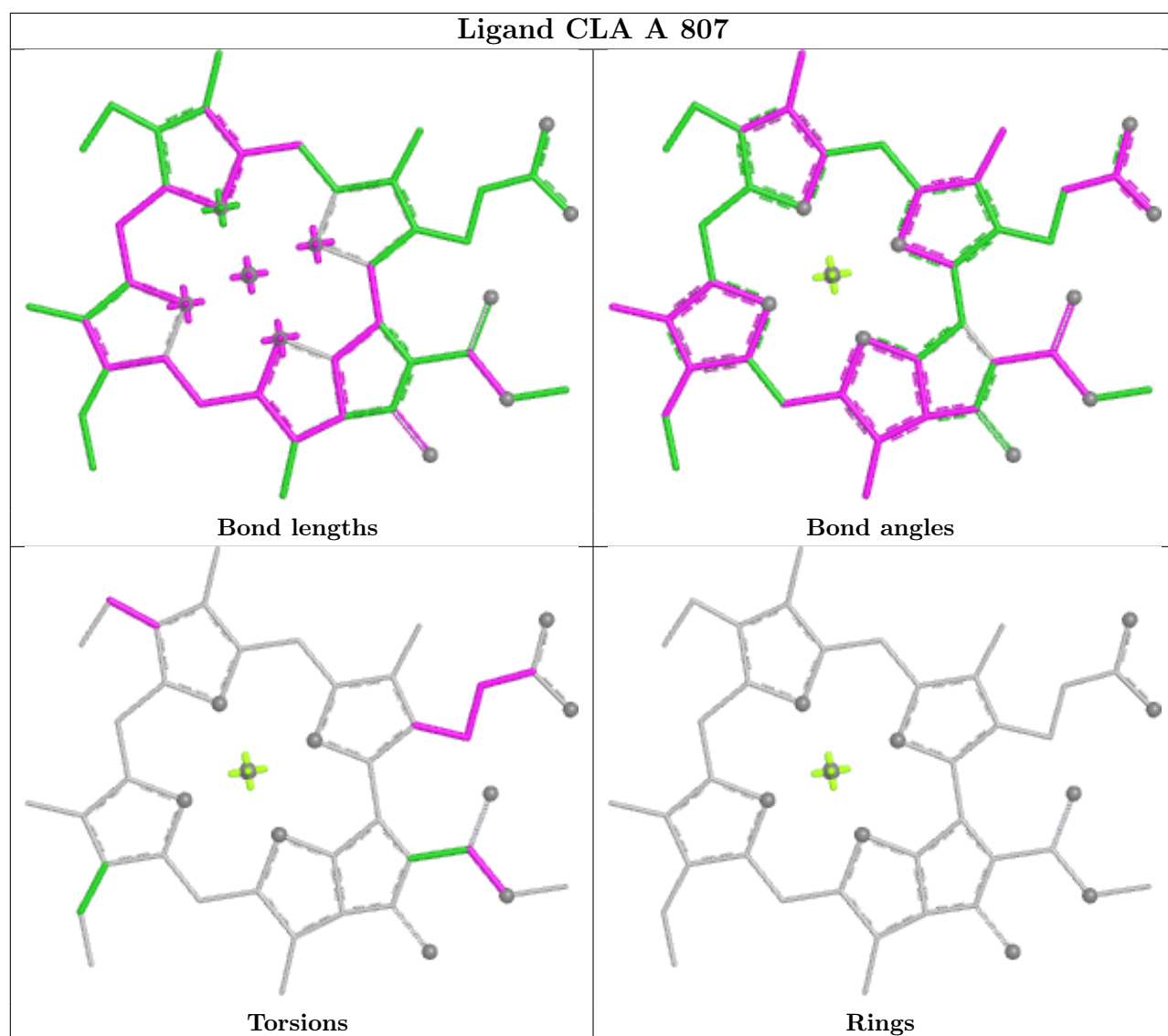
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	841	CLA	1	0
9	B	808	CLA	1	0
9	A	806	CLA	1	0
9	B	817	CLA	1	0
9	B	819	CLA	1	0
12	A	850	BCR	3	0
9	B	802	CLA	5	0
9	A	829	CLA	1	0
9	B	839	CLA	2	0
12	A	848	BCR	2	0
13	A	852	LHG	3	0
14	B	848	LMG	6	0
9	B	824	CLA	1	0
12	B	843	BCR	2	0
9	B	834	CLA	1	0
9	A	808	CLA	1	0
9	B	815	CLA	3	0
12	B	844	BCR	4	0
10	B	841	PQN	4	0
10	A	845	PQN	3	0
9	A	831	CLA	1	0
9	B	804	CLA	1	0
9	B	840	CLA	1	0
9	A	814	CLA	1	0
9	I	101	CLA	1	0
9	A	830	CLA	2	0
9	A	827	CLA	1	0
9	B	828	CLA	5	0
9	A	840	CLA	1	0
9	B	801	CLA	2	0
9	B	829	CLA	1	0
9	B	826	CLA	1	0
9	A	818	CLA	1	0
9	B	832	CLA	1	0
9	A	805	CLA	2	0
9	A	820	CLA	1	0

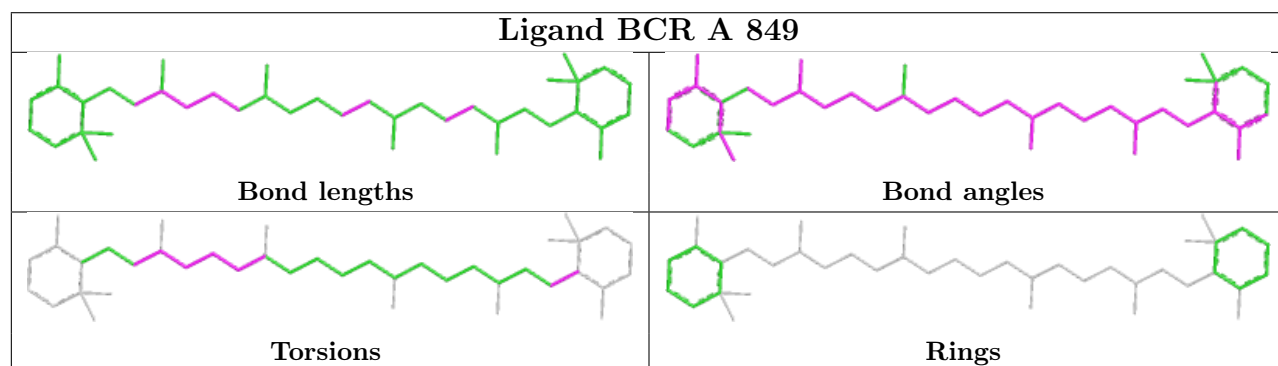
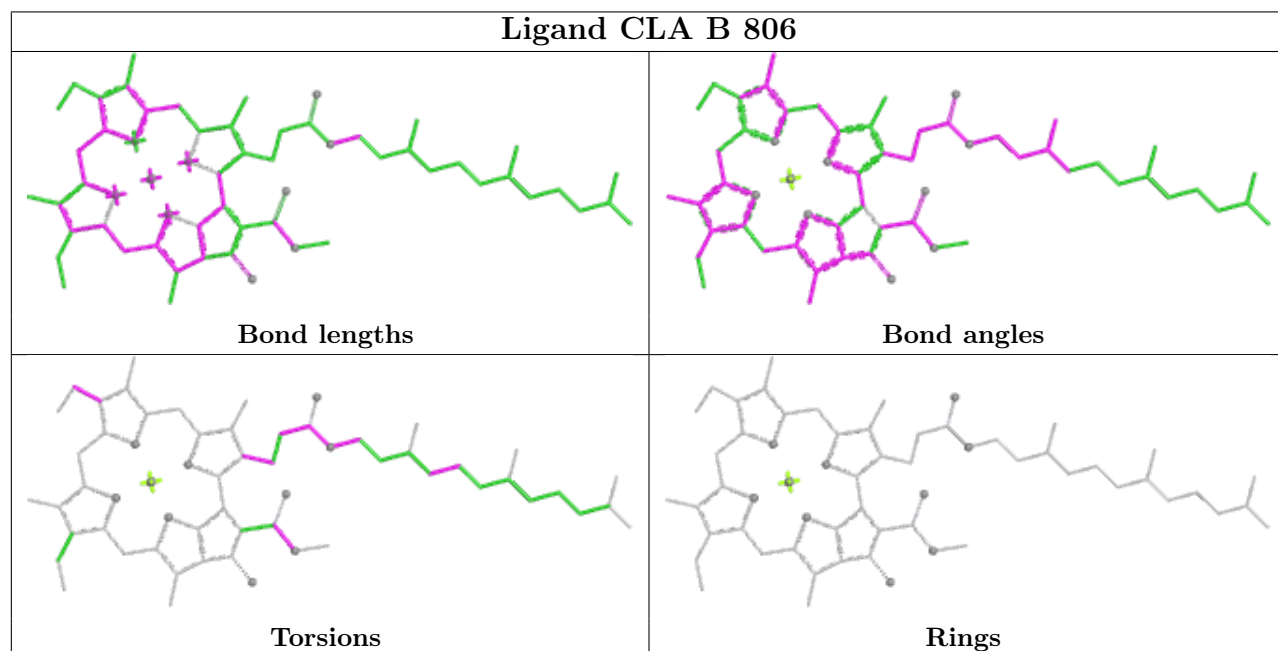
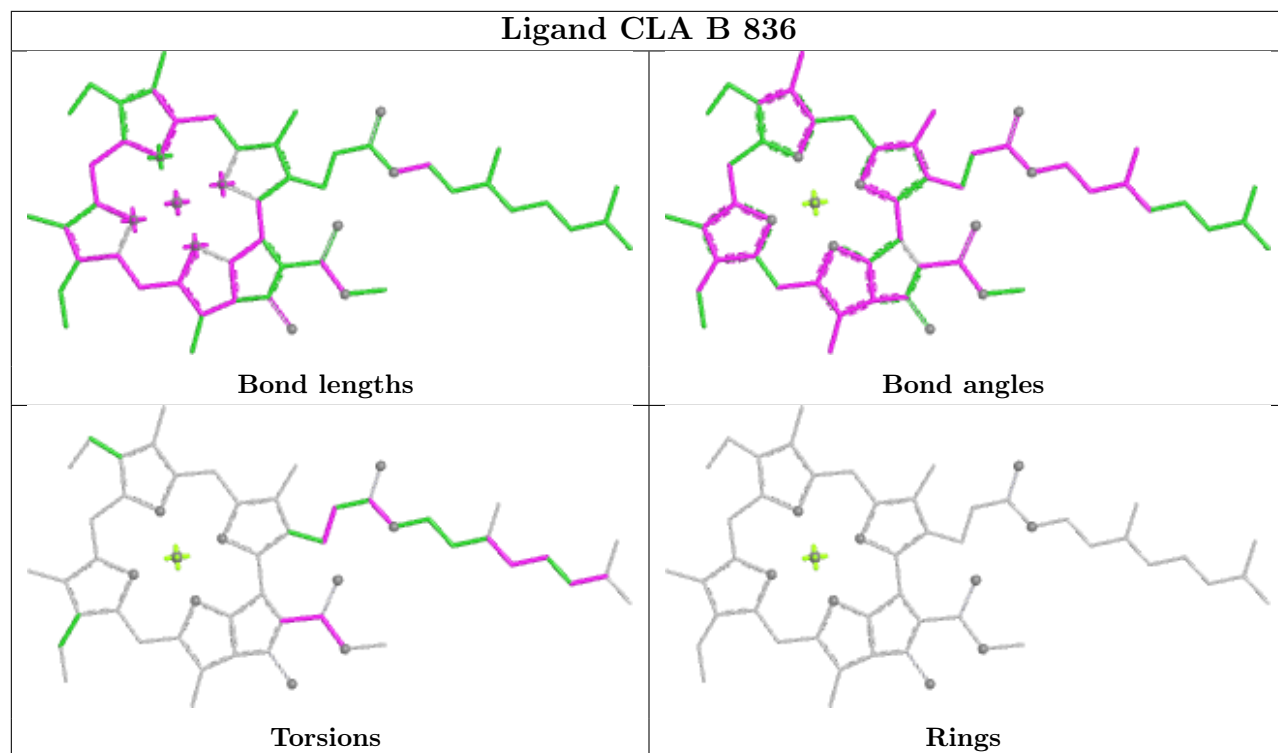
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

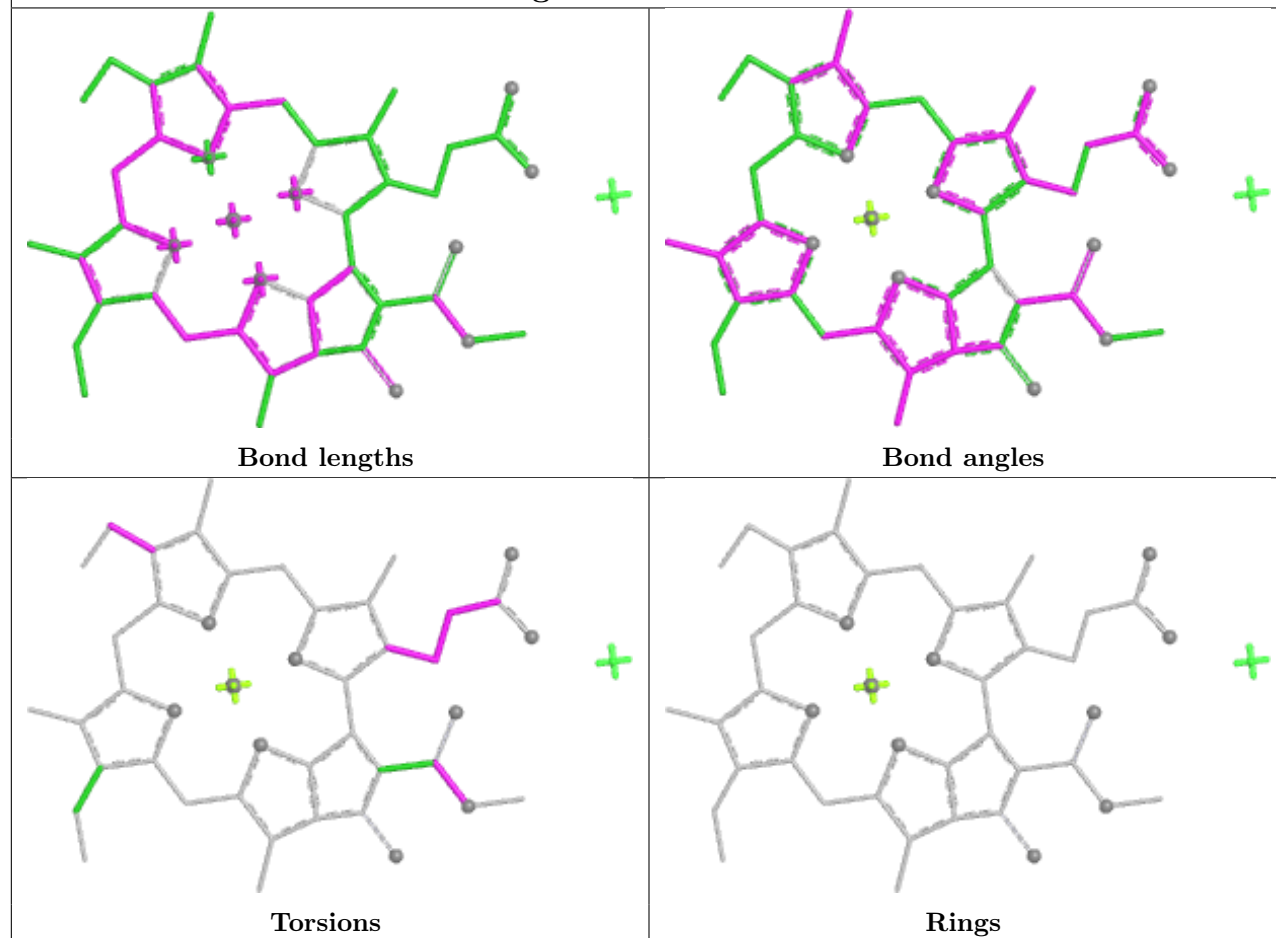




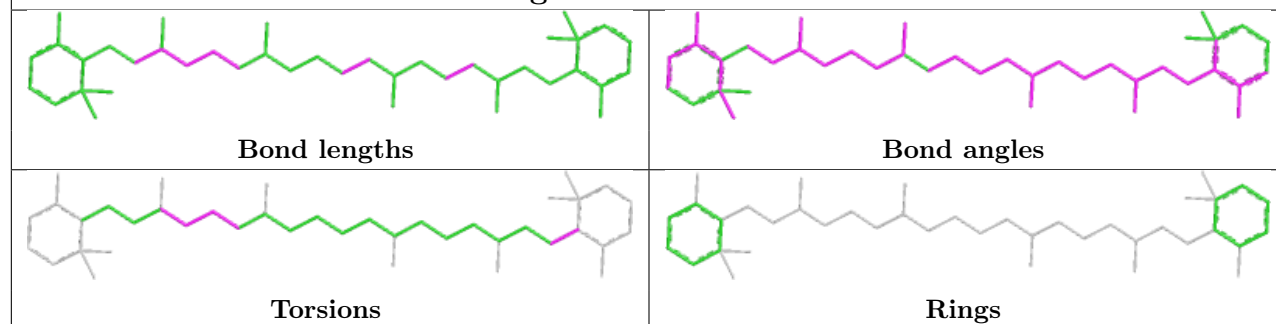


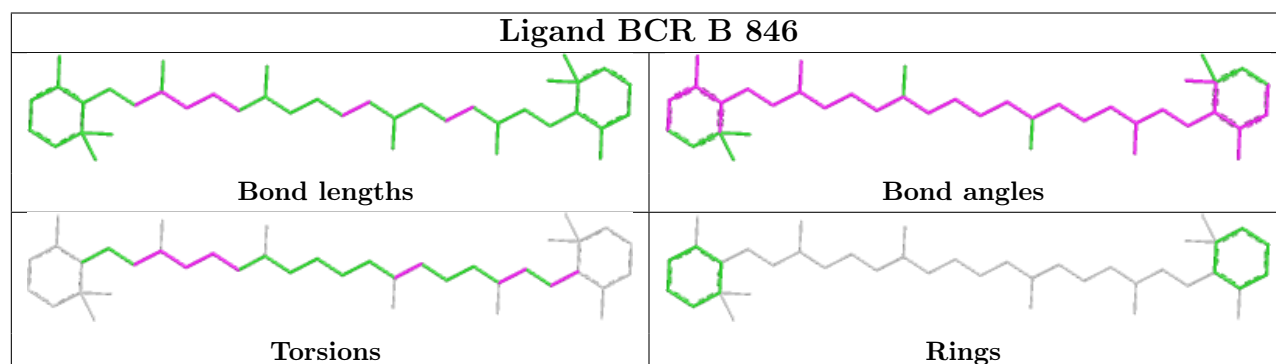
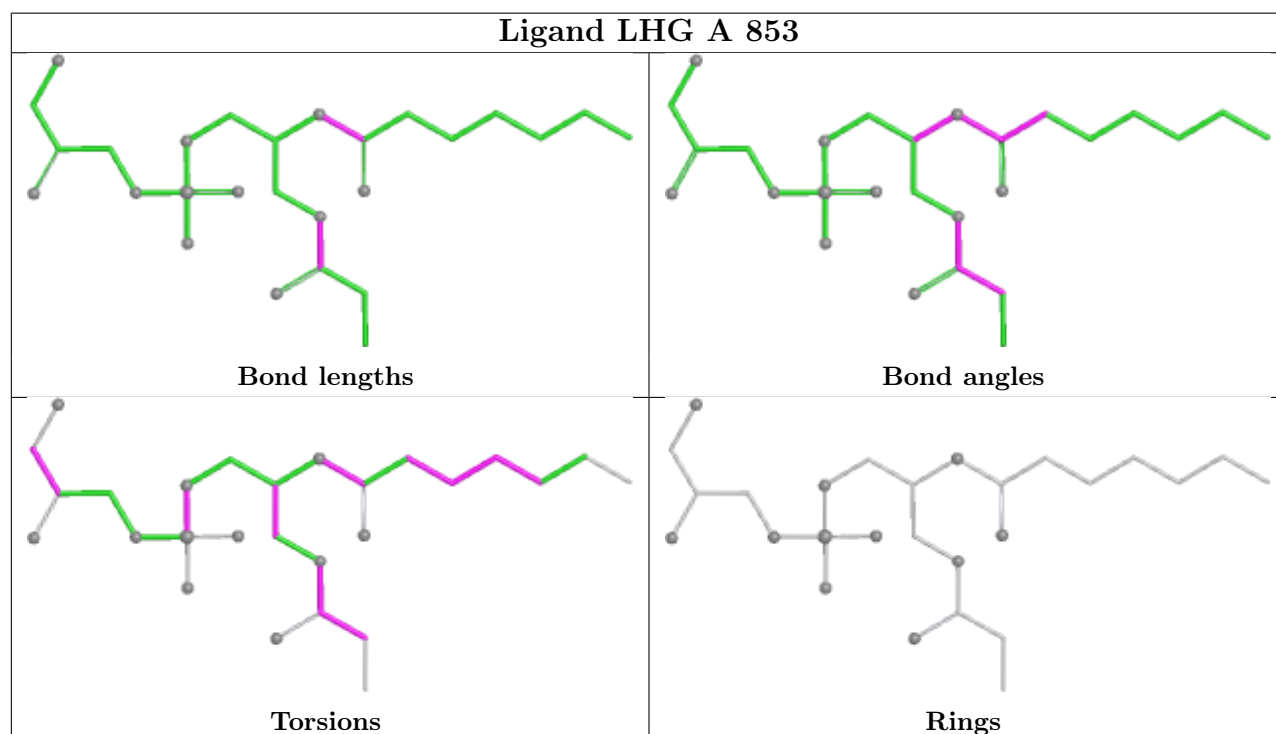
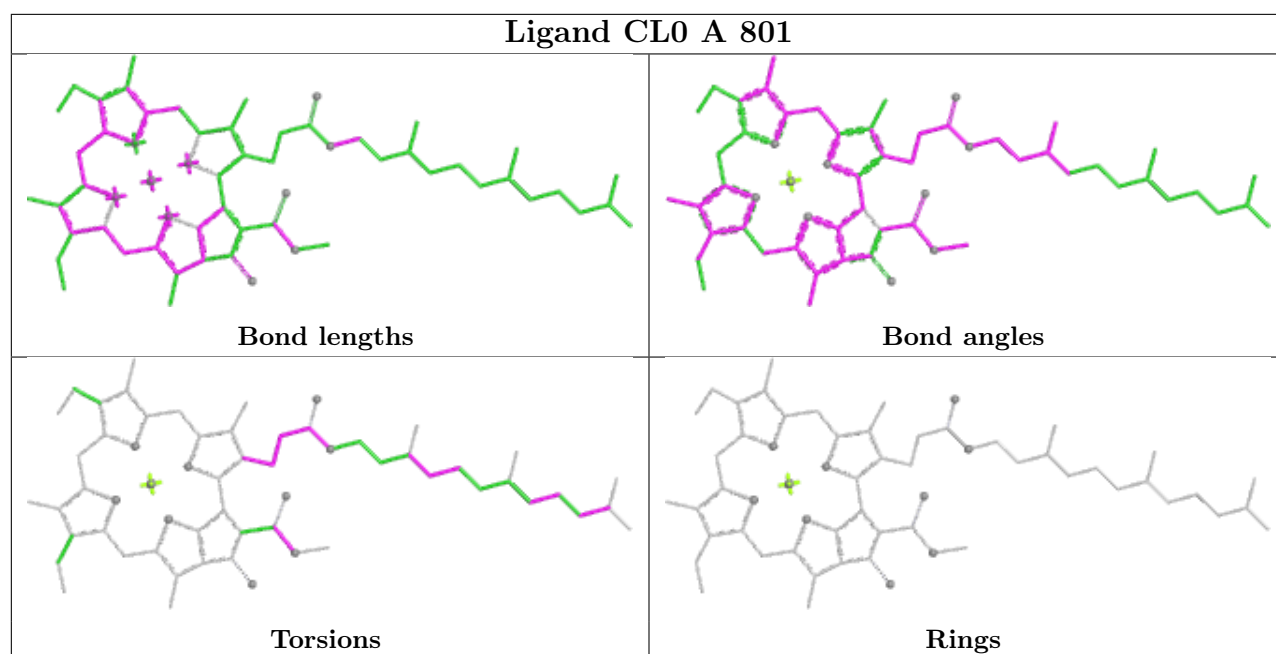


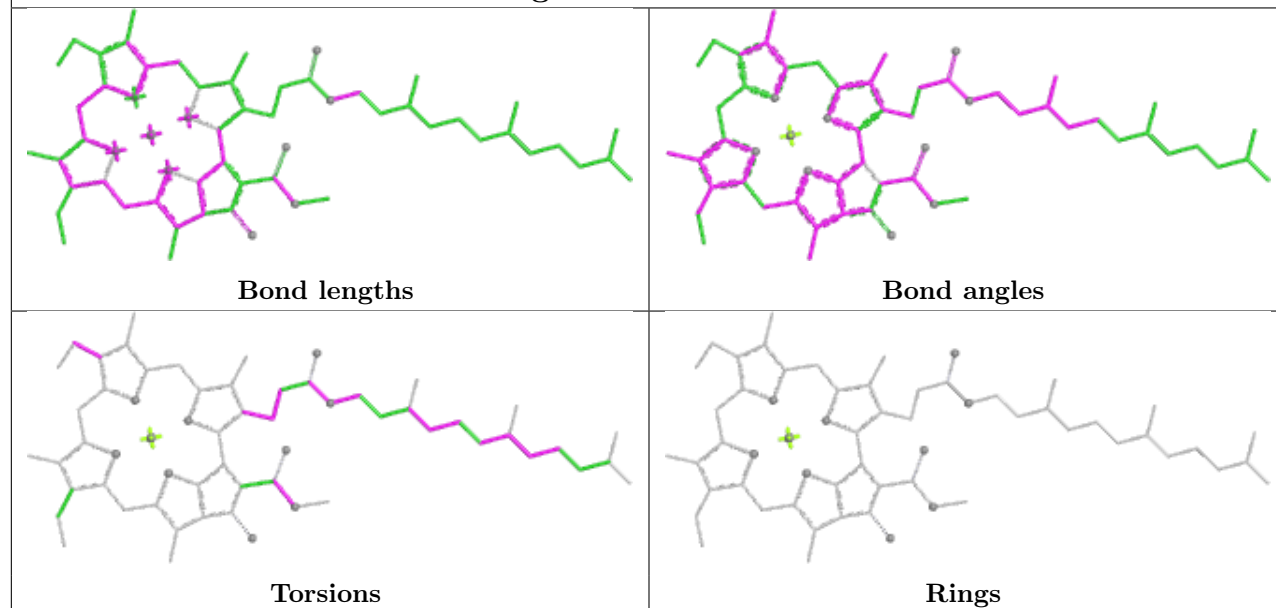
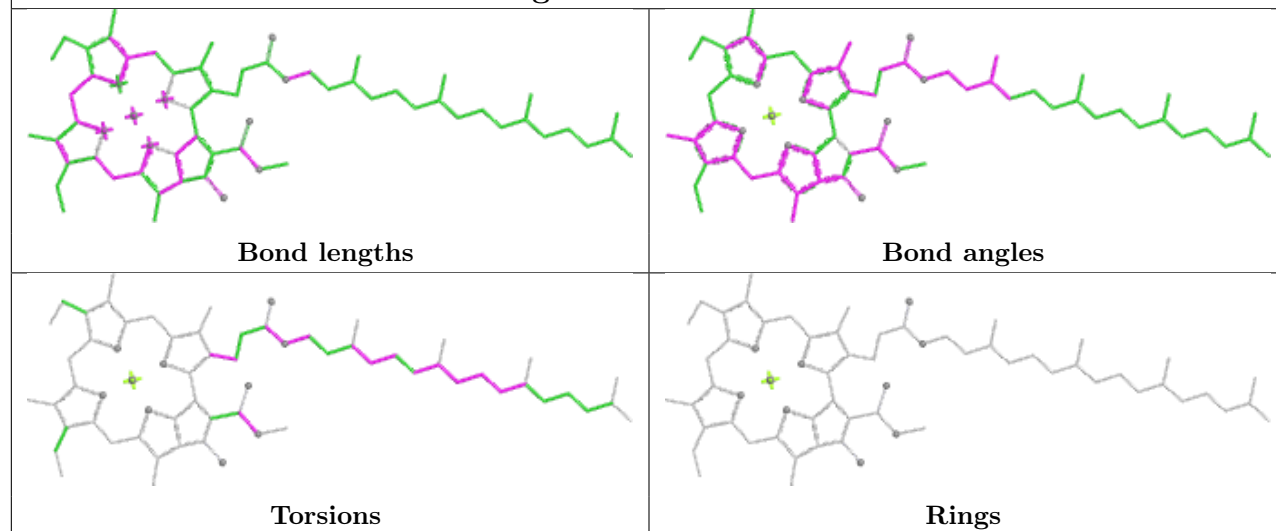
Ligand CLA B 810



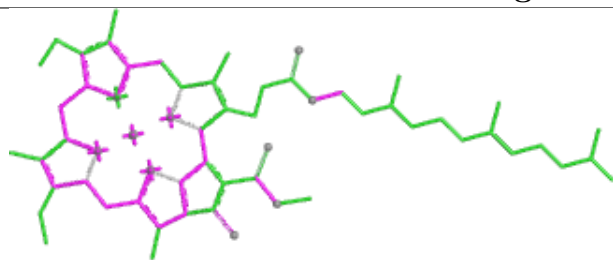
Ligand BCR A 847



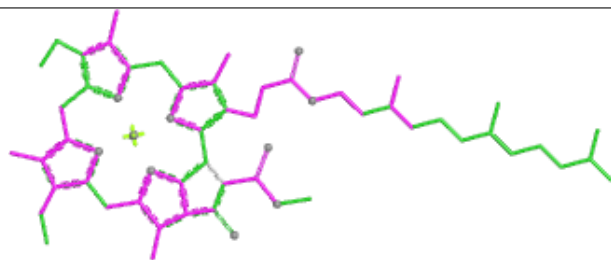


Ligand CLA A 813**Ligand CLA B 803**

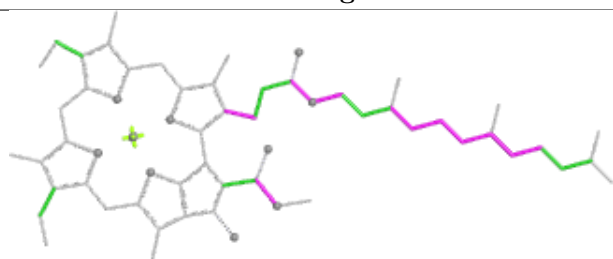
Ligand CLA B 818



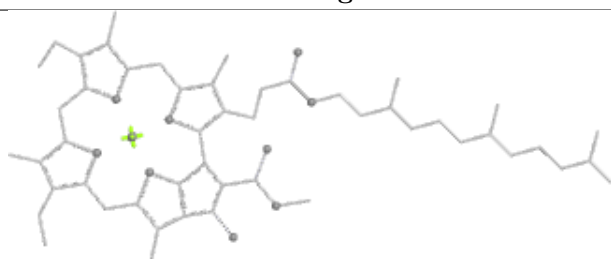
Bond lengths



Bond angles

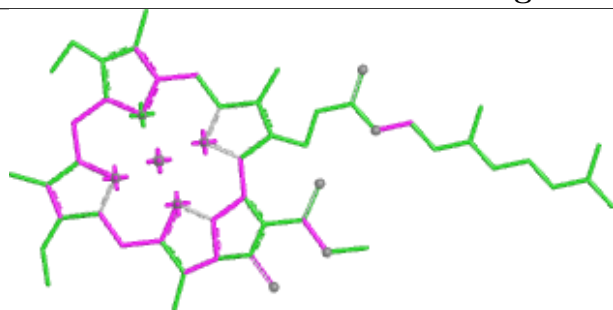


Torsions

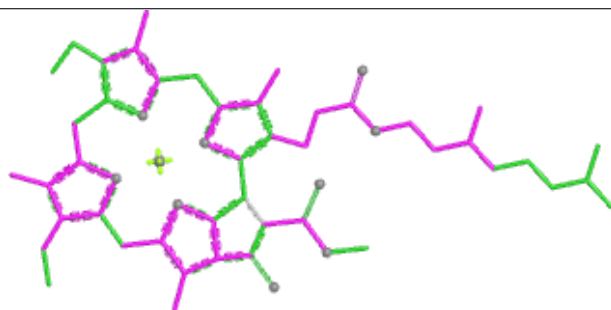


Rings

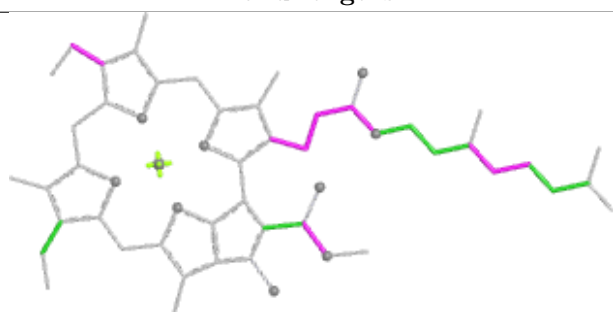
Ligand CLA B 827



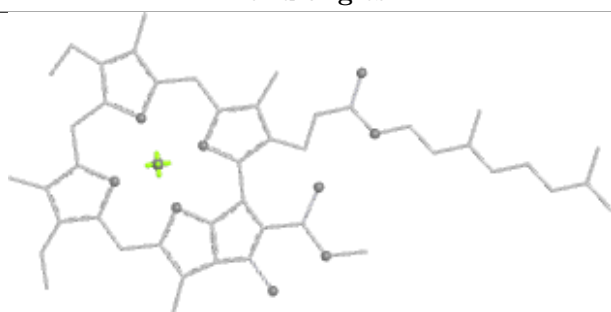
Bond lengths



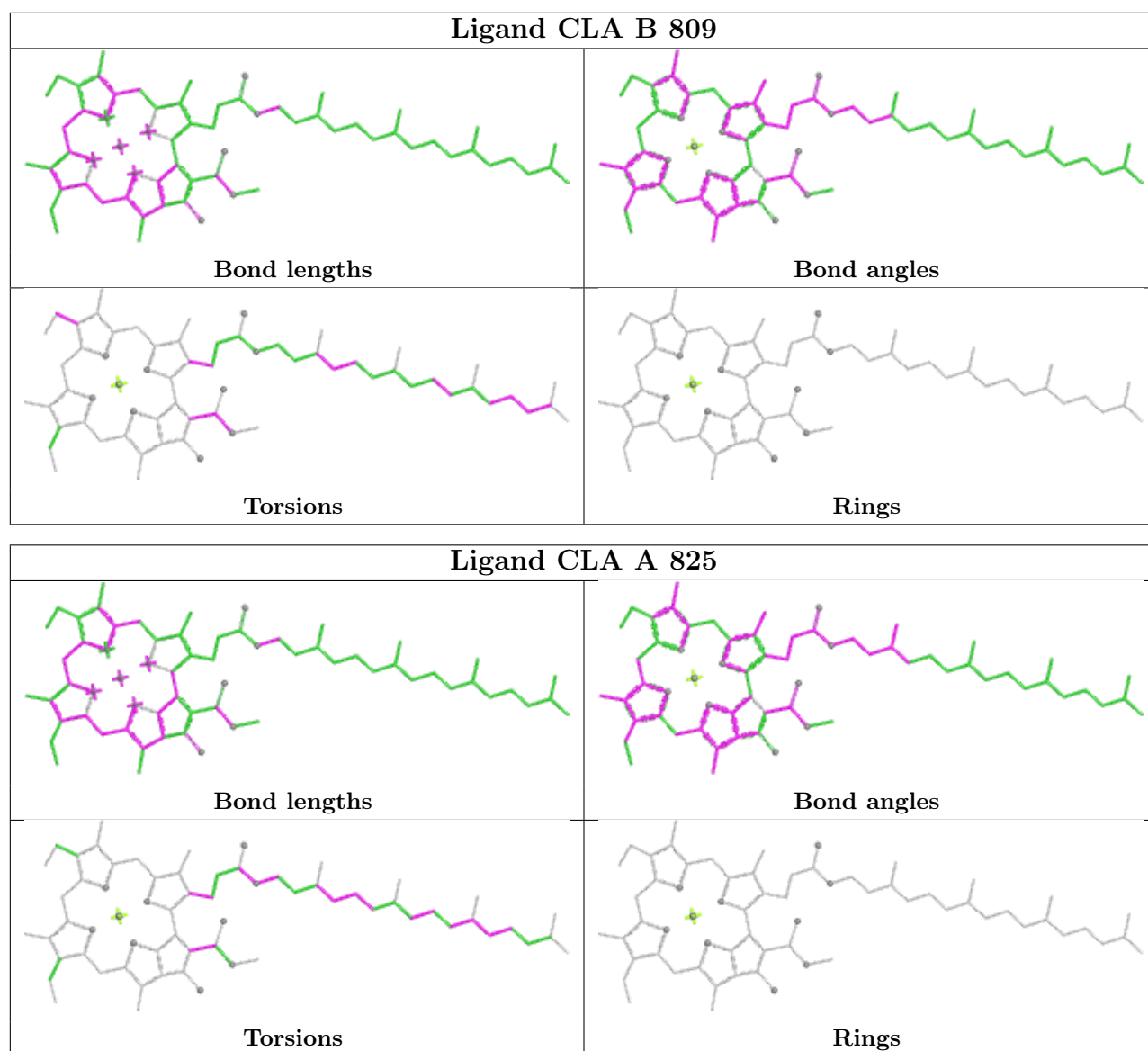
Bond angles



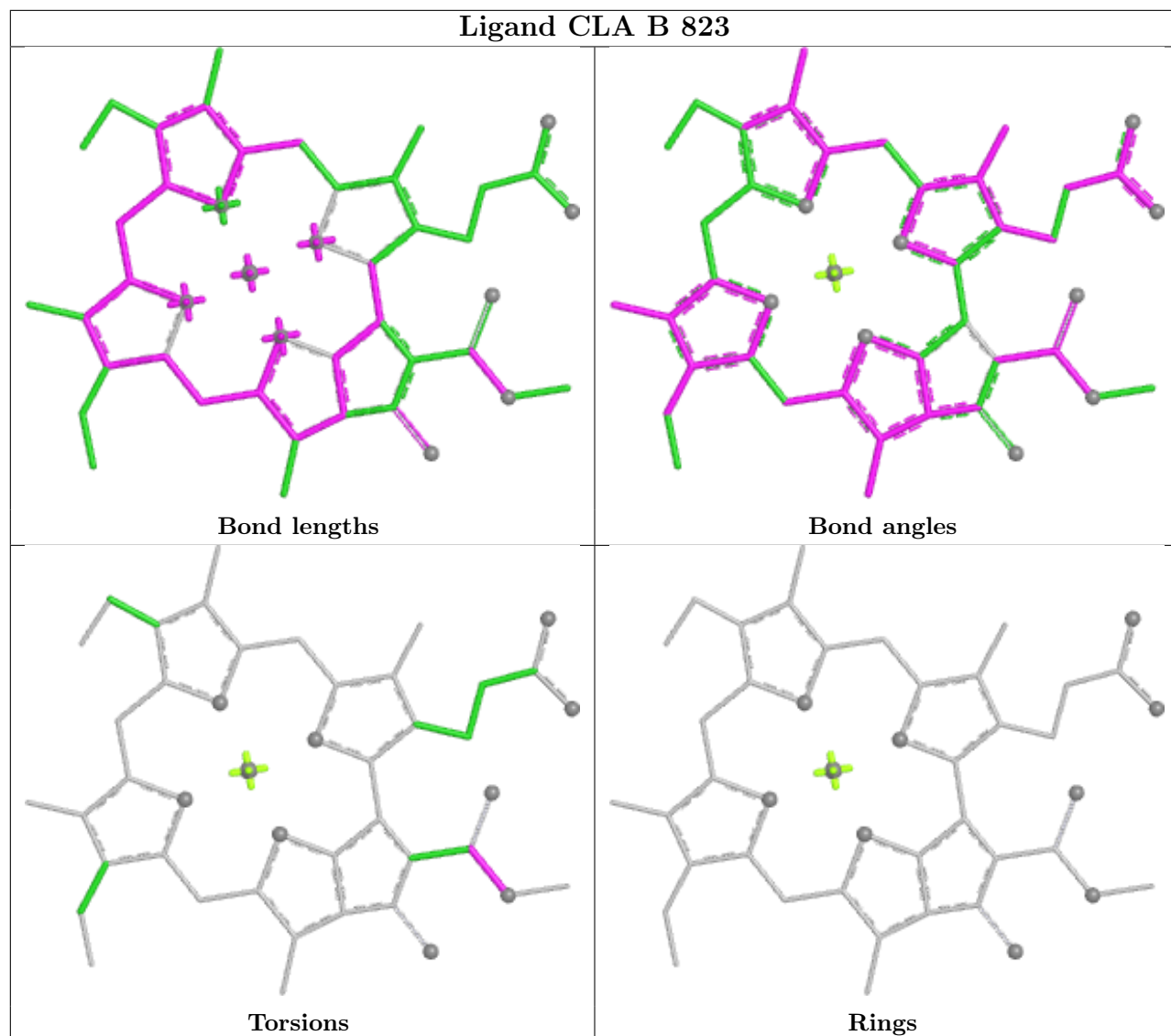
Torsions



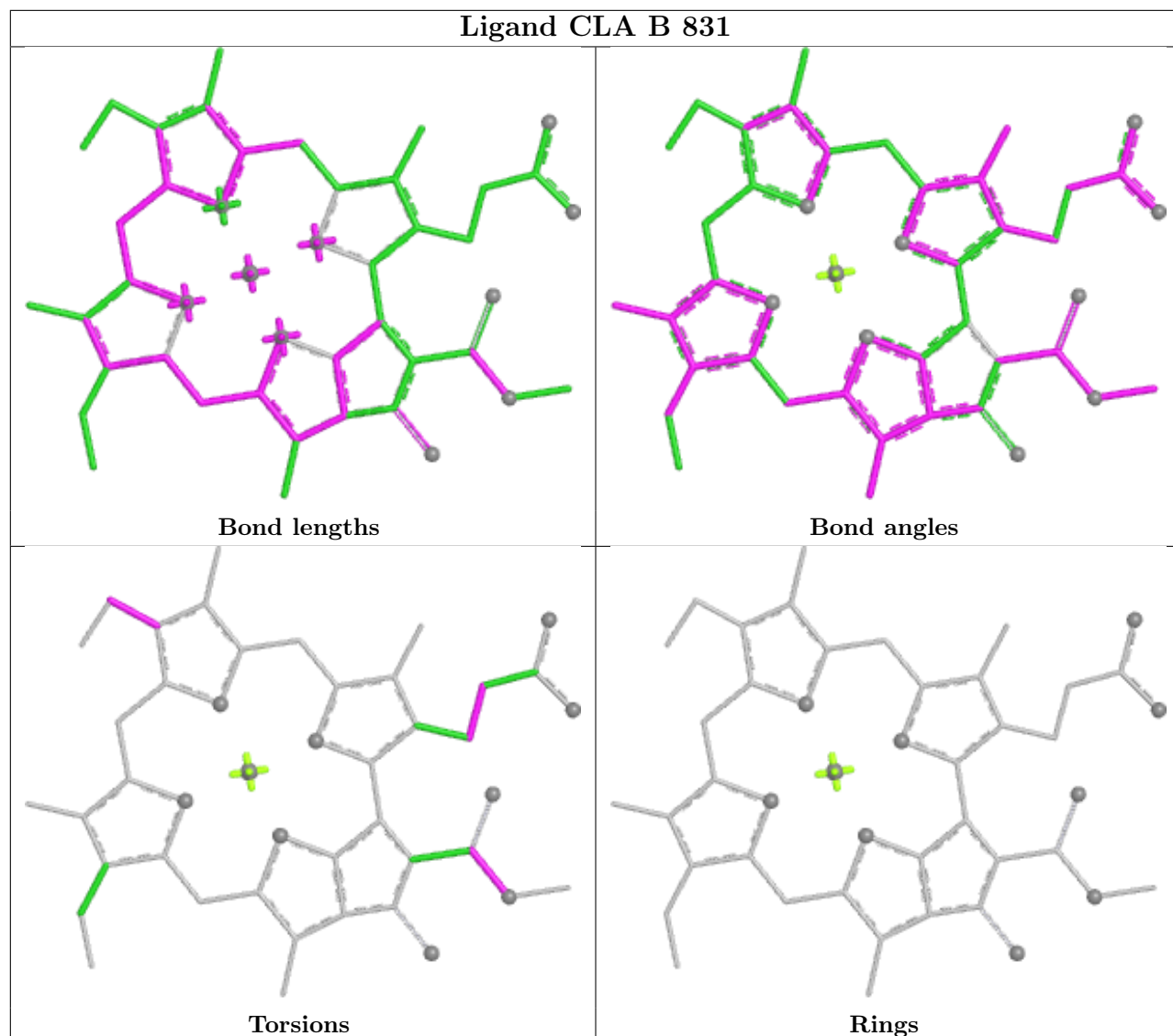
Rings



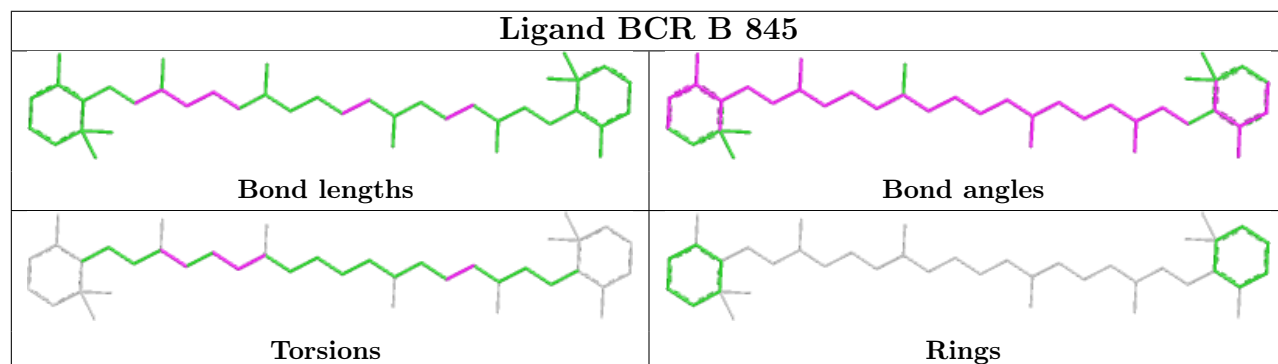
Ligand CLA B 823

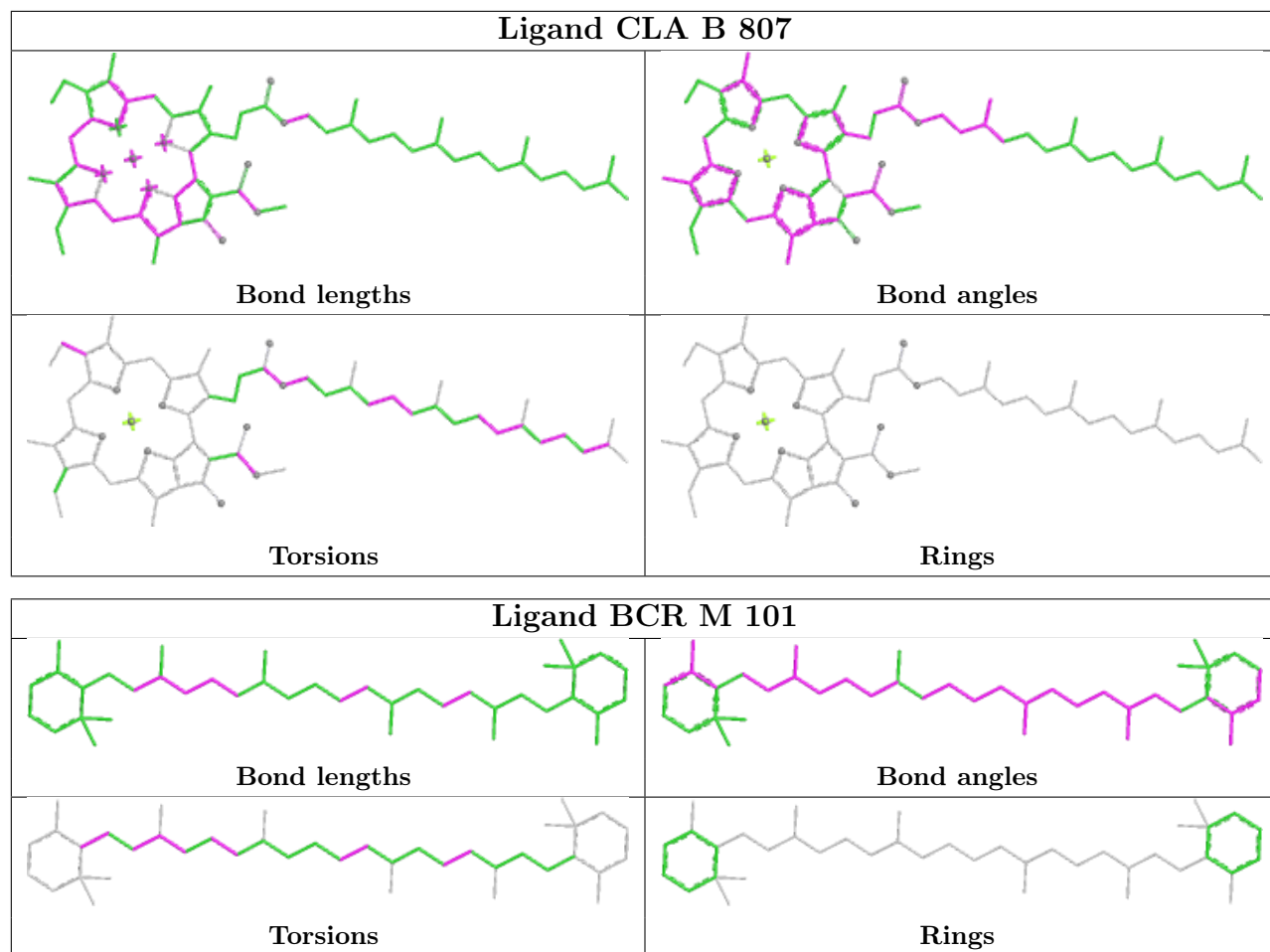


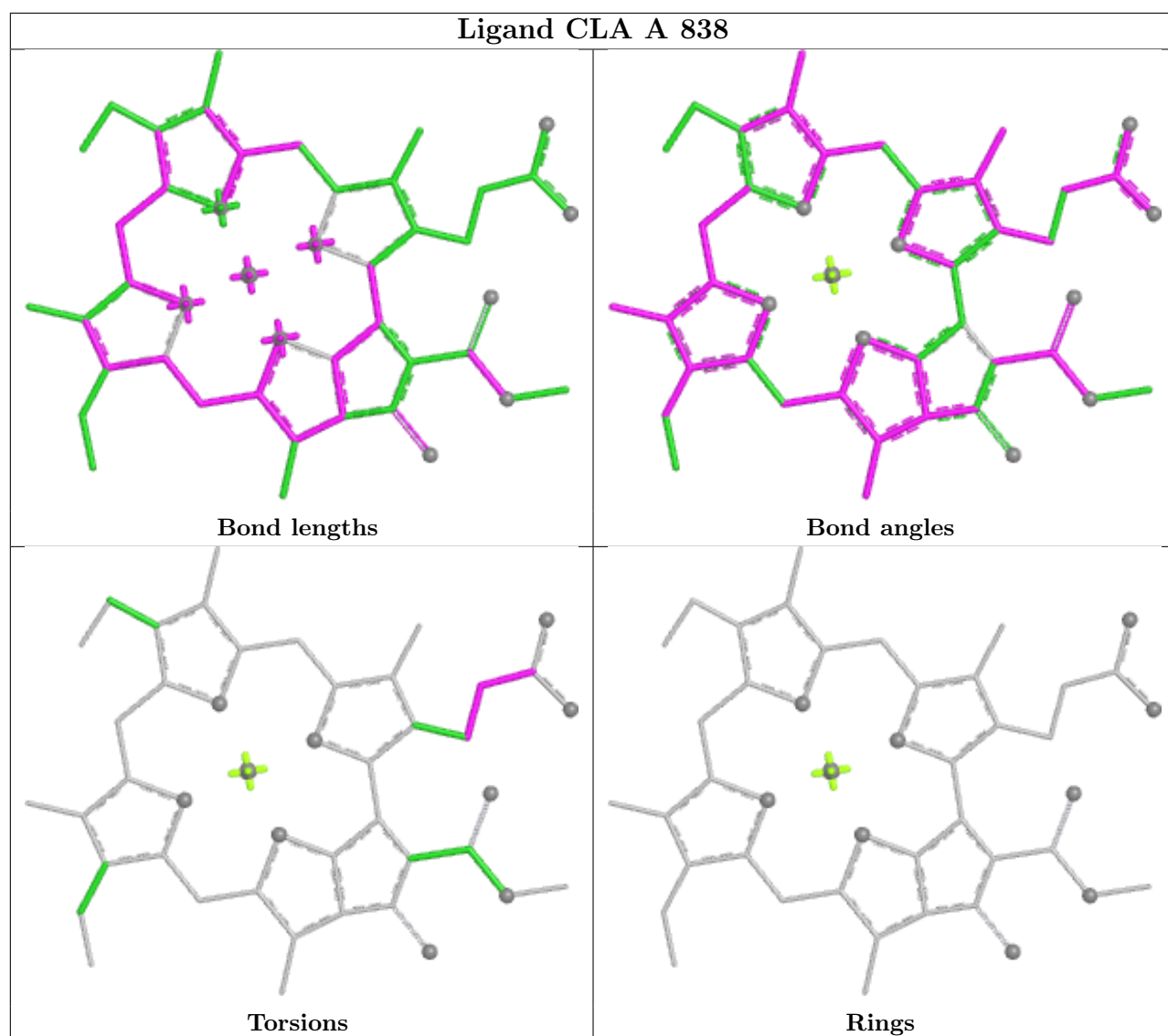
Ligand CLA B 831

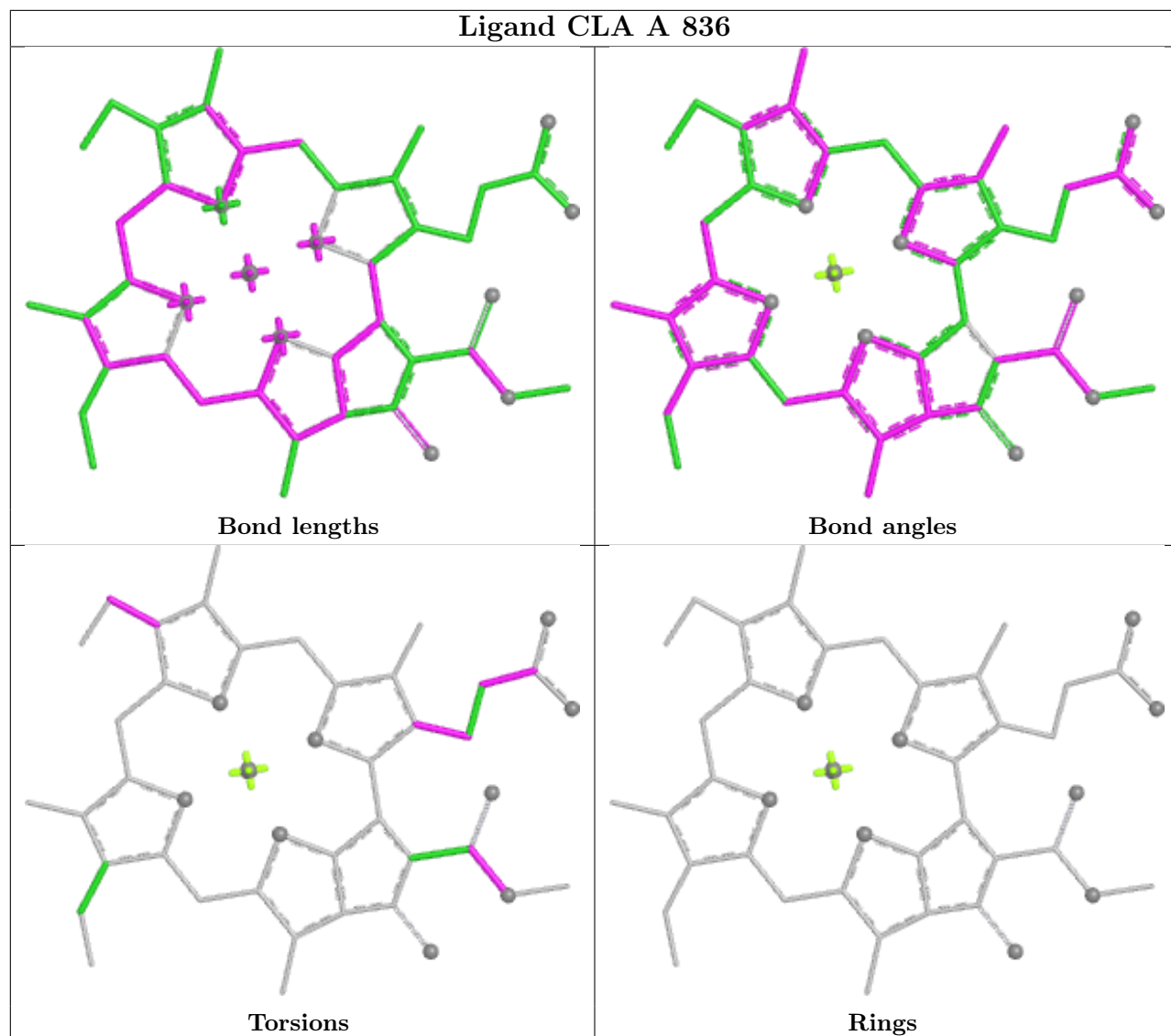


Ligand BCR B 845

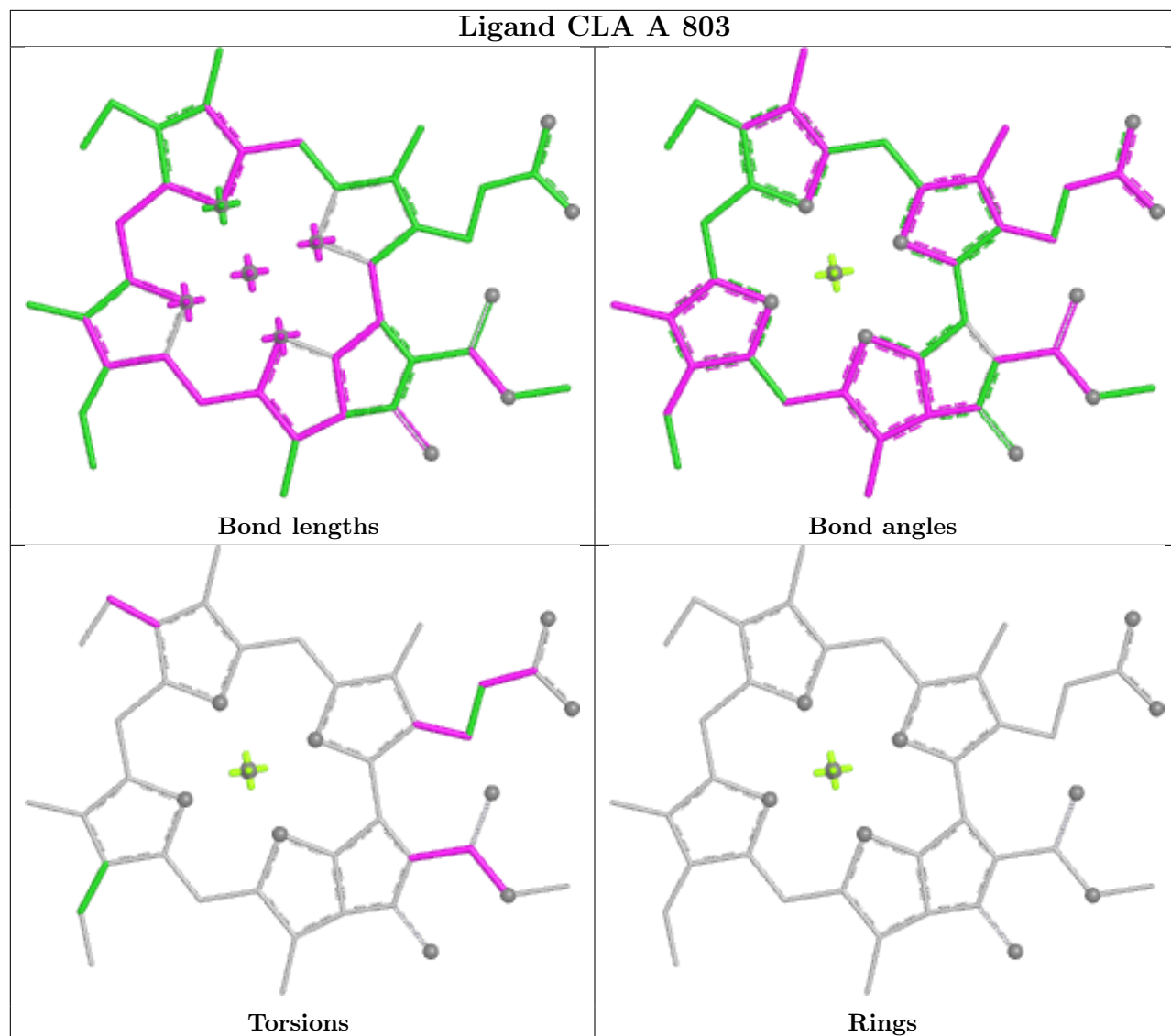




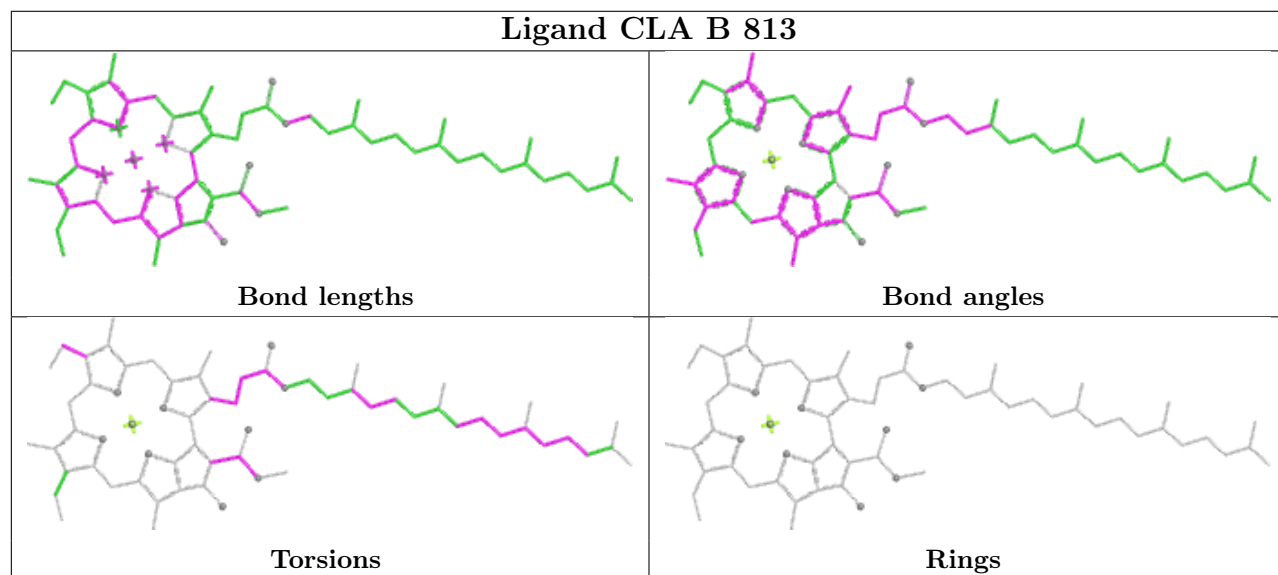


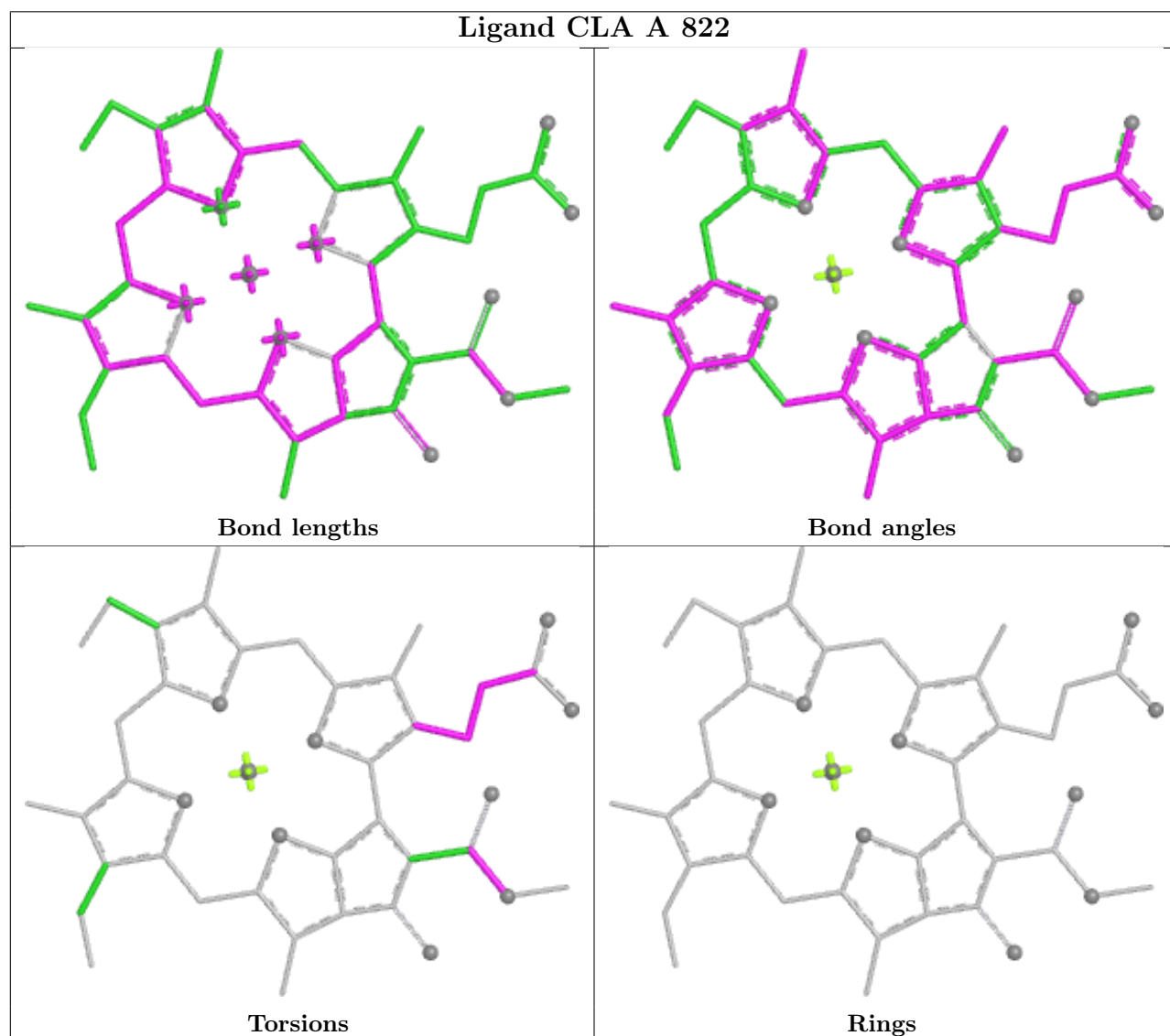
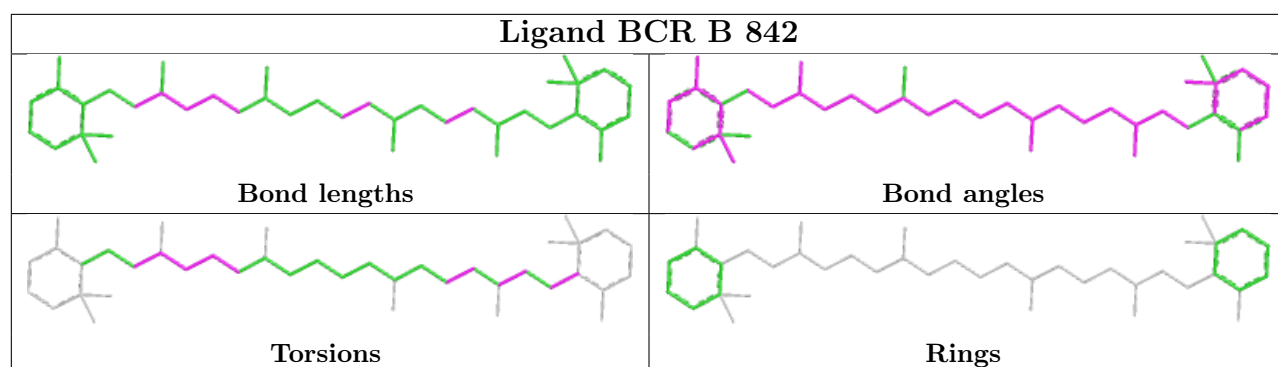


Ligand CLA A 803

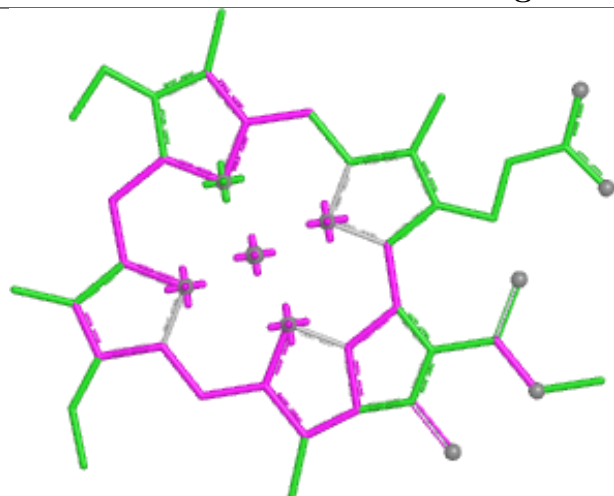


Ligand CLA B 813

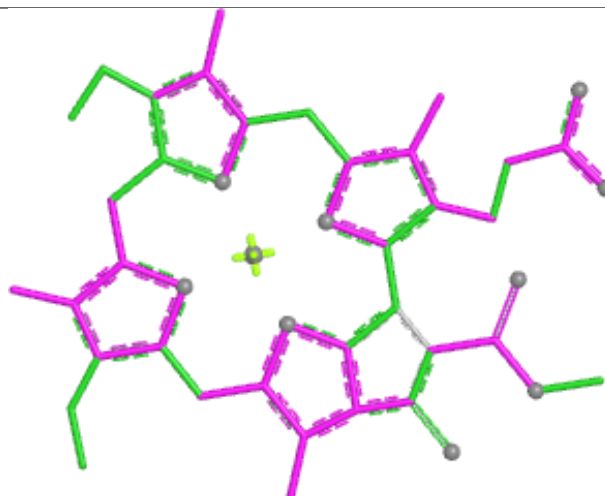




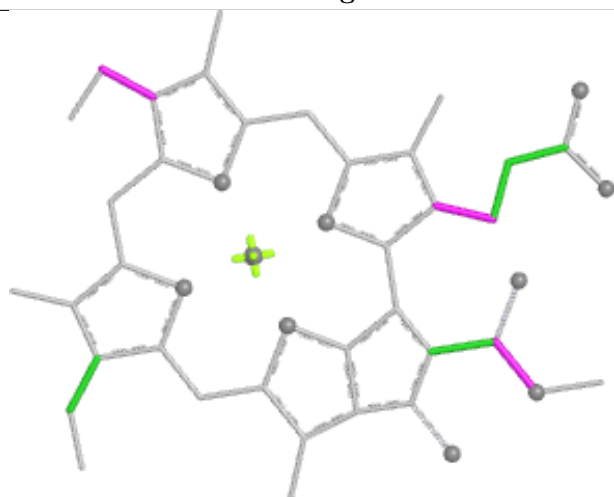
Ligand CLA B 811



Bond lengths



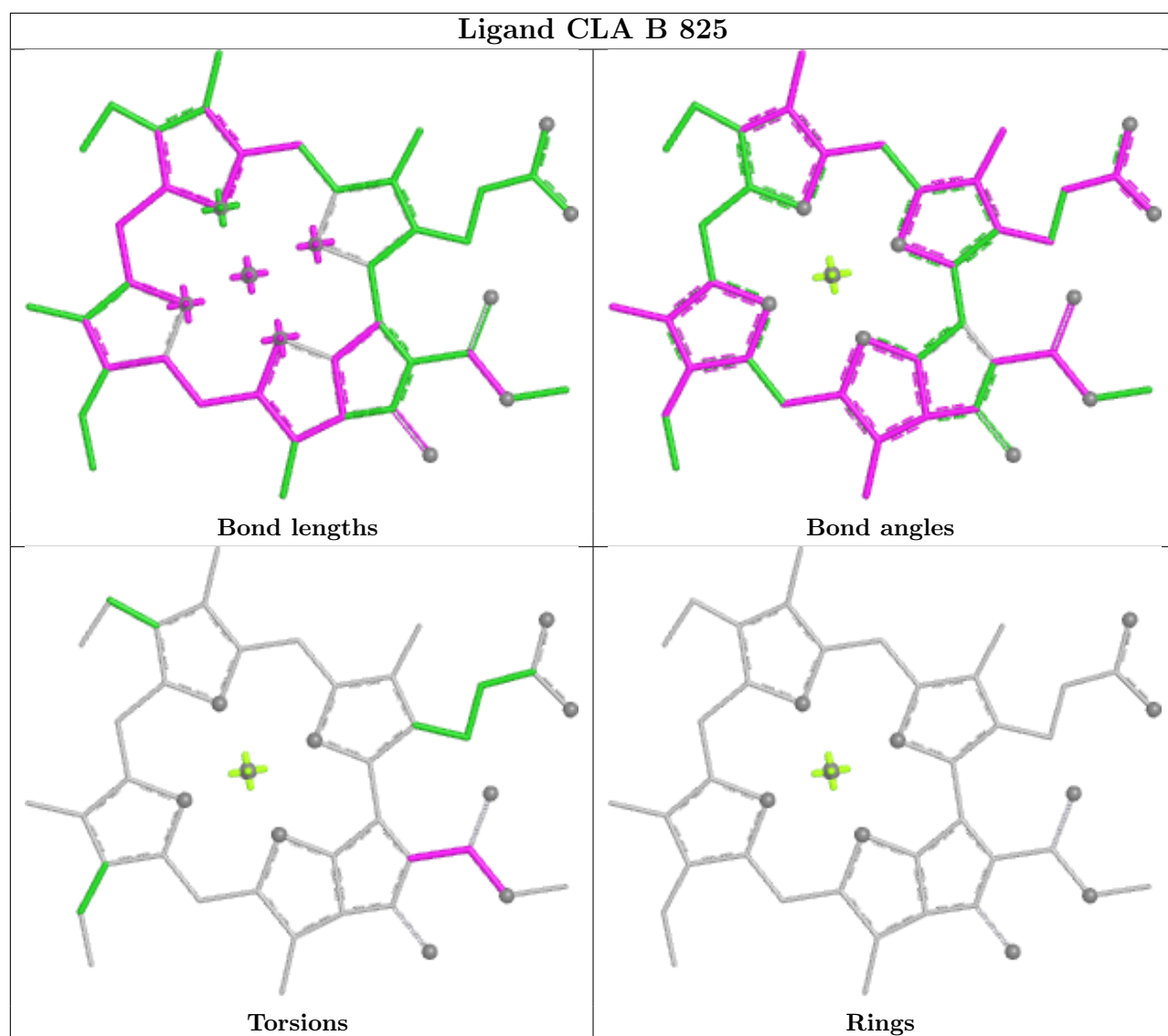
Bond angles



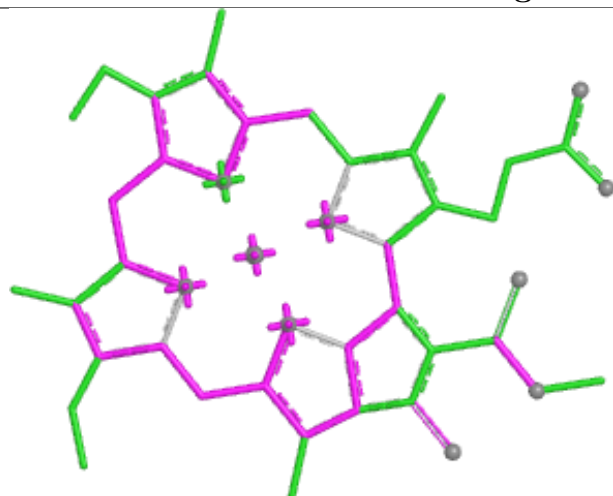
Torsions



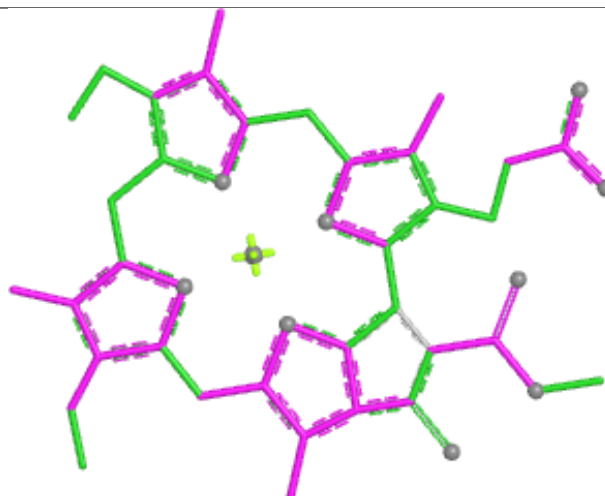
Rings



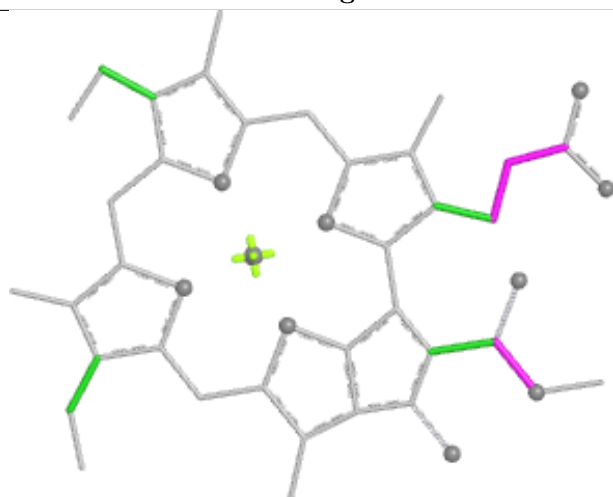
Ligand CLA B 805



Bond lengths



Bond angles

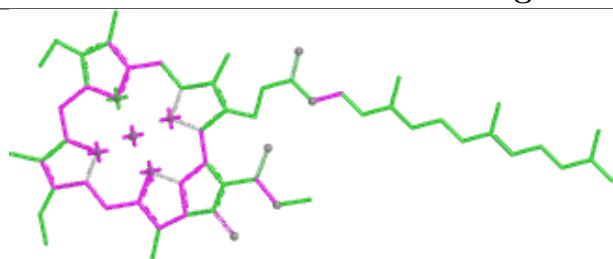


Torsions

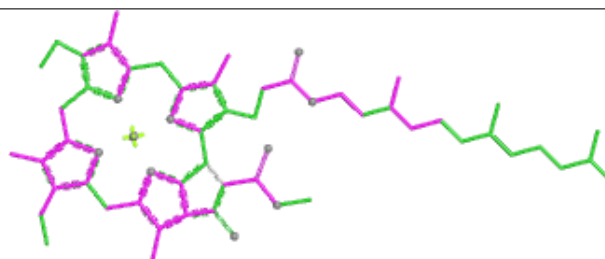


Rings

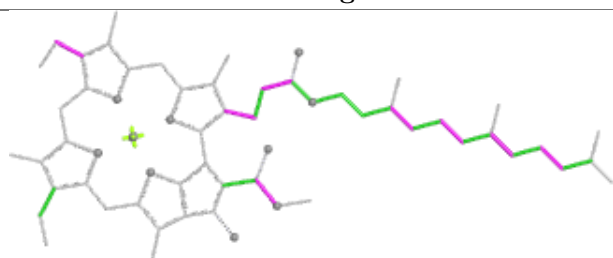
Ligand CLA B 837



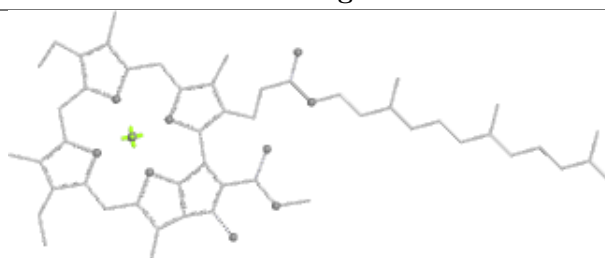
Bond lengths



Bond angles

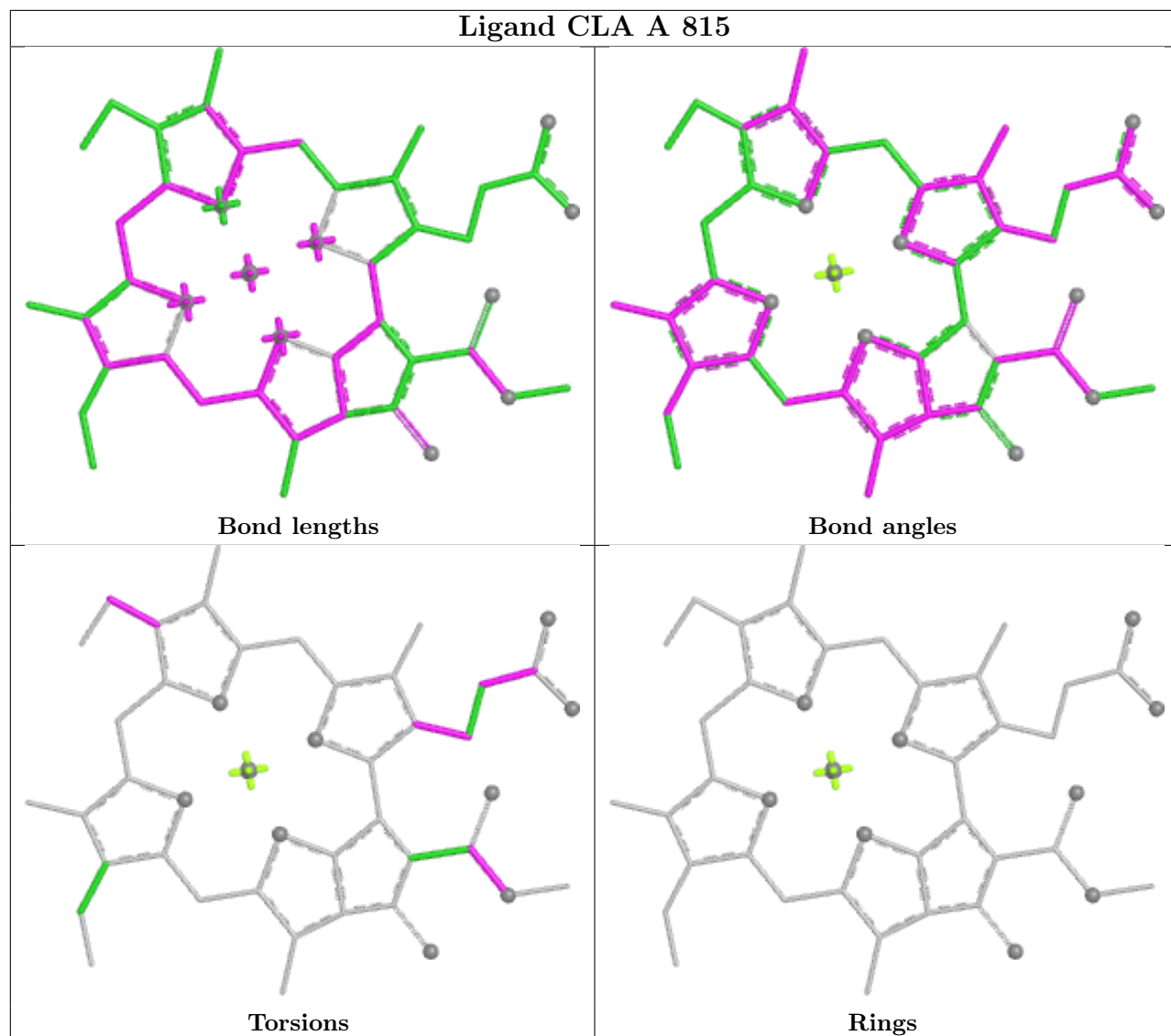


Torsions

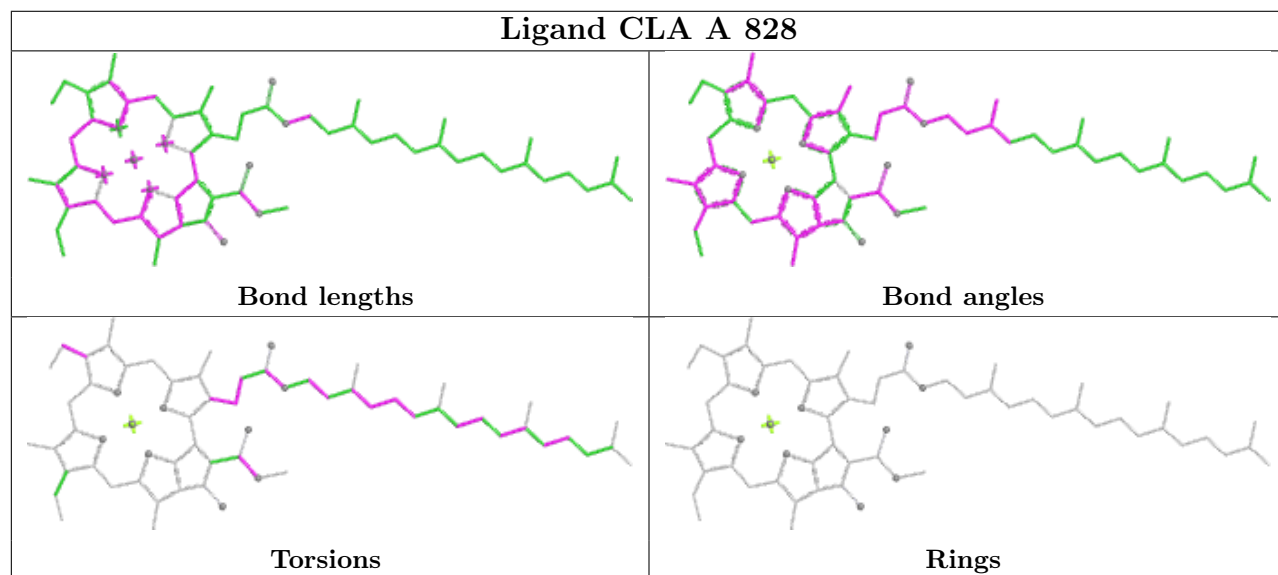


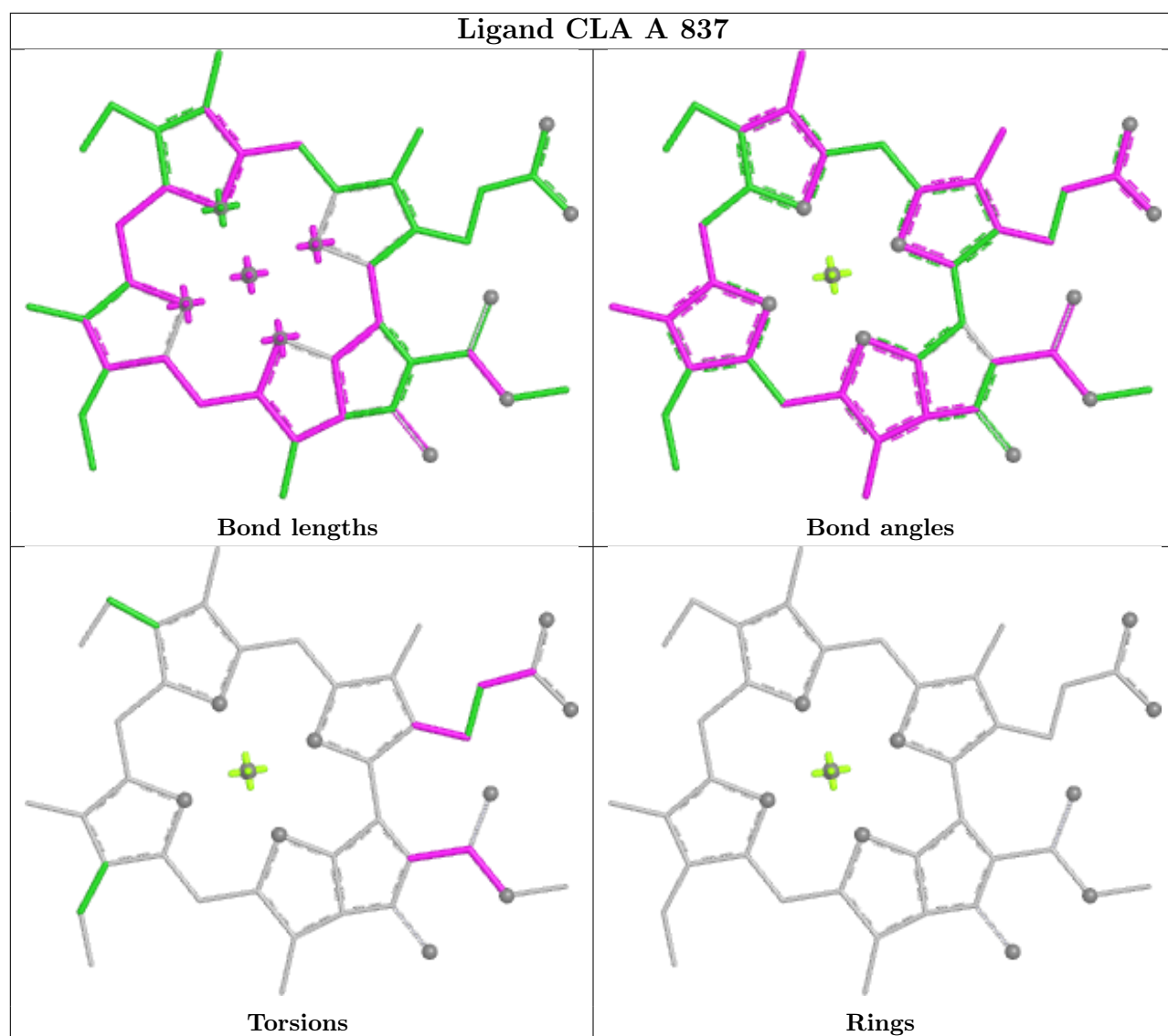
Rings

Ligand CLA A 815

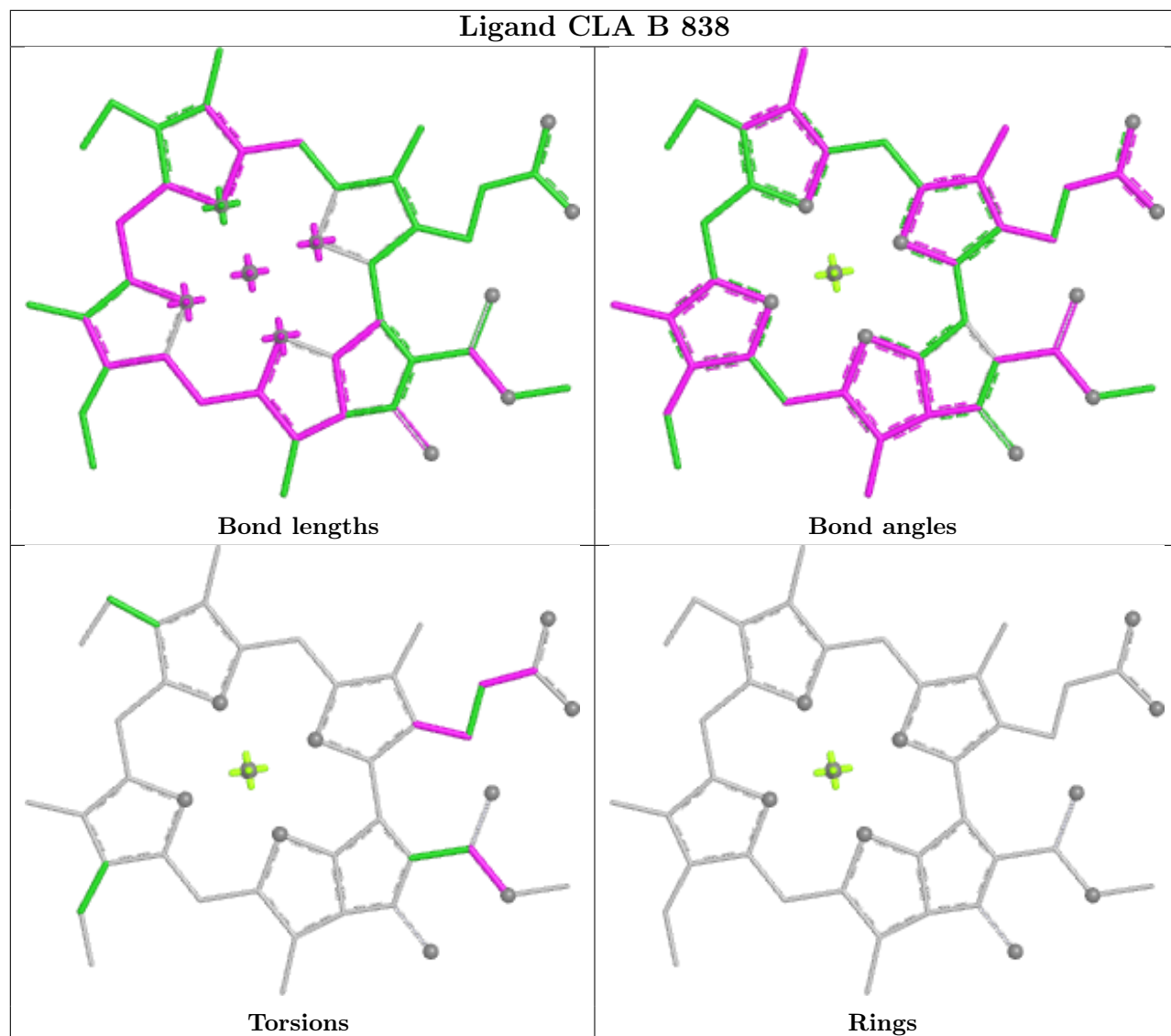


Ligand CLA A 828

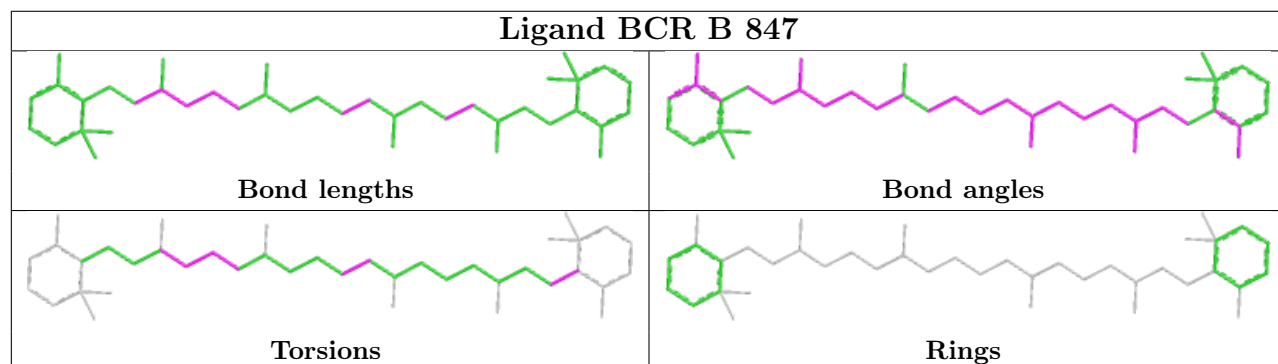


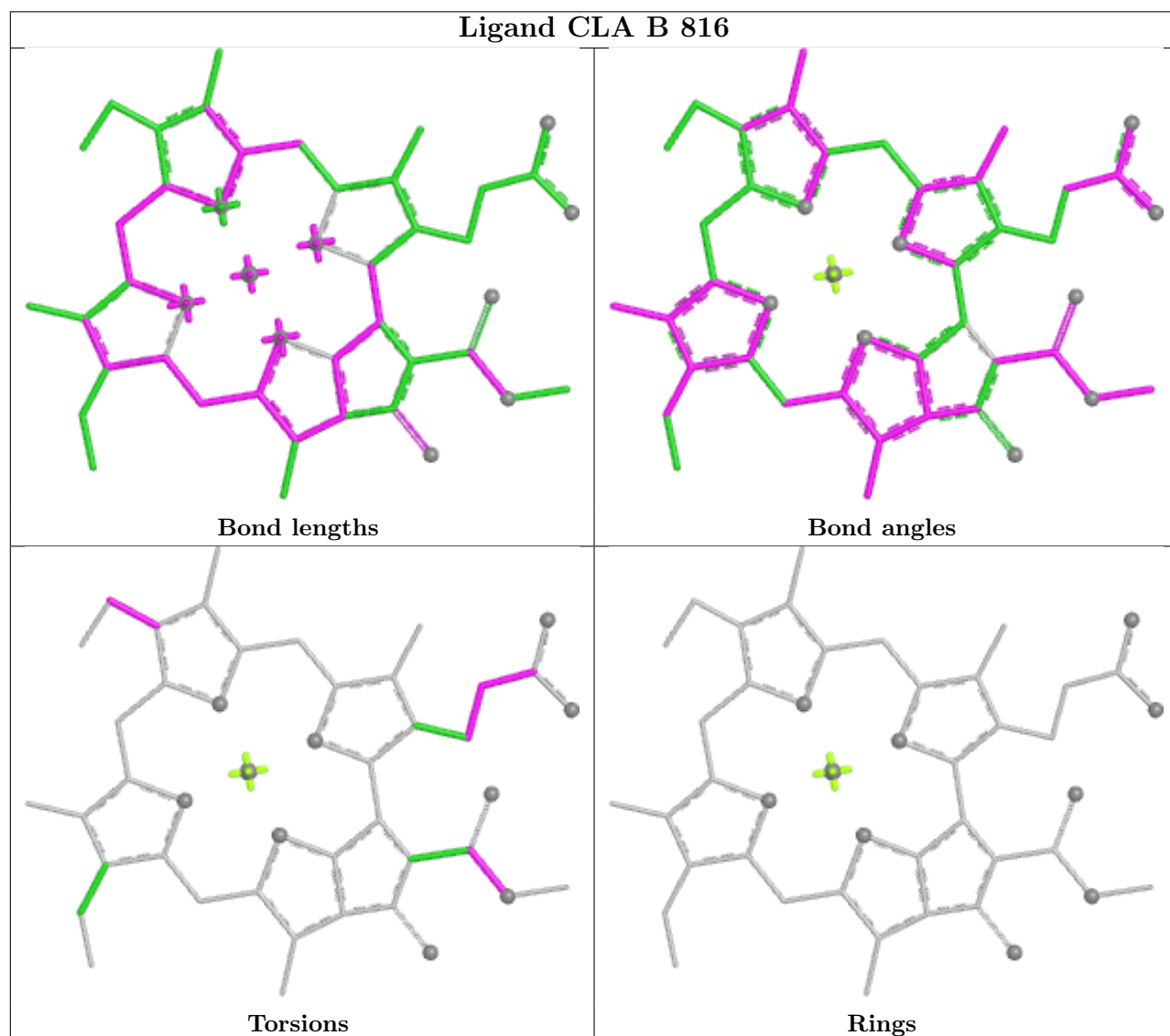
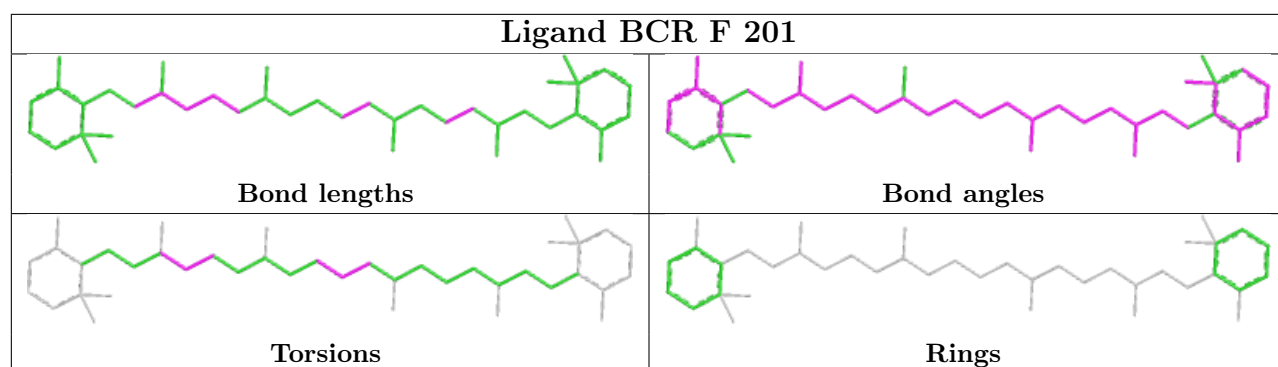


Ligand CLA B 838

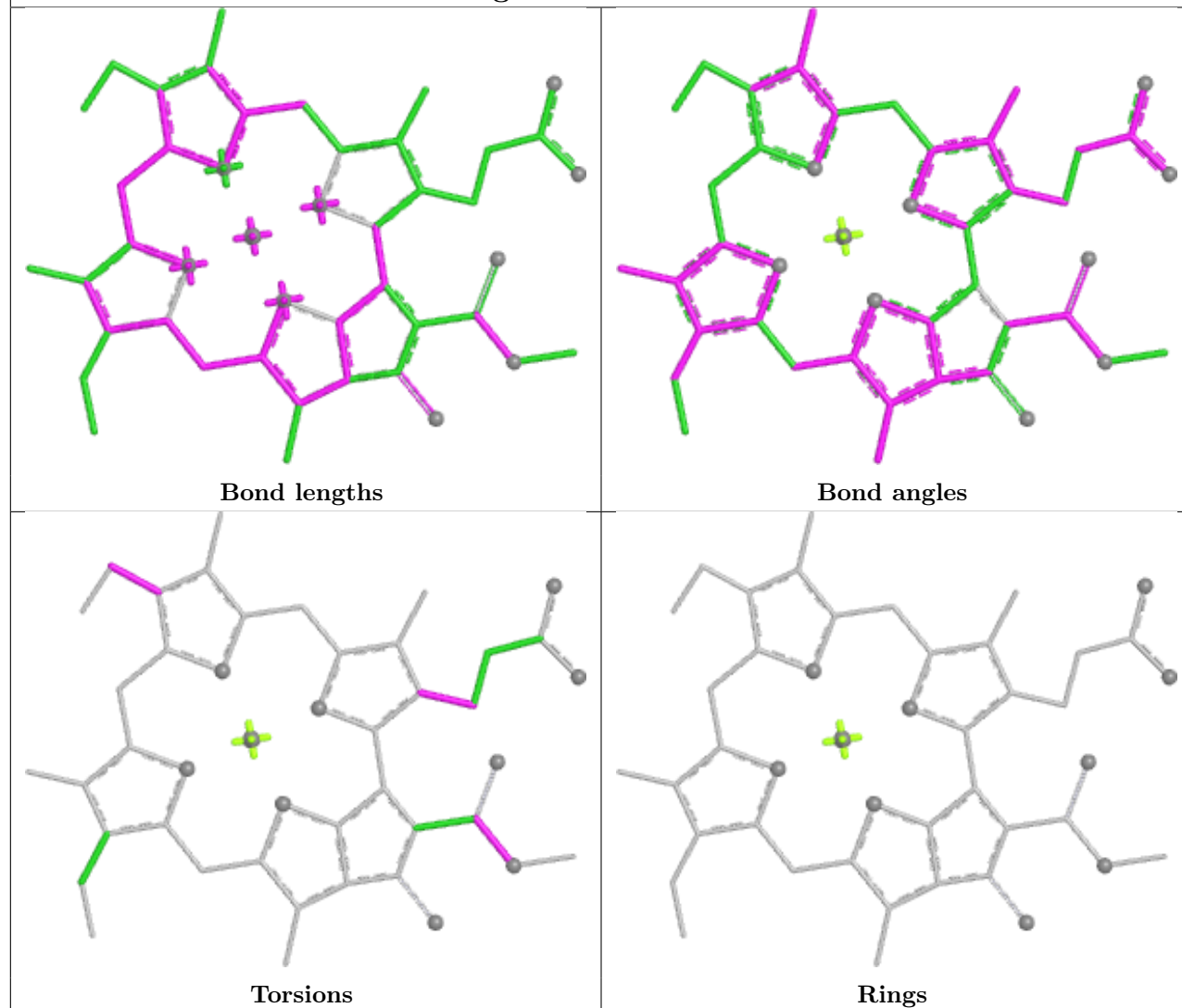


Ligand BCR B 847

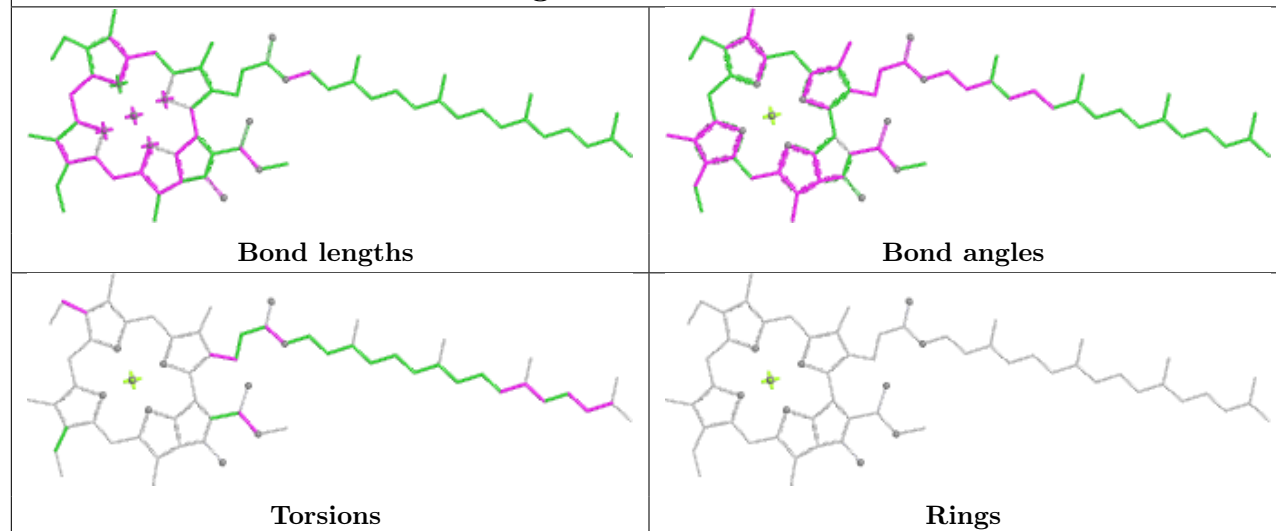


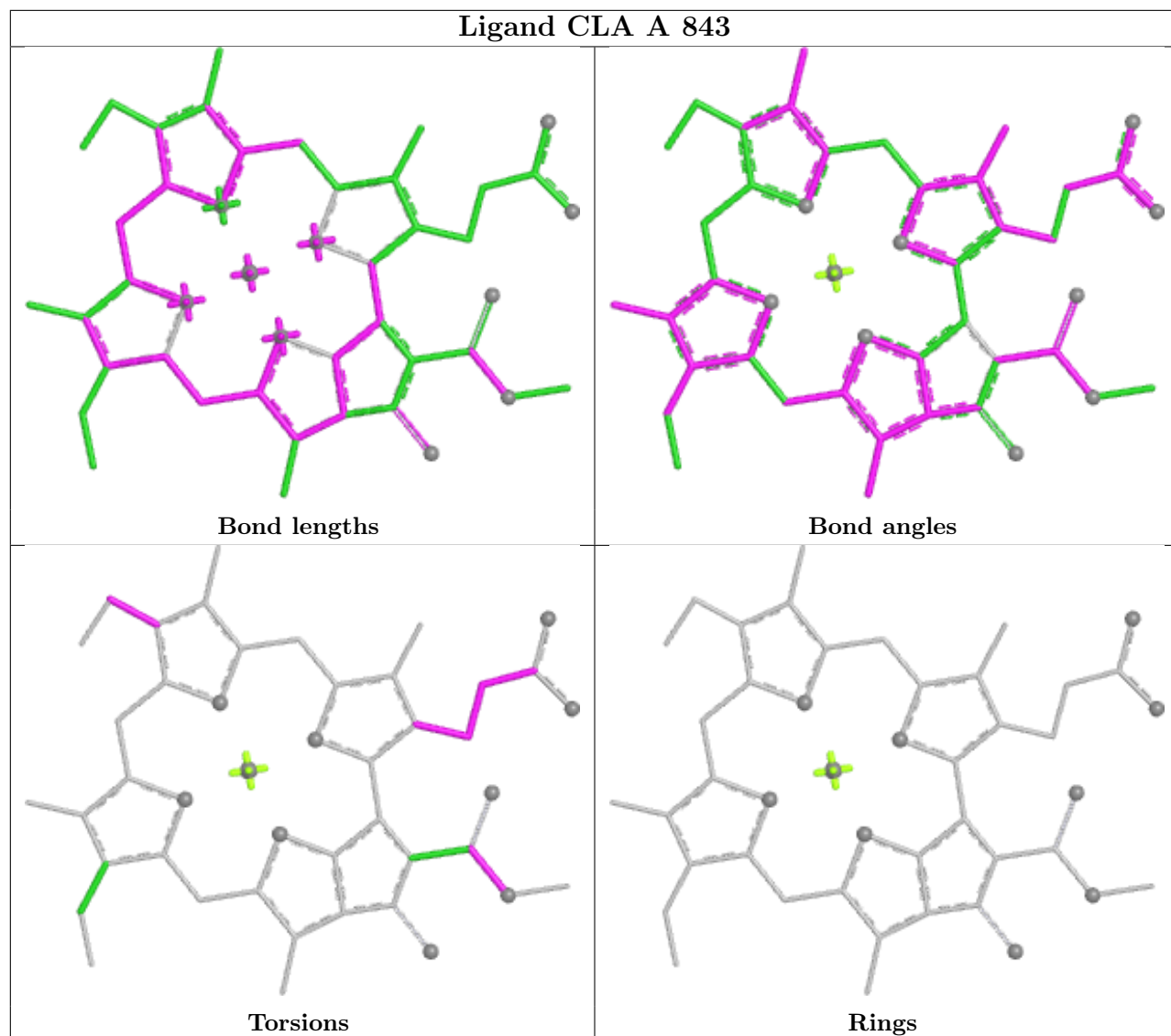


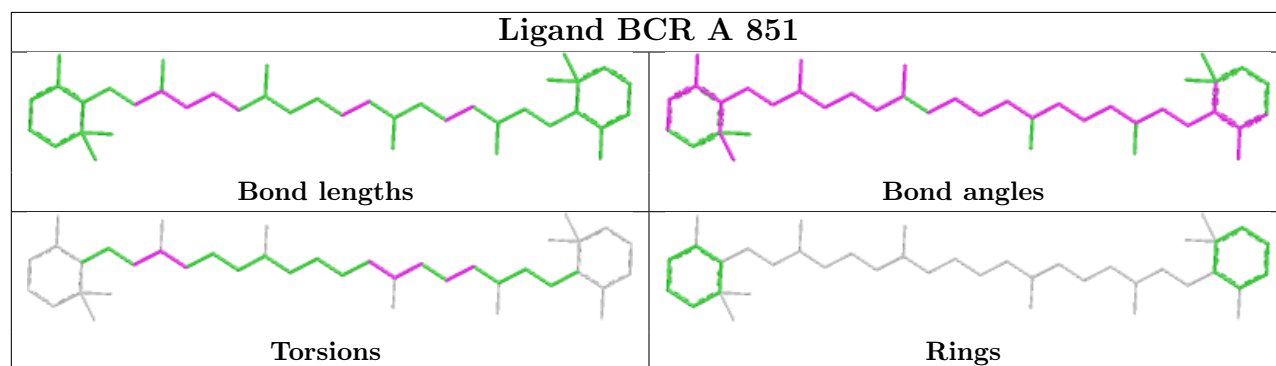
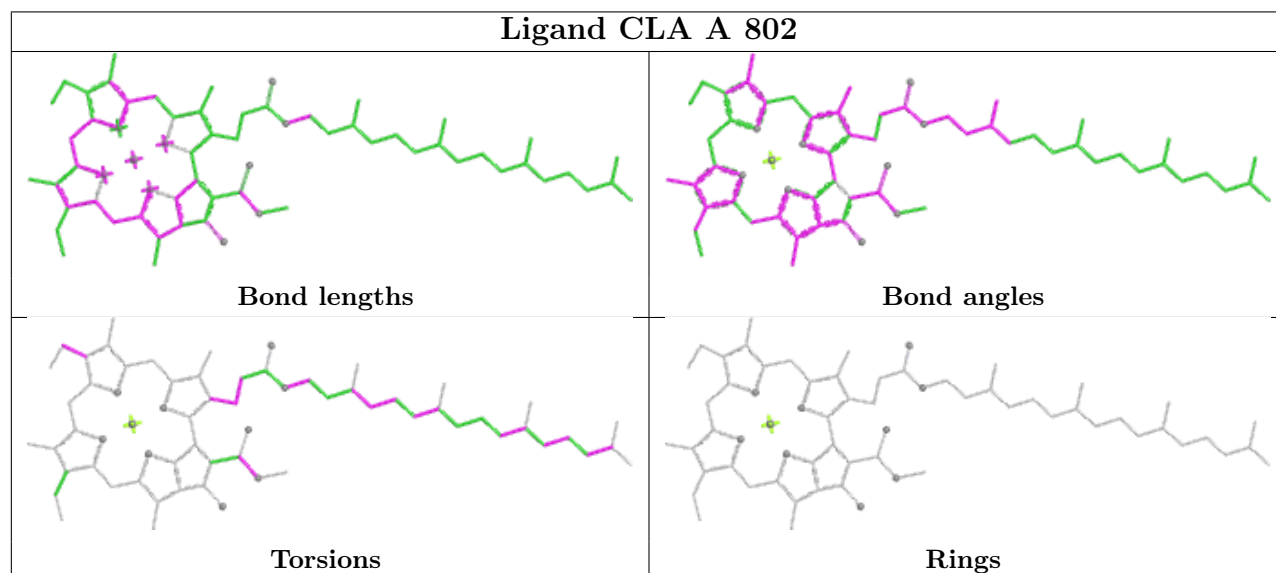
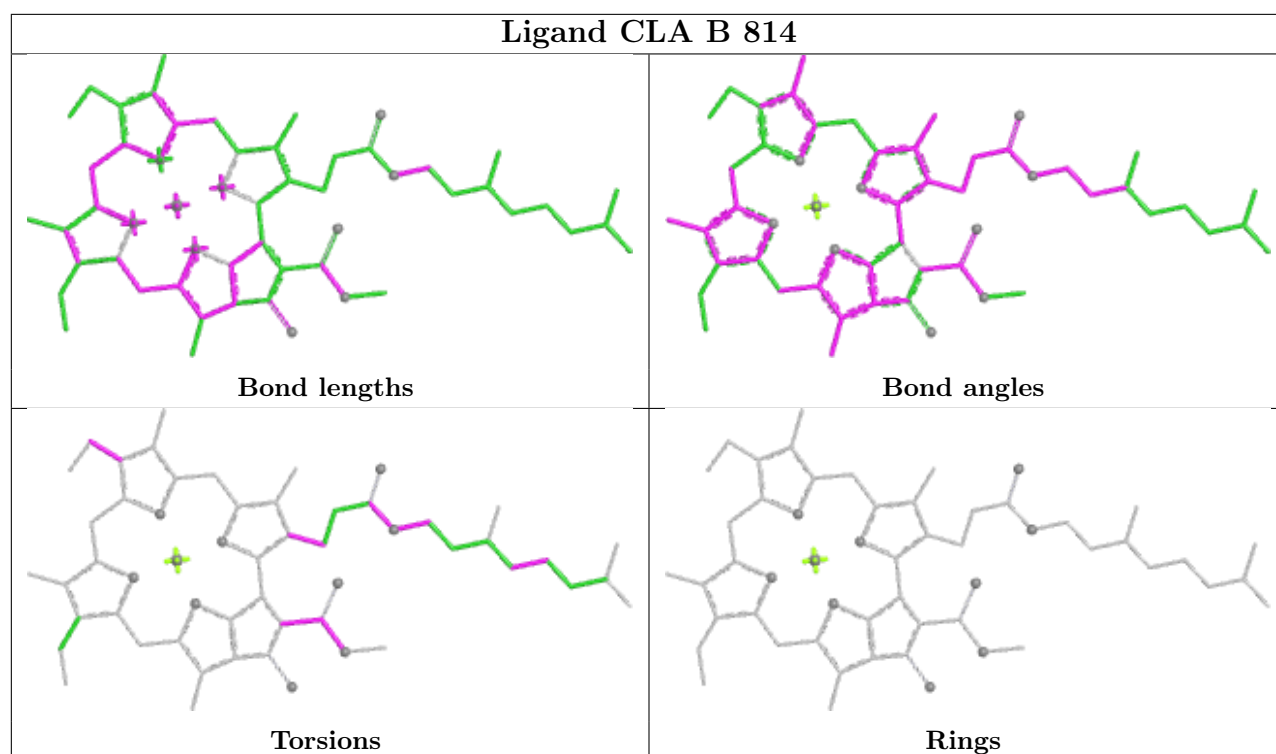
Ligand CLA B 835

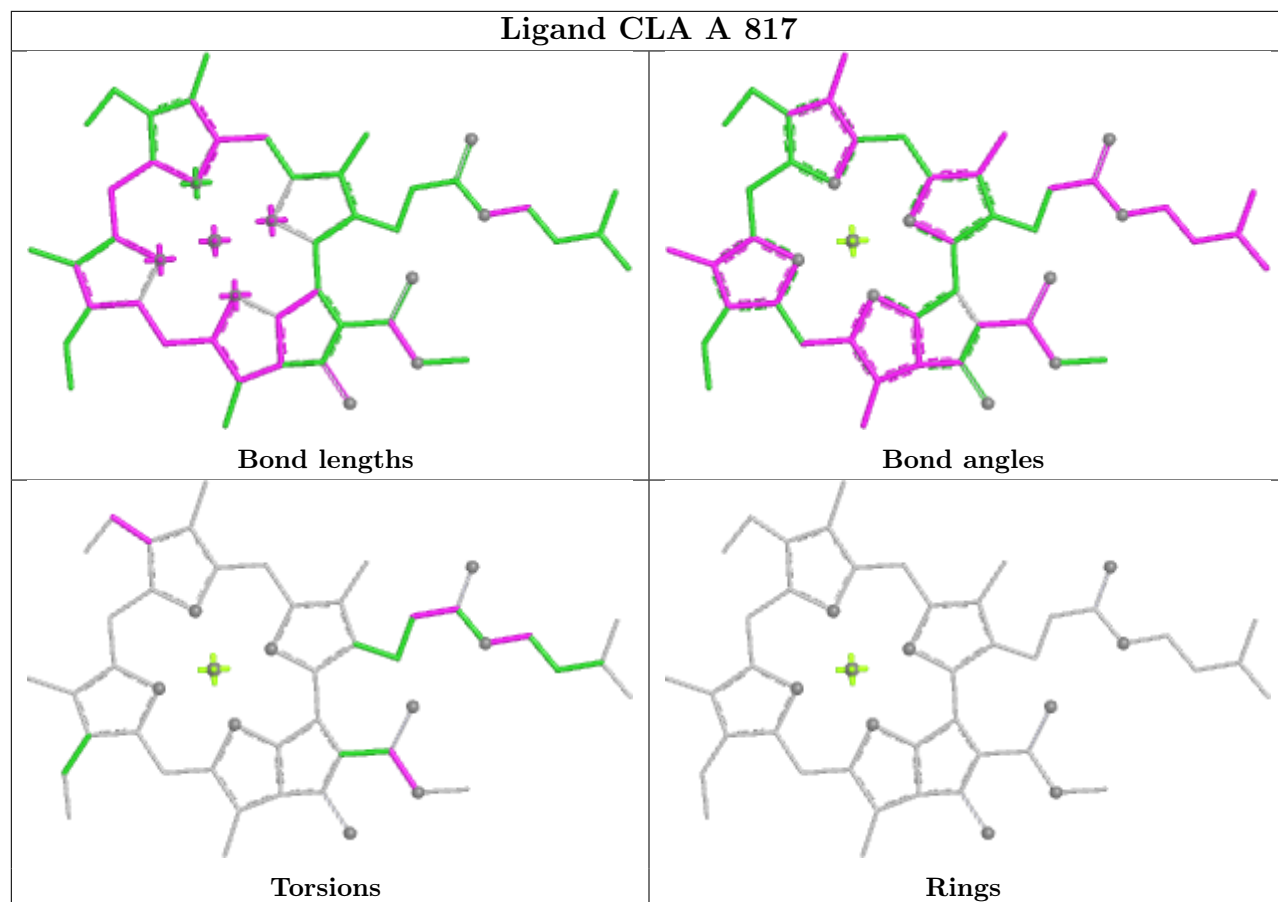


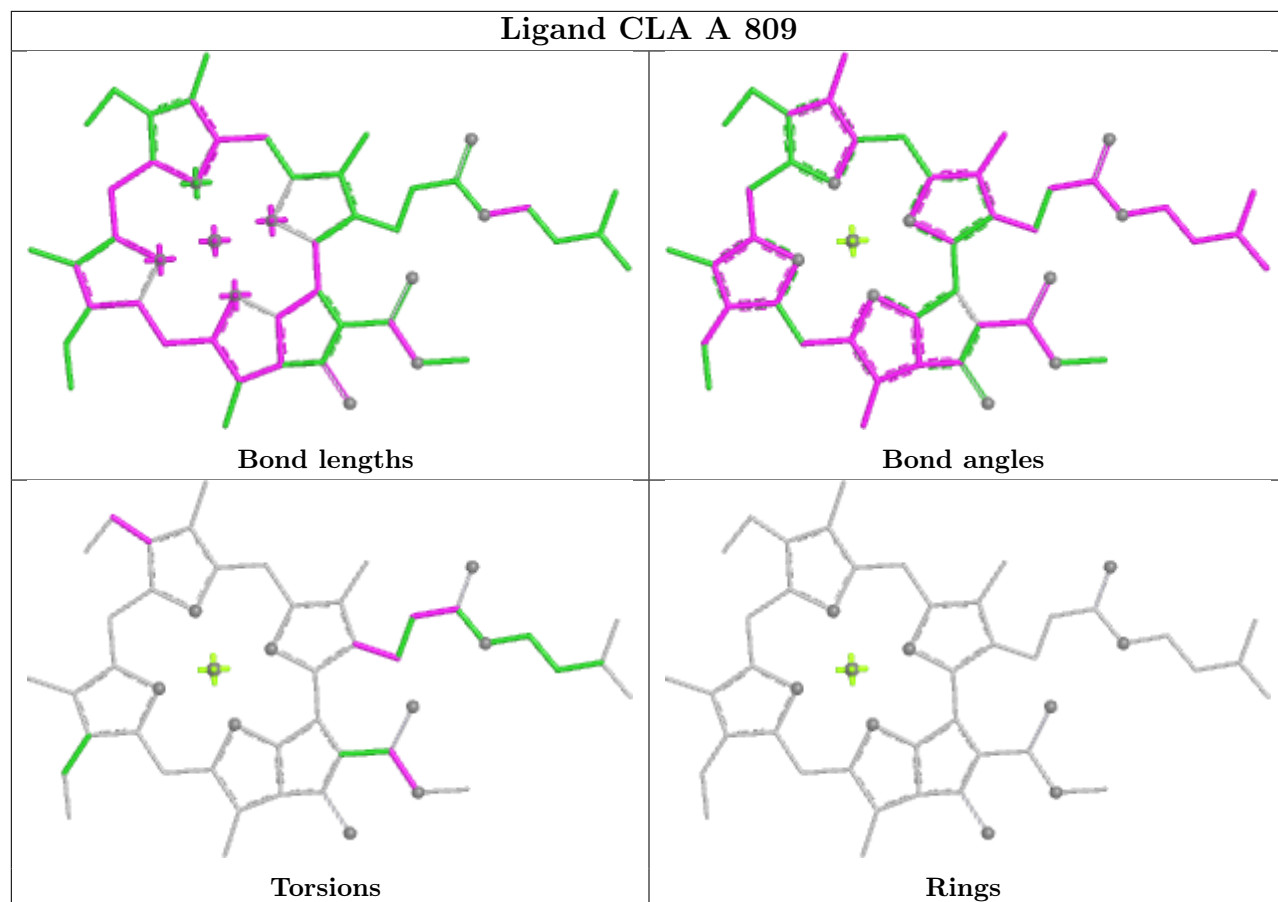
Ligand CLA A 819



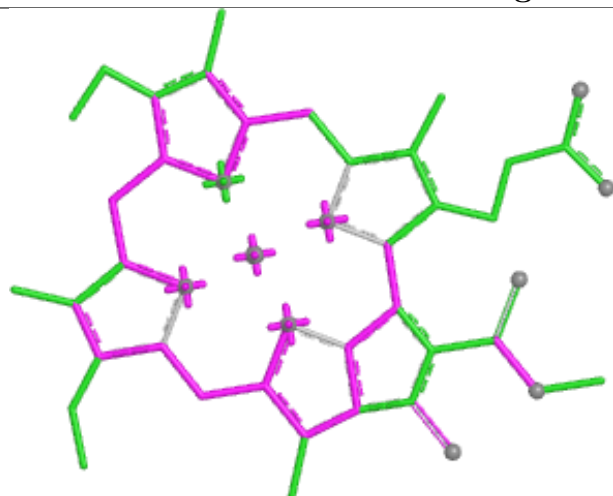




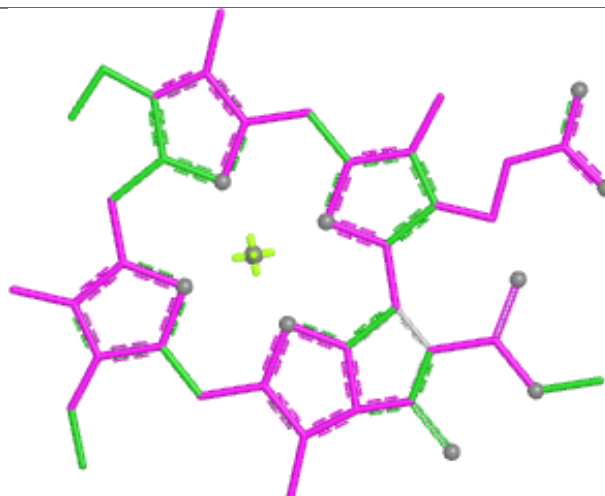




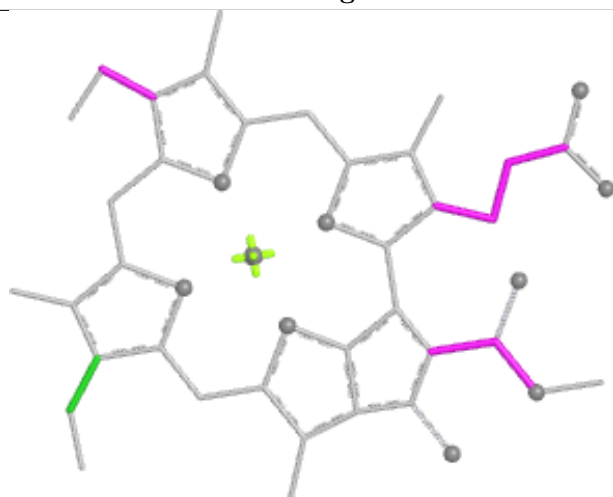
Ligand CLA B 830



Bond lengths



Bond angles

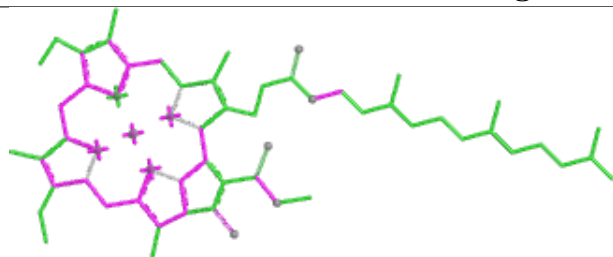


Torsions

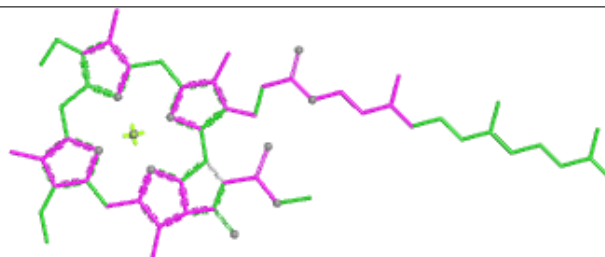


Rings

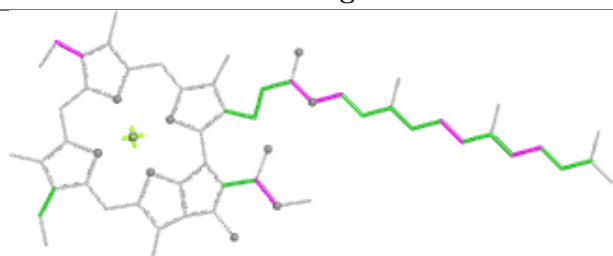
Ligand CLA A 826



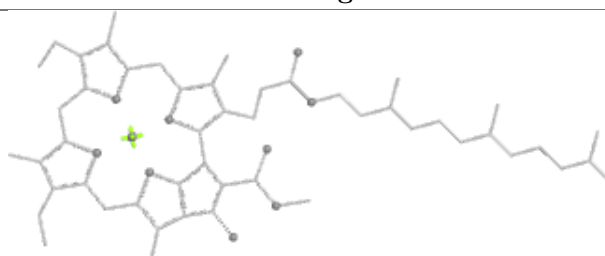
Bond lengths



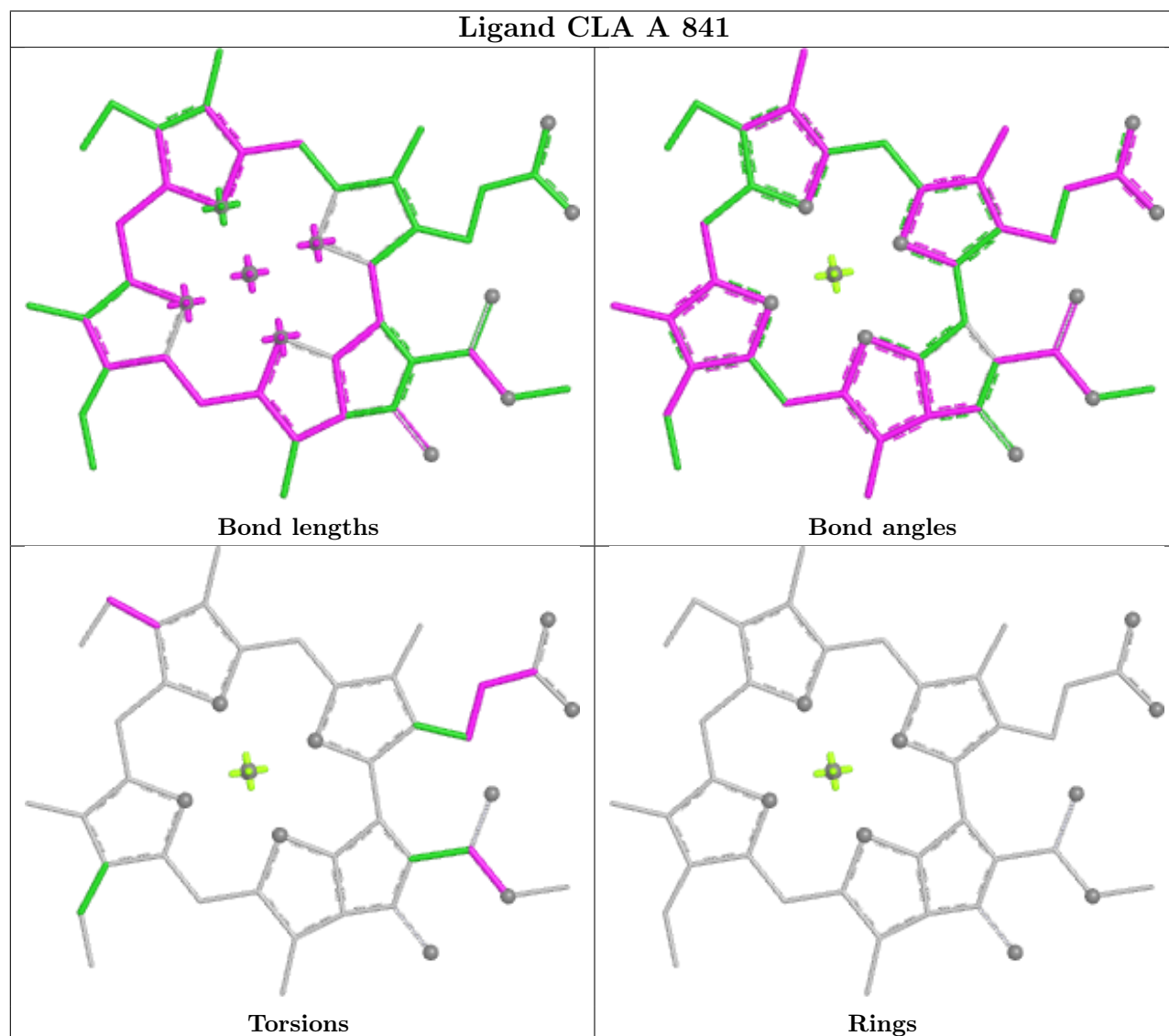
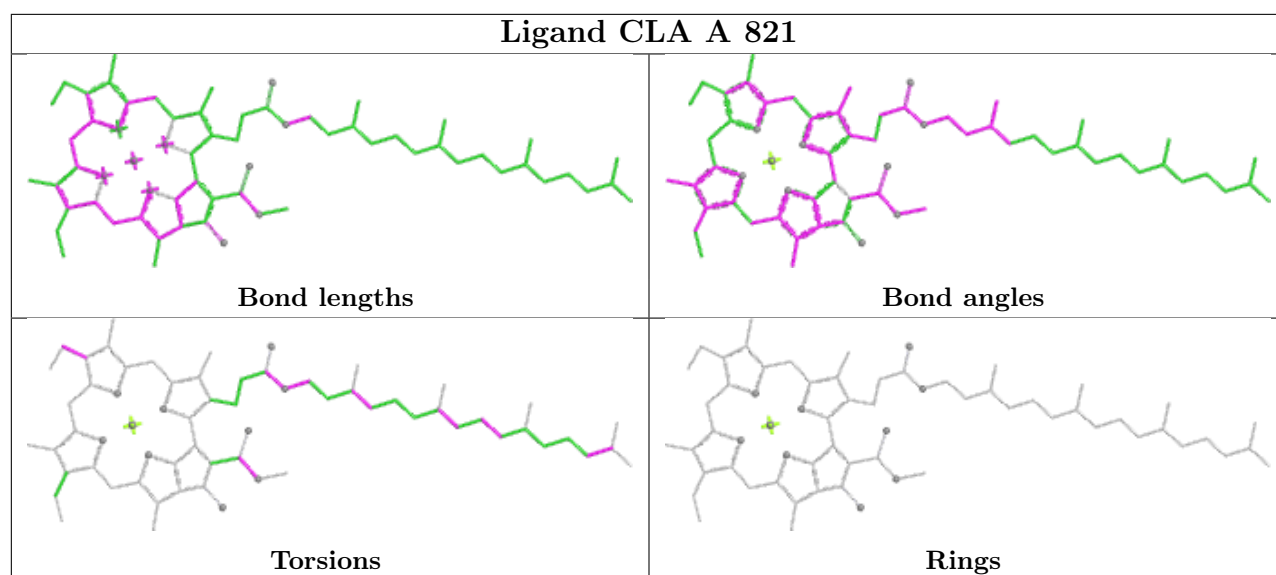
Bond angles



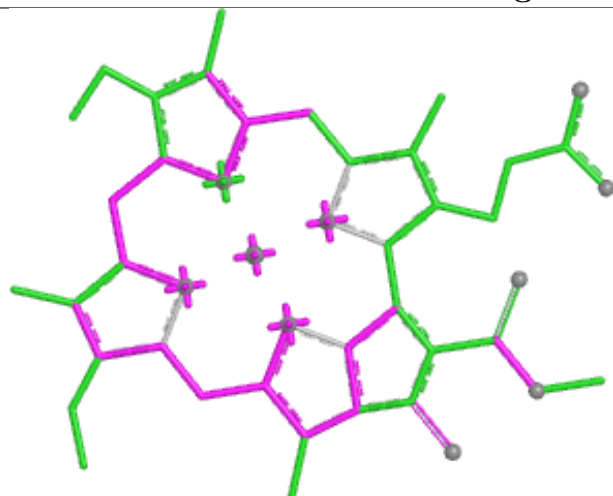
Torsions



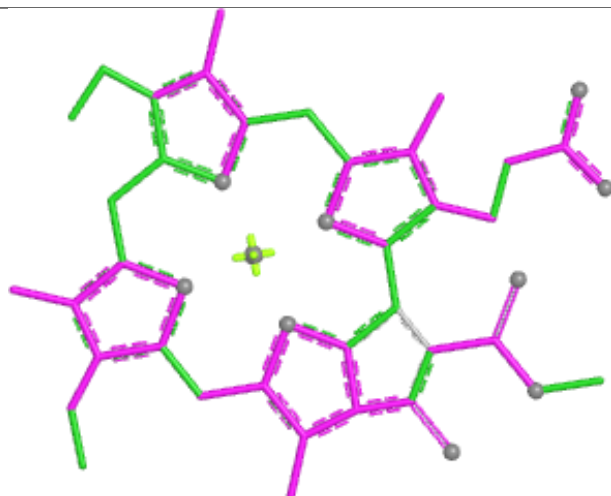
Rings



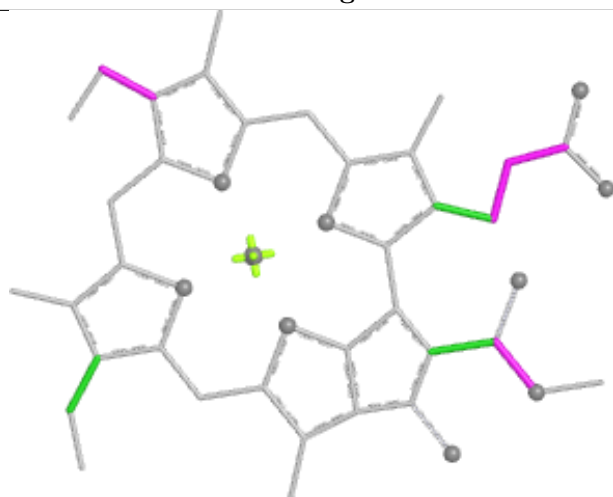
Ligand CLA B 808



Bond lengths



Bond angles

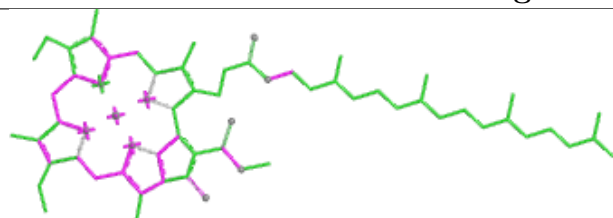


Torsions

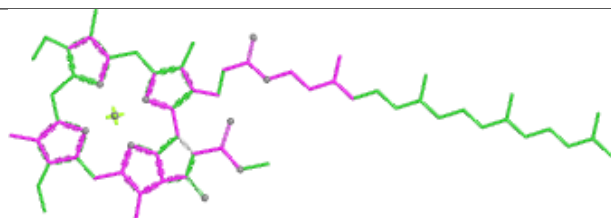


Rings

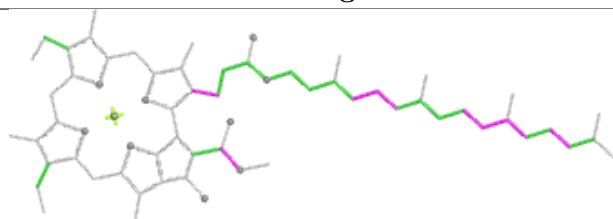
Ligand CLA A 806



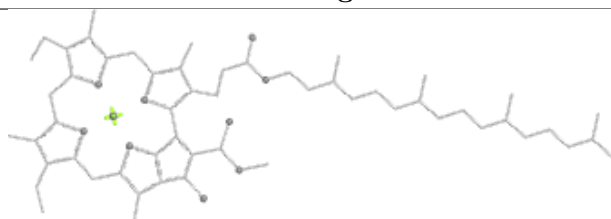
Bond lengths



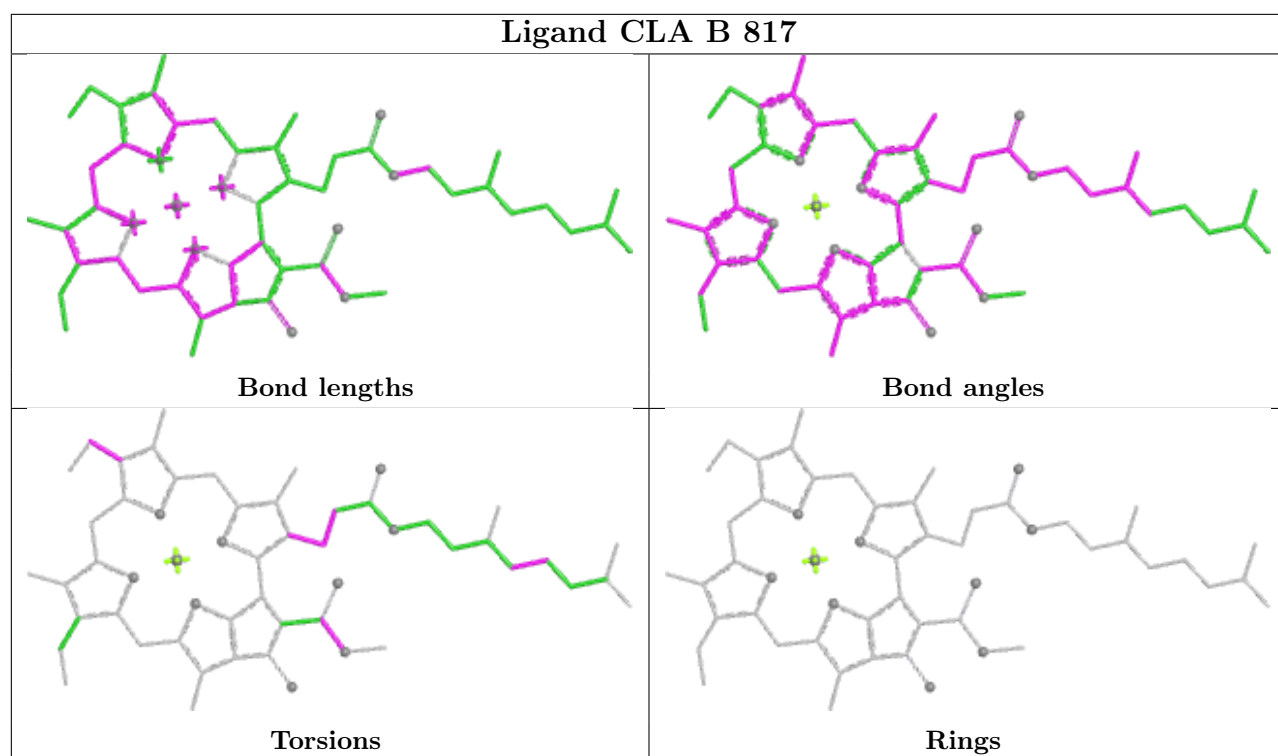
Bond angles

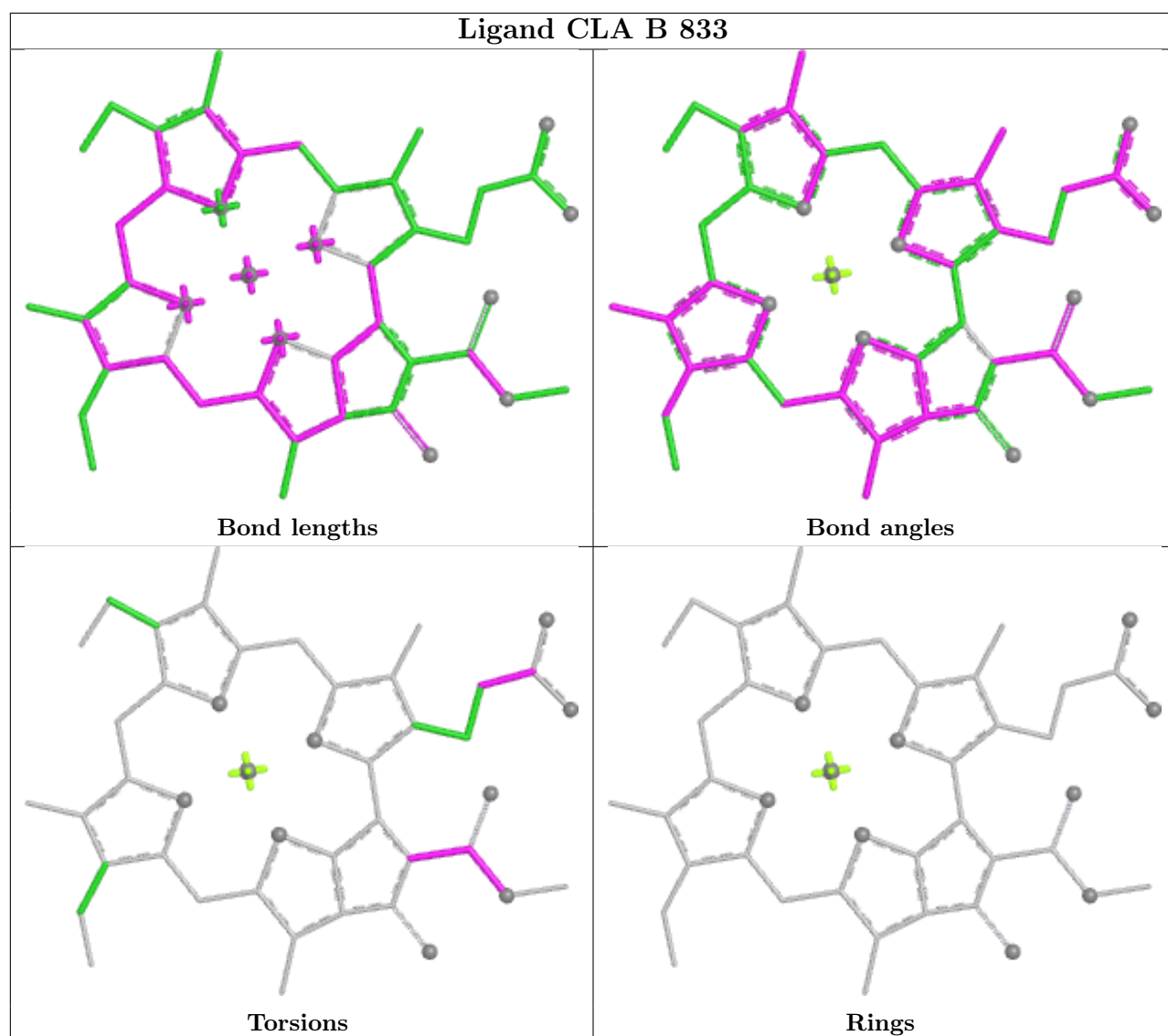


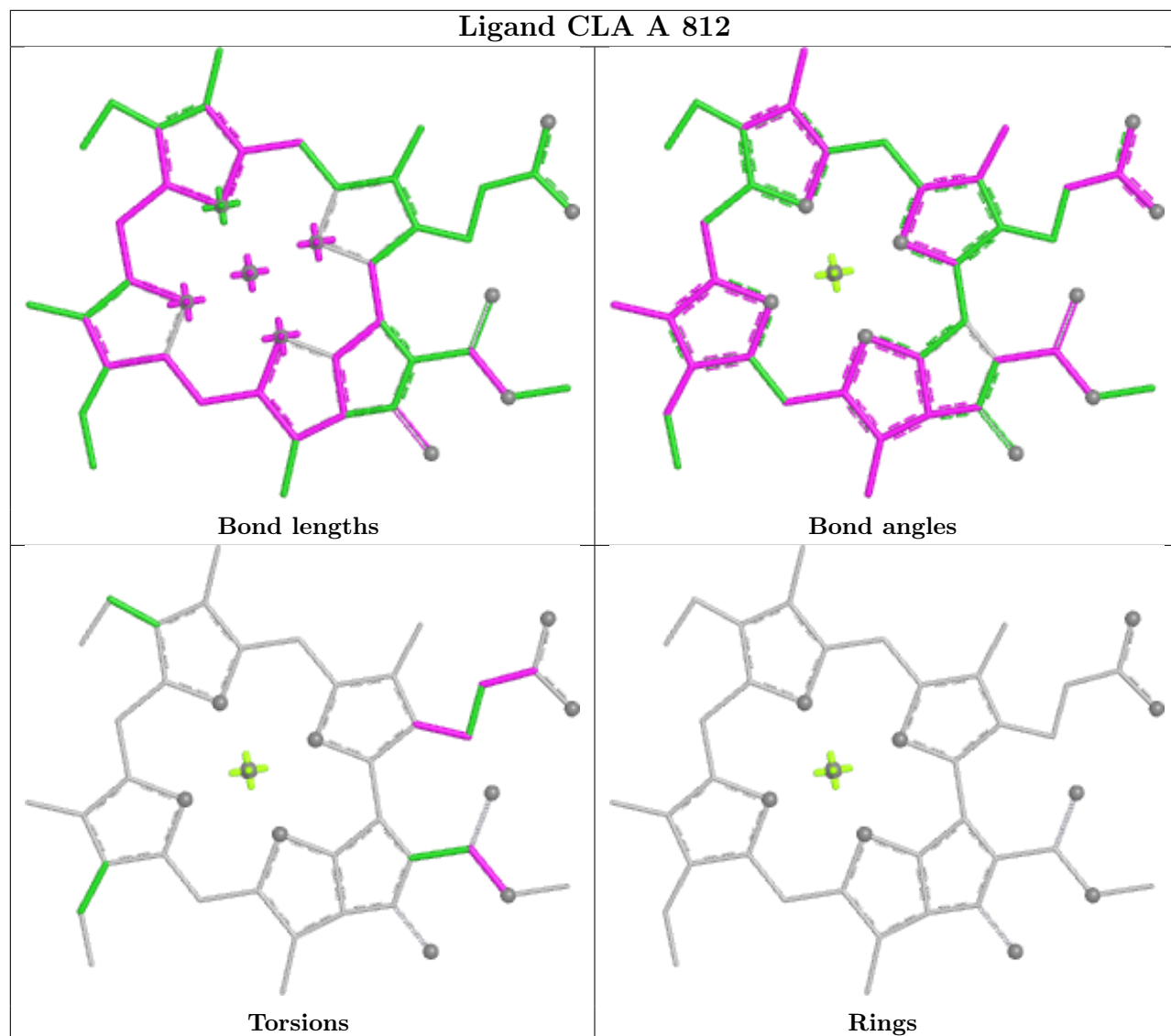
Torsions

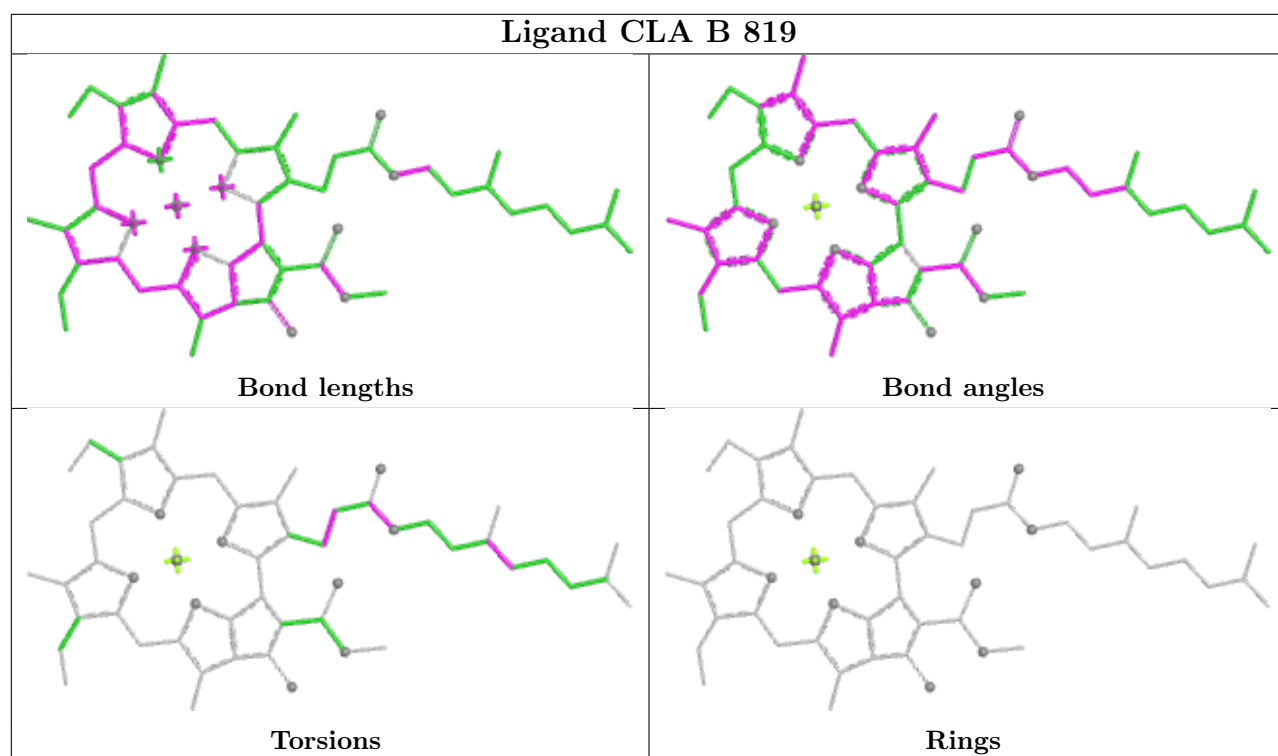


Rings

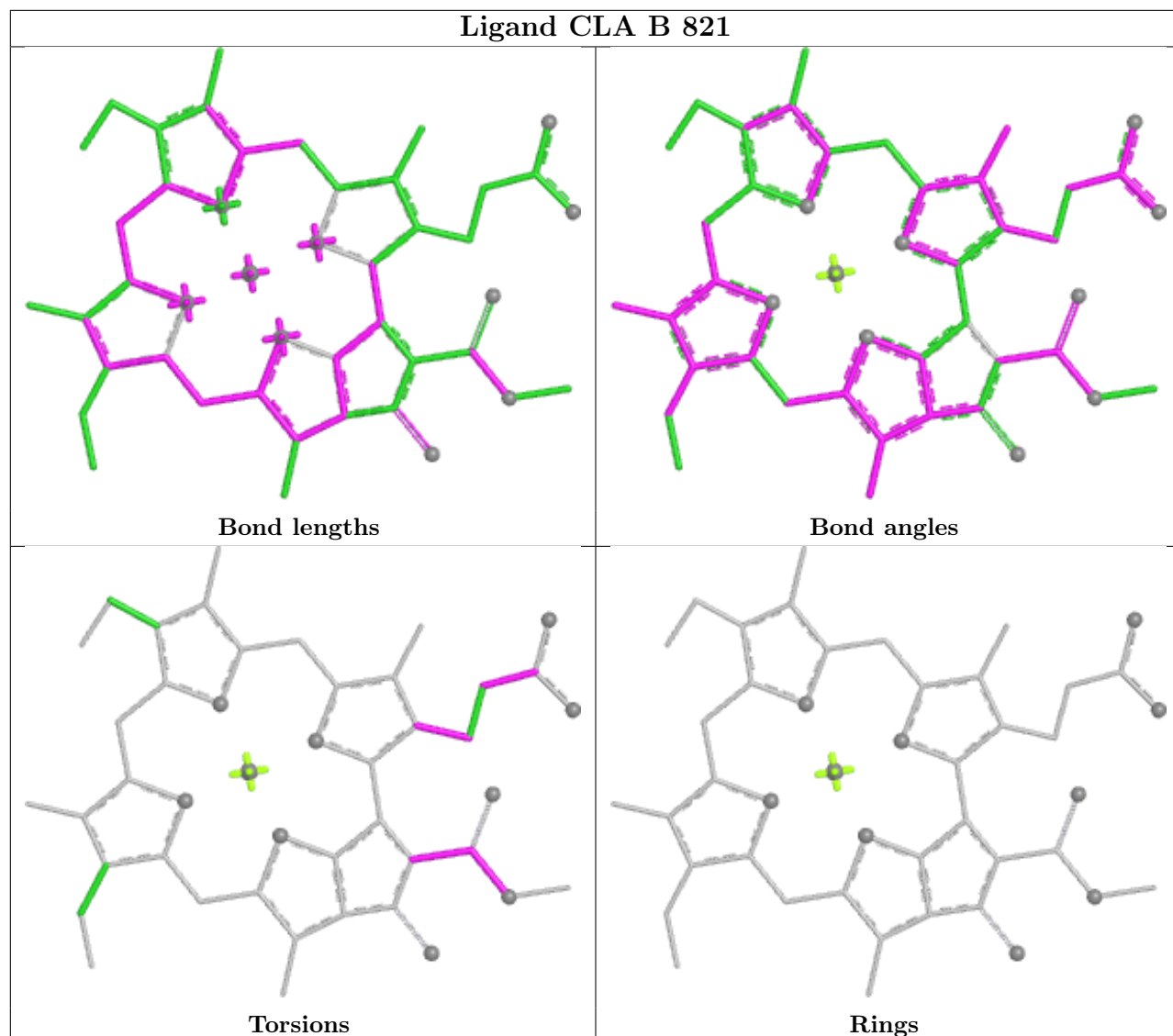




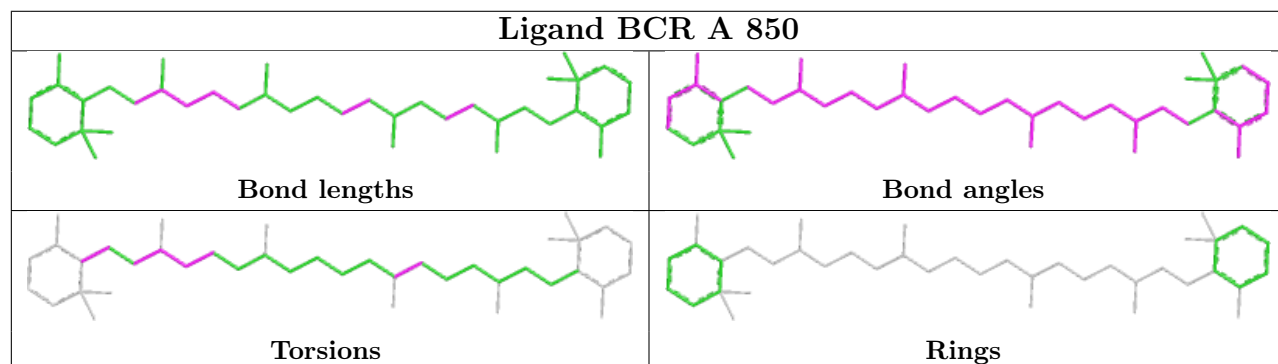


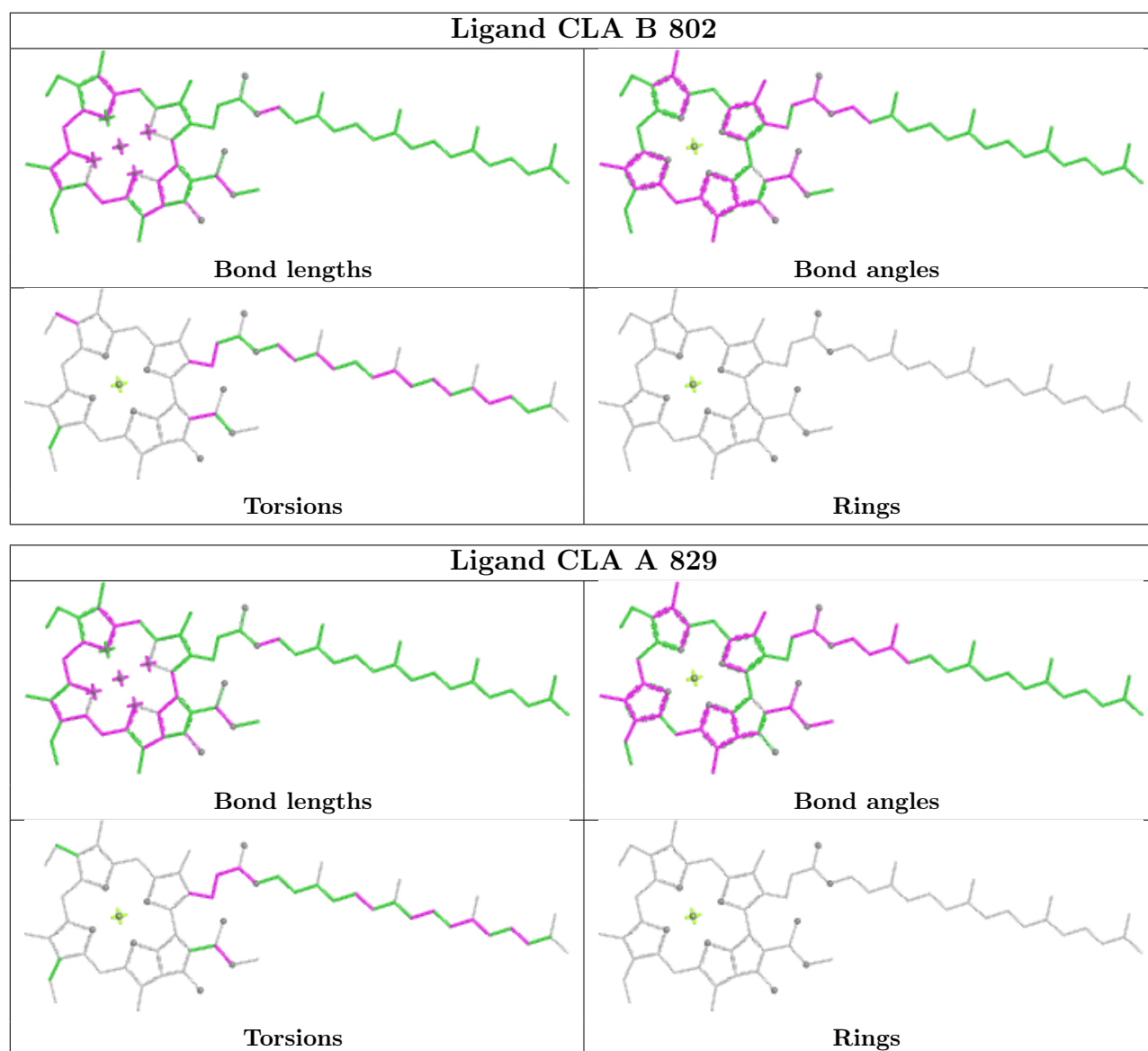


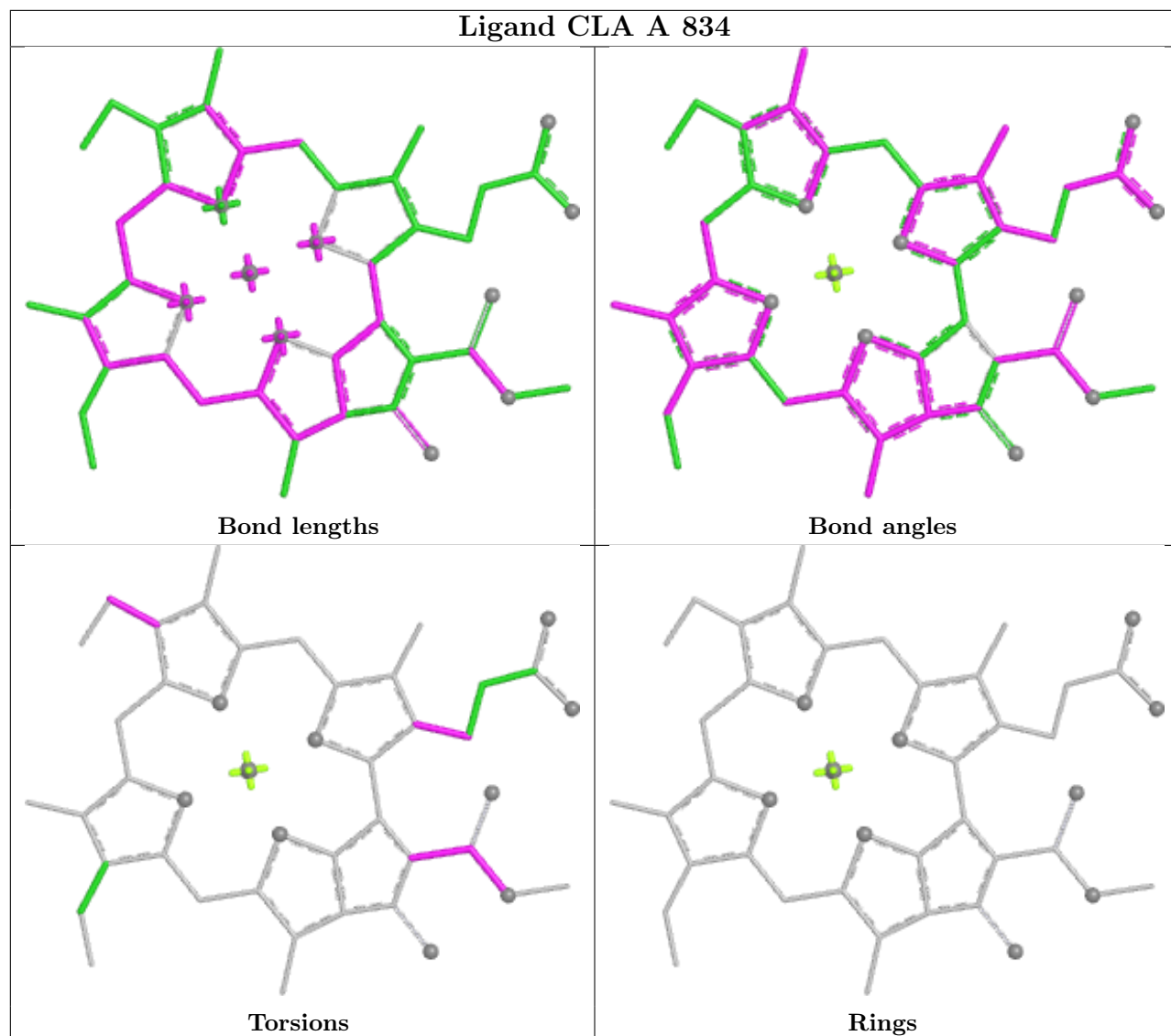
Ligand CLA B 821



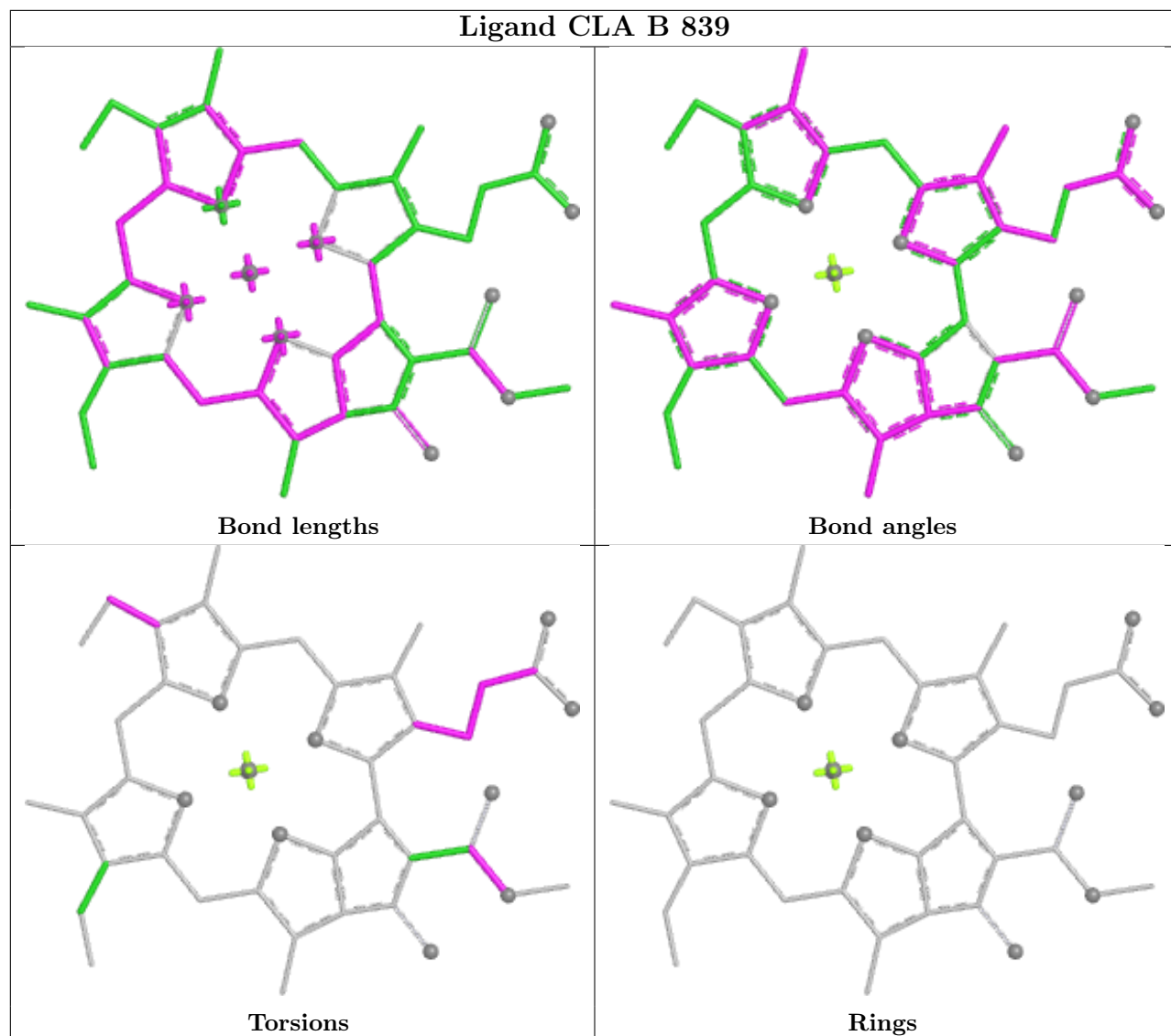
Ligand BCR A 850



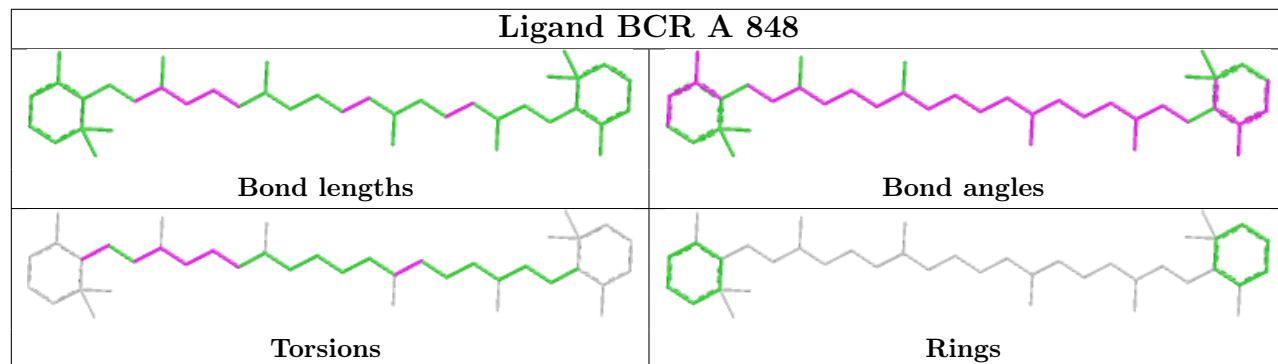


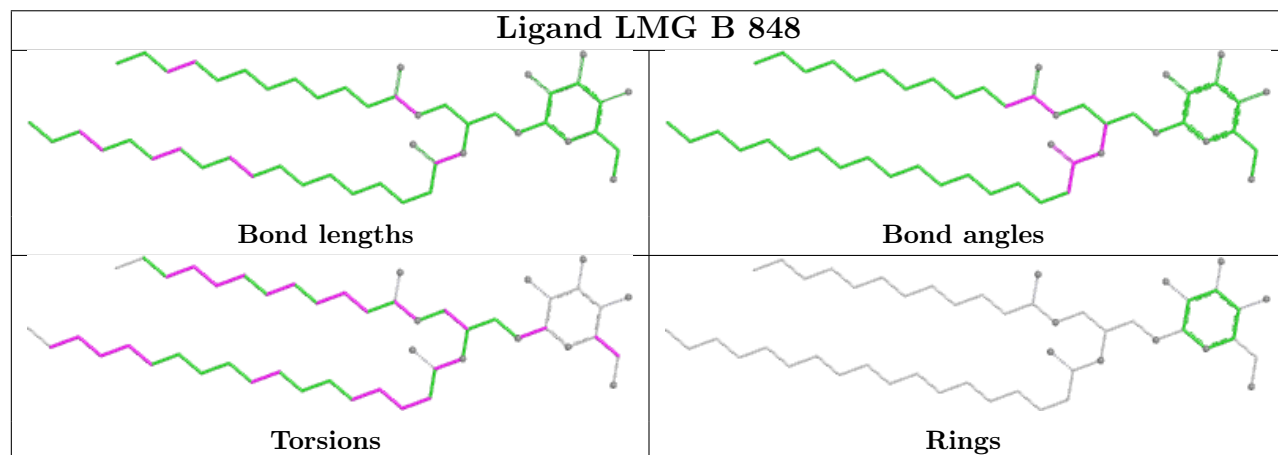
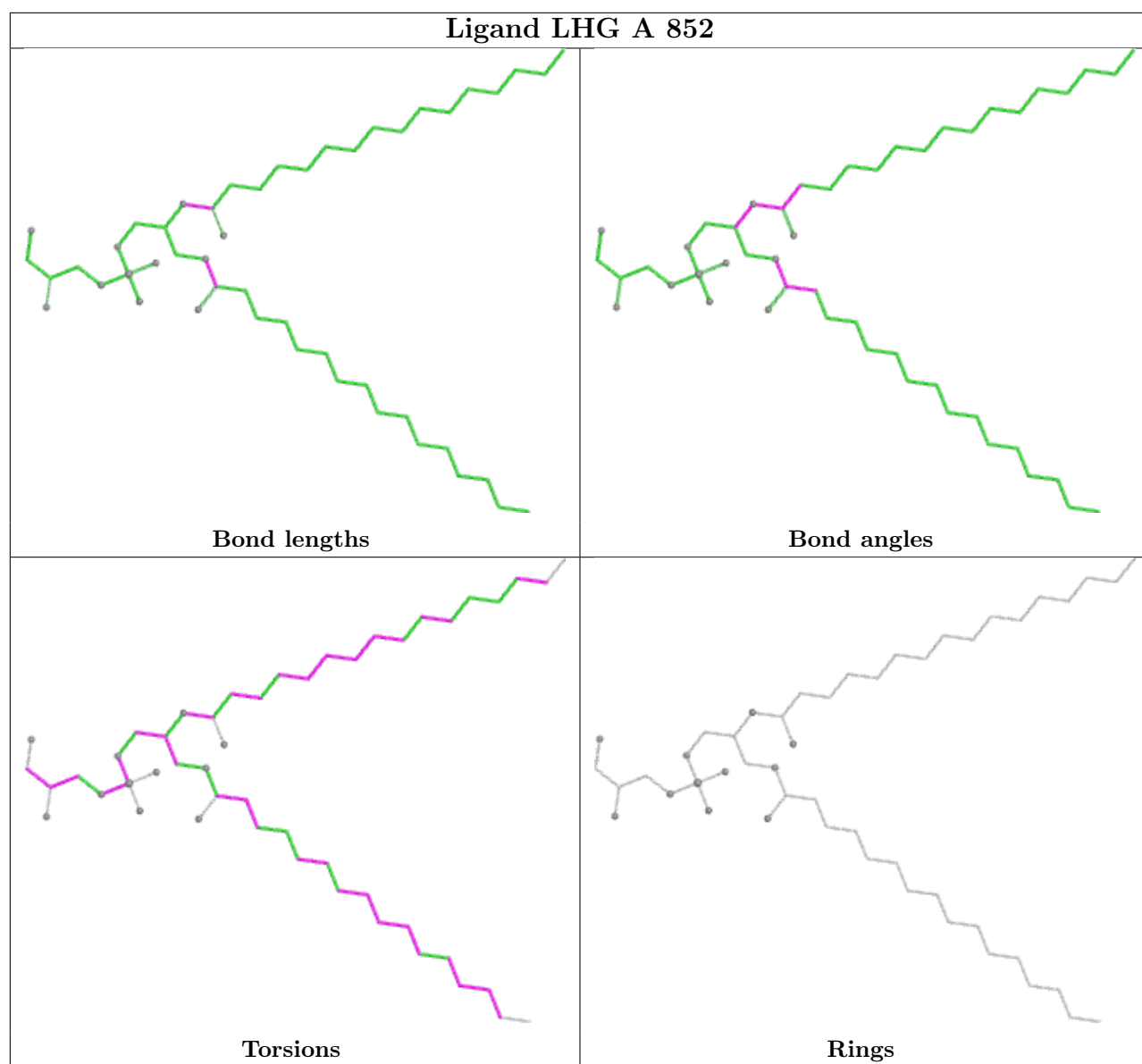


Ligand CLA B 839

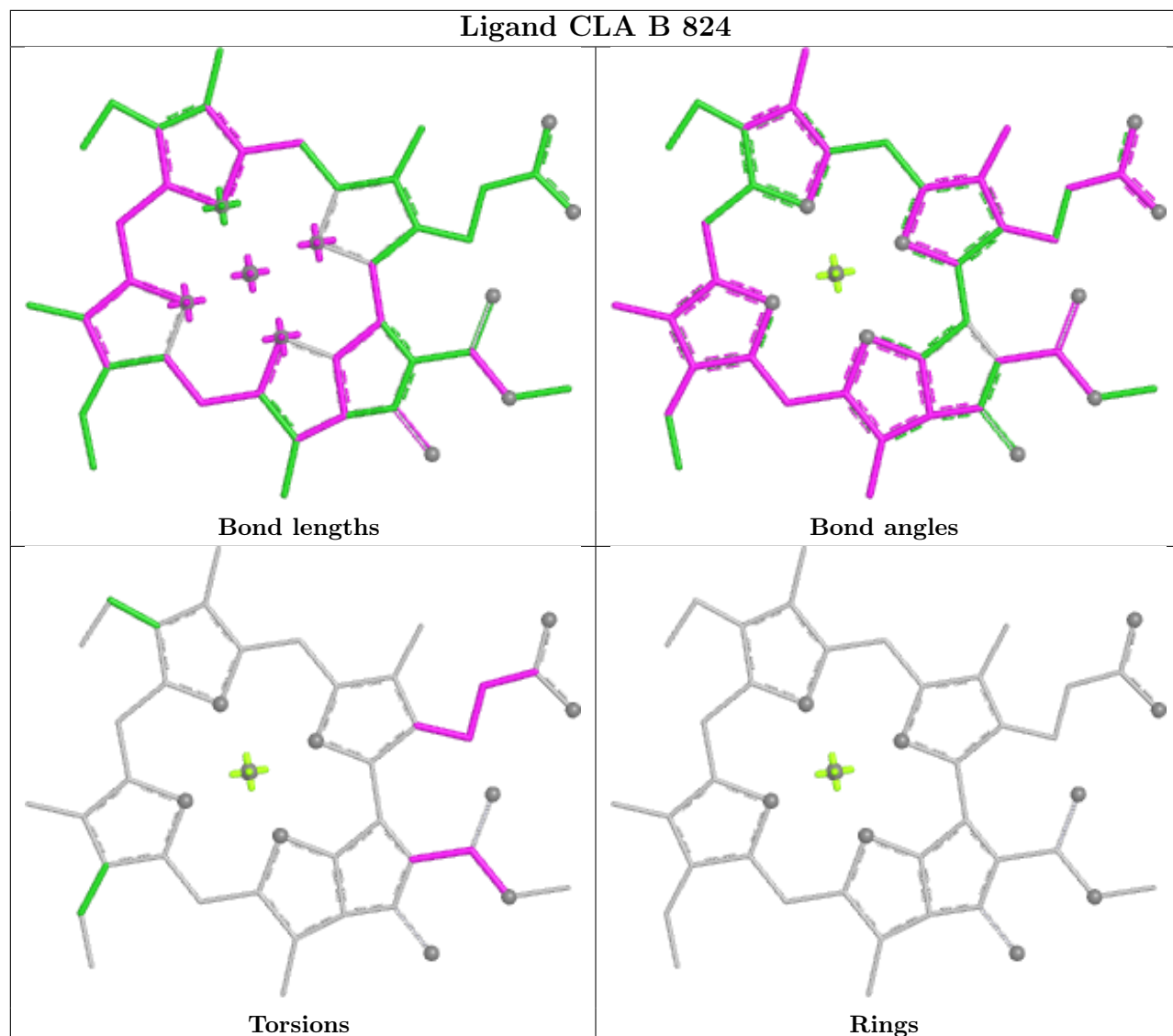


Ligand BCR A 848

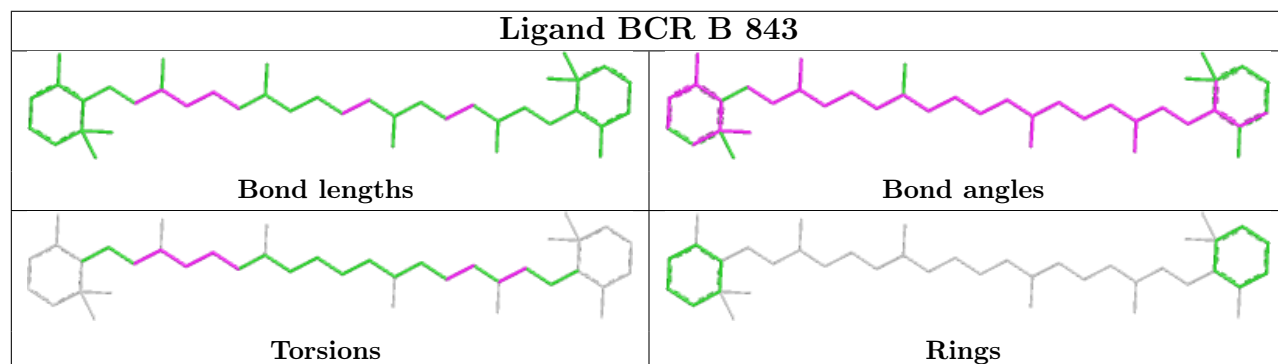




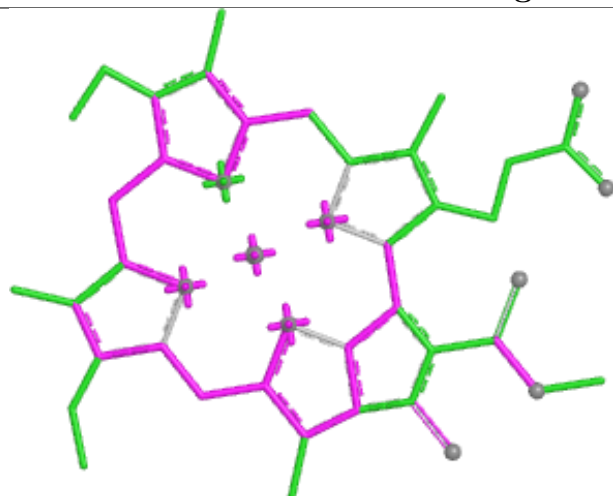
Ligand CLA B 824



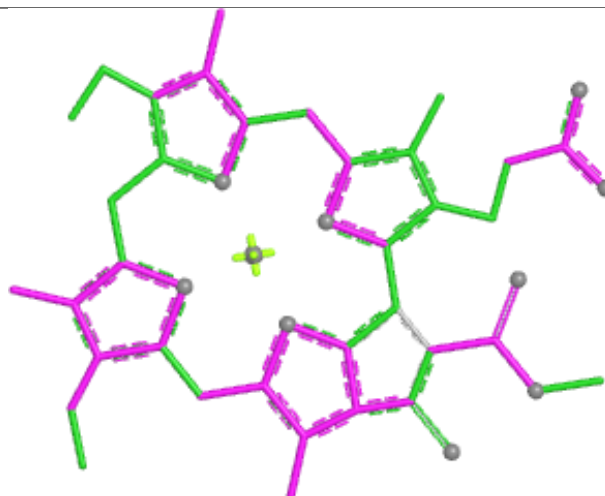
Ligand BCR B 843



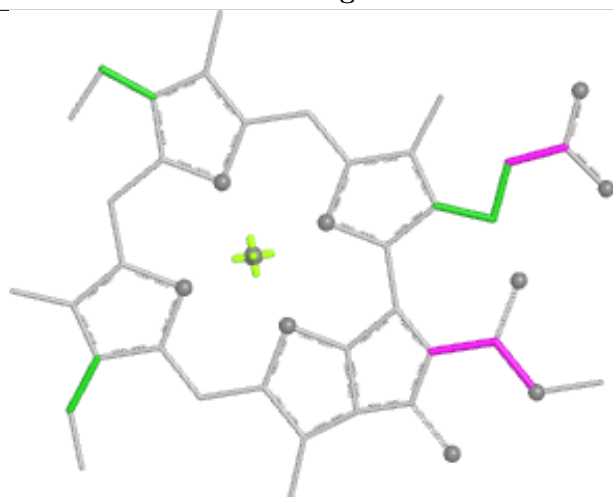
Ligand CLA B 834



Bond lengths



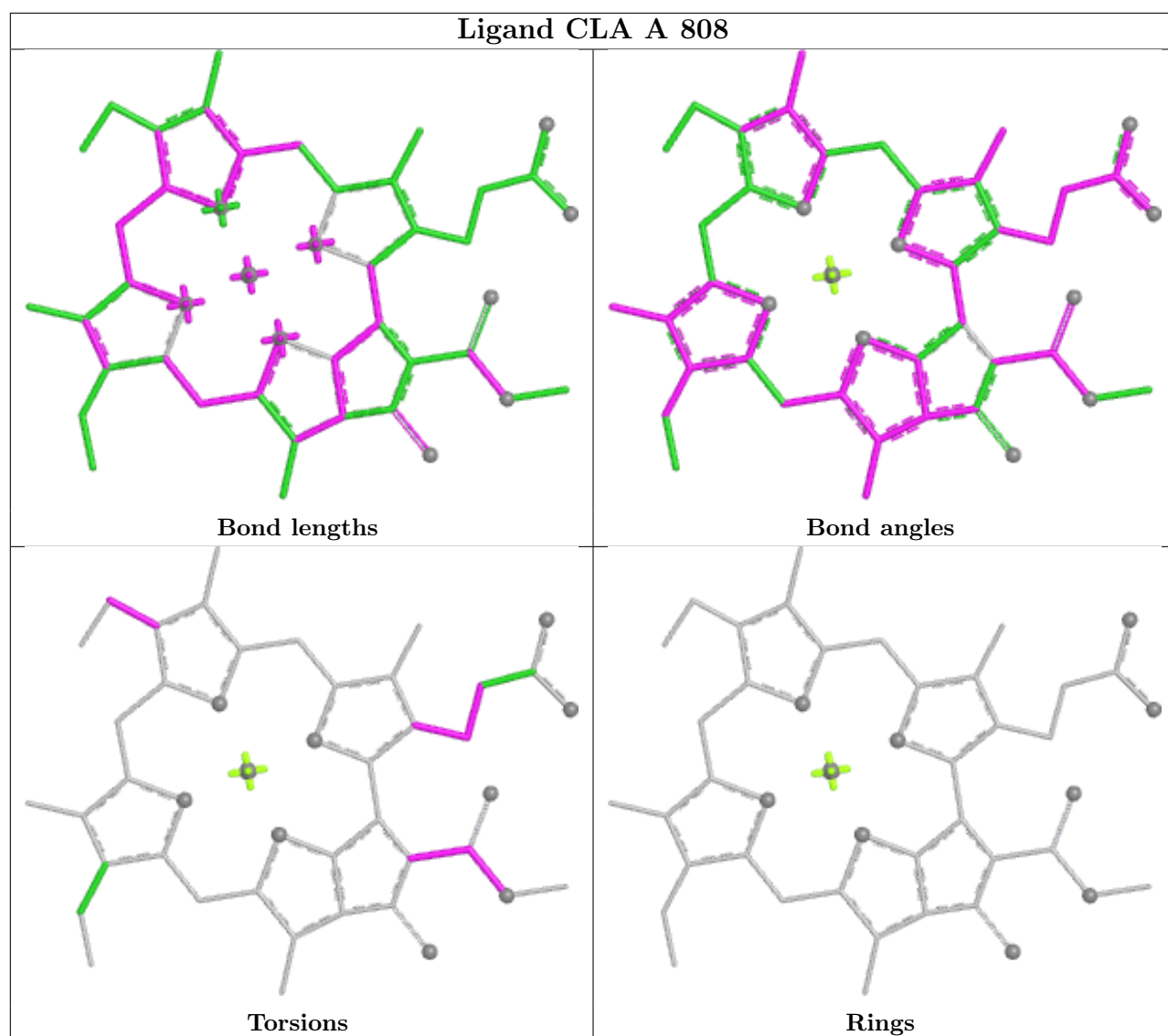
Bond angles



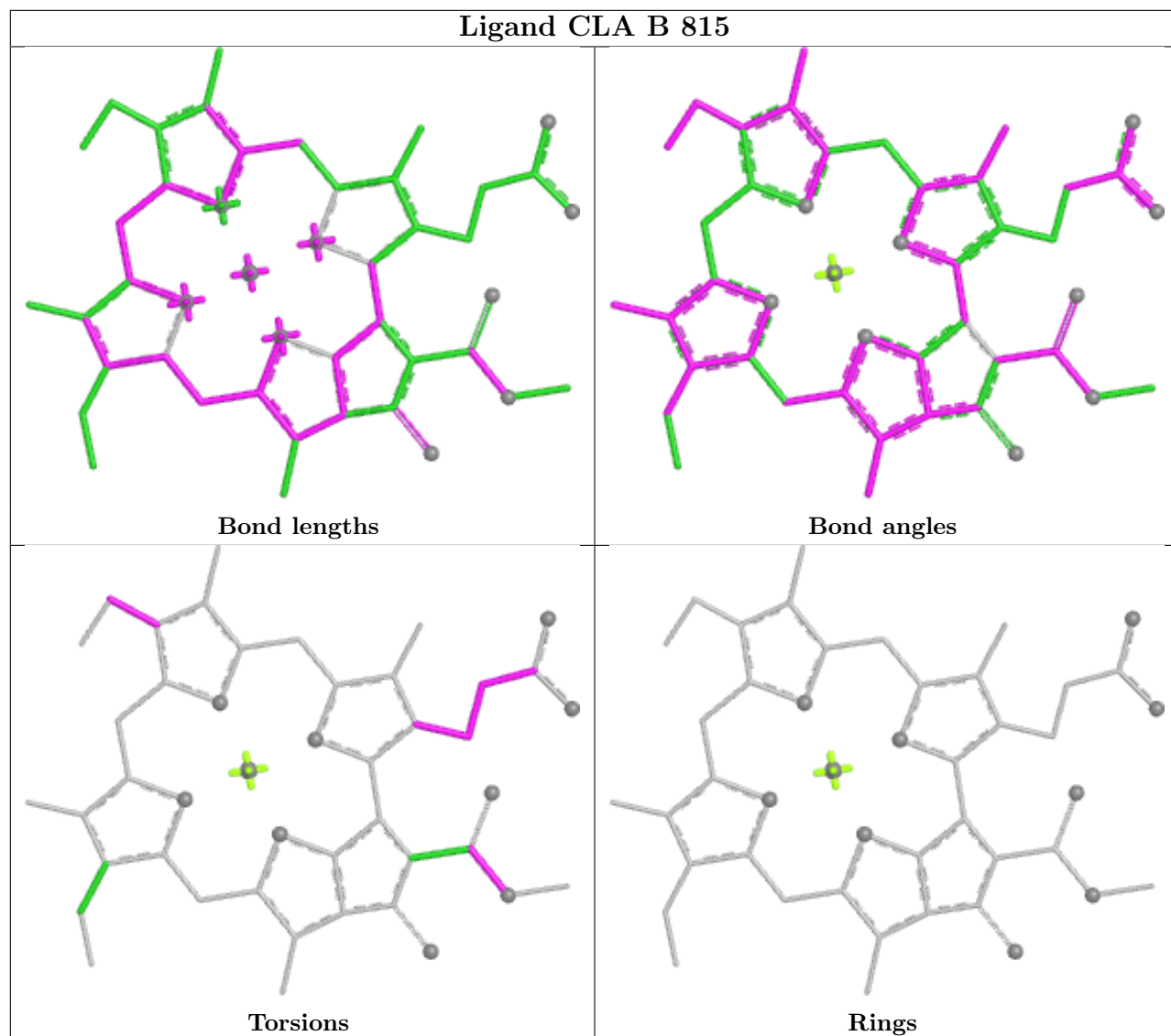
Torsions



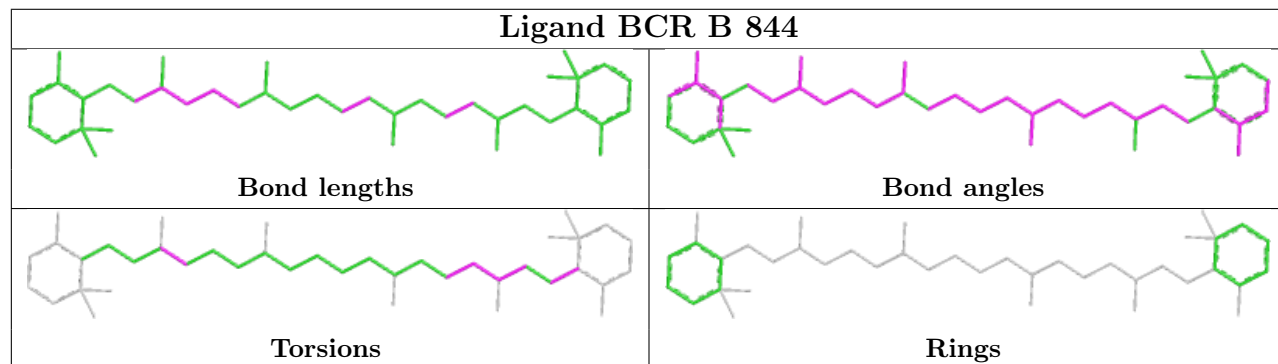
Rings

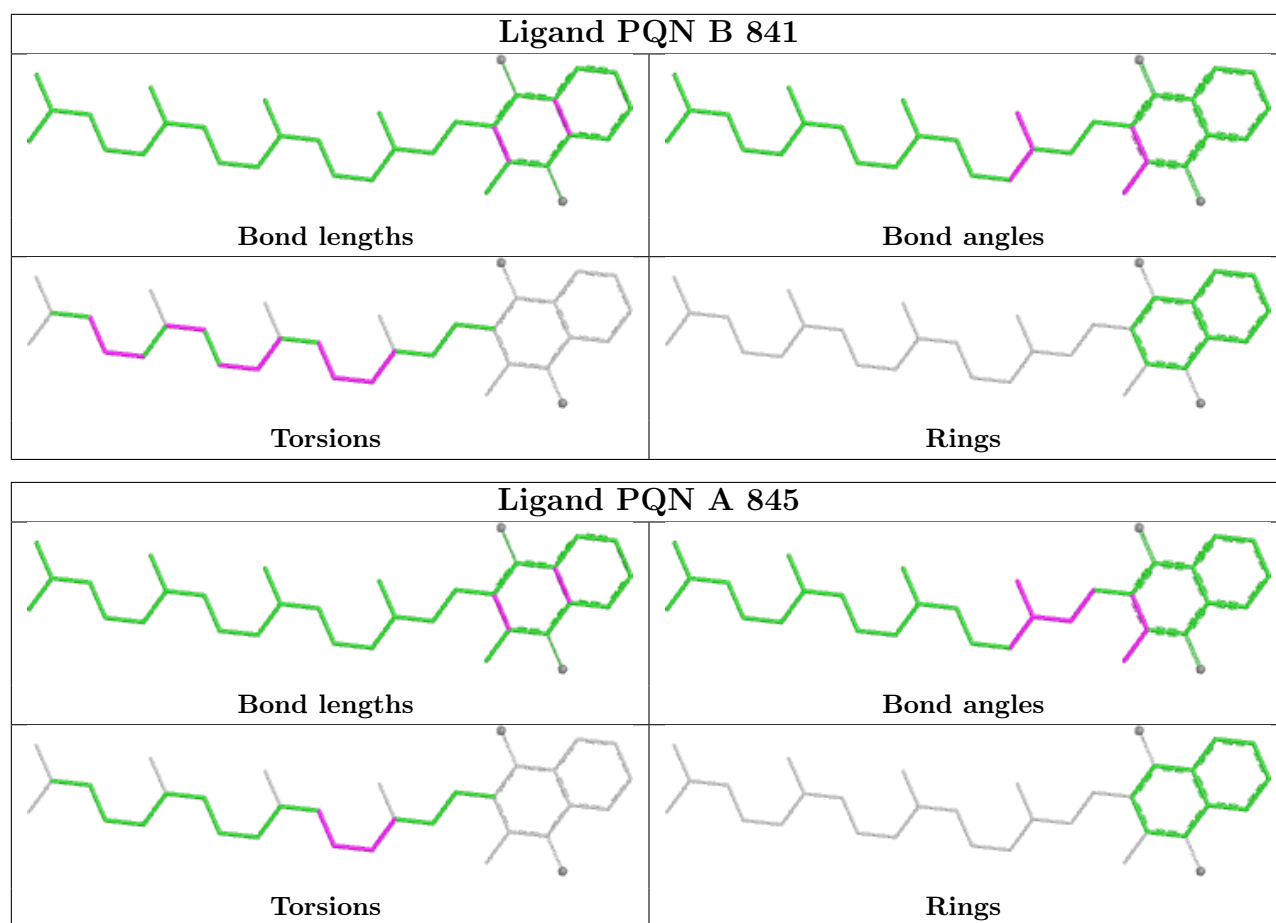


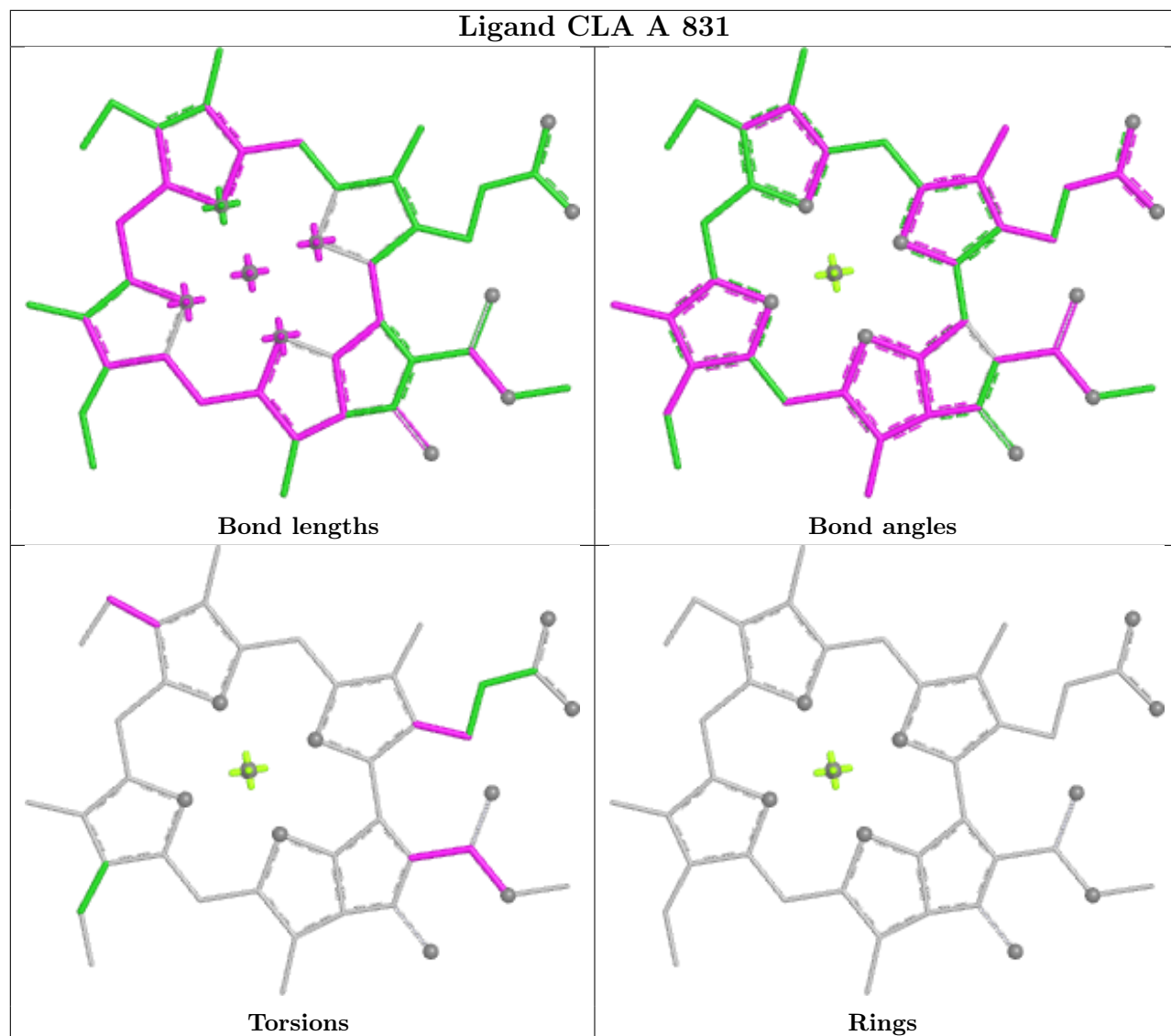
Ligand CLA B 815



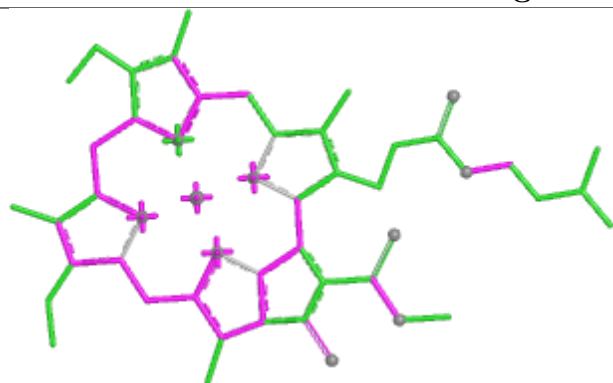
Ligand BCR B 844



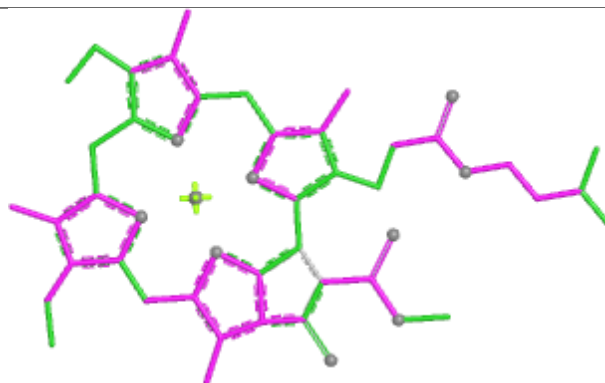




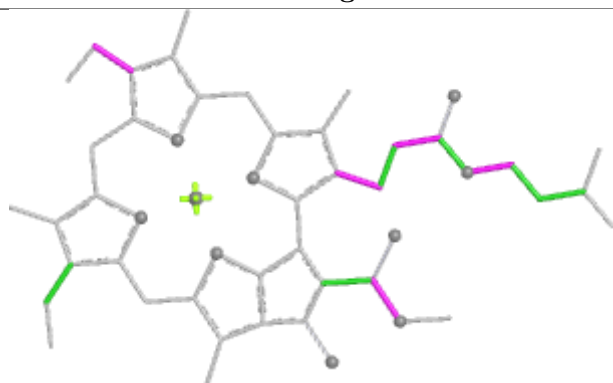
Ligand CLA A 842



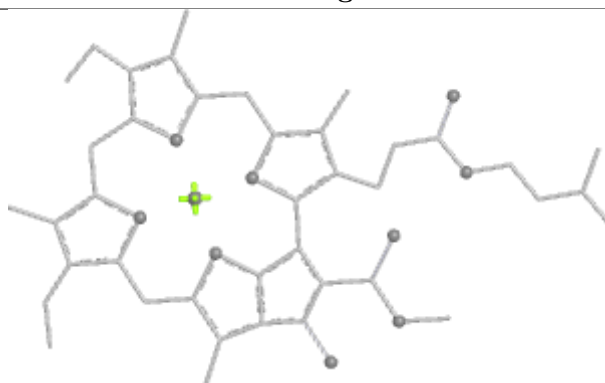
Bond lengths



Bond angles

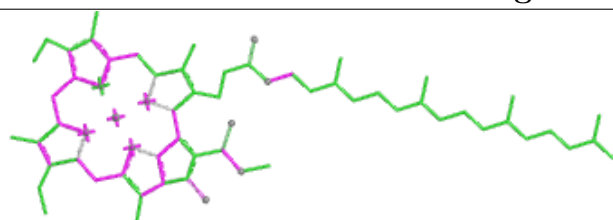


Torsions

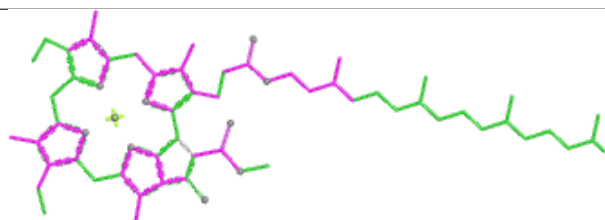


Rings

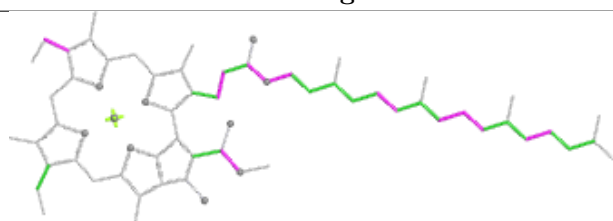
Ligand CLA B 804



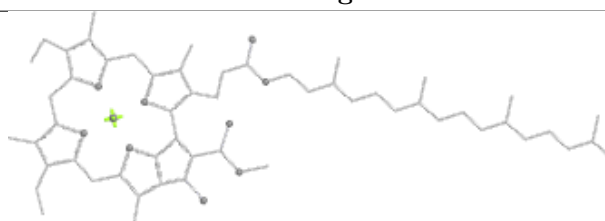
Bond lengths



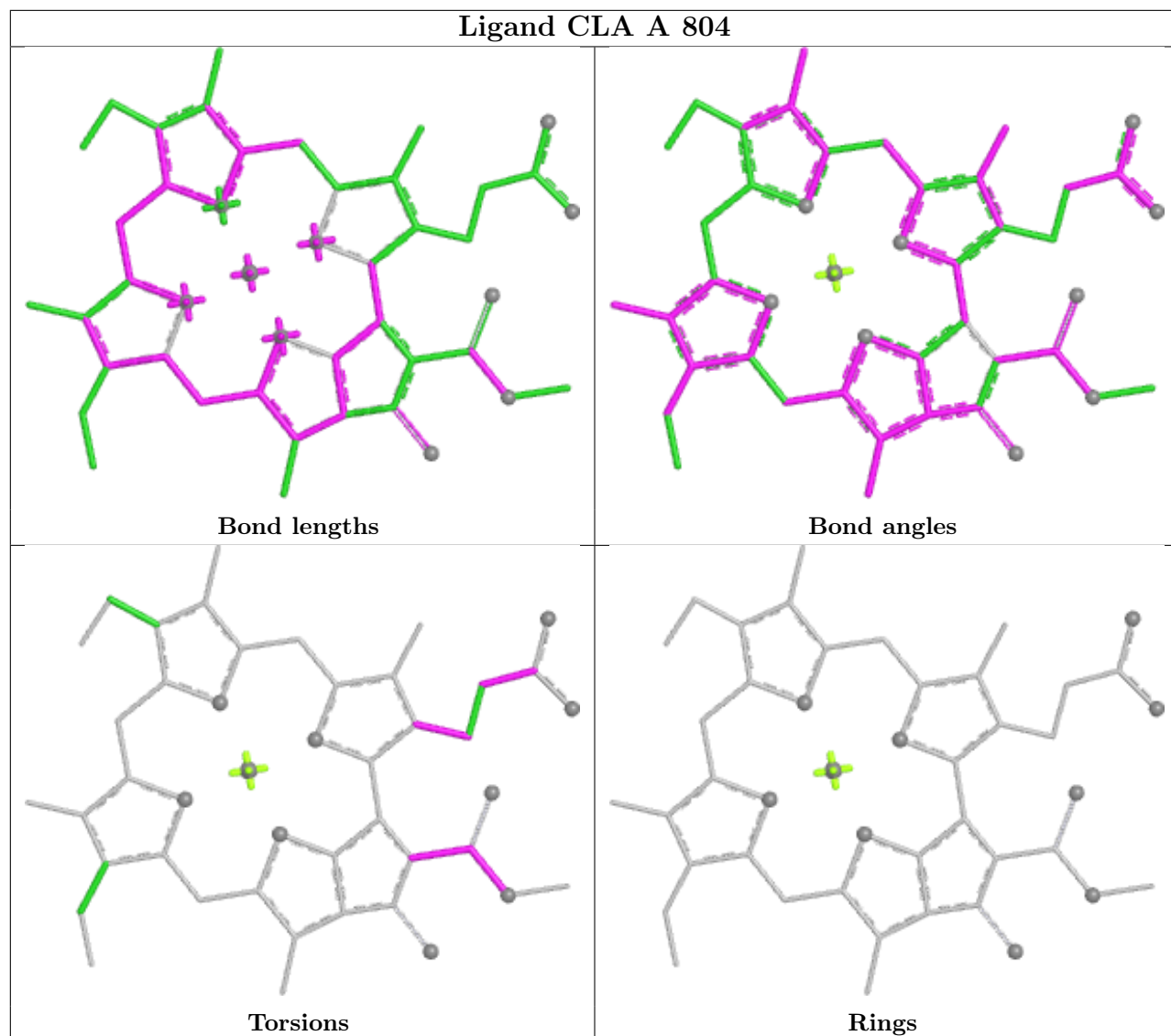
Bond angles



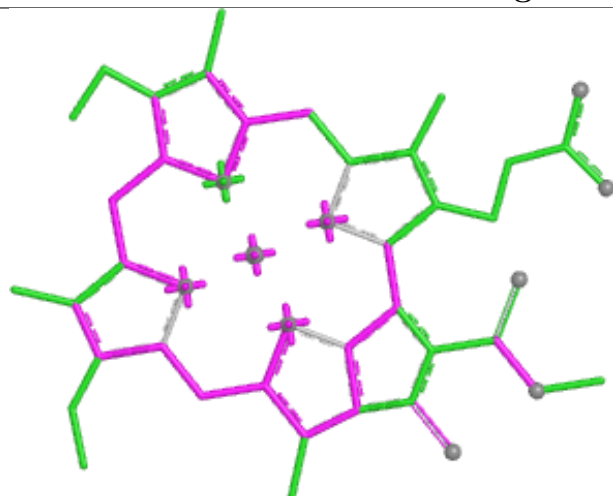
Torsions



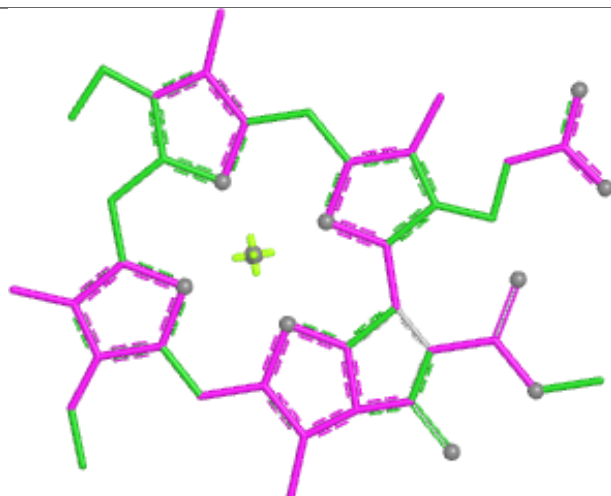
Rings



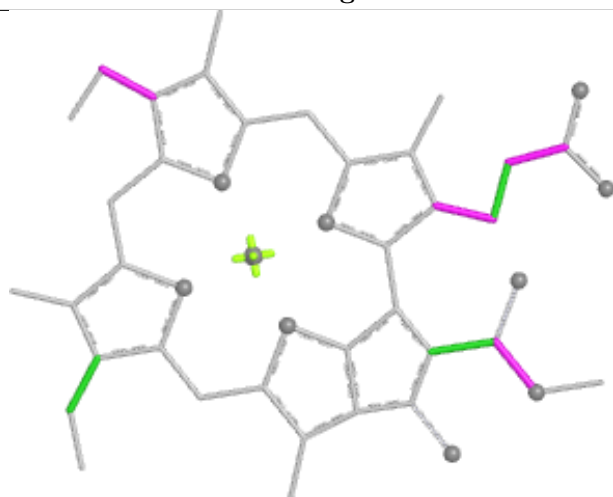
Ligand CLA B 822



Bond lengths



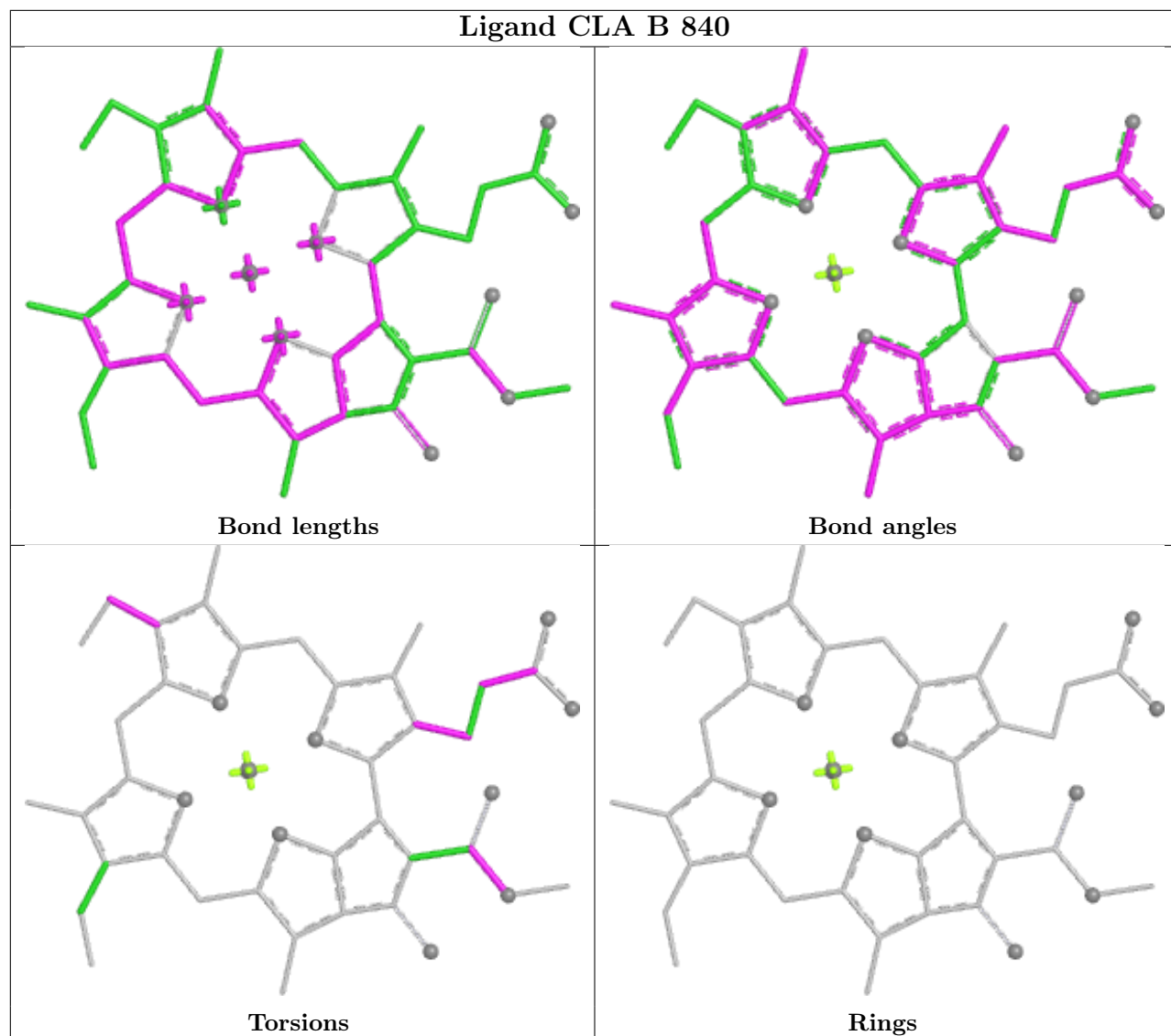
Bond angles

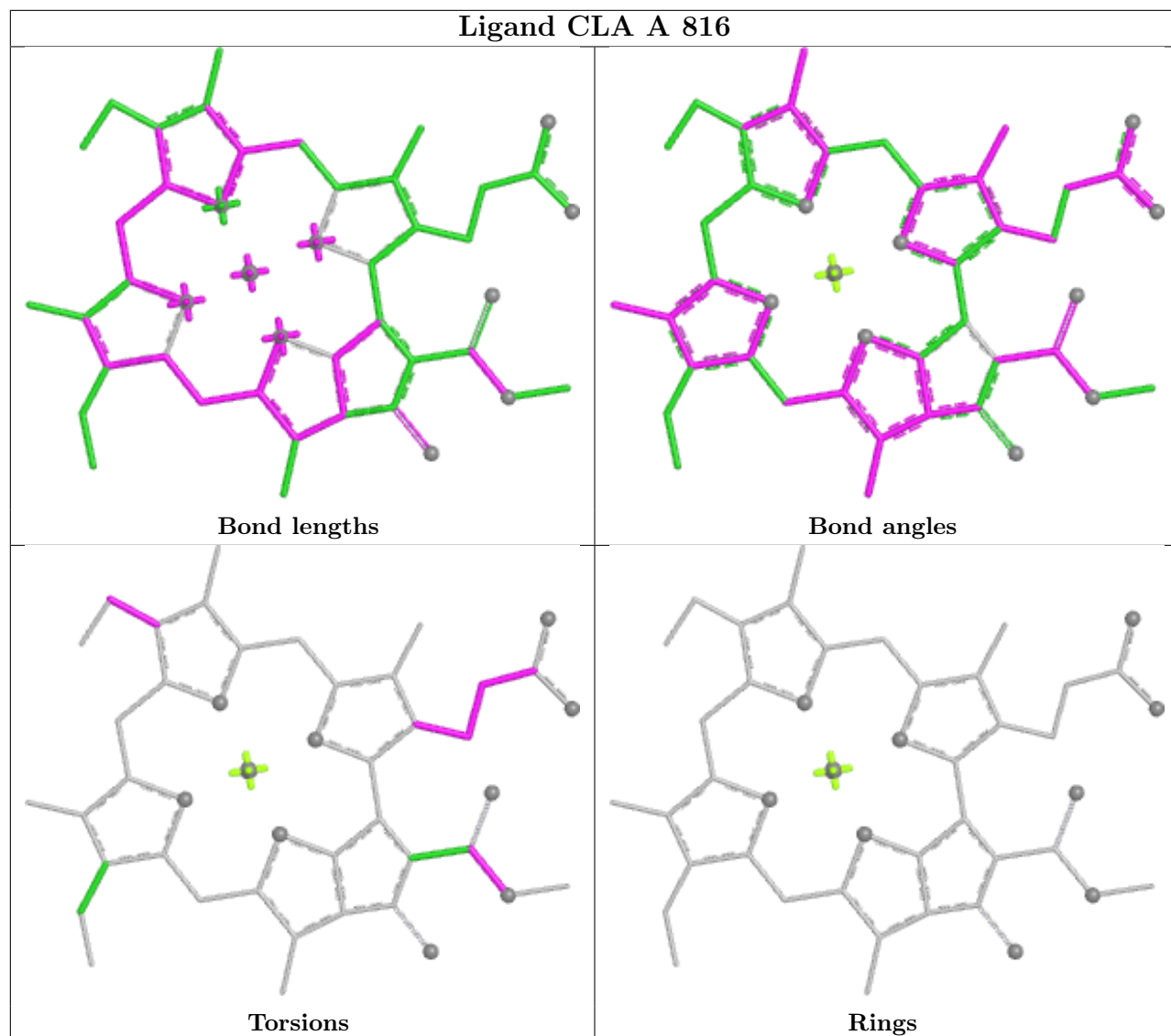


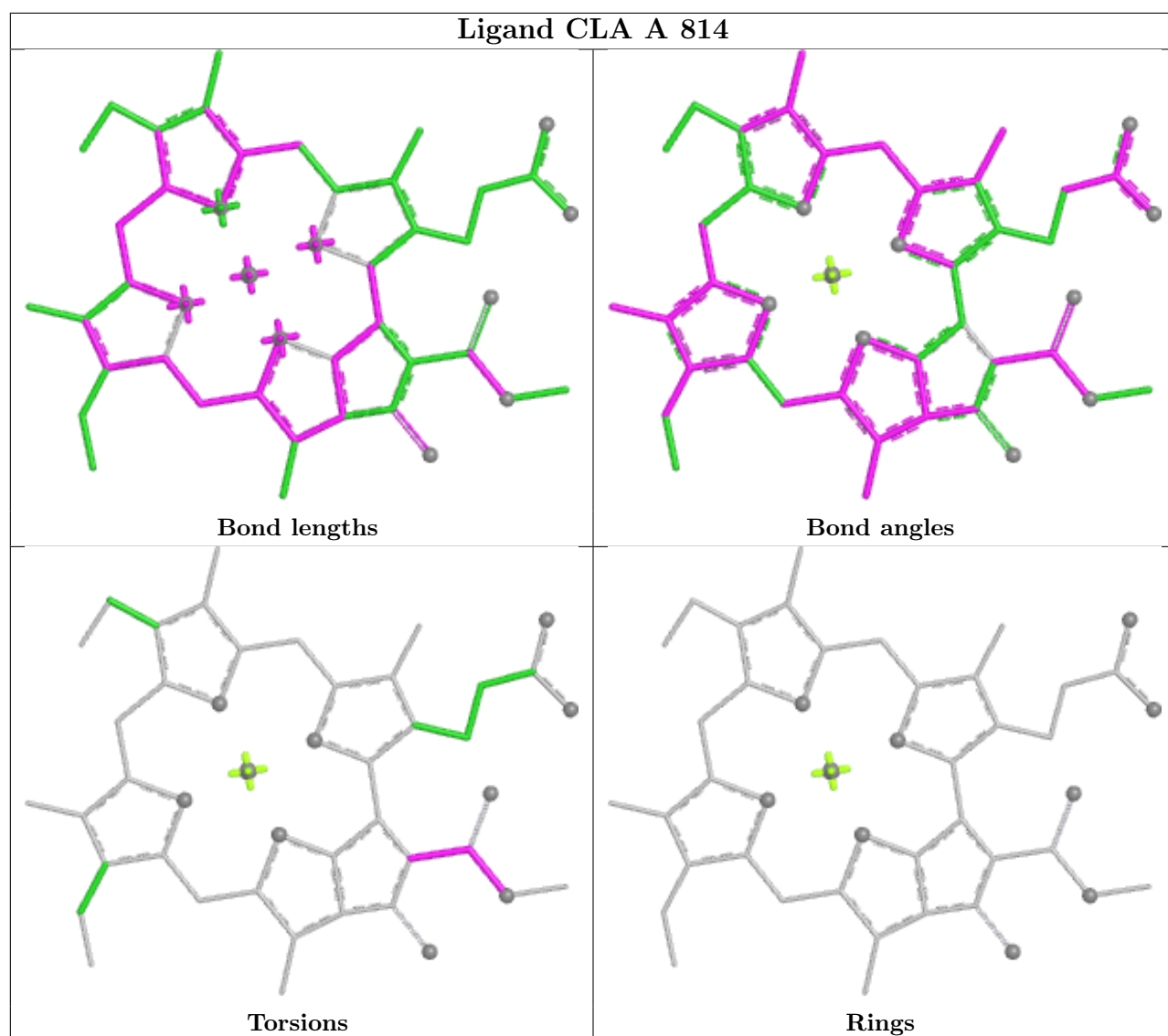
Torsions



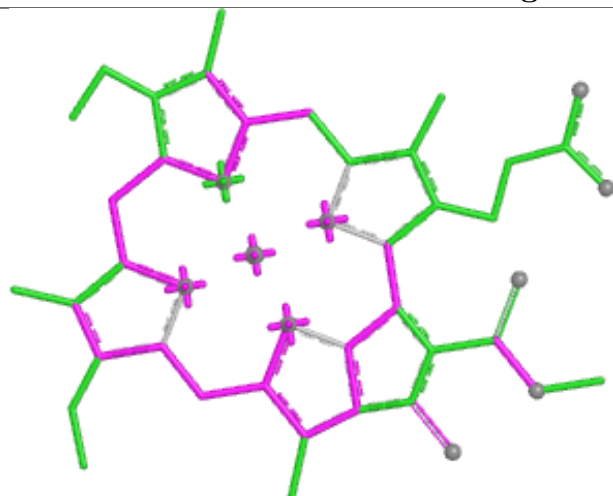
Rings



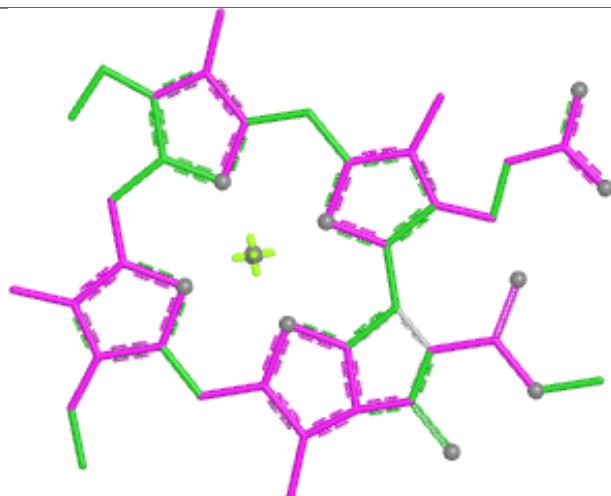




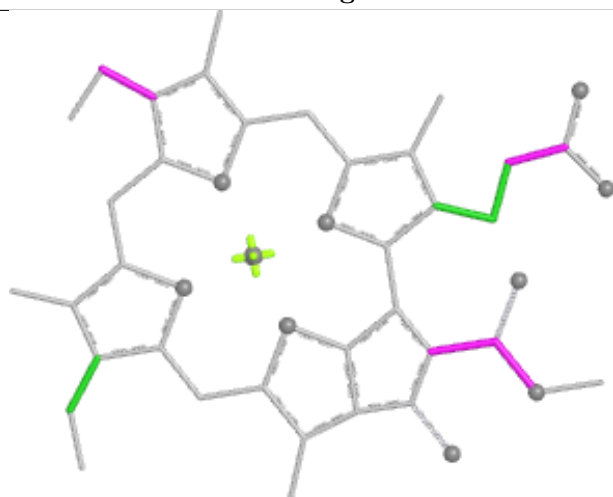
Ligand CLA I 101



Bond lengths



Bond angles

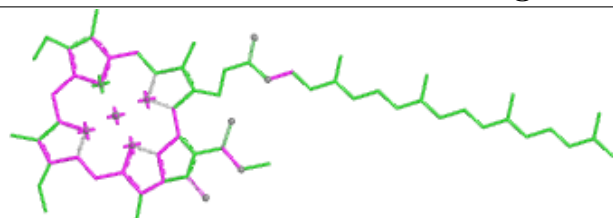


Torsions

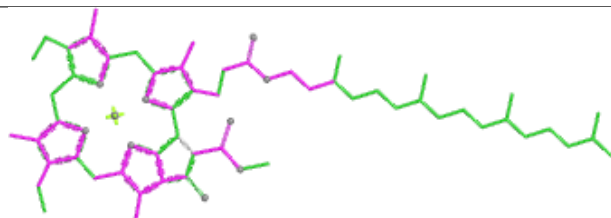


Rings

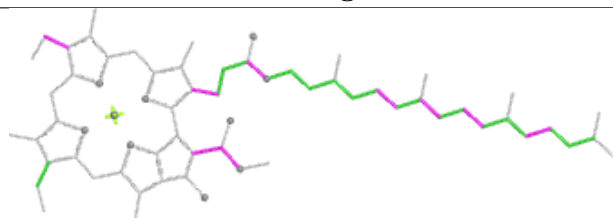
Ligand CLA A 830



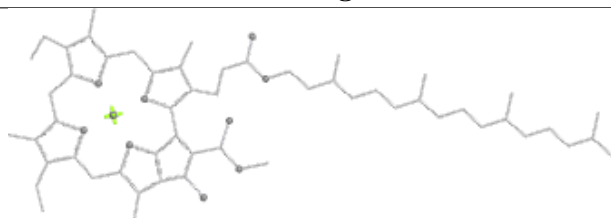
Bond lengths



Bond angles

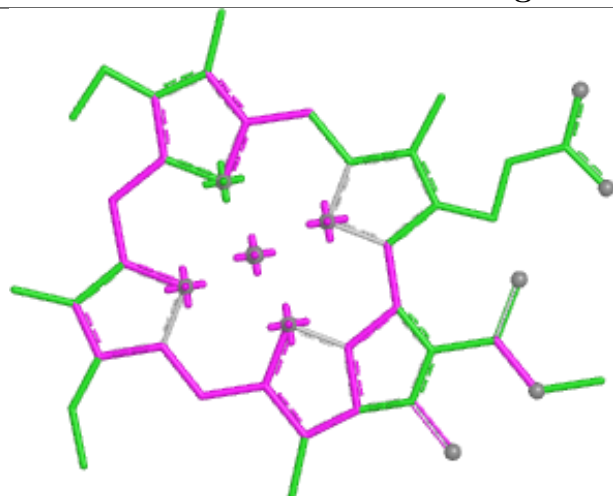


Torsions

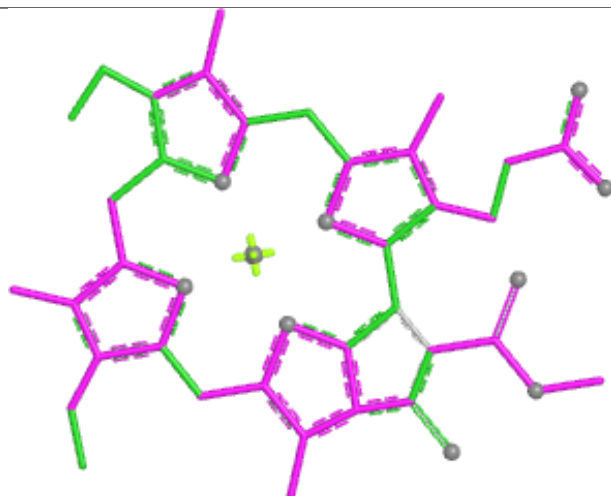


Rings

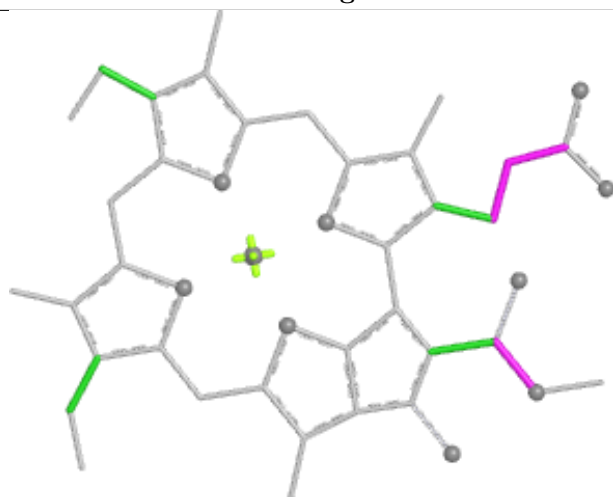
Ligand CLA B 812



Bond lengths



Bond angles

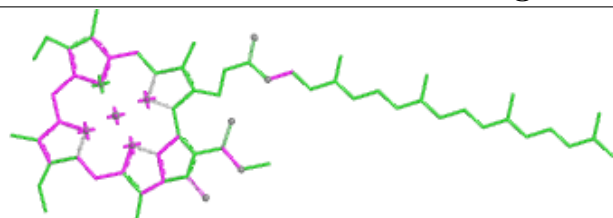


Torsions

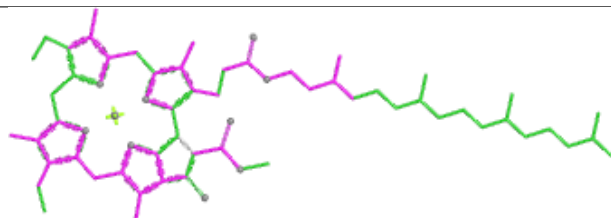


Rings

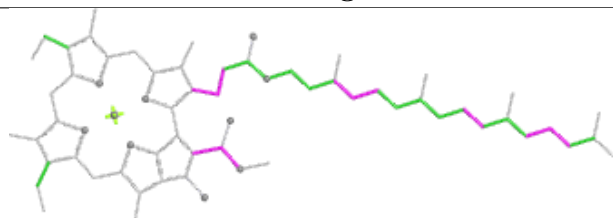
Ligand CLA A 827



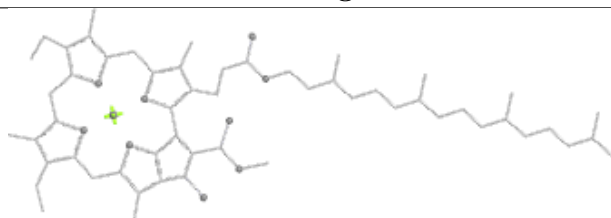
Bond lengths



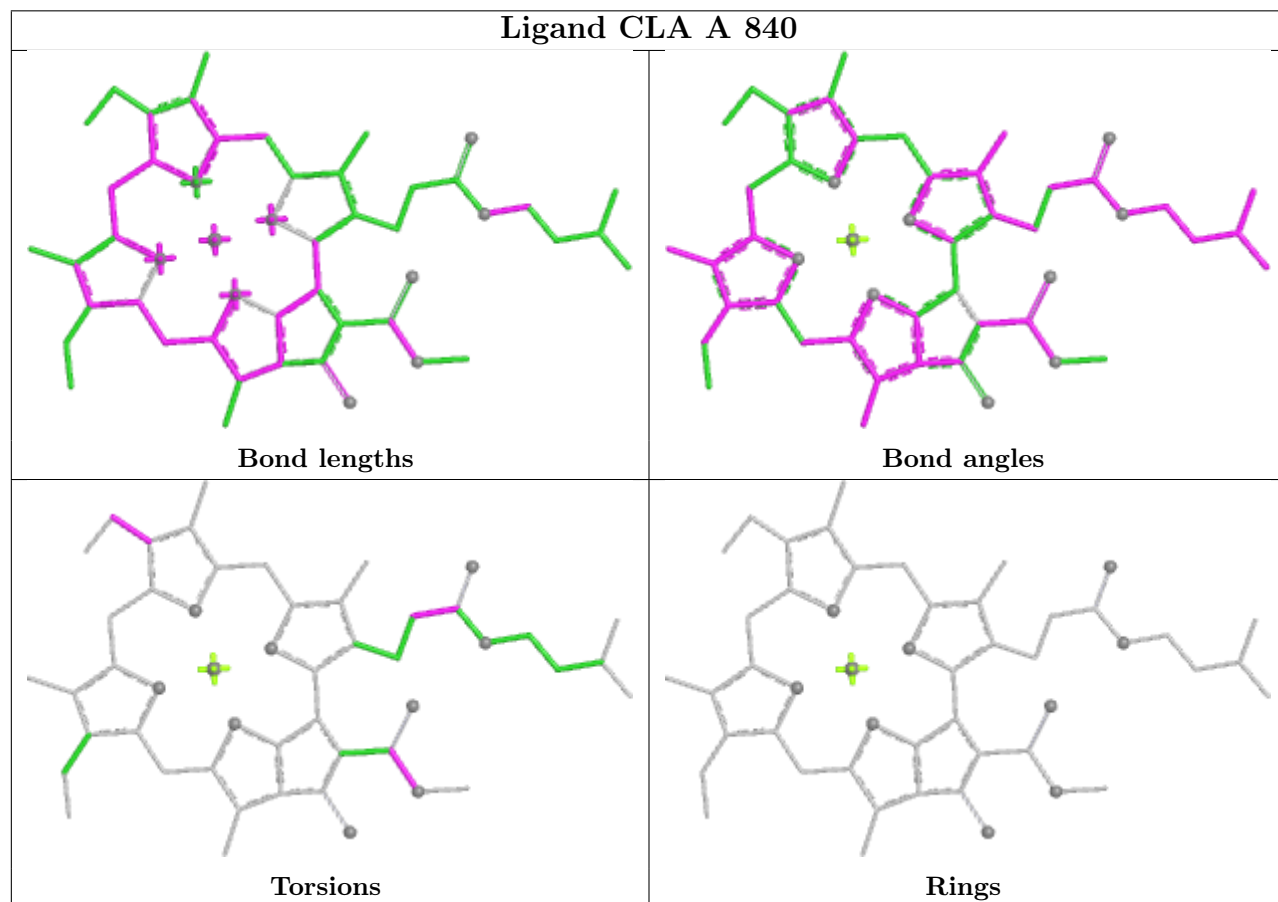
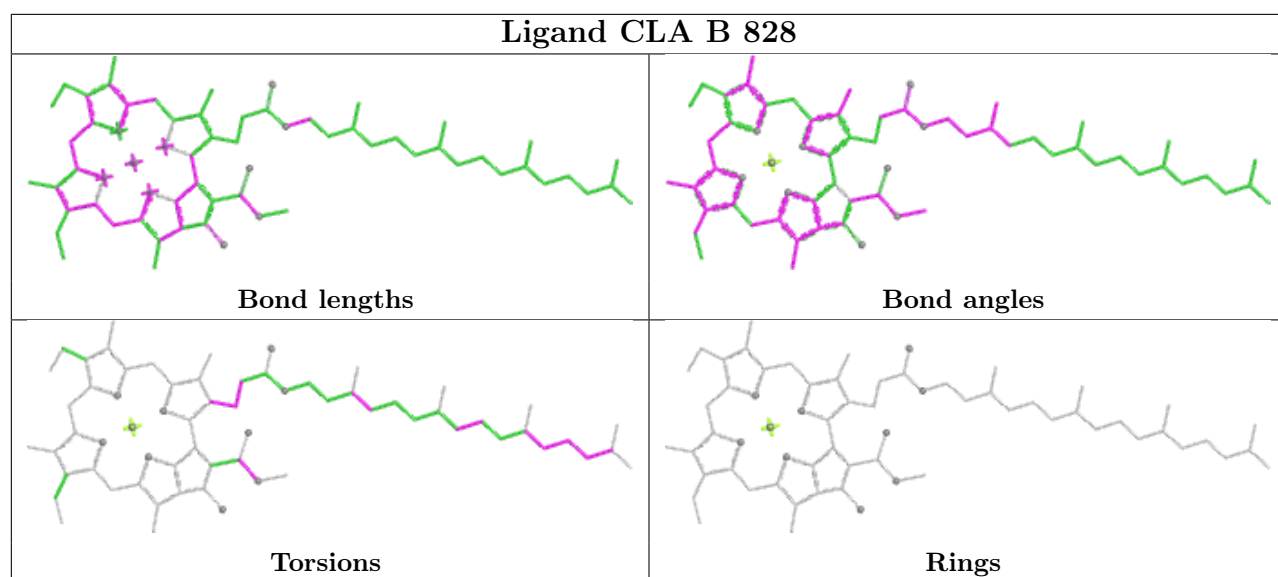
Bond angles



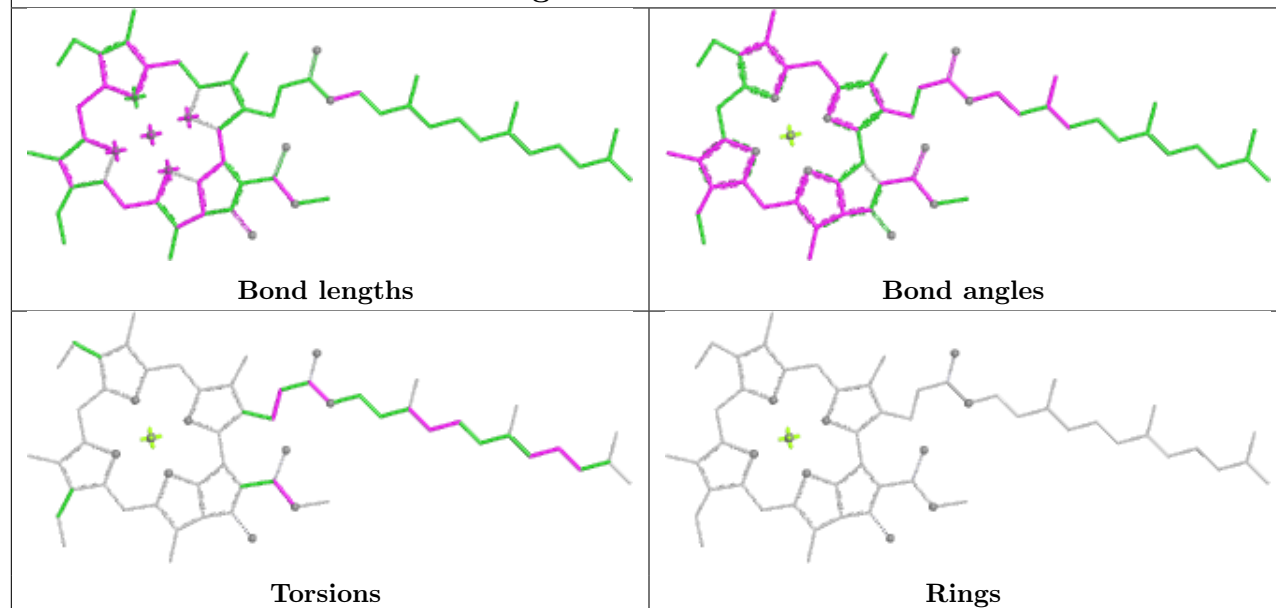
Torsions



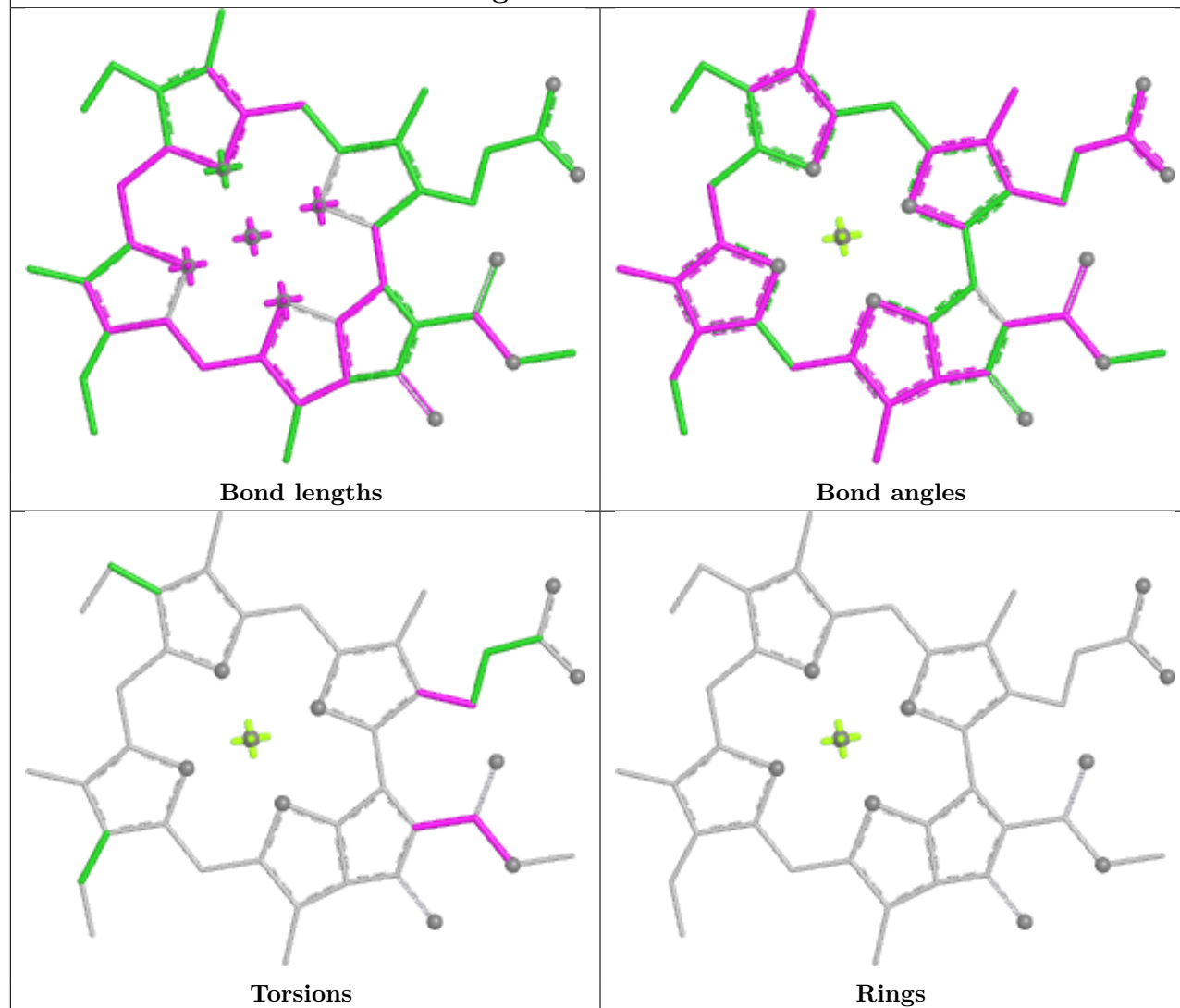
Rings

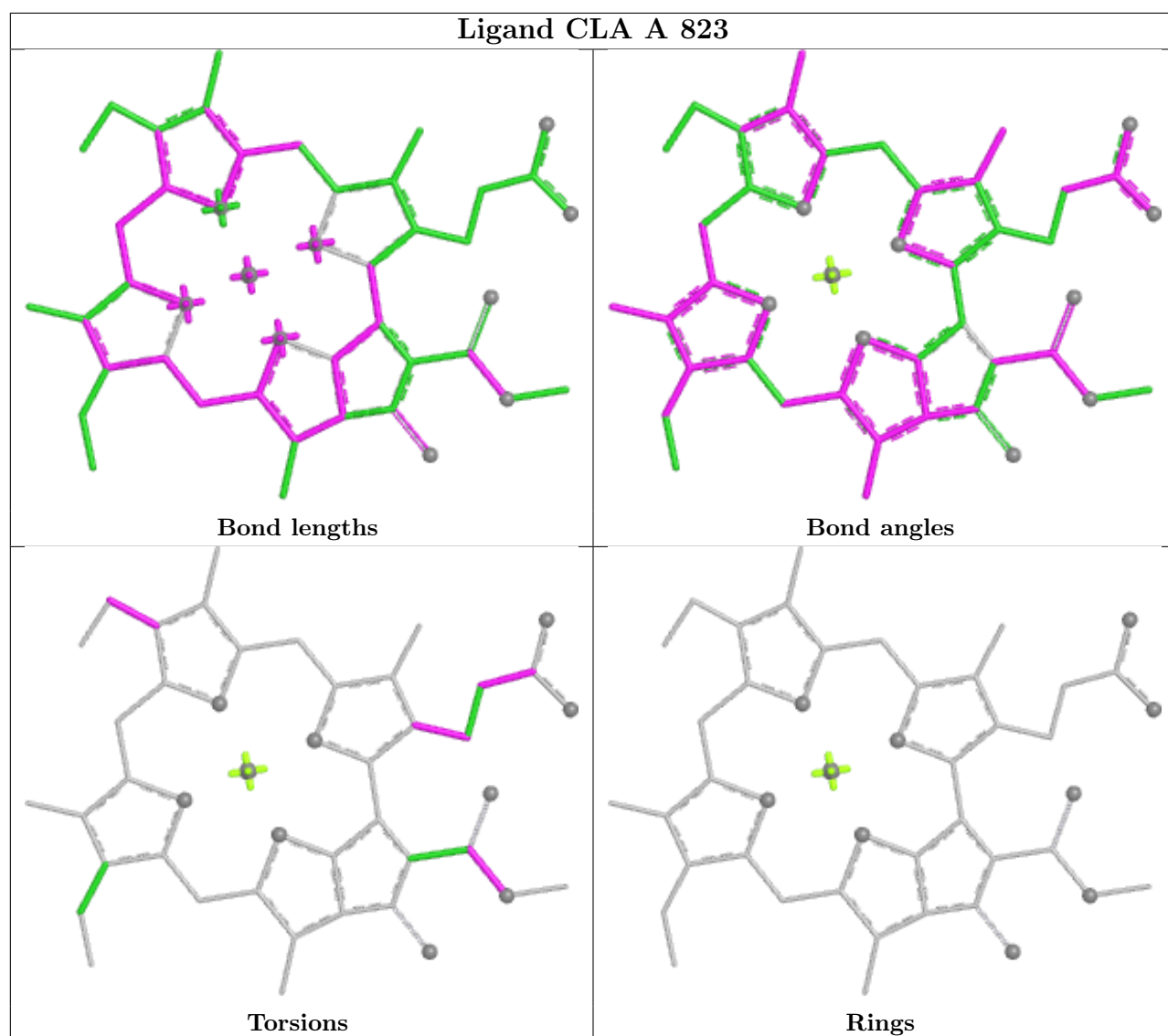


Ligand CLA B 801

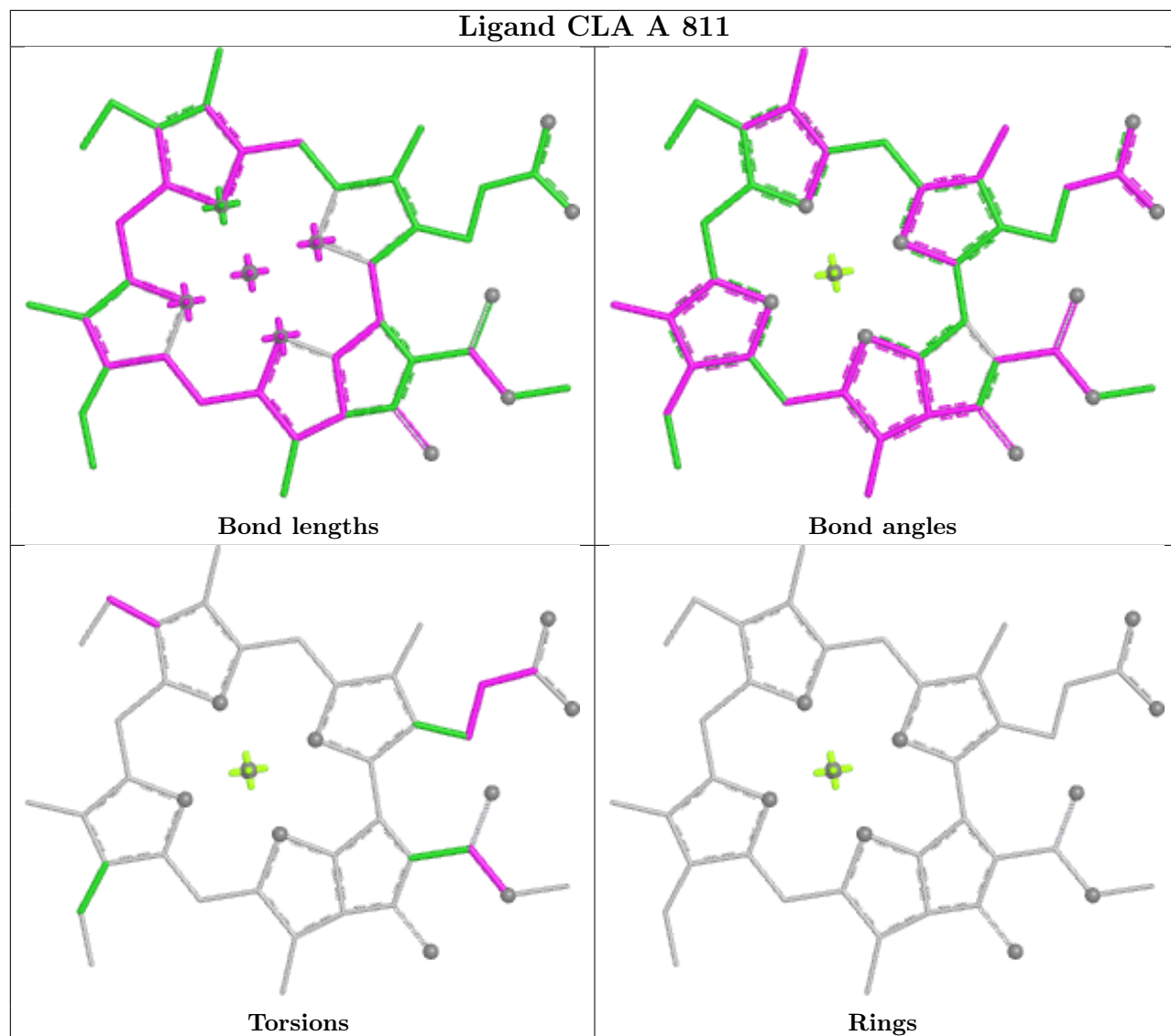


Ligand CLA B 829

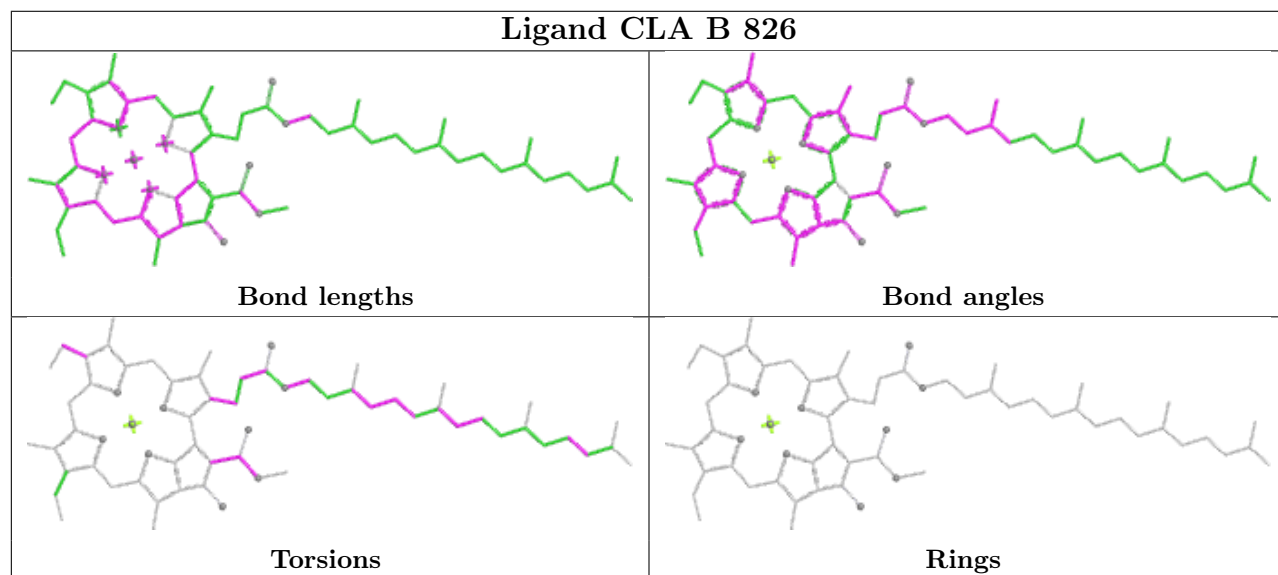


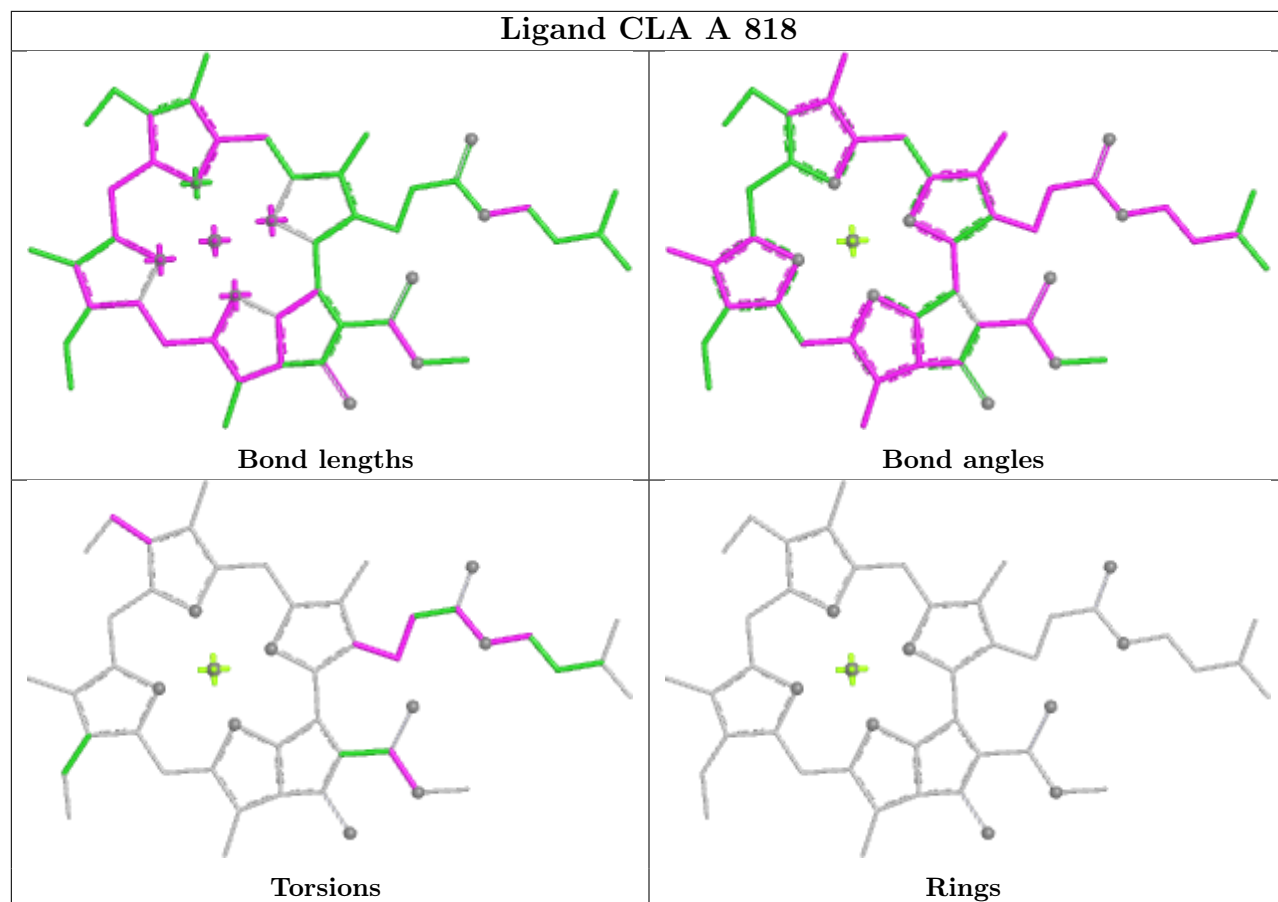


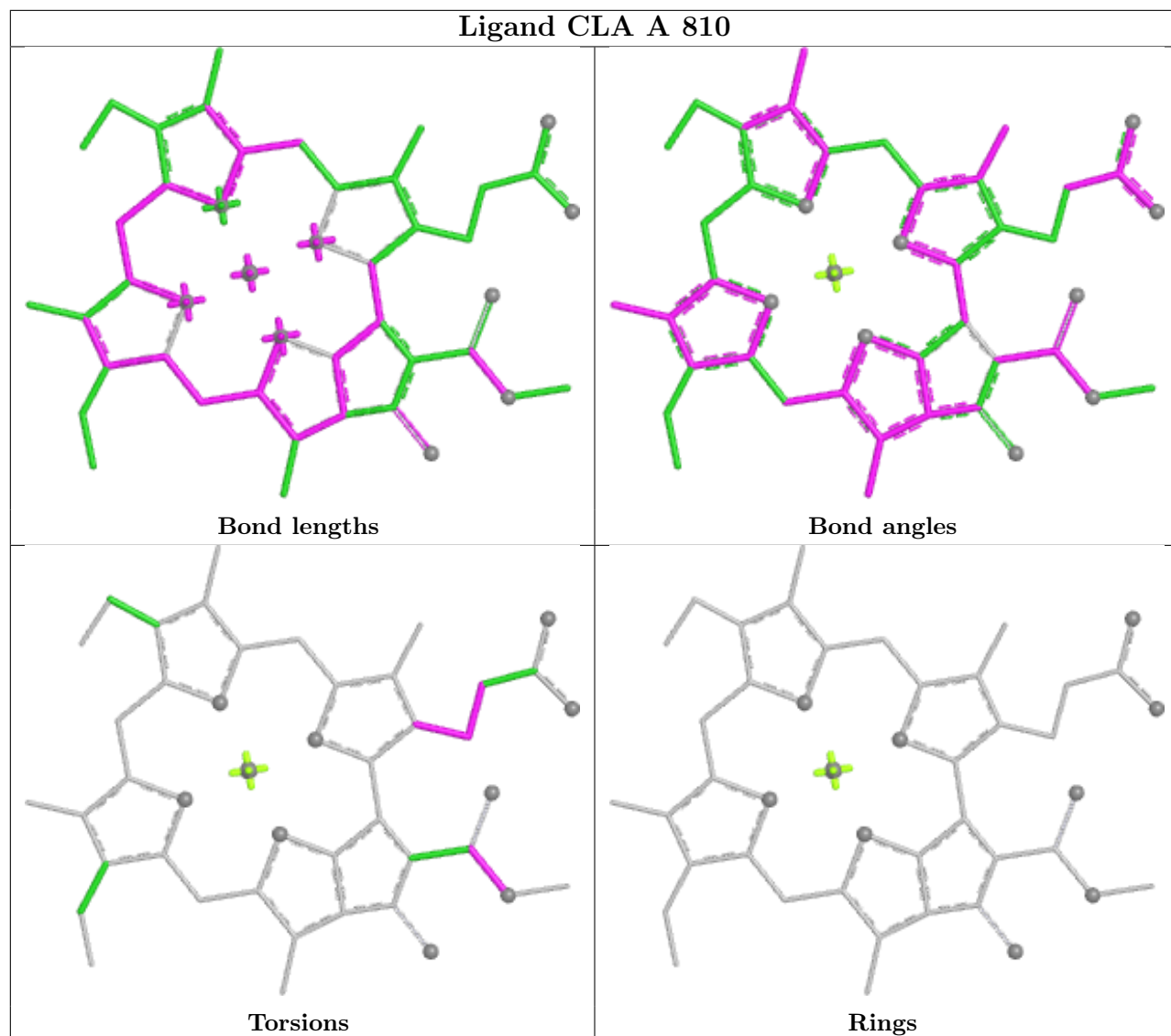
Ligand CLA A 811

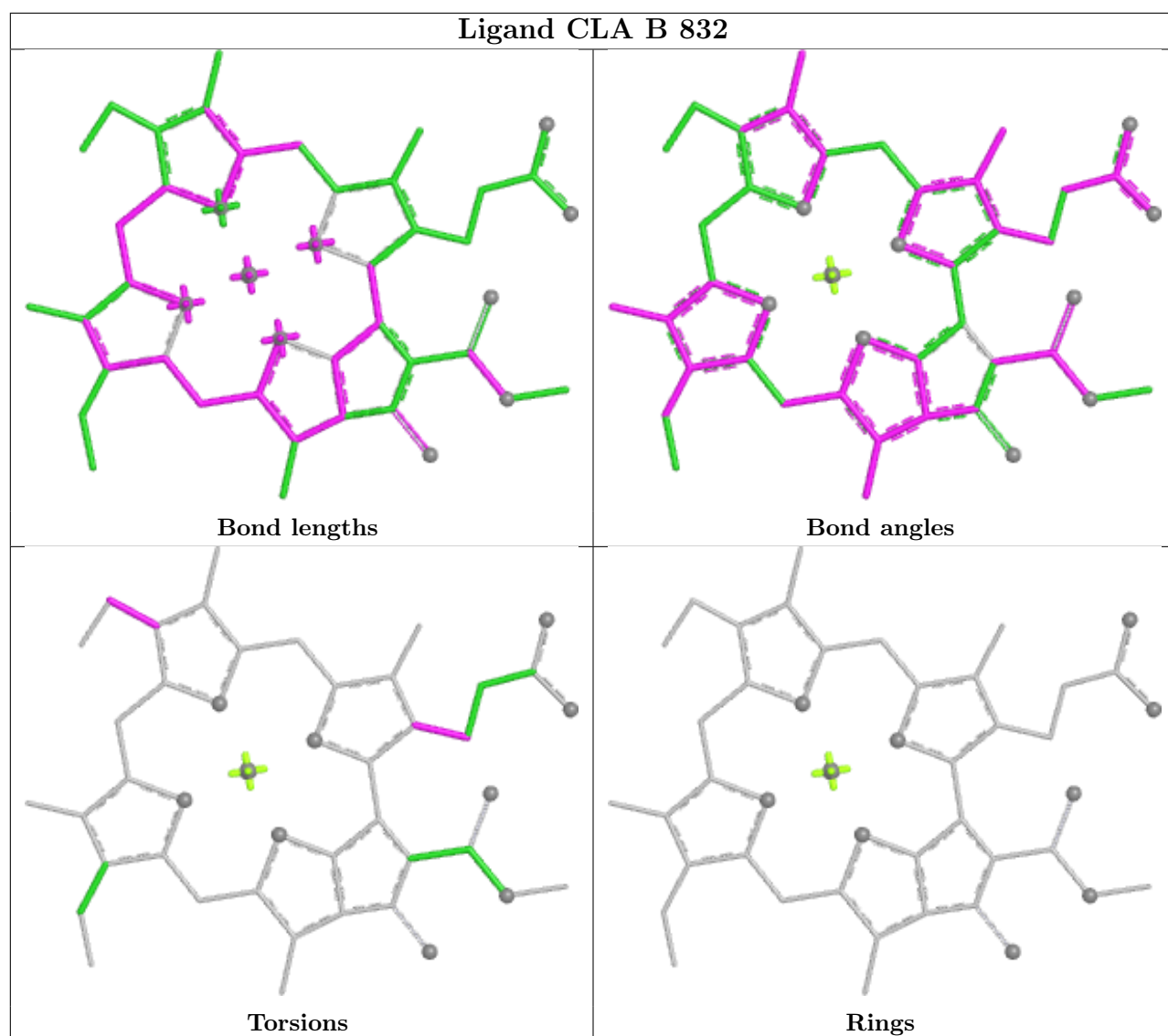


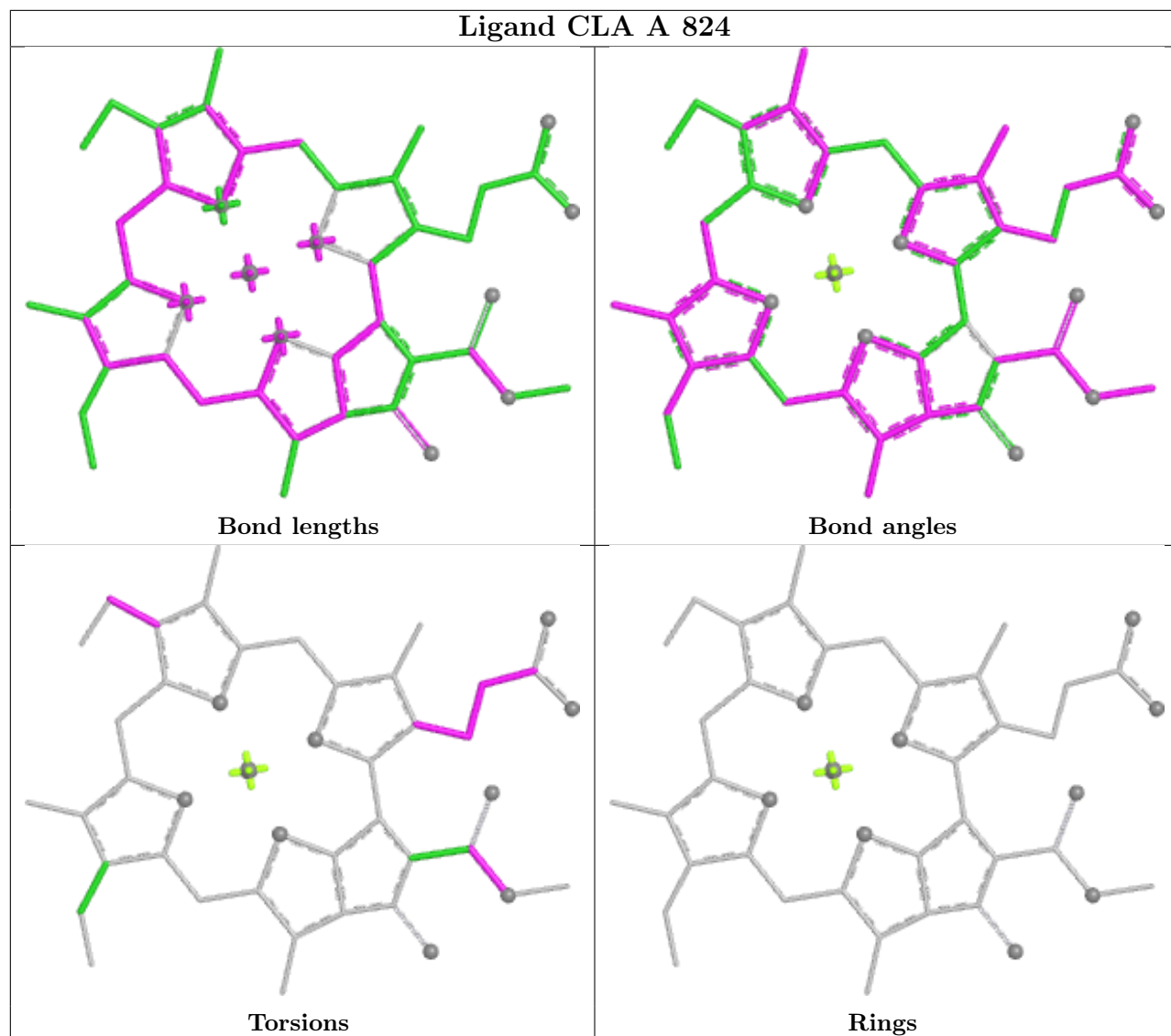
Ligand CLA B 826



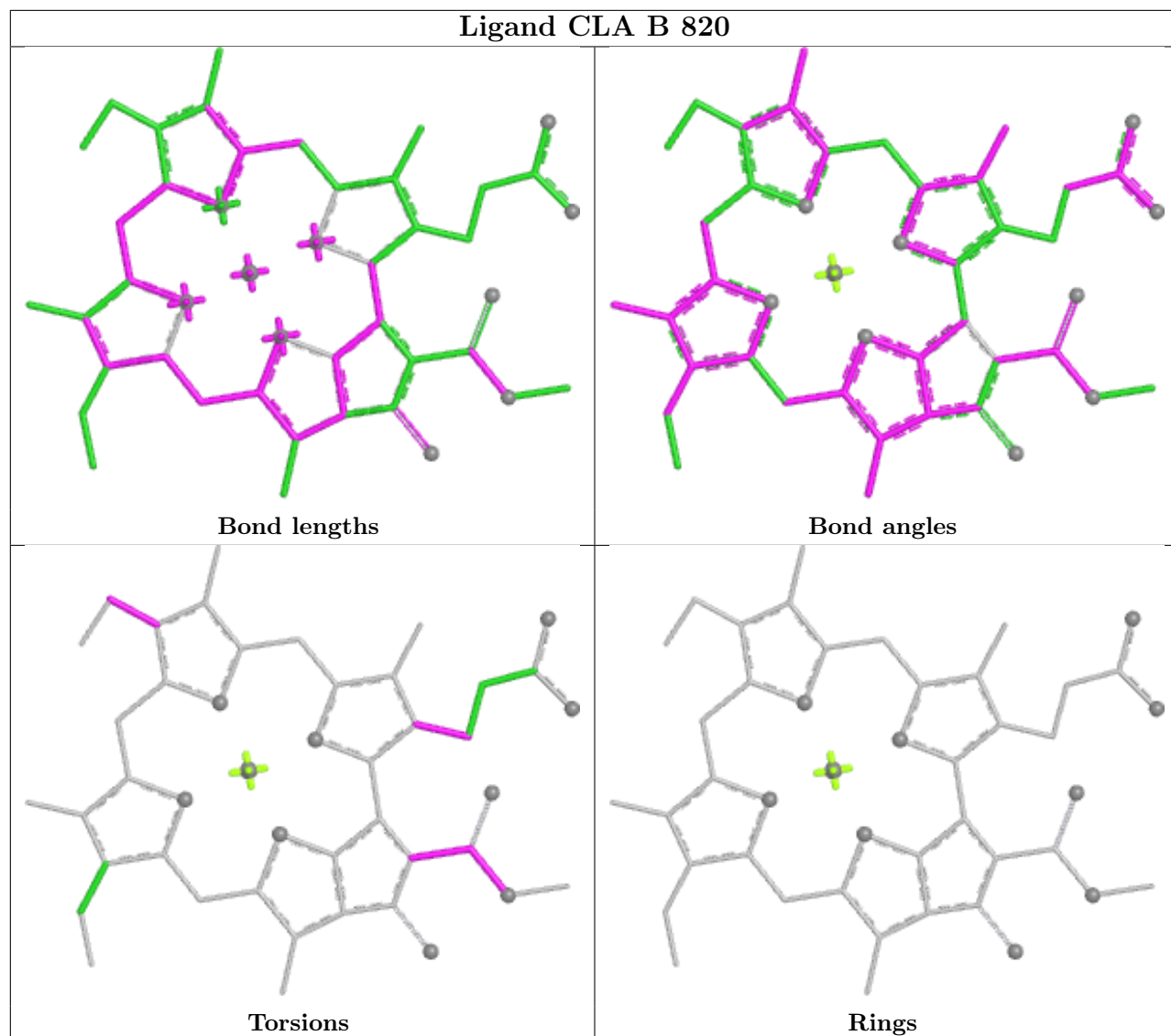




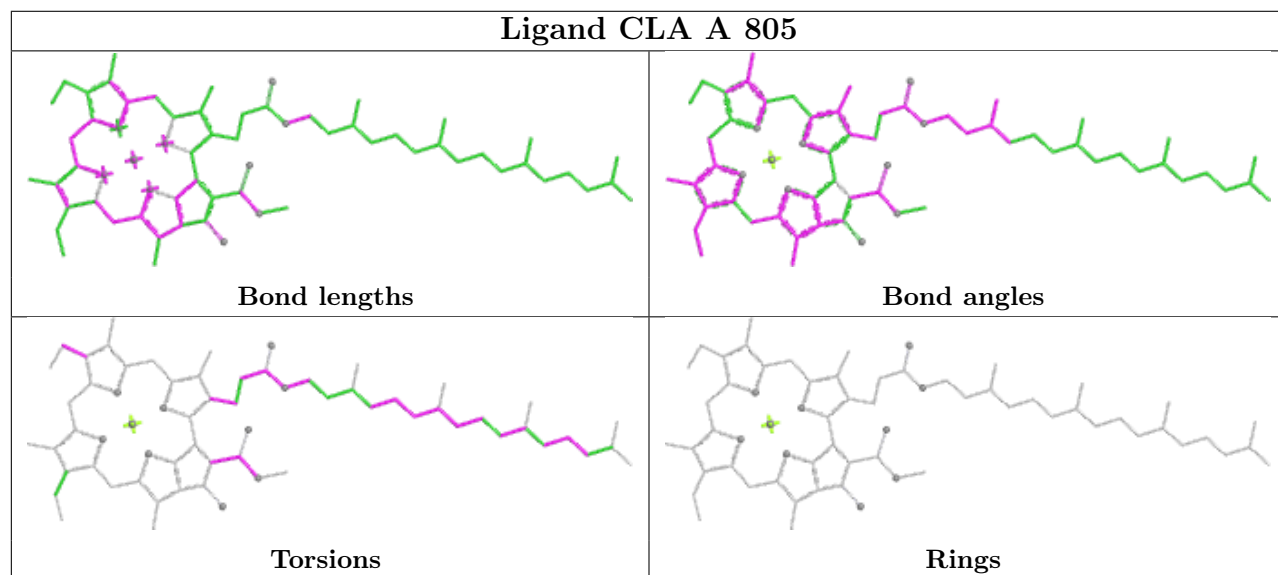


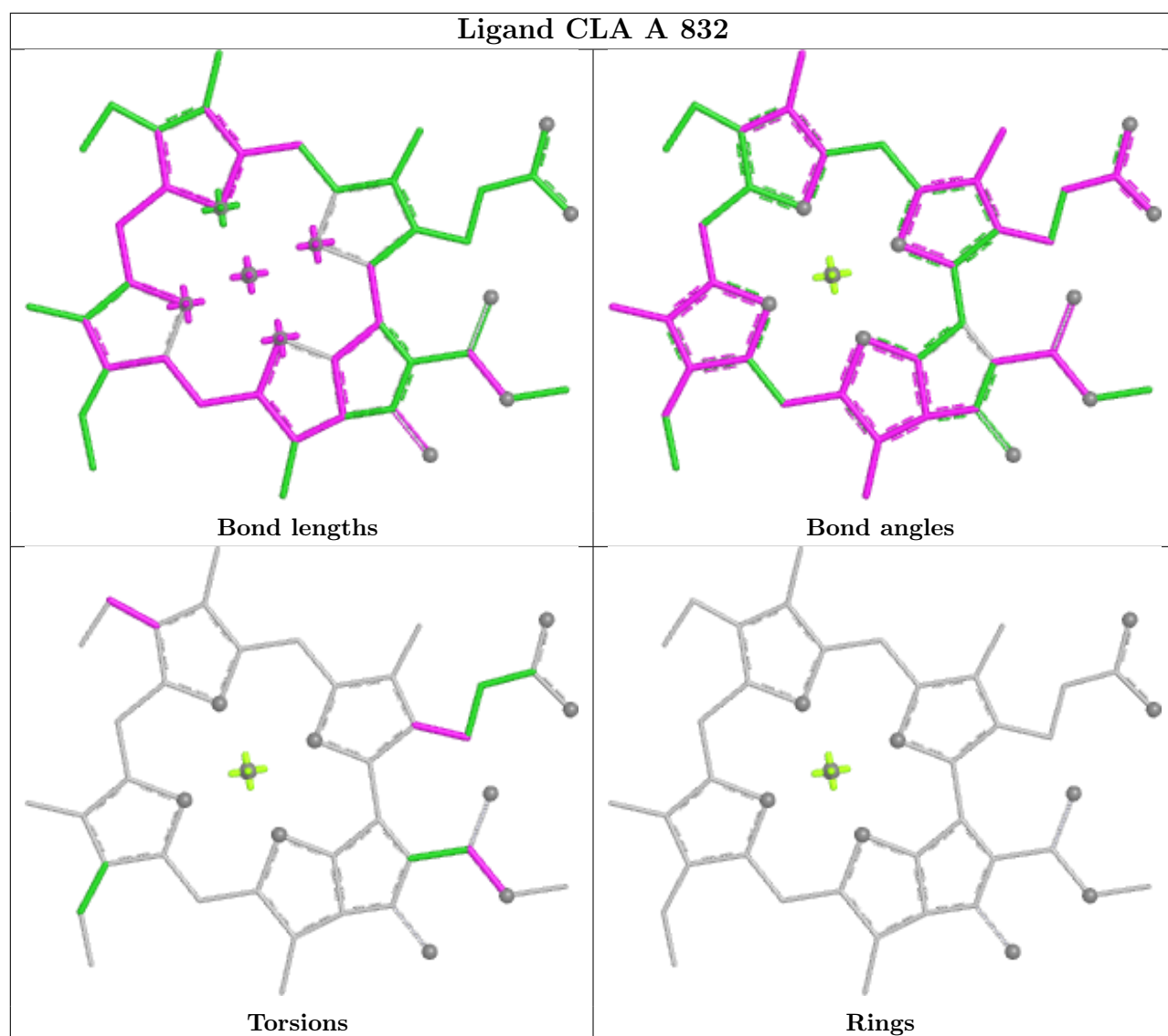


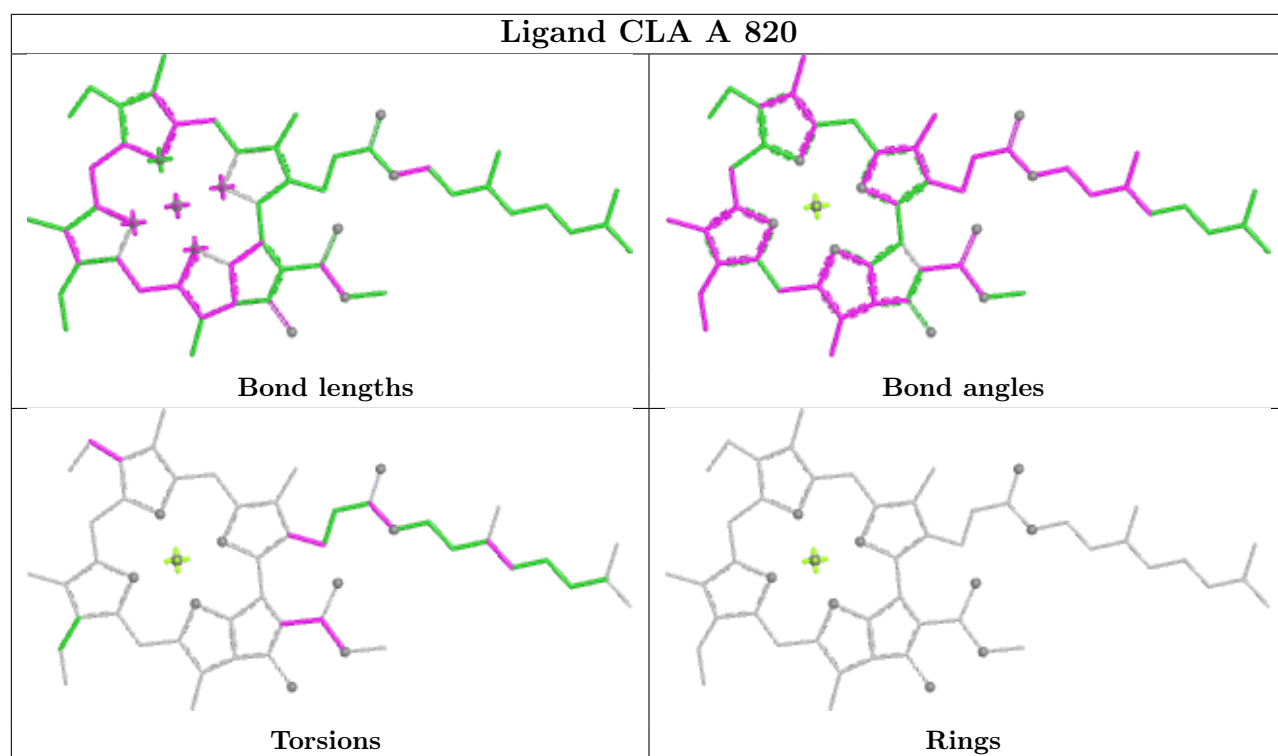
Ligand CLA B 820

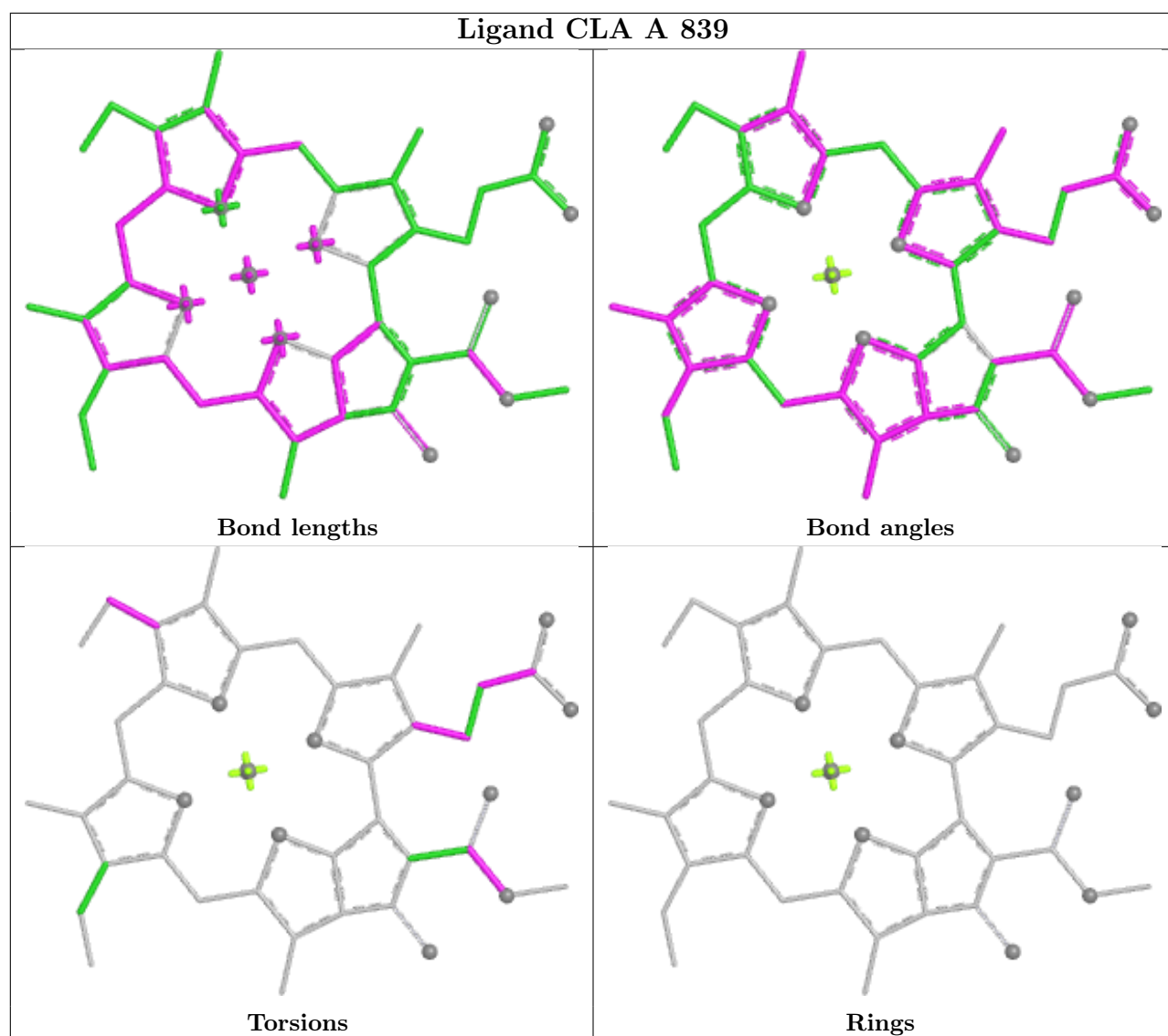


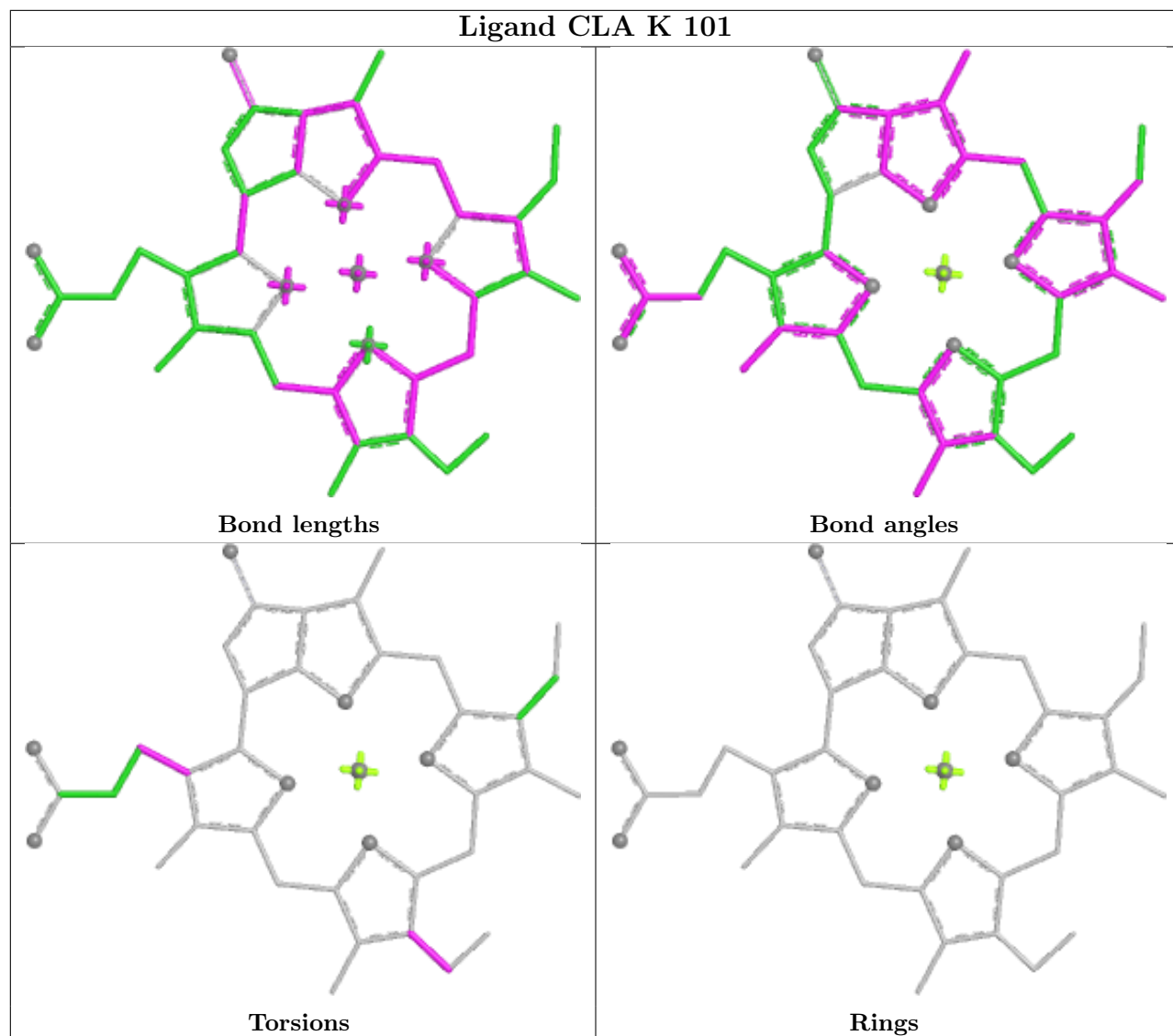
Ligand CLA A 805

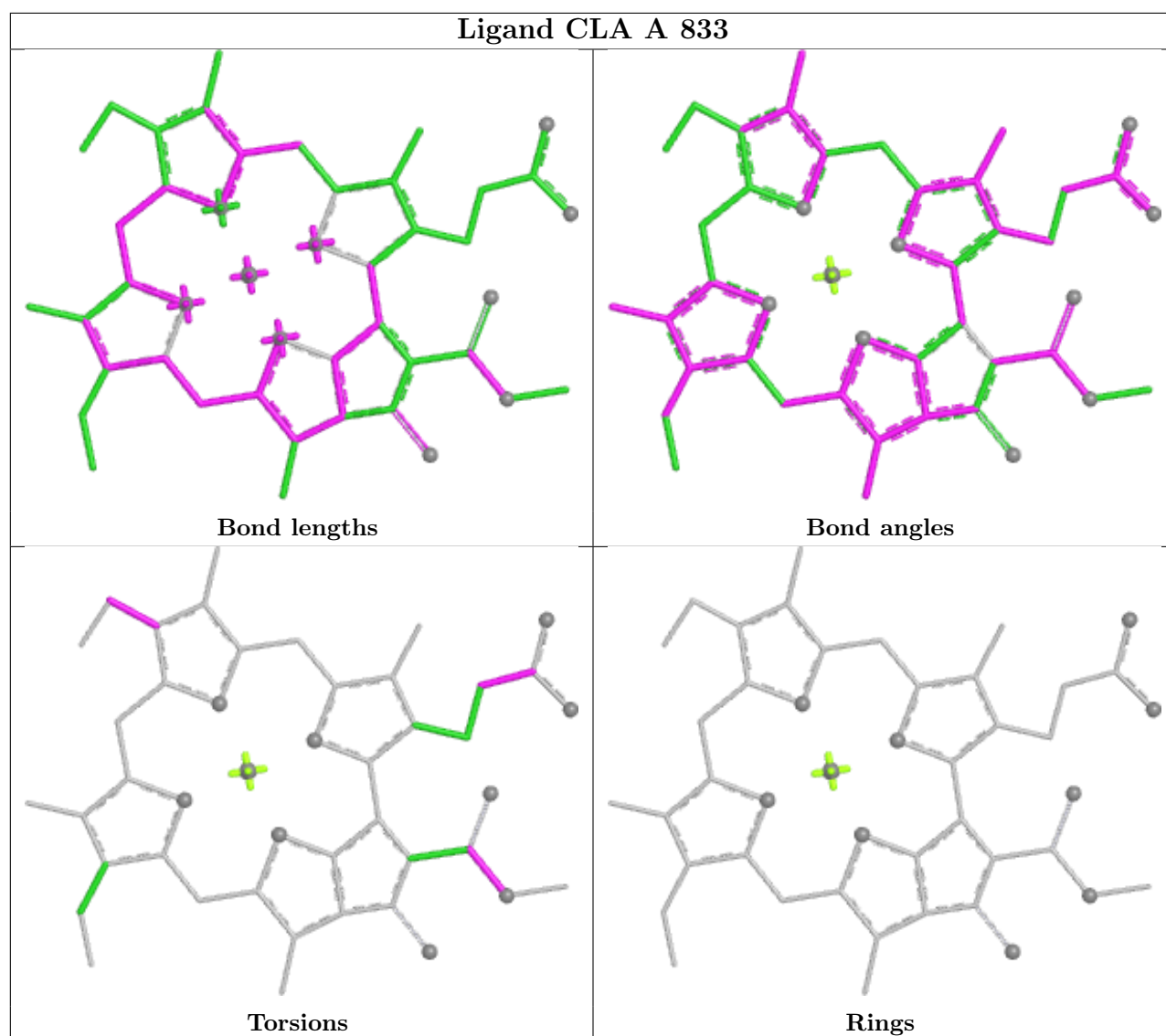












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

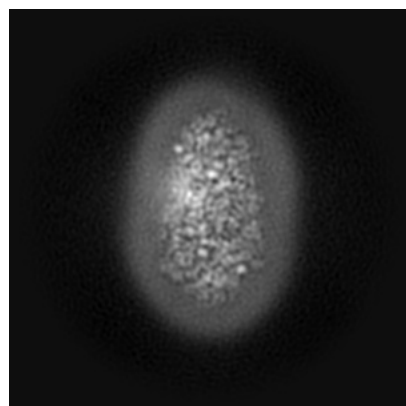
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-75232. These allow visual inspection of the internal detail of the map and identification of artifacts.

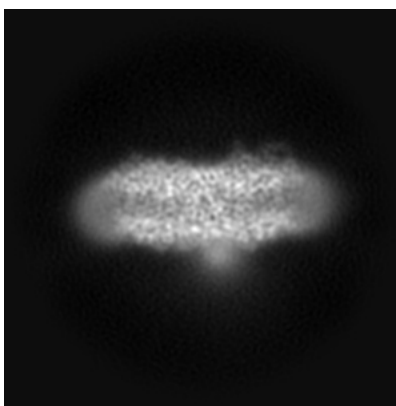
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

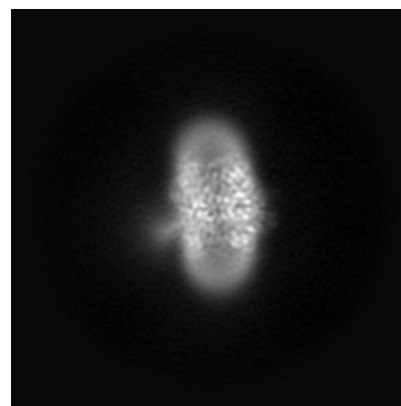
6.1.1 Primary map



X

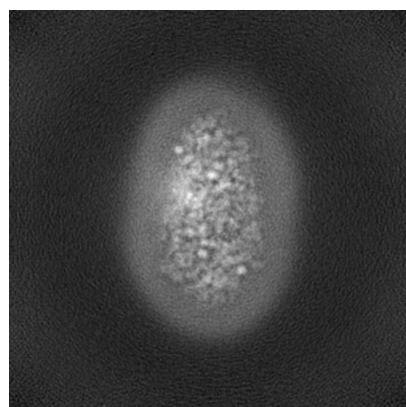


Y

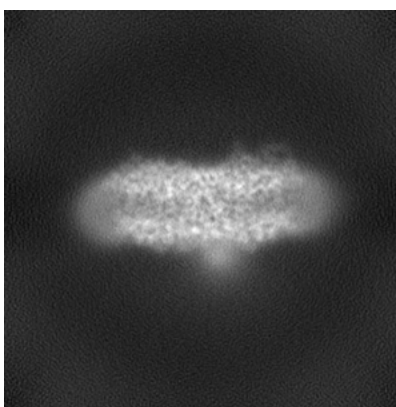


Z

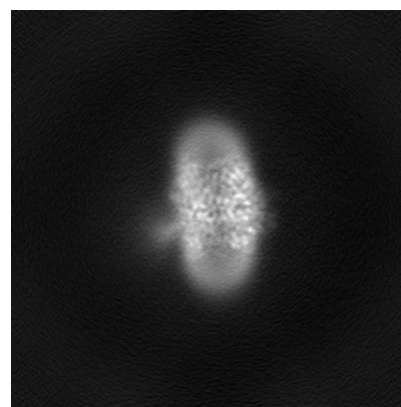
6.1.2 Raw map



X



Y

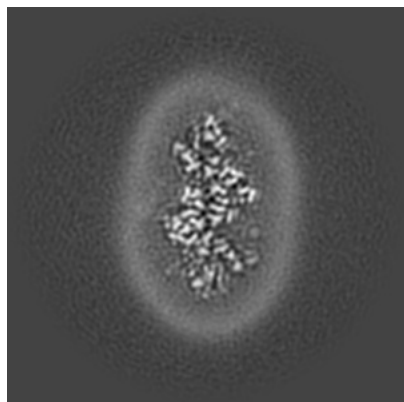


Z

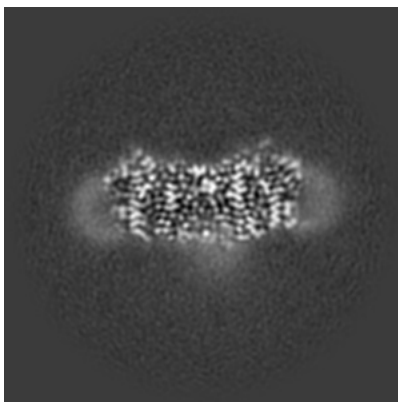
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

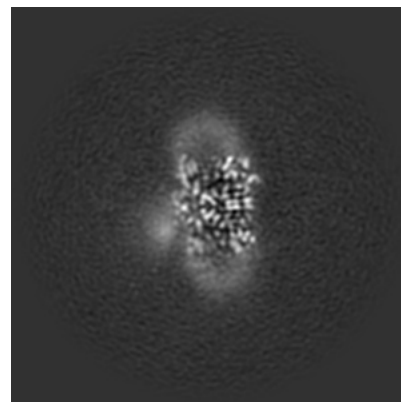
6.2.1 Primary map



X Index: 128

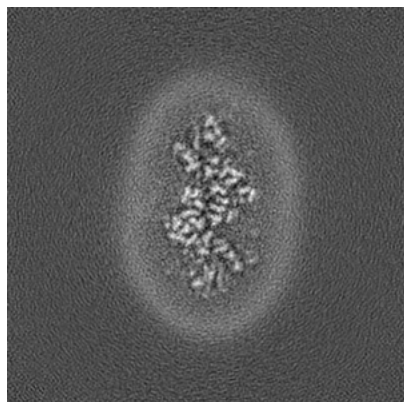


Y Index: 128

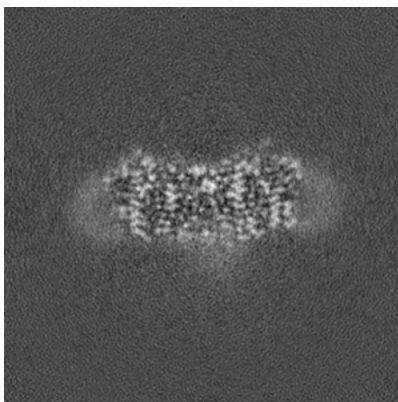


Z Index: 128

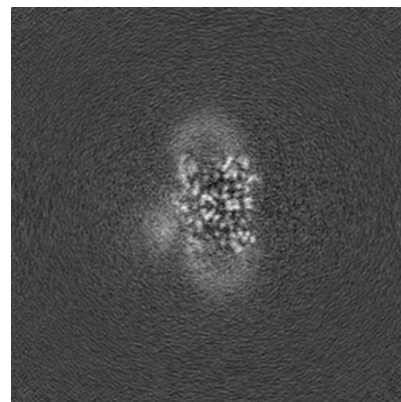
6.2.2 Raw map



X Index: 128



Y Index: 128

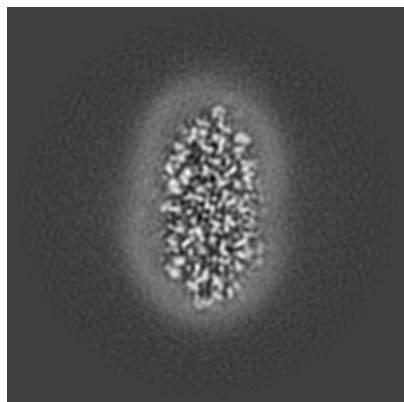


Z Index: 128

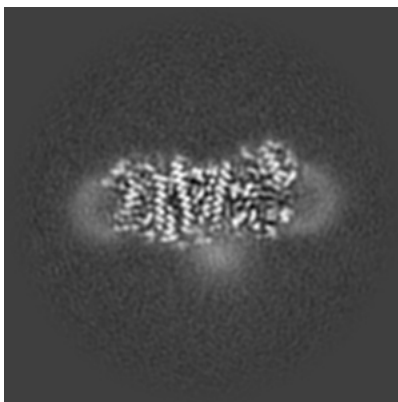
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

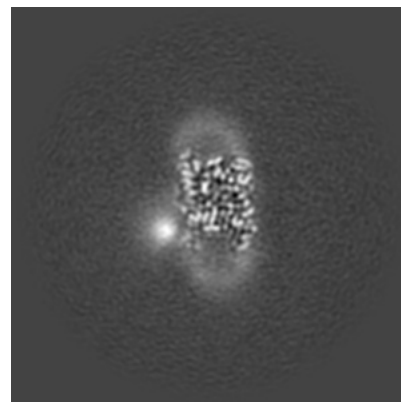
6.3.1 Primary map



X Index: 144

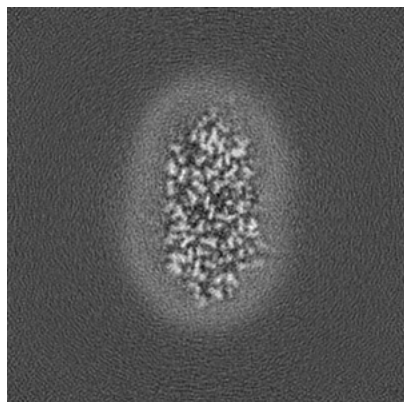


Y Index: 123

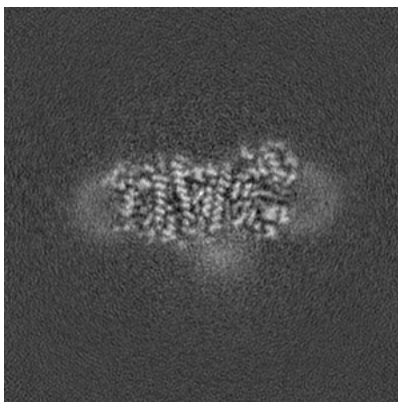


Z Index: 135

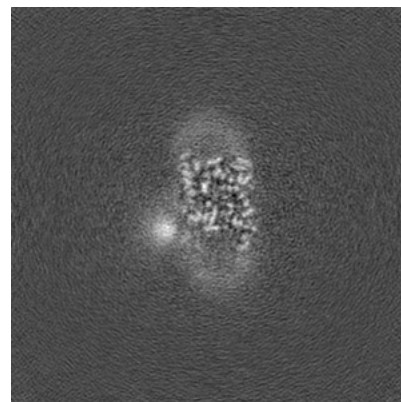
6.3.2 Raw map



X Index: 142



Y Index: 122

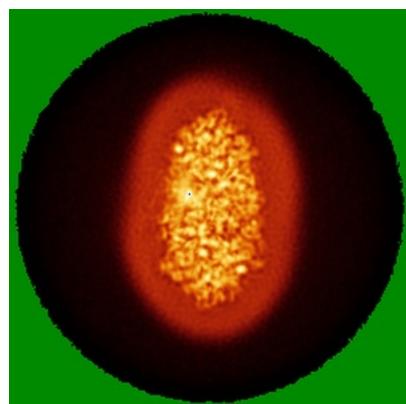


Z Index: 135

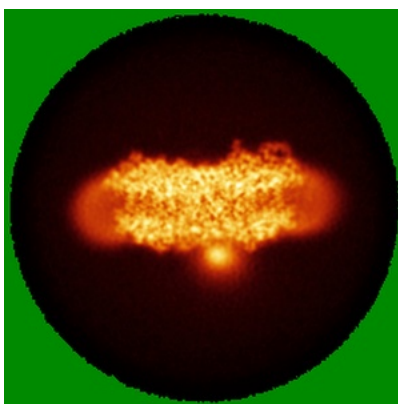
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

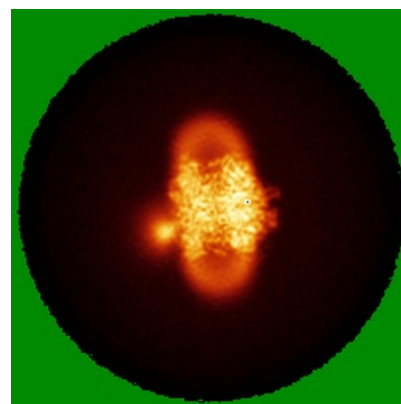
6.4.1 Primary map



X

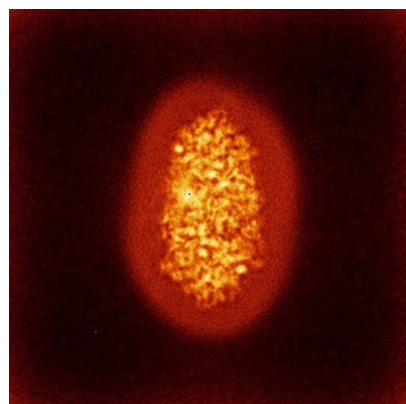


Y

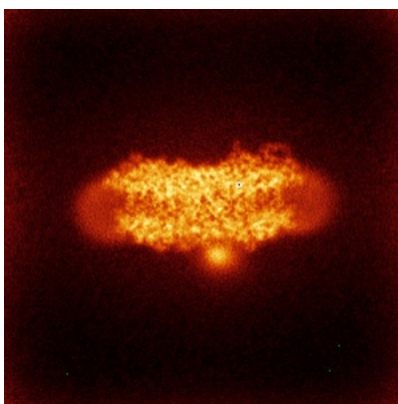


Z

6.4.2 Raw map



X



Y

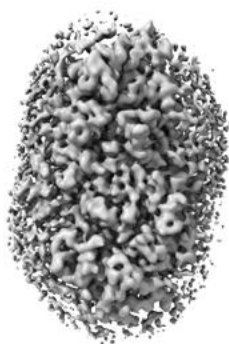


Z

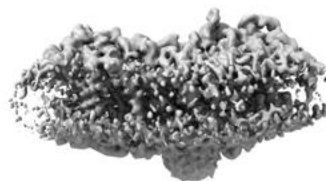
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



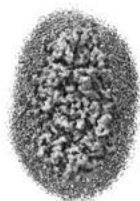
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.164. 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



X



Y



Z

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.

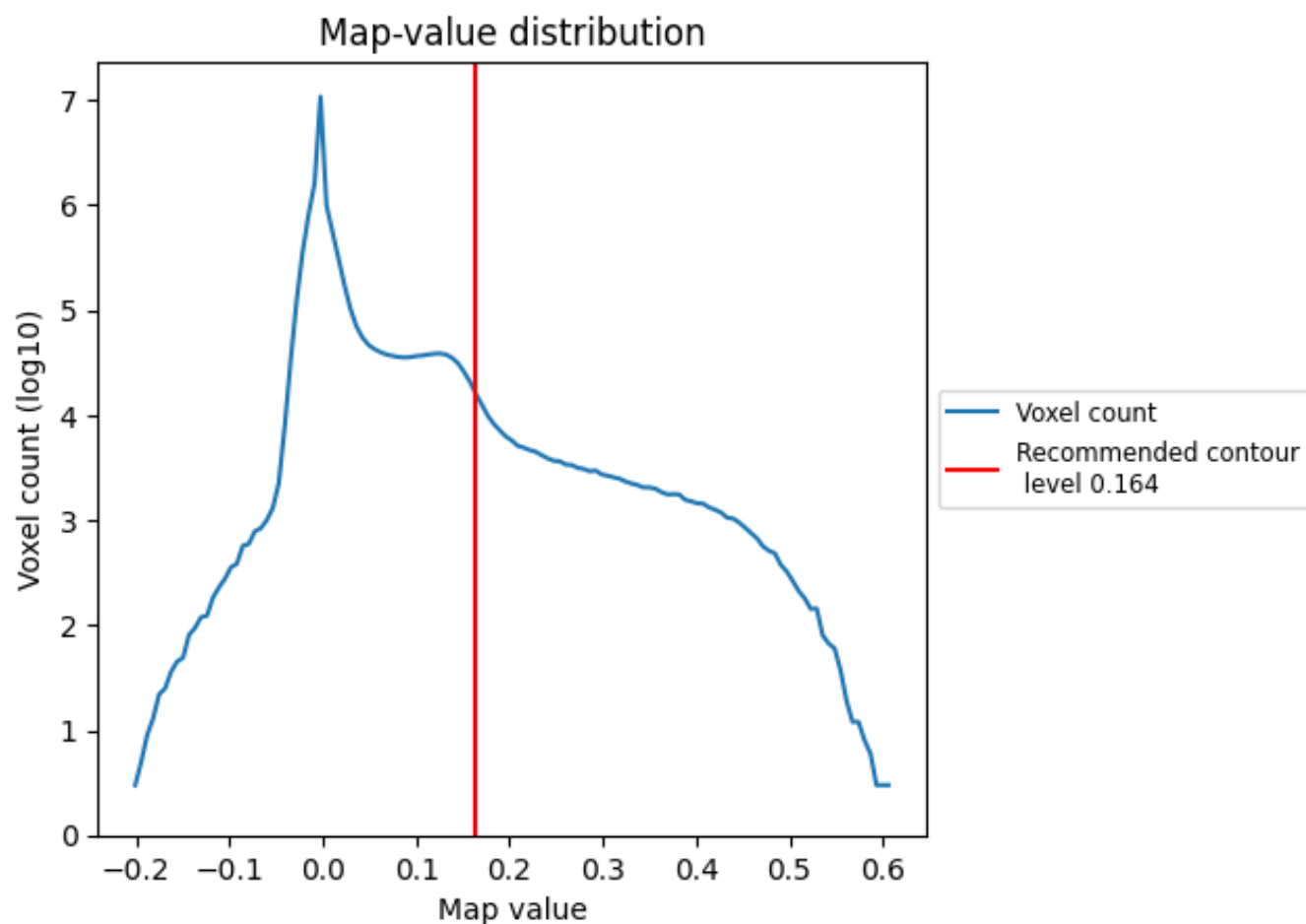
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

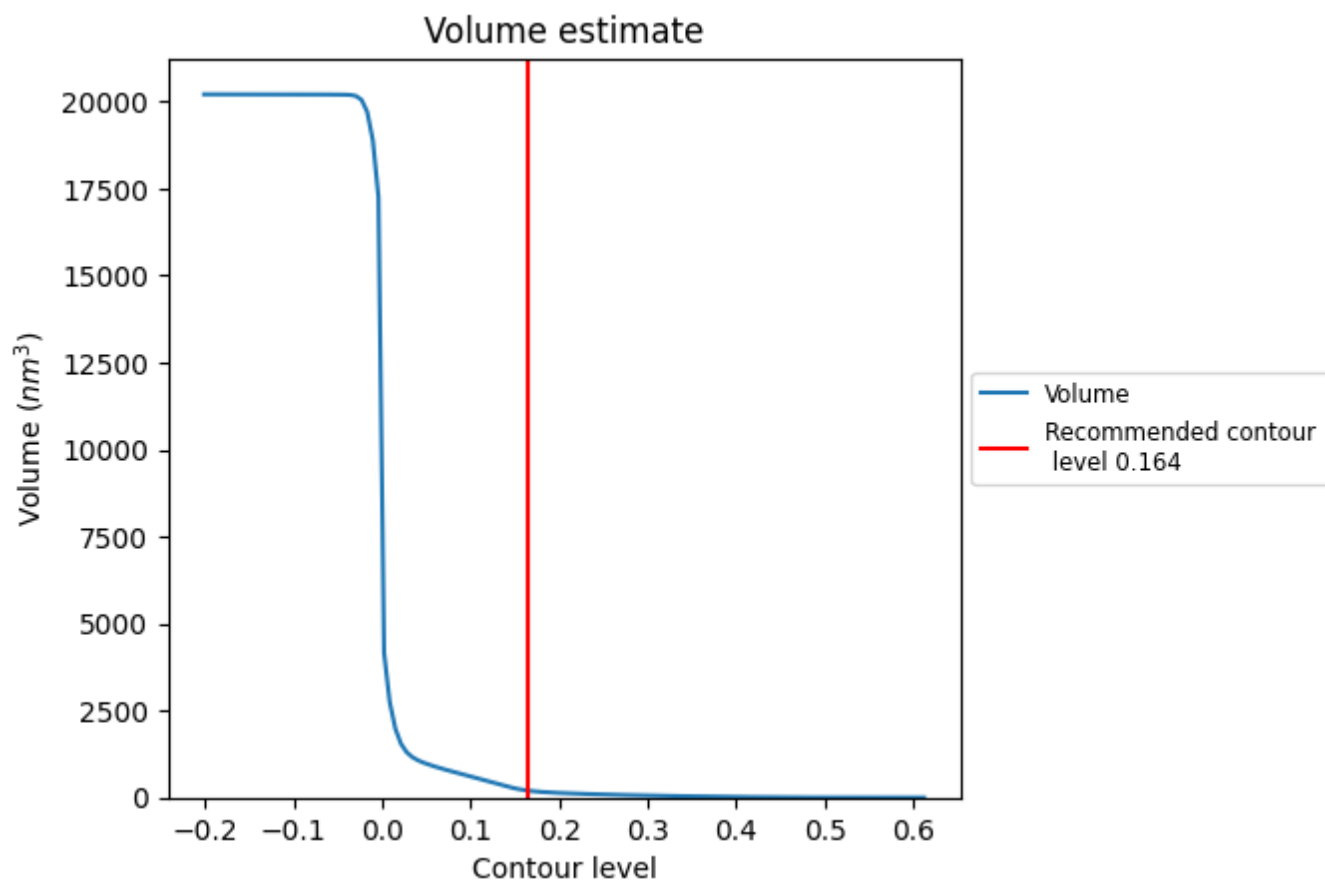
This section contains the results of statistical analysis of the map.

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.

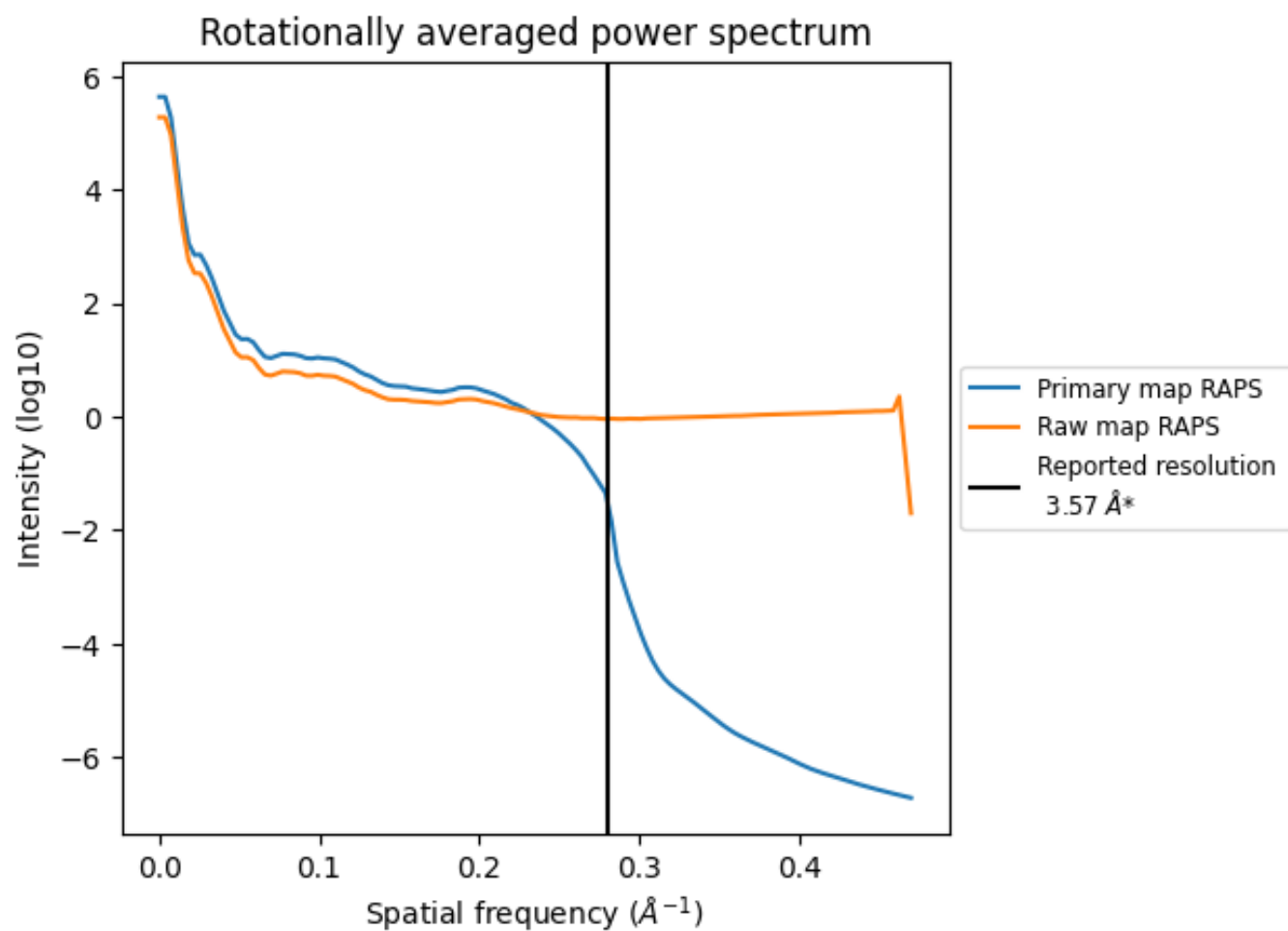
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 203 nm³; this corresponds to an approximate mass of 184 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 ⓘ

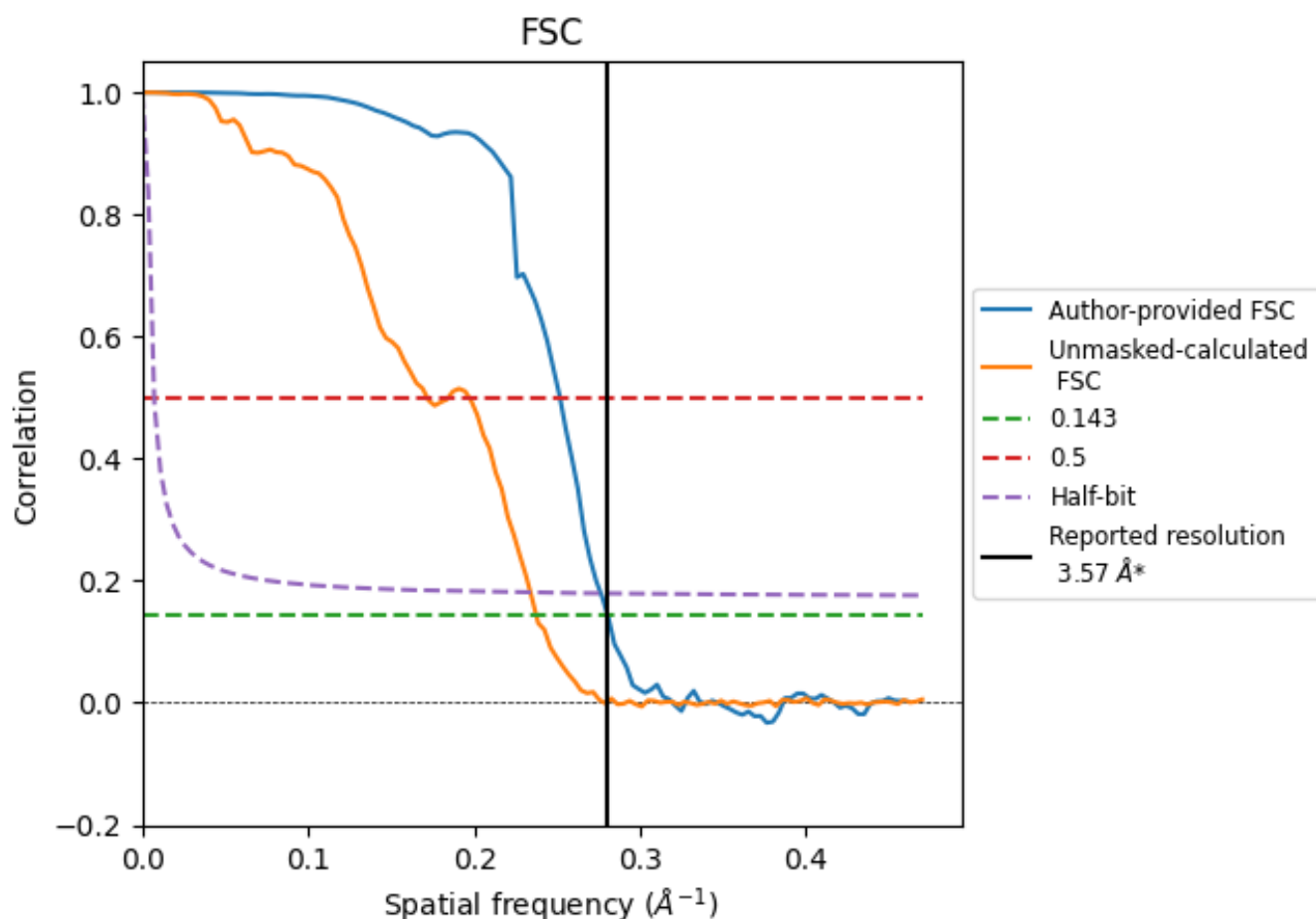


*Reported resolution corresponds to spatial frequency of 0.280 $\text{\AA}^{-1}$

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 0.280 Å⁻¹

8.2 Resolution estimates [i](#)

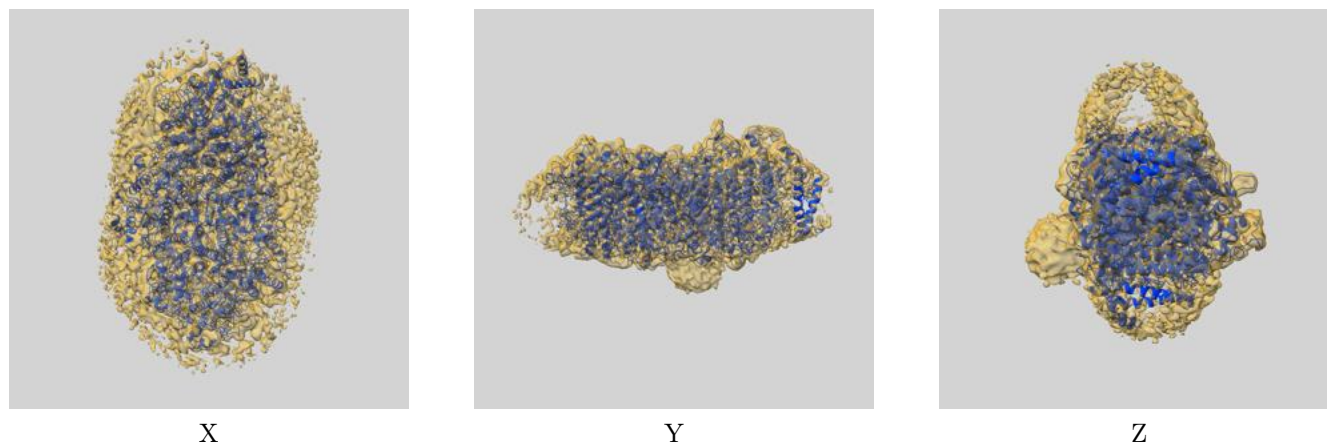
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.57	-	-
Author-provided FSC curve	3.57	3.97	3.62
Unmasked-calculated*	4.21	5.82	4.28

*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 4.21 differs from the reported value 3.57 by more than 10 %

9 Map-model fit [i](#)

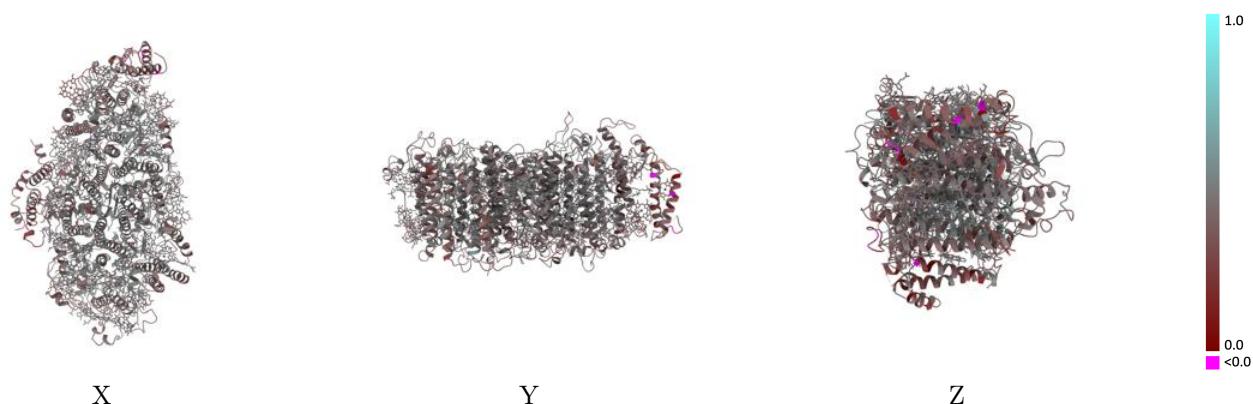
This section contains information regarding the fit between EMDB map EMD-75232 and PDB model 10KF. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



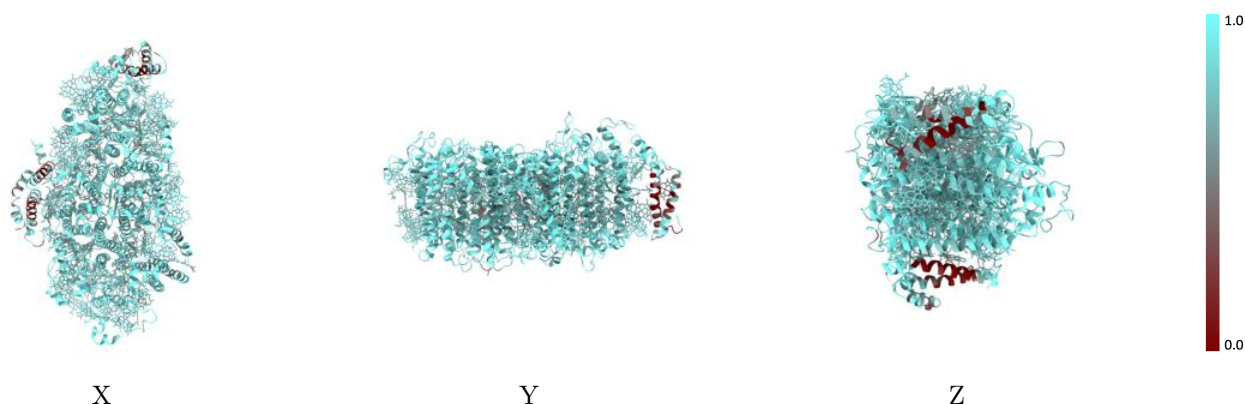
The images above show the 3D surface view of the map at the recommended contour level 0.164 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



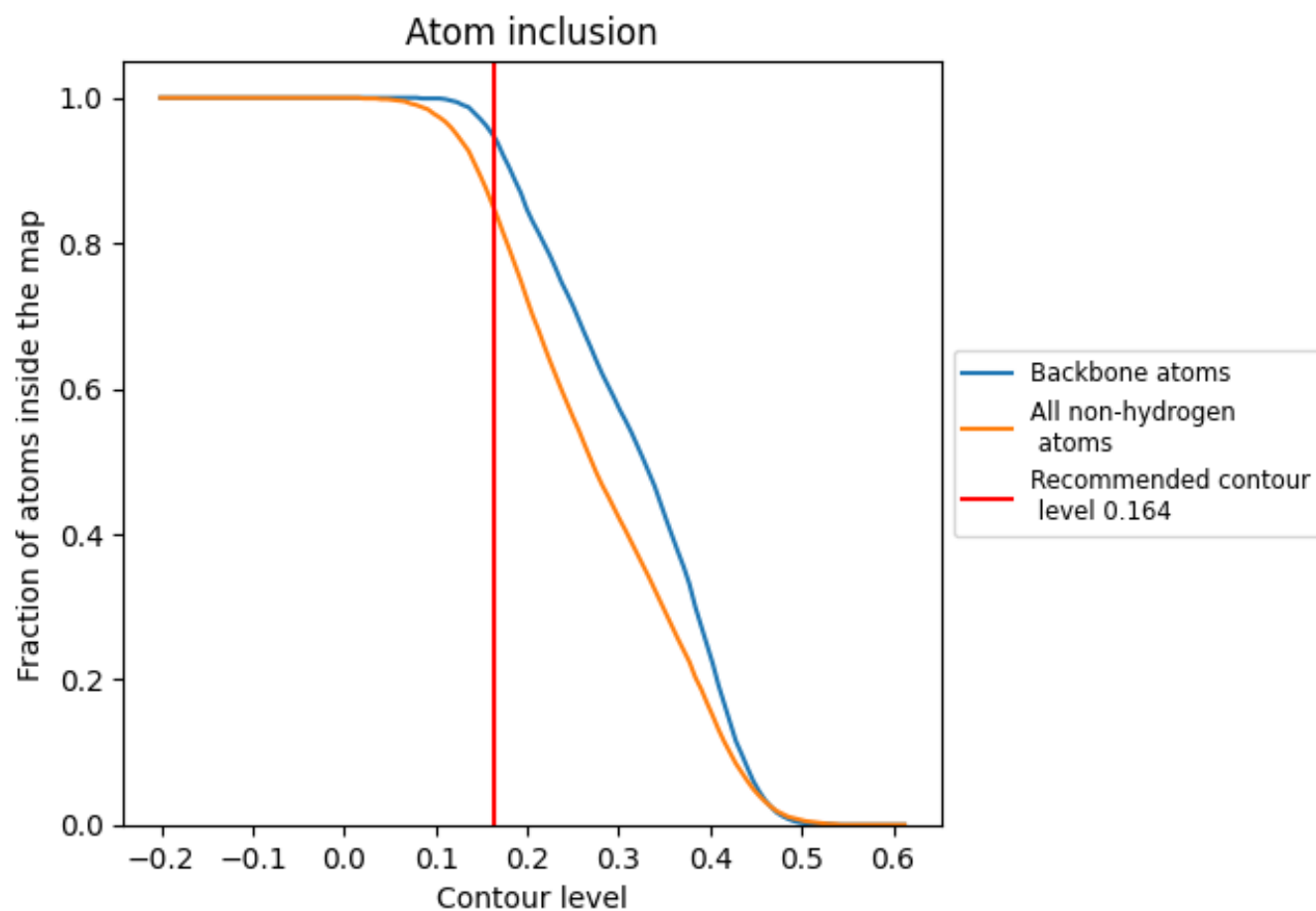
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.164).

9.4 Atom inclusion ⓘ



At the recommended contour level, 95% of all backbone atoms, 85% 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 (0.164) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8470	0.4230
A	0.8660	0.4280
B	0.8690	0.4340
F	0.5850	0.3130
I	0.7780	0.3760
J	0.5740	0.3120
K	0.5210	0.2990
M	0.7710	0.3930

1.0

0.0

<0.0