



Full wwPDB EM Validation Report ⓘ

Oct 5, 2026 – 08:36 PM EDT

PDB ID : 9YL7 / pdb_00009yl7
EMDB ID : EMD-73077
Title : Structure of photosystem I with plastoquinone-9 bound
Authors : Brininger, C.M.; Gisriel, C.J.
Deposited on : 2025-10-08
Resolution : 1.68 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:

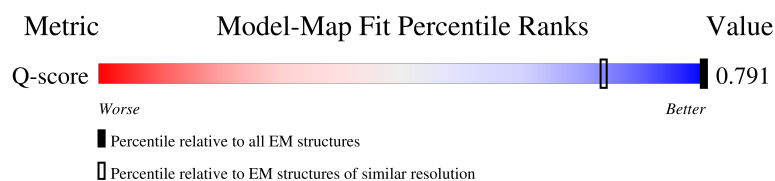
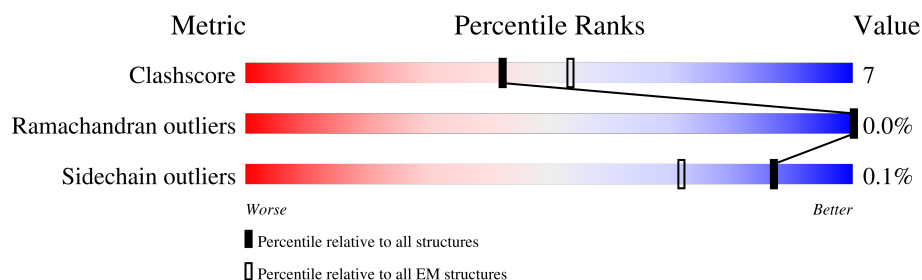
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.2
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.51

1 Overall quality at a glance

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

The reported resolution of this entry is 1.68 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	466 (1.19 - 2.18)

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

Mol	Chain	Length	Quality of chain
1	A	751	 91% 8% .
2	B	731	 87% 12%
3	C	81	 85% 14% .
4	D	141	 84% 12% ..

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Mol	Chain	Length	Quality of chain
5	E	74	 81% 11% • 7%
6	F	165	 73% 12% 15%
7	I	40	 85% 10% 5%
8	J	40	 72% 22% • •
9	K	86	 74% 15% • 9%
10	L	157	 86% 11% • •
11	M	31	 84% 13% •

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 25616 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	742	Total	C	N	O	S	0	0
			5783	3791	981	984	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	729	Total	C	N	O	S	0	0
			5759	3792	967	986	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			600	369	103	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	139	Total	C	N	O	S	0	0
			1075	680	186	206	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	69	Total	C	N	O	0	0
			537	337	95	105		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	141	Total	C	N	O	S	0	0
			1084	700	180	199	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	38	Total	C	N	O	S	0	0
			297	202	42	50	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	39	Total	C	N	O	S	0	0
			311	210	46	53	2		

- Molecule 9 is a protein called Photosystem I reaction center subunit PsaK 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	78	Total	C	N	O	S	0	0
			545	358	89	94	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	37	PHE	LEU	conflict	UNP P72712
K	43	SER	ASN	conflict	UNP P72712

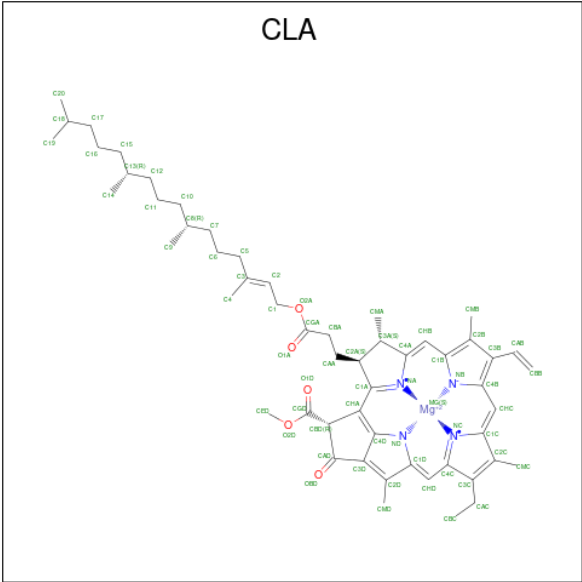
- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	154	Total	C	N	O	S	0	0
			1152	751	188	211	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total	C	N	O	S	0	0
			238	159	36	42	1		

- Molecule 12 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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

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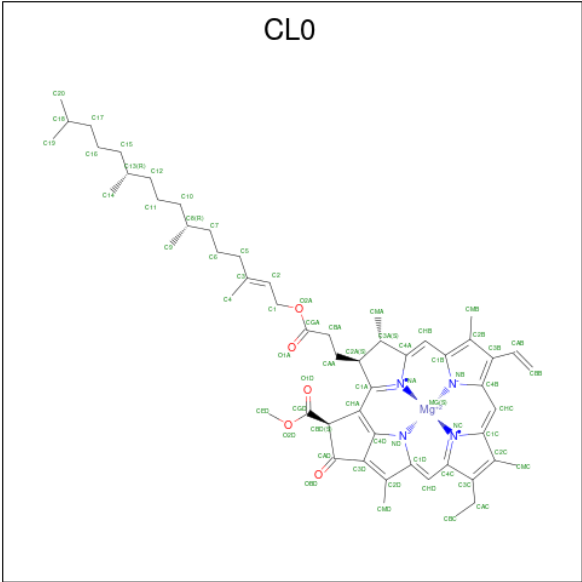
Mol	Chain	Residues	Atoms					AltConf
12	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total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

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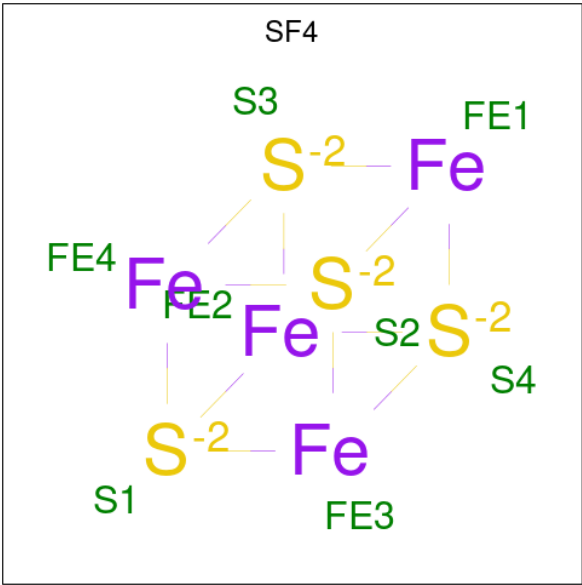
Mol	Chain	Residues	Atoms					AltConf
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	F	1	Total	C	Mg	N	O	0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

- Molecule 13 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



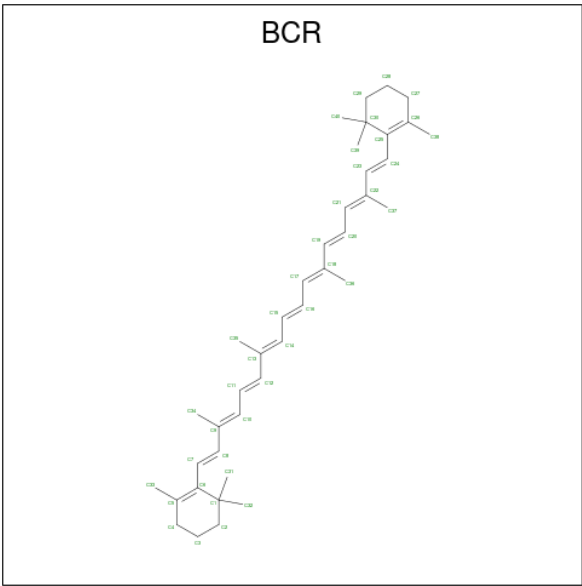
Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 14 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

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



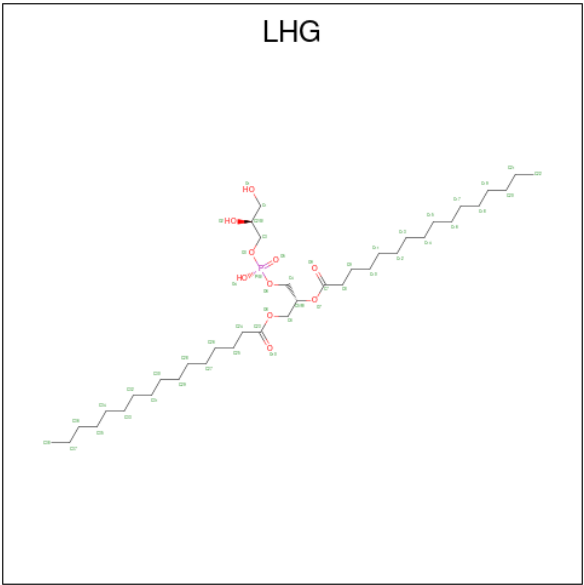
Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total	C	0
			40	40	
15	A	1	Total	C	0
			40	40	
15	A	1	Total	C	0
			40	40	
15	A	1	Total	C	0
			40	40	
15	B	1	Total	C	0
			40	40	
15	B	1	Total	C	0
			40	40	
15	B	1	Total	C	0
			40	40	
15	B	1	Total	C	0
			25	25	
15	B	1	Total	C	0
			40	40	
15	F	1	Total	C	0
			40	40	
15	F	1	Total	C	0
			40	40	
15	I	1	Total	C	0
			40	40	
15	J	1	Total	C	0
			14	14	

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Mol	Chain	Residues	Atoms		AltConf
15	J	1	Total	C	0
			40	40	
15	J	1	Total	C	0
			40	40	
15	K	1	Total	C	0
			40	40	
15	K	1	Total	C	0
			40	40	
15	L	1	Total	C	0
			40	40	
15	L	1	Total	C	0
			40	40	

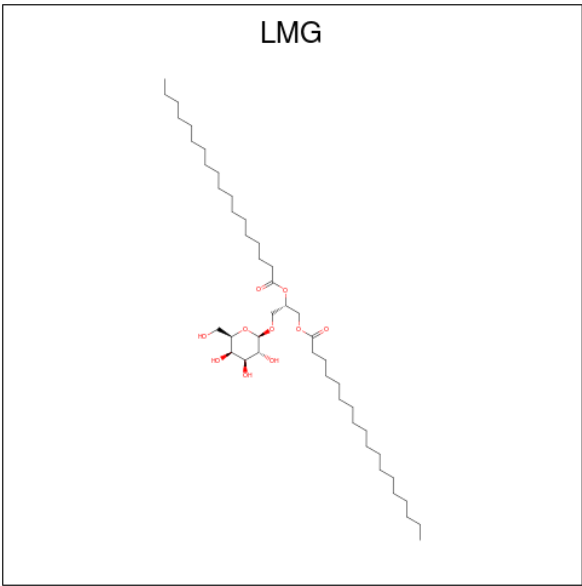
- Molecule 16 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
16	A	1	Total	C	O	P	0
			49	38	10	1	
16	A	1	Total	C	O	P	0
			37	26	10	1	
16	B	1	Total	C	O	P	0
			49	38	10	1	
16	M	1	Total	C	O	P	0
			44	33	10	1	

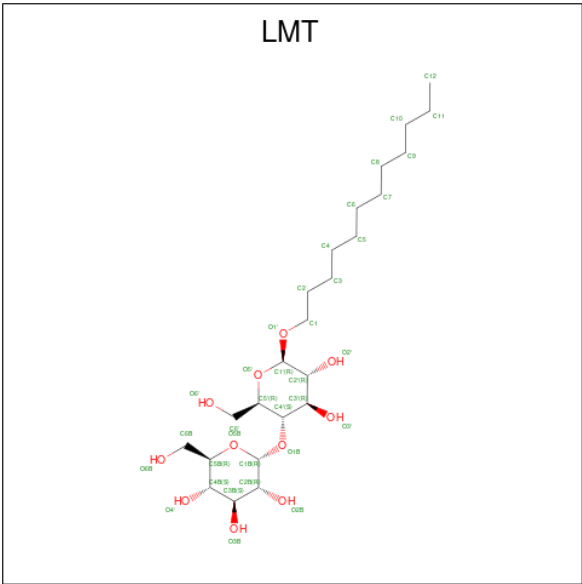
- Molecule 17 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID:

LMG) (formula: C₄₅H₈₆O₁₀).



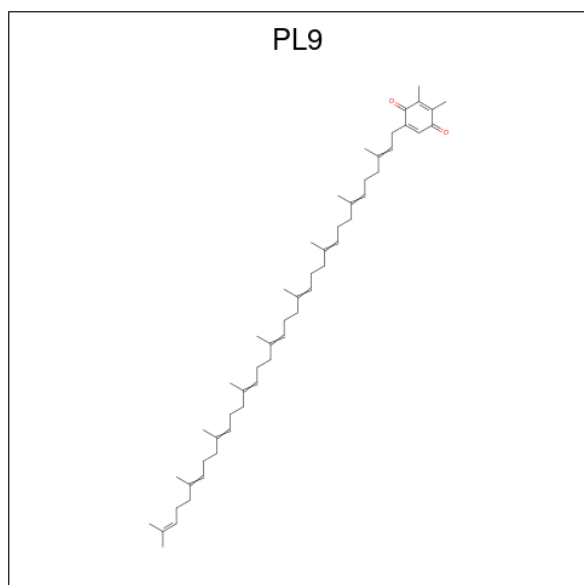
Mol	Chain	Residues	Atoms			AltConf
17	A	1	Total	C	O	0
			50	40	10	
17	A	1	Total	C	O	0
			46	36	10	
17	B	1	Total	C	O	0
			51	41	10	

- Molecule 18 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



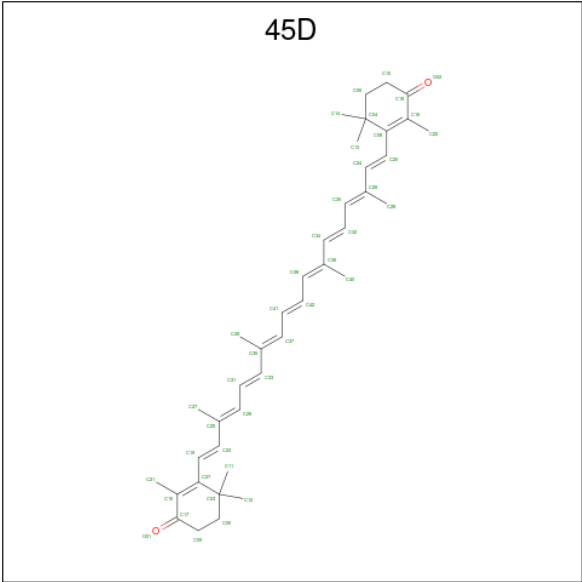
Mol	Chain	Residues	Atoms			AltConf
18	A	1	Total	C	O	0
			35	24	11	
18	A	1	Total	C	O	0
			35	24	11	
18	A	1	Total	C	O	0
			35	24	11	
18	B	1	Total	C	O	0
			29	18	11	
18	B	1	Total	C	O	0
			35	24	11	
18	F	1	Total	C	O	0
			31	20	11	
18	J	1	Total	C	O	0
			31	20	11	
18	L	1	Total	C	O	0
			35	24	11	

- Molecule 19 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
19	A	1	Total	C	O	0
			30	28	2	

- Molecule 20 is beta,beta-carotene-4,4'-dione (CCD ID: 45D) (formula: C₄₀H₅₂O₂).

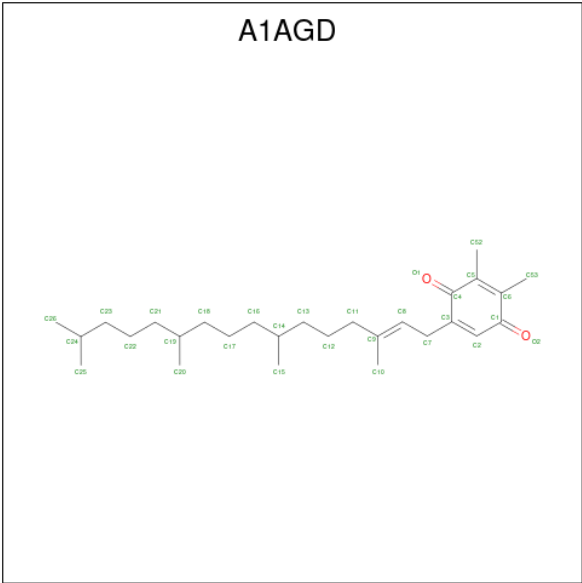


Mol	Chain	Residues	Atoms			AltConf
20	A	1	Total	C	O	0
			42	40	2	

- Molecule 21 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

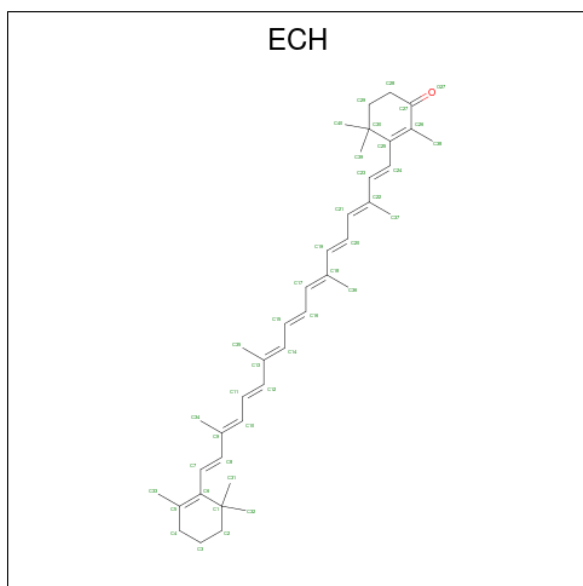
Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total	Cl	0
			1	1	

- Molecule 22 is 2,3-dimethyl-5-[(2E,7R,11R)-3,7,11,15-tetramethylhexadec-2-en-1-yl]cyclohexa-2,5-diene-1,4-dione (CCD ID: A1AGD) (formula: C₂₈H₄₆O₂).



Mol	Chain	Residues	Atoms			AltConf
22	B	1	Total	C	O	0
			30	28	2	

- Molecule 23 is beta,beta-caroten-4-one (CCD ID: ECH) (formula: $C_{40}H_{54}O$).

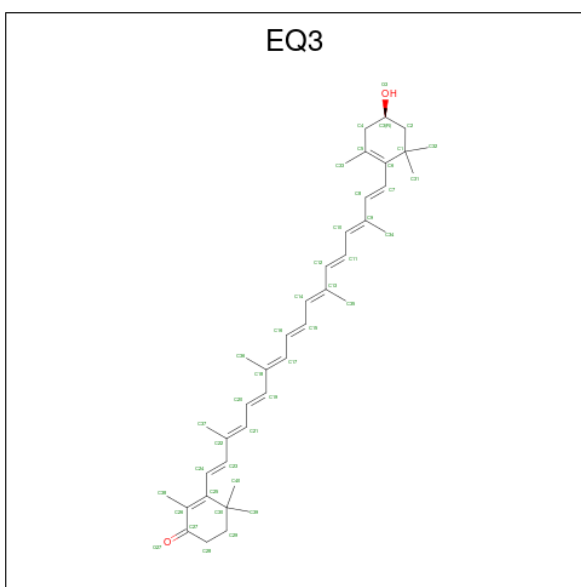


Mol	Chain	Residues	Atoms			AltConf
23	B	1	Total	C	O	0
			41	40	1	
23	M	1	Total	C	O	0
			41	40	1	

- Molecule 24 is CALCIUM ION (CCD ID: CA) (formula: Ca).

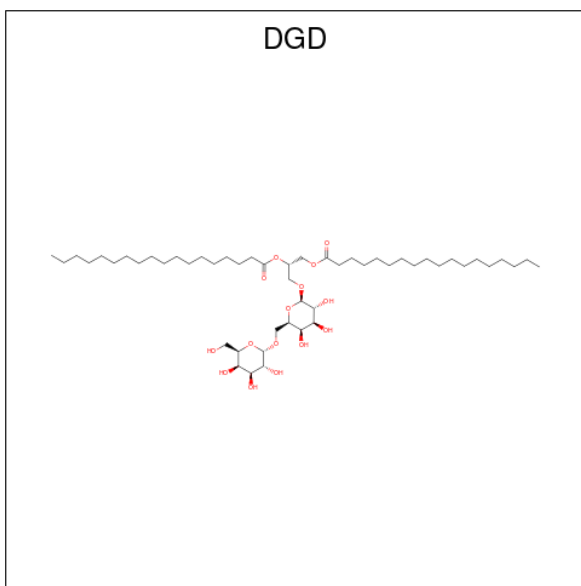
Mol	Chain	Residues	Atoms		AltConf
24	B	1	Total	Ca	0
			1	1	
24	L	1	Total	Ca	0
			1	1	

- Molecule 25 is (3'R)-3'-hydroxy-beta,beta-caroten-4-one (CCD ID: EQ3) (formula: $C_{40}H_{54}O_2$).



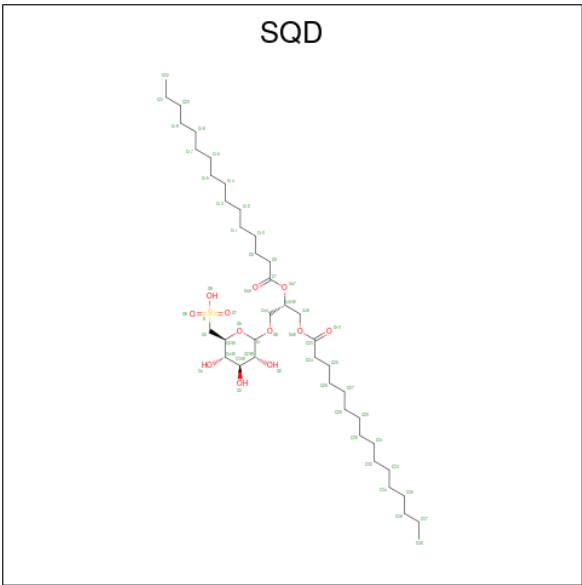
Mol	Chain	Residues	Atoms			AltConf
25	L	1	Total	C	O	0
			42	40	2	

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
26	L	1	Total	C	O	0
			49	39	10	

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
27	M	1	Total	C	O	S	0
			54	41	12	1	

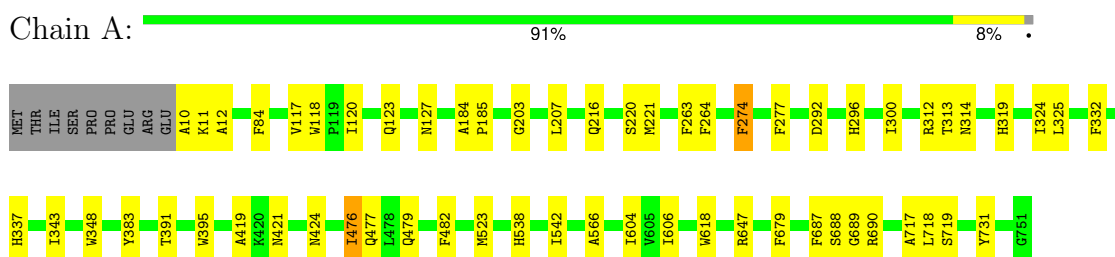
- Molecule 28 is water.

Mol	Chain	Residues	Atoms		AltConf
28	A	267	Total	O	0
			267	267	
28	B	291	Total	O	0
			291	291	
28	C	68	Total	O	0
			68	68	
28	D	68	Total	O	0
			68	68	
28	E	26	Total	O	0
			26	26	
28	F	11	Total	O	0
			11	11	
28	I	6	Total	O	0
			6	6	
28	J	3	Total	O	0
			3	3	
28	K	7	Total	O	0
			7	7	
28	L	39	Total	O	0
			39	39	
28	M	7	Total	O	0
			7	7	

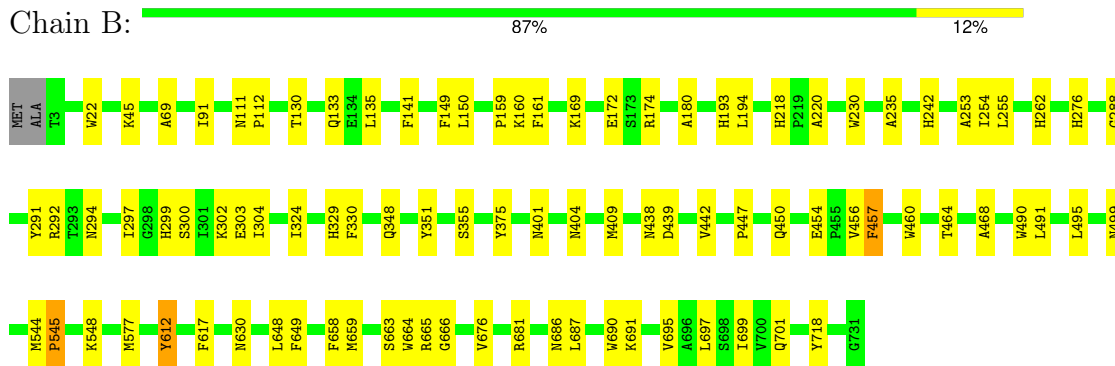
3 Residue-property plots

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

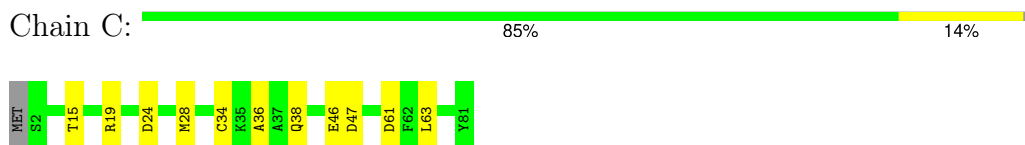
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



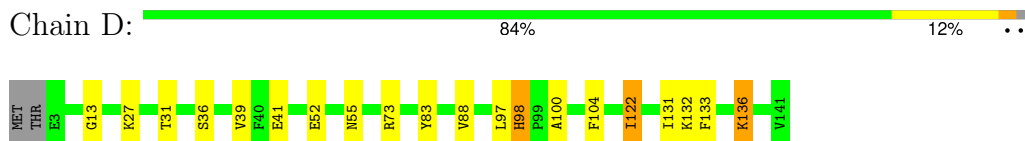
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 3: Photosystem I iron-sulfur center



- Molecule 4: Photosystem I reaction center subunit II



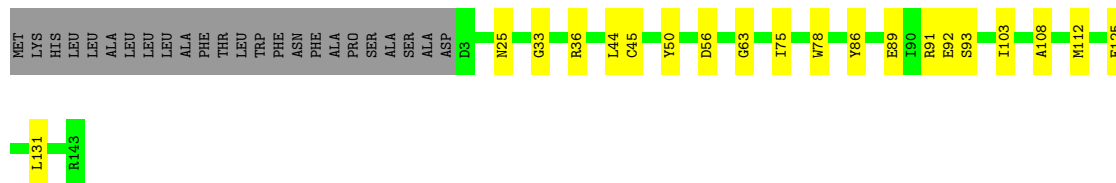
- Molecule 5: Photosystem I reaction center subunit IV

Chain E:  81% 11% 7%



- Molecule 6: Photosystem I reaction center subunit III

Chain F:  73% 12% 15%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain I:  85% 10% 5%



- Molecule 8: Photosystem I reaction center subunit IX

Chain J:  72% 22% 6%



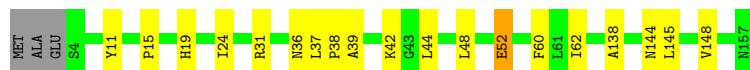
- Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain K:  74% 15% 9%



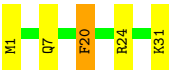
- Molecule 10: Photosystem I reaction center subunit XI

Chain L:  86% 11% 3%



- Molecule 11: Photosystem I reaction center subunit XII

Chain M:  84% 13% 3%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1243569	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.571	Depositor
Minimum map value	-1.161	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.0353	Depositor
Map size (Å)	350.28, 350.28, 350.28	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.834, 0.834, 0.834	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, A1AGD, BCR, DGD, LHG, CA, EQ3, ECH, CL0, CL, CLA, SF4, SQD, LMG, 45D, PL9

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	0.68	20/5981 (0.3%)	0.69	8/8156 (0.1%)
2	B	0.93	46/5970 (0.8%)	0.97	17/8165 (0.2%)
3	C	0.65	2/610 (0.3%)	1.01	1/826 (0.1%)
4	D	0.64	4/1099 (0.4%)	0.94	7/1484 (0.5%)
5	E	0.86	2/546 (0.4%)	1.23	5/740 (0.7%)
6	F	0.72	1/1114 (0.1%)	1.07	3/1518 (0.2%)
7	I	0.38	0/308	0.78	0/421
8	J	0.65	0/320	1.08	3/433 (0.7%)
9	K	0.82	3/557 (0.5%)	1.01	1/754 (0.1%)
10	L	0.56	3/1182 (0.3%)	0.81	1/1606 (0.1%)
11	M	0.67	2/241 (0.8%)	0.62	0/326
All	All	0.77	83/17928 (0.5%)	0.89	46/24429 (0.2%)

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
2	B	0	2
3	C	0	1
4	D	0	2
5	E	0	3
6	F	0	1
7	I	0	1
10	L	0	1
All	All	0	11

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	313	THR	CA-C	16.23	1.60	1.52
1	A	731	TYR	C-O	-13.06	1.08	1.24
2	B	695	VAL	C-O	-13.02	1.09	1.23
2	B	649	PHE	C-O	-11.44	1.10	1.24
2	B	297	ILE	C-O	-11.44	1.10	1.24
2	B	665	ARG	C-O	-11.12	1.11	1.24
2	B	276	HIS	C-O	-11.06	1.11	1.24
2	B	161	PHE	C-O	-11.00	1.08	1.24
2	B	666	GLY	C-O	-10.56	1.11	1.23
2	B	658	PHE	C-O	-10.20	1.11	1.24
2	B	150	LEU	C-O	-9.97	1.12	1.24
2	B	686	ASN	C-O	-9.96	1.11	1.24
2	B	659	MET	C-O	-9.66	1.12	1.24
2	B	242	HIS	C-O	-9.53	1.12	1.23
2	B	699	ILE	C-O	-9.26	1.13	1.24
2	B	194	LEU	C-O	-8.97	1.13	1.24
2	B	691	LYS	C-O	-8.83	1.12	1.24
2	B	329	HIS	C-O	-8.83	1.13	1.24
2	B	375	TYR	C-O	-8.77	1.13	1.24
4	D	98	HIS	C-O	-8.63	1.13	1.24
1	A	277	PHE	C-O	-8.40	1.15	1.23
1	A	690	ARG	C-O	-8.32	1.13	1.24
2	B	697	LEU	C-O	-8.31	1.13	1.24
2	B	612	TYR	C-O	-8.19	1.13	1.23
1	A	312	ARG	CA-C	-8.05	1.42	1.52
2	B	375	TYR	CA-C	7.88	1.63	1.52
5	E	17	TYR	C-O	-7.84	1.14	1.24
10	L	37	LEU	C-O	-7.70	1.13	1.23
2	B	664	TRP	C-O	-7.66	1.14	1.23
2	B	457	PHE	C-O	-7.60	1.15	1.24
2	B	649	PHE	N-CA	7.50	1.55	1.46
2	B	193	HIS	C-N	-7.42	1.24	1.33
2	B	545	PRO	C-O	-7.38	1.14	1.24
1	A	476	ILE	C-O	-7.26	1.14	1.23
1	A	679	PHE	C-O	-7.20	1.15	1.24
2	B	663	SER	C-O	-7.08	1.15	1.24
1	A	476	ILE	CA-CB	7.06	1.60	1.53
2	B	45	LYS	C-O	-7.02	1.15	1.24
1	A	263	PHE	C-O	-6.91	1.16	1.24
2	B	330	PHE	N-CA	6.82	1.54	1.46
1	A	84	PHE	C-O	-6.70	1.15	1.24
3	C	61	ASP	C-O	-6.67	1.16	1.24
1	A	719	SER	C-O	-6.42	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	689	GLY	C-O	-6.33	1.17	1.24
11	M	20	PHE	C-O	-6.31	1.16	1.24
2	B	490	TRP	CA-CB	6.30	1.64	1.53
10	L	36	ASN	CA-C	6.18	1.61	1.52
1	A	688	SER	C-O	-6.15	1.15	1.24
10	L	60	PHE	C-O	-6.13	1.16	1.24
3	C	63	LEU	C-O	-6.04	1.16	1.23
2	B	617	PHE	C-O	-5.87	1.17	1.24
2	B	329	HIS	C-N	-5.79	1.26	1.33
2	B	149	PHE	C-N	-5.75	1.26	1.33
4	D	122	ILE	C-O	-5.75	1.16	1.24
1	A	264	PHE	N-CA	5.72	1.53	1.46
1	A	687	PHE	C-O	-5.72	1.16	1.24
2	B	686	ASN	N-CA	5.71	1.53	1.46
2	B	648	LEU	C-N	-5.67	1.26	1.33
9	K	13	THR	C-O	-5.65	1.17	1.23
4	D	122	ILE	N-CA	5.62	1.54	1.46
1	A	718	LEU	C-O	-5.60	1.17	1.23
2	B	658	PHE	N-CA	5.58	1.53	1.46
2	B	169	LYS	C-O	-5.58	1.16	1.24
2	B	612	TYR	CA-C	5.57	1.59	1.52
2	B	686	ASN	C-N	-5.56	1.26	1.33
1	A	717	ALA	C-O	-5.55	1.17	1.23
2	B	324	ILE	C-O	-5.52	1.18	1.24
9	K	20	VAL	C-O	-5.51	1.18	1.24
2	B	194	LEU	C-N	-5.47	1.26	1.33
2	B	160	LYS	C-O	-5.46	1.17	1.24
2	B	159	PRO	C-N	-5.39	1.26	1.33
4	D	97	LEU	C-O	-5.38	1.15	1.23
1	A	476	ILE	CA-C	5.35	1.58	1.53
1	A	313	THR	N-CA	-5.28	1.39	1.45
2	B	45	LYS	C-N	-5.27	1.27	1.33
5	E	35	TYR	C-O	-5.24	1.18	1.24
2	B	691	LYS	CA-C	5.24	1.59	1.52
9	K	15	SER	C-O	-5.23	1.17	1.23
6	F	86	TYR	C-O	-5.21	1.18	1.24
2	B	330	PHE	C-O	-5.17	1.18	1.24
1	A	274	PHE	C-O	-5.13	1.17	1.24
2	B	150	LEU	N-CA	5.07	1.52	1.46
11	M	20	PHE	CA-CB	-5.06	1.45	1.53

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	92	GLU	N-CA-C	-8.45	104.02	112.97
2	B	665	ARG	N-CA-C	8.26	120.28	111.28
4	D	136	LYS	CA-CB-CG	8.18	130.46	114.10
9	K	14	LEU	N-CA-C	8.04	122.74	109.95
3	C	63	LEU	CA-C-O	-6.90	113.60	121.19
2	B	544	MET	O-C-N	6.88	126.49	121.12
2	B	686	ASN	CA-C-N	6.79	131.47	120.60
2	B	686	ASN	C-N-CA	6.79	131.47	120.60
4	D	104	PHE	N-CA-C	6.79	117.41	109.60
2	B	454	GLU	CA-C-N	6.54	128.01	119.84
2	B	454	GLU	C-N-CA	6.54	128.01	119.84
1	A	566	ALA	CA-C-N	6.45	129.80	120.38
1	A	566	ALA	C-N-CA	6.45	129.80	120.38
6	F	103	ILE	N-CA-C	6.40	117.30	109.30
2	B	442	VAL	CA-CB-CG1	6.22	120.97	110.40
5	E	69	VAL	CA-C-N	6.17	132.81	121.70
5	E	69	VAL	C-N-CA	6.17	132.81	121.70
1	A	10	ALA	CA-C-N	6.14	133.28	121.54
1	A	10	ALA	C-N-CA	6.14	133.28	121.54
6	F	45	CYS	CA-CB-SG	6.03	128.27	114.40
1	A	679	PHE	N-CA-CB	5.94	118.85	109.82
4	D	100	ALA	N-CA-C	5.92	118.49	111.33
10	L	52	GLU	N-CA-C	5.89	117.50	111.14
2	B	545	PRO	CA-C-N	5.65	131.57	122.14
2	B	545	PRO	C-N-CA	5.65	131.57	122.14
2	B	666	GLY	O-C-N	-5.62	116.80	122.19
4	D	41	GLU	CB-CG-CD	5.55	122.03	112.60
2	B	262	HIS	N-CA-C	-5.47	102.89	109.83
4	D	136	LYS	CB-CG-CD	-5.41	98.86	111.30
2	B	659	MET	N-CA-CB	5.36	117.78	110.01
5	E	37	VAL	CA-C-N	-5.35	115.47	122.37
5	E	37	VAL	C-N-CA	-5.35	115.47	122.37
8	J	5	LYS	CD-CE-NZ	-5.33	94.83	111.90
1	A	679	PHE	N-CA-C	-5.30	104.55	111.02
2	B	548	LYS	CA-CB-CG	5.30	124.69	114.10
2	B	548	LYS	CD-CE-NZ	-5.17	95.35	111.90
1	A	476	ILE	N-CA-CB	5.15	117.46	111.90
8	J	33	TYR	CA-C-N	-5.15	115.29	120.85
8	J	33	TYR	C-N-CA	-5.15	115.29	120.85
4	D	36	SER	CA-C-N	-5.14	115.36	122.30
4	D	36	SER	C-N-CA	-5.14	115.36	122.30
2	B	490	TRP	CA-C-O	-5.14	112.53	119.11
2	B	130	THR	CA-CB-OG1	-5.08	101.98	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	664	TRP	N-CA-C	5.06	118.20	110.36
5	E	37	VAL	N-CA-C	5.05	116.02	108.54
1	A	690	ARG	N-CA-C	5.01	117.47	111.71

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	292	ARG	Sidechain
2	B	294	ASN	Mainchain
3	C	19	ARG	Sidechain
4	D	122	ILE	Mainchain
4	D	52	GLU	Sidechain
5	E	43	ARG	Sidechain
5	E	46	TYR	Mainchain
5	E	5	ARG	Sidechain
6	F	36	ARG	Sidechain
7	I	2	ASP	Sidechain
10	L	31	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5783	0	5630	30	0
2	B	5759	0	5532	41	0
3	C	600	0	581	5	0
4	D	1075	0	1056	8	0
5	E	537	0	511	2	0
6	F	1084	0	1059	9	0
7	I	297	0	295	2	0
8	J	311	0	316	10	0
9	K	545	0	567	8	0
10	L	1152	0	1123	12	0
11	M	238	0	260	8	0
12	A	2530	0	2581	83	0
12	B	2530	0	2667	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	F	90	0	66	3	0
12	J	150	0	124	4	0
12	K	150	0	123	10	0
12	L	260	0	288	6	0
13	A	65	0	72	1	0
14	A	8	0	0	0	0
14	C	16	0	0	0	0
15	A	160	0	224	6	0
15	B	185	0	257	10	0
15	F	80	0	112	6	0
15	I	40	0	56	4	0
15	J	94	0	132	7	0
15	K	80	0	112	5	0
15	L	80	0	112	4	0
16	A	86	0	118	9	0
16	B	49	0	74	5	0
16	M	44	0	61	1	0
17	A	96	0	135	4	0
17	B	51	0	75	1	0
18	A	105	0	138	5	0
18	B	64	0	77	4	0
18	F	31	0	35	1	0
18	J	31	0	35	1	0
18	L	35	0	46	3	0
19	A	30	0	37	10	0
20	A	42	0	52	3	0
21	A	1	0	0	0	0
22	B	30	0	0	0	0
23	B	41	0	54	1	0
23	M	41	0	54	0	0
24	B	1	0	0	0	0
24	L	1	0	0	0	0
25	L	42	0	0	0	0
26	L	49	0	70	2	0
27	M	54	0	78	5	0
28	A	267	0	0	0	0
28	B	291	0	0	0	0
28	C	68	0	0	0	0
28	D	68	0	0	0	0
28	E	26	0	0	1	0
28	F	11	0	0	0	0
28	I	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	J	3	0	0	0	0
28	K	7	0	0	0	0
28	L	39	0	0	0	0
28	M	7	0	0	0	0
All	All	25616	0	24995	334	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 (334) 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)
8:J:31:ARG:HD3	15:J:105:BCR:H313	1.48	0.95
12:B:847:CLA:HHC	12:B:847:CLA:HBB1	1.49	0.94
1:A:12:ALA:H	1:A:314:ASN:HD21	1.03	0.93
12:A:843:CLA:H92	12:A:846:CLA:C6	2.05	0.86
8:J:31:ARG:HD3	15:J:105:BCR:C31	2.08	0.83
12:A:843:CLA:H92	12:A:846:CLA:H61	1.58	0.83
12:B:823:CLA:HAB	12:B:824:CLA:H202	1.61	0.83
2:B:401:ASN:HD22	2:B:404:ASN:HD21	1.25	0.81
16:A:850:LHG:H281	16:A:850:LHG:H322	1.62	0.80
12:B:803:CLA:HBB1	12:B:803:CLA:HMB3	1.64	0.79
12:A:844:CLA:H142	12:A:844:CLA:H102	1.66	0.77
12:B:824:CLA:HMB1	12:B:824:CLA:HBB1	1.69	0.74
19:A:854:PL9:H162	19:A:854:PL9:H202	1.70	0.73
1:A:12:ALA:H	1:A:314:ASN:ND2	1.84	0.72
1:A:117:VAL:H	1:A:127:ASN:HD21	1.38	0.71
12:A:858:CLA:H143	15:B:835:BCR:H362	1.74	0.69
12:A:814:CLA:HAB	12:A:814:CLA:H8	1.74	0.68
12:A:815:CLA:HBB1	15:K:4005:BCR:H342	1.75	0.68
2:B:133:GLN:HE22	11:M:7:GLN:HE22	1.40	0.67
16:B:851:LHG:H242	16:B:851:LHG:HC81	1.76	0.67
19:A:854:PL9:H18	19:A:854:PL9:C23	2.25	0.67
1:A:421:ASN:HD22	1:A:424:ASN:HD21	1.44	0.66
1:A:12:ALA:N	1:A:314:ASN:HD21	1.87	0.66
1:A:343:ILE:HD11	1:A:421:ASN:HD21	1.61	0.65
12:B:824:CLA:HHD	12:B:824:CLA:HBC2	1.77	0.65
12:A:821:CLA:H52	20:A:856:45D:H221	1.78	0.64
6:F:125:GLU:HG3	6:F:131:LEU:HB2	1.80	0.64
2:B:456:VAL:HG21	6:F:56:ASP:HB3	1.78	0.64
2:B:718:TYR:HB2	12:B:853:CLA:HED2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:819:CLA:H112	15:B:834:BCR:H17C	1.82	0.62
19:A:854:PL9:C21	12:B:801:CLA:H202	2.29	0.62
2:B:235:ALA:O	2:B:253:ALA:HB2	1.99	0.62
9:K:20:VAL:HG13	9:K:77:ILE:HD13	1.81	0.61
11:M:20:PHE:CE2	11:M:24:ARG:HD2	2.35	0.60
12:B:827:CLA:HBC1	12:B:845:CLA:H93	1.84	0.60
12:B:807:CLA:H193	27:M:102:SQD:H382	1.84	0.60
8:J:24:GLY:HA3	12:J:102:CLA:HBB1	1.85	0.59
16:A:850:LHG:H281	16:A:850:LHG:C32	2.32	0.59
18:A:842:LMT:H41	12:A:843:CLA:HBA2	1.85	0.58
6:F:75:ILE:HG23	12:F:203:CLA:HAA1	1.84	0.58
1:A:477:GLN:HE21	1:A:479:GLN:HE21	1.51	0.58
12:A:830:CLA:H111	12:A:830:CLA:HAB	1.85	0.58
2:B:230:TRP:H	18:B:840:LMT:H12	1.70	0.57
12:A:829:CLA:H92	16:A:850:LHG:H321	1.87	0.56
1:A:395:TRP:CD1	12:A:821:CLA:HAB	2.40	0.56
12:B:802:CLA:H61	12:B:850:CLA:H12	1.87	0.56
12:B:803:CLA:HBB1	12:B:803:CLA:CMB	2.35	0.56
12:B:818:CLA:H112	12:B:850:CLA:H42	1.88	0.56
12:K:4003:CLA:HAA2	12:K:4003:CLA:HED2	1.87	0.56
2:B:439:ASP:OD1	2:B:612:TYR:HB2	2.06	0.56
12:K:4003:CLA:HHC	12:K:4003:CLA:HBB1	1.88	0.56
1:A:221:MET:HE1	1:A:274:PHE:HB2	1.87	0.56
10:L:44:LEU:HD22	10:L:48:LEU:HD23	1.87	0.56
1:A:482:PHE:HB3	12:A:849:CLA:H12	1.88	0.55
12:A:848:CLA:HBA1	12:K:4004:CLA:H92	1.88	0.55
1:A:216:GLN:HA	1:A:220:SER:HB2	1.89	0.55
2:B:174:ARG:HB2	12:B:816:CLA:HBC2	1.87	0.55
12:B:819:CLA:H13	15:B:834:BCR:H15C	1.88	0.55
12:B:848:CLA:H61	12:B:848:CLA:H142	1.89	0.54
12:A:855:CLA:H93	12:A:855:CLA:HBB1	1.89	0.54
8:J:31:ARG:CD	15:J:105:BCR:C31	2.83	0.54
19:A:854:PL9:H211	12:B:801:CLA:H202	1.89	0.54
12:B:824:CLA:HBC2	12:B:824:CLA:CHD	2.38	0.54
2:B:409:MET:HE3	15:B:836:BCR:H282	1.90	0.54
12:A:816:CLA:H122	12:A:847:CLA:H93	1.90	0.53
12:A:844:CLA:OBD	12:A:848:CLA:HED2	2.07	0.53
12:B:810:CLA:H192	27:M:102:SQD:H221	1.90	0.53
12:B:828:CLA:H8	15:I:101:BCR:H383	1.89	0.53
12:L:206:CLA:H2	18:L:210:LMT:H42	1.91	0.53
1:A:348:TRP:HB3	12:A:804:CLA:HAC1	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:810:CLA:H71	15:I:101:BCR:HC31	1.89	0.53
8:J:5:LYS:HB3	18:J:106:LMT:H12	1.89	0.53
12:A:844:CLA:H93	15:K:4005:BCR:HC22	1.89	0.53
9:K:71:ILE:HG22	12:K:4004:CLA:HBC1	1.91	0.52
2:B:348:GLN:HA	2:B:351:TYR:HE1	1.74	0.52
12:A:825:CLA:HBC2	12:A:829:CLA:HMC2	1.91	0.52
11:M:31:LYS:HD2	27:M:102:SQD:H2	1.91	0.52
1:A:118:TRP:HB3	15:J:105:BCR:HC21	1.90	0.52
12:B:818:CLA:H13	12:B:850:CLA:H42	1.92	0.52
9:K:73:GLY:O	9:K:77:ILE:HG13	2.10	0.52
19:A:854:PL9:H162	19:A:854:PL9:C20	2.39	0.51
2:B:468:ALA:H	2:B:499:ASN:HD21	1.57	0.51
3:C:15:THR:HG22	3:C:28:MET:HG3	1.92	0.51
12:A:844:CLA:H142	12:A:844:CLA:C10	2.30	0.51
12:B:848:CLA:H201	12:B:849:CLA:H91	1.92	0.50
7:I:13:ILE:O	7:I:17:MET:HG3	2.10	0.50
2:B:355:SER:HB2	12:B:817:CLA:HAA2	1.93	0.50
12:B:824:CLA:HAB	15:F:201:BCR:H323	1.94	0.50
12:A:843:CLA:H92	12:A:846:CLA:H62	1.91	0.50
12:A:844:CLA:C9	15:K:4005:BCR:HC22	2.42	0.50
1:A:319:HIS:HB3	1:A:324:ILE:HD11	1.93	0.49
3:C:24:ASP:OD2	4:D:98:HIS:HD2	1.95	0.49
12:A:832:CLA:HBA2	16:A:839:LHG:H161	1.94	0.49
12:A:844:CLA:H171	12:A:844:CLA:H143	1.93	0.48
15:A:835:BCR:H363	15:A:836:BCR:HC8	1.94	0.48
12:A:823:CLA:H62	16:A:839:LHG:H181	1.95	0.48
10:L:145:LEU:HD11	18:L:210:LMT:H6E	1.95	0.48
2:B:180:ALA:HB2	2:B:288:GLY:HA3	1.96	0.48
12:A:824:CLA:H42	16:A:850:LHG:H241	1.96	0.48
12:A:849:CLA:H61	12:A:849:CLA:H41	1.56	0.48
18:B:840:LMT:H42	18:B:840:LMT:H71	1.54	0.48
12:A:809:CLA:H41	12:A:809:CLA:H62	1.51	0.47
12:A:832:CLA:HBA1	19:A:854:PL9:C26	2.44	0.47
2:B:111:ASN:HD22	7:I:3:GLY:HA2	1.79	0.47
2:B:681:ARG:NE	10:L:19:HIS:HB2	2.29	0.47
12:B:828:CLA:H111	12:B:828:CLA:H71	1.80	0.47
12:B:811:CLA:H143	12:B:811:CLA:H161	1.79	0.47
12:K:4003:CLA:HED2	12:K:4003:CLA:HBD	1.67	0.47
12:A:826:CLA:HAB	12:L:201:CLA:HHB	1.97	0.47
12:B:844:CLA:HMB1	12:B:844:CLA:HBB1	1.96	0.47
2:B:491:LEU:HD23	2:B:491:LEU:HA	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:206:CLA:H151	12:L:206:CLA:H111	1.48	0.47
11:M:1:MET:HB3	11:M:1:MET:HE2	1.84	0.47
1:A:419:ALA:HA	4:D:39:VAL:HG11	1.96	0.47
12:A:825:CLA:H61	12:A:825:CLA:H41	1.57	0.47
2:B:457:PHE:CE2	12:F:204:CLA:HBB1	2.50	0.47
12:A:825:CLA:H62	12:A:825:CLA:H92	1.72	0.46
6:F:75:ILE:O	6:F:78:TRP:HB3	2.15	0.46
1:A:647:ARG:HD2	2:B:630:ASN:HD21	1.81	0.46
15:F:202:BCR:H11C	15:F:202:BCR:H341	1.85	0.46
12:A:846:CLA:H61	12:A:846:CLA:H41	1.62	0.46
12:B:813:CLA:H122	12:B:813:CLA:H8	1.63	0.46
1:A:332:PHE:CE1	12:A:833:CLA:HED2	2.51	0.46
2:B:300:SER:HB3	2:B:303:GLU:HG3	1.97	0.46
4:D:31:THR:HA	4:D:55:ASN:O	2.16	0.46
15:K:4005:BCR:H15C	15:K:4005:BCR:H351	1.84	0.46
2:B:348:GLN:HA	2:B:351:TYR:CE1	2.51	0.46
12:B:803:CLA:HMB3	12:B:803:CLA:CBB	2.42	0.46
18:B:840:LMT:H22	18:B:840:LMT:H51	1.55	0.46
15:B:841:BCR:HC8	12:B:848:CLA:H93	1.97	0.46
12:B:846:CLA:H3A	12:B:846:CLA:HBA1	1.47	0.46
15:A:835:BCR:C36	15:A:836:BCR:HC8	2.46	0.46
12:B:808:CLA:H41	15:B:832:BCR:H383	1.98	0.45
2:B:457:PHE:CZ	12:F:204:CLA:HBB1	2.51	0.45
6:F:91:ARG:C	6:F:93:SER:H	2.23	0.45
12:A:815:CLA:H91	12:A:815:CLA:H112	1.71	0.45
12:A:824:CLA:H61	12:A:824:CLA:H41	1.57	0.45
12:A:848:CLA:H13	12:A:848:CLA:H171	1.79	0.45
12:B:803:CLA:OBD	12:B:853:CLA:HMB3	2.17	0.45
2:B:133:GLN:NE2	11:M:7:GLN:HE22	2.12	0.45
12:A:816:CLA:H2	12:A:816:CLA:H62	1.72	0.45
12:B:802:CLA:H11	12:B:850:CLA:H2	1.99	0.45
12:B:821:CLA:H92	12:B:821:CLA:H61	1.84	0.45
9:K:48:MET:HB3	9:K:48:MET:HE3	1.73	0.45
1:A:325:LEU:O	1:A:337:HIS:HB2	2.16	0.45
12:A:843:CLA:H62	12:A:843:CLA:H41	1.59	0.45
12:B:806:CLA:H143	12:B:806:CLA:H111	1.78	0.45
4:D:131:ILE:HD12	4:D:136:LYS:O	2.16	0.45
1:A:120:ILE:O	1:A:123:GLN:HG2	2.17	0.45
8:J:39:HIS:HA	15:J:107:BCR:H10C	1.99	0.45
10:L:144:ASN:O	10:L:148:VAL:HG23	2.16	0.45
12:B:807:CLA:H141	12:B:807:CLA:H162	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:847:CLA:HBB1	12:B:847:CLA:CHC	2.31	0.45
16:B:851:LHG:H251	12:B:852:CLA:HBA2	1.98	0.45
12:A:831:CLA:HMC1	15:F:201:BCR:H381	1.98	0.45
12:B:848:CLA:H62	12:B:848:CLA:H101	1.68	0.45
10:L:11:TYR:CD1	10:L:19:HIS:HD2	2.35	0.45
12:A:814:CLA:H171	12:A:827:CLA:H41	1.99	0.44
15:L:207:BCR:H15C	15:L:207:BCR:H351	1.87	0.44
10:L:62:ILE:HG21	10:L:138:ALA:HB1	1.99	0.44
1:A:383:TYR:CE2	1:A:618:TRP:HB3	2.53	0.44
12:A:813:CLA:HBA2	12:A:813:CLA:H3A	1.74	0.44
3:C:36:ALA:HB1	3:C:38:GLN:HE21	1.82	0.44
11:M:20:PHE:HB2	16:M:103:LHG:H321	1.99	0.44
2:B:91:ILE:HB	2:B:112:PRO:HB2	2.00	0.44
2:B:133:GLN:HE22	11:M:7:GLN:NE2	2.10	0.44
2:B:438:ASN:HB3	2:B:450:GLN:HE21	1.82	0.44
12:A:803:CLA:HBA1	12:A:803:CLA:H3A	1.60	0.44
12:A:821:CLA:H62	12:A:821:CLA:H41	1.79	0.44
12:A:828:CLA:H92	12:A:828:CLA:H61	1.86	0.44
12:B:819:CLA:H111	15:B:836:BCR:H373	2.00	0.44
8:J:16:MET:O	8:J:20:THR:HG23	2.17	0.44
12:L:204:CLA:H62	12:L:204:CLA:H2	1.72	0.44
1:A:538:HIS:O	1:A:542:ILE:HG13	2.18	0.44
12:A:809:CLA:H112	12:A:809:CLA:H71	1.28	0.44
12:A:810:CLA:HAB	15:A:835:BCR:C14	2.48	0.44
2:B:141:PHE:HZ	12:B:842:CLA:H142	1.83	0.44
12:B:811:CLA:HBA1	12:B:820:CLA:OBD	2.18	0.44
12:B:845:CLA:H142	12:B:845:CLA:H112	1.76	0.44
12:A:820:CLA:H61	12:A:820:CLA:H2	1.72	0.44
12:A:828:CLA:H43	12:A:849:CLA:H71	2.00	0.44
15:A:837:BCR:H20C	15:A:837:BCR:H361	1.86	0.44
16:A:839:LHG:H131	19:A:854:PL9:H251	1.99	0.44
16:A:850:LHG:HC81	16:A:850:LHG:H112	1.49	0.44
15:B:836:BCR:H351	15:B:836:BCR:H15C	1.70	0.44
12:K:4003:CLA:HBB2	15:K:4005:BCR:C19	2.48	0.44
1:A:476:ILE:HG23	17:A:840:LMG:HC8	2.00	0.43
15:A:837:BCR:H15C	15:A:837:BCR:H351	1.76	0.43
12:A:846:CLA:H62	12:A:846:CLA:H92	1.60	0.43
12:B:819:CLA:H61	12:B:819:CLA:H101	1.89	0.43
12:B:806:CLA:H3A	12:B:806:CLA:HBA2	1.60	0.43
6:F:108:ALA:O	6:F:112:MET:HG3	2.18	0.43
12:A:815:CLA:H143	12:A:815:CLA:H111	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:813:CLA:HED2	12:B:813:CLA:H43	2.00	0.43
12:B:819:CLA:HBD	12:B:843:CLA:HED2	2.00	0.43
12:B:820:CLA:H61	12:B:820:CLA:H102	1.86	0.43
12:B:844:CLA:HBD	12:B:844:CLA:HAA2	2.01	0.43
11:M:20:PHE:CZ	11:M:24:ARG:HD2	2.53	0.43
12:B:827:CLA:HBA2	16:B:851:LHG:H383	1.98	0.43
12:J:101:CLA:HBB1	12:J:101:CLA:HMB1	2.00	0.43
12:B:850:CLA:HAB	12:B:852:CLA:HBC2	2.01	0.43
3:C:46:GLU:HG2	3:C:47:ASP:N	2.31	0.43
20:A:856:45D:H311	20:A:856:45D:H273	1.85	0.43
2:B:218:HIS:HD2	2:B:220:ALA:H	1.65	0.43
12:B:802:CLA:H42	12:B:819:CLA:H101	1.99	0.43
12:B:806:CLA:H61	12:B:806:CLA:H41	1.51	0.43
12:B:802:CLA:H62	16:B:851:LHG:H202	2.01	0.43
4:D:13:GLY:HA2	10:L:15:PRO:O	2.19	0.43
12:A:831:CLA:H41	12:A:831:CLA:H61	1.63	0.43
12:B:806:CLA:H141	12:B:806:CLA:H161	1.69	0.43
12:A:814:CLA:H141	12:A:820:CLA:H192	2.01	0.43
12:A:827:CLA:H62	12:K:4004:CLA:H141	2.00	0.43
4:D:73:ARG:HG3	4:D:83:TYR:HE1	1.83	0.43
12:B:842:CLA:H143	12:B:842:CLA:H111	1.80	0.43
8:J:36:LEU:HD23	8:J:36:LEU:HA	1.90	0.43
12:A:809:CLA:H203	12:A:809:CLA:H161	1.89	0.42
2:B:172:GLU:HG3	2:B:291:TYR:HB3	2.00	0.42
10:L:38:PRO:HB3	10:L:52:GLU:OE2	2.19	0.42
12:A:801:CLA:HBD	12:A:809:CLA:O1A	2.18	0.42
12:A:828:CLA:H143	12:A:828:CLA:H162	1.84	0.42
19:A:854:PL9:H102	15:F:201:BCR:H271	1.99	0.42
12:B:802:CLA:H193	12:B:802:CLA:H162	1.90	0.42
12:B:843:CLA:H93	12:B:843:CLA:H111	1.86	0.42
1:A:523:MET:HE3	1:A:523:MET:HB2	1.92	0.42
12:A:826:CLA:H112	12:A:826:CLA:H71	1.49	0.42
12:A:858:CLA:H143	12:A:858:CLA:H111	1.60	0.42
2:B:302:LYS:HE3	2:B:302:LYS:HB2	1.79	0.42
2:B:545:PRO:HB3	28:E:124:HOH:O	2.19	0.42
12:B:844:CLA:HBB1	12:B:844:CLA:CMB	2.50	0.42
12:A:809:CLA:C4A	12:A:809:CLA:HBA2	2.48	0.42
12:A:849:CLA:H142	12:A:849:CLA:H111	1.92	0.42
2:B:254:ILE:HG13	2:B:255:LEU:HG	2.00	0.42
12:B:809:CLA:H152	12:B:809:CLA:H112	1.69	0.42
12:L:204:CLA:H3A	12:L:204:CLA:HBA2	1.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:THR:HG23	1:A:606:ILE:HG21	2.00	0.42
12:A:844:CLA:C1A	12:A:844:CLA:CGA	2.97	0.42
12:B:845:CLA:H161	12:B:845:CLA:H192	1.81	0.42
12:A:827:CLA:H2	12:K:4004:CLA:H142	2.01	0.42
12:A:844:CLA:H162	12:A:844:CLA:H141	1.67	0.42
2:B:447:PRO:HB2	6:F:50:TYR:CZ	2.55	0.42
2:B:468:ALA:H	2:B:499:ASN:ND2	2.17	0.42
12:B:810:CLA:HHB	12:B:811:CLA:HMB3	2.02	0.42
12:B:853:CLA:H122	12:B:853:CLA:H8	1.91	0.42
12:A:846:CLA:CHB	12:A:846:CLA:H42	2.50	0.42
12:B:814:CLA:H122	15:B:832:BCR:H312	2.02	0.42
18:B:840:LMT:H2'	18:B:840:LMT:H11	1.67	0.42
12:A:823:CLA:H41	12:A:823:CLA:H61	1.65	0.42
12:A:827:CLA:H203	15:A:837:BCR:H19C	2.01	0.42
12:A:830:CLA:H203	12:A:831:CLA:H51	2.02	0.42
12:A:848:CLA:H61	12:A:848:CLA:H41	1.85	0.42
2:B:676:VAL:HG13	2:B:690:TRP:CH2	2.55	0.42
15:B:834:BCR:H15C	15:B:834:BCR:H351	1.90	0.42
3:C:34:CYS:HA	5:E:33:ILE:HG23	2.00	0.42
10:L:42:LYS:HA	10:L:42:LYS:HD3	1.91	0.42
15:L:208:BCR:H11C	15:L:208:BCR:H341	1.87	0.42
1:A:604:ILE:HG13	13:A:802:CL0:H66	2.01	0.42
18:A:842:LMT:H122	12:A:843:CLA:CAB	2.50	0.42
12:B:805:CLA:HMB2	12:B:826:CLA:HBA2	2.02	0.42
12:B:807:CLA:H161	12:B:807:CLA:H202	1.84	0.42
12:B:809:CLA:H161	12:B:809:CLA:H193	1.77	0.42
12:B:814:CLA:H203	23:B:833:ECH:H35B	2.00	0.42
12:B:842:CLA:H61	12:B:842:CLA:H41	1.80	0.42
12:B:847:CLA:H142	12:B:847:CLA:H111	1.80	0.42
18:A:842:LMT:H111	18:A:842:LMT:H82	1.55	0.41
20:A:856:45D:H131	20:A:856:45D:H201	1.86	0.41
9:K:39:ILE:HB	9:K:42:GLN:HG2	2.02	0.41
9:K:48:MET:HA	9:K:49:PRO:HD3	1.82	0.41
10:L:145:LEU:HD21	18:L:210:LMT:H6E	2.01	0.41
27:M:102:SQD:H241	27:M:102:SQD:H272	1.73	0.41
1:A:296:HIS:O	1:A:300:ILE:HG12	2.20	0.41
12:A:845:CLA:H52	12:A:845:CLA:H12	1.77	0.41
4:D:132:LYS:HE3	4:D:133:PHE:CE2	2.55	0.41
12:A:809:CLA:H93	12:A:809:CLA:H61	1.89	0.41
12:A:843:CLA:H52	12:A:846:CLA:ND	2.35	0.41
12:B:811:CLA:H162	12:B:811:CLA:H202	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:63:GLY:HA3	8:J:39:HIS:HB3	2.03	0.41
9:K:36:LYS:HG2	12:K:4003:CLA:HBA2	2.02	0.41
26:L:209:DGD:HAN1	26:L:209:DGD:HB61	2.01	0.41
12:A:830:CLA:HAB	12:A:830:CLA:C11	2.50	0.41
12:B:823:CLA:H93	15:F:202:BCR:H15C	2.02	0.41
15:F:202:BCR:H14C	18:F:205:LMT:H52	2.03	0.41
18:A:842:LMT:H22	18:A:842:LMT:H51	1.76	0.41
12:B:847:CLA:H3A	12:B:847:CLA:HBA2	1.76	0.41
12:B:848:CLA:H62	12:B:848:CLA:H41	1.60	0.41
12:A:807:CLA:HAB	12:A:821:CLA:H93	2.02	0.41
19:A:854:PL9:C20	19:A:854:PL9:C16	2.99	0.41
2:B:69:ALA:HB2	2:B:135:LEU:HB2	2.02	0.41
15:I:101:BCR:H15C	15:I:101:BCR:H351	1.93	0.41
12:J:102:CLA:CHA	12:J:102:CLA:HBA1	2.50	0.41
9:K:16:TRP:CZ2	9:K:21:ALA:HB2	2.55	0.41
12:K:4003:CLA:HAA2	12:K:4003:CLA:HBD	2.01	0.41
1:A:292:ASP:HB3	12:A:813:CLA:HMA1	2.01	0.41
12:A:846:CLA:H3A	12:A:846:CLA:HBA2	1.59	0.41
2:B:495:LEU:HD23	2:B:495:LEU:HA	1.75	0.41
2:B:577:MET:HE3	2:B:577:MET:HB3	1.92	0.41
12:B:847:CLA:HBB2	12:B:849:CLA:CHD	2.51	0.41
17:A:840:LMG:C10	26:L:209:DGD:HA72	2.51	0.41
17:A:851:LMG:H112	17:A:851:LMG:H141	1.64	0.41
12:B:825:CLA:CMB	15:J:107:BCR:H19C	2.51	0.41
12:J:101:CLA:H11	12:J:101:CLA:H52	1.77	0.41
10:L:24:ILE:HD13	10:L:24:ILE:HA	1.81	0.41
1:A:203:GLY:O	1:A:207:LEU:HB2	2.21	0.41
12:A:819:CLA:CHB	12:A:829:CLA:HAA2	2.50	0.41
18:A:841:LMT:H102	18:A:841:LMT:H71	1.69	0.41
12:A:846:CLA:H42	12:A:846:CLA:C1B	2.51	0.41
12:B:844:CLA:H93	12:B:844:CLA:H112	1.53	0.41
6:F:25:ASN:HD22	6:F:33:GLY:H	1.69	0.41
15:L:207:BCR:H11C	15:L:207:BCR:H341	1.90	0.41
27:M:102:SQD:H152	27:M:102:SQD:H182	1.78	0.41
1:A:421:ASN:ND2	1:A:424:ASN:HD21	2.15	0.41
2:B:687:LEU:HD11	10:L:39:ALA:HB1	2.03	0.41
12:B:820:CLA:HBC3	17:B:837:LMG:H441	2.03	0.41
12:B:827:CLA:NC	16:B:851:LHG:H352	2.35	0.41
4:D:27:LYS:HG2	4:D:88:VAL:HB	2.03	0.41
15:L:207:BCR:H20C	15:L:207:BCR:H361	1.95	0.41
12:A:847:CLA:H41	12:A:847:CLA:H62	1.71	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:824:CLA:HBB1	12:B:824:CLA:CMB	2.44	0.40
8:J:8:LEU:O	8:J:14:MET:HE3	2.20	0.40
16:A:839:LHG:H131	19:A:854:PL9:C26	2.51	0.40
2:B:22:TRP:CG	2:B:701:GLN:HE22	2.40	0.40
12:B:806:CLA:H152	12:B:806:CLA:H18	1.92	0.40
15:J:107:BCR:H371	15:J:107:BCR:H24C	1.74	0.40
12:A:843:CLA:H93	12:A:843:CLA:H61	1.79	0.40
2:B:299:HIS:HB3	2:B:304:ILE:HD11	2.02	0.40
12:B:822:CLA:H141	12:B:822:CLA:H161	1.67	0.40
15:I:101:BCR:H392	15:I:101:BCR:H24C	1.80	0.40
1:A:184:ALA:HA	1:A:185:PRO:HD3	1.95	0.40
12:A:804:CLA:H3A	12:A:804:CLA:HBA1	1.87	0.40
12:A:827:CLA:H93	12:A:827:CLA:H111	1.83	0.40
2:B:460:TRP:O	2:B:464:THR:HG23	2.22	0.40
5:E:3:LEU:HD13	5:E:37:VAL:HG11	2.03	0.40
12:L:204:CLA:H202	12:L:204:CLA:H161	1.91	0.40
17:A:851:LMG:H162	17:A:851:LMG:H132	1.77	0.40
12:B:827:CLA:HAA2	12:B:843:CLA:CHB	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	740/751 (98%)	722 (98%)	17 (2%)	1 (0%)	48	31
2	B	727/731 (100%)	695 (96%)	32 (4%)	0	100	100
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
4	D	137/141 (97%)	134 (98%)	3 (2%)	0	100	100
5	E	67/74 (90%)	64 (96%)	3 (4%)	0	100	100
6	F	139/165 (84%)	133 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	I	36/40 (90%)	34 (94%)	2 (6%)	0	100	100
8	J	37/40 (92%)	37 (100%)	0	0	100	100
9	K	76/86 (88%)	73 (96%)	3 (4%)	0	100	100
10	L	152/157 (97%)	145 (95%)	7 (5%)	0	100	100
11	M	29/31 (94%)	29 (100%)	0	0	100	100
All	All	2218/2297 (97%)	2142 (97%)	75 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	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	589/603 (98%)	589 (100%)	0	100	100
2	B	579/583 (99%)	579 (100%)	0	100	100
3	C	68/69 (99%)	68 (100%)	0	100	100
4	D	111/116 (96%)	111 (100%)	0	100	100
5	E	56/60 (93%)	56 (100%)	0	100	100
6	F	114/137 (83%)	112 (98%)	2 (2%)	51	27
7	I	31/32 (97%)	31 (100%)	0	100	100
8	J	34/35 (97%)	34 (100%)	0	100	100
9	K	55/62 (89%)	55 (100%)	0	100	100
10	L	115/118 (98%)	115 (100%)	0	100	100
11	M	25/25 (100%)	25 (100%)	0	100	100
All	All	1777/1840 (97%)	1775 (100%)	2 (0%)	87	83

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

Mol	Chain	Res	Type
6	F	44	LEU
6	F	89	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	61	GLN
1	A	115	GLN
1	A	127	ASN
1	A	267	ASN
1	A	314	ASN
1	A	421	ASN
1	A	439	HIS
1	A	477	GLN
1	A	488	HIS
1	A	500	ASN
1	A	567	ASN
1	A	637	GLN
1	A	643	ASN
1	A	659	ASN
1	A	714	GLN
2	B	14	GLN
2	B	29	HIS
2	B	76	GLN
2	B	83	ASN
2	B	111	ASN
2	B	133	GLN
2	B	158	GLN
2	B	218	HIS
2	B	294	ASN
2	B	306	ASN
2	B	319	ASN
2	B	326	ASN
2	B	331	GLN
2	B	401	ASN
2	B	437	HIS
2	B	450	GLN
2	B	499	ASN
2	B	518	HIS
2	B	595	HIS
2	B	624	ASN
2	B	630	ASN

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Mol	Chain	Res	Type
2	B	679	HIS
3	C	38	GLN
4	D	7	GLN
4	D	98	HIS
4	D	115	GLN
6	F	13	ASN
6	F	25	ASN
9	K	28	ASN
9	K	70	HIS
10	L	12	ASN
10	L	19	HIS
10	L	77	GLN
10	L	108	GLN
10	L	144	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 144 ligands modelled in this entry, 3 are monoatomic - leaving 141 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	A	828	1	69,73,73	2.18	23 (33%)	82,113,113	2.42	24 (29%)
12	CLA	A	817	1	54,58,73	2.52	22 (40%)	64,95,113	2.69	23 (35%)
12	CLA	F	203	28	49,53,73	2.54	20 (40%)	58,89,113	2.61	23 (39%)
12	CLA	B	823	2	59,63,73	2.45	24 (40%)	70,101,113	2.52	24 (34%)
12	CLA	A	843	1	64,68,73	2.28	22 (34%)	76,107,113	2.58	28 (36%)
12	CLA	B	852	2	54,58,73	2.60	23 (42%)	64,95,113	2.75	25 (39%)
16	LHG	M	103	-	43,43,48	1.04	2 (4%)	46,49,54	1.26	5 (10%)
17	LMG	A	840	-	50,50,55	1.49	8 (16%)	58,58,63	1.52	8 (13%)
12	CLA	A	808	1	54,58,73	2.52	21 (38%)	64,95,113	2.75	27 (42%)
12	CLA	B	807	2	69,73,73	2.22	23 (33%)	82,113,113	2.44	25 (30%)
12	CLA	F	204	6	49,53,73	2.58	22 (44%)	58,89,113	2.81	25 (43%)
15	BCR	B	835	-	41,41,41	4.66	24 (58%)	56,56,56	2.24	23 (41%)
14	SF4	A	834	1,2	0,12,12	-	-	-	-	-
12	CLA	A	823	1	69,73,73	2.22	22 (31%)	82,113,113	2.43	25 (30%)
12	CLA	B	846	2	59,63,73	2.28	21 (35%)	70,101,113	2.96	29 (41%)
15	BCR	B	832	-	41,41,41	4.80	24 (58%)	56,56,56	2.06	18 (32%)
16	LHG	A	839	-	48,48,48	0.92	2 (4%)	51,54,54	0.97	3 (5%)
15	BCR	F	201	-	41,41,41	4.80	24 (58%)	56,56,56	2.17	23 (41%)
12	CLA	A	804	1	69,73,73	2.19	23 (33%)	82,113,113	2.45	25 (30%)
12	CLA	B	828	28	69,73,73	2.21	22 (31%)	82,113,113	2.36	23 (28%)
15	BCR	A	835	-	41,41,41	4.74	24 (58%)	56,56,56	2.25	23 (41%)
27	SQD	M	102	-	52,54,54	1.52	7 (13%)	62,65,65	1.53	10 (16%)
12	CLA	B	809	2	69,73,73	2.23	20 (28%)	82,113,113	2.32	23 (28%)
12	CLA	A	818	28	69,73,73	2.24	22 (31%)	82,113,113	2.51	25 (30%)
12	CLA	A	846	1	59,63,73	2.45	20 (33%)	70,101,113	2.79	25 (35%)
12	CLA	B	830	16	49,53,73	2.55	22 (44%)	58,89,113	2.81	24 (41%)
12	CLA	A	849	1	69,73,73	2.21	22 (31%)	82,113,113	2.37	25 (30%)
12	CLA	A	811	1	49,53,73	2.51	21 (42%)	58,89,113	2.71	22 (37%)
12	CLA	B	814	2	69,73,73	2.26	24 (34%)	82,113,113	2.41	24 (29%)
18	LMT	A	842	-	36,36,36	0.55	0	47,47,47	0.87	1 (2%)
12	CLA	B	812	2	69,73,73	2.20	22 (31%)	82,113,113	2.45	27 (32%)
12	CLA	B	826	28	69,73,73	2.24	23 (33%)	82,113,113	2.47	26 (31%)
15	BCR	L	207	-	41,41,41	4.72	24 (58%)	56,56,56	2.37	25 (44%)
16	LHG	A	850	12	36,36,48	1.20	4 (11%)	39,42,54	1.65	6 (15%)
25	EQ3	L	202	-	43,43,43	1.31	8 (18%)	55,60,60	1.57	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	BCR	B	836	-	25,25,41	4.34	12 (48%)	33,33,56	2.81	16 (48%)
12	CLA	B	802	28	69,73,73	2.22	22 (31%)	82,113,113	2.45	26 (31%)
12	CLA	A	809	1,12	69,73,73	2.16	21 (30%)	82,113,113	2.69	31 (37%)
12	CLA	A	845	1	69,73,73	2.21	22 (31%)	82,113,113	2.41	26 (31%)
18	LMT	B	839	-	30,30,36	0.59	0	41,41,47	0.82	1 (2%)
12	CLA	A	810	1	54,58,73	2.50	20 (37%)	64,95,113	2.70	23 (35%)
12	CLA	B	805	28	49,53,73	2.54	22 (44%)	58,89,113	4.41	21 (36%)
18	LMT	A	853	-	36,36,36	0.55	0	47,47,47	0.85	3 (6%)
23	ECH	M	101	-	42,42,42	0.44	0	55,58,58	0.90	3 (5%)
12	CLA	B	819	2	69,73,73	2.19	21 (30%)	82,113,113	2.40	23 (28%)
12	CLA	A	830	1	69,73,73	2.24	23 (33%)	82,113,113	2.36	27 (32%)
12	CLA	A	814	1	69,73,73	2.21	22 (31%)	82,113,113	2.30	25 (30%)
18	LMT	J	106	-	32,32,36	0.56	0	43,43,47	1.09	3 (6%)
12	CLA	B	804	2	69,73,73	2.25	22 (31%)	82,113,113	2.45	26 (31%)
12	CLA	A	848	1	69,73,73	2.20	22 (31%)	82,113,113	2.45	25 (30%)
12	CLA	B	825	2	59,63,73	2.42	23 (38%)	70,101,113	2.62	27 (38%)
13	CL0	A	802	1	69,73,73	2.20	23 (33%)	82,113,113	2.40	23 (28%)
12	CLA	B	843	28	69,73,73	2.22	22 (31%)	82,113,113	2.41	25 (30%)
12	CLA	B	808	2	69,73,73	2.24	23 (33%)	82,113,113	2.34	21 (25%)
12	CLA	A	819	28	64,68,73	2.32	23 (35%)	76,107,113	2.54	25 (32%)
12	CLA	B	811	2	69,73,73	2.17	21 (30%)	82,113,113	2.57	28 (34%)
12	CLA	B	849	2	64,68,73	2.29	21 (32%)	76,107,113	2.71	26 (34%)
14	SF4	C	101	3	0,12,12	-	-	-	-	-
17	LMG	B	837	-	51,51,55	1.44	7 (13%)	59,59,63	1.07	5 (8%)
12	CLA	A	822	1	69,73,73	2.24	21 (30%)	82,113,113	2.30	20 (24%)
12	CLA	B	853	2	69,73,73	2.21	22 (31%)	82,113,113	2.80	26 (31%)
12	CLA	K	4003	9	49,53,73	1.44	8 (16%)	58,89,113	1.09	5 (8%)
12	CLA	L	204	-	69,73,73	2.24	23 (33%)	82,113,113	2.44	24 (29%)
12	CLA	A	855	28	69,73,73	2.21	23 (33%)	82,113,113	2.56	28 (34%)
12	CLA	B	815	2	49,53,73	2.55	22 (44%)	58,89,113	2.64	21 (36%)
15	BCR	A	837	-	41,41,41	4.69	24 (58%)	56,56,56	2.46	22 (39%)
12	CLA	A	816	28	69,73,73	2.25	23 (33%)	82,113,113	2.34	26 (31%)
14	SF4	C	102	3	0,12,12	-	-	-	-	-
12	CLA	B	829	2	69,73,73	2.19	23 (33%)	82,113,113	2.46	23 (28%)
12	CLA	A	826	1	69,73,73	2.20	22 (31%)	82,113,113	2.41	24 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	A	833	16	54,58,73	2.53	23 (42%)	64,95,113	2.74	25 (39%)
18	LMT	B	840	-	36,36,36	0.48	0	47,47,47	1.47	6 (12%)
12	CLA	K	4002	9	49,53,73	2.54	21 (42%)	58,89,113	2.80	28 (48%)
12	CLA	J	102	-	49,53,73	2.54	22 (44%)	58,89,113	2.70	22 (37%)
12	CLA	A	831	28	69,73,73	2.22	22 (31%)	82,113,113	2.59	26 (31%)
12	CLA	L	201	1	69,73,73	2.22	22 (31%)	82,113,113	2.49	22 (26%)
12	CLA	A	852	28	59,63,73	2.58	24 (40%)	70,101,113	2.79	28 (40%)
12	CLA	A	844	1	69,73,73	2.12	19 (27%)	82,113,113	2.78	28 (34%)
12	CLA	B	827	2	49,53,73	2.51	20 (40%)	58,89,113	2.82	19 (32%)
15	BCR	K	4001	-	41,41,41	4.79	24 (58%)	56,56,56	2.30	21 (37%)
12	CLA	B	847	2	69,73,73	2.04	19 (27%)	82,113,113	2.49	24 (29%)
12	CLA	A	825	1	64,68,73	2.28	23 (35%)	76,107,113	2.59	27 (35%)
12	CLA	B	803	28	69,73,73	2.22	20 (28%)	82,113,113	2.85	28 (34%)
18	LMT	A	841	-	36,36,36	0.56	0	47,47,47	0.71	0
12	CLA	A	858	-	69,73,73	2.17	21 (30%)	82,113,113	2.53	27 (32%)
12	CLA	B	824	2	69,73,73	2.10	18 (26%)	82,113,113	2.66	27 (32%)
15	BCR	J	105	-	41,41,41	4.77	25 (60%)	56,56,56	3.14	28 (50%)
12	CLA	A	832	1	54,58,73	2.53	22 (40%)	64,95,113	2.71	24 (37%)
12	CLA	B	820	2	69,73,73	2.21	21 (30%)	82,113,113	2.41	24 (29%)
16	LHG	B	851	12	48,48,48	0.98	2 (4%)	51,54,54	1.34	7 (13%)
12	CLA	B	817	2	69,73,73	2.19	21 (30%)	82,113,113	2.48	29 (35%)
12	CLA	K	4004	28	64,68,73	2.25	22 (34%)	76,107,113	3.03	32 (42%)
12	CLA	B	813	2	69,73,73	2.22	23 (33%)	82,113,113	2.53	26 (31%)
18	LMT	F	205	-	32,32,36	0.58	0	43,43,47	0.88	2 (4%)
12	CLA	B	850	2	69,73,73	2.26	23 (33%)	82,113,113	2.37	29 (35%)
12	CLA	A	847	1	69,73,73	2.19	22 (31%)	82,113,113	2.39	25 (30%)
12	CLA	A	821	1	69,73,73	2.23	22 (31%)	82,113,113	2.46	24 (29%)
12	CLA	B	816	2	69,73,73	2.22	23 (33%)	82,113,113	2.40	25 (30%)
12	CLA	J	101	1	64,68,73	2.41	23 (35%)	76,107,113	2.65	28 (36%)
12	CLA	B	818	28	69,73,73	2.21	22 (31%)	82,113,113	2.49	29 (35%)
12	CLA	A	824	1	59,63,73	2.39	23 (38%)	70,101,113	2.61	27 (38%)
12	CLA	A	829	1	69,73,73	2.24	24 (34%)	82,113,113	2.55	28 (34%)
15	BCR	B	841	-	41,41,41	4.73	24 (58%)	56,56,56	2.34	20 (35%)
12	CLA	A	820	1	69,73,73	2.20	21 (30%)	82,113,113	2.44	26 (31%)
12	CLA	A	803	1	69,73,73	2.24	22 (31%)	82,113,113	2.47	27 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	A	813	1	64,68,73	2.32	23 (35%)	76,107,113	2.48	27 (35%)
15	BCR	F	202	-	41,41,41	4.79	24 (58%)	56,56,56	2.27	21 (37%)
12	CLA	A	812	28	49,53,73	2.55	23 (46%)	58,89,113	2.72	23 (39%)
15	BCR	K	4005	-	41,41,41	4.77	24 (58%)	56,56,56	2.12	28 (50%)
12	CLA	A	801	1,12	64,68,73	2.29	23 (35%)	76,107,113	2.62	28 (36%)
12	CLA	B	810	2	69,73,73	2.22	22 (31%)	82,113,113	2.33	23 (28%)
15	BCR	B	834	-	41,41,41	4.74	24 (58%)	56,56,56	2.25	25 (44%)
15	BCR	J	107	-	41,41,41	4.72	24 (58%)	56,56,56	2.60	24 (42%)
22	A1AGD	B	831	-	30,30,30	0.84	1 (3%)	38,39,39	1.45	5 (13%)
15	BCR	A	836	-	41,41,41	4.75	24 (58%)	56,56,56	2.29	23 (41%)
17	LMG	A	851	-	46,46,55	1.42	6 (13%)	54,54,63	1.75	11 (20%)
12	CLA	B	842	2	69,73,73	2.22	23 (33%)	82,113,113	2.41	24 (29%)
12	CLA	B	845	2	69,73,73	2.23	22 (31%)	82,113,113	2.44	26 (31%)
26	DGD	L	209	-	49,49,67	1.42	6 (12%)	57,57,81	1.16	3 (5%)
12	CLA	B	821	2	69,73,73	2.23	22 (31%)	82,113,113	2.35	25 (30%)
12	CLA	A	827	1	69,73,73	2.21	23 (33%)	82,113,113	2.42	27 (32%)
19	PL9	A	854	-	30,30,55	0.93	2 (6%)	38,39,69	2.03	15 (39%)
15	BCR	J	104	-	14,14,41	5.39	8 (57%)	20,20,56	2.81	9 (45%)
12	CLA	B	844	2	64,68,73	2.24	23 (35%)	76,107,113	3.15	27 (35%)
12	CLA	B	801	-	69,73,73	2.20	22 (31%)	82,113,113	2.51	27 (32%)
12	CLA	A	807	1	59,63,73	2.39	23 (38%)	70,101,113	2.70	25 (35%)
12	CLA	A	805	1	69,73,73	2.24	22 (31%)	82,113,113	2.57	30 (36%)
12	CLA	B	848	2	69,73,73	2.27	23 (33%)	82,113,113	2.48	25 (30%)
12	CLA	B	822	2	69,73,73	2.21	22 (31%)	82,113,113	2.45	27 (32%)
15	BCR	A	838	-	41,41,41	4.75	24 (58%)	56,56,56	2.25	20 (35%)
12	CLA	B	806	2	69,73,73	2.24	22 (31%)	82,113,113	2.42	25 (30%)
12	CLA	L	206	28	69,73,73	2.24	23 (33%)	82,113,113	2.46	24 (29%)
18	LMT	L	210	-	36,36,36	0.50	0	47,47,47	1.07	4 (8%)
15	BCR	I	101	-	41,41,41	4.81	24 (58%)	56,56,56	2.18	19 (33%)
12	CLA	A	815	1	69,73,73	2.23	22 (31%)	82,113,113	2.44	24 (29%)
12	CLA	J	103	8	49,53,73	2.59	24 (48%)	58,89,113	3.04	26 (44%)
20	45D	A	856	-	43,43,43	1.50	8 (18%)	54,60,60	1.80	17 (31%)
12	CLA	L	205	10	69,73,73	2.20	21 (30%)	82,113,113	2.52	25 (30%)
15	BCR	L	208	-	41,41,41	4.80	24 (58%)	56,56,56	2.27	20 (35%)
12	CLA	A	806	1	49,53,73	2.52	21 (42%)	58,89,113	2.77	22 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	ECH	B	833	-	42,42,42	0.40	0	55,58,58	0.75	1 (1%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	A	828	1	-	16/39/115/115	-
12	CLA	A	817	1	-	6/21/97/115	-
12	CLA	F	203	28	-	1/15/91/115	-
12	CLA	B	823	2	-	9/27/103/115	-
12	CLA	A	843	1	-	13/33/109/115	-
12	CLA	B	852	2	-	3/21/97/115	-
16	LHG	M	103	-	-	25/48/48/53	-
17	LMG	A	840	-	-	18/45/65/70	0/1/1/1
12	CLA	A	808	1	-	8/21/97/115	-
12	CLA	B	807	2	-	9/39/115/115	-
12	CLA	F	204	6	-	9/15/91/115	-
15	BCR	B	835	-	-	2/29/63/63	0/2/2/2
14	SF4	A	834	1,2	-	-	0/6/5/5
12	CLA	A	823	1	-	15/39/115/115	-
12	CLA	B	846	2	-	12/27/103/115	-
15	BCR	B	832	-	-	4/29/63/63	0/2/2/2
16	LHG	A	839	-	-	24/53/53/53	-
15	BCR	F	201	-	-	5/29/63/63	0/2/2/2
12	CLA	A	804	1	-	19/39/115/115	-
12	CLA	B	828	28	-	6/39/115/115	-
15	BCR	A	835	-	-	8/29/63/63	0/2/2/2
27	SQD	M	102	-	-	28/49/69/69	0/1/1/1
12	CLA	B	809	2	-	10/39/115/115	-
12	CLA	A	818	28	-	7/39/115/115	-
12	CLA	A	846	1	-	11/27/103/115	-
12	CLA	B	830	16	-	4/15/91/115	-
12	CLA	A	849	1	-	14/39/115/115	-
12	CLA	A	811	1	-	3/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	B	814	2	-	17/39/115/115	-
18	LMT	A	842	-	-	12/21/61/61	0/2/2/2
12	CLA	B	812	2	-	6/39/115/115	-
12	CLA	B	826	28	-	11/39/115/115	-
15	BCR	L	207	-	-	6/29/63/63	0/2/2/2
16	LHG	A	850	12	-	14/41/41/53	-
25	EQ3	L	202	-	-	5/29/68/68	0/2/2/2
15	BCR	B	836	-	-	8/18/35/63	0/1/1/2
12	CLA	B	802	28	-	10/39/115/115	-
12	CLA	A	809	1,12	-	17/39/115/115	-
12	CLA	A	845	1	-	11/39/115/115	-
18	LMT	B	839	-	-	5/15/55/61	0/2/2/2
12	CLA	A	810	1	-	5/21/97/115	-
12	CLA	B	805	28	-	3/15/91/115	-
18	LMT	A	853	-	-	4/21/61/61	0/2/2/2
23	ECH	M	101	-	-	6/29/66/66	0/2/2/2
12	CLA	B	819	2	-	4/39/115/115	-
12	CLA	A	830	1	-	6/39/115/115	-
12	CLA	A	814	1	-	6/39/115/115	-
18	LMT	J	106	-	-	10/17/57/61	0/2/2/2
12	CLA	B	804	2	-	13/39/115/115	-
12	CLA	A	848	1	-	21/39/115/115	-
12	CLA	B	825	2	-	11/27/103/115	-
13	CL0	A	802	1	-	5/39/115/115	-
12	CLA	B	843	28	-	19/39/115/115	-
12	CLA	B	808	2	-	11/39/115/115	-
12	CLA	A	819	28	-	8/33/109/115	-
12	CLA	B	811	2	-	7/39/115/115	-
12	CLA	B	849	2	-	11/33/109/115	-
17	LMG	B	837	-	-	12/46/66/70	0/1/1/1
14	SF4	C	101	3	-	-	0/6/5/5
12	CLA	A	822	1	-	5/39/115/115	-
12	CLA	B	853	2	-	5/39/115/115	-
12	CLA	K	4003	9	-	2/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	L	204	-	-	16/39/115/115	-
12	CLA	A	855	28	-	7/39/115/115	-
12	CLA	B	815	2	-	3/15/91/115	-
15	BCR	A	837	-	-	4/29/63/63	0/2/2/2
12	CLA	A	816	28	-	5/39/115/115	-
14	SF4	C	102	3	-	-	0/6/5/5
12	CLA	B	829	2	-	15/39/115/115	-
12	CLA	A	826	1	-	13/39/115/115	-
12	CLA	A	833	16	-	6/21/97/115	-
18	LMT	B	840	-	-	12/21/61/61	0/2/2/2
12	CLA	K	4002	9	-	9/15/91/115	-
12	CLA	J	102	-	-	7/15/91/115	-
12	CLA	A	831	28	-	15/39/115/115	-
12	CLA	L	201	1	-	7/39/115/115	-
12	CLA	A	852	28	-	4/27/103/115	-
12	CLA	A	844	1	-	12/39/115/115	-
12	CLA	B	827	2	-	3/15/91/115	-
15	BCR	K	4001	-	-	4/29/63/63	0/2/2/2
12	CLA	B	847	2	-	4/39/115/115	-
12	CLA	A	825	1	-	12/33/109/115	-
12	CLA	B	803	28	-	3/39/115/115	-
18	LMT	A	841	-	-	9/21/61/61	0/2/2/2
12	CLA	A	858	-	-	10/39/115/115	-
12	CLA	B	824	2	-	9/39/115/115	-
15	BCR	J	105	-	-	7/29/63/63	0/2/2/2
12	CLA	A	832	1	-	7/21/97/115	-
12	CLA	B	820	2	-	19/39/115/115	-
16	LHG	B	851	12	-	26/53/53/53	-
12	CLA	B	817	2	-	14/39/115/115	-
12	CLA	K	4004	28	-	9/33/109/115	-
12	CLA	B	813	2	-	9/39/115/115	-
18	LMT	F	205	-	-	4/17/57/61	0/2/2/2
12	CLA	B	850	2	-	9/39/115/115	-
12	CLA	A	847	1	-	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	A	821	1	-	10/39/115/115	-
12	CLA	B	816	2	-	19/39/115/115	-
12	CLA	J	101	1	-	16/33/109/115	-
12	CLA	B	818	28	-	14/39/115/115	-
12	CLA	A	824	1	-	14/27/103/115	-
12	CLA	A	829	1	-	12/39/115/115	-
15	BCR	B	841	-	-	9/29/63/63	0/2/2/2
12	CLA	A	820	1	-	6/39/115/115	-
12	CLA	A	803	1	-	12/39/115/115	-
12	CLA	A	813	1	-	11/33/109/115	-
15	BCR	F	202	-	-	2/29/63/63	0/2/2/2
12	CLA	A	812	28	-	6/15/91/115	-
15	BCR	K	4005	-	-	8/29/63/63	0/2/2/2
12	CLA	A	801	1,12	-	12/33/109/115	-
12	CLA	B	810	2	-	10/39/115/115	-
15	BCR	B	834	-	-	2/29/63/63	0/2/2/2
15	BCR	J	107	-	-	10/29/63/63	0/2/2/2
22	A1AGD	B	831	-	-	10/23/43/43	0/1/1/1
15	BCR	A	836	-	-	1/29/63/63	0/2/2/2
17	LMG	A	851	-	-	21/41/61/70	0/1/1/1
12	CLA	B	842	2	-	17/39/115/115	-
12	CLA	B	845	2	-	13/39/115/115	-
26	DGD	L	209	-	-	23/44/64/95	0/1/1/2
12	CLA	B	821	2	-	6/39/115/115	-
12	CLA	A	827	1	-	16/39/115/115	-
19	PL9	A	854	-	-	5/23/43/73	0/1/1/1
15	BCR	J	104	-	-	3/5/22/63	0/1/1/2
12	CLA	B	844	2	-	11/33/109/115	-
12	CLA	B	801	-	-	6/39/115/115	-
12	CLA	A	807	1	-	8/27/103/115	-
12	CLA	A	805	1	-	10/39/115/115	-
12	CLA	B	848	2	-	23/39/115/115	-
12	CLA	B	822	2	-	14/39/115/115	-
15	BCR	A	838	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	B	806	2	-	21/39/115/115	-
12	CLA	L	206	28	-	19/39/115/115	-
18	LMT	L	210	-	-	14/21/61/61	0/2/2/2
15	BCR	I	101	-	-	4/29/63/63	0/2/2/2
12	CLA	A	815	1	-	12/39/115/115	-
12	CLA	J	103	8	-	7/15/91/115	-
20	45D	A	856	-	-	5/29/69/69	0/2/2/2
12	CLA	L	205	10	-	10/39/115/115	-
15	BCR	L	208	-	-	2/29/63/63	0/2/2/2
12	CLA	A	806	1	-	6/15/91/115	-
23	ECH	B	833	-	-	5/29/66/66	0/2/2/2

All (2593) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	K	4001	BCR	C26-C25	16.71	1.62	1.34
15	F	201	BCR	C26-C25	16.11	1.61	1.34
15	I	101	BCR	C26-C25	16.09	1.61	1.34
15	A	836	BCR	C26-C25	16.02	1.61	1.34
15	B	834	BCR	C26-C25	15.90	1.61	1.34
15	A	837	BCR	C26-C25	15.82	1.61	1.34
15	A	838	BCR	C26-C25	15.67	1.60	1.34
15	B	835	BCR	C26-C25	15.62	1.60	1.34
15	J	105	BCR	C26-C25	15.60	1.60	1.34
15	B	832	BCR	C26-C25	15.57	1.60	1.34
15	L	208	BCR	C26-C25	15.56	1.60	1.34
15	K	4005	BCR	C26-C25	15.52	1.60	1.34
15	F	202	BCR	C26-C25	15.52	1.60	1.34
15	L	207	BCR	C26-C25	15.47	1.60	1.34
15	B	841	BCR	C26-C25	15.45	1.60	1.34
15	J	107	BCR	C26-C25	15.39	1.60	1.34
15	I	101	BCR	C5-C6	15.39	1.60	1.34
15	L	207	BCR	C5-C6	15.37	1.60	1.34
15	L	208	BCR	C5-C6	15.32	1.60	1.34
15	A	835	BCR	C26-C25	15.31	1.60	1.34
15	B	832	BCR	C5-C6	15.29	1.60	1.34
15	F	202	BCR	C5-C6	15.18	1.60	1.34
15	K	4005	BCR	C5-C6	15.13	1.59	1.34
15	J	107	BCR	C5-C6	15.08	1.59	1.34
15	J	104	BCR	C26-C25	15.04	1.59	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	J	105	BCR	C5-C6	14.92	1.59	1.34
15	B	834	BCR	C5-C6	14.92	1.59	1.34
15	A	836	BCR	C5-C6	14.91	1.59	1.34
15	B	836	BCR	C26-C25	14.85	1.59	1.34
15	F	201	BCR	C5-C6	14.82	1.59	1.34
15	A	838	BCR	C5-C6	14.80	1.59	1.34
15	B	835	BCR	C5-C6	14.77	1.59	1.34
15	B	841	BCR	C5-C6	14.70	1.59	1.34
15	A	835	BCR	C5-C6	14.57	1.58	1.34
15	K	4001	BCR	C5-C6	14.54	1.58	1.34
15	A	837	BCR	C5-C6	14.27	1.58	1.34
12	B	803	CLA	MG-NA	9.36	2.28	2.06
12	A	846	CLA	MG-NA	8.20	2.25	2.06
12	B	852	CLA	MG-NA	7.96	2.25	2.06
12	A	832	CLA	MG-NA	7.90	2.25	2.06
12	A	852	CLA	MG-NA	7.89	2.25	2.06
12	A	818	CLA	MG-NA	7.82	2.24	2.06
12	F	203	CLA	MG-NA	7.77	2.24	2.06
12	B	812	CLA	MG-NA	7.75	2.24	2.06
12	A	831	CLA	MG-NA	7.74	2.24	2.06
12	A	829	CLA	MG-NA	7.72	2.24	2.06
12	J	101	CLA	MG-NA	7.72	2.24	2.06
12	A	855	CLA	MG-NA	7.68	2.24	2.06
12	A	822	CLA	MG-NA	7.67	2.24	2.06
12	A	849	CLA	MG-NA	7.66	2.24	2.06
12	B	806	CLA	MG-NA	7.65	2.24	2.06
12	B	804	CLA	MG-NA	7.65	2.24	2.06
12	A	815	CLA	MG-NA	7.64	2.24	2.06
12	B	814	CLA	MG-NA	7.64	2.24	2.06
12	J	103	CLA	MG-NA	7.64	2.24	2.06
12	L	204	CLA	MG-NA	7.64	2.24	2.06
12	B	830	CLA	MG-NA	7.63	2.24	2.06
12	B	818	CLA	MG-NA	7.63	2.24	2.06
12	A	830	CLA	MG-NA	7.62	2.24	2.06
12	A	812	CLA	MG-NA	7.61	2.24	2.06
12	B	828	CLA	MG-NA	7.61	2.24	2.06
12	B	802	CLA	MG-NA	7.60	2.24	2.06
12	L	206	CLA	MG-NA	7.60	2.24	2.06
12	A	826	CLA	MG-NA	7.58	2.24	2.06
12	A	823	CLA	MG-NA	7.57	2.24	2.06
12	A	821	CLA	MG-NA	7.57	2.24	2.06
12	B	819	CLA	MG-NA	7.57	2.24	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	819	CLA	MG-NA	7.57	2.24	2.06
12	B	853	CLA	MG-NA	7.57	2.24	2.06
12	B	842	CLA	MG-NA	7.56	2.24	2.06
12	B	805	CLA	MG-NA	7.55	2.24	2.06
12	B	816	CLA	MG-NA	7.54	2.24	2.06
12	B	829	CLA	MG-NA	7.54	2.24	2.06
12	B	815	CLA	MG-NA	7.52	2.24	2.06
12	A	813	CLA	MG-NA	7.52	2.24	2.06
12	B	810	CLA	MG-NA	7.52	2.24	2.06
12	B	848	CLA	MG-NA	7.52	2.24	2.06
12	B	817	CLA	MG-NA	7.51	2.24	2.06
12	B	823	CLA	MG-NA	7.50	2.24	2.06
12	B	813	CLA	MG-NA	7.50	2.24	2.06
12	B	849	CLA	MG-NA	7.50	2.24	2.06
13	A	802	CL0	MG-NA	7.50	2.24	2.06
12	B	809	CLA	MG-NA	7.50	2.24	2.06
12	B	808	CLA	MG-NA	7.49	2.24	2.06
12	A	833	CLA	MG-NA	7.49	2.24	2.06
12	A	844	CLA	MG-NA	7.49	2.24	2.06
12	B	827	CLA	MG-NA	7.48	2.24	2.06
12	A	824	CLA	MG-NA	7.48	2.24	2.06
12	J	102	CLA	MG-NA	7.48	2.24	2.06
12	B	807	CLA	MG-NA	7.48	2.24	2.06
12	B	826	CLA	MG-NA	7.48	2.24	2.06
12	A	803	CLA	MG-NA	7.47	2.24	2.06
12	B	821	CLA	MG-NA	7.47	2.24	2.06
12	A	820	CLA	MG-NA	7.47	2.24	2.06
12	A	845	CLA	MG-NA	7.47	2.24	2.06
12	A	847	CLA	MG-NA	7.46	2.24	2.06
15	J	105	BCR	C2-C3	-7.46	1.34	1.52
12	B	811	CLA	MG-NA	7.46	2.24	2.06
12	A	806	CLA	MG-NA	7.45	2.24	2.06
12	B	822	CLA	MG-NA	7.45	2.24	2.06
12	B	850	CLA	MG-NA	7.45	2.24	2.06
12	K	4002	CLA	MG-NA	7.45	2.24	2.06
12	B	825	CLA	MG-NA	7.42	2.23	2.06
12	L	201	CLA	MG-NA	7.42	2.23	2.06
12	L	205	CLA	MG-NA	7.40	2.23	2.06
12	F	204	CLA	MG-NA	7.39	2.23	2.06
12	B	845	CLA	MG-NA	7.38	2.23	2.06
12	A	825	CLA	MG-NA	7.38	2.23	2.06
12	A	808	CLA	MG-NA	7.37	2.23	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	816	CLA	MG-NA	7.37	2.23	2.06
15	J	105	BCR	C1-C6	-7.36	1.44	1.53
12	B	843	CLA	MG-NA	7.35	2.23	2.06
12	A	811	CLA	MG-NA	7.33	2.23	2.06
12	A	810	CLA	MG-NA	7.33	2.23	2.06
12	B	820	CLA	MG-NA	7.31	2.23	2.06
12	A	843	CLA	MG-NA	7.30	2.23	2.06
12	A	817	CLA	MG-NA	7.29	2.23	2.06
12	A	827	CLA	MG-NA	7.28	2.23	2.06
12	A	801	CLA	MG-NA	7.25	2.23	2.06
12	A	848	CLA	MG-NA	7.25	2.23	2.06
12	B	824	CLA	MG-NA	7.24	2.23	2.06
12	A	828	CLA	MG-NA	7.23	2.23	2.06
12	A	814	CLA	MG-NA	7.23	2.23	2.06
15	A	835	BCR	C30-C25	-7.22	1.44	1.53
12	A	805	CLA	MG-NA	7.20	2.23	2.06
15	L	207	BCR	C2-C3	-7.19	1.35	1.52
12	A	807	CLA	MG-NA	7.18	2.23	2.06
15	K	4005	BCR	C2-C3	-7.13	1.35	1.52
15	B	832	BCR	C2-C3	-7.12	1.35	1.52
15	B	834	BCR	C30-C25	-7.12	1.44	1.53
15	I	101	BCR	C2-C3	-7.12	1.35	1.52
15	L	208	BCR	C2-C3	-7.11	1.35	1.52
15	B	834	BCR	C29-C28	-7.11	1.35	1.52
12	B	801	CLA	MG-NA	7.11	2.23	2.06
12	B	846	CLA	MG-NA	7.09	2.23	2.06
15	A	838	BCR	C2-C3	-7.08	1.35	1.52
15	B	841	BCR	C2-C3	-7.06	1.35	1.52
12	A	804	CLA	MG-NA	7.06	2.23	2.06
15	F	202	BCR	C2-C3	-7.05	1.35	1.52
12	A	858	CLA	MG-NA	7.04	2.23	2.06
15	K	4001	BCR	C29-C28	-7.01	1.36	1.52
15	J	107	BCR	C2-C3	-7.00	1.36	1.52
15	A	838	BCR	C1-C6	-6.98	1.44	1.53
15	B	834	BCR	C2-C3	-6.97	1.36	1.52
15	B	835	BCR	C2-C3	-6.97	1.36	1.52
15	J	104	BCR	C29-C28	-6.96	1.36	1.52
12	K	4004	CLA	MG-NA	6.96	2.22	2.06
15	A	837	BCR	C1-C6	-6.92	1.44	1.53
15	A	837	BCR	C30-C25	-6.90	1.44	1.53
15	A	836	BCR	C2-C3	-6.90	1.36	1.52
15	F	201	BCR	C30-C25	-6.89	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	835	BCR	C30-C25	-6.88	1.45	1.53
15	A	835	BCR	C2-C3	-6.87	1.36	1.52
15	F	201	BCR	C2-C3	-6.86	1.36	1.52
12	A	809	CLA	MG-NA	6.86	2.22	2.06
15	K	4005	BCR	C1-C6	-6.85	1.45	1.53
15	L	207	BCR	C29-C28	-6.85	1.36	1.52
15	B	832	BCR	C30-C25	-6.84	1.45	1.53
15	A	838	BCR	C29-C28	-6.80	1.36	1.52
15	J	105	BCR	C29-C28	-6.79	1.36	1.52
15	B	836	BCR	C30-C25	-6.76	1.45	1.53
15	B	841	BCR	C29-C28	-6.73	1.36	1.52
12	B	847	CLA	MG-NA	6.73	2.22	2.06
15	F	201	BCR	C29-C28	-6.72	1.36	1.52
15	J	107	BCR	C29-C28	-6.72	1.36	1.52
15	A	836	BCR	C29-C28	-6.69	1.36	1.52
15	I	101	BCR	C29-C28	-6.68	1.36	1.52
15	J	107	BCR	C30-C25	-6.68	1.45	1.53
15	K	4001	BCR	C1-C6	-6.68	1.45	1.53
15	K	4001	BCR	C2-C3	-6.66	1.36	1.52
15	A	837	BCR	C2-C3	-6.66	1.36	1.52
15	A	837	BCR	C29-C28	-6.66	1.36	1.52
15	F	202	BCR	C30-C25	-6.65	1.45	1.53
15	A	836	BCR	C30-C25	-6.64	1.45	1.53
15	K	4005	BCR	C29-C28	-6.59	1.37	1.52
15	B	832	BCR	C29-C28	-6.57	1.37	1.52
15	B	835	BCR	C29-C28	-6.56	1.37	1.52
15	I	101	BCR	C30-C25	-6.54	1.45	1.53
15	B	841	BCR	C1-C6	-6.54	1.45	1.53
15	B	841	BCR	C30-C25	-6.53	1.45	1.53
15	F	202	BCR	C29-C28	-6.50	1.37	1.52
15	A	835	BCR	C1-C6	-6.50	1.45	1.53
15	K	4001	BCR	C30-C25	-6.46	1.45	1.53
15	B	836	BCR	C29-C28	-6.43	1.37	1.52
15	L	208	BCR	C29-C28	-6.42	1.37	1.52
15	L	208	BCR	C1-C6	-6.40	1.45	1.53
15	A	835	BCR	C29-C28	-6.39	1.37	1.52
15	I	101	BCR	C1-C6	-6.29	1.45	1.53
15	A	838	BCR	C30-C25	-6.29	1.45	1.53
15	B	832	BCR	C1-C6	-6.29	1.45	1.53
12	A	809	CLA	O2A-C1	6.25	1.63	1.46
15	B	834	BCR	C1-C6	-6.25	1.45	1.53
15	K	4005	BCR	C30-C25	-6.25	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	844	CLA	MG-NA	6.23	2.21	2.06
15	J	105	BCR	C29-C30	6.20	1.68	1.54
15	F	201	BCR	C1-C6	-6.13	1.45	1.53
15	B	835	BCR	C1-C6	-6.13	1.45	1.53
15	J	104	BCR	C30-C25	-6.12	1.45	1.53
15	L	208	BCR	C30-C25	-6.09	1.46	1.53
15	F	202	BCR	C1-C6	-6.09	1.46	1.53
15	J	107	BCR	C1-C6	-6.02	1.46	1.53
15	A	836	BCR	C1-C6	-5.98	1.46	1.53
15	L	207	BCR	C1-C6	-5.98	1.46	1.53
15	L	208	BCR	C29-C30	5.77	1.67	1.54
15	J	104	BCR	C29-C30	5.71	1.67	1.54
12	B	821	CLA	O2A-C1	5.69	1.61	1.46
12	A	829	CLA	O2A-C1	5.66	1.61	1.46
15	K	4005	BCR	C29-C30	5.64	1.67	1.54
12	A	852	CLA	O2A-C1	5.62	1.61	1.46
15	A	835	BCR	C29-C30	5.61	1.67	1.54
12	A	805	CLA	O2A-C1	5.58	1.61	1.46
12	B	824	CLA	O2A-C1	5.58	1.61	1.46
15	L	207	BCR	C30-C25	-5.52	1.46	1.53
12	A	820	CLA	O2A-C1	5.51	1.61	1.46
15	L	207	BCR	C29-C30	5.51	1.66	1.54
12	A	803	CLA	O2A-C1	5.51	1.61	1.46
12	A	858	CLA	O2A-C1	5.50	1.60	1.46
12	B	820	CLA	O2A-C1	5.49	1.60	1.46
12	A	821	CLA	O2A-C1	5.47	1.60	1.46
12	A	807	CLA	O2A-C1	5.46	1.60	1.46
12	A	831	CLA	O2A-C1	5.45	1.60	1.46
15	B	832	BCR	C29-C30	5.45	1.66	1.54
12	B	842	CLA	O2A-C1	5.44	1.60	1.46
15	I	101	BCR	C29-C30	5.43	1.66	1.54
12	B	803	CLA	C1D-ND	-5.43	1.30	1.37
12	L	206	CLA	O2A-C1	5.42	1.60	1.46
12	A	843	CLA	O2A-C1	5.41	1.60	1.46
12	B	823	CLA	O2A-C1	5.41	1.60	1.46
15	F	202	BCR	C29-C30	5.41	1.66	1.54
12	A	846	CLA	O2A-C1	5.39	1.60	1.46
15	B	836	BCR	C29-C30	5.39	1.66	1.54
12	A	827	CLA	O2A-C1	5.38	1.60	1.46
12	A	855	CLA	O2A-C1	5.38	1.60	1.46
12	A	830	CLA	O2A-C1	5.38	1.60	1.46
15	A	838	BCR	C29-C30	5.37	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	822	CLA	O2A-C1	5.37	1.60	1.46
15	J	105	BCR	C30-C25	-5.37	1.46	1.53
12	A	817	CLA	O2A-C1	5.37	1.60	1.46
15	B	841	BCR	C29-C30	5.37	1.66	1.54
12	A	810	CLA	O2A-C1	5.36	1.60	1.46
12	B	811	CLA	O2A-C1	5.36	1.60	1.46
12	B	826	CLA	O2A-C1	5.35	1.60	1.46
12	B	812	CLA	O2A-C1	5.33	1.60	1.46
12	B	802	CLA	O2A-C1	5.33	1.60	1.46
15	A	837	BCR	C29-C30	5.33	1.66	1.54
12	L	205	CLA	O2A-C1	5.32	1.60	1.46
15	B	835	BCR	C29-C30	5.31	1.66	1.54
15	F	201	BCR	C29-C30	5.31	1.66	1.54
12	A	833	CLA	O2A-C1	5.30	1.60	1.46
12	A	814	CLA	O2A-C1	5.30	1.60	1.46
15	F	201	BCR	C2-C1	5.30	1.66	1.54
12	B	813	CLA	O2A-C1	5.30	1.60	1.46
12	B	804	CLA	O2A-C1	5.30	1.60	1.46
12	A	823	CLA	O2A-C1	5.29	1.60	1.46
12	B	806	CLA	O2A-C1	5.28	1.60	1.46
12	B	814	CLA	O2A-C1	5.28	1.60	1.46
15	B	832	BCR	C8-C9	5.27	1.57	1.46
15	A	836	BCR	C2-C1	5.27	1.66	1.54
12	A	804	CLA	O2A-C1	5.27	1.60	1.46
12	A	816	CLA	O2A-C1	5.26	1.60	1.46
12	B	845	CLA	O2A-C1	5.26	1.60	1.46
12	A	808	CLA	O2A-C1	5.25	1.60	1.46
12	L	204	CLA	O2A-C1	5.25	1.60	1.46
12	B	809	CLA	O2A-C1	5.25	1.60	1.46
12	A	803	CLA	O2D-CGD	5.25	1.46	1.33
15	K	4001	BCR	C2-C1	5.24	1.66	1.54
12	A	824	CLA	O2A-C1	5.24	1.60	1.46
12	B	816	CLA	O2A-C1	5.23	1.60	1.46
12	B	852	CLA	O2A-C1	5.23	1.60	1.46
12	A	813	CLA	O2A-C1	5.22	1.60	1.46
12	A	815	CLA	O2A-C1	5.22	1.60	1.46
12	F	203	CLA	O2D-CGD	5.22	1.46	1.33
12	B	847	CLA	O2A-C1	5.21	1.60	1.46
12	B	808	CLA	O2A-C1	5.21	1.60	1.46
12	B	801	CLA	O2A-C1	5.19	1.60	1.46
12	A	813	CLA	O2D-CGD	5.19	1.46	1.33
12	B	848	CLA	O2A-C1	5.18	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	847	CLA	O2A-C1	5.18	1.60	1.46
12	A	844	CLA	O2D-CGD	5.17	1.45	1.33
12	B	850	CLA	O2D-CGD	5.17	1.45	1.33
12	L	201	CLA	O2A-C1	5.16	1.60	1.46
12	B	830	CLA	O2D-CGD	5.16	1.45	1.33
12	B	819	CLA	O2A-C1	5.16	1.60	1.46
12	B	843	CLA	O2A-C1	5.16	1.60	1.46
12	A	822	CLA	O2A-C1	5.16	1.60	1.46
12	K	4002	CLA	O2D-CGD	5.15	1.45	1.33
12	A	818	CLA	O2A-C1	5.15	1.60	1.46
12	B	809	CLA	O2D-CGD	5.14	1.45	1.33
12	B	852	CLA	O2D-CGD	5.14	1.45	1.33
15	F	202	BCR	C2-C1	5.14	1.65	1.54
12	B	810	CLA	O2A-C1	5.14	1.60	1.46
12	B	807	CLA	O2A-C1	5.14	1.60	1.46
12	J	101	CLA	O2A-C1	5.13	1.59	1.46
12	B	805	CLA	O2D-CGD	5.13	1.45	1.33
12	B	845	CLA	O2D-CGD	5.13	1.45	1.33
12	A	816	CLA	O2D-CGD	5.12	1.45	1.33
12	J	103	CLA	O2D-CGD	5.12	1.45	1.33
12	A	822	CLA	O2D-CGD	5.12	1.45	1.33
12	B	829	CLA	O2D-CGD	5.11	1.45	1.33
15	A	836	BCR	C29-C30	5.11	1.65	1.54
12	B	828	CLA	O2A-C1	5.11	1.59	1.46
15	K	4005	BCR	C2-C1	5.11	1.65	1.54
12	A	845	CLA	O2A-C1	5.10	1.59	1.46
12	B	825	CLA	O2A-C1	5.10	1.59	1.46
12	F	204	CLA	O2D-CGD	5.10	1.45	1.33
12	B	820	CLA	O2D-CGD	5.09	1.45	1.33
12	B	812	CLA	O2D-CGD	5.09	1.45	1.33
12	B	818	CLA	O2A-C1	5.09	1.59	1.46
12	A	845	CLA	O2D-CGD	5.09	1.45	1.33
13	A	802	CL0	O2D-CGD	5.08	1.45	1.33
12	B	804	CLA	O2D-CGD	5.08	1.45	1.33
12	J	101	CLA	CHD-C1D	5.07	1.48	1.38
12	A	806	CLA	O2D-CGD	5.07	1.45	1.33
12	K	4004	CLA	O2A-C1	5.07	1.59	1.46
12	A	849	CLA	O2A-C1	5.07	1.59	1.46
12	B	803	CLA	C1B-NB	-5.07	1.31	1.37
15	A	838	BCR	C2-C1	5.07	1.65	1.54
12	A	848	CLA	O2A-C1	5.07	1.59	1.46
15	J	107	BCR	C29-C30	5.06	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	846	CLA	O2A-C1	5.06	1.59	1.46
12	A	852	CLA	MG-ND	-5.06	1.95	2.05
15	B	834	BCR	C29-C30	5.06	1.65	1.54
12	L	204	CLA	O2D-CGD	5.06	1.45	1.33
12	A	832	CLA	O2A-C1	5.06	1.59	1.46
12	B	827	CLA	O2D-CGD	5.06	1.45	1.33
12	B	821	CLA	O2D-CGD	5.05	1.45	1.33
12	A	812	CLA	O2D-CGD	5.05	1.45	1.33
12	A	817	CLA	O2D-CGD	5.04	1.45	1.33
12	B	814	CLA	CHC-C1C	5.04	1.48	1.38
12	B	815	CLA	O2D-CGD	5.04	1.45	1.33
12	A	830	CLA	O2D-CGD	5.04	1.45	1.33
12	A	811	CLA	O2D-CGD	5.03	1.45	1.33
12	A	826	CLA	O2D-CGD	5.03	1.45	1.33
12	B	823	CLA	O2D-CGD	5.03	1.45	1.33
15	J	107	BCR	C2-C1	5.03	1.65	1.54
12	A	804	CLA	O2D-CGD	5.02	1.45	1.33
12	A	832	CLA	O2D-CGD	5.02	1.45	1.33
12	B	849	CLA	O2A-C1	5.02	1.59	1.46
12	A	825	CLA	O2D-CGD	5.02	1.45	1.33
12	A	814	CLA	O2D-CGD	5.02	1.45	1.33
12	B	810	CLA	O2D-CGD	5.02	1.45	1.33
15	L	207	BCR	C8-C9	5.02	1.56	1.46
12	A	828	CLA	O2A-C1	5.02	1.59	1.46
12	A	801	CLA	CHC-C1C	5.02	1.48	1.38
12	L	201	CLA	O2D-CGD	5.02	1.45	1.33
12	A	801	CLA	O2A-C1	5.00	1.59	1.46
15	A	836	BCR	C8-C9	5.00	1.56	1.46
12	A	827	CLA	O2D-CGD	5.00	1.45	1.33
12	B	817	CLA	O2D-CGD	5.00	1.45	1.33
12	B	853	CLA	O2A-C1	5.00	1.59	1.46
15	B	834	BCR	C2-C1	5.00	1.65	1.54
12	A	819	CLA	O2A-C1	4.99	1.59	1.46
15	A	837	BCR	C2-C1	4.99	1.65	1.54
12	B	828	CLA	O2D-CGD	4.99	1.45	1.33
12	A	843	CLA	O2D-CGD	4.99	1.45	1.33
15	A	835	BCR	C2-C1	4.99	1.65	1.54
12	A	818	CLA	O2D-CGD	4.99	1.45	1.33
15	F	201	BCR	C8-C9	4.99	1.56	1.46
12	A	831	CLA	O2D-CGD	4.98	1.45	1.33
15	L	207	BCR	C2-C1	4.98	1.65	1.54
12	B	807	CLA	O2D-CGD	4.98	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	202	BCR	C8-C9	4.98	1.56	1.46
15	B	841	BCR	C2-C1	4.97	1.65	1.54
13	A	802	CL0	O2A-C1	4.97	1.59	1.46
12	A	808	CLA	O2D-CGD	4.97	1.45	1.33
12	B	823	CLA	CHC-C1C	4.97	1.48	1.38
12	A	821	CLA	O2D-CGD	4.97	1.45	1.33
12	A	847	CLA	O2D-CGD	4.96	1.45	1.33
12	B	825	CLA	O2D-CGD	4.96	1.45	1.33
15	L	208	BCR	C2-C1	4.96	1.65	1.54
12	L	206	CLA	O2D-CGD	4.96	1.45	1.33
12	A	819	CLA	O2D-CGD	4.96	1.45	1.33
15	K	4001	BCR	C29-C30	4.96	1.65	1.54
12	K	4004	CLA	O2D-CGD	4.95	1.45	1.33
12	B	802	CLA	O2D-CGD	4.95	1.45	1.33
12	B	826	CLA	O2D-CGD	4.95	1.45	1.33
12	B	844	CLA	C1B-NB	-4.94	1.31	1.37
12	A	824	CLA	O2D-CGD	4.94	1.45	1.33
15	B	832	BCR	C2-C1	4.94	1.65	1.54
12	B	814	CLA	O2D-CGD	4.94	1.45	1.33
12	A	801	CLA	O2D-CGD	4.93	1.45	1.33
12	B	850	CLA	O2A-C1	4.93	1.59	1.46
12	A	815	CLA	O2D-CGD	4.93	1.45	1.33
12	J	102	CLA	CHC-C1C	4.93	1.48	1.38
12	A	828	CLA	O2D-CGD	4.93	1.45	1.33
12	J	103	CLA	CHC-C1C	4.92	1.48	1.38
12	A	826	CLA	O2A-C1	4.92	1.59	1.46
15	J	107	BCR	C8-C9	4.92	1.56	1.46
12	A	833	CLA	O2D-CGD	4.92	1.45	1.33
12	A	855	CLA	O2D-CGD	4.92	1.45	1.33
15	L	208	BCR	C8-C9	4.92	1.56	1.46
12	K	4003	CLA	C4C-C3C	-4.91	1.36	1.45
12	B	818	CLA	O2D-CGD	4.91	1.45	1.33
12	B	849	CLA	O2D-CGD	4.90	1.45	1.33
12	A	810	CLA	O2D-CGD	4.89	1.45	1.33
12	A	805	CLA	O2D-CGD	4.89	1.45	1.33
12	F	203	CLA	CHC-C1C	4.89	1.48	1.38
12	A	807	CLA	O2D-CGD	4.89	1.45	1.33
12	A	825	CLA	O2A-C1	4.88	1.59	1.46
12	B	848	CLA	CHC-C1C	4.88	1.48	1.38
12	B	830	CLA	CHC-C1C	4.87	1.48	1.38
12	B	804	CLA	CHC-C1C	4.87	1.48	1.38
12	B	816	CLA	O2D-CGD	4.87	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	823	CLA	O2D-CGD	4.86	1.45	1.33
12	B	829	CLA	O2A-C1	4.86	1.59	1.46
12	B	843	CLA	O2D-CGD	4.86	1.45	1.33
12	A	807	CLA	CHC-C1C	4.86	1.48	1.38
12	B	819	CLA	CHC-C1C	4.86	1.48	1.38
15	I	101	BCR	C2-C1	4.85	1.65	1.54
12	A	820	CLA	O2D-CGD	4.85	1.45	1.33
12	B	848	CLA	O2D-CGD	4.85	1.45	1.33
12	A	852	CLA	CHB-C1B	4.85	1.50	1.39
12	B	844	CLA	O2A-C1	4.85	1.59	1.46
12	B	850	CLA	C3D-C4D	-4.84	1.33	1.44
12	J	101	CLA	CHC-C1C	4.84	1.48	1.38
15	B	841	BCR	C8-C9	4.84	1.56	1.46
12	B	850	CLA	CHD-C1D	4.84	1.47	1.38
12	J	101	CLA	O2D-CGD	4.84	1.45	1.33
12	A	813	CLA	CHC-C1C	4.84	1.48	1.38
12	A	805	CLA	CHC-C1C	4.84	1.48	1.38
12	L	205	CLA	O2D-CGD	4.83	1.45	1.33
12	B	819	CLA	O2D-CGD	4.83	1.45	1.33
12	B	806	CLA	O2D-CGD	4.83	1.45	1.33
12	K	4004	CLA	CHD-C1D	4.82	1.47	1.38
12	B	808	CLA	O2D-CGD	4.82	1.45	1.33
12	B	813	CLA	O2D-CGD	4.82	1.45	1.33
15	K	4001	BCR	C8-C9	4.82	1.56	1.46
12	B	807	CLA	CHC-C1C	4.81	1.48	1.38
12	B	852	CLA	CHC-C1C	4.81	1.48	1.38
12	B	847	CLA	C1B-NB	-4.81	1.31	1.37
15	A	835	BCR	C8-C9	4.79	1.56	1.46
12	L	205	CLA	CHC-C1C	4.79	1.48	1.38
15	B	834	BCR	C8-C9	4.79	1.56	1.46
12	B	826	CLA	CHC-C1C	4.78	1.48	1.38
12	B	822	CLA	O2D-CGD	4.78	1.45	1.33
12	B	817	CLA	O2A-C1	4.78	1.59	1.46
12	A	852	CLA	O2D-CGD	4.78	1.45	1.33
12	A	832	CLA	CHC-C1C	4.78	1.48	1.38
12	B	845	CLA	CHC-C1C	4.77	1.48	1.38
12	A	845	CLA	CHC-C1C	4.77	1.48	1.38
15	B	835	BCR	C2-C1	4.77	1.65	1.54
12	A	819	CLA	CHC-C1C	4.77	1.48	1.38
12	A	849	CLA	O2D-CGD	4.77	1.44	1.33
12	B	842	CLA	CHC-C1C	4.76	1.48	1.38
12	B	801	CLA	CHC-C1C	4.76	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	848	CLA	CHC-C1C	4.75	1.48	1.38
12	A	816	CLA	CHC-C1C	4.75	1.48	1.38
12	B	801	CLA	O2D-CGD	4.75	1.44	1.33
12	B	850	CLA	CHC-C1C	4.75	1.48	1.38
12	J	102	CLA	O2D-CGD	4.75	1.44	1.33
12	B	846	CLA	C3D-C4D	-4.75	1.33	1.44
12	B	828	CLA	CHC-C1C	4.74	1.48	1.38
12	A	858	CLA	O2D-CGD	4.74	1.44	1.33
12	A	817	CLA	CHC-C1C	4.73	1.48	1.38
12	F	204	CLA	CHC-C1C	4.73	1.48	1.38
12	A	803	CLA	CHC-C1C	4.73	1.48	1.38
15	I	101	BCR	C8-C9	4.73	1.56	1.46
12	A	806	CLA	CHC-C1C	4.73	1.48	1.38
12	L	201	CLA	CHD-C1D	4.73	1.47	1.38
12	A	852	CLA	C3C-C2C	4.72	1.46	1.36
12	A	820	CLA	CHC-C1C	4.72	1.47	1.38
12	B	842	CLA	O2D-CGD	4.71	1.44	1.33
12	A	814	CLA	CHC-C1C	4.71	1.47	1.38
12	A	852	CLA	CHC-C1C	4.71	1.47	1.38
13	A	802	CL0	CHC-C1C	4.71	1.47	1.38
12	A	843	CLA	CHC-C1C	4.71	1.47	1.38
12	B	818	CLA	CHC-C1C	4.71	1.47	1.38
12	A	829	CLA	O2D-CGD	4.71	1.44	1.33
12	B	811	CLA	O2D-CGD	4.71	1.44	1.33
12	L	205	CLA	C3C-C2C	4.71	1.46	1.36
12	L	204	CLA	CHC-C1C	4.70	1.47	1.38
12	A	833	CLA	CHC-C1C	4.70	1.47	1.38
12	A	824	CLA	CHC-C1C	4.70	1.47	1.38
12	B	802	CLA	CHD-C1D	4.69	1.47	1.38
15	A	838	BCR	C8-C9	4.69	1.56	1.46
12	A	830	CLA	CHD-C1D	4.69	1.47	1.38
15	B	836	BCR	C19-C18	4.68	1.56	1.46
12	A	821	CLA	CHC-C1C	4.67	1.47	1.38
12	K	4002	CLA	CHC-C1C	4.67	1.47	1.38
12	A	848	CLA	O2D-CGD	4.67	1.44	1.33
12	B	808	CLA	CHC-C1C	4.65	1.47	1.38
12	A	822	CLA	C3C-C2C	4.65	1.46	1.36
12	A	812	CLA	CHD-C1D	4.65	1.47	1.38
12	A	830	CLA	CHC-C1C	4.65	1.47	1.38
12	B	825	CLA	CHC-C1C	4.65	1.47	1.38
12	B	806	CLA	CHC-C1C	4.64	1.47	1.38
12	A	822	CLA	CHC-C1C	4.64	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	853	CLA	O2D-CGD	4.64	1.44	1.33
15	A	837	BCR	C8-C9	4.64	1.55	1.46
15	F	202	BCR	C19-C18	4.64	1.55	1.46
12	B	816	CLA	CHC-C1C	4.63	1.47	1.38
27	M	102	SQD	O48-C23	4.63	1.46	1.33
12	J	103	CLA	CHD-C1D	4.63	1.47	1.38
16	M	103	LHG	O7-C7	4.63	1.47	1.34
12	B	848	CLA	C1D-ND	-4.62	1.31	1.37
12	B	843	CLA	CHC-C1C	4.62	1.47	1.38
12	B	822	CLA	CHC-C1C	4.62	1.47	1.38
12	A	809	CLA	CHC-C1C	4.62	1.47	1.38
12	A	811	CLA	CHC-C1C	4.62	1.47	1.38
12	A	808	CLA	CHC-C1C	4.61	1.47	1.38
12	B	809	CLA	CHC-C1C	4.61	1.47	1.38
12	A	831	CLA	CHC-C1C	4.61	1.47	1.38
15	K	4005	BCR	C8-C9	4.60	1.55	1.46
15	L	208	BCR	C23-C22	4.60	1.55	1.46
12	B	815	CLA	CHC-C1C	4.60	1.47	1.38
12	A	818	CLA	CHC-C1C	4.59	1.47	1.38
12	J	103	CLA	C3C-C2C	4.59	1.46	1.36
12	B	803	CLA	C3D-C4D	-4.58	1.33	1.44
15	A	835	BCR	C19-C18	4.58	1.55	1.46
12	J	101	CLA	C3C-C2C	4.58	1.46	1.36
12	L	206	CLA	CHC-C1C	4.58	1.47	1.38
12	A	826	CLA	CHC-C1C	4.58	1.47	1.38
12	A	832	CLA	C3C-C2C	4.57	1.46	1.36
12	A	816	CLA	C3C-C2C	4.57	1.46	1.36
12	B	853	CLA	CHC-C1C	4.56	1.47	1.38
17	A	840	LMG	O8-C28	4.56	1.46	1.33
12	B	823	CLA	C3C-C2C	4.56	1.46	1.36
12	J	102	CLA	C3D-C4D	-4.56	1.33	1.44
12	F	204	CLA	CHD-C1D	4.55	1.47	1.38
12	B	848	CLA	C3C-C2C	4.54	1.46	1.36
12	A	810	CLA	CHC-C1C	4.54	1.47	1.38
12	B	821	CLA	CHC-C1C	4.54	1.47	1.38
12	B	808	CLA	C3C-C2C	4.54	1.46	1.36
12	B	823	CLA	CHD-C1D	4.54	1.47	1.38
12	A	812	CLA	C3C-C2C	4.54	1.46	1.36
12	A	846	CLA	C3D-C4D	-4.54	1.34	1.44
17	A	851	LMG	O8-C28	4.54	1.46	1.33
12	B	830	CLA	CHD-C1D	4.53	1.47	1.38
12	B	809	CLA	C3C-C2C	4.53	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	849	CLA	CHC-C1C	4.53	1.47	1.38
12	A	807	CLA	C3C-C2C	4.52	1.46	1.36
12	A	815	CLA	CHC-C1C	4.52	1.47	1.38
12	B	843	CLA	C3C-C2C	4.51	1.46	1.36
12	A	816	CLA	CHD-C1D	4.51	1.47	1.38
12	B	849	CLA	C3C-C2C	4.51	1.46	1.36
12	B	802	CLA	CHC-C1C	4.51	1.47	1.38
12	B	842	CLA	C3C-C2C	4.51	1.46	1.36
15	J	104	BCR	C23-C22	4.50	1.54	1.47
12	J	102	CLA	C3C-C2C	4.50	1.46	1.36
12	K	4002	CLA	CHD-C1D	4.50	1.47	1.38
12	A	803	CLA	CHD-C1D	4.50	1.47	1.38
12	A	814	CLA	CHD-C1D	4.50	1.47	1.38
12	J	101	CLA	CHD-C4C	4.50	1.49	1.39
12	J	101	CLA	C3D-C4D	-4.49	1.34	1.44
13	A	802	CL0	C3C-C2C	4.49	1.46	1.36
12	B	829	CLA	C3C-C2C	4.49	1.46	1.36
12	A	817	CLA	C3C-C2C	4.49	1.46	1.36
12	B	845	CLA	C3C-C2C	4.49	1.46	1.36
15	L	208	BCR	C19-C18	4.48	1.55	1.46
12	A	824	CLA	C3C-C2C	4.47	1.46	1.36
12	A	858	CLA	CHC-C1C	4.47	1.47	1.38
12	B	826	CLA	CHD-C1D	4.47	1.47	1.38
12	A	811	CLA	CHD-C1D	4.47	1.47	1.38
12	B	814	CLA	C3C-C2C	4.46	1.46	1.36
12	A	821	CLA	C3C-C2C	4.46	1.46	1.36
12	B	828	CLA	C3C-C2C	4.46	1.46	1.36
12	B	801	CLA	C3C-C2C	4.46	1.46	1.36
12	B	825	CLA	C3C-C2C	4.45	1.46	1.36
12	B	805	CLA	C3C-C2C	4.44	1.46	1.36
12	B	804	CLA	C3D-C4D	-4.44	1.34	1.44
12	B	807	CLA	C3C-C2C	4.44	1.46	1.36
12	A	827	CLA	C3C-C2C	4.44	1.46	1.36
12	B	847	CLA	C1D-ND	-4.44	1.32	1.37
12	A	845	CLA	C3D-C4D	-4.44	1.34	1.44
12	A	819	CLA	CHD-C1D	4.43	1.47	1.38
12	A	848	CLA	C3C-C2C	4.43	1.46	1.36
12	A	810	CLA	C3C-C2C	4.43	1.46	1.36
12	A	823	CLA	C3C-C2C	4.43	1.46	1.36
12	B	813	CLA	CHD-C1D	4.43	1.47	1.38
12	A	804	CLA	CHC-C1C	4.43	1.47	1.38
12	A	825	CLA	CHC-C1C	4.43	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	801	CLA	C3C-C2C	4.42	1.46	1.36
12	B	804	CLA	C3C-C2C	4.42	1.46	1.36
12	B	824	CLA	C1D-ND	-4.42	1.32	1.37
12	A	804	CLA	CHD-C1D	4.42	1.47	1.38
12	A	855	CLA	CHD-C1D	4.42	1.47	1.38
12	L	201	CLA	CHC-C1C	4.42	1.47	1.38
12	B	814	CLA	CHD-C1D	4.41	1.47	1.38
12	A	829	CLA	CHC-C1C	4.41	1.47	1.38
12	B	820	CLA	CHC-C1C	4.41	1.47	1.38
12	B	817	CLA	CHC-C1C	4.41	1.47	1.38
12	L	204	CLA	C3C-C2C	4.41	1.46	1.36
12	B	811	CLA	C3C-C2C	4.41	1.46	1.36
12	A	847	CLA	C3C-C2C	4.41	1.46	1.36
12	B	805	CLA	CHC-C1C	4.40	1.47	1.38
15	F	201	BCR	C19-C18	4.40	1.55	1.46
12	A	811	CLA	C3C-C2C	4.40	1.46	1.36
12	A	813	CLA	C3C-C2C	4.40	1.46	1.36
12	B	826	CLA	C3C-C2C	4.40	1.46	1.36
12	B	822	CLA	C3C-C2C	4.40	1.46	1.36
12	A	807	CLA	CHD-C1D	4.40	1.47	1.38
12	B	805	CLA	CHD-C1D	4.40	1.47	1.38
15	B	836	BCR	C23-C22	4.40	1.55	1.46
12	A	818	CLA	C3C-C2C	4.40	1.46	1.36
12	B	849	CLA	CHC-C1C	4.39	1.47	1.38
12	A	826	CLA	C3C-C2C	4.39	1.46	1.36
17	A	840	LMG	O7-C10	4.39	1.46	1.34
12	A	828	CLA	CHC-C1C	4.39	1.47	1.38
12	B	815	CLA	C3C-C2C	4.39	1.46	1.36
12	A	808	CLA	C3C-C2C	4.39	1.46	1.36
12	A	823	CLA	CHD-C1D	4.38	1.47	1.38
15	A	838	BCR	C19-C18	4.38	1.55	1.46
12	A	824	CLA	C3D-C4D	-4.38	1.34	1.44
12	A	811	CLA	C3D-C4D	-4.38	1.34	1.44
12	B	827	CLA	C3C-C2C	4.38	1.46	1.36
15	J	105	BCR	C19-C18	4.38	1.55	1.46
12	A	819	CLA	C3C-C2C	4.37	1.46	1.36
12	B	830	CLA	C3C-C2C	4.37	1.46	1.36
12	A	829	CLA	CHD-C1D	4.37	1.47	1.38
12	B	825	CLA	CHD-C1D	4.37	1.47	1.38
12	A	806	CLA	C3C-C2C	4.37	1.46	1.36
12	B	810	CLA	C3C-C2C	4.37	1.46	1.36
12	B	809	CLA	C3D-C4D	-4.37	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	J	102	CLA	CHD-C1D	4.37	1.46	1.38
12	A	818	CLA	C3D-C4D	-4.37	1.34	1.44
12	A	814	CLA	C3C-C2C	4.37	1.46	1.36
12	B	850	CLA	C3C-C2C	4.36	1.46	1.36
12	B	815	CLA	CHD-C1D	4.36	1.46	1.38
12	K	4002	CLA	C3C-C2C	4.36	1.46	1.36
12	B	827	CLA	CHC-C1C	4.36	1.47	1.38
26	L	209	DGD	O1G-C1A	4.36	1.46	1.33
12	B	822	CLA	C3D-C4D	-4.36	1.34	1.44
12	B	828	CLA	CHD-C1D	4.36	1.46	1.38
12	A	808	CLA	CHD-C1D	4.36	1.46	1.38
12	A	823	CLA	CHC-C1C	4.36	1.47	1.38
12	B	820	CLA	C3C-C2C	4.35	1.46	1.36
12	F	203	CLA	C3C-C2C	4.35	1.46	1.36
12	A	812	CLA	CHC-C1C	4.35	1.47	1.38
15	I	101	BCR	C19-C18	4.35	1.55	1.46
12	F	204	CLA	C3D-C4D	-4.35	1.34	1.44
12	B	823	CLA	C3D-C4D	-4.35	1.34	1.44
12	L	206	CLA	C3C-C2C	4.35	1.46	1.36
15	J	105	BCR	C8-C9	4.35	1.55	1.46
16	B	851	LHG	O8-C23	4.35	1.46	1.33
12	B	813	CLA	CHC-C1C	4.35	1.47	1.38
12	A	827	CLA	CHC-C1C	4.35	1.47	1.38
12	B	821	CLA	C3C-C2C	4.34	1.46	1.36
12	A	815	CLA	C3C-C2C	4.34	1.46	1.36
12	B	806	CLA	C3C-C2C	4.34	1.46	1.36
12	A	805	CLA	C3C-C2C	4.33	1.46	1.36
12	A	848	CLA	CHD-C1D	4.33	1.46	1.38
12	L	204	CLA	CHD-C1D	4.33	1.46	1.38
12	B	842	CLA	CHD-C1D	4.33	1.46	1.38
12	A	803	CLA	C3D-C4D	-4.33	1.34	1.44
12	A	809	CLA	C3C-C2C	4.32	1.46	1.36
12	B	817	CLA	C3C-C2C	4.32	1.46	1.36
12	B	808	CLA	C3D-C4D	-4.32	1.34	1.44
12	B	810	CLA	CHD-C1D	4.32	1.46	1.38
12	A	830	CLA	C3C-C2C	4.32	1.46	1.36
12	A	849	CLA	CHD-C1D	4.32	1.46	1.38
12	B	808	CLA	CHD-C1D	4.32	1.46	1.38
12	B	818	CLA	C3C-C2C	4.32	1.46	1.36
12	L	204	CLA	C3D-C4D	-4.32	1.34	1.44
12	A	847	CLA	CHD-C1D	4.32	1.46	1.38
12	A	833	CLA	C3C-C2C	4.31	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	853	CLA	C3C-C2C	4.31	1.46	1.36
12	B	842	CLA	C3D-C4D	-4.31	1.34	1.44
12	A	822	CLA	CHD-C1D	4.31	1.46	1.38
12	B	846	CLA	O2D-CGD	4.31	1.43	1.33
15	B	841	BCR	C19-C18	4.31	1.55	1.46
12	A	847	CLA	CHC-C1C	4.30	1.47	1.38
12	A	810	CLA	CHD-C1D	4.30	1.46	1.38
12	A	845	CLA	CHD-C1D	4.30	1.46	1.38
12	A	805	CLA	C3D-C4D	-4.30	1.34	1.44
12	A	814	CLA	C3D-C4D	-4.30	1.34	1.44
12	B	819	CLA	C3D-C4D	-4.30	1.34	1.44
15	F	202	BCR	C23-C22	4.30	1.55	1.46
12	A	828	CLA	CHD-C1D	4.30	1.46	1.38
12	L	206	CLA	CHD-C1D	4.30	1.46	1.38
15	B	841	BCR	C3-C4	4.30	1.65	1.52
15	J	105	BCR	C3-C4	4.30	1.65	1.52
12	A	803	CLA	C3C-C2C	4.30	1.46	1.36
12	B	809	CLA	CHD-C1D	4.29	1.46	1.38
15	B	836	BCR	C28-C27	4.29	1.65	1.52
12	A	832	CLA	CHD-C1D	4.29	1.46	1.38
15	B	832	BCR	C19-C18	4.29	1.55	1.46
12	B	845	CLA	C3D-C4D	-4.29	1.34	1.44
15	B	835	BCR	C28-C27	4.29	1.65	1.52
12	A	855	CLA	C3C-C2C	4.29	1.46	1.36
12	B	813	CLA	C3C-C2C	4.29	1.46	1.36
12	A	825	CLA	C3D-C4D	-4.29	1.34	1.44
12	A	806	CLA	CHD-C1D	4.28	1.46	1.38
12	B	852	CLA	CHD-C1D	4.28	1.46	1.38
12	A	820	CLA	C3D-C4D	-4.28	1.34	1.44
15	A	835	BCR	C3-C4	4.28	1.65	1.52
12	B	819	CLA	C3C-C2C	4.28	1.46	1.36
12	B	845	CLA	CHD-C1D	4.28	1.46	1.38
16	M	103	LHG	O8-C23	4.28	1.45	1.33
12	A	827	CLA	CHD-C1D	4.28	1.46	1.38
12	B	812	CLA	CHD-C1D	4.28	1.46	1.38
12	A	804	CLA	C3D-C4D	-4.27	1.34	1.44
12	B	824	CLA	C3D-C4D	-4.27	1.34	1.44
12	B	811	CLA	CHC-C1C	4.27	1.47	1.38
15	F	202	BCR	C28-C27	4.27	1.65	1.52
12	A	813	CLA	C3D-C4D	-4.27	1.34	1.44
15	K	4001	BCR	C19-C18	4.27	1.55	1.46
12	K	4002	CLA	C3D-C4D	-4.27	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	804	CLA	CHD-C1D	4.26	1.46	1.38
15	K	4005	BCR	C23-C22	4.26	1.55	1.46
12	A	852	CLA	C3D-C4D	-4.26	1.34	1.44
12	B	825	CLA	C3D-C4D	-4.26	1.34	1.44
12	B	827	CLA	CHD-C1D	4.26	1.46	1.38
12	A	815	CLA	C3D-C4D	-4.26	1.34	1.44
12	B	810	CLA	CHC-C1C	4.26	1.47	1.38
12	F	204	CLA	C3C-C2C	4.26	1.46	1.36
12	B	826	CLA	C3D-C4D	-4.26	1.34	1.44
12	A	831	CLA	C3C-C2C	4.25	1.45	1.36
12	B	843	CLA	C3D-C4D	-4.25	1.34	1.44
15	K	4001	BCR	C3-C4	4.25	1.65	1.52
12	A	828	CLA	C3C-C2C	4.25	1.45	1.36
12	B	807	CLA	CHD-C1D	4.25	1.46	1.38
12	B	810	CLA	C3D-C4D	-4.25	1.34	1.44
12	A	830	CLA	C3D-C4D	-4.25	1.34	1.44
15	L	208	BCR	C3-C4	4.25	1.65	1.52
12	A	827	CLA	C3D-C4D	-4.24	1.34	1.44
15	F	201	BCR	C28-C27	4.24	1.65	1.52
12	A	844	CLA	O2A-C1	4.24	1.57	1.46
16	B	851	LHG	O7-C7	4.24	1.46	1.34
12	A	845	CLA	C3C-C2C	4.24	1.45	1.36
12	A	829	CLA	C3C-C2C	4.24	1.45	1.36
12	A	825	CLA	CHD-C1D	4.24	1.46	1.38
15	A	835	BCR	C28-C27	4.24	1.65	1.52
12	B	817	CLA	CHD-C1D	4.24	1.46	1.38
12	A	819	CLA	C3D-C4D	-4.24	1.34	1.44
12	L	201	CLA	C3C-C2C	4.23	1.45	1.36
12	A	846	CLA	C1D-ND	-4.23	1.32	1.37
15	A	837	BCR	C28-C27	4.23	1.65	1.52
12	B	816	CLA	CHD-C1D	4.23	1.46	1.38
12	A	833	CLA	C3D-C4D	-4.23	1.34	1.44
12	A	813	CLA	CHD-C1D	4.23	1.46	1.38
12	B	843	CLA	CHD-C1D	4.23	1.46	1.38
12	B	848	CLA	CHD-C1D	4.23	1.46	1.38
12	B	821	CLA	C3D-C4D	-4.22	1.34	1.44
16	A	839	LHG	O8-C23	4.22	1.45	1.33
12	A	815	CLA	CHD-C1D	4.22	1.46	1.38
12	A	849	CLA	C3C-C2C	4.22	1.45	1.36
12	B	852	CLA	C3D-C4D	-4.21	1.34	1.44
12	A	806	CLA	C3D-C4D	-4.21	1.34	1.44
12	B	822	CLA	CHD-C1D	4.21	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	825	CLA	C3C-C2C	4.21	1.45	1.36
12	A	846	CLA	C1B-NB	-4.21	1.32	1.37
12	A	826	CLA	CHD-C1D	4.21	1.46	1.38
15	B	834	BCR	C3-C4	4.20	1.65	1.52
12	A	821	CLA	C3D-C4D	-4.20	1.34	1.44
12	A	817	CLA	C3D-C4D	-4.20	1.34	1.44
12	A	843	CLA	CHD-C1D	4.20	1.46	1.38
15	J	107	BCR	C3-C4	4.20	1.65	1.52
12	B	852	CLA	C3C-C2C	4.20	1.45	1.36
12	A	821	CLA	CHD-C1D	4.20	1.46	1.38
12	B	827	CLA	C3D-C4D	-4.20	1.34	1.44
12	B	807	CLA	C3D-C4D	-4.20	1.34	1.44
12	A	822	CLA	C3D-C4D	-4.20	1.34	1.44
12	B	844	CLA	CHC-C1C	4.20	1.46	1.38
12	B	814	CLA	C3D-C4D	-4.20	1.34	1.44
15	B	835	BCR	C3-C4	4.19	1.65	1.52
15	A	835	BCR	C16-C17	4.19	1.56	1.43
12	B	820	CLA	CHB-C1B	4.19	1.48	1.39
12	K	4004	CLA	C3C-C2C	4.19	1.45	1.36
15	B	832	BCR	C3-C4	4.19	1.65	1.52
12	A	855	CLA	C3D-C4D	-4.19	1.34	1.44
12	B	844	CLA	O2D-CGD	4.19	1.43	1.33
12	B	816	CLA	C3C-C2C	4.19	1.45	1.36
12	B	802	CLA	C3C-C2C	4.19	1.45	1.36
12	B	847	CLA	C3D-C4D	-4.19	1.34	1.44
15	I	101	BCR	C23-C22	4.19	1.54	1.46
15	I	101	BCR	C3-C4	4.18	1.65	1.52
12	B	853	CLA	CHB-C1B	4.18	1.48	1.39
15	J	107	BCR	C23-C22	4.18	1.54	1.46
12	B	847	CLA	O2D-CGD	4.18	1.43	1.33
15	J	107	BCR	C19-C18	4.18	1.54	1.46
12	B	806	CLA	CHD-C1D	4.17	1.46	1.38
12	L	205	CLA	C3D-C4D	-4.17	1.34	1.44
12	A	817	CLA	CHD-C1D	4.17	1.46	1.38
15	A	835	BCR	C23-C22	4.17	1.54	1.46
12	A	855	CLA	CHC-C1C	4.17	1.46	1.38
12	J	103	CLA	C3D-C4D	-4.17	1.34	1.44
12	J	103	CLA	CHD-C4C	4.17	1.48	1.39
15	K	4005	BCR	C19-C18	4.17	1.54	1.46
15	J	105	BCR	C2-C1	4.17	1.63	1.54
12	B	821	CLA	CHD-C1D	4.16	1.46	1.38
12	B	806	CLA	C3D-C4D	-4.16	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	812	CLA	C3D-C4D	-4.16	1.34	1.44
12	B	818	CLA	C3D-C4D	-4.16	1.34	1.44
12	L	206	CLA	C3D-C4D	-4.15	1.34	1.44
12	B	817	CLA	C3D-C4D	-4.15	1.34	1.44
15	B	836	BCR	C20-C21	4.15	1.56	1.43
12	A	808	CLA	C3D-C4D	-4.15	1.34	1.44
12	B	820	CLA	C3D-C4D	-4.15	1.34	1.44
15	B	832	BCR	C28-C27	4.15	1.65	1.52
12	F	203	CLA	CHD-C1D	4.15	1.46	1.38
15	F	201	BCR	C23-C22	4.15	1.54	1.46
15	F	202	BCR	C3-C4	4.15	1.65	1.52
12	A	849	CLA	C3D-C4D	-4.14	1.34	1.44
12	J	101	CLA	CHC-C4B	4.14	1.48	1.39
12	A	848	CLA	C3D-C4D	-4.14	1.34	1.44
15	A	838	BCR	C3-C4	4.14	1.65	1.52
15	J	107	BCR	C28-C27	4.13	1.65	1.52
12	L	201	CLA	C3D-C4D	-4.13	1.34	1.44
12	B	812	CLA	CHB-C1B	4.13	1.48	1.39
12	B	820	CLA	CHD-C1D	4.13	1.46	1.38
17	B	837	LMG	O8-C28	4.13	1.45	1.33
15	B	832	BCR	C23-C22	4.12	1.54	1.46
13	A	802	CL0	C3D-C4D	-4.12	1.34	1.44
12	A	833	CLA	CHD-C1D	4.12	1.46	1.38
12	A	810	CLA	C3D-C4D	-4.12	1.34	1.44
15	L	207	BCR	C3-C4	4.12	1.65	1.52
12	A	801	CLA	CHD-C1D	4.12	1.46	1.38
12	A	831	CLA	CHB-C1B	4.12	1.48	1.39
15	A	836	BCR	C3-C4	4.12	1.65	1.52
12	A	843	CLA	C3D-C4D	-4.11	1.34	1.44
15	B	834	BCR	C19-C18	4.11	1.54	1.46
12	A	820	CLA	C3C-C2C	4.11	1.45	1.36
15	F	201	BCR	C3-C4	4.11	1.65	1.52
12	A	801	CLA	C3D-C4D	-4.11	1.34	1.44
12	B	805	CLA	C3D-C4D	-4.11	1.34	1.44
15	L	208	BCR	C28-C27	4.11	1.65	1.52
15	K	4005	BCR	C28-C27	4.11	1.65	1.52
12	A	829	CLA	C3D-C4D	-4.11	1.34	1.44
12	B	815	CLA	C3D-C4D	-4.10	1.35	1.44
12	A	807	CLA	C3D-C4D	-4.10	1.35	1.44
15	I	101	BCR	C28-C27	4.10	1.65	1.52
15	K	4005	BCR	C3-C4	4.10	1.65	1.52
12	B	813	CLA	C3D-C4D	-4.10	1.35	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	J	104	BCR	C28-C27	4.10	1.65	1.52
12	A	828	CLA	C3D-C4D	-4.09	1.35	1.44
12	F	204	CLA	CHD-C4C	4.09	1.48	1.39
12	A	843	CLA	C3C-C2C	4.09	1.45	1.36
15	A	838	BCR	C23-C22	4.09	1.54	1.46
12	A	846	CLA	CHD-C1D	4.09	1.46	1.38
12	B	801	CLA	C3D-C4D	-4.08	1.35	1.44
15	A	837	BCR	C3-C4	4.08	1.65	1.52
12	A	823	CLA	C3D-C4D	-4.08	1.35	1.44
12	A	844	CLA	C1D-ND	-4.08	1.32	1.37
12	F	203	CLA	CHC-C4B	4.08	1.48	1.39
12	A	816	CLA	C3D-C4D	-4.08	1.35	1.44
12	B	830	CLA	C3D-C4D	-4.08	1.35	1.44
12	B	812	CLA	C3C-C2C	4.07	1.45	1.36
15	K	4001	BCR	C28-C27	4.07	1.65	1.52
15	B	841	BCR	C28-C27	4.07	1.65	1.52
12	B	814	CLA	CHC-C4B	4.06	1.48	1.39
12	B	818	CLA	CHD-C1D	4.06	1.46	1.38
12	B	828	CLA	C3D-C4D	-4.06	1.35	1.44
12	L	201	CLA	CHD-C4C	4.05	1.48	1.39
15	J	105	BCR	C23-C22	4.05	1.54	1.46
12	A	809	CLA	C3D-C4D	-4.05	1.35	1.44
12	B	802	CLA	C3D-C4D	-4.05	1.35	1.44
12	A	804	CLA	C3C-C2C	4.05	1.45	1.36
12	A	852	CLA	CHC-C4B	4.05	1.48	1.39
12	B	844	CLA	C3D-C4D	-4.05	1.35	1.44
12	B	850	CLA	CHD-C4C	4.04	1.48	1.39
12	A	847	CLA	C3D-C4D	-4.04	1.35	1.44
13	A	802	CL0	CHB-C1B	4.04	1.48	1.39
12	B	852	CLA	CHB-C1B	4.04	1.48	1.39
12	J	103	CLA	CHC-C4B	4.03	1.48	1.39
12	B	829	CLA	C3D-C4D	-4.03	1.35	1.44
12	B	830	CLA	CHD-C4C	4.03	1.48	1.39
12	B	816	CLA	C3D-C4D	-4.03	1.35	1.44
12	B	804	CLA	CHC-C4B	4.02	1.48	1.39
15	A	836	BCR	C28-C27	4.02	1.65	1.52
12	A	831	CLA	C3D-C4D	-4.01	1.35	1.44
15	B	832	BCR	C11-C10	4.01	1.55	1.43
12	A	803	CLA	CHD-C4C	4.01	1.48	1.39
12	A	830	CLA	CHD-C4C	4.00	1.48	1.39
15	A	836	BCR	C11-C10	4.00	1.55	1.43
15	A	838	BCR	C28-C27	4.00	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	846	CLA	CHB-C1B	4.00	1.48	1.39
12	A	826	CLA	C3D-C4D	-4.00	1.35	1.44
15	B	835	BCR	C19-C18	4.00	1.54	1.46
12	B	846	CLA	CHD-C1D	4.00	1.46	1.38
15	B	835	BCR	C8-C9	3.99	1.54	1.46
12	A	818	CLA	CHB-C1B	3.99	1.48	1.39
12	A	805	CLA	CHD-C1D	3.99	1.46	1.38
15	A	835	BCR	C20-C21	3.99	1.55	1.43
12	K	4004	CLA	CHC-C1C	3.99	1.46	1.38
12	B	823	CLA	CHD-C4C	3.99	1.48	1.39
15	A	835	BCR	C11-C10	3.98	1.55	1.43
12	B	811	CLA	CHD-C1D	3.98	1.46	1.38
12	B	824	CLA	C1B-NB	-3.98	1.32	1.37
15	A	836	BCR	C19-C18	3.98	1.54	1.46
12	A	832	CLA	CHC-C4B	3.97	1.48	1.39
15	F	202	BCR	C11-C10	3.97	1.55	1.43
12	B	812	CLA	CHC-C1C	3.97	1.46	1.38
26	L	209	DGD	O2G-C1B	3.97	1.45	1.34
12	A	824	CLA	CHD-C1D	3.97	1.46	1.38
12	B	852	CLA	CHC-C4B	3.97	1.48	1.39
17	B	837	LMG	O7-C10	3.97	1.45	1.34
12	J	103	CLA	CHB-C1B	3.97	1.48	1.39
12	A	820	CLA	CHC-C4B	3.97	1.48	1.39
12	A	831	CLA	CHD-C1D	3.97	1.46	1.38
15	F	202	BCR	C20-C21	3.97	1.55	1.43
12	A	812	CLA	CHD-C4C	3.96	1.48	1.39
15	B	841	BCR	C23-C22	3.96	1.54	1.46
15	L	207	BCR	C28-C27	3.96	1.64	1.52
12	A	844	CLA	MG-NC	3.96	2.15	2.06
12	B	801	CLA	CHC-C4B	3.96	1.48	1.39
12	A	818	CLA	CHD-C1D	3.96	1.46	1.38
15	F	201	BCR	C11-C10	3.96	1.55	1.43
12	B	848	CLA	CHB-C1B	3.95	1.48	1.39
12	A	858	CLA	C3C-C2C	3.95	1.45	1.36
15	A	837	BCR	C19-C18	3.95	1.54	1.46
12	A	858	CLA	CHB-C1B	3.95	1.48	1.39
12	A	832	CLA	C3D-C4D	-3.95	1.35	1.44
12	B	802	CLA	CHD-C4C	3.95	1.48	1.39
12	B	849	CLA	CHD-C4C	3.95	1.48	1.39
12	B	812	CLA	C3D-C4D	-3.94	1.35	1.44
12	B	846	CLA	CHC-C1C	3.94	1.46	1.38
12	B	823	CLA	CHC-C4B	3.94	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	813	CLA	CHD-C4C	3.94	1.48	1.39
12	B	829	CLA	CHD-C1D	3.94	1.46	1.38
12	F	204	CLA	CHB-C1B	3.94	1.48	1.39
12	B	829	CLA	CHC-C1C	3.94	1.46	1.38
13	A	802	CL0	CHD-C1D	3.93	1.46	1.38
12	A	858	CLA	CHD-C1D	3.93	1.46	1.38
12	A	828	CLA	CHB-C1B	3.93	1.48	1.39
12	B	853	CLA	C3D-C4D	-3.93	1.35	1.44
17	A	851	LMG	O7-C10	3.92	1.45	1.34
12	B	812	CLA	CHD-C4C	3.92	1.48	1.39
15	J	107	BCR	C20-C21	3.92	1.55	1.43
12	A	829	CLA	CHC-C4B	3.92	1.48	1.39
15	L	207	BCR	C23-C22	3.92	1.54	1.46
12	B	848	CLA	CHC-C4B	3.92	1.48	1.39
12	A	831	CLA	CHC-C4B	3.92	1.48	1.39
12	B	853	CLA	CHD-C1D	3.92	1.46	1.38
12	A	816	CLA	CHC-C4B	3.92	1.48	1.39
15	L	208	BCR	C20-C21	3.91	1.55	1.43
12	A	855	CLA	CHD-C4C	3.91	1.48	1.39
15	K	4005	BCR	C11-C10	3.91	1.55	1.43
12	A	801	CLA	CHC-C4B	3.91	1.48	1.39
12	A	858	CLA	C3D-C4D	-3.91	1.35	1.44
12	B	849	CLA	CHB-C1B	3.91	1.48	1.39
12	A	819	CLA	CHD-C4C	3.91	1.48	1.39
12	J	102	CLA	CHC-C4B	3.90	1.48	1.39
12	B	804	CLA	CHB-C1B	3.90	1.48	1.39
12	K	4003	CLA	C1C-C2C	-3.90	1.36	1.44
12	A	844	CLA	CHB-C1B	3.90	1.48	1.39
12	A	833	CLA	CHC-C4B	3.90	1.48	1.39
12	B	807	CLA	CHC-C4B	3.90	1.48	1.39
12	A	804	CLA	CHD-C4C	3.89	1.48	1.39
12	A	826	CLA	CHB-C1B	3.89	1.48	1.39
12	A	815	CLA	CHB-C1B	3.89	1.48	1.39
12	B	826	CLA	CHD-C4C	3.88	1.48	1.39
12	B	815	CLA	CHD-C4C	3.88	1.48	1.39
12	B	806	CLA	CHB-C1B	3.88	1.48	1.39
12	A	844	CLA	C3D-C4D	-3.88	1.35	1.44
16	A	839	LHG	O7-C7	3.88	1.45	1.34
12	B	819	CLA	CHD-C1D	3.88	1.46	1.38
12	A	832	CLA	CHB-C1B	3.88	1.48	1.39
12	L	204	CLA	CHC-C4B	3.88	1.48	1.39
12	A	805	CLA	CHC-C4B	3.87	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	K	4002	CLA	CHB-C1B	3.87	1.48	1.39
27	M	102	SQD	O47-C45	-3.87	1.37	1.46
13	A	802	CL0	CHC-C4B	3.87	1.48	1.39
12	A	813	CLA	CHC-C4B	3.87	1.48	1.39
12	B	850	CLA	CHC-C4B	3.87	1.48	1.39
15	I	101	BCR	C20-C21	3.87	1.55	1.43
12	K	4004	CLA	C1D-ND	-3.87	1.32	1.37
15	A	837	BCR	C23-C22	3.87	1.54	1.46
12	A	816	CLA	CHD-C4C	3.87	1.48	1.39
12	A	805	CLA	CHB-C1B	3.86	1.48	1.39
12	A	817	CLA	CHD-C4C	3.86	1.48	1.39
15	B	841	BCR	C11-C10	3.86	1.55	1.43
12	B	802	CLA	CHC-C4B	3.86	1.48	1.39
12	B	829	CLA	CHB-C1B	3.86	1.48	1.39
12	A	809	CLA	O2D-CGD	3.86	1.42	1.33
12	B	817	CLA	CHB-C1B	3.86	1.48	1.39
12	A	833	CLA	CHB-C1B	3.86	1.48	1.39
12	A	846	CLA	CHC-C1C	3.86	1.46	1.38
12	B	828	CLA	CHD-C4C	3.86	1.48	1.39
12	A	845	CLA	CHC-C4B	3.85	1.48	1.39
12	B	811	CLA	C3D-C4D	-3.85	1.35	1.44
15	A	838	BCR	C20-C21	3.85	1.55	1.43
12	B	849	CLA	CHC-C4B	3.85	1.48	1.39
12	K	4004	CLA	CHB-C1B	3.85	1.48	1.39
12	F	203	CLA	CHB-C1B	3.85	1.48	1.39
15	A	838	BCR	C11-C10	3.85	1.55	1.43
12	B	829	CLA	CHC-C4B	3.85	1.48	1.39
12	B	849	CLA	CHD-C1D	3.85	1.45	1.38
12	A	803	CLA	CHC-C4B	3.84	1.48	1.39
12	L	205	CLA	CHC-C4B	3.84	1.48	1.39
12	A	827	CLA	CHD-C4C	3.84	1.47	1.39
12	B	810	CLA	CHB-C1B	3.84	1.48	1.39
12	L	206	CLA	CHB-C1B	3.84	1.48	1.39
15	L	208	BCR	C11-C10	3.83	1.55	1.43
12	B	825	CLA	CHD-C4C	3.83	1.47	1.39
15	B	834	BCR	C28-C27	3.83	1.64	1.52
12	A	805	CLA	CHD-C4C	3.83	1.47	1.39
12	A	848	CLA	CHD-C4C	3.83	1.47	1.39
12	B	816	CLA	CHB-C1B	3.83	1.48	1.39
12	A	826	CLA	CHC-C4B	3.82	1.48	1.39
15	F	201	BCR	C20-C21	3.82	1.55	1.43
12	A	848	CLA	CHC-C4B	3.82	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	811	CLA	CHD-C4C	3.82	1.47	1.39
12	A	849	CLA	CHD-C4C	3.82	1.47	1.39
15	F	202	BCR	C16-C17	3.82	1.55	1.43
12	A	825	CLA	CHC-C4B	3.82	1.48	1.39
12	A	843	CLA	CHC-C4B	3.82	1.48	1.39
12	A	833	CLA	CHD-C4C	3.82	1.47	1.39
12	B	853	CLA	CHC-C4B	3.81	1.48	1.39
12	B	804	CLA	CHD-C4C	3.81	1.47	1.39
12	A	820	CLA	CHD-C1D	3.81	1.45	1.38
12	B	845	CLA	CHD-C4C	3.81	1.47	1.39
12	B	808	CLA	CHD-C4C	3.81	1.47	1.39
15	B	836	BCR	C16-C17	3.81	1.55	1.43
15	B	834	BCR	C23-C22	3.81	1.54	1.46
12	B	814	CLA	CHD-C4C	3.81	1.47	1.39
12	A	810	CLA	CHD-C4C	3.81	1.47	1.39
12	B	830	CLA	CHC-C4B	3.81	1.48	1.39
12	B	828	CLA	CHC-C4B	3.81	1.48	1.39
12	B	845	CLA	CHC-C4B	3.81	1.48	1.39
12	A	809	CLA	C1B-NB	-3.81	1.32	1.37
12	B	849	CLA	C3D-C4D	-3.81	1.35	1.44
17	B	837	LMG	C19-C18	-3.80	1.32	1.51
15	J	105	BCR	C20-C21	3.80	1.55	1.43
12	B	819	CLA	CHC-C4B	3.80	1.47	1.39
12	A	814	CLA	CHD-C4C	3.80	1.47	1.39
12	B	806	CLA	CHC-C4B	3.80	1.47	1.39
12	L	206	CLA	CHC-C4B	3.80	1.47	1.39
15	L	207	BCR	C11-C10	3.80	1.55	1.43
12	A	820	CLA	CHB-C1B	3.80	1.47	1.39
12	B	801	CLA	CHD-C4C	3.80	1.47	1.39
12	A	817	CLA	CHB-C1B	3.79	1.47	1.39
12	J	102	CLA	CHD-C4C	3.79	1.47	1.39
12	A	807	CLA	CHD-C4C	3.79	1.47	1.39
12	A	852	CLA	CHD-C1D	3.79	1.45	1.38
12	B	826	CLA	CHC-C4B	3.79	1.47	1.39
12	B	844	CLA	C1D-ND	-3.79	1.32	1.37
12	B	805	CLA	CHB-C1B	3.79	1.47	1.39
12	A	852	CLA	CHD-C4C	3.79	1.47	1.39
15	K	4001	BCR	C23-C22	3.79	1.54	1.46
12	B	819	CLA	CHB-C1B	3.79	1.47	1.39
15	J	107	BCR	C11-C10	3.79	1.54	1.43
12	A	829	CLA	CHD-C4C	3.78	1.47	1.39
12	B	825	CLA	CHB-C1B	3.78	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	850	LHG	O8-C23	3.78	1.44	1.33
12	A	808	CLA	CHC-C4B	3.78	1.47	1.39
12	A	808	CLA	CHB-C1B	3.78	1.47	1.39
12	B	843	CLA	CHD-C4C	3.78	1.47	1.39
12	A	815	CLA	CHC-C4B	3.78	1.47	1.39
26	L	209	DGD	CDA-CCA	-3.77	1.33	1.51
12	A	806	CLA	CHC-C4B	3.77	1.47	1.39
12	F	204	CLA	CHC-C4B	3.77	1.47	1.39
17	B	837	LMG	C43-C42	-3.77	1.33	1.51
12	B	818	CLA	CHC-C4B	3.77	1.47	1.39
12	A	819	CLA	CHC-C4B	3.77	1.47	1.39
12	L	204	CLA	CHB-C1B	3.77	1.47	1.39
15	B	832	BCR	C20-C21	3.77	1.54	1.43
15	K	4001	BCR	C11-C10	3.77	1.54	1.43
12	A	818	CLA	CHC-C4B	3.77	1.47	1.39
12	B	805	CLA	CHD-C4C	3.77	1.47	1.39
12	A	824	CLA	CHC-C4B	3.77	1.47	1.39
12	B	803	CLA	O2D-CGD	3.77	1.42	1.33
12	A	828	CLA	CHD-C4C	3.77	1.47	1.39
15	A	837	BCR	C4-C5	-3.76	1.44	1.51
12	B	809	CLA	CHB-C1B	3.76	1.47	1.39
12	A	821	CLA	CHD-C4C	3.76	1.47	1.39
12	B	807	CLA	CHD-C4C	3.76	1.47	1.39
12	A	823	CLA	CHB-C1B	3.76	1.47	1.39
12	B	822	CLA	CHB-C1B	3.76	1.47	1.39
12	A	814	CLA	CHC-C4B	3.76	1.47	1.39
12	A	829	CLA	CHB-C1B	3.76	1.47	1.39
12	A	826	CLA	CHD-C4C	3.76	1.47	1.39
15	L	207	BCR	C19-C18	3.76	1.54	1.46
15	L	208	BCR	C16-C17	3.76	1.54	1.43
12	B	843	CLA	CHB-C1B	3.76	1.47	1.39
12	A	803	CLA	CHB-C1B	3.75	1.47	1.39
12	A	830	CLA	CHC-C4B	3.75	1.47	1.39
12	B	852	CLA	CHD-C4C	3.75	1.47	1.39
12	A	855	CLA	CHB-C1B	3.75	1.47	1.39
12	B	801	CLA	CHB-C1B	3.75	1.47	1.39
15	B	841	BCR	C20-C21	3.75	1.54	1.43
12	K	4004	CLA	CHD-C4C	3.75	1.47	1.39
12	A	817	CLA	CHC-C4B	3.75	1.47	1.39
12	B	825	CLA	CHC-C4B	3.74	1.47	1.39
12	B	842	CLA	CHC-C4B	3.74	1.47	1.39
15	K	4005	BCR	C20-C21	3.74	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	807	CLA	CHB-C1B	3.74	1.47	1.39
12	A	821	CLA	CHB-C1B	3.74	1.47	1.39
12	A	822	CLA	CHC-C4B	3.74	1.47	1.39
12	A	822	CLA	CHB-C1B	3.74	1.47	1.39
12	A	825	CLA	CHD-C4C	3.74	1.47	1.39
12	B	847	CLA	CHC-C1C	3.73	1.46	1.38
15	B	836	BCR	C15-C14	3.73	1.54	1.43
12	J	103	CLA	OBD-CAD	3.73	1.28	1.22
12	B	827	CLA	CHB-C1B	3.73	1.47	1.39
12	B	846	CLA	C1C-NC	-3.73	1.32	1.37
15	A	836	BCR	C23-C22	3.73	1.53	1.46
12	F	204	CLA	OBD-CAD	3.73	1.28	1.22
12	A	825	CLA	CHB-C1B	3.73	1.47	1.39
15	A	835	BCR	C15-C14	3.73	1.54	1.43
12	A	832	CLA	CHD-C4C	3.73	1.47	1.39
12	A	808	CLA	CHD-C4C	3.73	1.47	1.39
12	L	204	CLA	CHD-C4C	3.73	1.47	1.39
12	A	814	CLA	CHB-C1B	3.72	1.47	1.39
12	B	808	CLA	CHB-C1B	3.72	1.47	1.39
17	B	837	LMG	C40-C39	-3.72	1.33	1.51
12	B	830	CLA	CHB-C1B	3.72	1.47	1.39
26	L	209	DGD	CGA-CFA	-3.72	1.33	1.51
15	I	101	BCR	C11-C10	3.72	1.54	1.43
15	B	834	BCR	C20-C21	3.72	1.54	1.43
12	A	806	CLA	CHB-C1B	3.72	1.47	1.39
12	A	849	CLA	CHB-C1B	3.72	1.47	1.39
12	B	803	CLA	O2A-C1	3.72	1.56	1.46
12	A	810	CLA	CHB-C1B	3.71	1.47	1.39
12	K	4002	CLA	CHD-C4C	3.71	1.47	1.39
12	B	811	CLA	CHB-C1B	3.71	1.47	1.39
12	B	806	CLA	CHD-C4C	3.71	1.47	1.39
12	B	801	CLA	CHD-C1D	3.71	1.45	1.38
12	B	821	CLA	CHC-C4B	3.71	1.47	1.39
17	A	851	LMG	C19-C18	-3.70	1.33	1.51
12	B	848	CLA	C3D-C4D	-3.70	1.35	1.44
12	A	811	CLA	CHB-C1B	3.70	1.47	1.39
15	B	834	BCR	C11-C10	3.70	1.54	1.43
12	A	815	CLA	CHD-C4C	3.70	1.47	1.39
12	B	842	CLA	CHD-C4C	3.70	1.47	1.39
15	B	841	BCR	C16-C17	3.70	1.54	1.43
12	B	843	CLA	CHC-C4B	3.70	1.47	1.39
15	B	835	BCR	C23-C22	3.70	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	809	CLA	C1D-ND	-3.70	1.33	1.37
12	B	827	CLA	CHD-C4C	3.70	1.47	1.39
12	A	806	CLA	CHD-C4C	3.70	1.47	1.39
12	A	821	CLA	CHC-C4B	3.70	1.47	1.39
12	B	818	CLA	CHB-C1B	3.70	1.47	1.39
17	A	851	LMG	C22-C21	-3.70	1.33	1.51
26	L	209	DGD	CAB-C9B	-3.70	1.33	1.51
12	A	830	CLA	CHB-C1B	3.69	1.47	1.39
12	B	816	CLA	CHC-C4B	3.69	1.47	1.39
12	A	801	CLA	CHB-C1B	3.69	1.47	1.39
12	B	844	CLA	C4B-NB	-3.69	1.33	1.37
12	A	848	CLA	OBD-CAD	3.69	1.28	1.22
15	F	202	BCR	C15-C14	3.69	1.54	1.43
17	A	840	LMG	C19-C18	-3.68	1.33	1.51
12	A	812	CLA	CHC-C4B	3.68	1.47	1.39
17	A	840	LMG	C40-C39	-3.68	1.33	1.51
12	B	813	CLA	CHB-C1B	3.68	1.47	1.39
12	B	852	CLA	MG-NC	3.68	2.15	2.06
15	B	832	BCR	C7-C6	3.68	1.57	1.45
15	J	105	BCR	C27-C26	-3.68	1.44	1.51
12	A	813	CLA	CHD-C4C	3.68	1.47	1.39
12	A	843	CLA	CHD-C4C	3.68	1.47	1.39
12	L	206	CLA	CHD-C4C	3.68	1.47	1.39
12	B	815	CLA	CHC-C4B	3.68	1.47	1.39
12	B	842	CLA	CHB-C1B	3.67	1.47	1.39
12	B	820	CLA	CHD-C4C	3.67	1.47	1.39
12	B	803	CLA	C3C-C2C	3.67	1.44	1.36
12	K	4003	CLA	MG-NA	3.67	2.15	2.06
12	B	823	CLA	CHB-C1B	3.67	1.47	1.39
12	A	808	CLA	OBD-CAD	3.67	1.28	1.22
12	A	852	CLA	C1C-NC	-3.67	1.32	1.37
12	A	846	CLA	O2D-CGD	3.67	1.42	1.33
15	A	837	BCR	C11-C10	3.66	1.54	1.43
12	F	203	CLA	CHD-C4C	3.66	1.47	1.39
12	K	4002	CLA	CHC-C4B	3.66	1.47	1.39
12	B	810	CLA	CHD-C4C	3.66	1.47	1.39
12	B	849	CLA	C1D-ND	-3.66	1.33	1.37
26	L	209	DGD	CAA-C9A	-3.66	1.33	1.51
12	A	858	CLA	CHC-C4B	3.66	1.47	1.39
15	J	105	BCR	C7-C6	3.66	1.57	1.45
12	A	801	CLA	CHD-C4C	3.66	1.47	1.39
15	K	4001	BCR	C20-C21	3.65	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	840	LMG	C43-C42	-3.65	1.33	1.51
16	A	850	LHG	O8-C6	-3.65	1.37	1.45
12	L	205	CLA	C1D-ND	-3.65	1.33	1.37
15	F	201	BCR	C16-C17	3.65	1.54	1.43
12	B	824	CLA	C4B-NB	-3.65	1.33	1.37
15	A	836	BCR	C20-C21	3.65	1.54	1.43
12	A	847	CLA	CHD-C4C	3.65	1.47	1.39
15	B	835	BCR	C16-C17	3.64	1.54	1.43
12	A	811	CLA	CHC-C4B	3.64	1.47	1.39
12	B	822	CLA	CHC-C4B	3.64	1.47	1.39
12	A	831	CLA	OBD-CAD	3.64	1.28	1.22
12	B	827	CLA	CHC-C4B	3.64	1.47	1.39
15	A	837	BCR	C20-C21	3.64	1.54	1.43
17	A	840	LMG	C37-C36	-3.64	1.33	1.51
12	A	812	CLA	OBD-CAD	3.64	1.28	1.22
12	A	849	CLA	CHC-C4B	3.64	1.47	1.39
15	L	207	BCR	C20-C21	3.64	1.54	1.43
12	A	807	CLA	CHC-C4B	3.63	1.47	1.39
12	B	809	CLA	CHC-C4B	3.63	1.47	1.39
15	A	836	BCR	C4-C5	-3.63	1.44	1.51
15	B	832	BCR	C16-C17	3.63	1.54	1.43
12	B	824	CLA	CHD-C4C	3.63	1.47	1.39
12	L	205	CLA	CHD-C4C	3.63	1.47	1.39
15	A	838	BCR	C16-C17	3.63	1.54	1.43
12	B	830	CLA	OBD-CAD	3.62	1.28	1.22
12	A	833	CLA	OBD-CAD	3.62	1.28	1.22
12	B	811	CLA	OBD-CAD	3.62	1.28	1.22
12	A	812	CLA	CHB-C1B	3.62	1.47	1.39
12	F	203	CLA	C3D-C4D	-3.62	1.36	1.44
12	B	824	CLA	O2D-CGD	3.62	1.42	1.33
12	A	845	CLA	CHD-C4C	3.61	1.47	1.39
12	A	804	CLA	CHC-C4B	3.61	1.47	1.39
15	J	105	BCR	C16-C17	3.61	1.54	1.43
12	A	827	CLA	CHC-C4B	3.61	1.47	1.39
17	B	837	LMG	C37-C36	-3.61	1.33	1.51
12	B	821	CLA	CHD-C4C	3.61	1.47	1.39
12	A	843	CLA	CHB-C1B	3.61	1.47	1.39
12	A	823	CLA	OBD-CAD	3.60	1.28	1.22
12	A	813	CLA	CHB-C1B	3.60	1.47	1.39
12	B	815	CLA	CHB-C1B	3.60	1.47	1.39
12	A	823	CLA	CHD-C4C	3.60	1.47	1.39
12	B	805	CLA	CHC-C4B	3.60	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	824	CLA	CHD-C1D	3.59	1.45	1.38
12	B	845	CLA	CHB-C1B	3.59	1.47	1.39
12	B	809	CLA	CHD-C4C	3.59	1.47	1.39
15	B	841	BCR	C15-C14	3.59	1.54	1.43
12	A	810	CLA	CHC-C4B	3.59	1.47	1.39
12	A	847	CLA	CHB-C1B	3.59	1.47	1.39
12	L	205	CLA	CHD-C1D	3.59	1.45	1.38
12	A	809	CLA	CHD-C1D	3.59	1.45	1.38
12	A	858	CLA	CHD-C4C	3.59	1.47	1.39
12	B	808	CLA	CHC-C4B	3.59	1.47	1.39
12	A	824	CLA	CHD-C4C	3.59	1.47	1.39
15	J	104	BCR	C27-C26	-3.59	1.44	1.51
12	A	806	CLA	OBD-CAD	3.58	1.28	1.22
12	B	803	CLA	MG-NC	3.58	2.14	2.06
15	A	837	BCR	C16-C17	3.58	1.54	1.43
12	L	206	CLA	OBD-CAD	3.58	1.28	1.22
12	A	824	CLA	CHB-C1B	3.58	1.47	1.39
12	J	101	CLA	OBD-CAD	3.58	1.28	1.22
12	A	822	CLA	CHD-C4C	3.58	1.47	1.39
15	K	4005	BCR	C16-C17	3.58	1.54	1.43
15	B	835	BCR	C20-C21	3.58	1.54	1.43
12	A	818	CLA	CHD-C4C	3.57	1.47	1.39
12	B	822	CLA	CHD-C4C	3.57	1.47	1.39
12	B	844	CLA	C3C-C2C	3.57	1.44	1.36
15	K	4001	BCR	C16-C17	3.57	1.54	1.43
12	B	825	CLA	OBD-CAD	3.57	1.28	1.22
12	A	845	CLA	CHB-C1B	3.57	1.47	1.39
12	A	847	CLA	CHC-C4B	3.56	1.47	1.39
12	B	846	CLA	C1B-NB	-3.56	1.33	1.37
15	J	107	BCR	C16-C17	3.56	1.54	1.43
12	B	853	CLA	C1D-ND	-3.56	1.33	1.37
12	K	4004	CLA	OBD-CAD	3.55	1.28	1.22
12	B	812	CLA	C1B-NB	-3.55	1.33	1.37
12	K	4002	CLA	OBD-CAD	3.55	1.28	1.22
12	B	826	CLA	CHB-C1B	3.55	1.47	1.39
12	B	814	CLA	CHB-C1B	3.55	1.47	1.39
12	B	817	CLA	CHC-C4B	3.55	1.47	1.39
12	L	201	CLA	CHC-C4B	3.55	1.47	1.39
12	B	814	CLA	OBD-CAD	3.55	1.28	1.22
15	A	836	BCR	C7-C6	3.55	1.57	1.45
12	A	819	CLA	CHB-C1B	3.55	1.47	1.39
12	B	805	CLA	OBD-CAD	3.55	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	816	CLA	CHB-C1B	3.54	1.47	1.39
12	B	818	CLA	CHD-C4C	3.54	1.47	1.39
12	A	831	CLA	CHD-C4C	3.54	1.47	1.39
15	J	107	BCR	C7-C6	3.54	1.57	1.45
12	A	844	CLA	CHC-C1C	3.54	1.45	1.38
15	J	105	BCR	C28-C27	3.54	1.63	1.52
12	A	823	CLA	CHC-C4B	3.54	1.47	1.39
12	B	852	CLA	OBD-CAD	3.54	1.28	1.22
12	B	820	CLA	CHC-C4B	3.54	1.47	1.39
15	I	101	BCR	C16-C17	3.53	1.54	1.43
12	B	824	CLA	CHB-C1B	3.53	1.47	1.39
12	A	801	CLA	OBD-CAD	3.53	1.28	1.22
15	F	201	BCR	C4-C5	-3.53	1.44	1.51
15	A	838	BCR	C15-C14	3.53	1.54	1.43
12	B	811	CLA	CHC-C4B	3.53	1.47	1.39
15	B	832	BCR	C15-C14	3.53	1.54	1.43
20	A	856	45D	C23-C25	-3.53	1.38	1.46
15	J	105	BCR	C11-C10	3.52	1.54	1.43
12	A	828	CLA	CHC-C4B	3.52	1.47	1.39
12	B	817	CLA	CHD-C4C	3.52	1.47	1.39
12	B	806	CLA	OBD-CAD	3.52	1.28	1.22
15	L	207	BCR	C7-C6	3.52	1.57	1.45
15	L	208	BCR	C7-C6	3.51	1.57	1.45
12	A	817	CLA	OBD-CAD	3.51	1.28	1.22
12	B	853	CLA	C1B-C2B	3.51	1.51	1.43
12	B	801	CLA	C1D-ND	-3.51	1.33	1.37
15	L	208	BCR	C15-C14	3.51	1.54	1.43
12	B	815	CLA	OBD-CAD	3.51	1.28	1.22
15	K	4005	BCR	C15-C14	3.51	1.54	1.43
12	A	844	CLA	CHD-C1D	3.51	1.45	1.38
15	B	841	BCR	C4-C5	-3.51	1.44	1.51
15	F	201	BCR	C24-C25	3.51	1.57	1.45
15	A	837	BCR	C15-C14	3.50	1.54	1.43
12	L	201	CLA	CHB-C1B	3.50	1.47	1.39
12	A	811	CLA	OBD-CAD	3.50	1.28	1.22
12	B	847	CLA	C3C-C2C	3.50	1.44	1.36
12	A	843	CLA	OBD-CAD	3.50	1.28	1.22
12	B	850	CLA	CHB-C1B	3.49	1.47	1.39
12	J	101	CLA	CHB-C1B	3.49	1.47	1.39
12	B	821	CLA	CHB-C1B	3.49	1.47	1.39
12	A	824	CLA	C1D-ND	-3.49	1.33	1.37
12	B	853	CLA	CHD-C4C	3.49	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	834	BCR	C16-C17	3.48	1.54	1.43
12	A	815	CLA	OBD-CAD	3.48	1.28	1.22
12	B	844	CLA	CHB-C1B	3.48	1.47	1.39
13	A	802	CL0	CHD-C4C	3.48	1.47	1.39
15	F	202	BCR	C7-C6	3.48	1.57	1.45
12	A	807	CLA	OBD-CAD	3.48	1.28	1.22
15	A	836	BCR	C16-C17	3.48	1.54	1.43
12	B	801	CLA	OBD-CAD	3.48	1.28	1.22
12	B	810	CLA	CHC-C4B	3.48	1.47	1.39
12	L	205	CLA	CHB-C1B	3.48	1.47	1.39
12	B	848	CLA	OBD-CAD	3.47	1.28	1.22
12	A	847	CLA	OBD-CAD	3.47	1.28	1.22
12	A	820	CLA	CHD-C4C	3.47	1.47	1.39
15	J	107	BCR	C15-C14	3.47	1.54	1.43
12	A	844	CLA	C1B-NB	-3.47	1.33	1.37
12	A	807	CLA	CHB-C1B	3.47	1.47	1.39
12	B	824	CLA	C1B-C2B	3.47	1.51	1.43
15	K	4001	BCR	C4-C5	-3.47	1.44	1.51
15	B	835	BCR	C11-C10	3.46	1.53	1.43
12	A	848	CLA	CHB-C1B	3.46	1.47	1.39
12	A	804	CLA	CHB-C1B	3.46	1.47	1.39
12	B	803	CLA	CHD-C1D	3.46	1.45	1.38
12	A	827	CLA	OBD-CAD	3.46	1.28	1.22
15	F	201	BCR	C15-C14	3.46	1.53	1.43
12	B	802	CLA	CHB-C1B	3.46	1.47	1.39
12	B	816	CLA	CHD-C4C	3.46	1.47	1.39
12	A	846	CLA	C3C-C2C	3.45	1.44	1.36
12	A	827	CLA	CHB-C1B	3.45	1.47	1.39
12	B	849	CLA	OBD-CAD	3.45	1.28	1.22
12	B	848	CLA	CHD-C4C	3.44	1.47	1.39
12	B	853	CLA	OBD-CAD	3.44	1.28	1.22
15	F	201	BCR	C7-C6	3.43	1.56	1.45
12	J	102	CLA	CHB-C1B	3.43	1.47	1.39
12	B	819	CLA	CHD-C4C	3.43	1.47	1.39
12	L	204	CLA	OBD-CAD	3.43	1.28	1.22
12	B	813	CLA	CHC-C4B	3.43	1.47	1.39
15	I	101	BCR	C15-C14	3.43	1.53	1.43
12	B	804	CLA	OBD-CAD	3.42	1.28	1.22
12	B	802	CLA	OBD-CAD	3.42	1.28	1.22
12	B	847	CLA	CHB-C1B	3.42	1.47	1.39
12	B	844	CLA	CHC-C4B	3.42	1.47	1.39
12	B	846	CLA	CHB-C1B	3.41	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	829	CLA	CHD-C4C	3.41	1.47	1.39
12	B	811	CLA	CHD-C4C	3.41	1.47	1.39
12	B	808	CLA	OBD-CAD	3.41	1.28	1.22
13	A	802	CL0	C1D-ND	-3.41	1.33	1.37
12	B	844	CLA	C1C-NC	-3.41	1.32	1.37
15	J	105	BCR	C4-C5	-3.40	1.44	1.51
12	J	102	CLA	OBD-CAD	3.40	1.28	1.22
12	B	809	CLA	C1D-ND	-3.40	1.33	1.37
15	I	101	BCR	C7-C6	3.40	1.56	1.45
15	F	202	BCR	C12-C13	3.40	1.53	1.46
12	B	810	CLA	OBD-CAD	3.40	1.28	1.22
15	B	834	BCR	C4-C5	-3.40	1.44	1.51
15	L	207	BCR	C15-C14	3.40	1.53	1.43
12	A	832	CLA	OBD-CAD	3.39	1.28	1.22
12	B	828	CLA	CHB-C1B	3.39	1.47	1.39
15	B	835	BCR	C15-C14	3.39	1.53	1.43
12	A	829	CLA	OBD-CAD	3.39	1.28	1.22
12	A	816	CLA	OBD-CAD	3.38	1.28	1.22
12	A	809	CLA	CHB-C1B	3.38	1.47	1.39
12	A	855	CLA	CHC-C4B	3.38	1.47	1.39
15	L	207	BCR	C27-C26	-3.38	1.44	1.51
12	B	823	CLA	OBD-CAD	3.38	1.28	1.22
15	A	836	BCR	C15-C14	3.38	1.53	1.43
16	A	850	LHG	O7-C7	3.38	1.43	1.34
15	L	208	BCR	C24-C25	3.38	1.56	1.45
12	A	805	CLA	OBD-CAD	3.38	1.28	1.22
12	A	844	CLA	C1C-NC	-3.37	1.32	1.37
12	A	849	CLA	OBD-CAD	3.37	1.28	1.22
15	K	4001	BCR	C7-C6	3.37	1.56	1.45
15	A	835	BCR	C4-C5	-3.37	1.44	1.51
15	B	835	BCR	C4-C5	-3.37	1.44	1.51
12	A	826	CLA	OBD-CAD	3.37	1.28	1.22
12	A	846	CLA	C4B-NB	-3.37	1.33	1.37
25	L	202	EQ3	C19-C18	-3.37	1.38	1.46
12	A	844	CLA	C3C-C2C	3.37	1.44	1.36
15	K	4005	BCR	C7-C6	3.37	1.56	1.45
12	B	824	CLA	CHC-C1C	3.36	1.45	1.38
12	K	4004	CLA	C1B-C2B	3.36	1.51	1.43
15	J	105	BCR	C15-C14	3.36	1.53	1.43
12	A	846	CLA	CHD-C4C	3.36	1.46	1.39
15	L	207	BCR	C16-C17	3.36	1.53	1.43
12	A	858	CLA	C1B-C2B	3.36	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	836	BCR	C24-C25	3.35	1.56	1.45
15	K	4001	BCR	C15-C14	3.35	1.53	1.43
15	B	841	BCR	C7-C6	3.35	1.56	1.45
12	B	849	CLA	C3D-C2D	3.35	1.48	1.39
12	B	821	CLA	C1D-ND	-3.35	1.33	1.37
15	K	4005	BCR	C4-C5	-3.34	1.44	1.51
12	A	846	CLA	MG-NC	3.34	2.14	2.06
12	A	809	CLA	C4B-NB	-3.34	1.33	1.37
12	A	846	CLA	CHC-C4B	3.34	1.46	1.39
15	B	834	BCR	C15-C14	3.34	1.53	1.43
12	B	850	CLA	OBD-CAD	3.33	1.28	1.22
12	A	852	CLA	MG-NC	3.33	2.14	2.06
12	B	805	CLA	C1B-NB	-3.33	1.33	1.37
15	A	835	BCR	C12-C13	3.32	1.53	1.46
12	A	845	CLA	OBD-CAD	3.32	1.28	1.22
12	B	820	CLA	C1D-ND	-3.32	1.33	1.37
12	A	814	CLA	OBD-CAD	3.32	1.28	1.22
12	B	846	CLA	CHC-C4B	3.31	1.46	1.39
12	B	822	CLA	OBD-CAD	3.31	1.28	1.22
12	F	203	CLA	OBD-CAD	3.31	1.28	1.22
12	B	844	CLA	MG-NC	3.31	2.14	2.06
15	B	832	BCR	C12-C13	3.31	1.53	1.46
15	B	834	BCR	C7-C6	3.31	1.56	1.45
12	A	809	CLA	CHC-C4B	3.31	1.46	1.39
15	L	208	BCR	C27-C26	-3.30	1.44	1.51
12	A	844	CLA	CHC-C4B	3.30	1.46	1.39
12	B	806	CLA	C1D-ND	-3.30	1.33	1.37
12	B	818	CLA	OBD-CAD	3.30	1.28	1.22
12	A	846	CLA	C1C-NC	-3.30	1.32	1.37
12	B	816	CLA	OBD-CAD	3.29	1.28	1.22
12	J	102	CLA	C1D-ND	-3.29	1.33	1.37
12	B	815	CLA	C1D-ND	-3.29	1.33	1.37
12	A	844	CLA	CHD-C4C	3.28	1.46	1.39
12	B	813	CLA	OBD-CAD	3.28	1.28	1.22
12	A	825	CLA	OBD-CAD	3.28	1.28	1.22
12	B	844	CLA	CHD-C1D	3.28	1.44	1.38
12	B	816	CLA	C3D-C2D	3.27	1.47	1.39
12	A	813	CLA	MG-NC	3.27	2.14	2.06
12	L	201	CLA	C3D-C2D	3.27	1.47	1.39
15	F	202	BCR	C4-C5	-3.26	1.44	1.51
12	B	801	CLA	C1B-NB	-3.26	1.33	1.37
15	A	838	BCR	C7-C6	3.26	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	829	CLA	C1C-NC	-3.26	1.32	1.37
12	B	812	CLA	OBD-CAD	3.26	1.28	1.22
12	A	820	CLA	C1D-ND	-3.26	1.33	1.37
12	A	822	CLA	C1D-ND	-3.26	1.33	1.37
12	L	205	CLA	OBD-CAD	3.26	1.28	1.22
15	A	835	BCR	C7-C6	3.26	1.56	1.45
12	A	823	CLA	C1B-NB	-3.26	1.33	1.37
12	B	808	CLA	C1D-ND	-3.25	1.33	1.37
15	I	101	BCR	C24-C25	3.25	1.56	1.45
12	K	4004	CLA	C3D-C2D	3.25	1.47	1.39
12	B	846	CLA	C3C-C2C	3.24	1.43	1.36
12	B	803	CLA	CHD-C4C	3.24	1.46	1.39
12	F	204	CLA	MG-NC	3.24	2.14	2.06
12	A	817	CLA	C1D-ND	-3.24	1.33	1.37
15	K	4005	BCR	C12-C13	3.24	1.52	1.46
12	B	813	CLA	C1B-C2B	3.24	1.50	1.43
12	B	845	CLA	OBD-CAD	3.23	1.28	1.22
12	B	822	CLA	C1D-ND	-3.23	1.33	1.37
15	J	105	BCR	C24-C25	3.23	1.56	1.45
15	L	207	BCR	C4-C5	-3.23	1.45	1.51
12	A	817	CLA	C3D-C2D	3.22	1.47	1.39
20	A	856	45D	C24-C26	-3.22	1.39	1.46
12	F	204	CLA	C3D-C2D	3.22	1.47	1.39
12	A	819	CLA	OBD-CAD	3.22	1.28	1.22
12	A	812	CLA	C1B-NB	-3.22	1.33	1.37
15	A	838	BCR	C4-C5	-3.22	1.45	1.51
12	B	817	CLA	OBD-CAD	3.22	1.28	1.22
12	B	843	CLA	OBD-CAD	3.22	1.28	1.22
12	A	816	CLA	C3D-C2D	3.21	1.47	1.39
12	A	818	CLA	MG-NC	3.21	2.13	2.06
12	A	815	CLA	C1D-ND	-3.21	1.33	1.37
12	A	804	CLA	OBD-CAD	3.21	1.28	1.22
12	L	201	CLA	OBD-CAD	3.21	1.28	1.22
12	B	802	CLA	C3D-C2D	3.20	1.47	1.39
15	B	841	BCR	C12-C13	3.20	1.52	1.46
12	B	816	CLA	C1D-ND	-3.20	1.33	1.37
12	B	842	CLA	OBD-CAD	3.20	1.28	1.22
12	B	818	CLA	C1D-ND	-3.20	1.33	1.37
12	A	810	CLA	OBD-CAD	3.20	1.28	1.22
12	B	822	CLA	C1B-NB	-3.19	1.33	1.37
15	K	4005	BCR	C24-C25	3.19	1.56	1.45
12	B	826	CLA	OBD-CAD	3.19	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	820	CLA	MG-NC	3.19	2.13	2.06
12	A	852	CLA	C1D-ND	-3.19	1.33	1.37
12	A	821	CLA	OBD-CAD	3.18	1.28	1.22
12	B	827	CLA	OBD-CAD	3.18	1.28	1.22
12	B	803	CLA	C1B-C2B	3.18	1.50	1.43
12	A	855	CLA	C1B-NB	-3.18	1.33	1.37
12	B	817	CLA	C1B-NB	-3.17	1.33	1.37
15	F	202	BCR	C24-C25	3.17	1.55	1.45
12	K	4004	CLA	C3D-C4D	-3.17	1.37	1.44
15	B	835	BCR	C7-C6	3.17	1.55	1.45
12	A	821	CLA	C1B-NB	-3.17	1.33	1.37
12	B	827	CLA	C1B-C2B	3.17	1.50	1.43
12	A	828	CLA	OBD-CAD	3.17	1.27	1.22
15	A	837	BCR	C7-C6	3.17	1.55	1.45
12	B	843	CLA	C1B-NB	-3.16	1.33	1.37
12	B	844	CLA	CHD-C4C	3.16	1.46	1.39
12	B	843	CLA	C1D-ND	-3.16	1.33	1.37
12	A	822	CLA	MG-NC	3.16	2.13	2.06
12	B	810	CLA	C1D-ND	-3.16	1.33	1.37
12	B	809	CLA	MG-NC	3.16	2.13	2.06
12	A	813	CLA	OBD-CAD	3.16	1.27	1.22
12	B	814	CLA	MG-NC	3.16	2.13	2.06
12	A	846	CLA	C1B-C2B	3.16	1.50	1.43
15	K	4001	BCR	C24-C25	3.15	1.55	1.45
12	B	808	CLA	C3D-C2D	3.15	1.47	1.39
12	A	831	CLA	C1B-C2B	3.15	1.50	1.43
12	B	829	CLA	OBD-CAD	3.15	1.27	1.22
12	A	852	CLA	C3D-C2D	3.15	1.47	1.39
12	B	848	CLA	MG-NC	3.15	2.13	2.06
27	M	102	SQD	O47-C7	3.15	1.43	1.34
12	B	824	CLA	C3C-C2C	3.15	1.43	1.36
15	K	4005	BCR	C27-C26	-3.15	1.45	1.51
12	A	814	CLA	C3D-C2D	3.15	1.47	1.39
15	A	836	BCR	C12-C13	3.15	1.52	1.46
27	M	102	SQD	O5-C1	3.15	1.49	1.41
12	A	825	CLA	MG-NC	3.14	2.13	2.06
12	B	812	CLA	CHC-C4B	3.14	1.46	1.39
15	F	201	BCR	C12-C13	3.14	1.52	1.46
12	A	823	CLA	C1D-ND	-3.14	1.33	1.37
12	A	855	CLA	C3D-C2D	3.14	1.47	1.39
12	B	846	CLA	C1D-ND	-3.14	1.33	1.37
12	A	852	CLA	OBD-CAD	3.14	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	810	CLA	C3D-C2D	3.14	1.47	1.39
12	B	818	CLA	MG-NC	3.13	2.13	2.06
12	A	818	CLA	OBD-CAD	3.13	1.27	1.22
12	B	802	CLA	C1B-NB	-3.13	1.33	1.37
12	A	804	CLA	C1B-NB	-3.13	1.33	1.37
12	A	827	CLA	C3D-C2D	3.13	1.47	1.39
12	B	816	CLA	MG-NC	3.13	2.13	2.06
12	A	815	CLA	MG-NC	3.13	2.13	2.06
12	J	102	CLA	C1B-NB	-3.13	1.33	1.37
15	J	107	BCR	C4-C5	-3.12	1.45	1.51
12	B	830	CLA	C3D-C2D	3.12	1.47	1.39
12	L	204	CLA	MG-NC	3.12	2.13	2.06
12	A	818	CLA	C1B-NB	-3.12	1.33	1.37
15	B	832	BCR	C27-C26	-3.12	1.45	1.51
12	B	806	CLA	MG-NC	3.12	2.13	2.06
12	A	830	CLA	C3D-C2D	3.12	1.47	1.39
12	A	808	CLA	C1D-ND	-3.12	1.33	1.37
12	A	805	CLA	C1B-C2B	3.11	1.50	1.43
13	A	802	CL0	MG-NC	3.11	2.13	2.06
15	A	837	BCR	C24-C25	3.11	1.55	1.45
12	B	807	CLA	OBD-CAD	3.11	1.27	1.22
12	B	813	CLA	C3D-C2D	3.11	1.47	1.39
15	I	101	BCR	C4-C5	-3.11	1.45	1.51
15	J	107	BCR	C12-C13	3.10	1.52	1.46
12	B	843	CLA	C3D-C2D	3.10	1.47	1.39
12	A	844	CLA	C4B-NB	-3.10	1.33	1.37
15	J	107	BCR	C24-C25	3.10	1.55	1.45
12	A	852	CLA	C1B-C2B	3.10	1.50	1.43
12	B	850	CLA	C1D-ND	-3.10	1.33	1.37
12	K	4004	CLA	CHC-C4B	3.10	1.46	1.39
12	A	823	CLA	C3D-C2D	3.10	1.47	1.39
12	B	810	CLA	C3D-C2D	3.10	1.47	1.39
12	B	809	CLA	OBD-CAD	3.10	1.27	1.22
12	A	804	CLA	C1D-ND	-3.09	1.33	1.37
12	F	203	CLA	MG-NC	3.09	2.13	2.06
12	A	833	CLA	C1D-ND	-3.09	1.33	1.37
12	B	852	CLA	C3D-C2D	3.09	1.47	1.39
12	A	809	CLA	CHD-C4C	3.09	1.46	1.39
15	A	838	BCR	C24-C25	3.09	1.55	1.45
12	A	816	CLA	C1B-NB	-3.09	1.33	1.37
15	J	104	BCR	C24-C25	3.09	1.55	1.45
12	L	201	CLA	C1B-NB	-3.08	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	824	CLA	OBD-CAD	3.08	1.27	1.22
12	A	801	CLA	C1B-C2B	3.08	1.50	1.43
12	A	818	CLA	C1B-C2B	3.08	1.50	1.43
15	A	835	BCR	C24-C25	3.08	1.55	1.45
15	L	207	BCR	C24-C25	3.08	1.55	1.45
12	F	203	CLA	C3D-C2D	3.08	1.47	1.39
12	B	847	CLA	MG-NC	3.08	2.13	2.06
12	A	805	CLA	C1D-ND	-3.08	1.33	1.37
12	A	849	CLA	C1D-ND	-3.08	1.33	1.37
12	B	811	CLA	C1B-NB	-3.08	1.33	1.37
12	B	807	CLA	MG-NC	3.08	2.13	2.06
12	B	806	CLA	C3D-C2D	3.08	1.47	1.39
12	B	829	CLA	C3D-C2D	3.08	1.47	1.39
12	A	849	CLA	C1B-NB	-3.08	1.33	1.37
12	B	827	CLA	C4B-NB	-3.08	1.33	1.37
15	L	208	BCR	C12-C13	3.07	1.52	1.46
12	B	823	CLA	C1B-NB	-3.07	1.33	1.37
12	B	829	CLA	C1B-C2B	3.07	1.50	1.43
12	B	847	CLA	CHD-C1D	3.07	1.44	1.38
12	A	824	CLA	C1B-NB	-3.07	1.33	1.37
12	B	828	CLA	C1B-NB	-3.07	1.33	1.37
15	L	208	BCR	C4-C5	-3.07	1.45	1.51
12	A	803	CLA	C1B-C2B	3.07	1.50	1.43
12	A	823	CLA	MG-NC	3.07	2.13	2.06
12	A	803	CLA	OBD-CAD	3.06	1.27	1.22
12	A	831	CLA	MG-NC	3.06	2.13	2.06
12	A	832	CLA	C3D-C2D	3.06	1.47	1.39
12	A	858	CLA	C1D-ND	-3.06	1.33	1.37
12	A	822	CLA	OBD-CAD	3.06	1.27	1.22
12	B	808	CLA	C1B-NB	-3.06	1.33	1.37
15	A	836	BCR	C24-C25	3.06	1.55	1.45
12	B	845	CLA	C1B-NB	-3.06	1.33	1.37
12	A	833	CLA	MG-NC	3.05	2.13	2.06
12	B	820	CLA	C3D-C2D	3.05	1.47	1.39
12	A	808	CLA	MG-NC	3.05	2.13	2.06
12	B	805	CLA	MG-NC	3.05	2.13	2.06
12	A	815	CLA	C1B-C2B	3.05	1.50	1.43
12	B	817	CLA	C1D-ND	-3.05	1.33	1.37
12	A	805	CLA	C3D-C2D	3.05	1.47	1.39
12	K	4004	CLA	C1B-NB	-3.05	1.33	1.37
12	A	848	CLA	C3D-C2D	3.05	1.47	1.39
12	B	853	CLA	C3D-C2D	3.05	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	849	CLA	MG-NC	3.05	2.13	2.06
12	A	810	CLA	MG-NC	3.04	2.13	2.06
12	A	828	CLA	C1B-C2B	3.04	1.50	1.43
12	B	845	CLA	C3D-C2D	3.04	1.47	1.39
15	B	832	BCR	C4-C5	-3.04	1.45	1.51
12	A	819	CLA	C3D-C2D	3.04	1.47	1.39
12	B	818	CLA	C3D-C2D	3.04	1.47	1.39
15	L	207	BCR	C12-C13	3.04	1.52	1.46
15	A	837	BCR	C12-C13	3.04	1.52	1.46
15	I	101	BCR	C27-C26	-3.04	1.45	1.51
12	A	803	CLA	MG-NC	3.04	2.13	2.06
12	B	813	CLA	C1D-ND	-3.04	1.33	1.37
15	A	838	BCR	C12-C13	3.04	1.52	1.46
12	B	822	CLA	C3D-C2D	3.04	1.47	1.39
12	B	820	CLA	OBD-CAD	3.03	1.27	1.22
12	B	819	CLA	C1B-NB	-3.03	1.33	1.37
12	A	822	CLA	C1B-NB	-3.03	1.33	1.37
12	B	812	CLA	C3D-C2D	3.03	1.47	1.39
15	B	841	BCR	C24-C25	3.03	1.55	1.45
12	A	808	CLA	C3D-C2D	3.03	1.47	1.39
12	B	830	CLA	MG-NC	3.03	2.13	2.06
12	A	847	CLA	C1D-ND	-3.03	1.33	1.37
12	B	849	CLA	C1B-NB	-3.03	1.33	1.37
12	A	810	CLA	C1B-NB	-3.03	1.33	1.37
12	B	828	CLA	C3D-C2D	3.03	1.47	1.39
12	A	855	CLA	MG-NC	3.02	2.13	2.06
12	K	4002	CLA	C3D-C2D	3.02	1.47	1.39
12	A	807	CLA	C3D-C2D	3.02	1.47	1.39
12	B	815	CLA	C3D-C2D	3.02	1.47	1.39
12	B	853	CLA	MG-NC	3.02	2.13	2.06
12	B	803	CLA	CHB-C1B	3.02	1.46	1.39
12	A	855	CLA	C4D-CHA	3.02	1.48	1.38
12	B	826	CLA	MG-NC	3.01	2.13	2.06
12	A	820	CLA	C3D-C2D	3.01	1.47	1.39
12	B	823	CLA	C3D-C2D	3.01	1.47	1.39
15	L	207	BCR	C33-C5	3.01	1.55	1.50
12	A	806	CLA	MG-NC	3.01	2.13	2.06
12	A	812	CLA	C3D-C2D	3.01	1.47	1.39
12	A	828	CLA	C1D-ND	-3.01	1.33	1.37
12	J	101	CLA	C1C-NC	-3.01	1.33	1.37
12	B	820	CLA	C1B-C2B	3.01	1.50	1.43
15	B	832	BCR	C24-C25	3.01	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	847	CLA	C1B-C2B	3.01	1.50	1.43
12	B	805	CLA	C3D-C2D	3.01	1.47	1.39
12	B	848	CLA	C1B-C2B	3.01	1.50	1.43
12	B	808	CLA	MG-NC	3.01	2.13	2.06
12	L	205	CLA	C3D-C2D	3.01	1.47	1.39
12	A	815	CLA	C3D-C2D	3.00	1.47	1.39
12	B	842	CLA	C3D-C2D	3.00	1.47	1.39
12	A	858	CLA	C1B-NB	-3.00	1.33	1.37
12	B	829	CLA	C1D-ND	-3.00	1.33	1.37
12	B	852	CLA	MG-ND	-3.00	1.99	2.05
12	A	819	CLA	MG-NC	3.00	2.13	2.06
12	B	827	CLA	C3D-C2D	3.00	1.47	1.39
12	A	845	CLA	C1D-ND	-3.00	1.33	1.37
12	B	815	CLA	MG-NC	3.00	2.13	2.06
12	A	828	CLA	C3D-C2D	3.00	1.47	1.39
12	B	803	CLA	C1C-NC	-2.99	1.33	1.37
13	A	802	CL0	C1B-C2B	2.99	1.50	1.43
12	B	804	CLA	MG-NC	2.99	2.13	2.06
12	L	204	CLA	C4D-CHA	2.99	1.48	1.38
15	B	841	BCR	C27-C26	-2.99	1.45	1.51
12	J	103	CLA	C3D-C2D	2.99	1.47	1.39
12	L	206	CLA	C1D-ND	-2.99	1.33	1.37
12	B	812	CLA	C1B-C2B	2.99	1.50	1.43
15	A	838	BCR	C27-C26	-2.99	1.45	1.51
12	B	846	CLA	MG-NC	2.99	2.13	2.06
12	B	821	CLA	MG-NC	2.99	2.13	2.06
15	B	836	BCR	C27-C26	-2.99	1.45	1.51
12	A	814	CLA	C1B-NB	-2.99	1.33	1.37
12	A	858	CLA	OBD-CAD	2.99	1.27	1.22
12	A	822	CLA	C3D-C2D	2.98	1.47	1.39
13	A	802	CL0	OBD-CAD	2.98	1.27	1.22
12	B	828	CLA	MG-NC	2.98	2.13	2.06
12	B	809	CLA	C1B-NB	-2.98	1.33	1.37
12	L	205	CLA	MG-NC	2.98	2.13	2.06
12	B	821	CLA	C1B-NB	-2.98	1.33	1.37
12	A	845	CLA	C1B-NB	-2.98	1.33	1.37
12	A	814	CLA	C1D-ND	-2.98	1.33	1.37
12	B	823	CLA	MG-NC	2.98	2.13	2.06
12	B	807	CLA	C3D-C2D	2.98	1.47	1.39
12	A	811	CLA	C3D-C2D	2.97	1.47	1.39
12	A	813	CLA	C3D-C2D	2.97	1.47	1.39
15	B	835	BCR	C24-C25	2.97	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	847	CLA	C1B-C2B	2.97	1.50	1.43
12	B	818	CLA	C1B-NB	-2.97	1.34	1.37
12	B	845	CLA	C1D-ND	-2.97	1.34	1.37
12	K	4004	CLA	C4D-CHA	2.97	1.48	1.38
12	B	825	CLA	C3D-C2D	2.97	1.47	1.39
12	A	822	CLA	C4D-CHA	2.97	1.48	1.38
12	A	829	CLA	C3D-C2D	2.97	1.47	1.39
12	B	852	CLA	C4D-CHA	2.97	1.48	1.38
12	A	821	CLA	C1B-C2B	2.97	1.50	1.43
12	F	203	CLA	C4D-CHA	2.97	1.48	1.38
12	B	810	CLA	MG-NC	2.96	2.13	2.06
12	J	103	CLA	MG-NC	2.96	2.13	2.06
15	I	101	BCR	C33-C5	2.96	1.55	1.50
12	B	812	CLA	MG-NC	2.96	2.13	2.06
12	A	825	CLA	C1D-ND	-2.96	1.34	1.37
12	B	814	CLA	C1D-ND	-2.96	1.34	1.37
12	A	829	CLA	C1B-C2B	2.96	1.50	1.43
12	A	844	CLA	C3D-C2D	2.96	1.47	1.39
12	B	826	CLA	C1B-NB	-2.96	1.34	1.37
12	A	846	CLA	C4D-CHA	2.96	1.48	1.38
12	A	819	CLA	C1B-NB	-2.96	1.34	1.37
12	B	825	CLA	C1D-ND	-2.95	1.34	1.37
12	B	819	CLA	OBD-CAD	2.95	1.27	1.22
12	J	101	CLA	MG-NC	2.95	2.13	2.06
12	A	848	CLA	C1D-ND	-2.95	1.34	1.37
12	B	849	CLA	MG-NC	2.95	2.13	2.06
12	B	804	CLA	C1D-ND	-2.95	1.34	1.37
12	A	817	CLA	C1B-NB	-2.95	1.34	1.37
12	A	847	CLA	C3D-C2D	2.95	1.47	1.39
15	A	835	BCR	C27-C26	-2.95	1.45	1.51
12	B	821	CLA	OBD-CAD	2.95	1.27	1.22
12	A	825	CLA	C4D-CHA	2.95	1.48	1.38
12	B	842	CLA	C1D-ND	-2.95	1.34	1.37
12	B	814	CLA	C3D-C2D	2.95	1.47	1.39
12	A	810	CLA	C1D-ND	-2.95	1.34	1.37
12	B	813	CLA	MG-NC	2.95	2.13	2.06
12	B	828	CLA	OBD-CAD	2.95	1.27	1.22
12	A	812	CLA	MG-NC	2.94	2.13	2.06
15	K	4001	BCR	C12-C13	2.94	1.52	1.46
12	A	820	CLA	OBD-CAD	2.94	1.27	1.22
12	B	816	CLA	C1B-C2B	2.94	1.50	1.43
12	A	804	CLA	C3D-C2D	2.94	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	858	CLA	C3D-C2D	2.94	1.47	1.39
12	B	803	CLA	CHC-C4B	2.94	1.46	1.39
17	A	851	LMG	C37-C36	-2.94	1.33	1.51
12	A	818	CLA	C1D-ND	-2.94	1.34	1.37
12	A	827	CLA	C1D-ND	-2.94	1.34	1.37
12	B	842	CLA	C1B-NB	-2.94	1.34	1.37
12	B	815	CLA	C1B-NB	-2.93	1.34	1.37
12	B	818	CLA	C4D-CHA	2.93	1.48	1.38
12	A	845	CLA	MG-NC	2.93	2.13	2.06
12	B	802	CLA	C4D-CHA	2.93	1.48	1.38
12	A	803	CLA	C1D-ND	-2.93	1.34	1.37
12	L	204	CLA	C3D-C2D	2.93	1.47	1.39
12	A	805	CLA	MG-NC	2.93	2.13	2.06
12	B	847	CLA	CHD-C4C	2.93	1.45	1.39
27	M	102	SQD	C24-C23	2.92	1.59	1.50
12	K	4002	CLA	C4D-CHA	2.92	1.48	1.38
20	A	856	45D	C33-C35	-2.92	1.39	1.46
12	A	847	CLA	MG-NC	2.92	2.13	2.06
17	B	837	LMG	C22-C21	-2.92	1.33	1.51
12	B	821	CLA	C3D-C2D	2.92	1.47	1.39
12	L	201	CLA	C1B-C2B	2.92	1.50	1.43
12	A	833	CLA	C3D-C2D	2.92	1.46	1.39
12	B	813	CLA	C4D-CHA	2.92	1.48	1.38
12	B	805	CLA	C4D-CHA	2.91	1.48	1.38
12	A	816	CLA	MG-NC	2.91	2.13	2.06
12	B	845	CLA	MG-NC	2.91	2.13	2.06
15	J	107	BCR	C27-C26	-2.91	1.45	1.51
12	B	830	CLA	C4D-CHA	2.91	1.48	1.38
12	B	804	CLA	C1B-C2B	2.91	1.50	1.43
12	B	846	CLA	C1B-C2B	2.91	1.50	1.43
12	A	821	CLA	MG-NC	2.91	2.13	2.06
12	L	206	CLA	C1B-NB	-2.91	1.34	1.37
12	L	206	CLA	C3D-C2D	2.91	1.46	1.39
12	B	826	CLA	C4D-CHA	2.91	1.48	1.38
12	A	825	CLA	C3D-C2D	2.91	1.46	1.39
12	F	204	CLA	C4B-NB	-2.91	1.34	1.37
12	B	811	CLA	C1C-NC	-2.91	1.33	1.37
12	B	817	CLA	C3D-C2D	2.90	1.46	1.39
12	B	810	CLA	C1B-NB	-2.90	1.34	1.37
12	B	842	CLA	MG-NC	2.90	2.13	2.06
12	B	801	CLA	C3D-C2D	2.90	1.46	1.39
12	A	847	CLA	C1B-NB	-2.90	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	826	CLA	C3D-C2D	2.90	1.46	1.39
12	A	824	CLA	MG-ND	-2.90	2.00	2.05
12	A	820	CLA	MG-NC	2.90	2.13	2.06
12	B	809	CLA	C4D-CHA	2.90	1.48	1.38
12	A	827	CLA	C1B-NB	-2.90	1.34	1.37
12	B	853	CLA	C1B-NB	-2.90	1.34	1.37
12	A	818	CLA	C4D-CHA	2.90	1.48	1.38
12	B	815	CLA	C4D-CHA	2.90	1.48	1.38
12	K	4002	CLA	MG-NC	2.90	2.13	2.06
12	B	849	CLA	C1B-C2B	2.89	1.49	1.43
12	A	830	CLA	C1B-C2B	2.89	1.49	1.43
12	A	827	CLA	C4D-CHA	2.89	1.48	1.38
12	B	806	CLA	C1B-C2B	2.89	1.49	1.43
12	A	819	CLA	C1D-ND	-2.89	1.34	1.37
12	A	804	CLA	MG-NC	2.89	2.13	2.06
12	B	811	CLA	C1B-C2B	2.89	1.49	1.43
12	A	813	CLA	C1D-ND	-2.89	1.34	1.37
12	A	826	CLA	C1D-ND	-2.89	1.34	1.37
12	A	832	CLA	C4D-CHA	2.88	1.48	1.38
12	A	855	CLA	C1D-ND	-2.88	1.34	1.37
12	A	830	CLA	OBD-CAD	2.88	1.27	1.22
12	A	849	CLA	C3D-C2D	2.88	1.46	1.39
12	A	806	CLA	C1D-ND	-2.88	1.34	1.37
19	A	854	PL9	C6-C5	2.88	1.49	1.35
12	A	810	CLA	C1B-C2B	2.88	1.49	1.43
12	A	821	CLA	C1D-ND	-2.88	1.34	1.37
12	A	821	CLA	C3D-C2D	2.88	1.46	1.39
12	L	206	CLA	C1B-C2B	2.88	1.49	1.43
12	L	201	CLA	MG-NC	2.88	2.13	2.06
12	B	809	CLA	C3D-C2D	2.88	1.46	1.39
12	A	829	CLA	MG-NC	2.88	2.13	2.06
12	J	101	CLA	C1B-C2B	2.88	1.49	1.43
12	A	832	CLA	MG-NC	2.88	2.13	2.06
12	B	802	CLA	MG-NC	2.88	2.13	2.06
12	A	809	CLA	MG-NC	2.88	2.13	2.06
12	A	815	CLA	C4D-CHA	2.88	1.48	1.38
12	A	812	CLA	C4D-CHA	2.88	1.48	1.38
12	L	206	CLA	MG-NC	2.87	2.13	2.06
12	B	848	CLA	MG-ND	-2.87	2.00	2.05
12	B	811	CLA	MG-NC	2.87	2.13	2.06
12	A	817	CLA	MG-NC	2.87	2.13	2.06
12	A	827	CLA	MG-NC	2.87	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	822	CLA	MG-NC	2.87	2.13	2.06
12	A	832	CLA	C1B-NB	-2.87	1.34	1.37
12	B	807	CLA	C1D-ND	-2.87	1.34	1.37
12	A	813	CLA	MG-ND	-2.87	2.00	2.05
12	A	819	CLA	C4D-CHA	2.87	1.48	1.38
12	B	825	CLA	MG-NC	2.87	2.13	2.06
12	B	806	CLA	MG-ND	-2.87	2.00	2.05
12	B	826	CLA	C3D-C2D	2.87	1.46	1.39
15	K	4001	BCR	C27-C26	-2.87	1.45	1.51
12	B	843	CLA	C4D-CHA	2.86	1.48	1.38
12	L	204	CLA	C1B-NB	-2.86	1.34	1.37
12	A	827	CLA	C1C-NC	-2.86	1.33	1.37
12	B	847	CLA	CHC-C4B	2.86	1.45	1.39
12	B	850	CLA	C1B-NB	-2.86	1.34	1.37
12	A	806	CLA	C1B-C2B	2.86	1.49	1.43
12	A	833	CLA	C1B-C2B	2.86	1.49	1.43
12	J	103	CLA	C1B-C2B	2.86	1.49	1.43
12	A	830	CLA	C4D-CHA	2.86	1.48	1.38
12	B	819	CLA	C1D-ND	-2.86	1.34	1.37
12	A	811	CLA	MG-NC	2.86	2.13	2.06
12	A	806	CLA	C3D-C2D	2.85	1.46	1.39
12	B	811	CLA	C3D-C2D	2.85	1.46	1.39
12	A	823	CLA	C4D-CHA	2.85	1.48	1.38
12	A	826	CLA	C1B-C2B	2.85	1.49	1.43
12	A	808	CLA	C4D-CHA	2.85	1.48	1.38
12	B	829	CLA	MG-NC	2.85	2.13	2.06
12	B	824	CLA	MG-NC	2.85	2.13	2.06
12	A	826	CLA	MG-NC	2.85	2.13	2.06
12	A	810	CLA	C4D-CHA	2.85	1.48	1.38
12	B	807	CLA	C4D-CHA	2.85	1.48	1.38
12	L	204	CLA	C1B-C2B	2.85	1.49	1.43
12	A	807	CLA	C4D-CHA	2.85	1.48	1.38
12	A	849	CLA	C4D-CHA	2.85	1.48	1.38
15	L	208	BCR	C33-C5	2.85	1.55	1.50
12	B	819	CLA	C3D-C2D	2.84	1.46	1.39
12	B	809	CLA	MG-ND	-2.84	2.00	2.05
12	A	829	CLA	C1C-NC	-2.84	1.33	1.37
13	A	802	CL0	C3D-C2D	2.84	1.46	1.39
12	A	831	CLA	C4D-CHA	2.84	1.48	1.38
12	B	844	CLA	C4C-C3C	2.84	1.49	1.45
12	A	843	CLA	C1D-ND	-2.84	1.34	1.37
12	B	816	CLA	C4D-CHA	2.84	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	806	CLA	C4D-CHA	2.84	1.48	1.38
12	A	843	CLA	C3D-C2D	2.84	1.46	1.39
12	B	852	CLA	C1B-C2B	2.84	1.49	1.43
12	A	848	CLA	MG-NC	2.84	2.13	2.06
15	A	836	BCR	C33-C5	2.84	1.55	1.50
15	I	101	BCR	C12-C13	2.83	1.52	1.46
12	A	813	CLA	C4D-CHA	2.83	1.48	1.38
12	B	850	CLA	C4D-CHA	2.83	1.48	1.38
12	B	814	CLA	C4D-CHA	2.83	1.48	1.38
12	A	832	CLA	C1B-C2B	2.83	1.49	1.43
12	A	824	CLA	MG-NC	2.83	2.13	2.06
12	A	820	CLA	C1B-C2B	2.83	1.49	1.43
12	A	830	CLA	MG-NC	2.83	2.13	2.06
12	F	204	CLA	C1B-C2B	2.83	1.49	1.43
12	A	811	CLA	C4D-CHA	2.83	1.48	1.38
12	B	852	CLA	C1B-NB	-2.83	1.34	1.37
15	B	841	BCR	C33-C5	2.83	1.55	1.50
12	A	803	CLA	C3D-C2D	2.83	1.46	1.39
12	B	808	CLA	C4D-CHA	2.83	1.48	1.38
12	B	843	CLA	C1B-C2B	2.83	1.49	1.43
12	A	846	CLA	C3D-C2D	2.83	1.46	1.39
12	A	848	CLA	C1B-NB	-2.82	1.34	1.37
12	B	812	CLA	C1D-ND	-2.82	1.34	1.37
12	B	821	CLA	C4D-CHA	2.82	1.48	1.38
12	A	828	CLA	MG-NC	2.82	2.13	2.06
12	B	850	CLA	C3D-C2D	2.82	1.46	1.39
12	J	102	CLA	MG-NC	2.82	2.13	2.06
12	B	811	CLA	C1D-ND	-2.82	1.34	1.37
12	B	825	CLA	C1B-NB	-2.82	1.34	1.37
12	A	816	CLA	C1D-ND	-2.82	1.34	1.37
12	B	825	CLA	C4D-CHA	2.82	1.48	1.38
12	A	801	CLA	C1B-NB	-2.82	1.34	1.37
12	L	205	CLA	C1B-NB	-2.82	1.34	1.37
15	J	105	BCR	C34-C9	2.82	1.56	1.50
12	B	819	CLA	MG-NC	2.82	2.13	2.06
12	F	204	CLA	C4D-CHA	2.82	1.48	1.38
12	J	103	CLA	C4D-CHA	2.81	1.48	1.38
12	B	823	CLA	C4D-CHA	2.81	1.48	1.38
12	B	819	CLA	C4D-CHA	2.81	1.48	1.38
12	B	848	CLA	C1B-NB	-2.81	1.34	1.37
12	A	821	CLA	C4D-CHA	2.81	1.48	1.38
12	A	822	CLA	C1B-C2B	2.81	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	K	4004	CLA	MG-NC	2.81	2.12	2.06
12	B	842	CLA	C1B-C2B	2.80	1.49	1.43
12	B	809	CLA	C1B-C2B	2.80	1.49	1.43
12	B	822	CLA	C4D-CHA	2.80	1.48	1.38
12	J	101	CLA	C1B-NB	-2.80	1.34	1.37
12	A	807	CLA	C1B-C2B	2.80	1.49	1.43
12	L	206	CLA	C4D-CHA	2.80	1.48	1.38
12	B	806	CLA	C1B-NB	-2.80	1.34	1.37
12	A	843	CLA	C1B-NB	-2.80	1.34	1.37
12	A	843	CLA	C4D-CHA	2.80	1.48	1.38
15	B	834	BCR	C24-C25	2.80	1.54	1.45
25	L	202	EQ3	C23-C22	-2.80	1.40	1.46
12	B	824	CLA	C3D-C2D	2.80	1.46	1.39
12	B	850	CLA	C1B-C2B	2.79	1.49	1.43
12	J	101	CLA	C3D-C2D	2.79	1.46	1.39
12	A	833	CLA	C4D-CHA	2.79	1.48	1.38
12	A	808	CLA	C1B-NB	-2.79	1.34	1.37
12	A	816	CLA	C4D-CHA	2.79	1.48	1.38
12	A	818	CLA	C3D-C2D	2.79	1.46	1.39
12	B	823	CLA	C1D-ND	-2.79	1.34	1.37
12	B	846	CLA	C3D-C2D	2.79	1.46	1.39
12	B	818	CLA	C1B-C2B	2.79	1.49	1.43
12	B	814	CLA	C1B-NB	-2.79	1.34	1.37
12	J	101	CLA	C4B-NB	-2.79	1.34	1.37
12	A	845	CLA	C3D-C2D	2.79	1.46	1.39
12	A	806	CLA	C1B-NB	-2.79	1.34	1.37
12	A	801	CLA	C3D-C2D	2.79	1.46	1.39
12	A	813	CLA	C1B-NB	-2.79	1.34	1.37
15	F	202	BCR	C27-C26	-2.79	1.45	1.51
12	B	828	CLA	C4D-CHA	2.78	1.47	1.38
12	B	827	CLA	MG-NC	2.78	2.12	2.06
12	B	843	CLA	MG-NC	2.78	2.12	2.06
12	B	817	CLA	MG-NC	2.78	2.12	2.06
12	B	850	CLA	MG-NC	2.78	2.12	2.06
12	B	808	CLA	MG-ND	-2.78	2.00	2.05
12	B	852	CLA	C4B-NB	-2.78	1.34	1.37
12	A	832	CLA	C1D-ND	-2.78	1.34	1.37
12	A	831	CLA	C3D-C2D	2.78	1.46	1.39
12	L	201	CLA	C4D-CHA	2.78	1.47	1.38
12	A	804	CLA	C1B-C2B	2.78	1.49	1.43
12	B	819	CLA	C1B-C2B	2.78	1.49	1.43
15	B	832	BCR	C33-C5	2.78	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	810	CLA	C1B-C2B	2.77	1.49	1.43
12	A	820	CLA	C4D-CHA	2.77	1.47	1.38
12	A	820	CLA	C1C-NC	-2.77	1.33	1.37
12	A	807	CLA	C1D-ND	-2.77	1.34	1.37
12	A	808	CLA	C1B-C2B	2.77	1.49	1.43
12	A	801	CLA	C1D-ND	-2.77	1.34	1.37
12	B	827	CLA	C1B-NB	-2.77	1.34	1.37
12	B	842	CLA	C4D-CHA	2.77	1.47	1.38
12	A	828	CLA	C1B-NB	-2.77	1.34	1.37
12	A	814	CLA	MG-NC	2.77	2.12	2.06
12	A	848	CLA	C4D-CHA	2.77	1.47	1.38
12	J	102	CLA	C3D-C2D	2.77	1.46	1.39
12	B	805	CLA	C1D-ND	-2.77	1.34	1.37
12	B	810	CLA	C1C-NC	-2.77	1.33	1.37
12	B	827	CLA	C4D-CHA	2.77	1.47	1.38
12	B	813	CLA	C1C-NC	-2.77	1.33	1.37
12	A	833	CLA	C1B-NB	-2.77	1.34	1.37
15	J	107	BCR	C33-C5	2.76	1.55	1.50
12	B	827	CLA	C1D-ND	-2.76	1.34	1.37
12	B	825	CLA	C1B-C2B	2.76	1.49	1.43
12	A	810	CLA	MG-ND	-2.76	2.00	2.05
12	B	846	CLA	C4B-NB	-2.76	1.34	1.37
12	B	844	CLA	C3D-C2D	2.76	1.46	1.39
12	A	825	CLA	C1B-C2B	2.76	1.49	1.43
12	A	858	CLA	C1C-NC	-2.76	1.33	1.37
12	B	829	CLA	C4D-CHA	2.76	1.47	1.38
12	B	807	CLA	C1B-C2B	2.76	1.49	1.43
12	A	807	CLA	C1B-NB	-2.76	1.34	1.37
12	A	830	CLA	C4B-NB	-2.76	1.34	1.37
12	A	845	CLA	C4D-CHA	2.76	1.47	1.38
12	K	4003	CLA	C1D-C2D	-2.75	1.39	1.45
12	K	4002	CLA	C1B-C2B	2.75	1.49	1.43
12	A	804	CLA	C4D-CHA	2.75	1.47	1.38
12	J	103	CLA	C1B-NB	-2.75	1.34	1.37
12	A	811	CLA	C1B-C2B	2.75	1.49	1.43
12	A	818	CLA	MG-ND	-2.75	2.00	2.05
12	B	827	CLA	C1C-NC	-2.75	1.33	1.37
12	A	809	CLA	C3D-C2D	2.75	1.46	1.39
12	A	849	CLA	C1B-C2B	2.75	1.49	1.43
12	A	811	CLA	C1B-NB	-2.75	1.34	1.37
12	A	803	CLA	C4D-CHA	2.75	1.47	1.38
12	B	811	CLA	C4D-CHA	2.75	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	817	CLA	C1B-C2B	2.75	1.49	1.43
12	B	845	CLA	C4D-CHA	2.74	1.47	1.38
12	A	829	CLA	C1D-ND	-2.74	1.34	1.37
12	B	852	CLA	C4C-C3C	2.74	1.49	1.45
12	A	825	CLA	C1B-NB	-2.74	1.34	1.37
12	B	820	CLA	C4D-CHA	2.74	1.47	1.38
12	B	812	CLA	C4D-CHA	2.74	1.47	1.38
12	A	815	CLA	MG-ND	-2.74	2.00	2.05
12	A	825	CLA	MG-ND	-2.74	2.00	2.05
12	B	822	CLA	MG-ND	-2.74	2.00	2.05
12	B	813	CLA	MG-ND	-2.74	2.00	2.05
15	B	835	BCR	C27-C26	-2.74	1.45	1.51
13	A	802	CL0	C1B-NB	-2.74	1.34	1.37
12	A	809	CLA	C1C-NC	-2.74	1.33	1.37
12	A	843	CLA	MG-NC	2.73	2.12	2.06
12	A	831	CLA	C1B-NB	-2.73	1.34	1.37
12	B	826	CLA	C1D-ND	-2.73	1.34	1.37
12	J	103	CLA	C1D-C2D	2.73	1.50	1.45
12	K	4002	CLA	C4C-C3C	2.73	1.49	1.45
12	B	826	CLA	C1B-C2B	2.73	1.49	1.43
12	A	801	CLA	C4D-CHA	2.73	1.47	1.38
15	B	835	BCR	C33-C5	2.73	1.55	1.50
15	A	836	BCR	C27-C26	-2.73	1.45	1.51
12	A	806	CLA	C4D-CHA	2.73	1.47	1.38
12	F	203	CLA	C1B-C2B	2.73	1.49	1.43
15	A	835	BCR	C33-C5	2.73	1.55	1.50
12	B	825	CLA	C1C-NC	-2.73	1.33	1.37
12	A	811	CLA	C1D-ND	-2.72	1.34	1.37
12	A	814	CLA	C4D-CHA	2.72	1.47	1.38
12	A	847	CLA	C1C-NC	-2.72	1.33	1.37
12	B	815	CLA	C1C-NC	-2.72	1.33	1.37
12	A	843	CLA	C1C-NC	-2.72	1.33	1.37
12	A	819	CLA	C1B-C2B	2.72	1.49	1.43
12	A	828	CLA	C4D-CHA	2.72	1.47	1.38
20	A	856	45D	C08-C16	2.72	1.39	1.35
12	B	804	CLA	C1B-NB	-2.71	1.34	1.37
12	B	814	CLA	C1B-C2B	2.71	1.49	1.43
12	B	828	CLA	C1D-ND	-2.71	1.34	1.37
12	A	807	CLA	MG-NC	2.71	2.12	2.06
12	A	826	CLA	C4D-CHA	2.71	1.47	1.38
12	B	830	CLA	C1B-C2B	2.71	1.49	1.43
12	B	817	CLA	C1C-NC	-2.71	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	849	CLA	C4D-CHA	2.71	1.47	1.38
12	B	801	CLA	C1B-C2B	2.71	1.49	1.43
12	B	808	CLA	C1B-C2B	2.71	1.49	1.43
15	A	837	BCR	C27-C26	-2.71	1.46	1.51
12	A	824	CLA	C3D-C2D	2.71	1.46	1.39
12	A	817	CLA	C1B-C2B	2.71	1.49	1.43
12	B	821	CLA	C4B-NB	-2.71	1.34	1.37
15	F	201	BCR	C33-C5	2.71	1.55	1.50
12	B	817	CLA	C4D-CHA	2.71	1.47	1.38
12	L	201	CLA	C4B-NB	-2.70	1.34	1.37
15	B	834	BCR	C27-C26	-2.70	1.46	1.51
15	B	834	BCR	C12-C13	2.70	1.51	1.46
12	B	821	CLA	MG-ND	-2.70	2.00	2.05
15	F	202	BCR	C33-C5	2.70	1.55	1.50
12	B	821	CLA	C1B-C2B	2.70	1.49	1.43
12	B	830	CLA	C1B-NB	-2.70	1.34	1.37
12	B	816	CLA	C1B-NB	-2.70	1.34	1.37
12	B	845	CLA	C1B-C2B	2.70	1.49	1.43
12	A	824	CLA	C4D-CHA	2.70	1.47	1.38
12	B	847	CLA	C3D-C2D	2.70	1.46	1.39
12	A	830	CLA	C1C-NC	-2.69	1.33	1.37
12	B	815	CLA	C1B-C2B	2.69	1.49	1.43
12	B	805	CLA	MG-ND	-2.69	2.00	2.05
12	B	852	CLA	C1D-ND	-2.69	1.34	1.37
12	A	817	CLA	C4D-CHA	2.69	1.47	1.38
12	A	820	CLA	C1B-NB	-2.69	1.34	1.37
12	A	801	CLA	MG-NC	2.69	2.12	2.06
12	A	858	CLA	C4D-CHA	2.69	1.47	1.38
12	A	813	CLA	C1B-C2B	2.68	1.49	1.43
12	A	847	CLA	C4D-CHA	2.68	1.47	1.38
15	A	838	BCR	C33-C5	2.68	1.55	1.50
13	A	802	CL0	C4D-CHA	2.68	1.47	1.38
12	L	204	CLA	C1D-ND	-2.68	1.34	1.37
12	A	843	CLA	C1B-C2B	2.68	1.49	1.43
12	A	804	CLA	C1C-NC	-2.68	1.33	1.37
12	A	829	CLA	C4D-CHA	2.68	1.47	1.38
12	F	204	CLA	C1D-ND	-2.68	1.34	1.37
12	A	826	CLA	C1B-NB	-2.68	1.34	1.37
12	A	845	CLA	C1B-C2B	2.67	1.49	1.43
12	A	811	CLA	C1C-NC	-2.67	1.33	1.37
12	L	201	CLA	C1D-ND	-2.67	1.34	1.37
12	A	808	CLA	C1C-NC	-2.67	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	829	CLA	C1B-NB	-2.67	1.34	1.37
12	B	810	CLA	C4D-CHA	2.67	1.47	1.38
12	A	819	CLA	C1C-NC	-2.67	1.33	1.37
12	B	815	CLA	MG-ND	-2.67	2.00	2.05
12	B	804	CLA	C3D-C2D	2.67	1.46	1.39
12	B	801	CLA	MG-NC	2.67	2.12	2.06
12	A	829	CLA	C1B-NB	-2.66	1.34	1.37
12	B	848	CLA	C4D-CHA	2.66	1.47	1.38
12	L	205	CLA	C4D-CHA	2.66	1.47	1.38
12	A	855	CLA	OBD-CAD	2.66	1.27	1.22
12	B	805	CLA	C1B-C2B	2.66	1.49	1.43
12	A	848	CLA	C1B-C2B	2.66	1.49	1.43
12	A	822	CLA	MG-ND	-2.66	2.00	2.05
12	A	845	CLA	MG-ND	-2.65	2.00	2.05
12	A	815	CLA	C1B-NB	-2.65	1.34	1.37
12	K	4004	CLA	C1C-NC	-2.65	1.33	1.37
12	A	816	CLA	C4B-NB	-2.65	1.34	1.37
12	B	804	CLA	C4D-CHA	2.65	1.47	1.38
15	F	201	BCR	C27-C26	-2.65	1.46	1.51
12	A	830	CLA	C1B-NB	-2.65	1.34	1.37
15	J	105	BCR	C12-C13	2.65	1.51	1.46
12	L	205	CLA	C1B-C2B	2.65	1.49	1.43
12	B	810	CLA	C4B-NB	-2.65	1.34	1.37
12	B	810	CLA	MG-ND	-2.65	2.00	2.05
12	A	816	CLA	C1C-NC	-2.65	1.33	1.37
12	K	4002	CLA	C1C-NC	-2.65	1.33	1.37
12	B	853	CLA	C4D-CHA	2.65	1.47	1.38
12	B	819	CLA	MG-ND	-2.64	2.00	2.05
12	A	844	CLA	C1B-C2B	2.64	1.49	1.43
12	F	203	CLA	C1D-ND	-2.64	1.34	1.37
12	B	848	CLA	C3D-C2D	2.64	1.46	1.39
12	A	821	CLA	C1C-NC	-2.64	1.33	1.37
12	B	813	CLA	C1B-NB	-2.63	1.34	1.37
12	L	206	CLA	C1C-NC	-2.63	1.33	1.37
12	A	852	CLA	C4D-CHA	2.63	1.47	1.38
15	K	4001	BCR	C34-C9	2.63	1.56	1.50
12	B	820	CLA	C1B-NB	-2.63	1.34	1.37
12	B	818	CLA	MG-ND	-2.63	2.00	2.05
12	B	825	CLA	MG-ND	-2.63	2.00	2.05
12	B	819	CLA	C1C-NC	-2.62	1.33	1.37
12	A	805	CLA	C4D-CHA	2.62	1.47	1.38
15	K	4005	BCR	C34-C9	2.62	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	805	CLA	C1C-NC	-2.62	1.33	1.37
12	A	823	CLA	C1B-C2B	2.62	1.49	1.43
15	B	834	BCR	C34-C9	2.62	1.56	1.50
12	A	833	CLA	MG-ND	-2.62	2.00	2.05
12	A	801	CLA	C1C-NC	-2.62	1.33	1.37
12	A	855	CLA	C1B-C2B	2.62	1.49	1.43
12	A	811	CLA	C4B-NB	-2.62	1.34	1.37
12	B	848	CLA	C1D-C2D	2.62	1.50	1.45
12	B	844	CLA	C1B-C2B	2.62	1.49	1.43
12	B	848	CLA	C1C-NC	-2.62	1.33	1.37
15	F	202	BCR	C34-C9	2.61	1.56	1.50
12	A	821	CLA	C4B-NB	-2.61	1.34	1.37
12	A	812	CLA	C1C-NC	-2.61	1.33	1.37
12	F	204	CLA	C4C-C3C	2.61	1.49	1.45
12	A	808	CLA	MG-ND	-2.61	2.00	2.05
12	A	822	CLA	C1C-NC	-2.61	1.33	1.37
12	B	850	CLA	C1C-NC	-2.61	1.33	1.37
12	F	203	CLA	C1B-NB	-2.60	1.34	1.37
12	B	846	CLA	OBD-CAD	2.60	1.27	1.22
12	B	822	CLA	C1C-NC	-2.60	1.33	1.37
12	K	4003	CLA	C3D-C4D	-2.60	1.38	1.44
12	A	807	CLA	C1C-NC	-2.60	1.33	1.37
12	B	802	CLA	C1D-ND	-2.60	1.34	1.37
12	B	820	CLA	MG-ND	-2.59	2.00	2.05
12	A	820	CLA	MG-ND	-2.59	2.00	2.05
12	J	102	CLA	C4D-CHA	2.59	1.47	1.38
12	A	810	CLA	C1C-NC	-2.59	1.33	1.37
12	A	804	CLA	MG-ND	-2.59	2.00	2.05
12	A	823	CLA	C1C-NC	-2.58	1.33	1.37
12	B	817	CLA	MG-ND	-2.58	2.00	2.05
12	B	803	CLA	C3B-C4B	2.58	1.50	1.42
12	A	827	CLA	C1B-C2B	2.58	1.49	1.43
12	J	101	CLA	C1D-C2D	2.58	1.50	1.45
12	J	102	CLA	C1C-NC	-2.58	1.33	1.37
12	A	827	CLA	C4B-NB	-2.57	1.34	1.37
12	A	826	CLA	C1D-C2D	2.57	1.50	1.45
12	B	826	CLA	C4B-NB	-2.57	1.34	1.37
12	A	812	CLA	C1B-C2B	2.57	1.49	1.43
12	B	804	CLA	MG-ND	-2.57	2.00	2.05
12	F	204	CLA	C1D-C2D	2.57	1.50	1.45
12	J	101	CLA	C3B-C4B	2.57	1.50	1.42
12	A	805	CLA	MG-ND	-2.56	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	823	CLA	MG-ND	-2.56	2.00	2.05
12	B	807	CLA	C1B-NB	-2.56	1.34	1.37
12	A	846	CLA	OBD-CAD	2.56	1.26	1.22
12	B	801	CLA	C4D-CHA	2.56	1.47	1.38
12	K	4002	CLA	C1B-NB	-2.56	1.34	1.37
13	A	802	CL0	C1C-NC	-2.56	1.33	1.37
15	B	834	BCR	C33-C5	2.56	1.55	1.50
12	B	802	CLA	C1C-NC	-2.56	1.33	1.37
12	B	816	CLA	C1C-NC	-2.56	1.33	1.37
12	A	812	CLA	C1D-ND	-2.56	1.34	1.37
12	B	824	CLA	CHC-C4B	2.56	1.45	1.39
12	B	801	CLA	C1C-NC	-2.56	1.33	1.37
12	A	829	CLA	C3B-C4B	2.55	1.50	1.42
12	B	850	CLA	MG-ND	-2.55	2.00	2.05
12	A	852	CLA	C1C-C2C	2.55	1.49	1.44
12	A	858	CLA	MG-NC	2.55	2.12	2.06
12	A	845	CLA	C1C-NC	-2.55	1.33	1.37
12	J	101	CLA	C4C-C3C	2.55	1.49	1.45
12	B	802	CLA	C1D-C2D	2.55	1.50	1.45
12	A	849	CLA	C4B-NB	-2.54	1.34	1.37
12	B	848	CLA	C4B-NB	-2.54	1.34	1.37
12	B	828	CLA	C1C-NC	-2.54	1.33	1.37
12	B	846	CLA	C4D-CHA	2.54	1.47	1.38
12	A	848	CLA	C4B-NB	-2.54	1.34	1.37
15	B	841	BCR	C34-C9	2.54	1.56	1.50
12	K	4002	CLA	MG-ND	-2.54	2.00	2.05
12	A	824	CLA	C1B-C2B	2.54	1.49	1.43
15	B	832	BCR	C34-C9	2.53	1.56	1.50
12	B	807	CLA	MG-ND	-2.53	2.00	2.05
12	A	828	CLA	C1C-NC	-2.53	1.33	1.37
12	A	807	CLA	C4B-NB	-2.53	1.34	1.37
12	K	4002	CLA	C4B-NB	-2.53	1.34	1.37
12	L	201	CLA	C1D-C2D	2.53	1.50	1.45
12	J	102	CLA	MG-ND	-2.53	2.00	2.05
12	J	101	CLA	MG-ND	-2.53	2.00	2.05
15	J	105	BCR	C33-C5	2.53	1.55	1.50
12	B	821	CLA	C1C-NC	-2.52	1.33	1.37
12	B	850	CLA	C4B-NB	-2.52	1.34	1.37
12	B	815	CLA	C4B-NB	-2.52	1.34	1.37
12	A	803	CLA	C1C-NC	-2.52	1.33	1.37
12	F	203	CLA	C3B-C4B	2.52	1.50	1.42
12	A	805	CLA	C1B-NB	-2.52	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	803	CLA	C4C-C3C	2.52	1.49	1.45
12	A	808	CLA	C4B-NB	-2.52	1.34	1.37
12	B	844	CLA	OBD-CAD	2.51	1.26	1.22
12	F	204	CLA	C1B-NB	-2.51	1.34	1.37
12	A	831	CLA	C3B-C4B	2.51	1.50	1.42
12	B	846	CLA	CHD-C4C	2.51	1.44	1.39
12	A	844	CLA	C4D-CHA	2.51	1.47	1.38
12	A	827	CLA	MG-ND	-2.51	2.00	2.05
12	J	101	CLA	C4D-CHA	2.51	1.47	1.38
12	A	830	CLA	MG-ND	-2.51	2.00	2.05
12	F	204	CLA	MG-ND	-2.51	2.00	2.05
12	A	818	CLA	C1C-NC	-2.51	1.34	1.37
12	A	847	CLA	C4B-NB	-2.51	1.34	1.37
12	A	830	CLA	C1D-ND	-2.51	1.34	1.37
12	B	843	CLA	MG-ND	-2.50	2.00	2.05
15	J	107	BCR	C34-C9	2.50	1.55	1.50
12	A	858	CLA	C4B-NB	-2.50	1.34	1.37
12	B	825	CLA	C4B-NB	-2.50	1.34	1.37
12	B	802	CLA	C3B-C4B	2.50	1.50	1.42
12	A	821	CLA	MG-ND	-2.50	2.00	2.05
15	K	4005	BCR	C33-C5	2.50	1.54	1.50
12	B	823	CLA	MG-ND	-2.50	2.00	2.05
12	A	824	CLA	C1C-NC	-2.50	1.34	1.37
12	A	805	CLA	C4B-NB	-2.50	1.34	1.37
12	B	817	CLA	C4B-NB	-2.50	1.34	1.37
12	A	817	CLA	C1C-NC	-2.49	1.34	1.37
12	A	814	CLA	C1B-C2B	2.49	1.49	1.43
12	A	814	CLA	C1C-NC	-2.49	1.34	1.37
12	B	803	CLA	CHC-C1C	2.49	1.43	1.38
12	L	206	CLA	C4B-NB	-2.49	1.34	1.37
12	A	849	CLA	MG-ND	-2.49	2.00	2.05
12	B	806	CLA	C1C-NC	-2.49	1.34	1.37
12	L	205	CLA	C1C-NC	-2.49	1.34	1.37
12	A	816	CLA	C1B-C2B	2.49	1.49	1.43
12	B	816	CLA	MG-ND	-2.48	2.00	2.05
12	A	843	CLA	C4B-NB	-2.48	1.34	1.37
12	A	826	CLA	C1C-NC	-2.48	1.34	1.37
12	B	823	CLA	C1B-C2B	2.48	1.49	1.43
15	A	838	BCR	C34-C9	2.48	1.55	1.50
12	A	833	CLA	C4B-NB	-2.48	1.34	1.37
12	B	807	CLA	C1C-NC	-2.48	1.34	1.37
12	A	849	CLA	C1C-NC	-2.48	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	827	CLA	MG-ND	-2.48	2.00	2.05
12	B	807	CLA	C4B-NB	-2.48	1.34	1.37
15	K	4001	BCR	C33-C5	2.48	1.54	1.50
12	A	830	CLA	C1D-C2D	2.47	1.50	1.45
15	B	835	BCR	C12-C13	2.47	1.51	1.46
12	B	826	CLA	MG-ND	-2.47	2.00	2.05
12	A	801	CLA	C4B-NB	-2.47	1.34	1.37
12	A	852	CLA	C1B-NB	-2.47	1.34	1.37
15	I	101	BCR	C34-C9	2.47	1.55	1.50
12	L	206	CLA	MG-ND	-2.47	2.00	2.05
12	A	825	CLA	C1C-NC	-2.46	1.34	1.37
12	B	843	CLA	C1C-NC	-2.46	1.34	1.37
12	B	801	CLA	MG-ND	-2.46	2.00	2.05
12	B	826	CLA	C1C-NC	-2.46	1.34	1.37
12	B	828	CLA	C1D-C2D	2.46	1.50	1.45
12	A	813	CLA	C4B-NB	-2.46	1.34	1.37
12	A	848	CLA	C1C-NC	-2.46	1.34	1.37
12	B	845	CLA	C4B-NB	-2.46	1.34	1.37
12	A	832	CLA	C1C-NC	-2.46	1.34	1.37
12	A	817	CLA	C4B-NB	-2.46	1.34	1.37
12	L	201	CLA	C1C-NC	-2.46	1.34	1.37
12	A	809	CLA	OBD-CAD	2.46	1.26	1.22
12	B	823	CLA	C1C-NC	-2.46	1.34	1.37
12	A	833	CLA	C1C-NC	-2.46	1.34	1.37
12	A	855	CLA	MG-ND	-2.46	2.00	2.05
12	B	842	CLA	C1C-NC	-2.45	1.34	1.37
12	B	822	CLA	C1B-C2B	2.45	1.48	1.43
12	B	801	CLA	C4B-NB	-2.45	1.34	1.37
12	B	843	CLA	C4B-NB	-2.45	1.34	1.37
12	L	204	CLA	C1C-NC	-2.45	1.34	1.37
12	A	813	CLA	C1C-NC	-2.45	1.34	1.37
12	K	4004	CLA	C1A-CHA	2.45	1.53	1.43
12	B	830	CLA	C1D-C2D	2.45	1.50	1.45
12	B	842	CLA	MG-ND	-2.45	2.00	2.05
12	A	811	CLA	MG-ND	-2.45	2.00	2.05
12	A	809	CLA	C1B-C2B	2.44	1.48	1.43
12	A	806	CLA	C1C-NC	-2.44	1.34	1.37
12	B	818	CLA	C1C-NC	-2.44	1.34	1.37
12	B	816	CLA	C4B-NB	-2.44	1.34	1.37
12	A	831	CLA	C1C-NC	-2.43	1.34	1.37
12	A	817	CLA	MG-ND	-2.43	2.01	2.05
12	A	812	CLA	C4C-C3C	2.43	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	L	207	BCR	C34-C9	2.43	1.55	1.50
12	B	805	CLA	C4B-NB	-2.43	1.34	1.37
12	B	828	CLA	C1B-C2B	2.43	1.48	1.43
12	L	205	CLA	C4B-NB	-2.43	1.34	1.37
12	K	4002	CLA	C1D-ND	-2.43	1.34	1.37
12	A	822	CLA	C4B-NB	-2.43	1.34	1.37
12	A	855	CLA	C4B-NB	-2.42	1.34	1.37
12	B	830	CLA	C1D-ND	-2.42	1.34	1.37
12	A	855	CLA	C4C-C3C	2.42	1.49	1.45
12	B	853	CLA	C1C-NC	-2.42	1.34	1.37
12	A	812	CLA	MG-ND	-2.42	2.01	2.05
12	A	810	CLA	C4B-NB	-2.42	1.34	1.37
12	L	204	CLA	MG-ND	-2.42	2.01	2.05
12	J	102	CLA	C4B-NB	-2.42	1.34	1.37
12	B	829	CLA	C4B-NB	-2.42	1.34	1.37
12	A	843	CLA	MG-ND	-2.42	2.01	2.05
12	A	828	CLA	C4B-NB	-2.42	1.34	1.37
12	K	4004	CLA	C4B-NB	-2.41	1.34	1.37
12	A	847	CLA	MG-ND	-2.41	2.01	2.05
12	A	816	CLA	MG-ND	-2.41	2.01	2.05
12	F	203	CLA	C1C-NC	-2.41	1.34	1.37
12	A	824	CLA	C4B-NB	-2.41	1.34	1.37
12	B	805	CLA	C1C-NC	-2.41	1.34	1.37
12	B	804	CLA	C4B-NB	-2.41	1.34	1.37
12	A	812	CLA	C1D-C2D	2.41	1.50	1.45
12	A	814	CLA	MG-ND	-2.41	2.01	2.05
15	A	837	BCR	C34-C9	2.40	1.55	1.50
12	B	845	CLA	MG-ND	-2.40	2.01	2.05
12	B	823	CLA	C4B-NB	-2.40	1.34	1.37
12	A	815	CLA	C4B-NB	-2.40	1.34	1.37
12	A	819	CLA	C1D-C2D	2.40	1.50	1.45
13	A	802	CL0	MG-ND	-2.40	2.01	2.05
12	B	814	CLA	MG-ND	-2.40	2.01	2.05
12	B	808	CLA	C1C-NC	-2.40	1.34	1.37
15	F	201	BCR	C34-C9	2.40	1.55	1.50
12	B	820	CLA	C1C-NC	-2.39	1.34	1.37
17	A	840	LMG	C22-C21	-2.39	1.33	1.50
12	B	844	CLA	C1C-C2C	2.39	1.49	1.44
19	A	854	PL9	C2-C1	-2.39	1.38	1.44
12	J	102	CLA	C3B-C4B	2.38	1.49	1.42
12	B	809	CLA	C1C-NC	-2.38	1.34	1.37
12	B	845	CLA	C1C-NC	-2.38	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	203	CLA	MG-ND	-2.38	2.01	2.05
12	A	819	CLA	MG-ND	-2.38	2.01	2.05
12	B	827	CLA	C1D-C2D	2.37	1.50	1.45
12	A	852	CLA	C4B-NB	-2.37	1.34	1.37
12	A	814	CLA	C1D-C2D	2.37	1.50	1.45
12	A	806	CLA	C4B-NB	-2.37	1.34	1.37
12	L	204	CLA	C4B-NB	-2.37	1.34	1.37
12	K	4004	CLA	MG-ND	-2.37	2.01	2.05
12	B	846	CLA	MG-ND	-2.36	2.01	2.05
17	A	851	LMG	C25-C24	-2.36	1.33	1.50
12	B	853	CLA	MG-ND	-2.36	2.01	2.05
12	A	832	CLA	C3B-C4B	2.36	1.49	1.42
12	A	816	CLA	C4C-C3C	2.36	1.49	1.45
12	B	804	CLA	C1C-NC	-2.36	1.34	1.37
20	A	856	45D	C07-C15	2.36	1.39	1.35
12	A	848	CLA	MG-ND	-2.36	2.01	2.05
12	A	811	CLA	C1D-C2D	2.36	1.50	1.45
12	B	814	CLA	C1C-NC	-2.36	1.34	1.37
12	A	812	CLA	C4B-NB	-2.36	1.34	1.37
15	A	836	BCR	C34-C9	2.36	1.55	1.50
12	A	806	CLA	C1D-C2D	2.36	1.50	1.45
15	A	835	BCR	C34-C9	2.36	1.55	1.50
12	B	823	CLA	C1D-C2D	2.36	1.50	1.45
12	B	812	CLA	C4B-NB	-2.36	1.34	1.37
12	L	205	CLA	MG-ND	-2.35	2.01	2.05
12	B	826	CLA	C1D-C2D	2.35	1.50	1.45
12	B	850	CLA	C1D-C2D	2.35	1.50	1.45
12	B	806	CLA	C4B-NB	-2.34	1.34	1.37
12	A	829	CLA	C1D-C2D	2.34	1.50	1.45
12	B	814	CLA	C4B-NB	-2.34	1.34	1.37
12	A	828	CLA	MG-ND	-2.34	2.01	2.05
12	A	815	CLA	C1C-NC	-2.34	1.34	1.37
12	A	819	CLA	C4B-NB	-2.34	1.34	1.37
12	A	826	CLA	C4B-NB	-2.34	1.34	1.37
25	L	202	EQ3	C12-C13	-2.34	1.40	1.46
12	B	819	CLA	C4B-NB	-2.33	1.34	1.37
12	A	806	CLA	MG-ND	-2.33	2.01	2.05
25	L	202	EQ3	C11-C10	-2.33	1.36	1.43
12	A	831	CLA	C1D-ND	-2.33	1.34	1.37
12	A	825	CLA	C4B-NB	-2.33	1.34	1.37
12	A	818	CLA	C4B-NB	-2.33	1.34	1.37
12	A	816	CLA	C1D-C2D	2.33	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	802	CLA	C1B-C2B	2.33	1.48	1.43
12	J	103	CLA	C1C-NC	-2.33	1.34	1.37
12	B	810	CLA	C4C-C3C	2.32	1.49	1.45
12	K	4003	CLA	C1B-C2B	-2.32	1.37	1.43
12	B	849	CLA	C1C-NC	-2.32	1.34	1.37
12	A	801	CLA	C3B-C4B	2.31	1.49	1.42
15	L	208	BCR	C34-C9	2.31	1.55	1.50
12	A	828	CLA	C1D-C2D	2.31	1.49	1.45
20	A	856	45D	C34-C36	-2.31	1.41	1.46
12	B	809	CLA	C4B-NB	-2.31	1.34	1.37
12	A	855	CLA	C1C-NC	-2.31	1.34	1.37
12	A	819	CLA	C4C-C3C	2.31	1.49	1.45
12	A	833	CLA	C4C-C3C	2.30	1.48	1.45
12	A	804	CLA	C4B-NB	-2.30	1.34	1.37
12	B	828	CLA	C3B-C4B	2.30	1.49	1.42
12	A	845	CLA	C4B-NB	-2.30	1.34	1.37
12	A	830	CLA	C4C-C3C	2.30	1.48	1.45
12	B	807	CLA	C3B-C4B	2.30	1.49	1.42
12	A	823	CLA	C4B-NB	-2.29	1.34	1.37
12	B	812	CLA	C1C-NC	-2.29	1.34	1.37
12	A	814	CLA	C4B-NB	-2.29	1.34	1.37
12	B	804	CLA	C1D-C2D	2.29	1.49	1.45
12	B	852	CLA	C1D-C2D	2.29	1.49	1.45
12	B	813	CLA	C1D-C2D	2.29	1.49	1.45
12	J	101	CLA	C1D-ND	-2.29	1.34	1.37
12	A	807	CLA	C1D-C2D	2.29	1.49	1.45
12	F	204	CLA	C1C-NC	-2.28	1.34	1.37
12	B	845	CLA	C1D-C2D	2.28	1.49	1.45
12	B	849	CLA	C1D-C2D	2.28	1.49	1.45
12	A	824	CLA	C1C-C2C	2.28	1.49	1.44
12	A	813	CLA	C4C-C3C	2.28	1.48	1.45
12	B	805	CLA	C1D-C2D	2.28	1.49	1.45
12	A	848	CLA	C1D-C2D	2.28	1.49	1.45
12	A	819	CLA	C3B-C4B	2.28	1.49	1.42
12	A	825	CLA	C1D-C2D	2.27	1.49	1.45
12	B	830	CLA	C1C-NC	-2.27	1.34	1.37
12	B	848	CLA	C1C-C2C	2.27	1.49	1.44
12	B	808	CLA	C4B-NB	-2.27	1.34	1.37
12	A	852	CLA	MG-NB	2.27	2.10	2.05
12	J	102	CLA	C1B-C2B	2.27	1.48	1.43
12	J	103	CLA	C1D-ND	-2.26	1.34	1.37
12	B	815	CLA	C4C-C3C	2.26	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	847	CLA	C4D-CHA	2.26	1.46	1.38
25	L	202	EQ3	C8-C9	-2.26	1.41	1.46
12	B	826	CLA	C4C-C3C	2.26	1.48	1.45
12	J	103	CLA	MG-ND	-2.26	2.01	2.05
12	B	849	CLA	MG-ND	-2.26	2.01	2.05
13	A	802	CL0	C4B-NB	-2.26	1.34	1.37
12	B	812	CLA	MG-ND	-2.25	2.01	2.05
12	K	4002	CLA	C1D-C2D	2.25	1.49	1.45
12	B	813	CLA	C4B-NB	-2.25	1.34	1.37
12	A	817	CLA	C1D-C2D	2.25	1.49	1.45
12	B	825	CLA	C1D-C2D	2.25	1.49	1.45
12	B	824	CLA	C1C-NC	-2.25	1.34	1.37
12	A	809	CLA	C4D-CHA	2.25	1.46	1.38
12	B	803	CLA	O1D-CGD	-2.25	1.15	1.21
12	B	811	CLA	C3B-C4B	2.25	1.49	1.42
12	A	809	CLA	C1C-C2C	2.24	1.49	1.44
12	B	808	CLA	C1D-C2D	2.24	1.49	1.45
12	B	830	CLA	C4B-NB	-2.24	1.34	1.37
27	M	102	SQD	O9-S	2.24	1.51	1.45
27	M	102	SQD	O7-S	2.24	1.51	1.45
12	B	829	CLA	C1D-C2D	2.24	1.49	1.45
12	K	4004	CLA	C4C-C3C	2.24	1.48	1.45
17	A	840	LMG	O1-C1	2.24	1.43	1.40
12	B	843	CLA	C1D-C2D	2.23	1.49	1.45
12	A	803	CLA	MG-ND	-2.23	2.01	2.05
12	A	843	CLA	C1D-C2D	2.23	1.49	1.45
12	B	814	CLA	C1D-C2D	2.23	1.49	1.45
12	A	803	CLA	C3B-C4B	2.23	1.49	1.42
12	B	829	CLA	MG-ND	-2.23	2.01	2.05
12	A	829	CLA	C4C-C3C	2.23	1.48	1.45
12	B	825	CLA	C4C-C3C	2.22	1.48	1.45
12	J	103	CLA	C4C-C3C	2.22	1.48	1.45
12	B	847	CLA	C1C-NC	-2.22	1.34	1.37
12	B	824	CLA	C4D-CHA	2.22	1.46	1.38
12	B	816	CLA	C4C-C3C	2.22	1.48	1.45
12	A	801	CLA	C1D-C2D	2.22	1.49	1.45
12	A	804	CLA	C1D-C2D	2.22	1.49	1.45
12	B	850	CLA	C4C-C3C	2.22	1.48	1.45
12	B	803	CLA	CHB-C4A	-2.22	1.32	1.37
12	B	844	CLA	C3B-C4B	2.21	1.49	1.42
12	A	832	CLA	C1D-C2D	2.21	1.49	1.45
12	A	803	CLA	C1B-NB	-2.21	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	844	CLA	C4D-CHA	2.21	1.46	1.38
12	A	827	CLA	C1D-C2D	2.20	1.49	1.45
12	B	830	CLA	MG-ND	-2.20	2.01	2.05
12	A	829	CLA	MG-ND	-2.20	2.01	2.05
12	A	827	CLA	C4C-C3C	2.20	1.48	1.45
12	A	823	CLA	C4C-C3C	2.20	1.48	1.45
12	A	831	CLA	C1C-C2C	2.20	1.49	1.44
12	L	206	CLA	C1D-C2D	2.19	1.49	1.45
12	L	204	CLA	C1D-C2D	2.19	1.49	1.45
12	A	815	CLA	C4C-C3C	2.19	1.48	1.45
12	B	828	CLA	C4C-C3C	2.19	1.48	1.45
12	B	830	CLA	C4C-C3C	2.19	1.48	1.45
12	A	858	CLA	MG-ND	-2.19	2.01	2.05
12	A	847	CLA	C1D-C2D	2.19	1.49	1.45
12	B	807	CLA	C1D-C2D	2.19	1.49	1.45
12	A	812	CLA	C3B-C4B	2.19	1.49	1.42
12	L	201	CLA	MG-ND	-2.19	2.01	2.05
12	B	813	CLA	C1A-CHA	2.19	1.52	1.43
20	A	856	45D	C38-C36	2.18	1.40	1.35
12	B	815	CLA	C1D-C2D	2.18	1.49	1.45
12	B	814	CLA	C3B-C4B	2.18	1.49	1.42
12	A	803	CLA	C1D-C2D	2.18	1.49	1.45
12	A	833	CLA	C1D-C2D	2.18	1.49	1.45
12	A	808	CLA	C4C-C3C	2.18	1.48	1.45
12	B	852	CLA	C3B-C4B	2.18	1.49	1.42
12	B	810	CLA	C1D-C2D	2.18	1.49	1.45
12	A	831	CLA	C1A-CHA	2.17	1.52	1.43
25	L	202	EQ3	C16-C17	-2.17	1.36	1.43
12	B	823	CLA	C3B-C4B	2.17	1.49	1.42
12	B	852	CLA	C1C-NC	-2.17	1.34	1.37
12	J	102	CLA	C1D-C2D	2.17	1.49	1.45
12	A	813	CLA	C1D-C2D	2.17	1.49	1.45
12	A	845	CLA	C3B-C4B	2.16	1.49	1.42
12	A	832	CLA	MG-ND	-2.16	2.01	2.05
12	A	828	CLA	C4C-C3C	2.16	1.48	1.45
12	A	816	CLA	C3B-C4B	2.16	1.49	1.42
12	B	853	CLA	C4B-NB	-2.16	1.35	1.37
12	A	855	CLA	C1D-C2D	2.16	1.49	1.45
12	A	805	CLA	C3B-C4B	2.16	1.49	1.42
15	J	105	BCR	C31-C1	-2.16	1.49	1.53
12	A	825	CLA	C1A-CHA	2.16	1.52	1.43
12	B	820	CLA	C4B-NB	-2.16	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	818	CLA	C1C-C2C	2.15	1.48	1.44
12	A	846	CLA	C4C-C3C	2.15	1.48	1.45
12	A	820	CLA	C4B-NB	-2.15	1.35	1.37
12	A	847	CLA	C4C-C3C	2.15	1.48	1.45
12	A	807	CLA	MG-ND	-2.15	2.01	2.05
22	B	831	A1AGD	C3-C4	-2.15	1.46	1.49
12	B	845	CLA	C3B-C4B	2.15	1.49	1.42
12	A	821	CLA	C1D-C2D	2.14	1.49	1.45
12	J	103	CLA	C4B-NB	-2.14	1.35	1.37
12	A	831	CLA	C1D-C2D	2.14	1.49	1.45
20	A	856	45D	C30-C26	2.14	1.40	1.35
12	B	808	CLA	C1C-C2C	2.14	1.48	1.44
12	A	820	CLA	C3B-C4B	2.14	1.49	1.42
12	B	842	CLA	C4B-NB	-2.14	1.35	1.37
12	B	821	CLA	C4C-C3C	2.14	1.48	1.45
12	A	832	CLA	C1A-CHA	2.13	1.51	1.43
12	L	204	CLA	C4C-C3C	2.13	1.48	1.45
12	A	806	CLA	C4C-C3C	2.13	1.48	1.45
12	B	847	CLA	C3B-C4B	2.13	1.49	1.42
12	A	829	CLA	C4B-NB	-2.13	1.35	1.37
12	B	818	CLA	C3B-C4B	2.13	1.48	1.42
12	A	858	CLA	C1D-C2D	2.13	1.49	1.45
12	A	807	CLA	C3B-C4B	2.13	1.48	1.42
12	B	811	CLA	MG-ND	-2.13	2.01	2.05
12	A	809	CLA	MG-ND	-2.13	2.01	2.05
12	B	844	CLA	C1D-C2D	2.13	1.49	1.45
13	A	802	CL0	C1C-C2C	2.12	1.48	1.44
12	B	803	CLA	C4B-NB	-2.12	1.35	1.37
16	A	850	LHG	P-O4	-2.12	1.45	1.55
12	B	807	CLA	C1C-C2C	2.12	1.48	1.44
12	A	801	CLA	MG-ND	-2.12	2.01	2.05
12	B	801	CLA	C4C-C3C	2.12	1.48	1.45
12	A	827	CLA	C3B-C4B	2.11	1.48	1.42
12	A	824	CLA	C3B-C4B	2.11	1.48	1.42
12	F	203	CLA	C1C-C2C	2.11	1.48	1.44
12	A	805	CLA	C1C-C2C	2.11	1.48	1.44
12	A	804	CLA	C4C-C3C	2.11	1.48	1.45
12	B	813	CLA	C4C-C3C	2.11	1.48	1.45
12	B	816	CLA	C1D-C2D	2.11	1.49	1.45
12	B	816	CLA	C3B-C4B	2.11	1.48	1.42
12	B	812	CLA	C4C-C3C	2.11	1.48	1.45
12	B	801	CLA	C3B-C4B	2.11	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	849	CLA	C1D-C2D	2.11	1.49	1.45
12	J	103	CLA	C3B-C4B	2.11	1.48	1.42
12	B	808	CLA	C4C-C3C	2.11	1.48	1.45
12	B	814	CLA	C4C-C3C	2.10	1.48	1.45
12	A	826	CLA	C3B-C4B	2.10	1.48	1.42
12	B	842	CLA	C3B-C4B	2.10	1.48	1.42
12	A	848	CLA	C3B-C4B	2.10	1.48	1.42
12	J	103	CLA	C1C-C2C	2.10	1.48	1.44
12	B	814	CLA	C1C-C2C	2.09	1.48	1.44
12	B	853	CLA	C3B-C4B	2.09	1.48	1.42
12	B	805	CLA	C4C-C3C	2.09	1.48	1.45
12	B	812	CLA	C1D-C2D	2.09	1.49	1.45
12	B	818	CLA	C1A-CHA	2.09	1.51	1.43
12	B	822	CLA	C4C-C3C	2.09	1.48	1.45
12	B	804	CLA	C1C-C2C	2.09	1.48	1.44
12	A	813	CLA	C1C-C2C	2.09	1.48	1.44
12	F	204	CLA	C3B-C4B	2.09	1.48	1.42
12	B	848	CLA	C1A-CHA	2.08	1.51	1.43
12	A	807	CLA	C4C-C3C	2.08	1.48	1.45
12	L	206	CLA	C4C-C3C	2.08	1.48	1.45
12	A	844	CLA	C4C-C3C	2.08	1.48	1.45
12	B	802	CLA	C1A-CHA	2.07	1.51	1.43
12	B	849	CLA	C3B-C4B	2.07	1.48	1.42
12	B	817	CLA	C1D-C2D	2.07	1.49	1.45
12	A	830	CLA	C3B-C4B	2.07	1.48	1.42
12	A	811	CLA	C4C-C3C	2.07	1.48	1.45
12	B	850	CLA	C3B-C4B	2.07	1.48	1.42
12	B	823	CLA	C4C-C3C	2.07	1.48	1.45
12	B	815	CLA	C3B-C4B	2.07	1.48	1.42
12	B	828	CLA	MG-ND	-2.07	2.01	2.05
15	B	835	BCR	C34-C9	2.06	1.55	1.50
12	A	817	CLA	C3B-C4B	2.06	1.48	1.42
13	A	802	CL0	C3B-C4B	2.06	1.48	1.42
12	B	853	CLA	C4C-C3C	2.06	1.48	1.45
12	B	818	CLA	C4B-NB	-2.06	1.35	1.37
12	A	824	CLA	C4C-C3C	2.06	1.48	1.45
12	A	825	CLA	C1C-C2C	2.06	1.48	1.44
12	L	205	CLA	C3B-C4B	2.05	1.48	1.42
12	B	830	CLA	C3B-C4B	2.05	1.48	1.42
12	K	4003	CLA	MG-NC	2.05	2.11	2.06
12	B	823	CLA	C1C-C2C	2.05	1.48	1.44
15	A	837	BCR	C33-C5	2.05	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	821	CLA	C3B-C4B	2.05	1.48	1.42
12	L	201	CLA	C4C-C3C	2.05	1.48	1.45
12	A	843	CLA	C3B-C4B	2.05	1.48	1.42
12	B	820	CLA	C1D-C2D	2.05	1.49	1.45
12	B	842	CLA	C4C-C3C	2.05	1.48	1.45
12	J	102	CLA	C4C-C3C	2.05	1.48	1.45
12	B	805	CLA	C1A-CHA	2.04	1.51	1.43
12	B	806	CLA	C3B-C4B	2.04	1.48	1.42
12	B	847	CLA	C4B-NB	-2.04	1.35	1.37
12	B	822	CLA	C4B-NB	-2.04	1.35	1.37
12	A	852	CLA	C4C-C3C	2.04	1.48	1.45
12	B	826	CLA	C3B-C4B	2.04	1.48	1.42
12	K	4003	CLA	MG-NB	2.04	2.09	2.05
12	A	855	CLA	C1A-CHA	2.04	1.51	1.43
12	L	204	CLA	C1A-CHA	2.04	1.51	1.43
12	A	833	CLA	C3B-C4B	2.04	1.48	1.42
12	L	206	CLA	C3B-C4B	2.04	1.48	1.42
25	L	202	EQ3	C21-C22	2.04	1.40	1.35
12	A	826	CLA	MG-ND	-2.03	2.01	2.05
12	B	842	CLA	C1D-C2D	2.03	1.49	1.45
12	A	818	CLA	C4C-C3C	2.03	1.48	1.45
12	B	819	CLA	C3B-C4B	2.03	1.48	1.42
12	B	843	CLA	C4C-C3C	2.03	1.48	1.45
12	A	852	CLA	C3B-C4B	2.03	1.48	1.42
12	B	803	CLA	C4C-C3C	2.03	1.48	1.45
12	A	814	CLA	C3B-C4B	2.03	1.48	1.42
12	A	823	CLA	C1D-C2D	2.03	1.49	1.45
25	L	202	EQ3	C17-C18	2.02	1.40	1.35
12	A	829	CLA	C1A-CHA	2.02	1.51	1.43
12	A	849	CLA	C3B-C4B	2.02	1.48	1.42
12	B	811	CLA	C4B-NB	-2.02	1.35	1.37
12	A	845	CLA	C1D-C2D	2.02	1.49	1.45
12	B	829	CLA	C3B-C4B	2.02	1.48	1.42
12	A	815	CLA	C1D-C2D	2.02	1.49	1.45
12	A	822	CLA	C4C-C3C	2.01	1.48	1.45
12	A	804	CLA	C3B-C4B	2.01	1.48	1.42
12	A	821	CLA	C3B-C4B	2.01	1.48	1.42
12	B	825	CLA	C3B-C4B	2.01	1.48	1.42
13	A	802	CL0	C4C-C3C	2.01	1.48	1.45
12	J	103	CLA	C1A-CHA	2.01	1.51	1.43
12	B	806	CLA	C1D-C2D	2.01	1.49	1.45
12	A	828	CLA	C3B-C4B	2.01	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	802	CLA	C4C-C3C	2.01	1.48	1.45
12	B	822	CLA	C3B-C4B	2.01	1.48	1.42
12	B	846	CLA	CAA-C2A	-2.00	1.50	1.54
12	A	801	CLA	C1C-C2C	2.00	1.48	1.44
12	A	812	CLA	C1A-CHA	2.00	1.51	1.43
12	B	829	CLA	C1A-CHA	2.00	1.51	1.43

All (2951) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	805	CLA	O2A-CGA-O1A	-20.40	70.86	123.33
12	B	844	CLA	C4A-NA-C1A	13.79	112.97	106.68
12	B	805	CLA	O2A-CGA-CBA	12.91	154.79	114.00
12	B	805	CLA	O1A-CGA-CBA	-12.34	83.95	123.09
12	B	803	CLA	C4A-NA-C1A	11.82	112.07	106.68
12	K	4004	CLA	O2D-CGD-CBD	11.09	130.62	111.23
12	A	846	CLA	C4A-NA-C1A	10.61	111.52	106.68
12	B	846	CLA	C4A-NA-C1A	10.37	111.41	106.68
15	J	105	BCR	C31-C1-C6	-10.06	94.46	110.24
12	B	803	CLA	O2D-CGD-CBD	9.74	128.26	111.23
12	A	844	CLA	C4A-NA-C1A	9.11	110.84	106.68
12	J	103	CLA	CMD-C2D-C1D	9.08	140.72	124.73
12	J	101	CLA	CMD-C2D-C1D	9.08	140.72	124.73
12	K	4004	CLA	C4A-NA-C1A	9.02	110.80	106.68
12	B	804	CLA	CMD-C2D-C1D	8.80	140.22	124.73
12	A	825	CLA	CMD-C2D-C1D	8.49	139.68	124.73
12	B	826	CLA	CMD-C2D-C1D	8.38	139.48	124.73
12	B	847	CLA	C4A-NA-C1A	8.35	110.49	106.68
12	A	831	CLA	CMD-C2D-C1D	8.16	139.10	124.73
12	A	845	CLA	CMD-C2D-C1D	8.05	138.91	124.73
12	B	827	CLA	CMD-C2D-C1D	8.02	138.86	124.73
12	B	852	CLA	CMD-C2D-C1D	8.02	138.85	124.73
12	J	102	CLA	CMD-C2D-C1D	8.02	138.84	124.73
12	A	843	CLA	CMD-C2D-C1D	8.01	138.84	124.73
12	A	813	CLA	CMD-C2D-C1D	7.99	138.81	124.73
12	A	801	CLA	CMD-C2D-C1D	7.97	138.77	124.73
12	B	830	CLA	CMD-C2D-C1D	7.97	138.77	124.73
12	A	806	CLA	CMD-C2D-C1D	7.95	138.72	124.73
12	B	850	CLA	CMD-C2D-C1D	7.94	138.71	124.73
12	A	812	CLA	CMD-C2D-C1D	7.92	138.68	124.73
12	F	204	CLA	CMD-C2D-C1D	7.92	138.68	124.73
12	B	823	CLA	CMD-C2D-C1D	7.91	138.66	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	845	CLA	CMD-C2D-C1D	7.89	138.62	124.73
12	A	811	CLA	CMD-C2D-C1D	7.86	138.57	124.73
12	L	204	CLA	CMD-C2D-C1D	7.86	138.57	124.73
12	A	826	CLA	CMD-C2D-C1D	7.86	138.56	124.73
12	B	825	CLA	CMD-C2D-C1D	7.86	138.56	124.73
12	A	848	CLA	CMD-C2D-C1D	7.84	138.54	124.73
12	A	803	CLA	CMD-C2D-C1D	7.84	138.53	124.73
12	K	4002	CLA	CMD-C2D-C1D	7.83	138.52	124.73
12	B	848	CLA	CMD-C2D-C1D	7.81	138.47	124.73
12	A	844	CLA	C2D-C1D-ND	7.79	117.83	110.13
12	B	805	CLA	CMD-C2D-C1D	7.79	138.44	124.73
12	A	804	CLA	CMD-C2D-C1D	7.76	138.38	124.73
12	A	852	CLA	CMD-C2D-C1D	7.74	138.37	124.73
12	A	819	CLA	CMD-C2D-C1D	7.73	138.34	124.73
12	B	846	CLA	O2D-CGD-CBD	7.72	124.73	111.23
12	A	829	CLA	CMD-C2D-C1D	7.70	138.29	124.73
12	B	828	CLA	CMD-C2D-C1D	7.68	138.26	124.73
12	A	830	CLA	CMD-C2D-C1D	7.66	138.22	124.73
12	B	843	CLA	CMD-C2D-C1D	7.64	138.18	124.73
12	B	813	CLA	CMD-C2D-C1D	7.64	138.18	124.73
12	A	815	CLA	CMD-C2D-C1D	7.63	138.16	124.73
12	B	802	CLA	CMD-C2D-C1D	7.62	138.16	124.73
12	A	821	CLA	CMD-C2D-C1D	7.62	138.14	124.73
12	B	814	CLA	CMD-C2D-C1D	7.60	138.11	124.73
12	L	206	CLA	CMD-C2D-C1D	7.59	138.10	124.73
12	B	819	CLA	CMD-C2D-C1D	7.57	138.05	124.73
12	B	824	CLA	CMD-C2D-C1D	7.56	138.04	124.73
12	A	833	CLA	CMD-C2D-C1D	7.55	138.03	124.73
12	A	818	CLA	CMD-C2D-C1D	7.53	137.99	124.73
12	A	847	CLA	CMD-C2D-C1D	7.53	137.99	124.73
12	B	818	CLA	CMD-C2D-C1D	7.52	137.96	124.73
12	B	807	CLA	CMD-C2D-C1D	7.48	137.90	124.73
12	A	807	CLA	CMD-C2D-C1D	7.47	137.89	124.73
15	J	107	BCR	C24-C23-C22	-7.47	115.19	126.23
12	B	820	CLA	CMD-C2D-C1D	7.45	137.85	124.73
12	B	822	CLA	CMD-C2D-C1D	7.45	137.84	124.73
12	A	832	CLA	CMD-C2D-C1D	7.44	137.83	124.73
12	B	817	CLA	CMD-C2D-C1D	7.44	137.83	124.73
12	A	827	CLA	CMD-C2D-C1D	7.42	137.80	124.73
12	A	849	CLA	CMD-C2D-C1D	7.37	137.71	124.73
12	B	829	CLA	CMD-C2D-C1D	7.35	137.68	124.73
12	B	808	CLA	CMD-C2D-C1D	7.35	137.67	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	809	CLA	CMD-C2D-C1D	7.32	137.62	124.73
12	A	814	CLA	CMD-C2D-C1D	7.29	137.57	124.73
12	L	201	CLA	CMD-C2D-C1D	7.29	137.56	124.73
12	A	805	CLA	CMD-C2D-C1D	7.28	137.55	124.73
15	B	836	BCR	C20-C21-C22	-7.28	117.07	127.28
12	A	828	CLA	CMD-C2D-C1D	7.27	137.53	124.73
12	B	806	CLA	CMD-C2D-C1D	7.26	137.52	124.73
12	B	853	CLA	O2D-CGD-CBD	7.23	123.86	111.23
12	A	858	CLA	CMD-C2D-C1D	7.23	137.45	124.73
12	B	809	CLA	CMD-C2D-C1D	7.22	137.44	124.73
12	B	842	CLA	CMD-C2D-C1D	7.22	137.44	124.73
12	A	855	CLA	CMD-C2D-C1D	7.20	137.41	124.73
12	A	816	CLA	CMD-C2D-C1D	7.18	137.37	124.73
12	B	813	CLA	C4A-NA-C1A	7.18	109.95	106.68
12	A	809	CLA	O2A-CGA-O1A	-7.12	105.83	123.63
15	A	838	BCR	C33-C5-C6	-7.07	116.77	124.48
12	B	811	CLA	CMD-C2D-C1D	7.07	137.18	124.73
12	B	824	CLA	C4A-NA-C1A	7.07	109.90	106.68
12	B	816	CLA	CMD-C2D-C1D	7.06	137.16	124.73
12	A	810	CLA	CMD-C2D-C1D	7.05	137.14	124.73
12	B	815	CLA	CMD-C2D-C1D	7.03	137.12	124.73
12	B	810	CLA	CMD-C2D-C1D	7.02	137.09	124.73
12	B	849	CLA	C4A-NA-C1A	7.02	109.88	106.68
12	A	820	CLA	CMD-C2D-C1D	7.00	137.06	124.73
12	B	824	CLA	C2C-C1C-NC	6.94	117.28	109.98
12	B	844	CLA	C2C-C1C-NC	6.94	117.27	109.98
12	B	812	CLA	CMD-C2D-C1D	6.93	136.94	124.73
12	A	808	CLA	CMD-C2D-C1D	6.93	136.93	124.73
12	F	203	CLA	CMD-C2D-C1D	6.91	136.89	124.73
12	A	817	CLA	CMD-C2D-C1D	6.89	136.86	124.73
12	B	844	CLA	O2D-CGD-CBD	6.85	123.21	111.23
12	B	849	CLA	C2D-C1D-ND	6.84	116.89	110.13
12	A	822	CLA	CMD-C2D-C1D	6.83	136.76	124.73
15	J	104	BCR	C27-C26-C25	-6.83	113.47	122.70
15	J	105	BCR	C4-C5-C6	-6.81	113.50	122.70
12	B	846	CLA	CMD-C2D-C1D	6.80	136.70	124.73
12	K	4004	CLA	C2C-C1C-NC	6.79	117.12	109.98
12	A	823	CLA	CMD-C2D-C1D	6.79	136.68	124.73
12	B	853	CLA	C4A-NA-C1A	6.78	109.77	106.68
12	L	201	CLA	O2D-CGD-CBD	6.78	123.08	111.23
12	A	828	CLA	C4A-NA-C1A	6.77	109.77	106.68
12	A	824	CLA	CMD-C2D-C1D	6.75	136.62	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	801	CLA	CMD-C2D-C1D	6.68	136.50	124.73
12	A	844	CLA	C1D-ND-C4D	-6.67	101.63	106.31
12	K	4004	CLA	CMD-C2D-C1D	6.67	136.47	124.73
12	B	853	CLA	C2D-C1D-ND	6.64	116.70	110.13
12	B	812	CLA	C2C-C1C-NC	6.64	116.96	109.98
12	B	821	CLA	CMD-C2D-C1D	6.63	136.41	124.73
13	A	802	CL0	CMD-C2D-C1D	6.61	136.37	124.73
12	B	830	CLA	O2D-CGD-CBD	6.61	122.79	111.23
12	B	849	CLA	CMD-C2D-C1D	6.59	136.34	124.73
12	B	801	CLA	C2D-C1D-ND	6.59	116.65	110.13
12	L	205	CLA	C2D-C1D-ND	6.58	116.64	110.13
12	A	818	CLA	O2D-CGD-CBD	6.58	122.73	111.23
12	A	844	CLA	C3D-C2D-C1D	-6.56	96.88	105.83
12	B	849	CLA	C1D-ND-C4D	-6.55	101.72	106.31
12	A	812	CLA	C2C-C1C-NC	6.51	116.82	109.98
12	B	848	CLA	C2D-C1D-ND	6.50	116.56	110.13
12	B	818	CLA	O2D-CGD-CBD	6.48	122.55	111.23
12	L	205	CLA	CMD-C2D-C1D	6.47	136.13	124.73
12	B	812	CLA	C1C-C2C-C3C	-6.45	100.19	106.98
12	B	820	CLA	C2C-C1C-NC	6.45	116.76	109.98
12	B	844	CLA	CMD-C2D-C1D	6.44	136.06	124.73
12	B	848	CLA	C1D-ND-C4D	-6.44	101.80	106.31
12	B	852	CLA	C2C-C1C-NC	6.42	116.73	109.98
12	A	820	CLA	C2D-C1D-ND	6.42	116.48	110.13
12	B	801	CLA	C1D-ND-C4D	-6.41	101.81	106.31
12	B	847	CLA	C2D-C1D-ND	6.39	116.45	110.13
12	B	853	CLA	C2C-C1C-NC	6.37	116.67	109.98
12	A	844	CLA	O2D-CGD-CBD	6.35	122.32	111.23
12	A	823	CLA	C2C-C1C-NC	6.29	116.59	109.98
12	A	844	CLA	C2C-C1C-NC	6.29	116.58	109.98
12	A	855	CLA	C2C-C1C-NC	6.28	116.58	109.98
12	B	811	CLA	C1D-ND-C4D	-6.25	101.93	106.31
12	B	844	CLA	C1C-C2C-C3C	-6.25	100.41	106.98
12	A	807	CLA	O2D-CGD-CBD	6.23	122.12	111.23
12	L	204	CLA	O2D-CGD-CBD	6.23	122.12	111.23
12	A	801	CLA	O2D-CGD-CBD	6.22	122.11	111.23
12	K	4002	CLA	C2C-C1C-NC	6.21	116.50	109.98
12	A	846	CLA	CMD-C2D-C1D	6.21	135.66	124.73
12	A	855	CLA	CMA-C3A-C2A	-6.21	89.99	113.98
12	A	852	CLA	C2C-C1C-NC	6.19	116.49	109.98
12	B	844	CLA	C3D-C2D-C1D	-6.19	97.39	105.83
12	B	853	CLA	CMD-C2D-C1D	6.18	135.62	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	811	CLA	C4A-NA-C1A	6.17	109.50	106.68
15	B	834	BCR	C33-C5-C6	-6.16	117.76	124.48
12	B	849	CLA	C1C-C2C-C3C	-6.15	100.51	106.98
12	B	822	CLA	C2C-C1C-NC	6.15	116.44	109.98
12	A	807	CLA	C4A-NA-C1A	6.15	109.48	106.68
12	A	849	CLA	C2C-C1C-NC	6.14	116.44	109.98
12	B	810	CLA	C2C-C1C-NC	6.14	116.43	109.98
12	B	847	CLA	C1D-ND-C4D	-6.14	102.00	106.31
12	B	844	CLA	C2D-C1D-ND	6.14	116.20	110.13
12	A	818	CLA	C2C-C1C-NC	6.13	116.42	109.98
12	B	853	CLA	C1-C2-C3	-6.12	116.16	126.20
12	F	204	CLA	C2C-C1C-NC	6.12	116.41	109.98
12	B	811	CLA	C2D-C1D-ND	6.12	116.18	110.13
12	A	805	CLA	C2D-C1D-ND	6.12	116.18	110.13
12	A	825	CLA	C2C-C1C-NC	6.12	116.41	109.98
12	B	803	CLA	CMD-C2D-C1D	6.11	135.49	124.73
12	B	829	CLA	C2D-C1D-ND	6.11	116.17	110.13
12	B	817	CLA	C2C-C1C-NC	6.10	116.39	109.98
12	L	205	CLA	C4A-NA-C1A	6.10	109.46	106.68
12	A	858	CLA	C2D-C1D-ND	6.10	116.16	110.13
12	B	822	CLA	C4A-NA-C1A	6.09	109.46	106.68
12	B	829	CLA	C4A-NA-C1A	6.08	109.45	106.68
12	B	827	CLA	C2C-C1C-NC	6.07	116.36	109.98
12	A	825	CLA	C4A-NA-C1A	6.07	109.45	106.68
12	K	4004	CLA	C1C-C2C-C3C	-6.06	100.61	106.98
12	B	805	CLA	C4A-NA-C1A	6.05	109.44	106.68
12	B	805	CLA	C2C-C1C-NC	6.05	116.34	109.98
12	B	824	CLA	C1C-C2C-C3C	-6.05	100.62	106.98
12	A	801	CLA	C4A-NA-C1A	6.05	109.44	106.68
13	A	802	CL0	C2D-C1D-ND	6.05	116.11	110.13
15	B	841	BCR	C38-C26-C25	-6.04	117.89	124.48
12	B	811	CLA	O2D-CGD-CBD	6.04	121.80	111.23
12	A	829	CLA	C4A-NA-C1A	6.04	109.44	106.68
12	A	831	CLA	C2D-C1D-ND	6.04	116.10	110.13
12	B	853	CLA	C1D-ND-C4D	-6.03	102.08	106.31
12	A	831	CLA	C1D-ND-C4D	-6.03	102.08	106.31
12	B	802	CLA	C2C-C1C-NC	6.03	116.31	109.98
12	A	808	CLA	CMA-C3A-C4A	6.02	127.96	111.77
12	A	820	CLA	O2D-CGD-CBD	6.02	121.75	111.23
12	B	824	CLA	C3D-C2D-C1D	-6.02	97.62	105.83
15	I	101	BCR	C24-C23-C22	-6.01	117.35	126.23
12	B	819	CLA	C4A-NA-C1A	6.01	109.42	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	810	CLA	C4A-NA-C1A	6.00	109.42	106.68
12	B	853	CLA	C1C-C2C-C3C	-5.99	100.68	106.98
12	A	830	CLA	C2C-C1C-NC	5.98	116.26	109.98
12	A	829	CLA	C2C-C1C-NC	5.97	116.25	109.98
12	A	809	CLA	C2D-C1D-ND	5.96	116.03	110.13
12	B	820	CLA	C1C-C2C-C3C	-5.96	100.71	106.98
12	A	823	CLA	O2D-CGD-CBD	5.96	121.65	111.23
12	B	808	CLA	C2C-C1C-NC	5.96	116.24	109.98
18	B	840	LMT	C1'-O5'-C5'	5.96	125.35	113.72
15	A	837	BCR	C15-C14-C13	-5.95	118.93	127.28
12	L	205	CLA	C1D-ND-C4D	-5.95	102.14	106.31
12	A	804	CLA	C2C-C1C-NC	5.95	116.23	109.98
12	A	804	CLA	C4A-NA-C1A	5.94	109.39	106.68
12	A	820	CLA	C3D-C2D-C1D	-5.94	97.73	105.83
12	L	204	CLA	C2C-C1C-NC	5.93	116.21	109.98
12	B	807	CLA	O2D-CGD-CBD	5.93	121.60	111.23
12	A	827	CLA	C2C-C1C-NC	5.93	116.21	109.98
12	B	829	CLA	C3D-C2D-C1D	-5.93	97.74	105.83
12	A	831	CLA	C4A-NA-C1A	5.92	109.38	106.68
12	A	847	CLA	C2C-C1C-NC	5.92	116.20	109.98
12	B	819	CLA	C2D-C1D-ND	5.92	115.98	110.13
13	A	802	CL0	C2C-C1C-NC	5.90	116.18	109.98
12	A	815	CLA	O2D-CGD-CBD	5.90	121.54	111.23
12	A	809	CLA	O2D-CGD-CBD	5.89	121.53	111.23
12	B	819	CLA	C3D-C2D-C1D	-5.88	97.80	105.83
12	A	815	CLA	C2C-C1C-NC	5.88	116.16	109.98
12	B	829	CLA	C2C-C1C-NC	5.88	116.16	109.98
12	A	811	CLA	O2D-CGD-CBD	5.87	121.49	111.23
12	J	101	CLA	C2C-C1C-NC	5.87	116.14	109.98
12	B	821	CLA	C2C-C1C-NC	5.87	116.14	109.98
12	B	813	CLA	C1-O2A-CGA	5.87	130.85	116.65
12	B	815	CLA	C2C-C1C-NC	5.86	116.14	109.98
12	K	4002	CLA	O2D-CGD-CBD	5.86	121.47	111.23
12	F	203	CLA	C2D-C1D-ND	5.86	115.92	110.13
12	B	807	CLA	C4A-NA-C1A	5.85	109.35	106.68
15	B	836	BCR	C15-C14-C13	-5.85	118.54	127.48
12	L	206	CLA	O2D-CGD-CBD	5.85	121.45	111.23
12	A	832	CLA	C2D-C1D-ND	5.85	115.91	110.13
12	L	201	CLA	C2C-C1C-NC	5.84	116.11	109.98
12	B	842	CLA	O2D-CGD-CBD	5.84	121.43	111.23
12	L	201	CLA	C1C-C2C-C3C	-5.83	100.85	106.98
12	A	819	CLA	O2D-CGD-CBD	5.83	121.42	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	827	CLA	C3D-C2D-C1D	-5.82	97.88	105.83
12	A	809	CLA	C3D-C2D-C1D	-5.82	97.89	105.83
12	B	844	CLA	C3B-C2B-C1B	-5.80	100.33	107.17
15	J	105	BCR	C16-C15-C14	-5.80	111.65	123.52
15	A	835	BCR	C33-C5-C6	-5.80	118.16	124.48
12	B	826	CLA	C2C-C1C-NC	5.80	116.07	109.98
12	J	101	CLA	O2D-CGD-CBD	5.80	121.36	111.23
12	A	803	CLA	O2D-CGD-CBD	5.79	121.35	111.23
12	B	809	CLA	C2C-C1C-NC	5.79	116.06	109.98
12	B	827	CLA	C2D-C1D-ND	5.79	115.85	110.13
12	B	811	CLA	C2C-C1C-NC	5.78	116.05	109.98
12	A	806	CLA	C2C-C1C-NC	5.76	116.03	109.98
12	B	849	CLA	C2C-C1C-NC	5.76	116.03	109.98
15	J	107	BCR	C16-C17-C18	-5.75	119.21	127.28
12	B	850	CLA	C1-O2A-CGA	5.75	130.57	116.65
12	B	816	CLA	C2C-C1C-NC	5.75	116.02	109.98
12	A	828	CLA	C2C-C1C-NC	5.75	116.02	109.98
15	A	837	BCR	C16-C17-C18	-5.74	119.22	127.28
12	B	806	CLA	C2C-C1C-NC	5.74	116.01	109.98
12	A	855	CLA	C3D-C2D-C1D	-5.74	98.00	105.83
12	L	205	CLA	C3D-C2D-C1D	-5.74	98.00	105.83
12	A	831	CLA	C2C-C1C-NC	5.74	116.01	109.98
12	A	858	CLA	C1D-ND-C4D	-5.74	102.29	106.31
12	A	810	CLA	C2C-C1C-NC	5.73	116.00	109.98
12	F	204	CLA	O2D-CGD-CBD	5.73	121.25	111.23
12	A	808	CLA	C2C-C1C-NC	5.73	116.00	109.98
12	L	205	CLA	C2C-C1C-NC	5.72	115.99	109.98
12	B	824	CLA	O2A-CGA-O1A	-5.72	109.33	123.63
12	B	852	CLA	C1C-C2C-C3C	-5.72	100.97	106.98
12	A	826	CLA	C4A-NA-C1A	5.71	109.29	106.68
12	A	822	CLA	C2C-C1C-NC	5.71	115.98	109.98
12	A	805	CLA	C1D-ND-C4D	-5.71	102.31	106.31
12	B	802	CLA	C1C-C2C-C3C	-5.71	100.98	106.98
16	A	850	LHG	O7-C7-C8	5.71	123.83	111.48
12	A	805	CLA	C3D-C2D-C1D	-5.71	98.04	105.83
12	A	825	CLA	C3D-C2D-C1D	-5.71	98.05	105.83
12	A	823	CLA	C4A-NA-C1A	5.70	109.28	106.68
12	B	825	CLA	O2D-CGD-CBD	5.70	121.19	111.23
12	B	817	CLA	C1C-C2C-C3C	-5.70	100.99	106.98
12	B	812	CLA	C2D-C1D-ND	5.69	115.76	110.13
12	A	829	CLA	C2D-C1D-ND	5.69	115.75	110.13
12	B	824	CLA	O2A-CGA-CBA	5.68	129.16	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	828	CLA	C3D-C2D-C1D	-5.67	98.09	105.83
12	A	844	CLA	CMD-C2D-C1D	5.67	134.72	124.73
12	A	806	CLA	C1D-ND-C4D	-5.67	102.33	106.31
15	A	837	BCR	C33-C5-C6	-5.67	118.30	124.48
12	A	809	CLA	O2A-CGA-CBA	5.66	129.11	111.83
12	B	842	CLA	C2C-C1C-NC	5.66	115.93	109.98
12	B	828	CLA	C2D-C1D-ND	5.66	115.73	110.13
12	A	832	CLA	C3D-C2D-C1D	-5.66	98.11	105.83
12	A	811	CLA	C2C-C1C-NC	5.66	115.92	109.98
12	A	820	CLA	C1D-ND-C4D	-5.66	102.34	106.31
15	J	105	BCR	C27-C26-C25	-5.65	115.06	122.70
12	A	803	CLA	C3D-C2D-C1D	-5.65	98.11	105.83
12	A	826	CLA	C2C-C1C-NC	5.65	115.92	109.98
12	A	826	CLA	C3D-C2D-C1D	-5.65	98.12	105.83
12	A	818	CLA	C4A-NA-C1A	5.65	109.25	106.68
15	J	107	BCR	C30-C25-C26	-5.64	114.92	122.64
12	A	849	CLA	C1C-C2C-C3C	-5.64	101.05	106.98
12	A	855	CLA	C1C-C2C-C3C	-5.64	101.05	106.98
12	B	803	CLA	C1C-C2C-C3C	-5.63	101.06	106.98
12	B	813	CLA	C3B-C2B-C1B	-5.63	100.53	107.17
12	L	201	CLA	C3B-C2B-C1B	-5.63	100.53	107.17
12	B	853	CLA	C3D-C2D-C1D	-5.63	98.15	105.83
12	A	805	CLA	C4A-NA-C1A	5.63	109.25	106.68
12	B	813	CLA	C2C-C1C-NC	5.63	115.89	109.98
12	B	822	CLA	O2D-CGD-CBD	5.63	121.07	111.23
12	B	849	CLA	C3D-C2D-C1D	-5.62	98.16	105.83
12	A	812	CLA	C1C-C2C-C3C	-5.62	101.07	106.98
12	B	803	CLA	C2D-C1D-ND	5.61	115.68	110.13
12	B	825	CLA	C2C-C1C-NC	5.61	115.88	109.98
12	L	206	CLA	C2C-C1C-NC	5.61	115.87	109.98
12	A	813	CLA	C2C-C1C-NC	5.60	115.87	109.98
12	A	830	CLA	C1C-C2C-C3C	-5.60	101.09	106.98
12	A	831	CLA	C3D-C2D-C1D	-5.60	98.19	105.83
12	A	852	CLA	O2A-CGA-O1A	-5.60	109.62	123.63
15	K	4001	BCR	C11-C10-C9	-5.60	119.43	127.28
12	B	816	CLA	C4A-NA-C1A	5.60	109.23	106.68
12	A	844	CLA	C1C-C2C-C3C	-5.60	101.09	106.98
12	A	826	CLA	C2D-C1D-ND	5.59	115.66	110.13
12	B	808	CLA	C1C-C2C-C3C	-5.59	101.10	106.98
12	B	845	CLA	C2C-C1C-NC	5.58	115.85	109.98
13	A	802	CL0	C4A-NA-C1A	5.58	109.23	106.68
12	A	818	CLA	C3D-C2D-C1D	-5.58	98.21	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	819	CLA	C2C-C1C-NC	5.58	115.84	109.98
15	F	202	BCR	C38-C26-C25	-5.58	118.40	124.48
12	B	801	CLA	C3D-C2D-C1D	-5.57	98.22	105.83
17	A	840	LMG	O7-C10-C11	5.57	123.54	111.48
12	J	101	CLA	C3B-C2B-C1B	-5.57	100.60	107.17
12	B	809	CLA	C1C-C2C-C3C	-5.57	101.12	106.98
12	B	827	CLA	C1C-C2C-C3C	-5.56	101.13	106.98
13	A	802	CL0	C1D-ND-C4D	-5.56	102.41	106.31
12	A	858	CLA	C3D-C2D-C1D	-5.56	98.25	105.83
12	A	852	CLA	C3D-C2D-C1D	-5.56	98.25	105.83
12	A	852	CLA	CMA-C3A-C4A	5.55	126.69	111.77
12	A	817	CLA	O2D-CGD-CBD	5.55	120.93	111.23
12	A	846	CLA	C2D-C1D-ND	5.55	115.62	110.13
12	B	810	CLA	C1C-C2C-C3C	-5.54	101.16	106.98
12	B	818	CLA	C2D-C1D-ND	5.53	115.60	110.13
12	B	827	CLA	C3B-C2B-C1B	-5.53	100.65	107.17
12	A	829	CLA	C3D-C2D-C1D	-5.51	98.31	105.83
12	B	847	CLA	C3D-C2D-C1D	-5.51	98.31	105.83
12	B	805	CLA	C1C-C2C-C3C	-5.51	101.19	106.98
12	F	203	CLA	C3D-C2D-C1D	-5.51	98.32	105.83
12	B	846	CLA	C1C-C2C-C3C	-5.50	101.19	106.98
12	A	806	CLA	C2D-C1D-ND	5.50	115.57	110.13
12	A	818	CLA	C2D-C1D-ND	5.50	115.57	110.13
12	A	805	CLA	O2A-CGA-CBA	5.50	128.60	111.83
12	A	828	CLA	C2D-C1D-ND	5.50	115.57	110.13
12	L	205	CLA	O2D-CGD-CBD	5.50	120.84	111.23
12	B	852	CLA	C3D-C2D-C1D	-5.49	98.34	105.83
12	A	855	CLA	O2D-CGD-CBD	5.49	120.83	111.23
15	L	208	BCR	C27-C26-C25	-5.49	115.29	122.70
15	B	832	BCR	C33-C5-C6	-5.49	118.50	124.48
12	B	822	CLA	C1C-C2C-C3C	-5.49	101.21	106.98
12	A	852	CLA	C1C-C2C-C3C	-5.48	101.21	106.98
12	B	830	CLA	C3D-C2D-C1D	-5.48	98.35	105.83
12	A	816	CLA	C2C-C1C-NC	5.48	115.74	109.98
12	B	818	CLA	C4A-NA-C1A	5.48	109.18	106.68
12	A	829	CLA	C1D-ND-C4D	-5.48	102.47	106.31
12	A	848	CLA	C2D-C1D-ND	5.47	115.54	110.13
12	B	803	CLA	C3D-C2D-C1D	-5.47	98.37	105.83
12	B	816	CLA	C2D-C1D-ND	5.47	115.53	110.13
12	B	818	CLA	C3D-C2D-C1D	-5.46	98.37	105.83
12	B	843	CLA	C2C-C1C-NC	5.46	115.71	109.98
12	B	846	CLA	C2D-C1D-ND	5.45	115.52	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	807	CLA	C2C-C1C-NC	5.45	115.70	109.98
12	A	852	CLA	C2D-C1D-ND	5.45	115.52	110.13
12	B	813	CLA	C3D-C2D-C1D	-5.45	98.40	105.83
12	B	818	CLA	C2C-C1C-NC	5.45	115.70	109.98
12	K	4004	CLA	O2D-CGD-O1D	-5.44	113.25	123.85
12	A	804	CLA	C1C-C2C-C3C	-5.44	101.25	106.98
12	A	845	CLA	C2C-C1C-NC	5.44	115.70	109.98
12	J	103	CLA	C4A-NA-C1A	5.44	109.16	106.68
12	A	833	CLA	C2C-C1C-NC	5.44	115.70	109.98
15	J	107	BCR	C20-C21-C22	-5.44	119.65	127.28
12	L	205	CLA	C3B-C2B-C1B	-5.43	100.77	107.17
12	A	833	CLA	C2D-C1D-ND	5.43	115.50	110.13
12	A	801	CLA	C2D-C1D-ND	5.43	115.50	110.13
12	B	806	CLA	O2D-CGD-CBD	5.43	120.72	111.23
12	A	824	CLA	C2C-C1C-NC	5.43	115.68	109.98
12	A	824	CLA	O2D-CGD-CBD	5.42	120.71	111.23
12	B	825	CLA	C4A-NA-C1A	5.42	109.15	106.68
12	A	807	CLA	C2D-C1D-ND	5.42	115.49	110.13
12	A	801	CLA	C3B-C2B-C1B	-5.42	100.78	107.17
12	B	822	CLA	O2A-CGA-O1A	-5.42	110.07	123.63
12	B	830	CLA	C3B-C2B-C1B	-5.42	100.78	107.17
12	B	811	CLA	C1C-C2C-C3C	-5.42	101.28	106.98
12	A	826	CLA	C1C-C2C-C3C	-5.42	101.28	106.98
12	B	821	CLA	C1C-C2C-C3C	-5.42	101.28	106.98
12	B	846	CLA	C3D-C2D-C1D	-5.41	98.44	105.83
12	A	821	CLA	C4A-NA-C1A	5.41	109.15	106.68
12	A	817	CLA	C2D-C1D-ND	5.41	115.48	110.13
12	A	810	CLA	O2D-CGD-CBD	5.41	120.69	111.23
12	B	817	CLA	C2D-C1D-ND	5.41	115.48	110.13
12	L	204	CLA	C1C-C2C-C3C	-5.41	101.29	106.98
12	B	804	CLA	C2C-C1C-NC	5.41	115.67	109.98
12	A	858	CLA	C4A-NA-C1A	5.41	109.15	106.68
12	B	845	CLA	C1C-C2C-C3C	-5.41	101.29	106.98
12	A	833	CLA	C3D-C2D-C1D	-5.40	98.46	105.83
12	A	820	CLA	C4A-NA-C1A	5.40	109.14	106.68
12	A	813	CLA	C3D-C2D-C1D	-5.40	98.46	105.83
12	A	847	CLA	C1C-C2C-C3C	-5.40	101.30	106.98
12	A	843	CLA	C3D-C2D-C1D	-5.40	98.46	105.83
12	A	807	CLA	C3B-C2B-C1B	-5.40	100.81	107.17
12	A	843	CLA	C2D-C1D-ND	5.40	115.47	110.13
12	B	812	CLA	C3D-C2D-C1D	-5.39	98.47	105.83
12	B	815	CLA	O2D-CGD-CBD	5.39	120.66	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	801	CLA	C3D-C2D-C1D	-5.39	98.47	105.83
12	A	855	CLA	C2D-C1D-ND	5.39	115.46	110.13
12	A	848	CLA	C3D-C2D-C1D	-5.39	98.47	105.83
12	A	848	CLA	C2C-C1C-NC	5.39	115.65	109.98
12	B	802	CLA	C3D-C2D-C1D	-5.39	98.47	105.83
12	B	846	CLA	C1D-ND-C4D	-5.39	102.53	106.31
12	B	816	CLA	C3D-C2D-C1D	-5.39	98.48	105.83
12	B	817	CLA	C4A-NA-C1A	5.39	109.14	106.68
12	A	827	CLA	C1C-C2C-C3C	-5.38	101.32	106.98
12	L	206	CLA	C4A-NA-C1A	5.38	109.13	106.68
12	J	103	CLA	C2C-C1C-NC	5.38	115.63	109.98
12	A	817	CLA	O2A-CGA-O1A	-5.38	110.18	123.63
12	B	850	CLA	C2C-C1C-NC	5.37	115.63	109.98
12	J	103	CLA	C3D-C2D-C1D	-5.37	98.50	105.83
12	B	814	CLA	C2C-C1C-NC	5.37	115.62	109.98
12	B	808	CLA	C3D-C2D-C1D	-5.37	98.50	105.83
12	B	827	CLA	C4A-NA-C1A	5.37	109.13	106.68
12	L	204	CLA	C4A-NA-C1A	5.37	109.13	106.68
12	A	812	CLA	O2D-CGD-CBD	5.37	120.62	111.23
12	A	815	CLA	C3D-C2D-C1D	-5.37	98.50	105.83
13	A	802	CL0	C3D-C2D-C1D	-5.37	98.51	105.83
12	B	817	CLA	O2D-CGD-CBD	5.36	120.61	111.23
12	A	806	CLA	C1C-C2C-C3C	-5.36	101.34	106.98
12	A	825	CLA	C1C-C2C-C3C	-5.36	101.34	106.98
12	A	849	CLA	C2D-C1D-ND	5.36	115.43	110.13
15	F	202	BCR	C11-C10-C9	-5.35	119.77	127.28
12	A	858	CLA	O2A-CGA-O1A	-5.35	110.25	123.63
12	A	803	CLA	C2D-C1D-ND	5.35	115.42	110.13
12	L	204	CLA	C3D-C2D-C1D	-5.34	98.54	105.83
12	A	817	CLA	C2C-C1C-NC	5.34	115.59	109.98
12	B	806	CLA	C1C-C2C-C3C	-5.34	101.36	106.98
12	A	817	CLA	C1C-C2C-C3C	-5.33	101.37	106.98
12	K	4002	CLA	C3D-C2D-C1D	-5.33	98.55	105.83
12	A	821	CLA	C2C-C1C-NC	5.33	115.58	109.98
12	B	843	CLA	O2D-CGD-CBD	5.33	120.55	111.23
12	B	807	CLA	C3D-C2D-C1D	-5.33	98.56	105.83
12	B	814	CLA	C3B-C2B-C1B	-5.33	100.89	107.17
12	B	804	CLA	C3D-C2D-C1D	-5.33	98.56	105.83
12	A	848	CLA	O2D-CGD-CBD	5.33	120.54	111.23
12	B	807	CLA	C3B-C2B-C1B	-5.33	100.89	107.17
12	J	102	CLA	C2C-C1C-NC	5.33	115.58	109.98
12	A	815	CLA	C1C-C2C-C3C	-5.32	101.38	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	827	CLA	C1D-ND-C4D	-5.32	102.58	106.31
12	B	845	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
12	B	805	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
12	A	827	CLA	O2A-CGA-O1A	-5.32	110.33	123.63
12	B	830	CLA	C2D-C1D-ND	5.32	115.39	110.13
12	B	817	CLA	C3D-C2D-C1D	-5.32	98.58	105.83
12	A	833	CLA	O2D-CGD-CBD	5.31	120.51	111.23
12	A	811	CLA	C3B-C2B-C1B	-5.31	100.91	107.17
13	A	802	CL0	C1C-C2C-C3C	-5.31	101.40	106.98
12	B	848	CLA	C2C-C1C-NC	5.31	115.56	109.98
12	A	821	CLA	C2D-C1D-ND	5.30	115.38	110.13
12	B	845	CLA	C2D-C1D-ND	5.30	115.38	110.13
12	A	806	CLA	C3D-C2D-C1D	-5.30	98.59	105.83
12	L	204	CLA	C2D-C1D-ND	5.30	115.38	110.13
12	L	205	CLA	C1C-C2C-C3C	-5.30	101.40	106.98
12	A	823	CLA	C1C-C2C-C3C	-5.30	101.40	106.98
12	A	828	CLA	C1D-ND-C4D	-5.30	102.59	106.31
12	A	847	CLA	C3B-C2B-C1B	-5.30	100.92	107.17
12	L	206	CLA	C2D-C1D-ND	5.30	115.37	110.13
12	B	843	CLA	C3D-C2D-C1D	-5.30	98.60	105.83
12	A	845	CLA	O2D-CGD-CBD	5.30	120.49	111.23
12	B	820	CLA	C3D-C2D-C1D	-5.30	98.60	105.83
12	A	828	CLA	C3D-C2D-C1D	-5.29	98.61	105.83
12	B	847	CLA	CMD-C2D-C1D	5.29	134.05	124.73
12	B	842	CLA	C2D-C1D-ND	5.29	115.36	110.13
12	A	848	CLA	C1C-C2C-C3C	-5.29	101.42	106.98
12	B	823	CLA	C2C-C1C-NC	5.29	115.54	109.98
12	A	847	CLA	C4A-NA-C1A	5.29	109.09	106.68
12	A	843	CLA	C3B-C2B-C1B	-5.29	100.94	107.17
12	F	203	CLA	O2A-CGA-O1A	-5.29	109.74	123.33
12	A	803	CLA	C2C-C1C-NC	5.28	115.53	109.98
12	A	852	CLA	O2D-CGD-CBD	5.28	120.46	111.23
12	B	848	CLA	O2D-CGD-CBD	5.28	120.46	111.23
12	B	848	CLA	C3D-C2D-C1D	-5.28	98.63	105.83
12	A	818	CLA	C1C-C2C-C3C	-5.28	101.43	106.98
12	B	804	CLA	C1D-ND-C4D	-5.28	102.61	106.31
12	B	816	CLA	O2D-CGD-CBD	5.28	120.46	111.23
12	A	815	CLA	C2D-C1D-ND	5.28	115.35	110.13
12	A	829	CLA	C1C-C2C-C3C	-5.28	101.43	106.98
12	B	824	CLA	C2D-C1D-ND	5.28	115.35	110.13
12	B	852	CLA	C2D-C1D-ND	5.28	115.35	110.13
12	A	828	CLA	C1C-C2C-C3C	-5.27	101.43	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	810	CLA	C4A-NA-C1A	5.27	109.08	106.68
12	B	820	CLA	C2D-C1D-ND	5.27	115.34	110.13
12	A	831	CLA	C1C-C2C-C3C	-5.27	101.44	106.98
12	A	810	CLA	C1C-C2C-C3C	-5.27	101.44	106.98
12	B	804	CLA	C1C-C2C-C3C	-5.27	101.44	106.98
12	A	858	CLA	C3B-C2B-C1B	-5.27	100.96	107.17
12	A	827	CLA	C3D-C2D-C1D	-5.27	98.64	105.83
12	A	805	CLA	C3B-C2B-C1B	-5.27	100.96	107.17
12	A	821	CLA	C1D-ND-C4D	-5.27	102.62	106.31
12	A	807	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
12	B	826	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
12	B	850	CLA	C3B-C2B-C1B	-5.26	100.97	107.17
15	A	836	BCR	C20-C21-C22	-5.26	119.90	127.28
12	B	849	CLA	O2D-CGD-CBD	5.26	120.42	111.23
12	A	849	CLA	C1D-ND-C4D	-5.26	102.62	106.31
17	A	851	LMG	O1-C1-C2	5.26	116.26	108.27
12	A	847	CLA	C2D-C1D-ND	5.26	115.33	110.13
12	A	814	CLA	C1C-C2C-C3C	-5.26	101.45	106.98
12	J	102	CLA	C3D-C2D-C1D	-5.26	98.66	105.83
12	J	103	CLA	C1C-C2C-C3C	-5.25	101.45	106.98
12	F	204	CLA	C3D-C2D-C1D	-5.25	98.66	105.83
12	A	807	CLA	C1D-ND-C4D	-5.25	102.63	106.31
12	B	806	CLA	C2D-C1D-ND	5.25	115.32	110.13
12	B	842	CLA	C3D-C2D-C1D	-5.25	98.67	105.83
12	B	805	CLA	O2D-CGD-CBD	5.25	120.40	111.23
12	B	801	CLA	C2C-C1C-NC	5.25	115.49	109.98
12	A	824	CLA	C2D-C1D-ND	5.25	115.32	110.13
12	B	807	CLA	C2D-C1D-ND	5.25	115.32	110.13
12	A	816	CLA	C3D-C2D-C1D	-5.24	98.67	105.83
12	A	827	CLA	C2D-C1D-ND	5.24	115.32	110.13
12	A	812	CLA	C4A-NA-C1A	5.24	109.07	106.68
12	A	852	CLA	O2A-CGA-CBA	5.24	127.82	111.83
12	J	101	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
12	A	810	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
12	A	819	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
12	A	816	CLA	C2D-C1D-ND	5.24	115.31	110.13
12	B	807	CLA	C2C-C1C-NC	5.23	115.48	109.98
12	A	801	CLA	O2A-CGA-O1A	-5.23	110.54	123.63
12	A	830	CLA	C3B-C2B-C1B	-5.23	101.00	107.17
12	A	830	CLA	C3D-C2D-C1D	-5.23	98.69	105.83
12	A	822	CLA	C1C-C2C-C3C	-5.23	101.48	106.98
12	A	810	CLA	C2D-C1D-ND	5.23	115.30	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	844	CLA	O2A-CGA-O1A	-5.23	110.55	123.63
12	A	815	CLA	C4A-NA-C1A	5.23	109.06	106.68
12	B	826	CLA	C3B-C2B-C1B	-5.23	101.01	107.17
12	L	206	CLA	O2A-CGA-O1A	-5.23	110.55	123.63
12	B	801	CLA	C3B-C2B-C1B	-5.23	101.01	107.17
12	A	804	CLA	C3D-C2D-C1D	-5.22	98.70	105.83
12	A	833	CLA	C3B-C2B-C1B	-5.22	101.01	107.17
12	A	807	CLA	C1C-C2C-C3C	-5.22	101.49	106.98
15	J	104	BCR	C29-C30-C25	5.22	118.02	110.44
12	A	848	CLA	C3B-C2B-C1B	-5.22	101.02	107.17
12	A	833	CLA	O2A-CGA-O1A	-5.22	110.58	123.63
12	L	206	CLA	C3D-C2D-C1D	-5.22	98.71	105.83
12	A	827	CLA	O2D-CGD-CBD	5.22	120.35	111.23
12	B	830	CLA	C2C-C1C-NC	5.21	115.46	109.98
12	B	814	CLA	O2A-CGA-O1A	-5.21	110.59	123.63
15	L	208	BCR	C7-C8-C9	-5.21	118.52	126.23
12	B	802	CLA	C2D-C1D-ND	5.20	115.28	110.13
12	K	4002	CLA	C2D-C1D-ND	5.20	115.28	110.13
12	B	829	CLA	C1D-ND-C4D	-5.20	102.66	106.31
12	A	814	CLA	C2C-C1C-NC	5.20	115.44	109.98
12	A	825	CLA	C2D-C1D-ND	5.20	115.27	110.13
12	B	826	CLA	C1C-C2C-C3C	-5.20	101.52	106.98
12	B	810	CLA	O2D-CGD-CBD	5.19	120.31	111.23
12	A	825	CLA	C3B-C2B-C1B	-5.19	101.05	107.17
12	B	821	CLA	C3B-C2B-C1B	-5.19	101.05	107.17
12	B	823	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
12	B	806	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
12	B	804	CLA	C2D-C1D-ND	5.18	115.25	110.13
12	A	811	CLA	C1C-C2C-C3C	-5.18	101.53	106.98
12	A	805	CLA	O2D-CGD-CBD	5.18	120.28	111.23
12	A	846	CLA	C3D-C2D-C1D	-5.18	98.77	105.83
12	A	823	CLA	C2D-C1D-ND	5.18	115.25	110.13
12	A	817	CLA	C1D-ND-C4D	-5.18	102.68	106.31
12	A	817	CLA	C3D-C2D-C1D	-5.17	98.77	105.83
12	A	813	CLA	C3B-C2B-C1B	-5.17	101.07	107.17
12	A	832	CLA	CMA-C3A-C2A	-5.17	93.98	113.98
12	B	809	CLA	C3B-C2B-C1B	-5.17	101.07	107.17
12	B	811	CLA	C3D-C2D-C1D	-5.17	98.78	105.83
12	B	843	CLA	C1C-C2C-C3C	-5.17	101.55	106.98
12	A	822	CLA	C4A-NA-C1A	5.16	109.03	106.68
12	A	815	CLA	O2A-CGA-O1A	-5.16	110.72	123.63
12	B	842	CLA	C1C-C2C-C3C	-5.16	101.55	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	801	CLA	CMA-C3A-C4A	5.16	125.64	111.77
12	B	848	CLA	C3B-C2B-C1B	-5.15	101.09	107.17
12	A	809	CLA	C1C-C2C-C3C	-5.15	101.56	106.98
12	J	102	CLA	O2D-CGD-CBD	5.15	120.24	111.23
12	B	828	CLA	C4A-NA-C1A	5.15	109.03	106.68
12	B	821	CLA	C2D-C1D-ND	5.15	115.22	110.13
12	A	823	CLA	O2A-CGA-O1A	-5.15	110.75	123.63
12	B	812	CLA	C1D-ND-C4D	-5.15	102.70	106.31
12	A	801	CLA	C1D-ND-C4D	-5.15	102.70	106.31
12	L	204	CLA	C1D-ND-C4D	-5.14	102.70	106.31
12	B	825	CLA	C3D-C2D-C1D	-5.14	98.81	105.83
12	L	206	CLA	C1C-C2C-C3C	-5.14	101.57	106.98
12	A	806	CLA	C4A-NA-C1A	5.14	109.02	106.68
12	A	845	CLA	C1C-C2C-C3C	-5.14	101.57	106.98
12	B	813	CLA	O2D-CGD-CBD	5.14	120.21	111.23
12	B	819	CLA	O2D-CGD-CBD	5.14	120.21	111.23
12	B	819	CLA	C1D-ND-C4D	-5.13	102.71	106.31
15	J	107	BCR	C33-C5-C6	-5.13	118.88	124.48
12	B	805	CLA	C2D-C1D-ND	5.13	115.20	110.13
12	A	821	CLA	C3B-C2B-C1B	-5.13	101.12	107.17
12	B	812	CLA	O2A-CGA-O1A	-5.13	110.80	123.63
12	L	201	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
12	A	808	CLA	C1C-C2C-C3C	-5.13	101.59	106.98
12	J	103	CLA	C3B-C2B-C1B	-5.13	101.13	107.17
12	B	815	CLA	C3B-C2B-C1B	-5.12	101.13	107.17
12	B	843	CLA	O2A-CGA-O1A	-5.12	110.83	123.63
12	A	827	CLA	C4A-NA-C1A	5.12	109.01	106.68
12	J	101	CLA	C1D-ND-C4D	-5.12	102.72	106.31
12	B	829	CLA	C1C-C2C-C3C	-5.12	101.60	106.98
12	A	821	CLA	C3D-C2D-C1D	-5.11	98.85	105.83
12	J	102	CLA	C2D-C1D-ND	5.11	115.18	110.13
12	A	819	CLA	C1C-C2C-C3C	-5.11	101.61	106.98
12	B	814	CLA	C2D-C1D-ND	5.11	115.18	110.13
12	A	803	CLA	C4A-NA-C1A	5.10	109.01	106.68
12	B	828	CLA	C2C-C1C-NC	5.10	115.34	109.98
12	A	848	CLA	C1D-ND-C4D	-5.10	102.73	106.31
12	B	828	CLA	C1D-ND-C4D	-5.10	102.73	106.31
12	J	102	CLA	C1C-C2C-C3C	-5.10	101.62	106.98
12	A	819	CLA	C3B-C2B-C1B	-5.10	101.16	107.17
12	B	829	CLA	O2D-CGD-CBD	5.09	120.14	111.23
12	B	803	CLA	C2C-C1C-NC	5.09	115.33	109.98
12	A	826	CLA	C1D-ND-C4D	-5.09	102.74	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	823	CLA	C1C-C2C-C3C	-5.09	101.62	106.98
12	K	4002	CLA	C1D-ND-C4D	-5.09	102.74	106.31
12	A	824	CLA	O2A-CGA-O1A	-5.09	110.90	123.63
12	A	813	CLA	C2D-C1D-ND	5.08	115.16	110.13
12	A	847	CLA	C3D-C2D-C1D	-5.08	98.89	105.83
12	J	103	CLA	O2D-CGD-CBD	5.08	120.11	111.23
12	A	811	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
12	A	812	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
12	F	204	CLA	C1C-C2C-C3C	-5.08	101.64	106.98
12	A	849	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
12	A	846	CLA	C2C-C1C-NC	5.08	115.32	109.98
12	A	804	CLA	C3B-C2B-C1B	-5.08	101.18	107.17
12	B	815	CLA	C1C-C2C-C3C	-5.08	101.64	106.98
12	A	815	CLA	C3B-C2B-C1B	-5.08	101.18	107.17
15	B	835	BCR	C16-C17-C18	-5.08	120.16	127.28
12	B	816	CLA	O2A-CGA-O1A	-5.08	110.93	123.63
12	L	201	CLA	C4A-NA-C1A	5.08	109.00	106.68
12	B	825	CLA	C1C-C2C-C3C	-5.08	101.64	106.98
12	B	850	CLA	C1C-C2C-C3C	-5.08	101.64	106.98
12	B	853	CLA	O2A-CGA-O1A	-5.07	110.94	123.63
12	A	810	CLA	O2A-CGA-O1A	-5.07	110.94	123.63
12	A	814	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
12	B	807	CLA	C1C-C2C-C3C	-5.06	101.65	106.98
12	B	853	CLA	C3B-C2B-C1B	-5.06	101.20	107.17
12	B	825	CLA	C2D-C1D-ND	5.06	115.14	110.13
12	A	804	CLA	C2D-C1D-ND	5.06	115.14	110.13
15	L	208	BCR	C11-C10-C9	-5.06	120.18	127.28
12	A	824	CLA	C1C-C2C-C3C	-5.06	101.66	106.98
12	A	803	CLA	C3B-C2B-C1B	-5.06	101.21	107.17
12	A	821	CLA	O2D-CGD-CBD	5.06	120.07	111.23
12	A	822	CLA	C3B-C2B-C1B	-5.06	101.21	107.17
12	B	814	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
12	A	823	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
12	B	814	CLA	O2D-CGD-CBD	5.05	120.06	111.23
12	B	808	CLA	C2D-C1D-ND	5.05	115.13	110.13
15	B	841	BCR	C33-C5-C6	-5.05	118.97	124.48
12	J	102	CLA	C1D-ND-C4D	-5.05	102.77	106.31
12	B	823	CLA	O2A-CGA-O1A	-5.05	111.00	123.63
12	A	858	CLA	C2C-C1C-NC	5.04	115.28	109.98
12	F	203	CLA	C2C-C1C-NC	5.04	115.28	109.98
15	B	835	BCR	C24-C23-C22	-5.04	118.78	126.23
12	B	820	CLA	O2A-CGA-O1A	-5.04	111.02	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	832	CLA	C1D-ND-C4D	-5.04	102.78	106.31
12	A	816	CLA	C1C-C2C-C3C	-5.04	101.68	106.98
12	A	847	CLA	C1D-ND-C4D	-5.04	102.78	106.31
12	B	849	CLA	C3B-C2B-C1B	-5.04	101.23	107.17
12	B	852	CLA	C3B-C2B-C1B	-5.04	101.23	107.17
12	A	843	CLA	C1D-ND-C4D	-5.04	102.78	106.31
12	F	204	CLA	C2D-C1D-ND	5.03	115.11	110.13
12	B	845	CLA	C1D-ND-C4D	-5.03	102.78	106.31
12	A	808	CLA	O2D-CGD-CBD	5.03	120.03	111.23
12	B	803	CLA	O1D-CGD-CBD	-5.03	114.60	124.52
12	B	819	CLA	C2C-C1C-NC	5.03	115.27	109.98
12	A	858	CLA	O2A-CGA-CBA	5.02	127.16	111.83
12	A	821	CLA	C1C-C2C-C3C	-5.02	101.70	106.98
12	B	812	CLA	C4A-NA-C1A	5.02	108.97	106.68
12	K	4002	CLA	C1C-C2C-C3C	-5.02	101.70	106.98
12	A	809	CLA	C2C-C1C-NC	5.02	115.26	109.98
12	B	827	CLA	O2D-CGD-CBD	5.02	120.00	111.23
12	A	804	CLA	O2D-CGD-CBD	5.02	120.00	111.23
12	A	843	CLA	C4A-NA-C1A	5.02	108.97	106.68
12	A	831	CLA	O2A-CGA-O1A	-5.01	111.08	123.63
12	B	806	CLA	C3B-C2B-C1B	-5.01	101.26	107.17
15	J	105	BCR	C33-C5-C6	-5.01	119.01	124.48
12	B	814	CLA	C1C-C2C-C3C	-5.01	101.71	106.98
12	B	823	CLA	O2D-CGD-CBD	5.01	119.99	111.23
12	B	810	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
12	B	815	CLA	C3D-C2D-C1D	-5.01	99.00	105.83
12	B	812	CLA	O2D-CGD-CBD	5.01	119.98	111.23
12	J	101	CLA	O2A-CGA-O1A	-5.01	111.10	123.63
12	B	809	CLA	C3D-C2D-C1D	-5.01	99.00	105.83
12	F	204	CLA	C1D-ND-C4D	-5.00	102.80	106.31
12	A	806	CLA	O2A-CGA-O1A	-5.00	110.47	123.33
12	L	206	CLA	C1D-ND-C4D	-5.00	102.81	106.31
12	B	845	CLA	O2A-CGA-O1A	-5.00	111.13	123.63
12	L	206	CLA	C3B-C2B-C1B	-4.99	101.28	107.17
12	A	822	CLA	O2D-CGD-CBD	4.99	119.96	111.23
12	B	821	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
12	A	826	CLA	C3B-C2B-C1B	-4.99	101.29	107.17
12	A	819	CLA	C2D-C1D-ND	4.99	115.06	110.13
15	F	201	BCR	C4-C5-C6	-4.99	115.97	122.70
12	B	817	CLA	C1D-ND-C4D	-4.99	102.81	106.31
12	B	804	CLA	C3B-C2B-C1B	-4.99	101.29	107.17
12	A	832	CLA	C2C-C1C-NC	4.98	115.21	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	843	CLA	O2A-CGA-O1A	-4.98	111.17	123.63
12	A	814	CLA	C2D-C1D-ND	4.98	115.05	110.13
12	B	811	CLA	O2A-CGA-O1A	-4.98	111.18	123.63
12	B	802	CLA	O2A-CGA-O1A	-4.97	111.18	123.63
12	A	809	CLA	C1D-ND-C4D	-4.97	102.82	106.31
12	B	843	CLA	C2D-C1D-ND	4.97	115.04	110.13
12	A	820	CLA	C3B-C2B-C1B	-4.96	101.32	107.17
12	B	823	CLA	C2D-C1D-ND	4.96	115.04	110.13
12	B	823	CLA	C3B-C2B-C1B	-4.96	101.32	107.17
12	B	815	CLA	C4A-NA-C1A	4.96	108.94	106.68
12	A	805	CLA	C2C-C1C-NC	4.96	115.19	109.98
12	B	842	CLA	C1D-ND-C4D	-4.96	102.83	106.31
12	B	818	CLA	O2A-CGA-O1A	-4.96	111.23	123.63
12	A	822	CLA	C2D-C1D-ND	4.96	115.03	110.13
12	B	808	CLA	C4A-NA-C1A	4.96	108.94	106.68
12	B	813	CLA	C2D-C1D-ND	4.95	115.03	110.13
12	A	824	CLA	C1D-ND-C4D	-4.94	102.84	106.31
12	B	826	CLA	C2D-C1D-ND	4.94	115.02	110.13
12	B	816	CLA	C3B-C2B-C1B	-4.94	101.34	107.17
12	A	816	CLA	C3B-C2B-C1B	-4.94	101.34	107.17
15	L	208	BCR	C33-C5-C6	-4.94	119.09	124.48
12	J	102	CLA	C3B-C2B-C1B	-4.93	101.35	107.17
12	B	801	CLA	C1C-C2C-C3C	-4.93	101.79	106.98
12	A	830	CLA	C2D-C1D-ND	4.93	115.01	110.13
12	B	844	CLA	C1D-ND-C4D	-4.93	102.85	106.31
12	A	831	CLA	O2D-CGD-CBD	4.92	119.84	111.23
15	K	4001	BCR	C4-C5-C6	-4.92	116.06	122.70
15	A	836	BCR	C4-C5-C6	-4.92	116.06	122.70
12	B	808	CLA	O2D-CGD-CBD	4.92	119.83	111.23
12	A	808	CLA	C2D-C1D-ND	4.92	114.99	110.13
12	B	815	CLA	C2D-C1D-ND	4.92	114.99	110.13
12	A	817	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
12	A	843	CLA	C2C-C1C-NC	4.91	115.14	109.98
12	A	817	CLA	C4A-NA-C1A	4.91	108.92	106.68
12	B	814	CLA	C1D-ND-C4D	-4.91	102.87	106.31
12	B	828	CLA	C1C-C2C-C3C	-4.91	101.82	106.98
12	A	810	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
12	A	824	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
12	B	845	CLA	O2D-CGD-CBD	4.91	119.81	111.23
12	B	810	CLA	C2D-C1D-ND	4.90	114.98	110.13
12	A	833	CLA	C1D-ND-C4D	-4.90	102.87	106.31
12	A	807	CLA	O2A-CGA-O1A	-4.90	111.37	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	845	CLA	C3B-C2B-C1B	-4.90	101.39	107.17
16	B	851	LHG	O7-C7-C8	4.90	122.08	111.48
12	A	812	CLA	C2D-C1D-ND	4.90	114.97	110.13
12	A	843	CLA	O2A-C1-C2	4.89	126.94	108.11
12	B	830	CLA	O2A-CGA-O1A	-4.89	110.75	123.33
12	B	842	CLA	C4A-NA-C1A	4.89	108.91	106.68
12	A	848	CLA	O2A-CGA-O1A	-4.89	111.39	123.63
12	A	808	CLA	O2A-CGA-O1A	-4.88	111.41	123.63
12	L	201	CLA	C2D-C1D-ND	4.88	114.96	110.13
12	B	801	CLA	O2A-CGA-O1A	-4.88	111.43	123.63
12	A	828	CLA	O2D-CGD-CBD	4.87	119.75	111.23
12	B	806	CLA	C4A-NA-C1A	4.87	108.90	106.68
15	B	841	BCR	C15-C14-C13	-4.87	120.44	127.28
12	A	814	CLA	C1D-ND-C4D	-4.87	102.89	106.31
12	B	809	CLA	C2D-C1D-ND	4.87	114.94	110.13
15	L	207	BCR	C16-C17-C18	-4.87	120.45	127.28
12	A	858	CLA	C11-C10-C8	-4.87	99.79	115.97
12	A	803	CLA	O2A-CGA-CBA	4.87	126.67	111.83
12	A	813	CLA	O2A-CGA-O1A	-4.86	111.46	123.63
12	A	832	CLA	O2A-CGA-O1A	-4.86	111.46	123.63
12	A	808	CLA	C3D-C2D-C1D	-4.86	99.19	105.83
12	A	843	CLA	CMA-C3A-C2A	-4.86	95.17	113.98
12	A	822	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
12	A	819	CLA	O2A-CGA-O1A	-4.86	111.48	123.63
12	B	848	CLA	C1C-C2C-C3C	-4.86	101.87	106.98
12	A	808	CLA	C3B-C2B-C1B	-4.85	101.45	107.17
12	A	828	CLA	C3B-C2B-C1B	-4.85	101.45	107.17
12	A	846	CLA	C1D-ND-C4D	-4.84	102.91	106.31
12	A	811	CLA	O2A-CGA-O1A	-4.84	110.88	123.33
12	A	818	CLA	C3B-C2B-C1B	-4.84	101.47	107.17
12	F	204	CLA	C3B-C2B-C1B	-4.83	101.47	107.17
12	B	824	CLA	C3B-C2B-C1B	-4.83	101.47	107.17
12	B	847	CLA	C1C-C2C-C3C	-4.83	101.90	106.98
12	B	825	CLA	C1D-ND-C4D	-4.83	102.92	106.31
12	A	812	CLA	O2A-CGA-O1A	-4.83	110.92	123.33
12	L	204	CLA	O2A-CGA-O1A	-4.82	111.56	123.63
12	J	101	CLA	C1C-C2C-C3C	-4.82	101.91	106.98
12	B	827	CLA	O2A-CGA-O1A	-4.82	110.93	123.33
12	A	827	CLA	C1D-ND-C4D	-4.82	102.93	106.31
15	A	838	BCR	C38-C26-C25	-4.82	119.22	124.48
12	B	822	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
12	A	803	CLA	O2A-CGA-O1A	-4.82	111.58	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	L	207	BCR	C33-C5-C6	-4.81	119.23	124.48
15	A	835	BCR	C27-C26-C25	-4.81	116.20	122.70
12	J	103	CLA	C2D-C1D-ND	4.81	114.89	110.13
12	A	824	CLA	C3B-C2B-C1B	-4.80	101.51	107.17
12	B	849	CLA	O2A-CGA-O1A	-4.80	111.61	123.63
12	A	811	CLA	C2D-C1D-ND	4.80	114.88	110.13
12	A	814	CLA	O2A-CGA-O1A	-4.80	111.61	123.63
12	B	802	CLA	C4A-NA-C1A	4.80	108.87	106.68
15	J	105	BCR	C32-C1-C6	4.80	117.77	110.24
12	B	829	CLA	C3B-C2B-C1B	-4.80	101.51	107.17
15	K	4005	BCR	C15-C14-C13	-4.80	120.55	127.28
12	B	823	CLA	C1D-ND-C4D	-4.79	102.95	106.31
12	B	830	CLA	C1D-ND-C4D	-4.79	102.95	106.31
12	A	806	CLA	C3B-C2B-C1B	-4.79	101.52	107.17
12	F	203	CLA	C1D-ND-C4D	-4.79	102.95	106.31
15	K	4001	BCR	C24-C23-C22	-4.79	119.16	126.23
12	B	810	CLA	C3B-C2B-C1B	-4.78	101.53	107.17
12	A	845	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
12	B	802	CLA	O2D-CGD-CBD	4.78	119.59	111.23
12	A	848	CLA	C4A-NA-C1A	4.78	108.86	106.68
12	B	845	CLA	C4A-NA-C1A	4.78	108.86	106.68
12	L	204	CLA	C3B-C2B-C1B	-4.78	101.54	107.17
12	A	833	CLA	C4A-NA-C1A	4.77	108.86	106.68
12	A	829	CLA	C3B-C2B-C1B	-4.77	101.54	107.17
12	B	819	CLA	C3B-C2B-C1B	-4.77	101.54	107.17
12	B	808	CLA	C3B-C2B-C1B	-4.77	101.55	107.17
12	B	807	CLA	C1D-ND-C4D	-4.77	102.97	106.31
12	A	846	CLA	C3B-C2B-C1B	-4.76	101.55	107.17
15	B	836	BCR	C38-C26-C25	-4.76	119.29	124.48
12	A	811	CLA	C1D-ND-C4D	-4.76	102.97	106.31
12	A	805	CLA	O2A-CGA-O1A	-4.76	111.73	123.63
12	A	825	CLA	O2D-CGD-CBD	4.76	119.54	111.23
15	J	107	BCR	C15-C14-C13	-4.75	120.61	127.28
12	A	801	CLA	C2C-C1C-NC	4.75	114.97	109.98
15	B	836	BCR	C27-C26-C25	-4.75	116.28	122.70
12	B	842	CLA	O2A-CGA-O1A	-4.75	111.75	123.63
12	A	809	CLA	C3B-C2B-C1B	-4.75	101.57	107.17
12	A	832	CLA	C4A-NA-C1A	4.75	108.84	106.68
12	A	812	CLA	C1D-ND-C4D	-4.75	102.98	106.31
12	A	806	CLA	O2D-CGD-CBD	4.75	119.53	111.23
15	A	835	BCR	C4-C5-C6	-4.74	116.29	122.70
12	A	816	CLA	C1D-ND-C4D	-4.74	102.98	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	852	CLA	CHD-C4C-C3C	-4.74	117.86	124.77
12	L	206	CLA	O2A-CGA-CBA	4.74	126.29	111.83
12	L	205	CLA	O2A-CGA-O1A	-4.74	111.78	123.63
12	A	845	CLA	O2A-CGA-O1A	-4.74	111.78	123.63
12	A	855	CLA	O2A-C1-C2	4.73	126.32	108.11
12	B	825	CLA	O2A-CGA-O1A	-4.73	111.79	123.63
12	B	824	CLA	O2D-CGD-CBD	4.73	119.50	111.23
12	A	813	CLA	C1C-C2C-C3C	-4.72	102.01	106.98
15	K	4001	BCR	C20-C21-C22	-4.72	120.65	127.28
13	A	802	CL0	O2D-CGD-CBD	4.72	119.48	111.23
12	A	833	CLA	C1C-C2C-C3C	-4.72	102.01	106.98
12	B	817	CLA	C3B-C2B-C1B	-4.72	101.61	107.17
12	B	844	CLA	CAC-C3C-C4C	4.72	130.93	124.79
12	A	818	CLA	O2A-CGA-O1A	-4.72	111.82	123.63
12	B	804	CLA	O2A-CGA-O1A	-4.72	111.83	123.63
12	B	830	CLA	C1C-C2C-C3C	-4.72	102.02	106.98
12	J	103	CLA	CHD-C1D-ND	-4.72	118.17	124.80
12	B	820	CLA	O2D-CGD-CBD	4.72	119.47	111.23
12	B	826	CLA	O2D-CGD-CBD	4.72	119.47	111.23
15	L	207	BCR	C11-C10-C9	-4.71	120.67	127.28
12	B	816	CLA	C1C-C2C-C3C	-4.71	102.02	106.98
12	A	828	CLA	O2A-CGA-O1A	-4.71	111.84	123.63
12	A	830	CLA	C1D-ND-C4D	-4.71	103.01	106.31
12	K	4002	CLA	C3B-C2B-C1B	-4.71	101.62	107.17
12	B	846	CLA	O2A-CGA-O1A	-4.70	111.88	123.63
12	B	818	CLA	C1C-C2C-C3C	-4.69	102.04	106.98
15	F	201	BCR	C20-C19-C18	-4.69	113.50	126.36
12	B	853	CLA	C5-C3-C2	-4.69	110.64	121.17
12	B	826	CLA	C4A-NA-C1A	4.69	108.82	106.68
12	B	803	CLA	C1D-ND-C4D	-4.69	103.02	106.31
12	B	829	CLA	C1-O2A-CGA	4.69	127.99	116.65
12	A	830	CLA	O2A-CGA-O1A	-4.68	111.93	123.63
12	B	825	CLA	C3B-C2B-C1B	-4.68	101.66	107.17
12	B	822	CLA	C2D-C1D-ND	4.68	114.75	110.13
12	B	804	CLA	O2D-CGD-CBD	4.67	119.40	111.23
12	B	848	CLA	C4A-NA-C1A	4.67	108.81	106.68
12	A	805	CLA	C1C-C2C-C3C	-4.67	102.07	106.98
12	B	853	CLA	C4-C3-C5	4.67	123.33	115.23
12	A	814	CLA	O2D-CGD-CBD	4.66	119.38	111.23
12	A	818	CLA	C1D-ND-C4D	-4.66	103.04	106.31
15	F	202	BCR	C15-C14-C13	-4.66	120.74	127.28
12	J	101	CLA	C2D-C1D-ND	4.66	114.73	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	832	CLA	O2D-CGD-CBD	4.66	119.37	111.23
12	A	852	CLA	C3B-C2B-C1B	-4.66	101.68	107.17
12	B	828	CLA	O2D-CGD-CBD	4.65	119.36	111.23
12	B	852	CLA	O2A-CGA-O1A	-4.65	111.99	123.63
12	B	813	CLA	O2A-CGA-O1A	-4.65	111.99	123.63
12	A	855	CLA	C3B-C2B-C1B	-4.65	101.69	107.17
12	B	809	CLA	O2D-CGD-CBD	4.65	119.36	111.23
12	B	802	CLA	C1D-ND-C4D	-4.64	103.05	106.31
12	B	820	CLA	C3B-C2B-C1B	-4.64	101.70	107.17
15	B	835	BCR	C33-C5-C6	-4.64	119.42	124.48
12	A	849	CLA	O2D-CGD-CBD	4.64	119.33	111.23
12	A	804	CLA	C1D-ND-C4D	-4.63	103.06	106.31
12	B	843	CLA	C3B-C2B-C1B	-4.63	101.71	107.17
12	A	803	CLA	C1D-ND-C4D	-4.63	103.07	106.31
12	L	201	CLA	O2A-CGA-O1A	-4.63	112.06	123.63
12	B	815	CLA	O2A-CGA-O1A	-4.63	111.44	123.33
12	B	847	CLA	CED-O2D-CGD	4.62	126.40	115.92
15	B	841	BCR	C20-C21-C22	-4.62	120.80	127.28
12	B	852	CLA	C1D-ND-C4D	-4.61	103.07	106.31
12	B	842	CLA	C3B-C2B-C1B	-4.61	101.73	107.17
12	K	4004	CLA	C1D-ND-C4D	-4.61	103.08	106.31
12	J	102	CLA	O2A-CGA-O1A	-4.61	111.48	123.33
12	A	824	CLA	C4A-NA-C1A	4.61	108.78	106.68
17	A	851	LMG	O7-C10-C11	4.61	121.45	111.48
12	B	826	CLA	O2A-CGA-O1A	-4.60	112.12	123.63
12	B	820	CLA	O2A-CGA-CBA	4.60	125.86	111.83
12	B	807	CLA	O2A-CGA-O1A	-4.60	112.13	123.63
15	B	834	BCR	C15-C14-C13	-4.59	120.84	127.28
12	B	818	CLA	C3B-C2B-C1B	-4.59	101.75	107.17
12	B	826	CLA	C1D-ND-C4D	-4.59	103.09	106.31
12	A	845	CLA	C3B-C2B-C1B	-4.59	101.76	107.17
12	B	813	CLA	C1C-C2C-C3C	-4.59	102.15	106.98
12	A	844	CLA	C3B-C2B-C1B	-4.59	101.76	107.17
15	F	202	BCR	C33-C5-C6	-4.59	119.48	124.48
12	A	813	CLA	O2D-CGD-CBD	4.58	119.24	111.23
12	A	845	CLA	C2D-C1D-ND	4.58	114.66	110.13
12	A	824	CLA	C1-C2-C3	-4.58	118.69	126.20
12	A	820	CLA	C2C-C1C-NC	4.58	114.79	109.98
19	A	854	PL9	C22-C23-C24	-4.58	112.38	127.64
12	K	4004	CLA	CMB-C2B-C1B	4.58	132.39	125.42
12	L	201	CLA	C1D-ND-C4D	-4.57	103.10	106.31
15	A	836	BCR	C38-C26-C25	-4.57	119.50	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	824	CLA	C1-C2-C3	-4.57	118.71	126.20
12	J	103	CLA	O2A-CGA-O1A	-4.56	111.60	123.33
12	K	4004	CLA	C3B-C2B-C1B	-4.56	101.79	107.17
12	J	103	CLA	C1D-ND-C4D	-4.55	103.12	106.31
12	A	845	CLA	C1D-ND-C4D	-4.55	103.12	106.31
15	A	836	BCR	C16-C17-C18	-4.55	120.90	127.28
15	A	837	BCR	C4-C5-C6	-4.55	116.56	122.70
12	A	819	CLA	C1D-ND-C4D	-4.54	103.12	106.31
12	B	821	CLA	O2A-C1-C2	4.54	125.57	108.11
12	A	820	CLA	O2A-CGA-O1A	-4.54	112.28	123.63
12	K	4004	CLA	O2A-CGA-O1A	-4.54	112.28	123.63
13	A	802	CL0	C3B-C2B-C1B	-4.53	101.83	107.17
12	A	855	CLA	O2A-CGA-CBA	4.53	125.64	111.83
12	B	821	CLA	O2D-CGD-CBD	4.52	119.14	111.23
12	A	814	CLA	C3B-C2B-C1B	-4.52	101.84	107.17
12	A	846	CLA	O2A-CGA-O1A	-4.52	112.32	123.63
12	F	203	CLA	C1C-C2C-C3C	-4.52	102.23	106.98
12	A	820	CLA	O2A-C1-C2	4.51	125.48	108.11
12	A	823	CLA	C1D-ND-C4D	-4.50	103.16	106.31
12	B	810	CLA	O2A-CGA-O1A	-4.50	112.38	123.63
12	B	810	CLA	C1D-ND-C4D	-4.50	103.16	106.31
12	B	803	CLA	O2A-CGA-O1A	-4.50	112.38	123.63
12	B	809	CLA	O2A-CGA-O1A	-4.50	112.38	123.63
12	A	832	CLA	C1C-C2C-C3C	-4.49	102.25	106.98
15	B	834	BCR	C15-C16-C17	-4.49	114.33	123.52
12	B	803	CLA	C3B-C2B-C1B	-4.49	101.87	107.17
12	B	818	CLA	C1D-ND-C4D	-4.49	103.16	106.31
12	A	808	CLA	C1D-ND-C4D	-4.49	103.16	106.31
12	B	847	CLA	CMC-C2C-C1C	4.49	132.05	125.03
12	J	101	CLA	O2A-CGA-CBA	4.49	125.51	111.83
15	J	104	BCR	C23-C24-C25	-4.48	115.03	127.00
12	B	846	CLA	C2C-C1C-NC	4.48	114.69	109.98
12	B	820	CLA	C4A-NA-C1A	4.48	108.72	106.68
15	B	835	BCR	C8-C7-C6	-4.48	115.03	127.00
12	A	849	CLA	C4A-NA-C1A	4.47	108.72	106.68
12	F	204	CLA	O2A-CGA-O1A	-4.47	111.83	123.33
12	B	809	CLA	C4A-NA-C1A	4.47	108.72	106.68
12	B	806	CLA	C1D-ND-C4D	-4.47	103.18	106.31
15	A	836	BCR	C2-C1-C6	4.47	116.92	110.44
15	A	837	BCR	C38-C26-C25	-4.46	119.61	124.48
12	B	805	CLA	C1D-ND-C4D	-4.46	103.18	106.31
12	A	827	CLA	O2A-CGA-CBA	4.46	125.44	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	816	CLA	C1D-ND-C4D	-4.46	103.18	106.31
12	A	816	CLA	O2D-CGD-CBD	4.46	119.03	111.23
12	A	805	CLA	O2A-C1-C2	4.46	125.26	108.11
12	A	827	CLA	C3B-C2B-C1B	-4.45	101.92	107.17
15	F	201	BCR	C2-C1-C6	4.45	116.91	110.44
12	A	849	CLA	C3B-C2B-C1B	-4.45	101.92	107.17
12	A	819	CLA	C4A-NA-C1A	4.45	108.71	106.68
12	A	844	CLA	C1-C2-C3	-4.44	118.92	126.20
12	B	821	CLA	O2A-CGA-O1A	-4.44	112.52	123.63
12	A	822	CLA	O2A-CGA-O1A	-4.43	112.53	123.63
12	A	803	CLA	C1C-C2C-C3C	-4.43	102.32	106.98
12	B	806	CLA	O2A-CGA-O1A	-4.43	112.54	123.63
12	B	821	CLA	C4A-NA-C1A	4.43	108.70	106.68
12	B	820	CLA	C1D-ND-C4D	-4.42	103.21	106.31
12	A	810	CLA	C1D-ND-C4D	-4.42	103.21	106.31
12	B	826	CLA	O2A-CGA-CBA	4.42	125.31	111.83
12	B	808	CLA	O2A-CGA-O1A	-4.42	112.57	123.63
12	A	809	CLA	CHD-C1D-ND	-4.42	118.59	124.80
15	A	835	BCR	C38-C26-C25	-4.41	119.67	124.48
15	F	202	BCR	C20-C21-C22	-4.41	121.10	127.28
15	L	207	BCR	C15-C14-C13	-4.40	121.10	127.28
12	J	103	CLA	CMA-C3A-C2A	4.40	131.00	113.98
12	B	847	CLA	O2D-CGD-CBD	4.40	118.93	111.23
12	A	817	CLA	O2A-CGA-CBA	4.40	125.25	111.83
15	J	107	BCR	C11-C10-C9	-4.40	121.11	127.28
12	B	843	CLA	C1-C2-C3	-4.40	118.99	126.20
12	A	815	CLA	O2A-CGA-CBA	4.40	125.25	111.83
15	L	208	BCR	C29-C30-C25	4.40	116.83	110.44
25	L	202	EQ3	C16-C15-C14	4.40	132.52	123.52
12	B	850	CLA	CHD-C1D-ND	-4.39	118.62	124.80
12	A	815	CLA	C1D-ND-C4D	-4.39	103.23	106.31
12	A	813	CLA	C1D-ND-C4D	-4.39	103.23	106.31
12	J	101	CLA	C2B-C1B-NB	4.39	114.87	110.33
12	A	822	CLA	C1D-ND-C4D	-4.39	103.23	106.31
12	A	826	CLA	O2A-CGA-O1A	-4.38	112.66	123.63
12	B	819	CLA	O2A-CGA-O1A	-4.38	112.67	123.63
12	K	4004	CLA	CMA-C3A-C2A	4.37	130.88	113.98
12	B	819	CLA	C1C-C2C-C3C	-4.37	102.39	106.98
13	A	802	CL0	CMA-C3A-C2A	-4.37	97.10	113.98
15	B	841	BCR	C16-C17-C18	-4.36	121.16	127.28
12	B	821	CLA	C1D-ND-C4D	-4.36	103.25	106.31
12	A	843	CLA	O2D-CGD-CBD	4.36	118.85	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	814	CLA	C4A-NA-C1A	4.36	108.67	106.68
12	J	101	CLA	C4-C3-C5	4.35	122.78	115.23
20	A	856	45D	C03-C07-C19	4.35	127.45	115.65
15	J	105	BCR	C20-C21-C22	-4.35	121.18	127.28
12	A	832	CLA	C3B-C2B-C1B	-4.33	102.06	107.17
12	A	809	CLA	CMC-C2C-C1C	4.33	131.80	125.03
12	A	846	CLA	O2A-CGA-CBA	4.33	125.04	111.83
15	L	208	BCR	C30-C25-C26	-4.32	116.73	122.64
12	A	846	CLA	CMA-C3A-C2A	-4.32	97.28	113.98
12	B	801	CLA	O2D-CGD-CBD	4.31	118.77	111.23
15	B	835	BCR	C10-C11-C12	-4.31	110.71	123.20
12	A	843	CLA	C1C-C2C-C3C	-4.31	102.45	106.98
12	K	4004	CLA	O1D-CGD-CBD	-4.30	116.03	124.52
12	B	846	CLA	C1-C2-C3	-4.29	119.17	126.20
12	A	801	CLA	C2B-C1B-NB	4.29	114.78	110.33
12	B	813	CLA	C2B-C1B-NB	4.29	114.77	110.33
12	B	846	CLA	C3B-C2B-C1B	-4.28	102.12	107.17
12	B	847	CLA	C3B-C2B-C1B	-4.28	102.12	107.17
15	J	105	BCR	C34-C9-C8	4.28	124.63	118.09
15	I	101	BCR	C11-C10-C9	-4.28	121.28	127.28
12	B	821	CLA	O2A-CGA-CBA	4.27	124.86	111.83
12	A	801	CLA	C1C-C2C-C3C	-4.27	102.49	106.98
12	A	858	CLA	C1C-C2C-C3C	-4.26	102.50	106.98
12	A	829	CLA	O2D-CGD-CBD	4.25	118.66	111.23
12	B	844	CLA	O2D-CGD-O1D	-4.25	115.57	123.85
12	A	808	CLA	C1-C2-C3	-4.25	119.88	126.76
12	A	852	CLA	C1D-ND-C4D	-4.25	103.33	106.31
15	K	4005	BCR	C24-C23-C22	-4.25	119.95	126.23
12	B	828	CLA	C3B-C2B-C1B	-4.24	102.17	107.17
12	A	858	CLA	CMA-C3A-C4A	4.24	123.17	111.77
15	B	832	BCR	C30-C25-C26	-4.24	116.84	122.64
12	B	802	CLA	C3B-C2B-C1B	-4.24	102.17	107.17
12	B	844	CLA	C2B-C1B-NB	4.24	114.72	110.33
12	B	811	CLA	CMA-C3A-C2A	-4.23	97.61	113.98
12	F	204	CLA	CHD-C1D-ND	-4.23	118.85	124.80
12	J	103	CLA	CMA-C3A-C4A	4.22	123.13	111.77
12	F	203	CLA	C3B-C2B-C1B	-4.22	102.19	107.17
15	A	835	BCR	C7-C8-C9	-4.22	119.99	126.23
15	J	105	BCR	C2-C1-C6	4.22	116.56	110.44
12	A	849	CLA	O2A-CGA-O1A	-4.21	113.09	123.63
12	A	843	CLA	O2A-CGA-CBA	4.21	124.67	111.83
12	B	822	CLA	C1D-ND-C4D	-4.21	103.36	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	849	CLA	CHD-C1D-ND	-4.21	118.88	124.80
12	B	815	CLA	C1D-ND-C4D	-4.20	103.36	106.31
15	B	836	BCR	C30-C25-C26	-4.20	116.89	122.64
15	I	101	BCR	C30-C25-C26	-4.20	116.90	122.64
12	A	825	CLA	C1D-ND-C4D	-4.20	103.37	106.31
12	A	810	CLA	O2A-CGA-CBA	4.20	124.63	111.83
12	B	823	CLA	O2A-CGA-CBA	4.19	124.62	111.83
12	B	808	CLA	C1D-ND-C4D	-4.19	103.37	106.31
12	B	811	CLA	C3B-C2B-C1B	-4.19	102.23	107.17
12	A	831	CLA	C3B-C2B-C1B	-4.19	102.23	107.17
13	A	802	CL0	C1-O2A-CGA	4.19	126.79	116.65
12	A	821	CLA	O2A-CGA-O1A	-4.19	113.16	123.63
12	A	809	CLA	C4A-NA-C1A	4.18	108.59	106.68
12	A	855	CLA	C4A-NA-C1A	4.18	108.58	106.68
12	A	831	CLA	O2A-CGA-CBA	4.17	124.56	111.83
15	I	101	BCR	C16-C17-C18	-4.17	121.42	127.28
12	A	811	CLA	C4A-NA-C1A	4.17	108.58	106.68
12	A	833	CLA	O2A-CGA-CBA	4.17	124.54	111.83
12	B	850	CLA	CAA-C2A-C3A	-4.15	101.77	113.00
15	A	838	BCR	C24-C23-C22	-4.15	120.09	126.23
12	A	818	CLA	CMA-C3A-C2A	4.14	129.99	113.98
12	A	824	CLA	O2A-C1-C2	4.14	124.04	108.11
12	F	203	CLA	C4A-NA-C1A	4.14	108.57	106.68
12	A	852	CLA	C2A-C3A-C4A	-4.13	95.20	101.87
15	B	841	BCR	C24-C23-C22	-4.13	120.13	126.23
12	B	848	CLA	O2A-CGA-O1A	-4.12	113.31	123.63
12	B	852	CLA	CHD-C1D-ND	-4.12	119.00	124.80
12	L	201	CLA	C2B-C1B-NB	4.12	114.60	110.33
12	B	847	CLA	C2C-C1C-NC	4.12	114.31	109.98
12	A	816	CLA	C4A-NA-C1A	4.12	108.56	106.68
12	B	812	CLA	O2A-CGA-CBA	4.11	124.37	111.83
15	L	207	BCR	C38-C26-C25	-4.11	120.00	124.48
12	B	845	CLA	O2A-CGA-CBA	4.11	124.36	111.83
12	A	831	CLA	O2A-C1-C2	4.11	123.91	108.11
15	J	105	BCR	C8-C9-C10	-4.10	112.56	119.01
12	J	101	CLA	CHD-C1D-ND	-4.10	119.03	124.80
12	A	826	CLA	O2D-CGD-CBD	4.10	118.40	111.23
12	A	845	CLA	C4A-NA-C1A	4.10	108.55	106.68
16	M	103	LHG	C6-C5-C4	-4.10	102.23	111.78
12	B	847	CLA	O2A-CGA-O1A	-4.10	113.38	123.63
12	A	855	CLA	C1D-ND-C4D	-4.10	103.44	106.31
12	A	808	CLA	C4A-NA-C1A	4.09	108.54	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	847	CLA	O2A-CGA-O1A	-4.09	113.41	123.63
12	B	828	CLA	O2A-CGA-O1A	-4.08	113.42	123.63
12	A	846	CLA	CAA-CBA-CGA	-4.08	101.63	113.21
15	J	105	BCR	C8-C7-C6	-4.07	116.11	127.00
12	B	802	CLA	CHD-C1D-ND	-4.07	119.07	124.80
25	L	202	EQ3	C15-C16-C17	4.07	131.85	123.52
15	I	101	BCR	C33-C5-C6	-4.07	120.05	124.48
12	B	846	CLA	O2A-CGA-CBA	4.07	124.24	111.83
12	B	843	CLA	C1D-ND-C4D	-4.07	103.46	106.31
15	J	105	BCR	C15-C14-C13	-4.06	121.58	127.28
12	B	809	CLA	C1D-ND-C4D	-4.06	103.46	106.31
12	A	848	CLA	C4-C3-C5	4.06	122.27	115.23
12	A	814	CLA	O2A-CGA-CBA	4.05	124.19	111.83
12	B	824	CLA	CMA-C3A-C4A	4.05	122.65	111.77
12	B	853	CLA	C7-C6-C5	-4.05	102.48	113.26
20	A	856	45D	C42-C41-C37	4.05	131.80	123.52
12	B	822	CLA	O2A-CGA-CBA	4.03	124.13	111.83
12	B	828	CLA	C1-O2A-CGA	4.03	126.41	116.65
15	B	832	BCR	C7-C8-C9	-4.03	120.27	126.23
12	B	816	CLA	O2A-CGA-CBA	4.03	124.12	111.83
12	B	817	CLA	CBA-CAA-C2A	4.02	125.76	113.79
19	A	854	PL9	O1-C4-C3	-4.02	116.49	120.73
12	K	4002	CLA	O2A-CGA-O1A	-4.02	112.99	123.33
12	A	813	CLA	C4A-NA-C1A	4.02	108.51	106.68
12	B	849	CLA	C4-C3-C5	4.02	122.20	115.23
15	A	838	BCR	C7-C8-C9	-4.01	120.31	126.23
12	L	201	CLA	C1-C2-C3	-4.01	119.63	126.20
15	L	207	BCR	C20-C21-C22	-4.00	121.67	127.28
12	B	818	CLA	C1-C2-C3	-4.00	119.65	126.20
12	B	805	CLA	C3B-C2B-C1B	-4.00	102.46	107.17
12	B	830	CLA	C2B-C1B-NB	3.99	114.47	110.33
12	A	844	CLA	O2D-CGD-O1D	-3.99	116.08	123.85
26	L	209	DGD	O2G-C1B-C2B	3.99	120.10	111.48
12	K	4002	CLA	CMA-C3A-C2A	3.98	129.37	113.98
12	A	807	CLA	O2A-CGA-CBA	3.98	123.97	111.83
12	A	809	CLA	O2A-C1-C2	3.98	123.41	108.11
12	B	814	CLA	O2A-CGA-CBA	3.98	123.96	111.83
15	B	836	BCR	C15-C16-C17	-3.98	115.38	123.52
12	K	4004	CLA	C3D-C4D-ND	3.97	116.45	109.99
15	K	4001	BCR	C15-C16-C17	-3.97	115.39	123.52
15	B	832	BCR	C27-C26-C25	-3.97	117.34	122.70
12	B	801	CLA	O2A-C1-C2	3.97	123.39	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	841	BCR	C11-C10-C9	-3.97	121.71	127.28
15	K	4005	BCR	C29-C30-C25	3.96	116.19	110.44
12	B	843	CLA	O2A-CGA-CBA	3.96	123.91	111.83
12	A	804	CLA	O2A-CGA-O1A	-3.96	113.72	123.63
12	A	823	CLA	C3B-C2B-C1B	-3.95	102.51	107.17
15	A	837	BCR	C23-C24-C25	-3.95	116.44	127.00
12	B	853	CLA	O2A-CGA-CBA	3.95	123.89	111.83
12	A	829	CLA	C4-C3-C5	3.95	122.08	115.23
15	F	201	BCR	C30-C25-C26	-3.94	117.25	122.64
12	A	844	CLA	C6-C7-C8	-3.94	102.88	115.97
12	A	823	CLA	O2A-CGA-CBA	3.94	123.84	111.83
12	A	807	CLA	C2B-C1B-NB	3.94	114.41	110.33
12	A	825	CLA	O2A-CGA-O1A	-3.93	113.79	123.63
12	A	807	CLA	O2A-C1-C2	3.93	123.22	108.11
12	A	852	CLA	CHD-C1D-ND	-3.92	119.28	124.80
12	A	847	CLA	O2D-CGD-CBD	3.92	118.08	111.23
12	A	846	CLA	O2D-CGD-CBD	3.92	118.08	111.23
15	L	207	BCR	C24-C25-C26	-3.92	112.53	121.56
15	K	4001	BCR	C16-C17-C18	-3.92	121.79	127.28
12	B	850	CLA	C3D-C2D-C1D	-3.91	100.49	105.83
27	M	102	SQD	O9-S-O7	-3.91	101.10	113.82
15	I	101	BCR	C20-C21-C22	-3.91	121.80	127.28
15	F	202	BCR	C16-C17-C18	-3.90	121.80	127.28
12	B	801	CLA	C4A-NA-C1A	3.90	108.46	106.68
12	A	844	CLA	O2A-CGA-O1A	-3.90	113.88	123.63
12	B	843	CLA	C4A-NA-C1A	3.90	108.46	106.68
12	A	855	CLA	O2A-CGA-O1A	-3.90	113.88	123.63
15	A	836	BCR	C15-C14-C13	-3.90	121.81	127.28
17	A	851	LMG	O8-C28-C29	3.89	123.71	111.83
12	A	816	CLA	O2A-CGA-O1A	-3.89	113.90	123.63
12	A	824	CLA	O2A-CGA-CBA	3.89	123.69	111.83
15	B	841	BCR	C4-C5-C6	-3.89	117.45	122.70
12	A	809	CLA	CMA-C3A-C4A	3.89	122.22	111.77
15	B	841	BCR	C8-C7-C6	-3.88	116.63	127.00
13	A	802	CL0	O2A-CGA-O1A	-3.88	113.92	123.63
12	A	814	CLA	C4A-NA-C1A	3.88	108.45	106.68
12	B	801	CLA	C2A-C3A-C4A	-3.88	95.60	101.87
12	B	852	CLA	O2A-CGA-CBA	3.88	123.65	111.83
12	A	805	CLA	CHD-C1D-ND	-3.88	119.35	124.80
12	A	829	CLA	O2A-CGA-CBA	3.88	123.65	111.83
15	A	838	BCR	C15-C14-C13	-3.87	121.84	127.28
17	A	851	LMG	C4-C3-C2	3.87	117.63	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	J	105	BCR	C30-C25-C26	-3.87	117.35	122.64
12	B	804	CLA	CHD-C1D-ND	-3.86	119.37	124.80
12	B	824	CLA	C4-C3-C5	3.86	121.93	115.23
12	B	830	CLA	C4A-NA-C1A	3.86	108.44	106.68
12	J	103	CLA	OBD-CAD-C3D	-3.86	119.39	128.42
15	A	837	BCR	C11-C10-C9	-3.86	121.87	127.28
12	A	819	CLA	C1-C2-C3	-3.86	119.88	126.20
12	A	846	CLA	C1C-C2C-C3C	-3.86	102.92	106.98
12	B	822	CLA	C3B-C2B-C1B	-3.86	102.62	107.17
12	A	832	CLA	CHD-C1D-ND	-3.86	119.38	124.80
12	A	833	CLA	C1-C2-C3	-3.85	120.54	126.76
12	A	832	CLA	O2A-CGA-CBA	3.85	123.56	111.83
12	F	204	CLA	C4A-NA-C1A	3.84	108.43	106.68
12	B	852	CLA	C1-C2-C3	-3.84	120.54	126.76
12	A	852	CLA	C1-C2-C3	-3.84	119.91	126.20
12	A	819	CLA	C2B-C1B-NB	3.84	114.31	110.33
12	A	848	CLA	CHD-C1D-ND	-3.82	119.42	124.80
15	K	4001	BCR	C7-C8-C9	-3.82	120.58	126.23
12	A	812	CLA	C3B-C2B-C1B	-3.82	102.67	107.17
12	A	821	CLA	O2A-C1-C2	3.82	122.79	108.11
12	A	820	CLA	O2A-CGA-CBA	3.81	123.47	111.83
15	J	105	BCR	C28-C27-C26	-3.81	107.26	114.06
15	B	834	BCR	C20-C21-C22	-3.81	121.94	127.28
15	B	835	BCR	C20-C21-C22	-3.80	121.94	127.28
12	A	825	CLA	CHD-C1D-ND	-3.80	119.45	124.80
12	A	801	CLA	CHD-C1D-ND	-3.80	119.45	124.80
15	I	101	BCR	C15-C14-C13	-3.80	121.95	127.28
15	A	835	BCR	C30-C25-C26	-3.80	117.45	122.64
17	A	840	LMG	O1-C7-C8	3.80	120.05	110.82
15	J	105	BCR	C11-C10-C9	-3.80	121.95	127.28
12	B	813	CLA	CHD-C1D-ND	-3.79	119.46	124.80
12	A	804	CLA	C2B-C1B-NB	3.79	114.26	110.33
12	B	852	CLA	CAC-C3C-C4C	3.79	129.73	124.79
12	A	829	CLA	CHD-C1D-ND	-3.79	119.47	124.80
12	A	826	CLA	CHD-C1D-ND	-3.79	119.47	124.80
12	A	831	CLA	CMC-C2C-C1C	3.79	130.95	125.03
12	B	844	CLA	CMC-C2C-C1C	3.78	130.94	125.03
12	A	804	CLA	C1-C2-C3	-3.78	120.00	126.20
12	A	808	CLA	O2A-CGA-CBA	3.78	123.35	111.83
12	B	815	CLA	C2B-C1B-NB	3.78	114.24	110.33
15	J	105	BCR	C29-C30-C25	3.77	115.92	110.44
12	A	844	CLA	CHD-C1D-ND	-3.77	119.49	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	J	105	BCR	C21-C20-C19	-3.77	112.28	123.20
12	B	853	CLA	O2D-CGD-O1D	-3.76	116.52	123.85
12	A	848	CLA	C2B-C1B-NB	3.76	114.22	110.33
12	B	806	CLA	O2A-C1-C2	3.76	122.56	108.11
12	K	4004	CLA	CMD-C2D-C3D	-3.75	119.08	127.69
12	A	821	CLA	O2A-CGA-CBA	3.75	123.27	111.83
12	A	830	CLA	O2D-CGD-CBD	3.75	117.78	111.23
12	B	830	CLA	CHD-C1D-ND	-3.74	119.54	124.80
12	A	820	CLA	C1C-C2C-C3C	-3.74	103.05	106.98
12	A	817	CLA	CHD-C1D-ND	-3.73	119.55	124.80
12	L	205	CLA	O2A-CGA-CBA	3.73	123.22	111.83
12	B	844	CLA	C4-C3-C5	3.73	121.70	115.23
12	B	812	CLA	O2A-C1-C2	3.73	122.46	108.11
12	B	828	CLA	C2B-C1B-NB	3.72	114.19	110.33
12	B	818	CLA	O2A-C1-C2	3.72	122.44	108.11
12	A	858	CLA	C16-C15-C13	-3.72	103.59	115.97
12	A	816	CLA	O2A-C1-C2	3.72	122.43	108.11
15	A	837	BCR	C8-C7-C6	-3.72	117.06	127.00
12	B	829	CLA	O2A-CGA-O1A	-3.72	114.33	123.63
12	B	822	CLA	C4-C3-C5	3.72	121.68	115.23
12	A	816	CLA	C2B-C1B-NB	3.72	114.18	110.33
12	A	822	CLA	C1-O2A-CGA	3.71	125.64	116.65
12	A	809	CLA	CMA-C3A-C2A	-3.71	99.64	113.98
12	B	807	CLA	C2B-C1B-NB	3.71	114.17	110.33
12	B	814	CLA	C2B-C1B-NB	3.71	114.17	110.33
12	B	802	CLA	C2B-C1B-NB	3.70	114.17	110.33
12	A	829	CLA	C1-O2A-CGA	3.70	125.61	116.65
12	B	847	CLA	C3D-C4D-ND	3.70	116.00	109.99
12	B	812	CLA	C3B-C2B-C1B	-3.70	102.81	107.17
12	B	828	CLA	CHD-C1D-ND	-3.70	119.60	124.80
27	M	102	SQD	O6-C1-C2	3.69	113.88	108.27
12	F	203	CLA	CED-O2D-CGD	3.69	124.30	115.92
19	A	854	PL9	C7-C3-C2	-3.69	119.04	123.39
12	B	825	CLA	O2A-CGA-CBA	3.69	123.08	111.83
12	B	850	CLA	C2B-C1B-NB	3.68	114.15	110.33
12	B	801	CLA	O2A-CGA-CBA	3.68	123.06	111.83
12	B	842	CLA	O2A-C1-C2	3.68	122.28	108.11
12	B	813	CLA	C1D-ND-C4D	-3.68	103.73	106.31
12	J	102	CLA	C2B-C1B-NB	3.67	114.13	110.33
12	A	829	CLA	CAA-CBA-CGA	-3.67	102.79	113.21
12	K	4004	CLA	O2A-CGA-CBA	3.67	123.02	111.83
12	L	205	CLA	C2B-C1B-NB	3.67	114.13	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	849	CLA	C4-C3-C5	3.66	121.59	115.23
12	A	829	CLA	C2B-C1B-NB	3.66	114.12	110.33
12	A	848	CLA	O2A-CGA-CBA	3.65	122.98	111.83
19	A	854	PL9	C15-C14-C16	3.65	121.57	115.23
17	B	837	LMG	O7-C10-C11	3.65	119.38	111.48
12	A	825	CLA	C2B-C1B-NB	3.65	114.11	110.33
12	L	201	CLA	CHD-C1D-ND	-3.65	119.67	124.80
12	B	826	CLA	CMA-C3A-C2A	-3.64	99.91	113.98
12	B	823	CLA	C2B-C1B-NB	3.64	114.10	110.33
12	B	843	CLA	O2A-C1-C2	3.63	122.09	108.11
12	L	205	CLA	C1-C2-C3	-3.63	120.24	126.20
12	B	825	CLA	C4-C3-C5	3.63	121.53	115.23
20	A	856	45D	C27-C25-C23	3.63	123.63	118.09
12	B	802	CLA	CMA-C3A-C2A	-3.63	99.95	113.98
15	B	841	BCR	C27-C26-C25	-3.63	117.80	122.70
12	B	848	CLA	C1-C2-C3	-3.63	120.26	126.20
12	A	845	CLA	O2A-CGA-CBA	3.62	122.89	111.83
16	M	103	LHG	O7-C7-C8	3.62	119.31	111.48
22	B	831	A1AGD	C13-C12-C11	-3.62	103.61	113.26
15	A	838	BCR	C20-C21-C22	-3.62	122.20	127.28
12	L	201	CLA	O2D-CGD-O1D	-3.62	116.81	123.85
12	B	823	CLA	CHD-C1D-ND	-3.62	119.71	124.80
15	K	4005	BCR	C27-C26-C25	-3.61	117.82	122.70
12	A	813	CLA	O2A-CGA-CBA	3.61	122.85	111.83
12	A	845	CLA	C1-C2-C3	-3.61	120.28	126.20
15	F	201	BCR	C8-C7-C6	-3.61	117.35	127.00
17	A	851	LMG	O6-C1-C2	-3.61	102.95	110.37
12	B	803	CLA	O2A-CGA-CBA	3.61	122.85	111.83
12	A	855	CLA	C1-C2-C3	-3.61	120.29	126.20
15	J	107	BCR	C38-C26-C25	-3.61	120.55	124.48
12	A	819	CLA	O2A-CGA-CBA	3.61	122.83	111.83
12	F	204	CLA	CHD-C4C-C3C	-3.60	119.52	124.77
12	A	830	CLA	O2A-CGA-CBA	3.60	122.82	111.83
12	A	830	CLA	CMA-C3A-C2A	-3.60	100.06	113.98
12	L	205	CLA	O2A-C1-C2	3.60	121.97	108.11
12	B	852	CLA	O2A-C1-C2	3.60	121.95	108.11
12	A	814	CLA	CHD-C1D-ND	-3.59	119.75	124.80
12	A	818	CLA	C1-C2-C3	-3.59	120.32	126.20
12	A	830	CLA	C2B-C1B-NB	3.58	114.04	110.33
12	A	807	CLA	CHD-C1D-ND	-3.58	119.76	124.80
12	B	845	CLA	CHD-C1D-ND	-3.58	119.76	124.80
15	K	4005	BCR	C11-C10-C9	-3.57	122.27	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	850	CLA	O2A-CGA-O1A	-3.57	114.69	123.63
12	A	847	CLA	C1-C2-C3	-3.57	120.34	126.20
15	K	4001	BCR	C27-C26-C25	-3.57	117.88	122.70
12	A	843	CLA	C2B-C1B-NB	3.57	114.03	110.33
12	B	842	CLA	C1-C2-C3	-3.56	120.36	126.20
12	A	805	CLA	C1-O2A-CGA	3.56	125.28	116.65
12	B	847	CLA	O2A-CGA-CBA	3.56	122.70	111.83
15	F	201	BCR	C12-C13-C14	-3.56	113.41	119.01
12	A	818	CLA	O2D-CGD-O1D	-3.56	116.92	123.85
12	A	846	CLA	C4-C3-C5	3.56	121.41	115.23
12	B	826	CLA	O2A-C1-C2	3.56	121.81	108.11
12	B	813	CLA	O2A-CGA-CBA	3.56	122.69	111.83
12	B	850	CLA	C4D-C3D-CAD	3.56	111.97	108.11
15	J	104	BCR	C38-C26-C25	-3.56	120.60	124.48
12	B	845	CLA	C1-C2-C3	-3.56	120.37	126.20
25	L	202	EQ3	C34-C9-C8	3.56	123.52	118.09
12	A	806	CLA	O2A-CGA-CBA	3.56	125.23	114.00
12	B	805	CLA	CHD-C1D-ND	-3.55	119.80	124.80
15	B	834	BCR	C23-C24-C25	-3.55	117.50	127.00
12	A	818	CLA	O2A-CGA-CBA	3.55	122.67	111.83
12	A	813	CLA	C1-C2-C3	-3.55	120.38	126.20
12	L	201	CLA	O2A-C1-C2	3.55	121.78	108.11
12	J	102	CLA	CHD-C1D-ND	-3.55	119.81	124.80
12	A	833	CLA	C2B-C1B-NB	3.55	114.00	110.33
12	A	810	CLA	O2A-C1-C2	3.55	121.75	108.11
12	A	831	CLA	C1-C2-C3	-3.54	120.39	126.20
15	A	836	BCR	C33-C5-C6	-3.54	120.62	124.48
12	A	803	CLA	C1-O2A-CGA	3.54	125.22	116.65
12	B	826	CLA	CHD-C1D-ND	-3.54	119.82	124.80
12	B	806	CLA	C4-C3-C5	3.54	121.37	115.23
15	A	837	BCR	C15-C16-C17	-3.54	116.28	123.52
15	J	104	BCR	C30-C25-C26	-3.54	117.80	122.64
12	A	827	CLA	O2A-C1-C2	3.54	121.71	108.11
12	B	801	CLA	CHD-C1D-ND	-3.53	119.83	124.80
15	A	835	BCR	C21-C20-C19	-3.53	112.96	123.20
12	A	830	CLA	CHD-C1D-ND	-3.53	119.83	124.80
25	L	202	EQ3	C34-C9-C10	-3.53	117.10	122.82
12	B	826	CLA	C2B-C1B-NB	3.53	113.99	110.33
12	A	804	CLA	CHD-C1D-ND	-3.52	119.84	124.80
12	A	819	CLA	O2A-C1-C2	3.52	121.67	108.11
12	A	829	CLA	CMA-C3A-C2A	-3.52	100.36	113.98
12	B	817	CLA	C4-C3-C5	3.52	121.34	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	803	CLA	C4D-C3D-CAD	3.52	111.93	108.11
15	K	4001	BCR	C30-C25-C26	-3.52	117.83	122.64
12	A	833	CLA	O2A-C1-C2	3.52	121.64	108.11
12	A	817	CLA	C1-C2-C3	-3.51	121.08	126.76
15	L	207	BCR	C24-C23-C22	-3.51	121.04	126.23
12	B	848	CLA	C4-C3-C5	3.51	121.32	115.23
15	A	836	BCR	C11-C10-C9	-3.51	122.36	127.28
12	B	820	CLA	CHD-C1D-ND	-3.51	119.86	124.80
12	B	842	CLA	O2A-CGA-CBA	3.51	122.53	111.83
12	B	809	CLA	O2A-CGA-CBA	3.51	122.52	111.83
12	A	803	CLA	C2B-C1B-NB	3.50	113.96	110.33
15	F	201	BCR	C29-C30-C25	3.50	115.53	110.44
12	A	816	CLA	C1-O2A-CGA	3.50	125.13	116.65
15	B	834	BCR	C21-C20-C19	-3.50	113.05	123.20
12	B	825	CLA	CHD-C1D-ND	-3.50	119.88	124.80
12	A	804	CLA	O2A-CGA-CBA	3.50	122.49	111.83
12	B	843	CLA	CHD-C1D-ND	-3.49	119.88	124.80
12	B	804	CLA	O2A-C1-C2	3.49	121.55	108.11
12	J	102	CLA	C4A-NA-C1A	3.49	108.27	106.68
12	B	806	CLA	CHD-C1D-ND	-3.49	119.89	124.80
12	A	806	CLA	CHD-C1D-ND	-3.49	119.89	124.80
12	A	811	CLA	C2B-C1B-NB	3.49	113.94	110.33
12	J	103	CLA	C4D-C3D-CAD	3.48	111.89	108.11
12	A	843	CLA	CHD-C1D-ND	-3.48	119.91	124.80
12	K	4004	CLA	C1-C2-C3	-3.48	120.50	126.20
12	A	821	CLA	CHD-C1D-ND	-3.47	119.91	124.80
15	F	201	BCR	C16-C15-C14	-3.47	116.41	123.52
12	B	801	CLA	C2B-C1B-NB	3.47	113.93	110.33
12	B	846	CLA	CAA-CBA-CGA	-3.47	103.35	113.21
12	B	827	CLA	CHD-C1D-ND	-3.47	119.92	124.80
12	B	802	CLA	O2A-CGA-CBA	3.47	122.42	111.83
12	A	808	CLA	O2A-C1-C2	3.47	121.47	108.11
12	B	849	CLA	C2B-C1B-NB	3.47	113.92	110.33
12	A	831	CLA	CHD-C1D-ND	-3.47	119.92	124.80
18	B	840	LMT	O5'-C5'-C4'	3.47	116.89	109.72
12	A	810	CLA	CHD-C1D-ND	-3.47	119.92	124.80
12	L	205	CLA	CHD-C1D-ND	-3.47	119.92	124.80
12	B	807	CLA	C1-O2A-CGA	3.46	125.04	116.65
12	B	819	CLA	O2A-CGA-CBA	3.46	122.39	111.83
12	A	823	CLA	CMA-C3A-C2A	-3.46	100.60	113.98
12	A	830	CLA	C4A-NA-C1A	3.46	108.26	106.68
12	B	845	CLA	C2B-C1B-NB	3.46	113.91	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	834	BCR	C2-C1-C6	3.45	115.45	110.44
12	B	803	CLA	O2D-CGD-O1D	-3.45	117.13	123.85
12	A	805	CLA	C2B-C1B-NB	3.45	113.90	110.33
12	J	103	CLA	CHD-C4C-NC	-3.44	118.90	124.23
27	M	102	SQD	O47-C7-C8	3.44	118.93	111.48
12	A	823	CLA	C1-C2-C3	-3.43	120.57	126.20
12	A	803	CLA	CHD-C1D-ND	-3.43	119.97	124.80
12	B	821	CLA	C2B-C1B-NB	3.43	113.88	110.33
12	L	204	CLA	O2A-CGA-CBA	3.43	122.30	111.83
15	B	835	BCR	C7-C8-C9	-3.43	121.16	126.23
12	A	825	CLA	C1-O2A-CGA	3.43	124.94	116.65
12	B	806	CLA	C2B-C1B-NB	3.43	113.88	110.33
12	B	823	CLA	O2A-C1-C2	3.42	121.29	108.11
15	F	202	BCR	C7-C8-C9	-3.42	121.17	126.23
12	A	820	CLA	C1-O2A-CGA	3.42	124.93	116.65
12	A	811	CLA	CHD-C1D-ND	-3.42	119.99	124.80
27	M	102	SQD	O7-S-C6	3.42	111.86	106.76
12	B	824	CLA	CMC-C2C-C1C	3.41	130.37	125.03
12	J	103	CLA	C2B-C1B-NB	3.41	113.87	110.33
12	A	819	CLA	O2D-CGD-O1D	-3.41	117.20	123.85
15	A	835	BCR	C23-C24-C25	-3.41	117.88	127.00
12	A	846	CLA	C1-C2-C3	-3.41	120.61	126.20
12	B	814	CLA	CHD-C1D-ND	-3.41	120.00	124.80
15	L	208	BCR	C4-C5-C6	-3.41	118.10	122.70
12	A	825	CLA	C4-C3-C5	3.41	121.14	115.23
12	A	821	CLA	C1-C2-C3	-3.40	120.62	126.20
12	B	849	CLA	C3D-C4D-ND	3.40	115.52	109.99
12	L	206	CLA	O2D-CGD-O1D	-3.40	117.23	123.85
12	J	103	CLA	C1D-CHD-C4C	-3.40	118.79	126.02
12	B	826	CLA	C1-C2-C3	-3.40	120.63	126.20
15	L	207	BCR	C29-C30-C25	3.40	115.38	110.44
12	B	849	CLA	O2A-CGA-CBA	3.40	122.20	111.83
12	A	829	CLA	O2A-CGA-O1A	-3.40	115.13	123.63
12	A	855	CLA	O2D-CGD-O1D	-3.40	117.23	123.85
18	B	840	LMT	O1'-C1'-C2'	3.40	113.43	108.27
12	B	807	CLA	CHD-C1D-ND	-3.40	120.02	124.80
12	A	847	CLA	CHD-C1D-ND	-3.39	120.03	124.80
12	B	809	CLA	O2A-C1-C2	3.39	121.16	108.11
12	B	842	CLA	CHD-C1D-ND	-3.39	120.03	124.80
12	L	206	CLA	O2A-C1-C2	3.39	121.14	108.11
12	A	823	CLA	O2A-C1-C2	3.38	121.13	108.11
12	A	858	CLA	C2B-C1B-NB	3.38	113.83	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	846	CLA	O2D-CGD-O1D	-3.38	117.27	123.85
12	A	826	CLA	C2B-C1B-NB	3.38	113.83	110.33
25	L	202	EQ3	C37-C22-C21	-3.38	117.34	122.82
12	A	817	CLA	O2A-C1-C2	3.38	121.10	108.11
12	A	801	CLA	O2A-CGA-CBA	3.38	122.13	111.83
12	A	824	CLA	C4-C3-C5	3.37	121.08	115.23
12	A	816	CLA	CHD-C1D-ND	-3.37	120.06	124.80
12	B	852	CLA	CMC-C2C-C1C	3.37	130.30	125.03
12	B	804	CLA	O2A-CGA-CBA	3.37	122.11	111.83
12	A	810	CLA	C2B-C1B-NB	3.37	113.82	110.33
12	A	817	CLA	C2B-C1B-NB	3.36	113.81	110.33
25	L	202	EQ3	C24-C23-C22	3.36	131.21	126.23
15	A	837	BCR	C7-C8-C9	-3.36	121.26	126.23
12	B	809	CLA	C1-C2-C3	-3.36	120.69	126.20
20	A	856	45D	C28-C26-C30	-3.36	117.37	122.82
15	F	202	BCR	C2-C1-C6	3.36	115.32	110.44
12	B	804	CLA	C1-C2-C3	-3.36	120.70	126.20
12	B	848	CLA	C3D-C4D-ND	3.36	115.44	109.99
12	A	828	CLA	C2B-C1B-NB	3.35	113.81	110.33
12	B	819	CLA	O2A-C1-C2	3.35	121.01	108.11
12	A	819	CLA	CHD-C1D-ND	-3.35	120.08	124.80
12	B	810	CLA	C1-O2A-CGA	3.35	124.76	116.65
12	F	203	CLA	C2B-C1B-NB	3.35	113.80	110.33
12	B	830	CLA	O2A-CGA-CBA	3.35	124.58	114.00
12	A	845	CLA	CMA-C3A-C4A	-3.34	102.78	111.77
12	A	811	CLA	O2A-CGA-CBA	3.34	124.57	114.00
12	A	821	CLA	C2B-C1B-NB	3.34	113.79	110.33
12	B	814	CLA	O2A-C1-C2	3.34	120.97	108.11
12	B	818	CLA	O2D-CGD-O1D	-3.34	117.34	123.85
12	B	817	CLA	CMA-C3A-C4A	3.34	120.75	111.77
12	B	816	CLA	CHD-C1D-ND	-3.34	120.10	124.80
12	B	823	CLA	C4A-NA-C1A	3.34	108.20	106.68
12	A	858	CLA	CHD-C1D-ND	-3.34	120.11	124.80
12	B	808	CLA	C2B-C1B-NB	3.33	113.78	110.33
12	L	206	CLA	C4-C3-C5	3.33	121.02	115.23
12	B	847	CLA	C1-O2A-CGA	3.33	124.72	116.65
12	L	206	CLA	C2B-C1B-NB	3.33	113.78	110.33
12	B	812	CLA	CHD-C1D-ND	-3.33	120.11	124.80
12	B	808	CLA	CHD-C1D-ND	-3.33	120.11	124.80
12	B	806	CLA	O2A-CGA-CBA	3.33	121.99	111.83
12	F	203	CLA	CMC-C2C-C1C	3.33	130.24	125.03
12	L	201	CLA	O2A-CGA-CBA	3.33	121.99	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	801	CLA	C4-C3-C5	3.33	121.00	115.23
15	A	836	BCR	C8-C7-C6	-3.32	118.12	127.00
15	A	835	BCR	C8-C7-C6	-3.32	118.12	127.00
16	A	850	LHG	C6-C5-C4	-3.32	104.04	111.78
12	A	816	CLA	C1-C2-C3	-3.32	120.75	126.20
12	B	809	CLA	C2B-C1B-NB	3.32	113.77	110.33
12	A	809	CLA	C3C-C4C-NC	3.32	114.68	110.43
12	B	813	CLA	C4-C3-C5	3.31	120.98	115.23
12	B	818	CLA	CHD-C1D-ND	-3.31	120.14	124.80
12	A	822	CLA	C2B-C1B-NB	3.31	113.76	110.33
12	F	203	CLA	O2A-CGA-CBA	3.31	124.47	114.00
12	B	853	CLA	CMB-C2B-C1B	3.31	130.46	125.42
15	I	101	BCR	C8-C7-C6	-3.31	118.15	127.00
15	F	201	BCR	C35-C13-C12	3.31	123.15	118.09
12	B	806	CLA	C1-C2-C3	-3.31	120.78	126.20
12	B	846	CLA	O1D-CGD-CBD	-3.31	118.00	124.52
15	B	834	BCR	C4-C5-C6	-3.30	118.24	122.70
12	A	823	CLA	CHD-C1D-ND	-3.30	120.15	124.80
12	B	829	CLA	CHD-C1D-ND	-3.30	120.15	124.80
15	B	835	BCR	C21-C20-C19	-3.30	113.63	123.20
12	A	818	CLA	O2A-C1-C2	3.30	120.81	108.11
12	B	812	CLA	CMC-C2C-C1C	3.30	130.19	125.03
12	B	849	CLA	CMC-C2C-C1C	3.30	130.19	125.03
15	J	105	BCR	C40-C30-C25	-3.30	105.07	110.24
12	A	813	CLA	CHD-C1D-ND	-3.29	120.17	124.80
15	K	4005	BCR	C8-C7-C6	-3.29	118.20	127.00
12	B	827	CLA	C2B-C1B-NB	3.29	113.74	110.33
12	B	846	CLA	CMC-C2C-C1C	3.29	130.18	125.03
12	L	204	CLA	O2A-C1-C2	3.29	120.77	108.11
12	B	829	CLA	CMA-C3A-C2A	-3.29	101.26	113.98
12	A	821	CLA	C4-C3-C5	3.29	120.93	115.23
20	A	856	45D	C27-C25-C29	-3.28	117.50	122.82
12	A	828	CLA	CHD-C1D-ND	-3.28	120.18	124.80
15	A	836	BCR	C27-C26-C25	-3.28	118.27	122.70
12	K	4004	CLA	O2A-C1-C2	3.28	120.73	108.11
15	K	4001	BCR	C1-C6-C5	-3.28	118.16	122.64
12	A	847	CLA	C1-O2A-CGA	3.28	124.59	116.65
15	B	836	BCR	C24-C23-C22	-3.28	121.39	126.23
12	A	852	CLA	O2A-C1-C2	3.27	120.71	108.11
12	B	852	CLA	CED-O2D-CGD	3.27	123.34	115.92
12	A	824	CLA	C2B-C1B-NB	3.27	113.72	110.33
12	K	4002	CLA	CAC-C3C-C4C	3.27	129.04	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	838	BCR	C8-C7-C6	-3.27	118.28	127.00
22	B	831	A1AGD	O1-C4-C3	-3.26	117.29	120.73
12	A	844	CLA	C6-C5-C3	-3.26	105.53	113.47
12	A	827	CLA	CHD-C1D-ND	-3.26	120.22	124.80
16	A	850	LHG	O8-C23-C24	3.26	121.77	111.83
12	A	849	CLA	CHD-C1D-ND	-3.26	120.22	124.80
12	B	822	CLA	CHD-C1D-ND	-3.26	120.22	124.80
15	A	837	BCR	C23-C22-C21	-3.25	113.89	119.01
15	B	832	BCR	C2-C1-C6	3.25	115.16	110.44
12	B	846	CLA	O2A-C1-C2	3.25	120.61	108.11
12	B	827	CLA	O2A-CGA-CBA	3.25	124.26	114.00
12	B	817	CLA	CHD-C1D-ND	-3.25	120.23	124.80
15	A	838	BCR	C4-C5-C6	-3.25	118.32	122.70
12	A	826	CLA	C1-C2-C3	-3.25	120.88	126.20
15	L	207	BCR	C21-C20-C19	-3.25	113.80	123.20
12	A	829	CLA	O2A-C1-C2	3.25	120.60	108.11
15	B	834	BCR	C8-C7-C6	-3.24	118.33	127.00
12	A	814	CLA	C2B-C1B-NB	3.24	113.69	110.33
12	A	845	CLA	O2A-C1-C2	3.24	120.59	108.11
12	A	812	CLA	CHD-C1D-ND	-3.24	120.24	124.80
12	A	844	CLA	CMA-C3A-C2A	-3.24	101.45	113.98
12	B	807	CLA	CMC-C2C-C1C	3.24	130.09	125.03
15	A	837	BCR	C2-C3-C4	3.24	118.39	111.28
12	B	824	CLA	CED-O2D-CGD	3.23	123.25	115.92
12	B	847	CLA	C2A-C3A-C4A	-3.23	96.65	101.87
12	B	850	CLA	O2D-CGD-CBD	3.23	116.88	111.23
15	B	836	BCR	C29-C30-C25	3.23	115.13	110.44
12	B	811	CLA	O2A-CGA-CBA	3.23	121.69	111.83
12	A	821	CLA	CMA-C3A-C2A	-3.23	101.50	113.98
12	L	206	CLA	CHD-C1D-ND	-3.23	120.26	124.80
15	B	832	BCR	C21-C20-C19	-3.23	113.85	123.20
12	A	847	CLA	C2B-C1B-NB	3.23	113.67	110.33
12	A	818	CLA	C3C-C4C-NC	3.23	114.56	110.43
12	A	808	CLA	CHD-C1D-ND	-3.22	120.27	124.80
12	A	845	CLA	CMC-C2C-C1C	3.22	130.07	125.03
12	B	829	CLA	C4-C3-C5	3.22	120.82	115.23
12	B	815	CLA	O2A-CGA-CBA	3.22	124.17	114.00
18	J	106	LMT	C6'-C5'-C4'	-3.22	104.33	113.38
12	F	204	CLA	CAC-C3C-C4C	3.22	128.97	124.79
12	L	204	CLA	CHD-C1D-ND	-3.22	120.28	124.80
15	J	107	BCR	C29-C30-C25	3.21	115.11	110.44
12	B	804	CLA	C4D-C3D-CAD	3.21	111.59	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	850	LHG	C5-O7-C7	-3.21	110.11	117.80
12	B	818	CLA	C2B-C1B-NB	3.21	113.66	110.33
12	B	850	CLA	CED-O2D-CGD	3.21	123.19	115.92
12	B	824	CLA	CMB-C2B-C1B	3.21	130.30	125.42
12	B	844	CLA	C1-O2A-CGA	3.20	124.41	116.65
12	A	831	CLA	CMB-C2B-C1B	3.20	130.30	125.42
12	A	821	CLA	C1-O2A-CGA	3.20	124.40	116.65
12	B	824	CLA	CHD-C1D-ND	-3.20	120.30	124.80
12	A	812	CLA	O2A-CGA-CBA	3.20	124.12	114.00
15	J	107	BCR	C7-C8-C9	-3.20	121.50	126.23
12	B	817	CLA	C2B-C1B-NB	3.20	113.64	110.33
12	B	850	CLA	C4-C3-C5	3.20	120.78	115.23
15	A	836	BCR	C16-C15-C14	-3.20	116.97	123.52
12	A	804	CLA	O2A-C1-C2	3.20	120.42	108.11
12	B	808	CLA	C1-O2A-CGA	3.20	124.39	116.65
12	A	815	CLA	CHD-C1D-ND	-3.20	120.30	124.80
12	B	817	CLA	O2A-CGA-O1A	-3.20	115.64	123.63
17	A	840	LMG	O1-C1-C2	3.19	113.12	108.27
12	B	818	CLA	O2A-CGA-CBA	3.19	121.56	111.83
15	K	4005	BCR	C33-C5-C6	-3.19	121.00	124.48
12	A	858	CLA	CAC-C3C-C4C	3.19	128.94	124.79
12	A	844	CLA	C3D-C4D-ND	3.19	115.17	109.99
19	A	854	PL9	C16-C14-C13	-3.19	114.01	121.17
12	A	855	CLA	CAA-CBA-CGA	-3.19	104.16	113.21
12	B	825	CLA	C2B-C1B-NB	3.19	113.63	110.33
12	A	845	CLA	C2B-C1B-NB	3.18	113.63	110.33
12	F	203	CLA	CHD-C1D-ND	-3.18	120.32	124.80
15	J	105	BCR	C38-C26-C27	3.18	120.37	113.60
12	B	845	CLA	CMA-C3A-C2A	-3.17	101.71	113.98
15	K	4001	BCR	C2-C1-C6	3.17	115.05	110.44
12	A	833	CLA	CHD-C1D-ND	-3.17	120.34	124.80
12	B	808	CLA	O2A-CGA-CBA	3.17	121.49	111.83
12	B	830	CLA	O2D-CGD-O1D	-3.17	117.69	123.85
12	B	807	CLA	O2A-CGA-CBA	3.16	121.48	111.83
12	A	820	CLA	C2B-C1B-NB	3.16	113.61	110.33
12	B	843	CLA	C2B-C1B-NB	3.16	113.61	110.33
12	B	829	CLA	C3C-C4C-NC	3.16	114.48	110.43
12	A	845	CLA	CHD-C1D-ND	-3.16	120.35	124.80
15	A	838	BCR	C10-C11-C12	-3.16	114.04	123.20
12	A	822	CLA	O2A-CGA-CBA	3.16	121.47	111.83
12	B	816	CLA	C2B-C1B-NB	3.16	113.60	110.33
15	B	836	BCR	C23-C24-C25	-3.16	118.57	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	842	CLA	C4-C3-C5	3.16	120.71	115.23
12	A	803	CLA	CMA-C3A-C4A	3.15	120.24	111.77
12	A	820	CLA	C1-C2-C3	-3.15	121.03	126.20
12	A	825	CLA	C1-C2-C3	-3.15	121.03	126.20
12	B	849	CLA	CMA-C3A-C2A	-3.15	101.80	113.98
12	A	846	CLA	C3C-C4C-NC	3.15	114.47	110.43
12	L	204	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
12	B	824	CLA	C1D-ND-C4D	-3.15	104.10	106.31
12	A	813	CLA	CMC-C2C-C1C	3.15	129.95	125.03
12	A	817	CLA	C3D-C4D-ND	3.15	115.10	109.99
12	A	855	CLA	CHD-C1D-ND	-3.15	120.38	124.80
12	B	846	CLA	C3D-C4D-ND	3.14	115.10	109.99
12	B	801	CLA	C3D-C4D-ND	3.14	115.09	109.99
15	B	832	BCR	C11-C10-C9	-3.14	122.87	127.28
12	B	842	CLA	C2B-C1B-NB	3.14	113.58	110.33
27	M	102	SQD	O9-S-C6	3.13	111.43	106.76
12	B	846	CLA	C4-C3-C5	3.13	120.66	115.23
12	A	832	CLA	C2B-C1B-NB	3.13	113.57	110.33
12	B	819	CLA	C2B-C1B-NB	3.13	113.57	110.33
12	A	852	CLA	C6-C5-C3	-3.13	105.85	113.47
12	B	814	CLA	CMA-C3A-C2A	-3.13	101.89	113.98
15	L	208	BCR	C16-C17-C18	-3.13	122.89	127.28
15	F	202	BCR	C24-C23-C22	-3.12	121.61	126.23
12	B	816	CLA	C3C-C4C-NC	3.12	114.43	110.43
12	A	844	CLA	C1-O2A-CGA	3.12	124.21	116.65
12	A	831	CLA	C3C-C4C-NC	3.12	114.43	110.43
12	J	101	CLA	C3D-C4D-ND	3.12	115.06	109.99
12	A	832	CLA	C5-C3-C4	3.12	121.77	114.59
12	A	827	CLA	C2B-C1B-NB	3.12	113.56	110.33
15	B	832	BCR	C16-C17-C18	-3.12	122.91	127.28
15	K	4005	BCR	C10-C11-C12	-3.11	114.18	123.20
12	A	806	CLA	C2B-C1B-NB	3.11	113.55	110.33
12	K	4002	CLA	C4A-NA-C1A	3.11	108.10	106.68
15	A	838	BCR	C29-C30-C25	3.10	114.95	110.44
15	B	834	BCR	C10-C11-C12	-3.10	114.20	123.20
12	B	848	CLA	C3C-C4C-NC	3.10	114.41	110.43
15	K	4001	BCR	C33-C5-C6	-3.10	121.11	124.48
12	K	4002	CLA	O2A-CGA-CBA	3.10	123.78	114.00
15	J	104	BCR	C40-C30-C25	-3.10	105.39	110.24
15	A	838	BCR	C15-C16-C17	-3.09	117.19	123.52
12	B	810	CLA	C2B-C1B-NB	3.09	113.53	110.33
12	B	810	CLA	CHD-C1D-ND	-3.09	120.45	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	J	101	CLA	CMD-C2D-C3D	-3.09	120.60	127.69
15	F	202	BCR	C4-C5-C6	-3.09	118.53	122.70
15	B	836	BCR	C36-C18-C17	-3.09	117.81	122.82
12	A	825	CLA	C3C-C4C-NC	3.09	114.39	110.43
12	B	850	CLA	CMD-C2D-C3D	-3.09	120.61	127.69
12	B	819	CLA	C3C-C4C-NC	3.09	114.39	110.43
15	L	207	BCR	C4-C5-C6	-3.09	118.53	122.70
12	B	803	CLA	C4-C3-C5	3.09	120.58	115.23
15	I	101	BCR	C29-C30-C25	3.08	114.92	110.44
12	B	802	CLA	O2A-C1-C2	3.08	119.96	108.11
15	A	838	BCR	C11-C10-C9	-3.08	122.96	127.28
12	B	846	CLA	C2B-C1B-NB	3.08	113.52	110.33
12	J	102	CLA	O2A-CGA-CBA	3.08	123.72	114.00
12	A	803	CLA	CAC-C3C-C4C	3.08	128.79	124.79
12	A	831	CLA	C4-C3-C5	3.08	120.57	115.23
12	B	848	CLA	CMC-C2C-C1C	3.07	129.84	125.03
12	K	4003	CLA	C4D-CHA-C1A	3.07	124.91	121.24
12	A	806	CLA	C3D-C4D-ND	3.07	114.98	109.99
15	A	837	BCR	C21-C20-C19	-3.07	114.30	123.20
12	A	807	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
12	A	814	CLA	C3D-C4D-ND	3.07	114.98	109.99
12	A	825	CLA	CMC-C2C-C1C	3.07	129.83	125.03
16	M	103	LHG	O8-C23-C24	3.07	121.20	111.83
12	J	101	CLA	C4-C3-C2	-3.07	115.75	123.63
15	B	836	BCR	C20-C19-C18	-3.07	117.95	126.36
13	A	802	CL0	C3C-C4C-NC	3.07	114.36	110.43
12	A	832	CLA	CAA-C2A-C1A	3.07	122.02	111.97
12	B	811	CLA	CMA-C3A-C4A	3.06	120.01	111.77
15	I	101	BCR	C10-C11-C12	-3.06	114.33	123.20
15	A	837	BCR	C37-C22-C23	3.06	122.76	118.09
12	B	849	CLA	C1-C2-C3	-3.06	121.19	126.20
12	A	852	CLA	CHC-C1C-NC	-3.06	119.71	124.31
15	I	101	BCR	C16-C15-C14	-3.06	117.27	123.52
12	A	831	CLA	C4D-C3D-CAD	3.05	111.42	108.11
15	B	832	BCR	C23-C24-C25	-3.05	118.84	127.00
12	J	103	CLA	CMC-C2C-C1C	3.05	129.81	125.03
12	A	813	CLA	C2B-C1B-NB	3.05	113.49	110.33
12	A	824	CLA	CMC-C2C-C1C	3.05	129.80	125.03
12	L	204	CLA	C2B-C1B-NB	3.05	113.49	110.33
12	B	818	CLA	C3C-C4C-NC	3.05	114.34	110.43
12	J	103	CLA	O2A-CGA-CBA	3.05	123.64	114.00
12	A	826	CLA	O2A-CGA-CBA	3.05	121.13	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	818	CLA	C2B-C1B-NB	3.05	113.49	110.33
15	A	836	BCR	C24-C23-C22	-3.05	121.72	126.23
12	A	828	CLA	C1-O2A-CGA	3.04	124.02	116.65
12	A	801	CLA	C3C-C4C-NC	3.04	114.33	110.43
12	L	201	CLA	CMC-C2C-C1C	3.04	129.78	125.03
12	B	811	CLA	C4D-C3D-CAD	3.04	111.41	108.11
12	K	4002	CLA	CHD-C1D-ND	-3.04	120.53	124.80
12	A	808	CLA	C2B-C1B-NB	3.04	113.47	110.33
15	K	4005	BCR	C16-C17-C18	-3.04	123.02	127.28
12	B	817	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
12	A	815	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
12	A	845	CLA	C4D-C3D-CAD	3.03	111.40	108.11
12	A	815	CLA	C2B-C1B-NB	3.03	113.47	110.33
12	A	855	CLA	CMC-C2C-C1C	3.03	129.77	125.03
12	B	806	CLA	CMC-C2C-C1C	3.03	129.77	125.03
12	B	847	CLA	CAA-C2A-C3A	-3.03	104.81	113.00
12	A	805	CLA	CMC-C2C-C1C	3.02	129.76	125.03
12	A	852	CLA	CMC-C2C-C1C	3.02	129.76	125.03
12	B	810	CLA	O2A-CGA-CBA	3.02	121.05	111.83
15	F	202	BCR	C11-C12-C13	-3.02	118.08	126.36
12	A	845	CLA	CMA-C3A-C2A	-3.02	102.30	113.98
15	K	4005	BCR	C36-C18-C19	3.02	122.70	118.09
12	A	831	CLA	C1-O2A-CGA	3.02	123.96	116.65
15	L	207	BCR	C15-C16-C17	-3.02	117.34	123.52
12	B	811	CLA	C4-C3-C5	3.02	120.47	115.23
12	J	103	CLA	CMD-C2D-C3D	-3.02	120.77	127.69
12	K	4004	CLA	C2D-C1D-ND	3.02	113.11	110.13
15	F	201	BCR	C27-C26-C25	-3.01	118.63	122.70
15	A	837	BCR	C1-C6-C5	-3.01	118.52	122.64
12	F	204	CLA	C3D-C4D-ND	3.01	114.88	109.99
12	B	853	CLA	CHD-C1D-ND	-3.01	120.56	124.80
12	A	813	CLA	O2A-C1-C2	3.01	119.70	108.11
12	A	824	CLA	C3C-C4C-NC	3.01	114.29	110.43
12	A	828	CLA	O2A-CGA-CBA	3.01	121.02	111.83
12	B	843	CLA	C2A-C3A-C4A	-3.01	97.01	101.87
12	A	821	CLA	CMC-C2C-C1C	3.01	129.74	125.03
12	B	822	CLA	O2A-C1-C2	3.01	119.67	108.11
15	A	836	BCR	C21-C20-C19	-3.00	114.50	123.20
15	B	834	BCR	C24-C23-C22	-3.00	121.79	126.23
12	B	803	CLA	CED-O2D-CGD	3.00	122.72	115.92
15	K	4001	BCR	C2-C3-C4	3.00	117.87	111.28
12	B	804	CLA	C2B-C1B-NB	3.00	113.44	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	823	CLA	C4-C3-C5	3.00	120.43	115.23
12	B	845	CLA	O2A-C1-C2	3.00	119.64	108.11
15	J	105	BCR	C23-C24-C25	-3.00	118.99	127.00
12	B	815	CLA	CHD-C1D-ND	-3.00	120.59	124.80
12	A	849	CLA	C2B-C1B-NB	3.00	113.43	110.33
15	B	836	BCR	C38-C26-C27	3.00	119.98	113.60
15	B	834	BCR	C11-C10-C9	-2.99	123.08	127.28
26	L	209	DGD	C2G-O2G-C1B	-2.99	110.64	117.80
12	B	842	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
15	J	105	BCR	C11-C12-C13	-2.99	118.17	126.36
15	J	107	BCR	C33-C5-C4	2.99	119.97	113.60
15	K	4001	BCR	C10-C11-C12	-2.99	114.54	123.20
12	A	831	CLA	C2B-C1B-NB	2.99	113.42	110.33
12	A	846	CLA	O2D-CGD-O1D	-2.99	118.04	123.85
12	A	827	CLA	C1-C2-C3	-2.99	121.31	126.20
12	B	853	CLA	C2B-C1B-NB	2.98	113.42	110.33
12	B	819	CLA	C1-C2-C3	-2.98	121.31	126.20
12	B	844	CLA	CHD-C1D-ND	-2.98	120.61	124.80
15	F	201	BCR	C10-C11-C12	-2.98	114.56	123.20
12	B	811	CLA	CHD-C1D-ND	-2.98	120.61	124.80
12	B	821	CLA	CMA-C3A-C4A	-2.98	103.77	111.77
12	A	828	CLA	C3D-C4D-ND	2.98	114.83	109.99
12	B	801	CLA	C1-C2-C3	-2.98	121.32	126.20
12	A	809	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
12	B	804	CLA	CMC-C2C-C1C	2.97	129.68	125.03
12	B	853	CLA	C3D-C4D-ND	2.97	114.82	109.99
12	A	813	CLA	C3C-C4C-NC	2.97	114.23	110.43
12	A	803	CLA	C4-C3-C5	2.97	120.38	115.23
15	B	832	BCR	C29-C30-C25	2.97	114.75	110.44
12	A	801	CLA	O2D-CGD-O1D	-2.97	118.08	123.85
15	J	104	BCR	C38-C26-C27	2.97	119.92	113.60
12	B	808	CLA	C4-C3-C5	2.96	120.37	115.23
12	B	821	CLA	C1-C2-C3	-2.96	121.34	126.20
20	A	856	45D	C06-C04-C08	2.96	114.74	110.44
12	A	808	CLA	CMA-C3A-C2A	2.96	125.44	113.98
12	B	811	CLA	C3D-C4D-ND	2.96	114.80	109.99
15	L	207	BCR	C16-C15-C14	-2.96	117.47	123.52
12	J	102	CLA	C3D-C4D-ND	2.96	114.79	109.99
15	F	201	BCR	C33-C5-C4	2.95	119.89	113.60
12	A	806	CLA	CMC-C2C-C1C	2.95	129.65	125.03
15	K	4001	BCR	C15-C14-C13	-2.95	123.14	127.28
12	L	201	CLA	C3D-C4D-ND	2.95	114.78	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	J	107	BCR	C21-C20-C19	-2.95	114.65	123.20
12	B	853	CLA	CMC-C2C-C1C	2.95	129.64	125.03
12	B	853	CLA	C2A-C3A-C4A	-2.95	97.11	101.87
15	B	841	BCR	C20-C19-C18	-2.94	118.29	126.36
12	B	811	CLA	C2B-C1B-NB	2.94	113.38	110.33
12	F	204	CLA	O2A-CGA-CBA	2.94	123.29	114.00
12	A	848	CLA	CMC-C2C-C1C	2.94	129.62	125.03
15	A	835	BCR	C16-C15-C14	-2.94	117.51	123.52
12	A	818	CLA	CMC-C2C-C1C	2.93	129.62	125.03
12	L	205	CLA	C3D-C4D-ND	2.93	114.76	109.99
15	A	837	BCR	C27-C26-C25	-2.93	118.74	122.70
15	B	832	BCR	C4-C5-C6	-2.93	118.74	122.70
12	A	816	CLA	CAA-CBA-CGA	2.93	121.54	113.21
12	A	844	CLA	CED-O2D-CGD	2.93	122.57	115.92
15	J	107	BCR	C16-C15-C14	-2.93	117.52	123.52
12	B	803	CLA	CBA-CAA-C2A	2.93	122.52	113.79
12	A	847	CLA	C3D-C4D-ND	2.93	114.75	109.99
12	A	858	CLA	C3D-C4D-ND	2.93	114.75	109.99
12	A	847	CLA	C4-C3-C5	2.93	120.31	115.23
15	B	835	BCR	C38-C26-C25	-2.93	121.29	124.48
15	A	837	BCR	C30-C25-C26	-2.93	118.64	122.64
12	B	811	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
12	B	810	CLA	C4-C3-C5	2.93	120.31	115.23
15	B	832	BCR	C15-C16-C17	-2.92	117.53	123.52
12	A	825	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
15	J	107	BCR	C38-C26-C27	2.92	119.83	113.60
12	L	204	CLA	C1-C2-C3	-2.92	121.41	126.20
12	K	4002	CLA	C2B-C1B-NB	2.92	113.35	110.33
12	A	846	CLA	O2A-C1-C2	2.92	119.34	108.11
12	A	805	CLA	CAA-CBA-CGA	-2.92	104.92	113.21
19	A	854	PL9	C7-C3-C4	2.92	119.31	116.91
12	A	804	CLA	CAC-C3C-C4C	2.92	128.59	124.79
17	A	851	LMG	C8-O7-C10	-2.92	110.82	117.80
12	A	848	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
12	F	204	CLA	C2B-C1B-NB	2.92	113.35	110.33
12	A	847	CLA	O2A-C1-C2	2.91	119.33	108.11
15	I	101	BCR	C1-C6-C5	-2.91	118.66	122.64
12	B	806	CLA	CHD-C4C-C3C	-2.91	120.53	124.77
12	A	814	CLA	CMA-C3A-C4A	2.91	119.60	111.77
12	B	817	CLA	C1-C2-C3	-2.91	121.43	126.20
12	B	810	CLA	C3D-C4D-ND	2.91	114.72	109.99
15	A	838	BCR	C16-C17-C18	-2.91	123.20	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	820	CLA	CMC-C2C-C1C	2.91	129.58	125.03
12	F	203	CLA	C4D-C3D-CAD	2.91	111.27	108.11
15	L	207	BCR	C34-C9-C8	2.91	122.53	118.09
12	A	847	CLA	CMB-C2B-C1B	2.91	129.85	125.42
12	B	847	CLA	C2B-C1B-NB	2.91	113.34	110.33
12	B	848	CLA	C2B-C1B-NB	2.91	113.34	110.33
12	B	803	CLA	C3D-C4D-ND	2.91	114.71	109.99
12	F	203	CLA	C3C-C4C-NC	2.90	114.15	110.43
12	A	852	CLA	CMA-C3A-C2A	2.90	125.21	113.98
15	I	101	BCR	C4-C5-C6	-2.90	118.78	122.70
12	B	813	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
12	B	804	CLA	C3D-C4D-ND	2.90	114.70	109.99
12	A	816	CLA	CMB-C2B-C3B	2.90	133.37	126.55
27	M	102	SQD	C1-O5-C5	-2.90	108.06	113.72
12	A	801	CLA	CAA-CBA-CGA	-2.90	104.98	113.21
12	B	811	CLA	O2A-C1-C2	2.90	119.26	108.11
12	B	817	CLA	CAA-C2A-C3A	2.90	120.83	113.00
12	B	823	CLA	CMC-C2C-C1C	2.90	129.56	125.03
12	A	849	CLA	C3D-C4D-ND	2.90	114.69	109.99
12	A	820	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
15	A	835	BCR	C24-C23-C22	-2.89	121.96	126.23
19	A	854	PL9	C2-C1-C6	2.89	122.43	119.00
15	I	101	BCR	C27-C26-C25	-2.88	118.81	122.70
12	A	807	CLA	C3D-C4D-ND	2.88	114.67	109.99
12	B	805	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
12	B	850	CLA	C4-C3-C2	-2.88	116.23	123.63
15	B	835	BCR	C16-C15-C14	-2.88	117.63	123.52
12	A	824	CLA	CHD-C1D-ND	-2.88	120.75	124.80
12	A	848	CLA	C3D-C4D-ND	2.88	114.66	109.99
12	B	820	CLA	O2A-C1-C2	2.87	119.17	108.11
12	B	820	CLA	C2B-C1B-NB	2.87	113.31	110.33
15	L	208	BCR	C1-C6-C5	-2.87	118.71	122.64
12	A	847	CLA	O2A-CGA-CBA	2.87	120.59	111.83
12	B	845	CLA	C3D-C4D-ND	2.87	114.65	109.99
12	B	804	CLA	C4A-NA-C1A	2.87	107.99	106.68
12	K	4003	CLA	CHA-C1A-NA	-2.87	119.90	126.39
12	A	805	CLA	C3D-C4D-ND	2.86	114.64	109.99
12	A	812	CLA	C2B-C1B-NB	2.86	113.29	110.33
12	L	206	CLA	CMC-C2C-C1C	2.86	129.50	125.03
12	B	821	CLA	C1-O2A-CGA	2.86	123.57	116.65
12	A	846	CLA	CAC-C3C-C4C	2.86	128.51	124.79
19	A	854	PL9	C53-C6-C1	2.86	121.13	115.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	830	CLA	CED-O2D-CGD	2.85	122.39	115.92
12	A	849	CLA	C1-O2A-CGA	2.85	123.55	116.65
12	A	846	CLA	C3D-C4D-ND	2.85	114.62	109.99
15	J	105	BCR	C10-C11-C12	-2.85	114.94	123.20
12	A	821	CLA	C3D-C4D-ND	2.85	114.62	109.99
12	A	811	CLA	C3D-C4D-ND	2.85	114.62	109.99
12	B	845	CLA	CMC-C2C-C1C	2.85	129.49	125.03
12	B	809	CLA	CHD-C1D-ND	-2.85	120.80	124.80
12	B	848	CLA	O2A-C1-C2	2.85	119.06	108.11
12	B	810	CLA	CMC-C2C-C1C	2.85	129.48	125.03
12	A	829	CLA	C3D-C4D-ND	2.84	114.61	109.99
12	A	849	CLA	O2A-CGA-CBA	2.84	120.50	111.83
12	A	833	CLA	CAC-C3C-C4C	2.84	128.49	124.79
12	B	807	CLA	C4-C3-C5	2.84	120.16	115.23
15	F	201	BCR	C23-C22-C21	-2.84	114.54	119.01
13	A	802	CL0	C1-C2-C3	-2.84	121.55	126.20
12	B	825	CLA	C3D-C4D-ND	2.83	114.59	109.99
12	B	803	CLA	C5-C3-C2	-2.83	114.81	121.17
12	B	847	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
15	A	835	BCR	C19-C18-C17	2.83	123.46	119.01
12	A	843	CLA	CMA-C3A-C4A	2.83	119.37	111.77
16	A	839	LHG	O8-C23-C24	2.83	120.46	111.83
12	K	4004	CLA	CBC-CAC-C3C	-2.82	104.76	112.42
12	A	820	CLA	C3C-C4C-NC	2.82	114.05	110.43
12	B	823	CLA	C3D-C4D-ND	2.82	114.58	109.99
20	A	856	45D	C22-C16-C08	2.82	128.64	124.11
12	A	827	CLA	CMA-C3A-C4A	-2.82	104.19	111.77
12	A	846	CLA	CED-O2D-CGD	2.82	122.31	115.92
12	B	823	CLA	C4-C3-C5	2.82	120.12	115.23
12	B	804	CLA	CMD-C2D-C3D	-2.82	121.22	127.69
15	B	834	BCR	C7-C8-C9	-2.82	122.07	126.23
16	A	839	LHG	O7-C7-C8	2.81	117.57	111.48
15	L	208	BCR	C15-C14-C13	-2.81	123.33	127.28
12	B	801	CLA	CAA-C2A-C1A	-2.81	102.76	111.97
22	B	831	A1AGD	C7-C8-C9	-2.81	121.99	126.83
12	A	827	CLA	C3D-C4D-ND	2.81	114.56	109.99
12	B	828	CLA	C1-C2-C3	-2.81	121.59	126.20
15	K	4005	BCR	C4-C5-C6	-2.81	118.91	122.70
12	B	844	CLA	C3D-C4D-ND	2.81	114.55	109.99
15	A	835	BCR	C1-C6-C5	-2.81	118.80	122.64
12	A	809	CLA	C3D-C4D-ND	2.81	114.55	109.99
12	A	823	CLA	C3C-C4C-NC	2.80	114.02	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	830	CLA	O2A-C1-C2	2.80	118.89	108.11
15	L	207	BCR	C8-C7-C6	-2.80	119.52	127.00
12	A	846	CLA	C2B-C1B-NB	2.80	113.23	110.33
12	B	814	CLA	C3D-C4D-ND	2.80	114.54	109.99
12	A	844	CLA	C2B-C1B-NB	2.80	113.23	110.33
12	K	4004	CLA	CMA-C3A-C4A	2.80	119.29	111.77
12	A	814	CLA	O2A-C1-C2	2.80	118.88	108.11
12	B	850	CLA	C1D-ND-C4D	-2.80	104.35	106.31
12	B	852	CLA	C2A-C3A-C4A	-2.80	97.35	101.87
15	L	207	BCR	C29-C28-C27	2.80	117.42	111.28
12	B	844	CLA	O2A-CGA-CBA	2.79	120.35	111.83
12	A	801	CLA	CMA-C3A-C4A	2.79	119.28	111.77
12	B	829	CLA	CMB-C2B-C1B	2.79	129.67	125.42
12	B	803	CLA	CMB-C2B-C1B	2.79	129.67	125.42
12	B	842	CLA	C3D-C4D-ND	2.79	114.52	109.99
12	K	4002	CLA	C3D-C4D-ND	2.79	114.52	109.99
12	B	828	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
12	B	818	CLA	CMA-C3A-C4A	-2.79	104.28	111.77
12	A	832	CLA	C3C-C4C-NC	2.79	114.00	110.43
12	A	816	CLA	C3D-C4D-ND	2.79	114.52	109.99
12	A	855	CLA	C2A-C3A-C4A	-2.79	97.37	101.87
15	K	4005	BCR	C38-C26-C27	2.79	119.54	113.60
12	B	822	CLA	C3D-C4D-ND	2.79	114.51	109.99
12	A	844	CLA	C3C-C4C-NC	2.78	114.00	110.43
12	A	818	CLA	CHD-C1D-ND	-2.78	120.89	124.80
12	A	845	CLA	C3D-C4D-ND	2.78	114.51	109.99
12	F	204	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
12	A	830	CLA	C3D-C4D-ND	2.78	114.51	109.99
12	A	852	CLA	C2B-C1B-NB	2.78	113.21	110.33
12	A	812	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
12	B	846	CLA	CHD-C1D-ND	-2.78	120.89	124.80
12	A	820	CLA	CHD-C1D-ND	-2.78	120.89	124.80
16	B	851	LHG	O8-C23-C24	2.78	120.30	111.83
12	A	823	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
12	L	206	CLA	C3D-C4D-ND	2.78	114.50	109.99
12	B	825	CLA	O2A-C1-C2	2.77	118.78	108.11
12	B	824	CLA	CHC-C1C-C2C	-2.77	119.06	126.95
12	B	817	CLA	C3D-C4D-ND	2.77	114.49	109.99
12	B	827	CLA	C3D-C4D-ND	2.77	114.49	109.99
12	B	849	CLA	O2A-C1-C2	2.77	118.77	108.11
15	B	832	BCR	C1-C6-C5	-2.77	118.85	122.64
12	A	808	CLA	C3D-C4D-ND	2.77	114.49	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	822	CLA	C1-C2-C3	-2.77	121.66	126.20
13	A	802	CL0	C3D-C4D-ND	2.77	114.49	109.99
12	A	804	CLA	CMC-C2C-C1C	2.77	129.36	125.03
12	B	848	CLA	C1-O2A-CGA	2.76	123.34	116.65
15	B	834	BCR	C34-C9-C8	2.76	122.31	118.09
12	B	805	CLA	CMC-C2C-C1C	2.76	129.35	125.03
15	B	835	BCR	C29-C30-C25	2.76	114.45	110.44
13	A	802	CL0	O2A-CGA-CBA	2.76	120.25	111.83
12	A	804	CLA	C3D-C4D-ND	2.76	114.47	109.99
15	B	834	BCR	C38-C26-C25	-2.76	121.47	124.48
12	A	855	CLA	C2B-C1B-NB	2.76	113.19	110.33
12	A	846	CLA	C4C-C3C-C2C	-2.76	102.88	106.89
15	A	836	BCR	C15-C16-C17	-2.76	117.88	123.52
12	A	822	CLA	C3C-C4C-NC	2.76	113.96	110.43
12	B	816	CLA	CMC-C2C-C1C	2.75	129.34	125.03
12	A	822	CLA	CHD-C1D-ND	-2.75	120.93	124.80
12	A	858	CLA	O2D-CGD-CBD	2.75	116.04	111.23
15	B	841	BCR	C15-C16-C17	-2.75	117.89	123.52
12	B	807	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
12	A	826	CLA	C4-C3-C5	2.75	120.01	115.23
18	L	210	LMT	C1B-O1B-C4'	2.75	124.50	117.98
12	A	815	CLA	CMC-C2C-C1C	2.75	129.33	125.03
12	A	833	CLA	C4D-C3D-CAD	2.75	111.09	108.11
12	A	812	CLA	C3D-C4D-ND	2.75	114.45	109.99
12	A	822	CLA	C4-C3-C5	2.75	120.00	115.23
12	B	825	CLA	C1-C2-C3	-2.74	121.70	126.20
15	F	201	BCR	C37-C22-C23	2.74	122.27	118.09
12	B	844	CLA	C3C-C4C-NC	2.74	113.94	110.43
12	B	806	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
12	K	4004	CLA	CHB-C4A-NA	2.74	128.35	124.40
12	J	103	CLA	O1D-CGD-CBD	-2.73	119.13	124.52
15	A	835	BCR	C11-C10-C9	-2.73	123.45	127.28
12	B	850	CLA	CAC-C3C-C4C	2.73	128.34	124.79
20	A	856	45D	C20-C24-C26	2.73	130.27	126.23
12	A	815	CLA	C4D-C3D-CAD	2.73	111.07	108.11
12	F	204	CLA	C4D-C3D-CAD	2.73	111.07	108.11
12	B	809	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
12	A	843	CLA	C4D-C3D-CAD	2.73	111.07	108.11
12	B	816	CLA	O2A-C1-C2	2.73	118.60	108.11
12	B	826	CLA	C4D-C3D-CAD	2.73	111.07	108.11
15	K	4001	BCR	C33-C5-C4	2.72	119.41	113.60
12	A	829	CLA	C4D-C3D-CAD	2.72	111.06	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	850	CLA	CMB-C2B-C1B	2.72	129.57	125.42
12	B	805	CLA	C2B-C1B-NB	2.72	113.15	110.33
12	B	822	CLA	C1D-CHD-C4C	-2.72	120.24	126.02
15	F	202	BCR	C23-C24-C25	-2.72	119.73	127.00
12	A	819	CLA	CAC-C3C-C4C	2.72	128.32	124.79
12	A	814	CLA	CMC-C2C-C1C	2.72	129.28	125.03
12	J	103	CLA	CMB-C2B-C1B	2.72	129.56	125.42
15	B	841	BCR	C23-C24-C25	-2.72	119.74	127.00
12	B	824	CLA	CAC-C3C-C4C	2.71	128.32	124.79
15	F	201	BCR	C33-C5-C6	-2.71	121.52	124.48
12	B	817	CLA	C2A-C3A-C4A	-2.71	97.49	101.87
12	B	844	CLA	C2A-C1A-CHA	-2.71	119.16	123.87
12	J	102	CLA	CMA-C3A-C4A	2.71	119.06	111.77
15	L	208	BCR	C2-C1-C6	2.71	114.38	110.44
17	A	840	LMG	C9-C8-C7	-2.71	105.47	111.78
12	F	204	CLA	CMC-C2C-C1C	2.70	129.26	125.03
16	A	850	LHG	O7-C7-O9	-2.70	117.38	123.70
12	J	102	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
12	A	826	CLA	C3D-C4D-ND	2.70	114.38	109.99
12	B	815	CLA	CAC-C3C-C4C	2.70	128.31	124.79
15	L	208	BCR	C23-C24-C25	-2.70	119.78	127.00
12	A	813	CLA	CMB-C2B-C1B	2.70	129.53	125.42
12	A	843	CLA	C3D-C4D-ND	2.70	114.37	109.99
12	A	809	CLA	C11-C10-C8	-2.70	107.00	115.97
12	B	808	CLA	CMA-C3A-C2A	-2.70	103.56	113.98
12	A	819	CLA	C3D-C4D-ND	2.70	114.37	109.99
12	B	829	CLA	C2B-C1B-NB	2.70	113.12	110.33
12	L	204	CLA	CMC-C2C-C1C	2.69	129.25	125.03
12	A	833	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
12	L	204	CLA	C3D-C4D-ND	2.69	114.36	109.99
12	B	848	CLA	CMB-C2B-C1B	2.69	129.52	125.42
12	A	824	CLA	CMA-C3A-C2A	-2.69	103.57	113.98
12	A	828	CLA	CMC-C2C-C1C	2.69	129.24	125.03
15	B	835	BCR	C38-C26-C27	2.69	119.33	113.60
15	K	4001	BCR	C8-C7-C6	-2.69	119.81	127.00
12	A	821	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
12	A	828	CLA	CAC-C3C-C4C	2.69	128.29	124.79
15	B	841	BCR	C29-C30-C25	2.69	114.34	110.44
12	B	825	CLA	CAA-CBA-CGA	-2.69	105.58	113.21
12	B	812	CLA	C3D-C4D-ND	2.69	114.36	109.99
12	A	805	CLA	C3C-C4C-NC	2.68	113.87	110.43
12	A	820	CLA	C3D-C4D-ND	2.68	114.35	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	802	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
12	B	814	CLA	C3C-C4C-NC	2.68	113.86	110.43
12	J	102	CLA	CMC-C2C-C1C	2.68	129.22	125.03
12	A	801	CLA	C3D-C4D-ND	2.68	114.34	109.99
12	A	826	CLA	CMA-C3A-C2A	-2.68	103.63	113.98
12	B	804	CLA	OB D-CAD-C3D	-2.68	122.16	128.42
12	A	829	CLA	CMC-C2C-C1C	2.68	129.22	125.03
15	B	835	BCR	C27-C26-C25	-2.68	119.09	122.70
26	L	209	DGD	O1G-C1A-C2A	2.68	119.99	111.83
12	B	819	CLA	C4-C3-C5	2.67	119.87	115.23
12	B	809	CLA	C1-O2A-CGA	2.67	123.12	116.65
12	B	813	CLA	C3C-C4C-NC	2.67	113.85	110.43
12	B	816	CLA	C3D-C4D-ND	2.67	114.33	109.99
13	A	802	CL0	CHD-C1D-ND	-2.67	121.04	124.80
12	J	101	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
12	B	817	CLA	C4D-C3D-CAD	2.67	111.00	108.11
12	B	802	CLA	C4-C3-C5	2.67	119.86	115.23
15	A	838	BCR	C38-C26-C27	2.66	119.28	113.60
12	J	101	CLA	O2A-C1-C2	2.66	118.36	108.11
12	A	807	CLA	C1-C2-C3	-2.66	121.83	126.20
12	B	807	CLA	C3D-C4D-ND	2.66	114.31	109.99
12	B	850	CLA	C3D-C4D-ND	2.66	114.31	109.99
15	L	207	BCR	C7-C8-C9	-2.66	122.30	126.23
15	L	207	BCR	C10-C11-C12	-2.66	115.49	123.20
12	A	824	CLA	C3D-C4D-ND	2.66	114.31	109.99
15	K	4005	BCR	C38-C26-C25	-2.66	121.58	124.48
12	A	831	CLA	C3D-C4D-ND	2.66	114.31	109.99
12	B	828	CLA	CMC-C2C-C1C	2.66	129.19	125.03
12	K	4004	CLA	CAA-C2A-C3A	-2.66	105.82	113.00
15	B	832	BCR	C38-C26-C25	-2.66	121.59	124.48
12	A	849	CLA	CBA-CAA-C2A	-2.66	105.89	113.79
15	L	208	BCR	C15-C16-C17	-2.66	118.08	123.52
12	B	852	CLA	C2B-C1B-NB	2.65	113.08	110.33
12	K	4002	CLA	C4D-C3D-CAD	2.65	110.99	108.11
12	B	814	CLA	C1-C2-C3	-2.65	121.85	126.20
12	A	811	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
15	A	836	BCR	C34-C9-C8	2.65	122.14	118.09
12	B	815	CLA	CMC-C2C-C1C	2.65	129.17	125.03
12	B	814	CLA	C4D-C3D-CAD	2.65	110.98	108.11
12	B	811	CLA	CMB-C2B-C1B	2.65	129.45	125.42
15	K	4005	BCR	C37-C22-C23	2.65	122.13	118.09
12	B	801	CLA	O2D-CGD-O1D	-2.65	118.70	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	808	CLA	C3D-C4D-ND	2.65	114.29	109.99
12	B	816	CLA	CAC-C3C-C4C	2.64	128.23	124.79
18	A	842	LMT	C1-O1'-C1'	2.64	118.19	113.68
12	B	821	CLA	CHD-C1D-ND	-2.64	121.09	124.80
12	A	813	CLA	C4-C3-C5	2.64	119.81	115.23
12	B	816	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
12	A	823	CLA	C3D-C4D-ND	2.64	114.28	109.99
12	B	820	CLA	C3D-C4D-ND	2.64	114.28	109.99
12	A	855	CLA	CAA-C2A-C3A	-2.64	105.87	113.00
12	K	4004	CLA	C4D-C3D-CAD	2.64	110.97	108.11
12	A	815	CLA	C4-C3-C5	2.64	119.81	115.23
15	J	107	BCR	C34-C9-C8	2.64	122.12	118.09
12	B	848	CLA	CAC-C3C-C4C	2.64	128.22	124.79
12	B	843	CLA	CMC-C2C-C1C	2.64	129.15	125.03
15	F	202	BCR	C8-C7-C6	-2.63	119.96	127.00
12	A	826	CLA	C3C-C4C-NC	2.63	113.81	110.43
12	A	845	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
12	A	806	CLA	C4D-C3D-CAD	2.63	110.97	108.11
12	L	205	CLA	C3C-C4C-NC	2.63	113.80	110.43
12	B	822	CLA	C2B-C1B-NB	2.63	113.06	110.33
12	A	805	CLA	C1-C2-C3	-2.63	121.89	126.20
12	L	205	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
15	F	202	BCR	C29-C28-C27	2.63	117.06	111.28
12	B	808	CLA	C3C-C4C-NC	2.63	113.80	110.43
15	B	836	BCR	C23-C22-C21	2.63	123.14	119.01
12	B	826	CLA	C4-C3-C5	2.63	119.79	115.23
12	B	817	CLA	O2A-C1-C2	2.63	118.22	108.11
12	B	830	CLA	CMC-C2C-C1C	2.63	129.14	125.03
12	L	206	CLA	C4D-C3D-CAD	2.62	110.96	108.11
12	L	201	CLA	CBC-CAC-C3C	-2.62	105.31	112.42
12	B	814	CLA	CMC-C2C-C1C	2.62	129.13	125.03
12	A	815	CLA	C3C-C4C-NC	2.62	113.79	110.43
12	B	848	CLA	O2A-CGA-CBA	2.62	119.83	111.83
12	K	4004	CLA	C2B-C1B-NB	2.62	113.05	110.33
12	B	802	CLA	C3D-C4D-ND	2.62	114.25	109.99
12	B	806	CLA	C3D-C4D-ND	2.62	114.24	109.99
15	L	208	BCR	C29-C28-C27	2.62	117.03	111.28
12	K	4002	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
12	A	849	CLA	CMC-C2C-C1C	2.62	129.12	125.03
12	B	847	CLA	C6-C5-C3	-2.62	107.09	113.47
15	A	837	BCR	C10-C11-C12	-2.61	115.63	123.20
12	B	829	CLA	O2D-CGD-O1D	-2.61	118.76	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	820	CLA	C1-C2-C3	-2.61	121.92	126.20
12	A	843	CLA	CAC-C3C-C4C	2.61	128.19	124.79
15	B	835	BCR	C4-C5-C6	-2.61	119.17	122.70
12	B	815	CLA	C3D-C4D-ND	2.61	114.23	109.99
12	B	802	CLA	CMC-C2C-C1C	2.61	129.12	125.03
13	A	802	CL0	C4-C3-C5	2.61	119.76	115.23
12	B	850	CLA	CMA-C3A-C4A	-2.61	104.75	111.77
12	B	826	CLA	CMC-C2C-C1C	2.61	129.11	125.03
12	B	848	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
12	A	833	CLA	C3D-C4D-ND	2.61	114.23	109.99
18	F	205	LMT	C1'-O5'-C5'	2.61	118.81	113.72
12	B	803	CLA	CMC-C2C-C1C	2.61	129.11	125.03
12	B	814	CLA	C6-C5-C3	-2.61	107.11	113.47
12	B	803	CLA	CMA-C3A-C2A	-2.61	103.90	113.98
15	B	834	BCR	C27-C26-C25	-2.61	119.18	122.70
12	B	828	CLA	C3D-C4D-ND	2.61	114.22	109.99
12	A	817	CLA	O2D-CGD-O1D	-2.61	118.78	123.85
15	B	836	BCR	C19-C18-C17	2.61	123.11	119.01
15	J	107	BCR	C27-C26-C25	-2.60	119.18	122.70
12	A	808	CLA	C2A-C3A-C4A	-2.60	97.66	101.87
16	B	851	LHG	P-O3-C3	2.60	136.27	121.35
12	A	822	CLA	C3D-C4D-ND	2.60	114.22	109.99
12	B	821	CLA	CMA-C3A-C2A	-2.60	103.92	113.98
13	A	802	CL0	C2B-C1B-NB	2.60	113.03	110.33
12	A	830	CLA	CMC-C2C-C1C	2.60	129.10	125.03
17	A	851	LMG	O8-C28-O10	-2.60	117.12	123.63
12	B	850	CLA	C2D-C1D-ND	2.60	112.70	110.13
12	B	820	CLA	C11-C10-C8	-2.60	107.33	115.97
12	L	204	CLA	C3C-C4C-NC	2.60	113.76	110.43
15	B	835	BCR	C8-C9-C10	-2.60	114.92	119.01
12	A	801	CLA	CMC-C2C-C1C	2.60	129.09	125.03
12	B	826	CLA	C3D-C4D-ND	2.59	114.20	109.99
12	B	817	CLA	CMC-C2C-C1C	2.59	129.09	125.03
16	B	851	LHG	O6-P-O5	-2.59	98.66	108.94
12	A	844	CLA	O2A-CGA-CBA	2.59	119.74	111.83
12	B	809	CLA	CMC-C2C-C1C	2.59	129.08	125.03
12	A	804	CLA	CMA-C3A-C2A	-2.59	103.97	113.98
12	J	103	CLA	C3D-C4D-ND	2.59	114.20	109.99
12	A	814	CLA	C1-O2A-CGA	2.59	122.92	116.65
12	B	821	CLA	CMC-C2C-C1C	2.59	129.08	125.03
12	B	809	CLA	C3C-C4C-NC	2.59	113.75	110.43
15	L	208	BCR	C37-C22-C23	2.59	122.04	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	J	101	CLA	CMB-C2B-C3B	2.59	132.63	126.55
17	A	851	LMG	C6-C5-C4	2.59	119.37	113.02
12	A	852	CLA	CHB-C4A-NA	-2.58	120.67	124.40
12	A	815	CLA	CMA-C3A-C2A	-2.58	104.00	113.98
18	A	853	LMT	C4B-C3B-C2B	-2.58	106.30	110.83
12	B	826	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
15	L	208	BCR	C30-C25-C24	2.58	122.65	115.65
20	A	856	45D	C41-C42-C38	2.58	128.80	123.52
12	B	808	CLA	CMC-C2C-C1C	2.58	129.07	125.03
12	L	205	CLA	C1-O2A-CGA	2.58	122.89	116.65
12	A	813	CLA	CED-O2D-CGD	2.58	121.76	115.92
20	A	856	45D	C19-C23-C25	2.58	130.05	126.23
12	B	811	CLA	C1-O2A-CGA	2.58	122.89	116.65
12	A	845	CLA	CMD-C2D-C3D	-2.58	121.78	127.69
15	J	105	BCR	C29-C28-C27	-2.58	105.61	111.28
12	A	845	CLA	C4-C3-C5	2.57	119.70	115.23
12	B	829	CLA	C3D-C4D-ND	2.57	114.17	109.99
27	M	102	SQD	C4-C3-C2	2.57	115.34	110.83
12	A	812	CLA	C4D-C3D-CAD	2.57	110.90	108.11
12	A	849	CLA	C4D-C3D-CAD	2.57	110.89	108.11
12	A	846	CLA	CHD-C1D-ND	-2.57	121.19	124.80
12	B	820	CLA	C3C-C4C-NC	2.57	113.72	110.43
15	A	838	BCR	C27-C26-C25	-2.57	119.23	122.70
12	B	818	CLA	C4D-C3D-CAD	2.57	110.89	108.11
12	A	858	CLA	C3C-C4C-NC	2.57	113.72	110.43
12	A	822	CLA	O2D-CGD-O1D	-2.57	118.86	123.85
12	A	843	CLA	C3C-C4C-NC	2.56	113.72	110.43
12	B	805	CLA	C3C-C4C-NC	2.56	113.72	110.43
15	J	107	BCR	C8-C7-C6	-2.56	120.15	127.00
12	A	808	CLA	CMC-C2C-C1C	2.56	129.04	125.03
12	A	810	CLA	C3D-C4D-ND	2.56	114.15	109.99
15	A	838	BCR	C20-C19-C18	-2.56	119.34	126.36
12	A	816	CLA	O2A-CGA-CBA	2.56	119.65	111.83
12	B	822	CLA	C3C-C4C-NC	2.56	113.71	110.43
12	B	818	CLA	CMC-C2C-C1C	2.56	129.03	125.03
12	B	814	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
12	A	855	CLA	CMA-C3A-C4A	2.55	118.64	111.77
15	J	107	BCR	C1-C6-C5	-2.55	119.15	122.64
12	B	830	CLA	C3D-C4D-ND	2.55	114.13	109.99
12	A	803	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
12	B	817	CLA	CMB-C2B-C3B	2.55	132.55	126.55
12	B	827	CLA	O2D-CGD-O1D	-2.55	118.89	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	819	CLA	CHD-C1D-ND	-2.55	121.22	124.80
12	B	806	CLA	C4D-C3D-CAD	2.55	110.87	108.11
12	A	808	CLA	C3C-C4C-NC	2.55	113.69	110.43
12	A	805	CLA	CMB-C2B-C1B	2.55	129.30	125.42
15	I	101	BCR	C34-C9-C8	2.54	121.97	118.09
12	B	815	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
12	A	858	CLA	O2A-C1-C2	2.54	117.89	108.11
18	B	839	LMT	O3'-C3'-C2'	-2.54	104.39	110.38
27	M	102	SQD	C44-O6-C1	-2.54	108.35	113.80
22	B	831	A1AGD	C11-C9-C8	-2.54	115.47	121.17
12	B	826	CLA	CMD-C2D-C3D	-2.54	121.87	127.69
15	A	835	BCR	C38-C26-C27	2.54	119.00	113.60
12	A	810	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
15	K	4005	BCR	C19-C18-C17	-2.54	115.02	119.01
12	J	102	CLA	CMB-C2B-C1B	2.53	129.28	125.42
18	B	840	LMT	C1-O1'-C1'	2.53	118.01	113.68
12	B	812	CLA	C6-C5-C3	-2.53	107.30	113.47
12	A	820	CLA	C4C-C3C-C2C	-2.53	103.21	106.89
12	B	817	CLA	O2A-CGA-CBA	2.53	119.56	111.83
12	A	813	CLA	C3D-C4D-ND	2.53	114.10	109.99
12	B	830	CLA	O1D-CGD-CBD	-2.53	119.53	124.52
12	B	801	CLA	CMB-C2B-C3B	2.53	132.50	126.55
12	A	820	CLA	CAC-C3C-C4C	2.53	128.08	124.79
12	B	804	CLA	C4-C3-C5	2.53	119.62	115.23
12	B	852	CLA	CMA-C3A-C2A	-2.53	104.21	113.98
12	A	828	CLA	C4D-C3D-CAD	2.53	110.85	108.11
15	A	837	BCR	C33-C5-C4	2.53	118.98	113.60
12	B	803	CLA	C2B-C1B-NB	2.53	112.95	110.33
12	A	843	CLA	CMC-C2C-C1C	2.53	128.98	125.03
12	A	805	CLA	C4-C3-C5	2.53	119.61	115.23
12	B	843	CLA	C3D-C4D-ND	2.52	114.09	109.99
12	B	815	CLA	C3C-C4C-NC	2.52	113.66	110.43
12	B	812	CLA	C1-C2-C3	-2.52	122.06	126.20
12	A	830	CLA	C7-C6-C5	-2.52	106.54	113.26
12	B	845	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
15	B	841	BCR	C38-C26-C27	2.52	118.97	113.60
17	B	837	LMG	O8-C28-C29	2.52	119.52	111.83
12	B	802	CLA	CMA-C3A-C4A	2.52	118.55	111.77
12	B	853	CLA	C3C-C4C-NC	2.52	113.66	110.43
12	B	805	CLA	C4D-C3D-CAD	2.52	110.84	108.11
12	A	808	CLA	CAA-C2A-C3A	-2.52	106.20	113.00
12	B	821	CLA	C3D-C4D-ND	2.51	114.07	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	844	CLA	CHC-C1C-C2C	-2.51	119.81	126.95
12	B	807	CLA	C3C-C4C-NC	2.51	113.65	110.43
15	I	101	BCR	C36-C18-C19	2.51	121.92	118.09
12	K	4003	CLA	C4A-NA-C1A	2.51	107.82	106.68
15	B	834	BCR	C38-C26-C27	2.51	118.95	113.60
12	A	826	CLA	CMC-C2C-C1C	2.51	128.96	125.03
12	B	849	CLA	C4D-C3D-CAD	2.51	110.83	108.11
12	J	102	CLA	C4D-C3D-CAD	2.51	110.83	108.11
12	A	817	CLA	CMC-C2C-C1C	2.51	128.95	125.03
12	B	844	CLA	CMB-C2B-C3B	2.50	132.44	126.55
12	K	4004	CLA	CHC-C1C-C2C	-2.50	119.83	126.95
12	B	824	CLA	C3C-C4C-NC	2.50	113.63	110.43
15	A	835	BCR	C10-C11-C12	-2.50	115.95	123.20
12	A	807	CLA	C4-C3-C5	2.50	119.57	115.23
12	B	813	CLA	CAA-C2A-C1A	2.50	120.15	111.97
12	A	809	CLA	C1-C2-C3	-2.49	122.11	126.20
12	B	843	CLA	O1D-CGD-CBD	-2.49	119.60	124.52
12	A	826	CLA	C4D-C3D-CAD	2.49	110.81	108.11
12	A	819	CLA	CAA-C2A-C3A	-2.49	106.26	113.00
12	B	826	CLA	C3C-C4C-NC	2.49	113.62	110.43
12	A	824	CLA	C1-O2A-CGA	2.49	122.68	116.65
12	B	843	CLA	CMA-C3A-C4A	2.49	118.47	111.77
12	B	812	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
12	B	849	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
12	B	801	CLA	CMC-C2C-C1C	2.49	128.92	125.03
12	B	843	CLA	C3C-C4C-NC	2.49	113.62	110.43
15	B	835	BCR	C15-C16-C17	-2.49	118.43	123.52
15	F	202	BCR	C30-C25-C26	-2.49	119.24	122.64
12	B	853	CLA	O1D-CGD-CBD	-2.49	119.61	124.52
12	A	819	CLA	C4D-C3D-CAD	2.49	110.81	108.11
12	A	819	CLA	CMC-C2C-C1C	2.49	128.92	125.03
12	B	817	CLA	C3C-C4C-NC	2.49	113.61	110.43
17	B	837	LMG	C7-O1-C1	-2.48	108.47	113.80
12	B	812	CLA	C4-C3-C5	2.48	119.54	115.23
15	B	841	BCR	C2-C1-C6	2.48	114.05	110.44
12	B	812	CLA	CHC-C1C-C2C	-2.48	119.89	126.95
12	B	850	CLA	OBD-CAD-C3D	-2.48	122.61	128.42
12	B	824	CLA	O2A-C1-C2	2.48	117.66	108.11
12	A	803	CLA	CMC-C2C-C1C	2.48	128.91	125.03
12	B	852	CLA	CHD-C4C-NC	-2.48	120.39	124.23
12	B	816	CLA	C4-C3-C5	2.48	119.53	115.23
15	L	207	BCR	C37-C22-C23	2.48	121.87	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	K	4002	CLA	CMB-C2B-C1B	2.48	129.19	125.42
12	B	850	CLA	CMC-C2C-C1C	2.48	128.91	125.03
12	B	811	CLA	C3C-C4C-NC	2.48	113.60	110.43
12	B	824	CLA	CBC-CAC-C3C	-2.48	105.71	112.42
12	A	806	CLA	C3C-C4C-NC	2.48	113.60	110.43
12	A	821	CLA	C4D-C3D-CAD	2.48	110.80	108.11
15	L	207	BCR	C2-C1-C6	2.48	114.03	110.44
12	A	809	CLA	C2B-C1B-NB	2.47	112.89	110.33
12	B	850	CLA	C1-C2-C3	-2.47	122.14	126.20
12	B	842	CLA	C3C-C4C-NC	2.47	113.60	110.43
12	B	846	CLA	C3B-C4B-NB	2.47	112.74	110.53
12	A	813	CLA	CAC-C3C-C4C	2.47	128.01	124.79
12	A	847	CLA	CED-O2D-CGD	2.47	121.52	115.92
12	B	827	CLA	CMC-C2C-C1C	2.47	128.90	125.03
12	A	858	CLA	C17-C16-C15	-2.47	102.20	113.28
18	L	210	LMT	C1B-O5B-C5B	2.47	118.55	113.72
12	K	4002	CLA	C2A-C3A-C4A	-2.47	97.88	101.87
12	A	816	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
12	B	805	CLA	C3D-C4D-ND	2.47	114.00	109.99
12	B	852	CLA	C3D-C4D-ND	2.47	114.00	109.99
12	A	832	CLA	C3D-C4D-ND	2.47	114.00	109.99
12	A	801	CLA	C4D-C3D-CAD	2.47	110.79	108.11
12	A	821	CLA	C3C-C4C-NC	2.47	113.59	110.43
12	A	833	CLA	CMA-C3A-C4A	2.46	118.40	111.77
12	A	823	CLA	C2B-C1B-NB	2.46	112.88	110.33
12	A	852	CLA	C3D-C4D-ND	2.46	113.99	109.99
15	B	835	BCR	C37-C22-C23	2.46	121.85	118.09
12	B	822	CLA	O2D-CGD-O1D	-2.46	119.05	123.85
12	A	852	CLA	C3C-C4C-NC	2.46	113.59	110.43
12	A	811	CLA	C4D-C3D-CAD	2.46	110.78	108.11
12	A	832	CLA	CMC-C2C-C1C	2.46	128.88	125.03
15	I	101	BCR	C7-C8-C9	-2.46	122.59	126.23
12	B	849	CLA	CMA-C3A-C4A	2.46	118.38	111.77
12	A	813	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
15	A	836	BCR	C10-C11-C12	-2.46	116.08	123.20
12	A	847	CLA	CMC-C2C-C1C	2.46	128.88	125.03
19	A	854	PL9	C22-C21-C19	-2.46	105.04	113.19
12	A	833	CLA	CMC-C2C-C1C	2.46	128.88	125.03
18	L	210	LMT	C1'-O5'-C5'	2.46	118.52	113.72
12	A	829	CLA	C1-C2-C3	-2.46	122.17	126.20
15	J	105	BCR	C37-C22-C23	2.46	121.84	118.09
12	L	204	CLA	C4D-C3D-CAD	2.46	110.78	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	206	CLA	C3C-C4C-NC	2.46	113.58	110.43
12	A	829	CLA	C4-C3-C2	-2.46	117.32	123.63
12	A	829	CLA	C3C-C4C-NC	2.46	113.58	110.43
12	A	833	CLA	C3C-C4C-NC	2.46	113.58	110.43
12	A	849	CLA	O2D-CGD-O1D	-2.46	119.07	123.85
12	A	852	CLA	CHD-C4C-C3C	-2.46	121.19	124.77
15	F	201	BCR	C16-C17-C18	-2.45	123.84	127.28
17	A	840	LMG	C7-O1-C1	-2.45	108.53	113.80
12	A	824	CLA	O2D-CGD-O1D	-2.45	119.07	123.85
12	A	852	CLA	O2D-CGD-O1D	-2.45	119.07	123.85
12	B	818	CLA	CHD-C4C-C3C	-2.45	121.20	124.77
12	J	101	CLA	C2A-C3A-C4A	-2.45	97.91	101.87
12	A	829	CLA	CMB-C2B-C1B	2.45	129.15	125.42
12	A	858	CLA	CMC-C2C-C1C	2.45	128.87	125.03
20	A	856	45D	C33-C35-C37	2.45	122.87	119.01
12	B	825	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
15	A	838	BCR	C24-C25-C26	-2.45	115.91	121.56
12	B	850	CLA	O2A-CGA-CBA	2.45	119.31	111.83
12	J	102	CLA	C3C-C4C-NC	2.45	113.57	110.43
12	B	806	CLA	CAA-CBA-CGA	-2.45	106.26	113.21
12	K	4004	CLA	C4-C3-C5	2.45	119.47	115.23
12	B	828	CLA	C4-C3-C5	2.45	119.47	115.23
12	B	804	CLA	C3C-C4C-NC	2.44	113.56	110.43
12	A	823	CLA	C4D-C3D-CAD	2.44	110.76	108.11
15	I	101	BCR	C15-C16-C17	-2.44	118.53	123.52
12	B	830	CLA	C4D-C3D-CAD	2.44	110.75	108.11
12	B	803	CLA	C1-C2-C3	-2.44	122.20	126.20
12	A	828	CLA	C4-C3-C5	2.44	119.46	115.23
15	K	4001	BCR	C21-C20-C19	-2.44	116.14	123.20
12	A	849	CLA	O2A-C1-C2	2.44	117.49	108.11
12	A	813	CLA	C4D-C3D-CAD	2.44	110.75	108.11
12	K	4003	CLA	CHD-C1D-ND	-2.44	121.37	124.80
12	K	4002	CLA	CHC-C1C-C2C	-2.44	120.03	126.95
12	A	858	CLA	C4-C3-C5	2.43	119.45	115.23
12	A	808	CLA	CMB-C2B-C1B	2.43	129.13	125.42
12	A	824	CLA	C4D-C3D-CAD	2.43	110.75	108.11
12	A	803	CLA	C3D-C4D-ND	2.43	113.94	109.99
12	A	826	CLA	O2A-C1-C2	2.43	117.47	108.11
12	B	801	CLA	C4-C3-C5	2.43	119.45	115.23
12	A	808	CLA	CAC-C3C-C4C	2.43	127.95	124.79
12	K	4002	CLA	CMA-C3A-C4A	2.43	118.31	111.77
12	B	825	CLA	O1D-CGD-CBD	-2.43	119.73	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	819	CLA	C4-C3-C5	2.43	119.44	115.23
12	B	809	CLA	C4-C3-C5	2.43	119.44	115.23
12	A	815	CLA	C3D-C4D-ND	2.43	113.93	109.99
15	A	837	BCR	C20-C19-C18	-2.43	119.71	126.36
12	A	808	CLA	C4D-C3D-CAD	2.43	110.74	108.11
15	B	834	BCR	C16-C17-C18	-2.43	123.88	127.28
18	B	840	LMT	O5'-C1'-O1'	-2.42	104.31	110.04
12	B	819	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
12	B	828	CLA	O2A-CGA-CBA	2.42	119.23	111.83
12	B	816	CLA	C1-O2A-CGA	2.42	122.52	116.65
12	B	808	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
12	A	843	CLA	C6-C7-C8	-2.42	107.92	115.97
20	A	856	45D	C39-C35-C37	-2.42	118.89	122.82
12	A	845	CLA	CMB-C2B-C1B	2.42	129.10	125.42
18	L	210	LMT	O1B-C4'-C3'	2.42	113.38	107.23
12	A	801	CLA	C4C-C3C-C2C	-2.42	103.37	106.89
12	A	814	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
12	B	814	CLA	C4-C3-C5	2.42	119.42	115.23
15	B	841	BCR	C1-C6-C5	-2.42	119.33	122.64
12	A	848	CLA	C4D-C3D-CAD	2.42	110.73	108.11
12	B	812	CLA	C4B-C3B-C2B	-2.42	104.30	107.30
12	A	808	CLA	O2D-CGD-O1D	-2.42	119.15	123.85
15	K	4005	BCR	C2-C1-C6	2.41	113.94	110.44
12	A	803	CLA	O1D-CGD-CBD	-2.41	119.76	124.52
12	B	804	CLA	C1-O2A-CGA	2.41	122.48	116.65
12	K	4002	CLA	O1D-CGD-CBD	-2.41	119.77	124.52
12	B	819	CLA	C3D-C4D-ND	2.41	113.90	109.99
12	L	205	CLA	CMA-C3A-C4A	-2.41	105.31	111.77
12	B	823	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
12	B	852	CLA	CMB-C2B-C3B	2.40	132.20	126.55
12	A	845	CLA	C3C-C4C-NC	2.40	113.51	110.43
12	B	821	CLA	C3C-C4C-NC	2.40	113.51	110.43
15	B	835	BCR	C15-C14-C13	-2.40	123.91	127.28
12	B	815	CLA	CMB-C2B-C3B	2.40	132.19	126.55
12	A	844	CLA	CAC-C3C-C4C	2.40	127.91	124.79
12	K	4004	CLA	CAC-C3C-C4C	2.40	127.91	124.79
12	B	846	CLA	C6-C5-C3	-2.40	107.63	113.47
12	A	810	CLA	C3C-C4C-NC	2.40	113.50	110.43
12	A	803	CLA	C3C-C4C-NC	2.40	113.50	110.43
12	A	831	CLA	O2D-CGD-O1D	-2.40	119.19	123.85
12	B	810	CLA	O2D-CGD-O1D	-2.39	119.19	123.85
12	A	803	CLA	O2A-C1-C2	2.39	117.31	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	845	CLA	C3C-C4C-NC	2.39	113.49	110.43
12	B	804	CLA	CED-O2D-CGD	2.39	121.34	115.92
12	B	844	CLA	C11-C10-C8	-2.39	108.02	115.97
12	A	809	CLA	CAC-C3C-C4C	2.39	127.90	124.79
12	B	850	CLA	C2A-C3A-C4A	-2.39	98.01	101.87
12	A	827	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
15	F	202	BCR	C27-C26-C25	-2.39	119.48	122.70
12	B	845	CLA	C6-C5-C3	-2.39	107.65	113.47
12	A	855	CLA	C3C-C4C-NC	2.39	113.49	110.43
12	B	801	CLA	C3C-C4C-NC	2.39	113.49	110.43
12	A	830	CLA	C1-O2A-CGA	2.39	122.43	116.65
18	J	106	LMT	O3'-C3'-C2'	-2.39	104.75	110.38
12	B	806	CLA	C3C-C4C-NC	2.39	113.49	110.43
12	A	801	CLA	O1D-CGD-CBD	-2.39	119.81	124.52
12	A	814	CLA	C2A-C3A-C4A	-2.38	98.02	101.87
12	B	809	CLA	C3D-C4D-ND	2.38	113.86	109.99
12	A	828	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
15	F	201	BCR	C3-C4-C5	-2.38	109.80	114.06
12	B	803	CLA	CHD-C4C-C3C	-2.38	121.30	124.77
12	A	807	CLA	CMA-C3A-C2A	-2.38	104.77	113.98
15	K	4005	BCR	C7-C8-C9	-2.38	122.71	126.23
12	A	811	CLA	O1D-CGD-CBD	-2.38	119.82	124.52
15	I	101	BCR	C20-C19-C18	-2.38	119.83	126.36
12	A	815	CLA	CMB-C2B-C1B	2.38	129.04	125.42
12	A	810	CLA	C1-C2-C3	-2.38	122.91	126.76
12	B	807	CLA	C6-C5-C3	-2.38	107.67	113.47
12	B	830	CLA	CMA-C3A-C2A	2.38	123.18	113.98
12	B	824	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
12	A	807	CLA	CMC-C2C-C1C	2.38	128.75	125.03
12	B	847	CLA	CAA-C2A-C1A	-2.38	104.19	111.97
12	A	803	CLA	OBD-CAD-C3D	-2.37	122.87	128.42
15	L	208	BCR	C20-C21-C22	-2.37	123.95	127.28
12	B	825	CLA	C4D-C3D-CAD	2.37	110.68	108.11
12	B	813	CLA	CAC-C3C-C4C	2.37	127.88	124.79
12	K	4002	CLA	C3C-C4C-NC	2.37	113.47	110.43
12	B	823	CLA	CMB-C2B-C3B	2.37	132.13	126.55
15	F	202	BCR	C30-C25-C24	2.37	122.08	115.65
12	J	101	CLA	C4D-C3D-CAD	2.37	110.68	108.11
12	B	842	CLA	C1-O2A-CGA	2.37	122.39	116.65
12	A	803	CLA	CED-O2D-CGD	2.37	121.29	115.92
12	B	823	CLA	C3C-C4C-NC	2.37	113.46	110.43
25	L	202	EQ3	C35-C13-C14	-2.37	118.98	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	805	CLA	CED-O2D-CGD	2.37	121.28	115.92
12	B	810	CLA	CAC-C3C-C4C	2.37	127.87	124.79
12	A	830	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
16	M	103	LHG	O8-C6-C5	2.36	115.21	108.40
15	F	201	BCR	C34-C9-C8	2.36	121.70	118.09
12	A	848	CLA	CMA-C3A-C4A	2.36	118.12	111.77
13	A	802	CL0	CMC-C2C-C1C	2.36	128.72	125.03
20	A	856	45D	C40-C36-C38	-2.36	118.99	122.82
12	A	825	CLA	CMD-C2D-C3D	-2.36	122.28	127.69
27	M	102	SQD	O48-C23-C24	2.36	119.03	111.83
12	A	849	CLA	C3C-C4C-NC	2.36	113.45	110.43
15	K	4005	BCR	C15-C16-C17	-2.36	118.69	123.52
12	A	827	CLA	CAC-C3C-C4C	2.36	127.86	124.79
12	K	4003	CLA	C3B-C4B-NB	-2.36	108.43	110.53
12	A	805	CLA	C2A-C3A-C4A	-2.36	98.06	101.87
15	J	107	BCR	C36-C18-C19	2.35	121.69	118.09
17	A	851	LMG	O7-C10-O9	-2.35	118.20	123.70
12	B	818	CLA	C11-C10-C8	-2.35	108.14	115.97
12	B	822	CLA	O1D-CGD-CBD	-2.35	119.88	124.52
12	A	803	CLA	C4D-C3D-CAD	2.35	110.66	108.11
12	A	833	CLA	CMB-C2B-C3B	2.35	132.08	126.55
12	B	818	CLA	C3D-C4D-ND	2.35	113.81	109.99
12	B	827	CLA	C3C-C4C-NC	2.35	113.44	110.43
16	A	839	LHG	O8-C23-O10	-2.35	117.75	123.63
12	A	848	CLA	CMB-C2B-C1B	2.35	129.00	125.42
12	K	4002	CLA	OBD-CAD-C3D	-2.35	122.93	128.42
12	B	819	CLA	C4C-C3C-C2C	-2.35	103.48	106.89
15	B	834	BCR	C36-C18-C19	2.35	121.67	118.09
15	A	836	BCR	C20-C19-C18	-2.35	119.93	126.36
12	B	820	CLA	C2A-C3A-C4A	-2.35	98.08	101.87
12	F	203	CLA	CHD-C4C-C3C	-2.35	121.35	124.77
12	A	807	CLA	CMB-C2B-C1B	2.35	128.99	125.42
15	B	834	BCR	C30-C25-C26	-2.34	119.43	122.64
12	A	823	CLA	O1D-CGD-CBD	-2.34	119.89	124.52
20	A	856	45D	C10-C06-C04	-2.34	109.78	113.21
12	B	821	CLA	CAC-C3C-C4C	2.34	127.84	124.79
15	K	4005	BCR	C30-C25-C24	2.34	122.00	115.65
12	A	810	CLA	C5-C3-C4	2.34	119.97	114.59
12	A	825	CLA	C3D-C4D-ND	2.34	113.79	109.99
12	A	818	CLA	C4D-C3D-CAD	2.34	110.64	108.11
12	K	4002	CLA	CED-O2D-CGD	2.34	121.22	115.92
12	B	807	CLA	O1D-CGD-CBD	-2.34	119.91	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	848	CLA	C3C-C4C-NC	2.33	113.42	110.43
15	A	835	BCR	C29-C30-C25	2.33	113.83	110.44
12	B	829	CLA	C4C-C3C-C2C	-2.33	103.50	106.89
12	B	822	CLA	C4D-C3D-CAD	2.33	110.64	108.11
12	A	847	CLA	C3C-C4C-NC	2.33	113.42	110.43
12	A	830	CLA	C2A-C3A-C4A	-2.33	98.10	101.87
12	F	203	CLA	C3D-C4D-ND	2.33	113.78	109.99
12	B	801	CLA	C4D-C3D-CAD	2.33	110.64	108.11
12	A	806	CLA	CAC-C3C-C4C	2.33	127.82	124.79
12	B	810	CLA	C3C-C4C-NC	2.33	113.41	110.43
12	J	103	CLA	CED-O2D-CGD	2.33	121.19	115.92
12	A	812	CLA	C3C-C4C-NC	2.33	113.41	110.43
12	B	828	CLA	C6-C5-C3	-2.32	107.81	113.47
12	J	101	CLA	C3C-C4C-NC	2.32	113.41	110.43
12	B	823	CLA	C4D-C3D-CAD	2.32	110.63	108.11
15	B	832	BCR	C35-C13-C12	2.32	121.64	118.09
15	B	841	BCR	C11-C12-C13	-2.32	120.01	126.36
12	B	812	CLA	C4D-C3D-CAD	2.32	110.62	108.11
12	B	817	CLA	C1-O2A-CGA	2.32	122.26	116.65
12	F	203	CLA	O2D-CGD-CBD	2.32	115.28	111.23
12	A	832	CLA	CMB-C2B-C1B	2.32	128.95	125.42
15	L	207	BCR	C30-C25-C26	-2.31	119.47	122.64
19	A	854	PL9	C21-C19-C18	-2.31	115.98	121.17
12	A	829	CLA	CAC-C3C-C4C	2.31	127.80	124.79
12	B	822	CLA	CMC-C2C-C1C	2.31	128.64	125.03
12	L	201	CLA	CMB-C2B-C3B	2.31	131.98	126.55
15	B	832	BCR	C15-C14-C13	-2.31	124.04	127.28
12	B	813	CLA	C6-C5-C3	-2.31	107.85	113.47
12	J	101	CLA	O1D-CGD-CBD	-2.31	119.97	124.52
12	A	825	CLA	C11-C10-C8	-2.31	108.30	115.97
12	F	204	CLA	CMB-C2B-C1B	2.31	128.93	125.42
12	B	803	CLA	C1-O2A-CGA	2.31	122.23	116.65
12	B	820	CLA	O2D-CGD-O1D	-2.30	119.36	123.85
12	A	816	CLA	C4-C3-C5	2.30	119.23	115.23
12	L	205	CLA	CMC-C2C-C1C	2.30	128.63	125.03
12	A	847	CLA	C4D-C3D-CAD	2.30	110.61	108.11
15	A	836	BCR	C35-C13-C12	2.30	121.61	118.09
12	B	802	CLA	C4-C3-C2	-2.30	117.71	123.63
12	A	845	CLA	CAC-C3C-C4C	2.30	127.79	124.79
12	B	844	CLA	C6-C7-C8	-2.30	108.32	115.97
12	A	812	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
12	B	824	CLA	C3D-C4D-ND	2.30	113.72	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	L	208	BCR	C10-C11-C12	-2.30	116.55	123.20
17	A	840	LMG	C19-C18-C17	2.29	125.96	114.37
12	B	816	CLA	C4C-C3C-C2C	-2.29	103.56	106.89
12	B	812	CLA	CED-O2D-CGD	2.29	121.11	115.92
18	J	106	LMT	C1'-O5'-C5'	2.29	118.20	113.72
12	B	825	CLA	C3C-C4C-NC	2.29	113.36	110.43
12	B	842	CLA	C4D-C3D-CAD	2.29	110.59	108.11
15	J	107	BCR	C10-C11-C12	-2.29	116.57	123.20
12	A	807	CLA	O1D-CGD-CBD	-2.29	120.01	124.52
12	B	801	CLA	C1-O2A-CGA	2.29	122.19	116.65
12	A	844	CLA	CAA-C2A-C3A	-2.29	106.82	113.00
12	A	832	CLA	O2A-C1-C2	2.29	116.90	108.11
12	B	846	CLA	CMB-C2B-C1B	2.29	128.90	125.42
15	K	4005	BCR	C16-C15-C14	-2.29	118.84	123.52
12	B	813	CLA	C3D-C4D-ND	2.29	113.70	109.99
12	A	815	CLA	CAA-CBA-CGA	-2.28	106.72	113.21
19	A	854	PL9	C16-C17-C18	-2.28	100.72	112.02
15	A	837	BCR	C34-C9-C8	2.28	121.57	118.09
12	A	848	CLA	O2A-C1-C2	2.28	116.88	108.11
23	M	101	ECH	C30-C25-C24	2.28	121.83	115.65
15	A	838	BCR	C30-C25-C26	-2.28	119.52	122.64
12	A	809	CLA	CHD-C4C-NC	-2.28	120.70	124.23
12	A	806	CLA	CED-O2D-CGD	2.28	121.08	115.92
12	L	206	CLA	C1-O2A-CGA	2.28	122.16	116.65
12	A	820	CLA	O1D-CGD-CBD	-2.27	120.03	124.52
12	B	829	CLA	CHC-C1C-NC	-2.27	120.89	124.31
12	B	819	CLA	CHD-C4C-C3C	-2.27	121.46	124.77
12	A	804	CLA	O2D-CGD-O1D	-2.27	119.42	123.85
12	B	843	CLA	CAA-C2A-C1A	-2.27	104.53	111.97
15	J	107	BCR	C11-C12-C13	-2.27	120.14	126.36
12	A	812	CLA	CMB-C2B-C1B	2.27	128.88	125.42
15	F	202	BCR	C15-C16-C17	-2.27	118.88	123.52
12	K	4004	CLA	C4D-CHA-C1A	-2.27	118.54	121.24
12	B	806	CLA	CMB-C2B-C3B	2.27	131.89	126.55
12	B	825	CLA	CAA-C2A-C1A	-2.27	104.55	111.97
12	B	811	CLA	CAA-CBA-CGA	2.27	119.64	113.21
12	A	832	CLA	C4D-C3D-CAD	2.27	110.57	108.11
12	B	811	CLA	O1D-CGD-CBD	-2.26	120.05	124.52
12	A	804	CLA	C4-C3-C5	2.26	119.16	115.23
12	A	816	CLA	C3C-C4C-NC	2.26	113.33	110.43
12	J	102	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
12	A	844	CLA	C4-C3-C5	2.26	119.16	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	844	CLA	C5-C3-C2	-2.26	116.09	121.17
12	B	802	CLA	C4D-C3D-CAD	2.26	110.56	108.11
12	B	812	CLA	C2B-C1B-NB	2.26	112.67	110.33
12	A	855	CLA	OBD-CAD-C3D	-2.26	123.13	128.42
12	A	828	CLA	C3C-C4C-NC	2.26	113.33	110.43
12	A	823	CLA	CHC-C1C-C2C	-2.26	120.52	126.95
17	A	851	LMG	O1-C7-C8	2.26	116.32	110.82
15	K	4005	BCR	C1-C6-C5	-2.26	119.55	122.64
12	B	815	CLA	C4D-C3D-CAD	2.26	110.56	108.11
12	A	824	CLA	CAC-C3C-C4C	2.26	127.73	124.79
12	B	812	CLA	CMA-C3A-C4A	2.26	117.84	111.77
12	A	824	CLA	CED-O2D-CGD	2.25	121.03	115.92
12	B	846	CLA	CED-O2D-CGD	2.25	121.02	115.92
12	A	818	CLA	CAC-C3C-C4C	2.25	127.72	124.79
12	B	830	CLA	CMA-C3A-C4A	2.25	117.82	111.77
12	A	811	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
12	B	845	CLA	C4D-C3D-CAD	2.25	110.55	108.11
12	A	825	CLA	CMB-C2B-C3B	2.25	131.84	126.55
12	F	204	CLA	CBA-CAA-C2A	-2.25	107.10	113.79
12	F	203	CLA	C4D-CHA-C1A	2.25	123.92	121.24
12	B	806	CLA	C1-O2A-CGA	2.25	122.09	116.65
15	J	107	BCR	C37-C22-C21	-2.25	119.18	122.82
12	A	830	CLA	CHC-C1C-C2C	-2.24	120.57	126.95
12	B	818	CLA	C16-C15-C13	-2.24	108.50	115.97
12	B	842	CLA	CMC-C2C-C1C	2.24	128.54	125.03
12	B	823	CLA	C1-C2-C3	-2.24	122.52	126.20
12	A	806	CLA	O2D-CGD-O1D	-2.24	119.48	123.85
12	A	812	CLA	CHC-C1C-C2C	-2.24	120.58	126.95
12	B	846	CLA	CHC-C1C-C2C	-2.24	120.58	126.95
12	B	808	CLA	CMB-C2B-C3B	2.24	131.82	126.55
12	A	816	CLA	CED-O2D-CGD	2.24	120.99	115.92
12	B	818	CLA	O1D-CGD-CBD	-2.24	120.11	124.52
12	A	827	CLA	CMC-C2C-C1C	2.24	128.53	125.03
12	A	832	CLA	C4C-C3C-C2C	-2.23	103.64	106.89
12	B	842	CLA	CAC-C3C-C4C	2.23	127.70	124.79
12	B	821	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
15	J	105	BCR	C3-C4-C5	-2.23	110.08	114.06
12	L	201	CLA	O1D-CGD-CBD	-2.23	120.12	124.52
15	F	201	BCR	C24-C25-C26	2.23	126.69	121.56
12	A	809	CLA	CHB-C4A-NA	2.23	127.62	124.40
12	B	821	CLA	C4D-C3D-CAD	2.23	110.53	108.11
12	B	823	CLA	CMD-C2D-C3D	-2.23	122.58	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	J	103	CLA	C3C-C4C-NC	2.23	113.28	110.43
15	B	834	BCR	C19-C18-C17	-2.23	115.50	119.01
12	B	846	CLA	C4B-C3B-C2B	-2.23	104.53	107.30
12	A	810	CLA	CMC-C2C-C1C	2.22	128.51	125.03
12	A	820	CLA	CMC-C2C-C1C	2.22	128.51	125.03
12	A	806	CLA	CMB-C2B-C1B	2.22	128.80	125.42
12	A	817	CLA	C5-C3-C4	2.22	119.70	114.59
12	B	812	CLA	CMA-C3A-C2A	-2.22	105.39	113.98
12	A	827	CLA	CMA-C3A-C2A	-2.22	105.39	113.98
15	J	104	BCR	C37-C22-C23	-2.22	116.55	118.57
12	B	810	CLA	C4D-C3D-CAD	2.22	110.52	108.11
12	A	807	CLA	C4D-C3D-CAD	2.22	110.52	108.11
22	B	831	A1AGD	C3-C4-C5	2.22	121.34	118.57
12	A	855	CLA	C4-C3-C5	2.22	119.08	115.23
12	B	845	CLA	C4-C3-C5	2.22	119.08	115.23
12	B	830	CLA	C3C-C4C-NC	2.22	113.27	110.43
12	A	809	CLA	CMB-C2B-C1B	2.22	128.79	125.42
19	A	854	PL9	C20-C19-C21	2.22	119.07	115.23
12	B	853	CLA	C6-C7-C8	-2.21	108.61	115.97
12	J	101	CLA	C4A-NA-C1A	2.21	107.69	106.68
12	B	826	CLA	CAC-C3C-C4C	2.21	127.67	124.79
12	B	813	CLA	C4C-C3C-C2C	-2.21	103.67	106.89
12	B	848	CLA	C4C-C3C-C2C	-2.21	103.67	106.89
12	L	204	CLA	O1D-CGD-CBD	-2.21	120.15	124.52
12	K	4004	CLA	CED-O2D-CGD	-2.21	110.89	115.92
12	B	818	CLA	C4C-C3C-C2C	-2.21	103.67	106.89
12	B	846	CLA	CHB-C4A-NA	2.21	127.59	124.40
12	J	101	CLA	CGD-CBD-CAD	-2.21	103.69	110.85
12	A	820	CLA	OBD-CAD-C3D	-2.21	123.25	128.42
12	A	805	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
12	B	821	CLA	CMB-C2B-C3B	2.21	131.75	126.55
15	B	835	BCR	C12-C13-C14	-2.21	115.53	119.01
20	A	856	45D	C28-C26-C24	2.21	121.46	118.09
15	A	836	BCR	C1-C6-C5	-2.21	119.62	122.64
15	F	201	BCR	C36-C18-C19	2.21	121.46	118.09
12	B	825	CLA	CMD-C2D-C3D	-2.21	122.62	127.69
12	A	805	CLA	O2D-CGD-O1D	-2.21	119.55	123.85
12	A	816	CLA	C4D-C3D-CAD	2.21	110.50	108.11
16	B	851	LHG	C6-C5-C4	-2.21	106.64	111.78
12	A	813	CLA	C4C-C3C-C2C	-2.21	103.68	106.89
12	A	804	CLA	C4D-C3D-CAD	2.21	110.50	108.11
12	B	846	CLA	C4D-C3D-CAD	2.20	110.50	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	L	207	BCR	C20-C19-C18	-2.20	120.32	126.36
12	B	820	CLA	CMB-C2B-C1B	2.20	128.77	125.42
16	B	851	LHG	O4-P-O5	2.20	122.69	112.44
12	A	855	CLA	CHC-C1C-C2C	-2.20	120.69	126.95
12	A	822	CLA	C1-C2-C3	-2.20	122.59	126.20
12	B	810	CLA	CMB-C2B-C1B	2.20	128.77	125.42
12	A	810	CLA	CMA-C3A-C4A	-2.20	105.86	111.77
12	A	844	CLA	CMB-C2B-C3B	2.20	131.72	126.55
12	B	844	CLA	CBA-CAA-C2A	-2.20	107.25	113.79
12	A	811	CLA	CMC-C2C-C1C	2.20	128.47	125.03
12	B	824	CLA	OBD-CAD-C3D	-2.20	123.28	128.42
12	A	805	CLA	C4D-C3D-CAD	2.20	110.49	108.11
12	A	818	CLA	C3D-C4D-ND	2.20	113.56	109.99
12	F	204	CLA	CMD-C2D-C3D	-2.20	122.65	127.69
12	A	855	CLA	C3D-C4D-ND	2.20	113.56	109.99
12	A	858	CLA	C4C-C3C-C2C	-2.19	103.70	106.89
12	B	816	CLA	C6-C5-C3	-2.19	108.12	113.47
17	A	851	LMG	C9-O8-C28	2.19	125.14	117.12
12	B	829	CLA	CED-O2D-CGD	2.19	120.89	115.92
12	B	807	CLA	CMB-C2B-C3B	2.19	131.71	126.55
15	B	835	BCR	C20-C19-C18	-2.19	120.35	126.36
12	A	847	CLA	CAC-C3C-C4C	2.19	127.64	124.79
12	L	206	CLA	CMB-C2B-C3B	2.19	131.70	126.55
16	M	103	LHG	O8-C23-O10	-2.19	118.16	123.63
12	A	827	CLA	C1-O2A-CGA	2.19	121.94	116.65
12	B	849	CLA	C4-C3-C2	-2.19	118.01	123.63
12	A	812	CLA	CAC-C3C-C4C	2.19	127.63	124.79
12	B	811	CLA	CHC-C1C-C2C	-2.18	120.74	126.95
12	A	806	CLA	CMD-C2D-C3D	-2.18	122.68	127.69
15	B	835	BCR	C11-C10-C9	-2.18	124.22	127.28
12	A	824	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
15	A	837	BCR	C11-C12-C13	-2.18	120.38	126.36
15	A	835	BCR	C35-C13-C12	2.18	121.42	118.09
12	A	825	CLA	CMA-C3A-C2A	-2.18	105.55	113.98
12	A	829	CLA	C4B-CHC-C1C	2.18	131.37	126.25
12	B	818	CLA	C4-C3-C5	2.18	119.01	115.23
13	A	802	CL0	O2D-CGD-O1D	-2.18	119.61	123.85
15	K	4001	BCR	C12-C13-C14	-2.18	115.58	119.01
12	A	826	CLA	CED-O2D-CGD	2.18	120.85	115.92
27	M	102	SQD	O8-S-C6	2.18	110.17	105.97
15	K	4005	BCR	C24-C25-C26	-2.17	116.55	121.56
12	A	843	CLA	CMD-C2D-C3D	-2.17	122.70	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	858	CLA	CMA-C3A-C2A	-2.17	105.58	113.98
15	L	208	BCR	C38-C26-C27	2.17	118.23	113.60
12	A	825	CLA	CED-O2D-CGD	2.17	120.85	115.92
15	F	201	BCR	C38-C26-C27	2.17	118.23	113.60
12	B	819	CLA	CMC-C2C-C1C	2.17	128.43	125.03
12	B	822	CLA	CAC-C3C-C4C	2.17	127.62	124.79
12	A	801	CLA	C1-O2A-CGA	2.17	121.91	116.65
12	A	810	CLA	C4D-C3D-CAD	2.17	110.46	108.11
12	F	203	CLA	CMB-C2B-C1B	2.17	128.72	125.42
12	A	831	CLA	CMD-C2D-C3D	-2.17	122.71	127.69
25	L	202	EQ3	C37-C22-C23	2.17	121.40	118.09
12	A	815	CLA	OBD-CAD-C3D	-2.17	123.35	128.42
12	A	827	CLA	C4D-C3D-CAD	2.17	110.46	108.11
12	A	814	CLA	C4D-C3D-CAD	2.17	110.46	108.11
12	B	827	CLA	C4D-C3D-CAD	2.17	110.46	108.11
12	B	827	CLA	CMB-C2B-C1B	2.17	128.72	125.42
12	B	804	CLA	O2D-CGD-O1D	-2.16	119.64	123.85
12	B	820	CLA	C4D-C3D-CAD	2.16	110.46	108.11
15	B	834	BCR	C1-C6-C5	-2.16	119.68	122.64
12	B	852	CLA	C5-C3-C4	2.16	119.57	114.59
12	L	204	CLA	C4-C3-C5	2.16	118.98	115.23
12	B	807	CLA	O2A-C1-C2	2.16	116.43	108.11
12	A	813	CLA	CMD-C2D-C3D	-2.16	122.73	127.69
12	L	205	CLA	C4D-C3D-CAD	2.16	110.45	108.11
12	B	802	CLA	C7-C6-C5	2.16	119.02	113.26
12	A	819	CLA	CAA-C2A-C1A	-2.16	104.90	111.97
15	K	4005	BCR	C20-C19-C18	-2.16	120.44	126.36
23	M	101	ECH	C20-C21-C22	2.16	130.31	127.28
17	A	840	LMG	C20-C19-C18	2.16	125.28	114.37
12	A	816	CLA	CMC-C2C-C1C	2.16	128.41	125.03
12	B	804	CLA	CMB-C2B-C3B	2.16	131.62	126.55
12	A	805	CLA	CBA-CAA-C2A	-2.15	107.38	113.79
17	B	837	LMG	O1-C1-C2	2.15	111.55	108.27
12	A	848	CLA	C5-C3-C2	-2.15	116.33	121.17
12	L	206	CLA	C1-C2-C3	-2.15	122.67	126.20
12	B	807	CLA	C4D-C3D-CAD	2.15	110.44	108.11
15	B	834	BCR	C37-C22-C23	2.15	121.38	118.09
12	B	819	CLA	C4D-C3D-CAD	2.15	110.44	108.11
12	A	801	CLA	CMD-C2D-C3D	-2.15	122.76	127.69
12	A	829	CLA	O2D-CGD-O1D	-2.15	119.66	123.85
15	K	4001	BCR	C35-C13-C12	2.15	121.37	118.09
19	A	854	PL9	C12-C11-C9	-2.15	106.07	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	823	CLA	CAC-C3C-C4C	2.15	127.58	124.79
12	A	809	CLA	C1-O2A-CGA	2.15	121.85	116.65
12	B	826	CLA	CMB-C2B-C3B	2.15	131.60	126.55
12	B	802	CLA	CHC-C1C-C2C	-2.15	120.85	126.95
12	A	827	CLA	C4-C3-C5	2.15	118.95	115.23
12	B	843	CLA	CED-O2D-CGD	2.15	120.78	115.92
12	B	803	CLA	CHD-C1D-ND	-2.15	121.78	124.80
15	K	4005	BCR	C39-C30-C25	-2.15	106.88	110.24
12	A	820	CLA	C4-C3-C5	2.14	118.95	115.23
12	A	817	CLA	O1D-CGD-CBD	-2.14	120.29	124.52
12	B	828	CLA	C4D-C3D-CAD	2.14	110.43	108.11
15	K	4005	BCR	C35-C13-C12	2.14	121.36	118.09
15	A	835	BCR	C33-C5-C4	2.14	118.16	113.60
12	A	832	CLA	O1D-CGD-CBD	-2.14	120.29	124.52
12	A	844	CLA	CHC-C1C-C2C	-2.14	120.87	126.95
12	J	101	CLA	C4C-C3C-C2C	-2.14	103.78	106.89
12	B	825	CLA	CAC-C3C-C4C	2.14	127.57	124.79
12	A	808	CLA	C5-C3-C4	2.14	119.51	114.59
12	A	811	CLA	C3C-C4C-NC	2.14	113.17	110.43
15	J	105	BCR	C7-C8-C9	-2.14	123.08	126.23
12	B	825	CLA	CMB-C2B-C1B	2.14	128.67	125.42
12	K	4004	CLA	C3C-C4C-NC	2.13	113.17	110.43
12	B	853	CLA	O2A-C1-C2	2.13	116.32	108.11
12	A	822	CLA	C4D-C3D-CAD	2.13	110.42	108.11
12	F	204	CLA	O1D-CGD-CBD	-2.13	120.31	124.52
15	L	207	BCR	C38-C26-C27	2.13	118.14	113.60
12	B	852	CLA	CMD-C2D-C3D	-2.13	122.80	127.69
12	B	845	CLA	CMD-C2D-C3D	-2.13	122.81	127.69
12	F	203	CLA	C4C-C3C-C2C	-2.13	103.79	106.89
12	A	807	CLA	C3C-C4C-NC	2.13	113.16	110.43
12	B	805	CLA	C4B-C3B-C2B	-2.13	104.66	107.30
12	J	102	CLA	CAC-C3C-C4C	2.13	127.56	124.79
12	A	825	CLA	O2A-CGA-CBA	2.13	118.32	111.83
12	A	801	CLA	CAA-C2A-C1A	-2.13	105.00	111.97
12	B	807	CLA	C1-C2-C3	-2.13	122.71	126.20
12	A	819	CLA	C3C-C4C-NC	2.13	113.15	110.43
12	B	802	CLA	CHB-C1B-C2B	-2.13	121.25	127.43
12	A	848	CLA	C1-C2-C3	-2.13	122.71	126.20
12	B	828	CLA	C3C-C4C-NC	2.12	113.15	110.43
12	A	812	CLA	C4B-C3B-C2B	-2.12	104.66	107.30
12	B	828	CLA	CAC-C3C-C4C	2.12	127.55	124.79
12	B	847	CLA	CMB-C2B-C1B	2.12	128.65	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	835	BCR	C36-C18-C19	-2.12	114.84	118.09
19	A	854	PL9	C2-C3-C4	2.12	121.63	118.78
12	B	850	CLA	CHA-C4D-ND	2.12	136.93	132.55
12	A	849	CLA	C1-C2-C3	-2.12	122.72	126.20
12	L	206	CLA	CAC-C3C-C4C	2.12	127.55	124.79
12	B	809	CLA	C4D-C3D-CAD	2.12	110.41	108.11
12	A	843	CLA	O2D-CGD-O1D	-2.12	119.72	123.85
12	A	828	CLA	CHC-C1C-C2C	-2.12	120.92	126.95
12	A	803	CLA	C4C-C3C-C2C	-2.12	103.81	106.89
12	A	818	CLA	O1D-CGD-CBD	-2.12	120.34	124.52
12	B	822	CLA	CMA-C3A-C2A	-2.12	105.80	113.98
12	B	803	CLA	C2A-C3A-C4A	-2.12	98.45	101.87
12	A	843	CLA	CMB-C2B-C3B	2.11	131.52	126.55
12	A	807	CLA	C1-O2A-CGA	2.11	121.77	116.65
12	A	817	CLA	C4D-C3D-CAD	2.11	110.40	108.11
12	L	205	CLA	CMB-C2B-C1B	2.11	128.64	125.42
12	A	843	CLA	C4C-C3C-C2C	-2.11	103.82	106.89
15	B	836	BCR	C37-C22-C21	-2.11	119.39	122.82
23	B	833	ECH	C20-C21-C22	2.11	130.24	127.28
12	B	817	CLA	C4-C3-C2	-2.11	118.21	123.63
12	B	852	CLA	CHC-C1C-C2C	-2.11	120.95	126.95
12	B	848	CLA	CHD-C1D-ND	-2.11	121.83	124.80
18	A	853	LMT	C1B-O5B-C5B	2.11	117.84	113.72
12	K	4004	CLA	CMC-C2C-C1C	2.11	128.33	125.03
12	A	827	CLA	C3C-C4C-NC	2.11	113.13	110.43
12	L	205	CLA	C4-C3-C5	2.11	118.88	115.23
12	B	845	CLA	CMB-C2B-C3B	2.11	131.50	126.55
15	A	836	BCR	C37-C22-C23	2.10	121.30	118.09
12	A	830	CLA	CMB-C2B-C1B	2.10	128.62	125.42
12	B	809	CLA	C6-C5-C3	-2.10	108.34	113.47
15	A	836	BCR	C33-C5-C4	2.10	118.08	113.60
15	F	201	BCR	C1-C6-C5	-2.10	119.76	122.64
15	K	4005	BCR	C21-C20-C19	-2.10	117.11	123.20
18	F	205	LMT	O3'-C3'-C2'	-2.10	105.43	110.38
17	A	840	LMG	O8-C28-C29	2.10	118.24	111.83
12	B	818	CLA	CHA-C1A-NA	-2.10	121.64	126.39
12	B	850	CLA	CHA-C1A-NA	-2.10	121.64	126.39
12	F	203	CLA	CHA-C1A-NA	-2.10	121.64	126.39
12	B	830	CLA	CMD-C2D-C3D	-2.10	122.88	127.69
12	F	204	CLA	CHC-C1C-C2C	-2.10	120.99	126.95
12	A	809	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
12	A	810	CLA	O1D-CGD-CBD	-2.09	120.39	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	825	CLA	CHD-C4C-C3C	-2.09	121.72	124.77
12	B	820	CLA	C11-C12-C13	-2.09	109.01	115.97
12	B	849	CLA	C1-O2A-CGA	2.09	121.71	116.65
12	L	204	CLA	CMD-C2D-C3D	-2.09	122.89	127.69
12	B	824	CLA	CAA-C2A-C3A	-2.09	107.35	113.00
12	B	848	CLA	CMD-C2D-C3D	-2.09	122.89	127.69
15	F	202	BCR	C33-C5-C4	2.09	118.05	113.60
12	A	827	CLA	CMB-C2B-C1B	2.09	128.60	125.42
12	A	849	CLA	CBC-CAC-C3C	-2.09	106.76	112.42
12	A	804	CLA	CHB-C4A-NA	2.09	127.41	124.40
12	A	858	CLA	C2A-C3A-C4A	-2.09	98.50	101.87
12	B	822	CLA	CMD-C2D-C3D	-2.09	122.91	127.69
15	J	105	BCR	C1-C6-C5	-2.09	119.78	122.64
12	A	828	CLA	O2A-C1-C2	2.09	116.13	108.11
12	A	804	CLA	CMD-C2D-C3D	-2.08	122.91	127.69
12	A	843	CLA	C4-C3-C5	2.08	118.84	115.23
12	A	826	CLA	C7-C6-C5	-2.08	107.71	113.26
12	A	813	CLA	C1-O2A-CGA	2.08	121.69	116.65
12	B	845	CLA	CED-O2D-CGD	2.08	120.64	115.92
23	M	101	ECH	C23-C24-C25	2.08	132.56	127.00
12	B	813	CLA	CMB-C2B-C1B	2.08	128.59	125.42
15	J	107	BCR	C4-C5-C6	-2.08	119.89	122.70
15	K	4005	BCR	C23-C22-C21	-2.08	115.74	119.01
12	A	816	CLA	CHB-C1B-C2B	-2.08	121.40	127.43
12	B	816	CLA	C6-C7-C8	-2.08	109.06	115.97
12	A	820	CLA	C4D-C3D-CAD	2.08	110.36	108.11
12	K	4002	CLA	CMD-C2D-C3D	-2.08	122.93	127.69
12	A	846	CLA	CMC-C2C-C1C	2.07	128.28	125.03
12	L	204	CLA	CAC-C3C-C4C	2.07	127.49	124.79
12	B	811	CLA	CBC-CAC-C3C	-2.07	106.80	112.42
20	A	856	45D	C10-C18-C16	2.07	120.50	118.64
15	K	4001	BCR	C29-C30-C25	2.07	113.45	110.44
12	L	205	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
17	B	837	LMG	O8-C28-O10	-2.07	118.44	123.63
15	F	201	BCR	C15-C16-C17	-2.07	119.28	123.52
12	K	4004	CLA	C11-C10-C8	-2.07	109.08	115.97
12	A	852	CLA	C4D-C3D-CAD	2.07	110.35	108.11
15	B	836	BCR	C35-C13-C12	2.07	119.35	114.59
12	B	815	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
12	J	101	CLA	C1-O2A-CGA	2.07	121.65	116.65
15	B	832	BCR	C38-C26-C27	2.07	118.00	113.60
15	B	834	BCR	C8-C9-C10	-2.07	115.76	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	J	107	BCR	C15-C16-C17	-2.07	119.29	123.52
12	A	824	CLA	C4C-C3C-C2C	-2.06	103.89	106.89
16	A	850	LHG	O8-C23-O10	-2.06	118.46	123.63
13	A	802	CL0	CMB-C2B-C1B	2.06	128.56	125.42
12	B	849	CLA	CHC-C1C-C2C	-2.06	121.08	126.95
12	A	827	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
15	B	841	BCR	C34-C9-C8	2.06	121.24	118.09
12	A	814	CLA	C1-C2-C3	-2.06	122.82	126.20
12	B	814	CLA	CMD-C2D-C3D	-2.06	122.96	127.69
12	A	852	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
12	B	847	CLA	C4-C3-C5	2.06	118.81	115.23
12	A	811	CLA	CAC-C3C-C4C	2.06	127.47	124.79
15	A	835	BCR	C16-C17-C18	-2.06	124.39	127.28
15	B	835	BCR	C30-C25-C26	-2.06	119.82	122.64
12	A	830	CLA	C4-C3-C5	2.06	118.80	115.23
12	A	833	CLA	C5-C3-C4	2.06	119.33	114.59
12	A	809	CLA	C4C-C3C-C2C	-2.06	103.89	106.89
15	A	835	BCR	C12-C13-C14	-2.06	115.77	119.01
12	B	843	CLA	O2D-CGD-O1D	-2.06	119.84	123.85
15	L	207	BCR	C11-C12-C13	-2.06	120.72	126.36
12	A	809	CLA	C4-C3-C5	2.06	118.80	115.23
12	A	814	CLA	CMB-C2B-C3B	2.06	131.39	126.55
12	A	819	CLA	CMD-C2D-C3D	-2.05	122.98	127.69
12	A	804	CLA	CHC-C1C-C2C	-2.05	121.11	126.95
12	A	818	CLA	C4C-C3C-C2C	-2.05	103.90	106.89
12	B	805	CLA	CMD-C2D-C3D	-2.05	122.98	127.69
12	A	844	CLA	O2A-C1-C2	2.05	116.01	108.11
12	L	201	CLA	CHC-C1C-C2C	-2.05	121.11	126.95
12	J	101	CLA	C4B-CHC-C1C	2.05	131.07	126.25
12	B	811	CLA	CBA-CAA-C2A	2.05	119.90	113.79
12	K	4002	CLA	C4C-C3C-C2C	-2.05	103.91	106.89
12	A	801	CLA	C11-C10-C8	-2.05	109.15	115.97
12	B	826	CLA	CAA-CBA-CGA	2.05	119.03	113.21
12	A	855	CLA	CBC-CAC-C3C	-2.05	106.86	112.42
12	A	848	CLA	CMD-C2D-C3D	-2.05	122.99	127.69
18	B	840	LMT	O5'-C1'-C2'	2.05	114.58	110.37
15	L	207	BCR	C23-C24-C25	-2.05	121.53	127.00
16	B	851	LHG	O7-C7-O9	-2.05	118.92	123.70
12	B	829	CLA	C4D-C3D-CAD	2.05	110.33	108.11
12	B	816	CLA	C1-C2-C3	-2.04	122.85	126.20
15	B	835	BCR	C2-C1-C6	2.04	113.41	110.44
12	B	830	CLA	CAC-C3C-C4C	2.04	127.45	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	836	BCR	C1-C6-C7	2.04	121.19	115.65
15	A	835	BCR	C29-C28-C27	2.04	115.77	111.28
15	A	838	BCR	C2-C1-C6	2.04	113.41	110.44
12	A	821	CLA	CMD-C2D-C3D	-2.04	123.00	127.69
12	A	849	CLA	C4-C3-C2	-2.04	118.39	123.63
12	B	818	CLA	CMB-C2B-C1B	2.04	128.53	125.42
12	A	823	CLA	C4C-C3C-C2C	-2.04	103.92	106.89
12	B	847	CLA	CHD-C1D-C2D	-2.04	121.25	125.49
12	B	810	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
12	B	843	CLA	C4D-C3D-CAD	2.04	110.32	108.11
12	B	813	CLA	CHA-C1A-NA	-2.04	121.78	126.39
12	B	822	CLA	CAA-C2A-C3A	-2.04	107.49	113.00
15	J	104	BCR	C21-C22-C23	2.04	122.04	119.65
12	F	204	CLA	C3C-C4C-NC	2.04	113.04	110.43
12	B	802	CLA	OBD-CAD-C3D	-2.04	123.66	128.42
12	A	830	CLA	C11-C10-C8	-2.03	109.20	115.97
12	A	843	CLA	C6-C5-C3	-2.03	108.52	113.47
19	A	854	PL9	O2-C1-C2	-2.03	117.21	121.83
12	A	814	CLA	CED-O2D-CGD	2.03	120.53	115.92
15	L	208	BCR	C21-C20-C19	-2.03	117.31	123.20
15	B	841	BCR	C10-C11-C12	-2.03	117.31	123.20
12	A	831	CLA	CMA-C3A-C2A	-2.03	106.13	113.98
12	B	813	CLA	C4D-C3D-CAD	2.03	110.31	108.11
20	A	856	45D	C06-C10-C18	-2.03	109.00	112.71
12	A	815	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
12	A	831	CLA	CMA-C3A-C4A	-2.03	106.32	111.77
12	B	812	CLA	C3B-C4B-NB	2.03	112.34	110.53
12	B	817	CLA	CHC-C1C-C2C	-2.03	121.19	126.95
12	A	818	CLA	C1-O2A-CGA	2.03	121.56	116.65
12	B	801	CLA	CAC-C3C-C4C	2.03	127.42	124.79
15	K	4005	BCR	C32-C1-C6	-2.03	107.07	110.24
15	J	105	BCR	C24-C23-C22	-2.03	123.24	126.23
12	A	825	CLA	C4D-C3D-CAD	2.02	110.31	108.11
15	B	834	BCR	C11-C12-C13	-2.02	120.81	126.36
12	B	825	CLA	CMC-C2C-C1C	2.02	128.19	125.03
15	A	836	BCR	C30-C25-C26	-2.02	119.87	122.64
15	F	202	BCR	C28-C27-C26	2.02	117.66	114.06
13	A	802	CL0	C4C-C3C-C2C	-2.02	103.95	106.89
12	B	830	CLA	CMB-C2B-C3B	2.02	131.30	126.55
12	B	842	CLA	O1D-CGD-CBD	-2.02	120.54	124.52
15	A	838	BCR	C23-C24-C25	-2.02	121.61	127.00
12	A	817	CLA	C3C-C4C-NC	2.02	113.01	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	832	BCR	C10-C11-C12	-2.01	117.36	123.20
12	A	858	CLA	CED-O2D-CGD	2.01	120.48	115.92
12	A	809	CLA	CBC-CAC-C3C	-2.01	106.96	112.42
12	B	823	CLA	CHB-C1B-C2B	-2.01	121.58	127.43
12	A	826	CLA	C1-O2A-CGA	2.01	121.52	116.65
12	A	847	CLA	CHC-C1C-C2C	-2.01	121.23	126.95
12	A	814	CLA	CAC-C3C-C4C	2.01	127.41	124.79
12	A	817	CLA	CED-O2D-CGD	2.01	120.47	115.92
12	A	812	CLA	CMC-C2C-C1C	2.01	128.17	125.03
12	A	805	CLA	C4C-C3C-C2C	-2.01	103.97	106.89
12	A	801	CLA	C2A-C3A-C4A	-2.01	98.62	101.87
18	A	853	LMT	O3'-C3'-C2'	-2.01	105.64	110.38
12	A	833	CLA	CAA-C2A-C3A	-2.01	107.57	113.00
12	A	852	CLA	CAA-CBA-CGA	-2.01	107.51	113.21
12	A	805	CLA	CHD-C4C-C3C	-2.01	121.85	124.77
12	B	813	CLA	CHC-C1C-C2C	-2.01	121.24	126.95
12	A	830	CLA	CMD-C2D-C3D	-2.00	123.09	127.69
12	B	849	CLA	O1D-CGD-CBD	-2.00	120.57	124.52
15	F	202	BCR	C29-C30-C25	2.00	113.35	110.44
12	A	811	CLA	CHC-C1C-C2C	-2.00	121.26	126.95
12	A	828	CLA	CMB-C2B-C3B	2.00	131.26	126.55

There are no chirality outliers.

All (1368) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	803	CLA	C1A-C2A-CAA-CBA
12	A	803	CLA	CBA-CGA-O2A-C1
12	A	803	CLA	O1A-CGA-O2A-C1
12	A	804	CLA	C1A-C2A-CAA-CBA
12	A	804	CLA	C3A-C2A-CAA-CBA
12	A	804	CLA	CAD-CBD-CGD-O2D
12	A	805	CLA	CBA-CGA-O2A-C1
12	A	805	CLA	O1A-CGA-O2A-C1
12	A	805	CLA	CBD-CGD-O2D-CED
12	A	807	CLA	CHA-CBD-CGD-O1D
12	A	807	CLA	CHA-CBD-CGD-O2D
12	A	808	CLA	C1A-C2A-CAA-CBA
12	A	810	CLA	C2-C1-O2A-CGA
12	A	812	CLA	C4B-C3B-CAB-CBB
12	A	813	CLA	C3A-C2A-CAA-CBA
12	A	813	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
12	A	815	CLA	C2-C1-O2A-CGA
12	A	817	CLA	CHA-CBD-CGD-O1D
12	A	817	CLA	CHA-CBD-CGD-O2D
12	A	818	CLA	CHA-CBD-CGD-O1D
12	A	818	CLA	CHA-CBD-CGD-O2D
12	A	823	CLA	CHA-CBD-CGD-O1D
12	A	823	CLA	CHA-CBD-CGD-O2D
12	A	826	CLA	C2B-C3B-CAB-CBB
12	A	827	CLA	C4B-C3B-CAB-CBB
12	A	829	CLA	C2-C1-O2A-CGA
12	A	832	CLA	C1A-C2A-CAA-CBA
12	A	832	CLA	C3A-C2A-CAA-CBA
12	A	833	CLA	CAD-CBD-CGD-O1D
12	A	833	CLA	CAD-CBD-CGD-O2D
12	A	843	CLA	O2A-C1-C2-C3
12	A	844	CLA	C14-C13-C15-C16
12	A	845	CLA	C4B-C3B-CAB-CBB
12	A	845	CLA	CBD-CGD-O2D-CED
12	A	845	CLA	O1D-CGD-O2D-CED
12	A	846	CLA	C1A-C2A-CAA-CBA
12	A	846	CLA	C3A-C2A-CAA-CBA
12	A	847	CLA	C1A-C2A-CAA-CBA
12	A	847	CLA	C2B-C3B-CAB-CBB
12	A	847	CLA	C4B-C3B-CAB-CBB
12	A	848	CLA	C4B-C3B-CAB-CBB
12	A	849	CLA	C11-C12-C13-C14
12	B	804	CLA	C1A-C2A-CAA-CBA
12	B	804	CLA	C11-C10-C8-C9
12	B	806	CLA	C3A-C2A-CAA-CBA
12	B	808	CLA	C1A-C2A-CAA-CBA
12	B	811	CLA	CHA-CBD-CGD-O1D
12	B	811	CLA	CHA-CBD-CGD-O2D
12	B	814	CLA	CBD-CGD-O2D-CED
12	B	816	CLA	C1A-C2A-CAA-CBA
12	B	817	CLA	C1A-C2A-CAA-CBA
12	B	817	CLA	C4-C3-C5-C6
12	B	818	CLA	CHA-CBD-CGD-O1D
12	B	818	CLA	CHA-CBD-CGD-O2D
12	B	820	CLA	C1A-C2A-CAA-CBA
12	B	820	CLA	C3A-C2A-CAA-CBA
12	B	820	CLA	C6-C7-C8-C10
12	B	821	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	B	821	CLA	C3A-C2A-CAA-CBA
12	B	822	CLA	CHA-CBD-CGD-O1D
12	B	822	CLA	CHA-CBD-CGD-O2D
12	B	825	CLA	CHA-CBD-CGD-O2D
12	B	842	CLA	C4-C3-C5-C6
12	B	843	CLA	CHA-CBD-CGD-O1D
12	B	843	CLA	CHA-CBD-CGD-O2D
12	B	846	CLA	C1A-C2A-CAA-CBA
12	B	846	CLA	C3A-C2A-CAA-CBA
12	B	848	CLA	C1A-C2A-CAA-CBA
12	B	848	CLA	CHA-CBD-CGD-O1D
12	B	848	CLA	CHA-CBD-CGD-O2D
12	B	848	CLA	C11-C10-C8-C9
12	F	204	CLA	C4B-C3B-CAB-CBB
12	F	204	CLA	CHA-CBD-CGD-O1D
12	F	204	CLA	CHA-CBD-CGD-O2D
12	J	101	CLA	CHA-CBD-CGD-O1D
12	J	101	CLA	CHA-CBD-CGD-O2D
12	J	102	CLA	C1A-C2A-CAA-CBA
12	J	103	CLA	C2B-C3B-CAB-CBB
12	J	103	CLA	C4B-C3B-CAB-CBB
12	K	4002	CLA	C1A-C2A-CAA-CBA
12	K	4002	CLA	C4B-C3B-CAB-CBB
12	K	4003	CLA	CBD-CGD-O2D-CED
12	K	4003	CLA	O1D-CGD-O2D-CED
12	K	4004	CLA	C1A-C2A-CAA-CBA
12	L	201	CLA	CHA-CBD-CGD-O1D
12	L	201	CLA	CHA-CBD-CGD-O2D
12	L	204	CLA	C1A-C2A-CAA-CBA
12	L	204	CLA	C3A-C2A-CAA-CBA
15	A	835	BCR	C11-C12-C13-C14
15	A	835	BCR	C15-C16-C17-C18
15	A	838	BCR	C21-C22-C23-C24
15	A	838	BCR	C37-C22-C23-C24
15	A	838	BCR	C23-C24-C25-C26
15	B	832	BCR	C7-C8-C9-C10
15	B	832	BCR	C21-C22-C23-C24
15	B	841	BCR	C7-C8-C9-C10
15	B	841	BCR	C7-C8-C9-C34
15	I	101	BCR	C17-C18-C19-C20
15	I	101	BCR	C36-C18-C19-C20
15	J	104	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
15	J	105	BCR	C5-C6-C7-C8
15	J	105	BCR	C17-C18-C19-C20
15	J	105	BCR	C36-C18-C19-C20
15	J	107	BCR	C5-C6-C7-C8
15	J	107	BCR	C9-C10-C11-C12
15	K	4001	BCR	C21-C22-C23-C24
15	K	4001	BCR	C23-C24-C25-C30
15	K	4005	BCR	C17-C18-C19-C20
15	L	207	BCR	C7-C8-C9-C10
15	L	207	BCR	C21-C22-C23-C24
15	L	207	BCR	C37-C22-C23-C24
15	L	208	BCR	C7-C8-C9-C10
16	A	850	LHG	C3-O3-P-O5
16	B	851	LHG	C3-O3-P-O5
16	B	851	LHG	O9-C7-O7-C5
16	B	851	LHG	C8-C7-O7-C5
16	M	103	LHG	O2-C2-C3-O3
16	M	103	LHG	C3-O3-P-O6
17	A	840	LMG	O6-C1-O1-C7
17	A	840	LMG	O9-C10-O7-C8
17	A	840	LMG	O10-C28-O8-C9
17	A	840	LMG	C29-C28-O8-C9
17	A	851	LMG	O6-C1-O1-C7
17	A	851	LMG	C11-C10-O7-C8
17	A	851	LMG	O10-C28-O8-C9
17	A	851	LMG	C29-C28-O8-C9
18	A	842	LMT	O5'-C1'-O1'-C1
18	B	840	LMT	C2'-C1'-O1'-C1
18	L	210	LMT	C2'-C1'-O1'-C1
18	L	210	LMT	O5'-C1'-O1'-C1
23	M	101	ECH	C11-C12-C13-C14
26	L	209	DGD	C2B-C1B-O2G-C2G
27	M	102	SQD	C5-C6-S-O7
12	A	805	CLA	O1D-CGD-O2D-CED
12	A	811	CLA	CBD-CGD-O2D-CED
12	B	805	CLA	CBD-CGD-O2D-CED
12	B	823	CLA	CBD-CGD-O2D-CED
12	J	102	CLA	CBD-CGD-O2D-CED
12	J	103	CLA	CBD-CGD-O2D-CED
12	A	855	CLA	O1A-CGA-O2A-C1
12	A	848	CLA	C13-C15-C16-C17
12	J	102	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	A	855	CLA	CBA-CGA-O2A-C1
12	B	820	CLA	CBD-CGD-O2D-CED
12	A	846	CLA	O1A-CGA-O2A-C1
12	B	846	CLA	O1A-CGA-O2A-C1
12	B	852	CLA	O1A-CGA-O2A-C1
12	J	101	CLA	O1A-CGA-O2A-C1
12	L	204	CLA	O1A-CGA-O2A-C1
12	B	814	CLA	O1D-CGD-O2D-CED
12	K	4004	CLA	CBD-CGD-O2D-CED
17	A	851	LMG	O9-C10-O7-C8
26	L	209	DGD	O1B-C1B-O2G-C2G
12	A	809	CLA	C3-C5-C6-C7
12	A	813	CLA	C3-C5-C6-C7
12	A	831	CLA	C3-C5-C6-C7
12	A	846	CLA	C3-C5-C6-C7
12	A	849	CLA	C3-C5-C6-C7
12	B	817	CLA	C3-C5-C6-C7
12	B	823	CLA	C3-C5-C6-C7
12	B	842	CLA	C3-C5-C6-C7
12	J	101	CLA	C3-C5-C6-C7
12	L	206	CLA	C3-C5-C6-C7
12	A	846	CLA	CBA-CGA-O2A-C1
12	B	823	CLA	CBA-CGA-O2A-C1
12	B	852	CLA	CBA-CGA-O2A-C1
12	L	204	CLA	CBA-CGA-O2A-C1
12	A	806	CLA	CBD-CGD-O2D-CED
12	A	808	CLA	CBD-CGD-O2D-CED
12	A	832	CLA	CBD-CGD-O2D-CED
12	B	817	CLA	CBD-CGD-O2D-CED
12	B	825	CLA	CBD-CGD-O2D-CED
12	B	826	CLA	CBD-CGD-O2D-CED
12	B	848	CLA	CBD-CGD-O2D-CED
12	L	201	CLA	CBD-CGD-O2D-CED
17	A	840	LMG	C11-C10-O7-C8
12	A	809	CLA	C4-C3-C5-C6
12	A	825	CLA	C4-C3-C5-C6
12	A	829	CLA	C4-C3-C5-C6
12	A	831	CLA	C4-C3-C5-C6
12	A	846	CLA	C4-C3-C5-C6
12	A	849	CLA	C4-C3-C5-C6
12	B	825	CLA	C4-C3-C5-C6
12	A	809	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
12	A	825	CLA	C2-C3-C5-C6
12	A	831	CLA	C2-C3-C5-C6
12	B	817	CLA	C2-C3-C5-C6
12	B	842	CLA	C2-C3-C5-C6
12	B	817	CLA	C2A-CAA-CBA-CGA
12	B	806	CLA	C3-C5-C6-C7
12	A	817	CLA	CBA-CGA-O2A-C1
12	A	827	CLA	CBA-CGA-O2A-C1
12	B	846	CLA	CBA-CGA-O2A-C1
12	J	101	CLA	CBA-CGA-O2A-C1
26	L	209	DGD	C2A-C1A-O1G-C1G
17	A	840	LMG	C38-C39-C40-C41
17	B	837	LMG	O6-C5-C6-O5
17	A	840	LMG	C17-C18-C19-C20
17	A	840	LMG	C41-C42-C43-C44
17	B	837	LMG	C35-C36-C37-C38
15	B	836	BCR	C19-C20-C21-C22
15	J	105	BCR	C19-C20-C21-C22
12	A	827	CLA	O1A-CGA-O2A-C1
26	L	209	DGD	C8B-C9B-CAB-CBB
26	L	209	DGD	C8A-C9A-CAA-CBA
18	L	210	LMT	O5'-C5'-C6'-O6'
12	A	824	CLA	C3-C5-C6-C7
12	B	804	CLA	C3-C5-C6-C7
16	A	839	LHG	C11-C12-C13-C14
18	B	840	LMT	C4-C5-C6-C7
12	A	811	CLA	O1D-CGD-O2D-CED
12	B	805	CLA	O1D-CGD-O2D-CED
12	B	823	CLA	O1D-CGD-O2D-CED
12	J	103	CLA	O1D-CGD-O2D-CED
18	A	841	LMT	O5'-C5'-C6'-O6'
18	J	106	LMT	O5'-C5'-C6'-O6'
12	B	823	CLA	O1A-CGA-O2A-C1
12	B	825	CLA	O1A-CGA-O2A-C1
16	A	839	LHG	C23-C24-C25-C26
18	J	106	LMT	O5B-C5B-C6B-O6B
12	A	823	CLA	C3-C5-C6-C7
12	A	825	CLA	C3-C5-C6-C7
12	A	823	CLA	CBD-CGD-O2D-CED
12	B	825	CLA	CBA-CGA-O2A-C1
12	A	824	CLA	C4-C3-C5-C6
12	A	848	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
12	B	822	CLA	C4-C3-C5-C6
12	B	848	CLA	C4-C3-C5-C6
12	A	824	CLA	C2-C3-C5-C6
12	A	846	CLA	C2-C3-C5-C6
12	A	848	CLA	C2-C3-C5-C6
12	A	849	CLA	C2-C3-C5-C6
12	B	822	CLA	C2-C3-C5-C6
12	B	825	CLA	C2-C3-C5-C6
12	B	848	CLA	C2-C3-C5-C6
12	B	849	CLA	C2-C3-C5-C6
12	A	817	CLA	O1A-CGA-O2A-C1
17	B	837	LMG	C4-C5-C6-O5
26	L	209	DGD	O1A-C1A-O1G-C1G
12	B	810	CLA	C3-C5-C6-C7
18	B	839	LMT	O5'-C1'-O1'-C1
26	L	209	DGD	O6D-C1D-O3G-C3G
18	B	840	LMT	C2-C3-C4-C5
12	A	832	CLA	CBA-CGA-O2A-C1
12	A	848	CLA	CBA-CGA-O2A-C1
12	B	802	CLA	CBA-CGA-O2A-C1
12	B	814	CLA	CBA-CGA-O2A-C1
12	A	810	CLA	CBD-CGD-O2D-CED
12	A	824	CLA	CBD-CGD-O2D-CED
12	A	825	CLA	CBD-CGD-O2D-CED
12	A	843	CLA	CBD-CGD-O2D-CED
12	B	807	CLA	CBD-CGD-O2D-CED
12	B	846	CLA	CBD-CGD-O2D-CED
12	K	4002	CLA	CBD-CGD-O2D-CED
18	A	842	LMT	C2-C3-C4-C5
12	B	809	CLA	CBD-CGD-O2D-CED
12	B	816	CLA	CBD-CGD-O2D-CED
18	J	106	LMT	C4'-C5'-C6'-O6'
17	A	840	LMG	C32-C33-C34-C35
12	A	832	CLA	O1A-CGA-O2A-C1
12	B	814	CLA	O1A-CGA-O2A-C1
12	A	808	CLA	CBA-CGA-O2A-C1
12	A	809	CLA	CBA-CGA-O2A-C1
12	A	810	CLA	CBA-CGA-O2A-C1
12	A	815	CLA	CBA-CGA-O2A-C1
12	A	833	CLA	CBA-CGA-O2A-C1
12	B	822	CLA	CBA-CGA-O2A-C1
12	L	206	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	B	851	LHG	C24-C23-O8-C6
16	A	850	LHG	C11-C10-C9-C8
12	B	817	CLA	O1D-CGD-O2D-CED
12	B	820	CLA	O1D-CGD-O2D-CED
18	A	841	LMT	C7-C8-C9-C10
18	L	210	LMT	C4'-C5'-C6'-O6'
12	A	823	CLA	C4-C3-C5-C6
12	A	843	CLA	C4-C3-C5-C6
12	B	806	CLA	C4-C3-C5-C6
12	B	849	CLA	C4-C3-C5-C6
12	L	206	CLA	C4-C3-C5-C6
12	A	823	CLA	C2-C3-C5-C6
12	A	829	CLA	C2-C3-C5-C6
12	A	843	CLA	C2-C3-C5-C6
12	B	806	CLA	C2-C3-C5-C6
12	L	206	CLA	C2-C3-C5-C6
12	A	821	CLA	CBD-CGD-O2D-CED
12	A	809	CLA	C6-C7-C8-C9
12	A	816	CLA	C11-C10-C8-C9
12	A	826	CLA	C6-C7-C8-C9
12	A	826	CLA	C14-C13-C15-C16
12	A	827	CLA	C14-C13-C15-C16
12	A	829	CLA	C6-C7-C8-C9
12	A	844	CLA	C11-C12-C13-C14
12	A	847	CLA	C11-C10-C8-C9
12	A	849	CLA	C6-C7-C8-C9
12	A	858	CLA	C11-C12-C13-C14
12	B	802	CLA	C11-C12-C13-C14
12	B	806	CLA	C11-C12-C13-C14
12	B	806	CLA	C14-C13-C15-C16
12	B	807	CLA	C11-C12-C13-C14
12	B	809	CLA	C11-C10-C8-C9
12	B	817	CLA	C6-C7-C8-C9
12	B	828	CLA	C6-C7-C8-C9
12	B	829	CLA	C14-C13-C15-C16
12	B	843	CLA	C6-C7-C8-C9
12	B	844	CLA	C11-C10-C8-C9
12	J	101	CLA	C6-C7-C8-C9
12	L	205	CLA	C6-C7-C8-C9
12	L	206	CLA	C14-C13-C15-C16
22	B	831	A1AGD	C20-C19-C21-C22
12	A	808	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	A	832	CLA	O1D-CGD-O2D-CED
18	B	839	LMT	C2'-C1'-O1'-C1
12	A	808	CLA	O1A-CGA-O2A-C1
16	B	851	LHG	O10-C23-O8-C6
18	L	210	LMT	C6-C7-C8-C9
15	A	835	BCR	C11-C12-C13-C35
15	B	832	BCR	C7-C8-C9-C34
15	B	832	BCR	C37-C22-C23-C24
15	B	836	BCR	C37-C22-C23-C24
15	B	841	BCR	C37-C22-C23-C24
15	F	201	BCR	C36-C18-C19-C20
15	I	101	BCR	C37-C22-C23-C24
15	K	4001	BCR	C37-C22-C23-C24
15	K	4005	BCR	C36-C18-C19-C20
15	L	207	BCR	C7-C8-C9-C34
15	L	208	BCR	C7-C8-C9-C34
23	M	101	ECH	C11-C12-C13-C35
15	B	836	BCR	C21-C22-C23-C24
15	B	841	BCR	C21-C22-C23-C24
15	F	201	BCR	C17-C18-C19-C20
15	I	101	BCR	C21-C22-C23-C24
15	J	107	BCR	C7-C8-C9-C10
18	J	106	LMT	C4B-C5B-C6B-O6B
16	B	851	LHG	C23-C24-C25-C26
17	A	851	LMG	C11-C12-C13-C14
12	A	810	CLA	O1A-CGA-O2A-C1
12	A	833	CLA	O1A-CGA-O2A-C1
12	J	101	CLA	CBD-CGD-O2D-CED
12	B	844	CLA	C8-C10-C11-C12
16	B	851	LHG	C7-C8-C9-C10
12	A	818	CLA	C2-C1-O2A-CGA
12	A	821	CLA	C2-C1-O2A-CGA
12	B	806	CLA	C2-C1-O2A-CGA
12	L	206	CLA	O1A-CGA-O2A-C1
12	B	825	CLA	O1D-CGD-O2D-CED
12	B	826	CLA	O1D-CGD-O2D-CED
12	B	848	CLA	O1D-CGD-O2D-CED
12	K	4004	CLA	O1D-CGD-O2D-CED
12	L	201	CLA	O1D-CGD-O2D-CED
18	A	841	LMT	C4'-C5'-C6'-O6'
12	A	807	CLA	CBD-CGD-O2D-CED
12	A	821	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
12	B	822	CLA	C13-C15-C16-C17
12	B	843	CLA	CBD-CGD-O2D-CED
12	B	849	CLA	CBD-CGD-O2D-CED
12	A	801	CLA	C6-C7-C8-C10
12	A	809	CLA	C11-C10-C8-C7
12	A	826	CLA	C11-C10-C8-C7
12	A	828	CLA	C11-C10-C8-C7
12	A	848	CLA	C11-C10-C8-C7
12	B	848	CLA	C6-C7-C8-C10
12	L	204	CLA	C6-C7-C8-C10
12	L	206	CLA	C11-C12-C13-C15
22	B	831	A1AGD	C13-C14-C16-C17
18	A	842	LMT	C11-C10-C9-C8
12	A	821	CLA	C4-C3-C5-C6
12	A	847	CLA	C4-C3-C5-C6
15	J	105	BCR	C15-C16-C17-C18
15	J	107	BCR	C13-C14-C15-C16
12	A	815	CLA	O1A-CGA-O2A-C1
12	B	848	CLA	C3-C5-C6-C7
12	A	848	CLA	C15-C16-C17-C18
12	A	858	CLA	C10-C11-C12-C13
12	B	816	CLA	C5-C6-C7-C8
12	B	818	CLA	C15-C16-C17-C18
16	A	850	LHG	C23-C24-C25-C26
17	A	840	LMG	C28-C29-C30-C31
17	A	851	LMG	C10-C11-C12-C13
12	B	822	CLA	O1A-CGA-O2A-C1
12	L	206	CLA	CBD-CGD-O2D-CED
12	A	806	CLA	O1D-CGD-O2D-CED
12	B	806	CLA	C13-C15-C16-C17
12	B	809	CLA	C15-C16-C17-C18
12	B	814	CLA	C15-C16-C17-C18
12	B	822	CLA	C5-C6-C7-C8
12	B	822	CLA	C8-C10-C11-C12
12	A	807	CLA	C2A-CAA-CBA-CGA
12	A	822	CLA	C2A-CAA-CBA-CGA
12	B	828	CLA	C2A-CAA-CBA-CGA
12	F	204	CLA	C2A-CAA-CBA-CGA
12	A	814	CLA	C15-C16-C17-C18
12	A	825	CLA	C5-C6-C7-C8
12	A	826	CLA	C15-C16-C17-C18
12	B	802	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
12	B	808	CLA	C15-C16-C17-C18
12	B	818	CLA	C13-C15-C16-C17
12	B	820	CLA	C8-C10-C11-C12
12	B	842	CLA	C5-C6-C7-C8
12	B	842	CLA	C8-C10-C11-C12
12	B	848	CLA	C8-C10-C11-C12
18	A	842	LMT	O1'-C1-C2-C3
12	A	848	CLA	O1A-CGA-O2A-C1
12	B	802	CLA	O1A-CGA-O2A-C1
18	A	841	LMT	C2-C3-C4-C5
12	A	821	CLA	C13-C15-C16-C17
12	A	828	CLA	C13-C15-C16-C17
12	A	829	CLA	C13-C15-C16-C17
12	A	843	CLA	C10-C11-C12-C13
12	A	849	CLA	C13-C15-C16-C17
12	A	849	CLA	C15-C16-C17-C18
12	B	801	CLA	C8-C10-C11-C12
12	B	817	CLA	C8-C10-C11-C12
12	B	818	CLA	C10-C11-C12-C13
12	B	842	CLA	C10-C11-C12-C13
12	B	842	CLA	C13-C15-C16-C17
12	B	845	CLA	C15-C16-C17-C18
12	L	204	CLA	C10-C11-C12-C13
12	L	204	CLA	C13-C15-C16-C17
12	A	812	CLA	CBD-CGD-O2D-CED
12	A	809	CLA	O1A-CGA-O2A-C1
12	A	849	CLA	C10-C11-C12-C13
12	B	845	CLA	C13-C15-C16-C17
12	L	204	CLA	C15-C16-C17-C18
17	B	837	LMG	C20-C21-C22-C23
12	A	858	CLA	C15-C16-C17-C18
12	B	810	CLA	C5-C6-C7-C8
12	B	843	CLA	C13-C15-C16-C17
12	A	805	CLA	C4-C3-C5-C6
12	A	821	CLA	C2-C3-C5-C6
27	M	102	SQD	C45-C46-O48-C23
18	B	839	LMT	O1'-C1-C2-C3
12	A	815	CLA	C8-C10-C11-C12
12	A	827	CLA	C3-C5-C6-C7
12	A	855	CLA	C3-C5-C6-C7
12	B	829	CLA	C3-C5-C6-C7
12	A	804	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
12	B	844	CLA	C5-C6-C7-C8
16	M	103	LHG	C23-C24-C25-C26
12	A	818	CLA	CBA-CGA-O2A-C1
12	A	823	CLA	CBA-CGA-O2A-C1
27	M	102	SQD	C24-C23-O48-C46
12	A	804	CLA	C15-C16-C17-C18
12	A	828	CLA	C15-C16-C17-C18
12	A	829	CLA	C5-C6-C7-C8
12	A	847	CLA	C13-C15-C16-C17
12	A	848	CLA	C8-C10-C11-C12
12	B	801	CLA	C15-C16-C17-C18
12	B	804	CLA	C5-C6-C7-C8
12	B	814	CLA	C10-C11-C12-C13
12	B	829	CLA	C13-C15-C16-C17
12	L	205	CLA	C13-C15-C16-C17
12	A	803	CLA	CBD-CGD-O2D-CED
26	L	209	DGD	C4B-C5B-C6B-C7B
12	A	823	CLA	O1D-CGD-O2D-CED
12	A	831	CLA	C15-C16-C17-C18
12	B	817	CLA	C5-C6-C7-C8
12	B	826	CLA	C5-C6-C7-C8
12	B	848	CLA	C10-C11-C12-C13
18	L	210	LMT	C5'-C4'-O1B-C1B
12	A	809	CLA	C8-C10-C11-C12
12	A	819	CLA	C8-C10-C11-C12
12	A	822	CLA	C5-C6-C7-C8
12	A	845	CLA	C10-C11-C12-C13
12	B	807	CLA	C15-C16-C17-C18
12	B	826	CLA	C13-C15-C16-C17
12	B	816	CLA	CBA-CGA-O2A-C1
18	B	840	LMT	C6-C7-C8-C9
15	J	104	BCR	C37-C22-C23-C24
18	B	840	LMT	O1'-C1-C2-C3
27	M	102	SQD	C8-C7-O47-C45
27	M	102	SQD	O49-C7-O47-C45
17	A	840	LMG	C2-C1-O1-C7
17	A	851	LMG	C2-C1-O1-C7
18	A	853	LMT	C2'-C1'-O1'-C1
26	L	209	DGD	C2D-C1D-O3G-C3G
12	A	831	CLA	CBA-CGA-O2A-C1
25	L	202	EQ3	C16-C17-C18-C36
12	L	206	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
15	A	837	BCR	C37-C22-C23-C24
15	J	107	BCR	C7-C8-C9-C34
15	J	107	BCR	C36-C18-C19-C20
17	A	840	LMG	C29-C30-C31-C32
18	A	853	LMT	O5B-C5B-C6B-O6B
15	J	107	BCR	C17-C18-C19-C20
12	B	820	CLA	C2A-CAA-CBA-CGA
12	B	821	CLA	C2A-CAA-CBA-CGA
12	A	813	CLA	C10-C11-C12-C13
12	A	827	CLA	C10-C11-C12-C13
16	B	851	LHG	O1-C1-C2-C3
16	M	103	LHG	O1-C1-C2-C3
18	L	210	LMT	C3'-C4'-O1B-C1B
12	B	818	CLA	C16-C17-C18-C19
18	A	853	LMT	O5'-C1'-O1'-C1
12	A	847	CLA	C2-C3-C5-C6
17	A	840	LMG	C34-C35-C36-C37
12	A	810	CLA	O1D-CGD-O2D-CED
12	L	205	CLA	CBA-CGA-O2A-C1
16	A	850	LHG	C24-C23-O8-C6
12	K	4004	CLA	C8-C10-C11-C12
12	A	809	CLA	C2-C1-O2A-CGA
12	B	809	CLA	C2-C1-O2A-CGA
12	B	826	CLA	C2-C1-O2A-CGA
12	A	803	CLA	C16-C17-C18-C20
12	A	845	CLA	C16-C17-C18-C20
12	B	849	CLA	C11-C12-C13-C14
13	A	802	CL0	C16-C17-C18-C20
18	F	205	LMT	C1-C2-C3-C4
18	J	106	LMT	C1-C2-C3-C4
16	B	851	LHG	C28-C29-C30-C31
16	M	103	LHG	C26-C27-C28-C29
27	M	102	SQD	C26-C27-C28-C29
12	B	821	CLA	C5-C6-C7-C8
12	A	813	CLA	CBA-CGA-O2A-C1
26	L	209	DGD	CCA-CDA-CEA-CFA
18	B	840	LMT	C2-C1-O1'-C1'
27	M	102	SQD	C14-C15-C16-C17
12	B	846	CLA	O1D-CGD-O2D-CED
18	A	841	LMT	O1'-C1-C2-C3
12	A	827	CLA	C16-C17-C18-C19
12	A	827	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
12	B	850	CLA	C16-C17-C18-C20
12	A	831	CLA	O1A-CGA-O2A-C1
16	A	839	LHG	C32-C33-C34-C35
12	A	826	CLA	C8-C10-C11-C12
12	B	804	CLA	C8-C10-C11-C12
12	B	807	CLA	C10-C11-C12-C13
12	B	811	CLA	C13-C15-C16-C17
12	B	820	CLA	C10-C11-C12-C13
12	B	824	CLA	C13-C15-C16-C17
18	B	840	LMT	C3-C4-C5-C6
12	A	824	CLA	O1D-CGD-O2D-CED
12	A	803	CLA	C11-C12-C13-C15
12	A	823	CLA	C6-C7-C8-C10
26	L	209	DGD	C3A-C4A-C5A-C6A
16	B	851	LHG	C18-C19-C20-C21
12	A	823	CLA	O1A-CGA-O2A-C1
12	B	844	CLA	C3-C5-C6-C7
12	A	805	CLA	C3A-C2A-CAA-CBA
12	B	808	CLA	C3A-C2A-CAA-CBA
12	B	816	CLA	C3A-C2A-CAA-CBA
12	B	848	CLA	C3A-C2A-CAA-CBA
12	F	204	CLA	C3A-C2A-CAA-CBA
12	J	101	CLA	C3A-C2A-CAA-CBA
12	J	102	CLA	C3A-C2A-CAA-CBA
12	K	4004	CLA	C3A-C2A-CAA-CBA
16	A	839	LHG	C14-C15-C16-C17
26	L	209	DGD	C1B-C2B-C3B-C4B
15	A	838	BCR	C19-C20-C21-C22
15	F	201	BCR	C19-C20-C21-C22
12	A	804	CLA	C16-C17-C18-C19
12	B	810	CLA	C16-C17-C18-C19
12	B	820	CLA	C16-C17-C18-C19
12	B	820	CLA	C16-C17-C18-C20
12	B	844	CLA	C11-C12-C13-C14
12	A	818	CLA	O1A-CGA-O2A-C1
12	B	816	CLA	O1A-CGA-O2A-C1
27	M	102	SQD	O10-C23-O48-C46
16	A	839	LHG	C31-C32-C33-C34
16	B	851	LHG	C34-C35-C36-C37
17	A	851	LMG	C19-C20-C21-C22
12	B	849	CLA	C8-C10-C11-C12
16	M	103	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
12	B	807	CLA	O1D-CGD-O2D-CED
12	K	4002	CLA	O1D-CGD-O2D-CED
12	A	824	CLA	CBA-CGA-O2A-C1
17	A	840	LMG	C10-C11-C12-C13
27	M	102	SQD	C7-C8-C9-C10
18	B	840	LMT	C7-C8-C9-C10
12	A	801	CLA	O1A-CGA-O2A-C1
27	M	102	SQD	C28-C29-C30-C31
12	A	843	CLA	O1D-CGD-O2D-CED
12	B	842	CLA	C16-C17-C18-C20
12	B	850	CLA	C16-C17-C18-C19
16	A	850	LHG	C7-C8-C9-C10
12	L	205	CLA	O1A-CGA-O2A-C1
12	A	813	CLA	C2B-C3B-CAB-CBB
12	A	848	CLA	C2B-C3B-CAB-CBB
12	K	4002	CLA	C2B-C3B-CAB-CBB
12	K	4004	CLA	C2B-C3B-CAB-CBB
15	A	835	BCR	C5-C6-C7-C8
15	A	838	BCR	C23-C24-C25-C30
15	B	836	BCR	C23-C24-C25-C30
15	B	841	BCR	C23-C24-C25-C26
15	J	104	BCR	C23-C24-C25-C26
15	J	105	BCR	C1-C6-C7-C8
15	J	107	BCR	C1-C6-C7-C8
15	L	207	BCR	C23-C24-C25-C26
15	L	207	BCR	C23-C24-C25-C30
23	M	101	ECH	C23-C24-C25-C26
18	L	210	LMT	C5-C6-C7-C8
12	L	204	CLA	CBD-CGD-O2D-CED
12	A	801	CLA	CBA-CGA-O2A-C1
12	A	828	CLA	C8-C10-C11-C12
27	M	102	SQD	C11-C10-C9-C8
12	J	101	CLA	O1D-CGD-O2D-CED
16	M	103	LHG	C30-C31-C32-C33
12	A	852	CLA	C2A-CAA-CBA-CGA
12	A	813	CLA	O1A-CGA-O2A-C1
12	A	824	CLA	O1A-CGA-O2A-C1
12	A	829	CLA	O1A-CGA-O2A-C1
18	J	106	LMT	C3-C4-C5-C6
12	A	805	CLA	C2-C3-C5-C6
18	B	840	LMT	O5'-C5'-C6'-O6'
12	B	849	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
18	B	839	LMT	C2-C3-C4-C5
12	A	829	CLA	CBA-CGA-O2A-C1
16	M	103	LHG	C13-C14-C15-C16
17	A	851	LMG	C12-C13-C14-C15
12	B	826	CLA	C8-C10-C11-C12
16	A	850	LHG	O10-C23-O8-C6
16	A	839	LHG	C34-C35-C36-C37
16	B	851	LHG	C30-C31-C32-C33
16	A	839	LHG	C13-C14-C15-C16
12	A	847	CLA	C3-C5-C6-C7
12	A	801	CLA	C11-C12-C13-C15
12	B	846	CLA	C6-C7-C8-C10
12	A	847	CLA	CBD-CGD-O2D-CED
16	M	103	LHG	C8-C7-O7-C5
16	M	103	LHG	C29-C30-C31-C32
12	B	819	CLA	C10-C11-C12-C13
16	M	103	LHG	O9-C7-O7-C5
16	M	103	LHG	C35-C36-C37-C38
18	F	205	LMT	C5-C6-C7-C8
12	B	824	CLA	C2C-C3C-CAC-CBC
15	A	835	BCR	C36-C18-C19-C20
15	K	4005	BCR	C7-C8-C9-C34
15	K	4005	BCR	C11-C12-C13-C35
16	M	103	LHG	C11-C12-C13-C14
15	A	835	BCR	C17-C18-C19-C20
12	A	803	CLA	C16-C17-C18-C19
12	A	843	CLA	C11-C12-C13-C14
12	A	845	CLA	C16-C17-C18-C19
12	B	842	CLA	C16-C17-C18-C19
12	A	828	CLA	C4-C3-C5-C6
12	B	804	CLA	C4-C3-C5-C6
18	A	842	LMT	C1-C2-C3-C4
12	B	804	CLA	C2-C3-C5-C6
16	M	103	LHG	C33-C34-C35-C36
12	A	845	CLA	C5-C6-C7-C8
12	A	801	CLA	C5-C6-C7-C8
12	A	801	CLA	C8-C10-C11-C12
12	A	823	CLA	C10-C11-C12-C13
12	A	844	CLA	C5-C6-C7-C8
12	A	846	CLA	C5-C6-C7-C8
12	B	818	CLA	C8-C10-C11-C12
12	B	819	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
27	M	102	SQD	C33-C34-C35-C36
12	B	801	CLA	C13-C15-C16-C17
12	B	814	CLA	C5-C6-C7-C8
12	B	847	CLA	C10-C11-C12-C13
12	B	823	CLA	C6-C7-C8-C9
13	A	802	CL0	C16-C17-C18-C19
26	L	209	DGD	C1A-C2A-C3A-C4A
12	A	847	CLA	C10-C11-C12-C13
12	A	855	CLA	C5-C6-C7-C8
22	B	831	A1AGD	C19-C21-C22-C23
12	A	825	CLA	O1D-CGD-O2D-CED
18	A	842	LMT	C6-C7-C8-C9
12	L	205	CLA	C3-C5-C6-C7
16	A	850	LHG	O7-C5-C6-O8
18	A	841	LMT	C5-C6-C7-C8
18	F	205	LMT	C2-C3-C4-C5
12	B	802	CLA	C13-C15-C16-C17
12	A	820	CLA	C2-C1-O2A-CGA
12	B	810	CLA	C16-C17-C18-C20
12	B	818	CLA	C16-C17-C18-C20
12	B	842	CLA	C15-C16-C17-C18
26	L	209	DGD	C4D-C5D-C6D-O5D
16	B	851	LHG	C26-C27-C28-C29
17	A	840	LMG	C37-C38-C39-C40
16	M	103	LHG	C28-C29-C30-C31
12	B	845	CLA	C3-C5-C6-C7
12	L	204	CLA	C3-C5-C6-C7
12	B	843	CLA	C2-C3-C5-C6
12	A	813	CLA	C2A-CAA-CBA-CGA
12	A	831	CLA	C2A-CAA-CBA-CGA
12	B	806	CLA	C2A-CAA-CBA-CGA
12	B	815	CLA	C2A-CAA-CBA-CGA
12	B	843	CLA	O1D-CGD-O2D-CED
18	B	840	LMT	C1-C2-C3-C4
16	M	103	LHG	O1-C1-C2-O2
12	A	805	CLA	C1A-C2A-CAA-CBA
12	A	811	CLA	C1A-C2A-CAA-CBA
12	A	813	CLA	C1A-C2A-CAA-CBA
12	A	814	CLA	C1A-C2A-CAA-CBA
12	A	817	CLA	C1A-C2A-CAA-CBA
12	A	825	CLA	C1A-C2A-CAA-CBA
12	A	843	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	A	855	CLA	C1A-C2A-CAA-CBA
12	B	802	CLA	C1A-C2A-CAA-CBA
12	B	806	CLA	C1A-C2A-CAA-CBA
12	B	822	CLA	C1A-C2A-CAA-CBA
12	B	823	CLA	C1A-C2A-CAA-CBA
12	B	829	CLA	C1A-C2A-CAA-CBA
12	B	842	CLA	C1A-C2A-CAA-CBA
12	F	204	CLA	C1A-C2A-CAA-CBA
12	A	847	CLA	C5-C6-C7-C8
17	A	840	LMG	C14-C15-C16-C17
16	M	103	LHG	O6-C4-C5-C6
27	M	102	SQD	C27-C28-C29-C30
12	A	815	CLA	C6-C7-C8-C10
12	A	828	CLA	C11-C12-C13-C15
12	A	844	CLA	C6-C7-C8-C10
12	A	848	CLA	C6-C7-C8-C10
12	A	848	CLA	C11-C12-C13-C15
12	B	802	CLA	C11-C12-C13-C15
12	B	804	CLA	C11-C10-C8-C7
12	B	812	CLA	C6-C7-C8-C10
12	B	829	CLA	C6-C7-C8-C10
12	B	844	CLA	C11-C10-C8-C7
12	J	101	CLA	C11-C10-C8-C7
12	L	204	CLA	C11-C12-C13-C15
12	B	806	CLA	C5-C6-C7-C8
12	B	816	CLA	O1D-CGD-O2D-CED
12	A	804	CLA	C13-C15-C16-C17
12	B	802	CLA	C5-C6-C7-C8
12	A	804	CLA	C2-C3-C5-C6
27	M	102	SQD	C9-C10-C11-C12
12	A	826	CLA	C13-C15-C16-C17
16	A	839	LHG	C8-C7-O7-C5
12	A	823	CLA	C6-C7-C8-C9
12	A	830	CLA	C11-C10-C8-C9
12	A	844	CLA	C6-C7-C8-C9
12	A	848	CLA	C11-C12-C13-C14
12	A	858	CLA	C11-C10-C8-C9
12	B	810	CLA	C11-C10-C8-C9
12	B	814	CLA	C14-C13-C15-C16
12	B	816	CLA	C6-C7-C8-C9
12	B	845	CLA	C6-C7-C8-C9
12	B	848	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
12	B	848	CLA	C11-C12-C13-C14
12	B	848	CLA	CBA-CGA-O2A-C1
12	B	809	CLA	O1D-CGD-O2D-CED
18	A	842	LMT	C2'-C1'-O1'-C1
16	B	851	LHG	C25-C26-C27-C28
18	A	842	LMT	C4-C5-C6-C7
17	A	851	LMG	C7-C8-C9-O8
12	B	846	CLA	C3-C5-C6-C7
12	A	807	CLA	O1D-CGD-O2D-CED
12	A	849	CLA	CBA-CGA-O2A-C1
12	B	842	CLA	CBA-CGA-O2A-C1
16	A	839	LHG	C11-C10-C9-C8
16	M	103	LHG	C31-C32-C33-C34
12	A	821	CLA	O1D-CGD-O2D-CED
17	B	837	LMG	C28-C29-C30-C31
12	A	804	CLA	C4-C3-C5-C6
12	B	843	CLA	C4-C3-C5-C6
12	A	828	CLA	C2-C3-C5-C6
15	A	838	BCR	C36-C18-C19-C20
18	L	210	LMT	C11-C10-C9-C8
12	B	812	CLA	C16-C17-C18-C20
18	B	840	LMT	C5-C6-C7-C8
12	A	822	CLA	C13-C15-C16-C17
12	A	844	CLA	C13-C15-C16-C17
12	A	855	CLA	C13-C15-C16-C17
12	B	829	CLA	C15-C16-C17-C18
12	J	101	CLA	C5-C6-C7-C8
18	A	841	LMT	C6-C7-C8-C9
12	B	829	CLA	CBA-CGA-O2A-C1
12	A	846	CLA	O2A-C1-C2-C3
12	A	830	CLA	C8-C10-C11-C12
15	J	105	BCR	C13-C14-C15-C16
12	B	802	CLA	C3-C5-C6-C7
25	L	202	EQ3	C16-C17-C18-C19
16	A	839	LHG	C33-C34-C35-C36
12	B	816	CLA	C2-C3-C5-C6
12	A	801	CLA	C11-C12-C13-C14
19	A	854	PL9	C16-C17-C18-C19
17	A	851	LMG	O1-C7-C8-O7
12	B	801	CLA	CBA-CGA-O2A-C1
12	B	808	CLA	CBA-CGA-O2A-C1
26	L	209	DGD	CFA-CGA-CHA-CIA

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Mol	Chain	Res	Type	Atoms
12	A	855	CLA	C2A-CAA-CBA-CGA
12	B	842	CLA	O1A-CGA-O2A-C1
12	A	830	CLA	CBA-CGA-O2A-C1
27	M	102	SQD	C34-C35-C36-C37
12	A	812	CLA	O1D-CGD-O2D-CED
12	B	824	CLA	C4C-C3C-CAC-CBC
12	B	808	CLA	C4-C3-C5-C6
12	B	810	CLA	C4-C3-C5-C6
12	B	816	CLA	C4-C3-C5-C6
12	B	821	CLA	C4-C3-C5-C6
19	A	854	PL9	C20-C19-C21-C22
27	M	102	SQD	C24-C25-C26-C27
12	A	819	CLA	CBA-CGA-O2A-C1
16	A	839	LHG	C29-C30-C31-C32
26	L	209	DGD	C7B-C8B-C9B-CAB
12	A	803	CLA	C11-C12-C13-C14
12	A	814	CLA	C14-C13-C15-C16
12	A	826	CLA	C11-C10-C8-C9
12	A	828	CLA	C11-C12-C13-C14
12	A	843	CLA	C11-C10-C8-C9
12	A	848	CLA	C6-C7-C8-C9
12	B	822	CLA	C14-C13-C15-C16
12	B	829	CLA	C6-C7-C8-C9
12	B	842	CLA	C11-C12-C13-C14
12	J	101	CLA	C11-C10-C8-C9
12	L	204	CLA	C14-C13-C15-C16
12	B	845	CLA	C10-C11-C12-C13
12	L	206	CLA	C5-C6-C7-C8
12	B	829	CLA	O1A-CGA-O2A-C1
12	A	809	CLA	C4B-C3B-CAB-CBB
12	A	826	CLA	C4B-C3B-CAB-CBB
12	B	829	CLA	C4B-C3B-CAB-CBB
12	K	4004	CLA	C4B-C3B-CAB-CBB
12	B	849	CLA	O1D-CGD-O2D-CED
12	B	823	CLA	C5-C6-C7-C8
12	A	821	CLA	C16-C17-C18-C20
12	B	848	CLA	C16-C17-C18-C20
16	A	850	LHG	C27-C28-C29-C30
18	J	106	LMT	C2'-C1'-O1'-C1
16	A	850	LHG	C25-C26-C27-C28
12	L	206	CLA	O1D-CGD-O2D-CED
12	A	804	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
12	A	814	CLA	C12-C13-C15-C16
12	A	826	CLA	C11-C12-C13-C15
12	A	827	CLA	C12-C13-C15-C16
12	A	830	CLA	C11-C10-C8-C7
12	A	831	CLA	C12-C13-C15-C16
12	A	858	CLA	C11-C10-C8-C7
12	A	858	CLA	C12-C13-C15-C16
12	B	810	CLA	C11-C10-C8-C7
12	B	813	CLA	C11-C10-C8-C7
12	B	813	CLA	C12-C13-C15-C16
12	B	817	CLA	C6-C7-C8-C10
12	B	820	CLA	C11-C10-C8-C7
12	B	822	CLA	C11-C10-C8-C7
12	B	828	CLA	C6-C7-C8-C10
12	B	844	CLA	C6-C7-C8-C10
12	B	845	CLA	C6-C7-C8-C10
12	B	848	CLA	C11-C10-C8-C7
12	B	848	CLA	C11-C12-C13-C15
12	L	204	CLA	C12-C13-C15-C16
12	L	206	CLA	C6-C7-C8-C10
12	L	206	CLA	C10-C11-C12-C13
16	B	851	LHG	C35-C36-C37-C38
18	B	840	LMT	C9-C10-C11-C12
12	A	803	CLA	C3A-C2A-CAA-CBA
12	A	808	CLA	C3A-C2A-CAA-CBA
12	A	809	CLA	C3A-C2A-CAA-CBA
12	B	814	CLA	C4-C3-C5-C6
12	B	817	CLA	C3A-C2A-CAA-CBA
12	B	850	CLA	C3A-C2A-CAA-CBA
12	A	822	CLA	C10-C11-C12-C13
12	B	824	CLA	C5-C6-C7-C8
12	L	204	CLA	O1D-CGD-O2D-CED
12	B	821	CLA	C2-C3-C5-C6
27	M	102	SQD	C35-C36-C37-C38
12	A	826	CLA	C10-C11-C12-C13
15	J	107	BCR	C19-C20-C21-C22
12	A	820	CLA	C16-C17-C18-C20
15	B	836	BCR	C36-C18-C19-C20
12	A	849	CLA	O1A-CGA-O2A-C1
12	B	848	CLA	O1A-CGA-O2A-C1
17	A	851	LMG	C31-C32-C33-C34
16	A	850	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
19	A	854	PL9	C19-C21-C22-C23
12	A	824	CLA	C6-C7-C8-C10
12	A	803	CLA	C8-C10-C11-C12
22	B	831	A1AGD	C14-C16-C17-C18
18	A	842	LMT	C3-C4-C5-C6
12	A	816	CLA	C4-C3-C5-C6
12	A	820	CLA	C4-C3-C5-C6
12	A	816	CLA	C2-C3-C5-C6
12	B	808	CLA	C2-C3-C5-C6
12	B	810	CLA	C2-C3-C5-C6
12	B	814	CLA	C2-C3-C5-C6
12	A	819	CLA	C11-C12-C13-C15
12	A	824	CLA	C6-C7-C8-C9
15	A	836	BCR	C23-C24-C25-C26
15	B	841	BCR	C23-C24-C25-C30
15	K	4001	BCR	C23-C24-C25-C26
15	K	4005	BCR	C23-C24-C25-C30
12	A	803	CLA	O1D-CGD-O2D-CED
12	A	849	CLA	C16-C17-C18-C20
12	A	844	CLA	C8-C10-C11-C12
12	B	843	CLA	C10-C11-C12-C13
16	B	851	LHG	O7-C5-C6-O8
17	A	851	LMG	O7-C8-C9-O8
16	B	851	LHG	C10-C11-C12-C13
12	A	815	CLA	C13-C15-C16-C17
12	B	813	CLA	C8-C10-C11-C12
19	A	854	PL9	C18-C19-C21-C22
12	A	804	CLA	C16-C17-C18-C20
12	A	804	CLA	C14-C13-C15-C16
12	A	826	CLA	C11-C12-C13-C14
12	A	828	CLA	C11-C10-C8-C9
12	A	831	CLA	C14-C13-C15-C16
12	A	858	CLA	C14-C13-C15-C16
12	B	813	CLA	C11-C10-C8-C9
12	B	813	CLA	C14-C13-C15-C16
12	B	820	CLA	C11-C10-C8-C9
12	B	822	CLA	C11-C10-C8-C9
12	B	843	CLA	C11-C12-C13-C14
12	L	204	CLA	C6-C7-C8-C9
12	L	204	CLA	C11-C12-C13-C14
12	L	206	CLA	C6-C7-C8-C9
12	L	206	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
26	L	209	DGD	O6D-C5D-C6D-O5D
12	A	807	CLA	C6-C7-C8-C9
12	B	823	CLA	C6-C7-C8-C10
12	B	846	CLA	C6-C7-C8-C9
12	B	806	CLA	C10-C11-C12-C13
12	A	847	CLA	C2A-CAA-CBA-CGA
17	A	851	LMG	C13-C14-C15-C16
18	J	106	LMT	C5-C6-C7-C8
15	K	4005	BCR	C19-C20-C21-C22
12	A	820	CLA	C2-C3-C5-C6
12	A	819	CLA	C11-C12-C13-C14
12	A	821	CLA	C16-C17-C18-C19
12	A	827	CLA	C5-C6-C7-C8
12	B	808	CLA	O1A-CGA-O2A-C1
12	B	853	CLA	O1A-CGA-O2A-C1
16	A	839	LHG	O9-C7-O7-C5
12	B	801	CLA	O1A-CGA-O2A-C1
12	A	825	CLA	CBA-CGA-O2A-C1
12	B	853	CLA	CBA-CGA-O2A-C1
18	L	210	LMT	O1'-C1-C2-C3
12	B	844	CLA	C11-C12-C13-C15
15	B	841	BCR	C36-C18-C19-C20
12	A	809	CLA	C6-C7-C8-C10
12	A	826	CLA	C6-C7-C8-C10
12	A	843	CLA	C11-C10-C8-C7
12	A	849	CLA	C11-C12-C13-C15
12	B	807	CLA	C11-C10-C8-C7
12	B	829	CLA	C12-C13-C15-C16
12	L	206	CLA	C12-C13-C15-C16
22	B	831	A1AGD	C12-C13-C14-C16
22	B	831	A1AGD	C17-C18-C19-C21
22	B	831	A1AGD	C18-C19-C21-C22
12	A	827	CLA	CBD-CGD-O2D-CED
15	A	837	BCR	C21-C22-C23-C24
15	A	838	BCR	C17-C18-C19-C20
15	F	201	BCR	C11-C12-C13-C14
12	A	819	CLA	O1A-CGA-O2A-C1
17	A	851	LMG	C8-C7-O1-C1
27	M	102	SQD	C5-C6-S-O8
12	A	805	CLA	C2A-CAA-CBA-CGA
12	B	807	CLA	C2A-CAA-CBA-CGA
16	M	103	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
12	A	807	CLA	C6-C7-C8-C10
12	L	205	CLA	C16-C17-C18-C20
12	A	815	CLA	C4-C3-C5-C6
17	A	851	LMG	C16-C17-C18-C19
12	A	845	CLA	C13-C15-C16-C17
12	A	804	CLA	C8-C10-C11-C12
12	A	815	CLA	C15-C16-C17-C18
12	A	820	CLA	C16-C17-C18-C19
12	A	843	CLA	C11-C12-C13-C15
12	A	830	CLA	O1A-CGA-O2A-C1
12	A	843	CLA	C3-C5-C6-C7
13	A	802	CL0	C3-C5-C6-C7
12	A	845	CLA	C15-C16-C17-C18
16	A	850	LHG	C30-C31-C32-C33
16	M	103	LHG	O6-C4-C5-O7
17	A	851	LMG	O1-C7-C8-C9
12	B	812	CLA	C16-C17-C18-C19
12	B	812	CLA	C3-C5-C6-C7
16	M	103	LHG	C32-C33-C34-C35
12	B	850	CLA	C5-C6-C7-C8
12	A	808	CLA	C2A-CAA-CBA-CGA
18	A	841	LMT	C4-C5-C6-C7
16	A	839	LHG	C30-C31-C32-C33
12	B	816	CLA	C3-C5-C6-C7
12	L	206	CLA	C11-C12-C13-C14
12	B	809	CLA	C16-C17-C18-C19
18	A	841	LMT	C11-C10-C9-C8
18	L	210	LMT	C1-C2-C3-C4
12	A	847	CLA	O1D-CGD-O2D-CED
12	B	824	CLA	C2-C1-O2A-CGA
12	B	825	CLA	C2-C1-O2A-CGA
12	A	814	CLA	C16-C17-C18-C20
12	A	846	CLA	C6-C7-C8-C9
12	B	848	CLA	C16-C17-C18-C19
12	K	4004	CLA	C10-C11-C12-C13
12	A	849	CLA	C16-C17-C18-C19
12	B	845	CLA	C5-C6-C7-C8
12	A	829	CLA	C3-C5-C6-C7
12	A	824	CLA	C1A-C2A-CAA-CBA
12	A	829	CLA	C4B-C3B-CAB-CBB
12	A	832	CLA	C4B-C3B-CAB-CBB
12	B	828	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
12	B	848	CLA	C4B-C3B-CAB-CBB
12	F	203	CLA	C4B-C3B-CAB-CBB
12	J	101	CLA	C1A-C2A-CAA-CBA
12	J	102	CLA	C4B-C3B-CAB-CBB
12	L	201	CLA	C1A-C2A-CAA-CBA
15	B	841	BCR	C17-C18-C19-C20
15	K	4005	BCR	C11-C12-C13-C14
12	L	205	CLA	C16-C17-C18-C19
27	M	102	SQD	C18-C19-C20-C21
12	A	820	CLA	C3-C5-C6-C7
12	A	809	CLA	C11-C12-C13-C15
12	A	825	CLA	C11-C10-C8-C7
12	A	844	CLA	C11-C12-C13-C15
12	A	847	CLA	C11-C10-C8-C7
12	A	849	CLA	C6-C7-C8-C10
12	B	804	CLA	C11-C12-C13-C15
12	B	807	CLA	C11-C12-C13-C15
12	B	814	CLA	C11-C12-C13-C15
12	B	816	CLA	C6-C7-C8-C10
12	B	842	CLA	C12-C13-C15-C16
12	B	843	CLA	C6-C7-C8-C10
12	J	101	CLA	C6-C7-C8-C10
18	A	842	LMT	C5-C6-C7-C8
17	B	837	LMG	C37-C38-C39-C40
16	A	839	LHG	C35-C36-C37-C38
12	A	825	CLA	O1A-CGA-O2A-C1
26	L	209	DGD	C4A-C5A-C6A-C7A
12	A	815	CLA	C2-C3-C5-C6
17	A	851	LMG	C34-C35-C36-C37
16	B	851	LHG	C19-C20-C21-C22
12	B	843	CLA	C3-C5-C6-C7
12	B	813	CLA	C13-C15-C16-C17
15	K	4005	BCR	C15-C16-C17-C18
12	A	848	CLA	CBD-CGD-O2D-CED
16	B	851	LHG	C4-C5-C6-O8
12	A	824	CLA	CAD-CBD-CGD-O2D
12	A	852	CLA	CAD-CBD-CGD-O2D
12	B	808	CLA	CAD-CBD-CGD-O2D
12	B	830	CLA	CAD-CBD-CGD-O2D
12	L	201	CLA	C13-C15-C16-C17
12	B	849	CLA	C3-C5-C6-C7
12	B	850	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
12	A	833	CLA	CAA-CBA-CGA-O2A
16	A	850	LHG	O7-C7-C8-C9
12	A	804	CLA	CAD-CBD-CGD-O1D
12	A	809	CLA	CHA-CBD-CGD-O1D
12	A	809	CLA	CHA-CBD-CGD-O2D
12	A	824	CLA	CAD-CBD-CGD-O1D
12	A	852	CLA	CAD-CBD-CGD-O1D
12	B	808	CLA	CAD-CBD-CGD-O1D
12	B	825	CLA	CHA-CBD-CGD-O1D
12	B	830	CLA	CAD-CBD-CGD-O1D
12	B	844	CLA	CAD-CBD-CGD-O1D
16	A	839	LHG	C3-O3-P-O5
16	M	103	LHG	C3-O3-P-O5
23	M	101	ECH	C9-C10-C11-C12
26	L	209	DGD	C2A-C3A-C4A-C5A
12	A	808	CLA	C2B-C3B-CAB-CBB
12	A	830	CLA	C2B-C3B-CAB-CBB
12	B	850	CLA	C2B-C3B-CAB-CBB
12	F	204	CLA	C2B-C3B-CAB-CBB
15	B	834	BCR	C5-C6-C7-C8
12	A	813	CLA	CAA-CBA-CGA-O2A
17	B	837	LMG	C39-C40-C41-C42
12	A	827	CLA	O1D-CGD-O2D-CED
12	B	819	CLA	C16-C17-C18-C20
12	B	843	CLA	C5-C6-C7-C8
16	A	850	LHG	C26-C27-C28-C29
17	B	837	LMG	C15-C16-C17-C18
26	L	209	DGD	C9A-CAA-CBA-CCA
12	B	806	CLA	O1A-CGA-O2A-C1
16	M	103	LHG	C9-C10-C11-C12
12	A	809	CLA	C5-C6-C7-C8
12	A	815	CLA	C5-C6-C7-C8
12	A	809	CLA	C11-C12-C13-C14
12	A	816	CLA	C6-C7-C8-C9
12	A	821	CLA	C11-C10-C8-C9
12	A	831	CLA	C6-C7-C8-C9
12	B	818	CLA	C11-C10-C8-C9
12	B	826	CLA	C6-C7-C8-C9
12	B	844	CLA	C6-C7-C8-C9
22	B	831	A1AGD	C12-C13-C14-C15
12	A	847	CLA	C12-C13-C15-C16
12	B	818	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
12	B	845	CLA	C16-C17-C18-C19
12	A	848	CLA	O1D-CGD-O2D-CED
12	B	813	CLA	C4-C3-C5-C6
27	M	102	SQD	C25-C26-C27-C28
12	B	845	CLA	C16-C17-C18-C20
16	A	839	LHG	O7-C5-C6-O8
12	B	847	CLA	CAA-CBA-CGA-O2A
12	B	813	CLA	C2A-CAA-CBA-CGA
12	B	824	CLA	CAA-CBA-CGA-O2A
13	A	802	CL0	CAA-CBA-CGA-O2A
15	B	835	BCR	C36-C18-C19-C20
15	F	201	BCR	C11-C12-C13-C35
12	A	804	CLA	CBA-CGA-O2A-C1
12	B	806	CLA	CBA-CGA-O2A-C1
16	A	850	LHG	C29-C30-C31-C32
12	B	843	CLA	C15-C16-C17-C18
25	L	202	EQ3	C9-C10-C11-C12
12	A	846	CLA	C6-C7-C8-C10
12	B	813	CLA	C2-C3-C5-C6
18	A	853	LMT	C2-C1-O1'-C1'
18	B	839	LMT	C2-C1-O1'-C1'
18	L	210	LMT	C2-C1-O1'-C1'
12	A	804	CLA	C11-C12-C13-C14
12	A	825	CLA	C11-C10-C8-C9
12	A	847	CLA	C14-C13-C15-C16
12	B	814	CLA	C11-C12-C13-C14
12	L	205	CLA	C14-C13-C15-C16
16	B	851	LHG	C12-C13-C14-C15
12	A	824	CLA	C4B-C3B-CAB-CBB
12	A	831	CLA	C4B-C3B-CAB-CBB
12	B	810	CLA	C4B-C3B-CAB-CBB
16	B	851	LHG	C16-C17-C18-C19
12	A	823	CLA	C13-C15-C16-C17
12	K	4002	CLA	C2A-CAA-CBA-CGA
12	A	828	CLA	O1D-CGD-O2D-CED
12	B	818	CLA	O1A-CGA-O2A-C1
12	A	814	CLA	C16-C17-C18-C19
16	M	103	LHG	C25-C26-C27-C28
12	A	823	CLA	C12-C13-C15-C16
12	A	858	CLA	C11-C12-C13-C15
12	B	817	CLA	C11-C12-C13-C15
12	B	845	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
12	B	843	CLA	O1A-CGA-O2A-C1
12	A	828	CLA	CBD-CGD-O2D-CED
26	L	209	DGD	C3B-C4B-C5B-C6B
12	A	848	CLA	C5-C6-C7-C8
12	B	806	CLA	C8-C10-C11-C12
27	M	102	SQD	O6-C44-C45-O47
12	B	826	CLA	C4-C3-C5-C6
15	B	836	BCR	C16-C17-C18-C36
15	F	202	BCR	C35-C13-C14-C15
20	A	856	45D	C28-C26-C30-C32
20	A	856	45D	C39-C35-C37-C41
23	B	833	ECH	C11-C10-C9-C34
23	B	833	ECH	C20-C21-C22-C37
23	M	101	ECH	C11-C10-C9-C34
12	B	852	CLA	C2C-C3C-CAC-CBC
12	A	831	CLA	C13-C15-C16-C17
12	B	849	CLA	C2-C1-O2A-CGA
12	A	827	CLA	C4-C3-C5-C6
12	A	827	CLA	C8-C10-C11-C12
12	A	817	CLA	C2A-CAA-CBA-CGA
12	B	843	CLA	CBA-CGA-O2A-C1
27	M	102	SQD	O6-C44-C45-C46
12	B	806	CLA	O1D-CGD-O2D-CED
12	B	815	CLA	CAA-CBA-CGA-O2A
12	A	801	CLA	C6-C7-C8-C9
12	A	819	CLA	C6-C7-C8-C9
12	A	819	CLA	C11-C10-C8-C9
12	A	825	CLA	C6-C7-C8-C9
12	A	848	CLA	C11-C10-C8-C9
12	B	804	CLA	C14-C13-C15-C16
12	B	811	CLA	C14-C13-C15-C16
12	B	817	CLA	C11-C12-C13-C14
12	B	819	CLA	C11-C10-C8-C9
12	B	820	CLA	C6-C7-C8-C9
12	B	843	CLA	C11-C10-C8-C9
12	B	845	CLA	C11-C12-C13-C14
12	B	845	CLA	C14-C13-C15-C16
12	B	826	CLA	C16-C17-C18-C20
16	A	839	LHG	C19-C20-C21-C22
12	A	828	CLA	C5-C6-C7-C8
12	J	103	CLA	C2A-CAA-CBA-CGA
12	A	806	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	B	850	CLA	C1A-C2A-CAA-CBA
15	B	836	BCR	C16-C17-C18-C19
15	F	202	BCR	C12-C13-C14-C15
20	A	856	45D	C24-C26-C30-C32
20	A	856	45D	C33-C35-C37-C41
23	B	833	ECH	C11-C10-C9-C8
23	B	833	ECH	C20-C21-C22-C23
23	M	101	ECH	C11-C10-C9-C8
12	A	812	CLA	CAA-CBA-CGA-O2A
12	A	806	CLA	C2B-C3B-CAB-CBB
12	A	807	CLA	C2B-C3B-CAB-CBB
12	A	815	CLA	C2B-C3B-CAB-CBB
12	A	823	CLA	C2B-C3B-CAB-CBB
12	B	802	CLA	C2B-C3B-CAB-CBB
12	B	811	CLA	C2B-C3B-CAB-CBB
12	B	814	CLA	C2B-C3B-CAB-CBB
12	B	822	CLA	C2B-C3B-CAB-CBB
12	B	828	CLA	C2B-C3B-CAB-CBB
12	B	842	CLA	C2B-C3B-CAB-CBB
12	B	846	CLA	C2B-C3B-CAB-CBB
12	B	848	CLA	C2B-C3B-CAB-CBB
12	B	853	CLA	C2B-C3B-CAB-CBB
12	L	205	CLA	C2B-C3B-CAB-CBB
13	A	802	CL0	C2B-C3B-CAB-CBB
15	B	834	BCR	C23-C24-C25-C26
15	B	841	BCR	C5-C6-C7-C8
15	J	107	BCR	C23-C24-C25-C26
23	B	833	ECH	C5-C6-C7-C8
16	B	851	LHG	C11-C12-C13-C14
12	A	806	CLA	CAA-CBA-CGA-O1A
12	A	828	CLA	C16-C17-C18-C20
12	B	844	CLA	C4-C3-C5-C6
12	B	826	CLA	C2-C3-C5-C6
12	A	812	CLA	CAA-CBA-CGA-O1A
12	K	4002	CLA	CAA-CBA-CGA-O2A
12	A	801	CLA	C11-C10-C8-C7
12	A	804	CLA	C11-C12-C13-C15
12	A	816	CLA	C6-C7-C8-C10
12	A	831	CLA	C6-C7-C8-C10
12	B	806	CLA	C12-C13-C15-C16
12	B	809	CLA	C12-C13-C15-C16
12	B	814	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
12	B	816	CLA	C12-C13-C15-C16
12	L	205	CLA	C12-C13-C15-C16
12	B	816	CLA	C8-C10-C11-C12
12	A	831	CLA	CBD-CGD-O2D-CED
12	A	844	CLA	C16-C17-C18-C19
17	B	837	LMG	C31-C32-C33-C34
12	B	846	CLA	C5-C6-C7-C8
12	J	103	CLA	CAA-CBA-CGA-O1A
12	B	853	CLA	C4-C3-C5-C6
12	A	831	CLA	O1D-CGD-O2D-CED
12	B	815	CLA	CAA-CBA-CGA-O1A
12	B	827	CLA	CAA-CBA-CGA-O1A
12	K	4002	CLA	CAA-CBA-CGA-O1A
12	A	847	CLA	C6-C7-C8-C9
12	B	846	CLA	C4-C3-C5-C6
12	A	827	CLA	C2-C3-C5-C6
12	B	853	CLA	C2-C3-C5-C6
12	A	806	CLA	CAA-CBA-CGA-O2A
17	A	840	LMG	O1-C7-C8-C9
12	J	103	CLA	CAA-CBA-CGA-O2A
12	A	858	CLA	C2A-CAA-CBA-CGA
16	A	839	LHG	C24-C25-C26-C27
12	B	847	CLA	O1A-CGA-O2A-C1
12	A	858	CLA	C8-C10-C11-C12
18	F	205	LMT	C2-C1-O1'-C1'
12	B	829	CLA	C16-C17-C18-C20
12	B	809	CLA	C4B-C3B-CAB-CBB
12	B	820	CLA	C4B-C3B-CAB-CBB
12	B	827	CLA	CAA-CBA-CGA-O2A
25	L	202	EQ3	C11-C10-C9-C34
12	A	801	CLA	C3-C5-C6-C7
18	L	210	LMT	C2-C3-C4-C5
16	A	839	LHG	C10-C11-C12-C13
12	B	806	CLA	CAA-CBA-CGA-O2A
16	A	839	LHG	C9-C10-C11-C12
12	A	805	CLA	C15-C16-C17-C18
12	B	820	CLA	C13-C15-C16-C17
12	A	819	CLA	C11-C10-C8-C7
12	B	806	CLA	C11-C12-C13-C15
22	B	831	A1AGD	C21-C22-C23-C24
12	A	828	CLA	C14-C13-C15-C16
12	B	829	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	B	831	A1AGD	C15-C14-C16-C17
12	A	804	CLA	CAA-CBA-CGA-O2A
12	F	204	CLA	CAA-CBA-CGA-O2A
12	A	818	CLA	C15-C16-C17-C18
12	A	824	CLA	C2-C1-O2A-CGA
12	A	833	CLA	C2-C1-O2A-CGA
12	B	818	CLA	CBA-CGA-O2A-C1
12	B	820	CLA	CBA-CGA-O2A-C1
12	B	804	CLA	C3A-C2A-CAA-CBA
12	B	805	CLA	C3A-C2A-CAA-CBA
12	K	4002	CLA	C3A-C2A-CAA-CBA
12	A	804	CLA	O1A-CGA-O2A-C1
12	B	830	CLA	CAA-CBA-CGA-O2A
17	A	851	LMG	C14-C15-C16-C17
12	B	825	CLA	C3-C5-C6-C7
18	J	106	LMT	C3'-C4'-O1B-C1B
12	B	814	CLA	C16-C17-C18-C20
18	A	842	LMT	C9-C10-C11-C12
12	B	806	CLA	C15-C16-C17-C18
25	L	202	EQ3	C11-C10-C9-C8
17	B	837	LMG	C16-C17-C18-C19
16	B	851	LHG	O6-C4-C5-O7
12	B	847	CLA	CBA-CGA-O2A-C1
19	A	854	PL9	C14-C16-C17-C18
12	B	820	CLA	O1A-CGA-O2A-C1
12	A	848	CLA	C3-C5-C6-C7
12	A	812	CLA	C2A-CAA-CBA-CGA
12	B	816	CLA	CAA-CBA-CGA-O2A
12	B	830	CLA	CAA-CBA-CGA-O1A
12	J	101	CLA	CAA-CBA-CGA-O2A
26	L	209	DGD	O2G-C2G-C3G-O3G
12	A	852	CLA	C5-C6-C7-C8
12	A	815	CLA	C11-C10-C8-C9
12	A	829	CLA	C11-C10-C8-C9
12	A	844	CLA	C11-C10-C8-C9
12	A	828	CLA	C16-C17-C18-C19
16	B	851	LHG	O6-C4-C5-C6
12	F	204	CLA	CAA-CBA-CGA-O1A
18	L	210	LMT	O5B-C5B-C6B-O6B
15	B	836	BCR	C17-C18-C19-C20
18	A	842	LMT	C7-C8-C9-C10
12	A	845	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
12	A	847	CLA	C6-C7-C8-C10
12	B	811	CLA	C11-C12-C13-C15
12	B	828	CLA	C11-C10-C8-C7
12	A	822	CLA	C2B-C3B-CAB-CBB
12	B	816	CLA	C2B-C3B-CAB-CBB
12	B	818	CLA	C2B-C3B-CAB-CBB
12	B	825	CLA	C2B-C3B-CAB-CBB
12	B	829	CLA	C2B-C3B-CAB-CBB
12	B	843	CLA	C2B-C3B-CAB-CBB
15	A	835	BCR	C1-C6-C7-C8
15	A	837	BCR	C5-C6-C7-C8
15	A	837	BCR	C23-C24-C25-C26
15	B	835	BCR	C5-C6-C7-C8
20	A	856	45D	C04-C08-C20-C24
12	B	812	CLA	CAA-CBA-CGA-O2A
12	A	803	CLA	C2-C1-O2A-CGA
12	B	814	CLA	C2-C1-O2A-CGA
12	A	844	CLA	C16-C17-C18-C20
12	L	201	CLA	C5-C6-C7-C8
27	M	102	SQD	C13-C14-C15-C16
12	A	818	CLA	C10-C11-C12-C13
12	L	206	CLA	CAA-CBA-CGA-O2A
17	B	837	LMG	O7-C10-C11-C12
12	B	849	CLA	CAA-CBA-CGA-O2A
16	A	839	LHG	O8-C23-C24-C25
12	A	848	CLA	C14-C13-C15-C16
12	B	804	CLA	C11-C12-C13-C14
12	B	814	CLA	C6-C7-C8-C9
16	A	839	LHG	C16-C17-C18-C19
12	B	826	CLA	C16-C17-C18-C19
12	B	811	CLA	C4B-C3B-CAB-CBB
12	B	824	CLA	C1A-C2A-CAA-CBA
12	B	827	CLA	C1A-C2A-CAA-CBA
16	B	851	LHG	O8-C23-C24-C25
27	M	102	SQD	O48-C23-C24-C25
12	K	4004	CLA	C2-C3-C5-C6
15	A	835	BCR	C13-C14-C15-C16
27	M	102	SQD	C31-C32-C33-C34
26	L	209	DGD	C6A-C7A-C8A-C9A
12	J	102	CLA	CAA-CBA-CGA-O2A
12	B	801	CLA	C16-C17-C18-C20
12	A	828	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
27	M	102	SQD	C5-C6-S-O9
12	B	803	CLA	C15-C16-C17-C18
12	B	803	CLA	C4-C3-C5-C6
12	A	845	CLA	C2-C1-O2A-CGA
12	B	804	CLA	C2-C1-O2A-CGA
12	B	843	CLA	C2-C1-O2A-CGA
12	A	829	CLA	C6-C7-C8-C10
12	A	844	CLA	C12-C13-C15-C16
12	A	848	CLA	C12-C13-C15-C16
12	B	809	CLA	C11-C10-C8-C7
12	B	820	CLA	C11-C12-C13-C15
12	B	824	CLA	C11-C10-C8-C7
12	B	850	CLA	C11-C12-C13-C15
12	B	808	CLA	C13-C15-C16-C17
12	B	806	CLA	CBD-CGD-O2D-CED
12	B	807	CLA	C13-C15-C16-C17
12	B	829	CLA	C16-C17-C18-C19
12	B	803	CLA	C3A-C2A-CAA-CBA
12	B	818	CLA	C4-C3-C5-C6
12	L	206	CLA	CAA-CBA-CGA-O1A
12	B	820	CLA	C15-C16-C17-C18
16	A	839	LHG	O10-C23-C24-C25
12	A	801	CLA	C11-C10-C8-C9
12	A	827	CLA	C11-C12-C13-C14
12	B	809	CLA	C14-C13-C15-C16
12	B	816	CLA	C14-C13-C15-C16
12	B	824	CLA	C11-C10-C8-C9
12	B	808	CLA	CAA-CBA-CGA-O2A
12	J	101	CLA	CAA-CBA-CGA-O1A
17	B	837	LMG	O9-C10-C11-C12
27	M	102	SQD	O5-C5-C6-S
16	B	851	LHG	O10-C23-C24-C25
12	B	850	CLA	C10-C11-C12-C13
12	B	816	CLA	CAA-CBA-CGA-O1A
12	B	845	CLA	C8-C10-C11-C12
17	A	840	LMG	O1-C7-C8-O7
18	J	106	LMT	C5'-C4'-O1B-C1B
12	B	812	CLA	CAA-CBA-CGA-O1A
16	A	839	LHG	O7-C7-C8-C9
12	J	102	CLA	CAA-CBA-CGA-O1A
12	A	801	CLA	CAD-CBD-CGD-O2D
12	A	843	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
12	B	816	CLA	CAD-CBD-CGD-O2D
12	B	842	CLA	CAD-CBD-CGD-O2D
12	A	813	CLA	C2-C1-O2A-CGA
17	A	851	LMG	C29-C30-C31-C32
12	B	810	CLA	CAA-CBA-CGA-O2A
12	B	849	CLA	CAA-CBA-CGA-O1A
27	M	102	SQD	O10-C23-C24-C25
16	M	103	LHG	C14-C15-C16-C17

There are no ring outliers.

113 monomers are involved in 242 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	828	CLA	3	0
12	F	203	CLA	1	0
12	B	823	CLA	2	0
12	A	843	CLA	8	0
12	B	852	CLA	2	0
16	M	103	LHG	1	0
17	A	840	LMG	2	0
12	B	807	CLA	3	0
12	F	204	CLA	2	0
15	B	835	BCR	1	0
12	A	823	CLA	2	0
12	B	846	CLA	1	0
15	B	832	BCR	2	0
16	A	839	LHG	4	0
15	F	201	BCR	3	0
12	A	804	CLA	2	0
12	B	828	CLA	2	0
15	A	835	BCR	3	0
27	M	102	SQD	5	0
12	B	809	CLA	2	0
12	A	846	CLA	9	0
12	A	849	CLA	4	0
12	B	814	CLA	2	0
18	A	842	LMT	4	0
12	B	826	CLA	1	0
15	L	207	BCR	3	0
16	A	850	LHG	5	0
15	B	836	BCR	3	0
12	B	802	CLA	5	0

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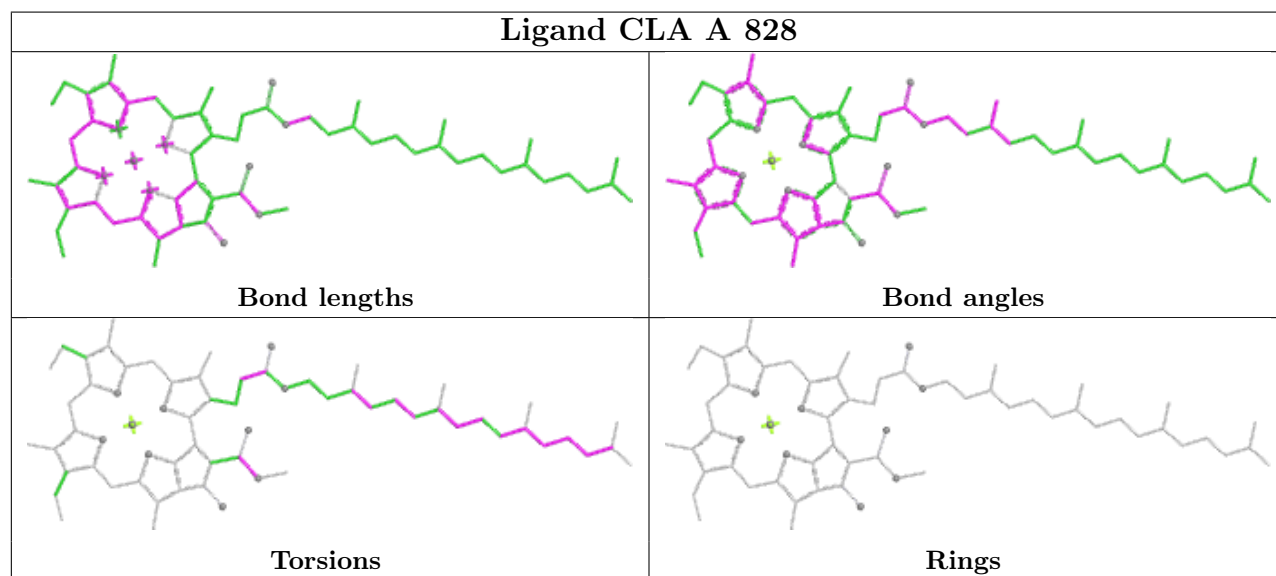
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	809	CLA	6	0
12	A	845	CLA	1	0
12	A	810	CLA	1	0
12	B	805	CLA	1	0
12	B	819	CLA	6	0
12	A	830	CLA	3	0
12	A	814	CLA	3	0
18	J	106	LMT	1	0
12	A	848	CLA	4	0
12	B	825	CLA	1	0
13	A	802	CL0	1	0
12	B	843	CLA	3	0
12	B	808	CLA	1	0
12	A	819	CLA	1	0
12	B	811	CLA	4	0
12	B	849	CLA	2	0
17	B	837	LMG	1	0
12	B	853	CLA	3	0
12	K	4003	CLA	6	0
12	L	204	CLA	3	0
12	A	855	CLA	1	0
15	A	837	BCR	3	0
12	A	816	CLA	2	0
12	A	826	CLA	2	0
12	A	833	CLA	1	0
18	B	840	LMT	4	0
12	J	102	CLA	2	0
12	A	831	CLA	3	0
12	L	201	CLA	1	0
12	A	844	CLA	8	0
12	B	827	CLA	4	0
12	B	847	CLA	5	0
12	A	825	CLA	3	0
12	B	803	CLA	4	0
18	A	841	LMT	1	0
12	A	858	CLA	2	0
12	B	824	CLA	6	0
15	J	105	BCR	4	0
12	A	832	CLA	2	0
12	B	820	CLA	3	0
16	B	851	LHG	5	0
12	B	817	CLA	1	0

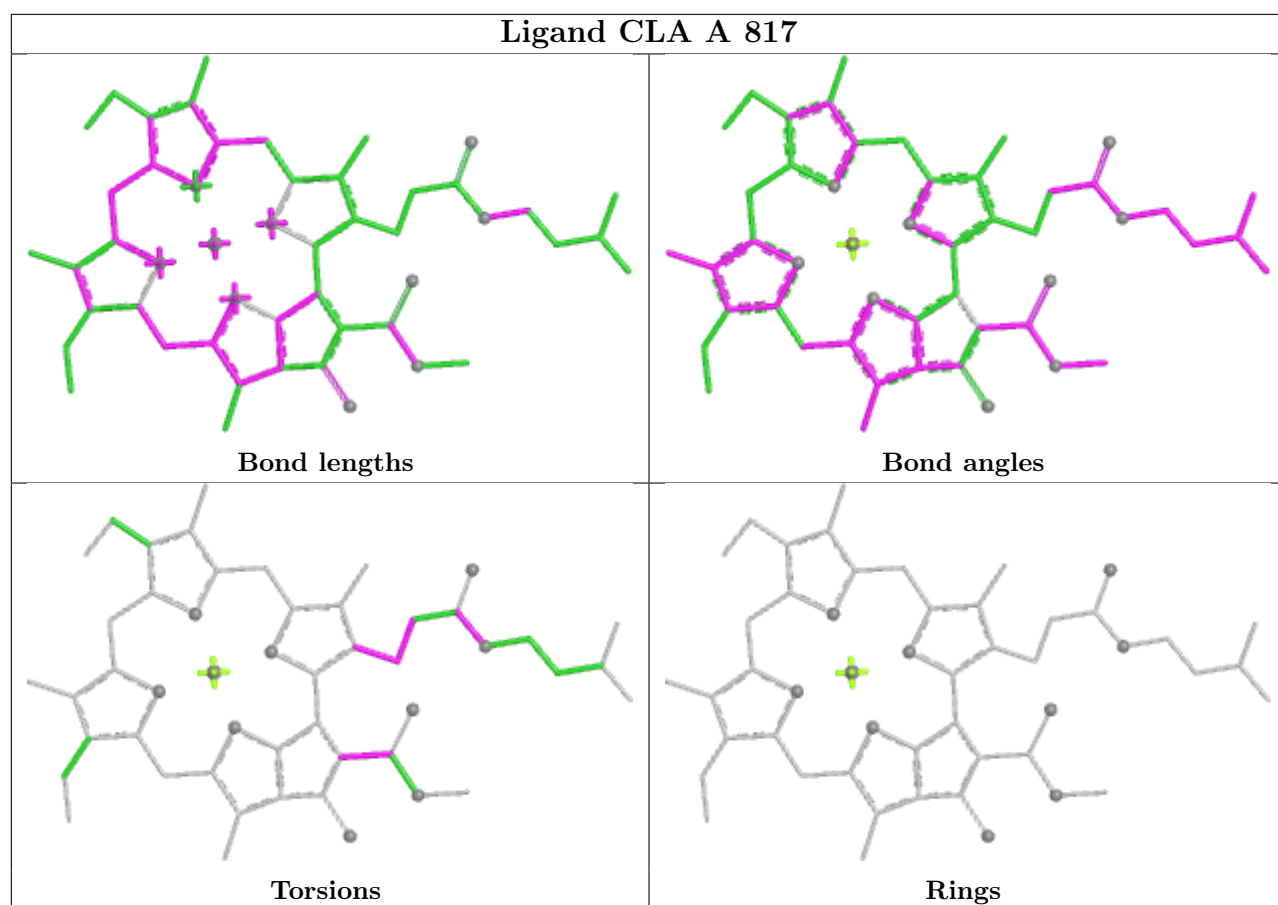
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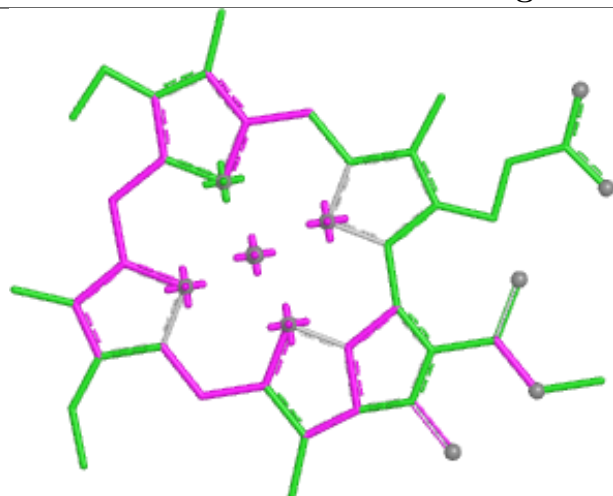
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	K	4004	CLA	4	0
12	B	813	CLA	2	0
18	F	205	LMT	1	0
12	B	850	CLA	5	0
12	A	847	CLA	2	0
12	A	821	CLA	4	0
12	B	816	CLA	1	0
12	J	101	CLA	2	0
12	B	818	CLA	2	0
12	A	824	CLA	2	0
12	A	829	CLA	3	0
15	B	841	BCR	1	0
12	A	820	CLA	2	0
12	A	803	CLA	1	0
12	A	813	CLA	2	0
15	F	202	BCR	3	0
15	K	4005	BCR	5	0
12	A	801	CLA	1	0
12	B	810	CLA	3	0
15	B	834	BCR	3	0
15	J	107	BCR	3	0
15	A	836	BCR	2	0
17	A	851	LMG	2	0
12	B	842	CLA	3	0
12	B	845	CLA	3	0
26	L	209	DGD	2	0
12	B	821	CLA	1	0
12	A	827	CLA	5	0
19	A	854	PL9	10	0
12	B	844	CLA	4	0
12	B	801	CLA	2	0
12	A	807	CLA	1	0
12	B	848	CLA	5	0
12	B	822	CLA	1	0
12	B	806	CLA	5	0
12	L	206	CLA	2	0
18	L	210	LMT	3	0
15	I	101	BCR	4	0
12	A	815	CLA	3	0
20	A	856	45D	3	0
15	L	208	BCR	1	0
23	B	833	ECH	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.

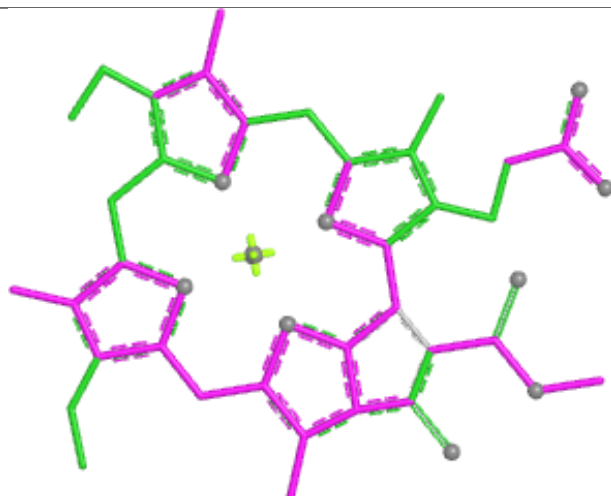




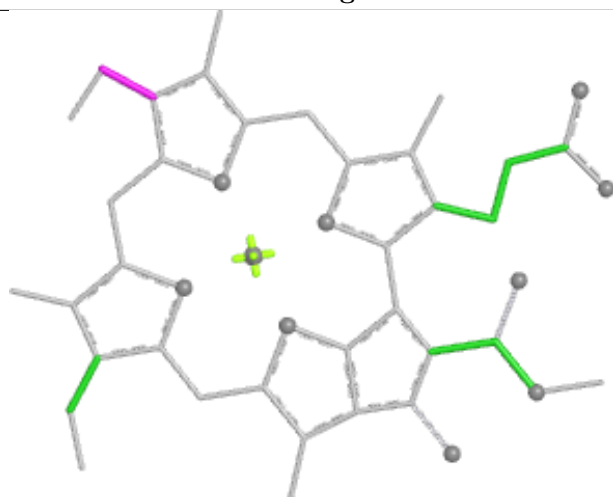
Ligand CLA F 203



Bond lengths



Bond angles

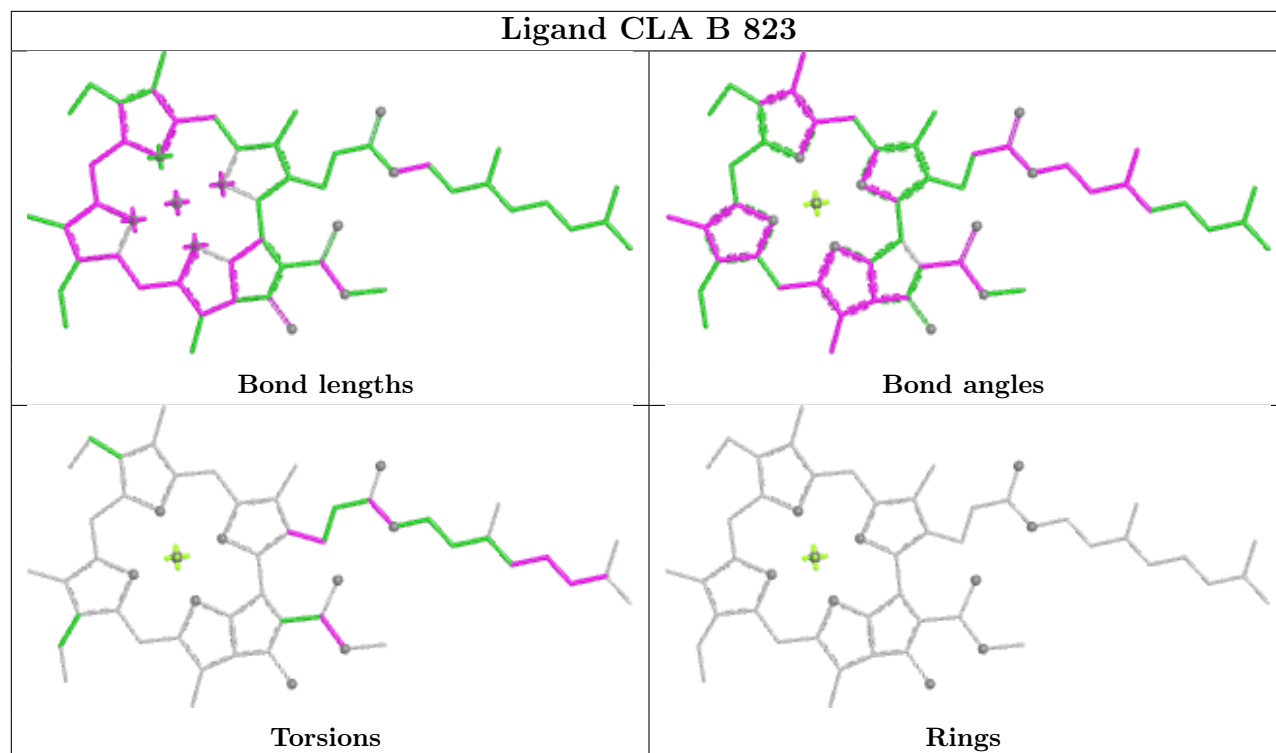


Torsions

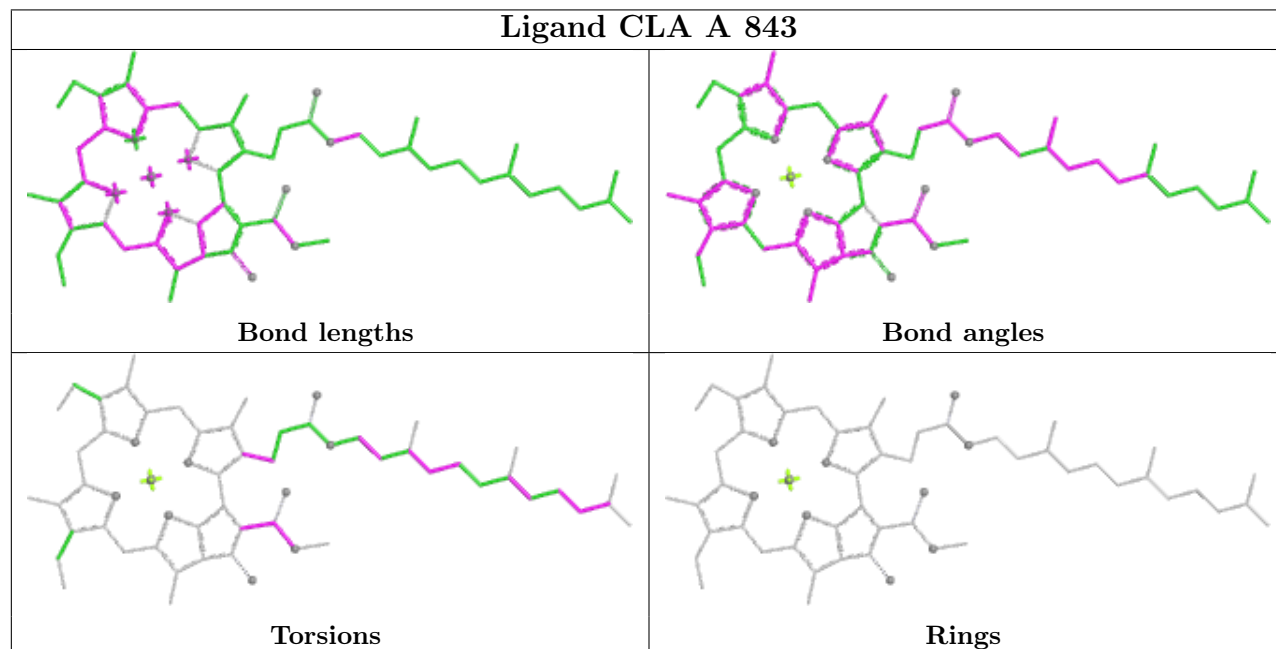


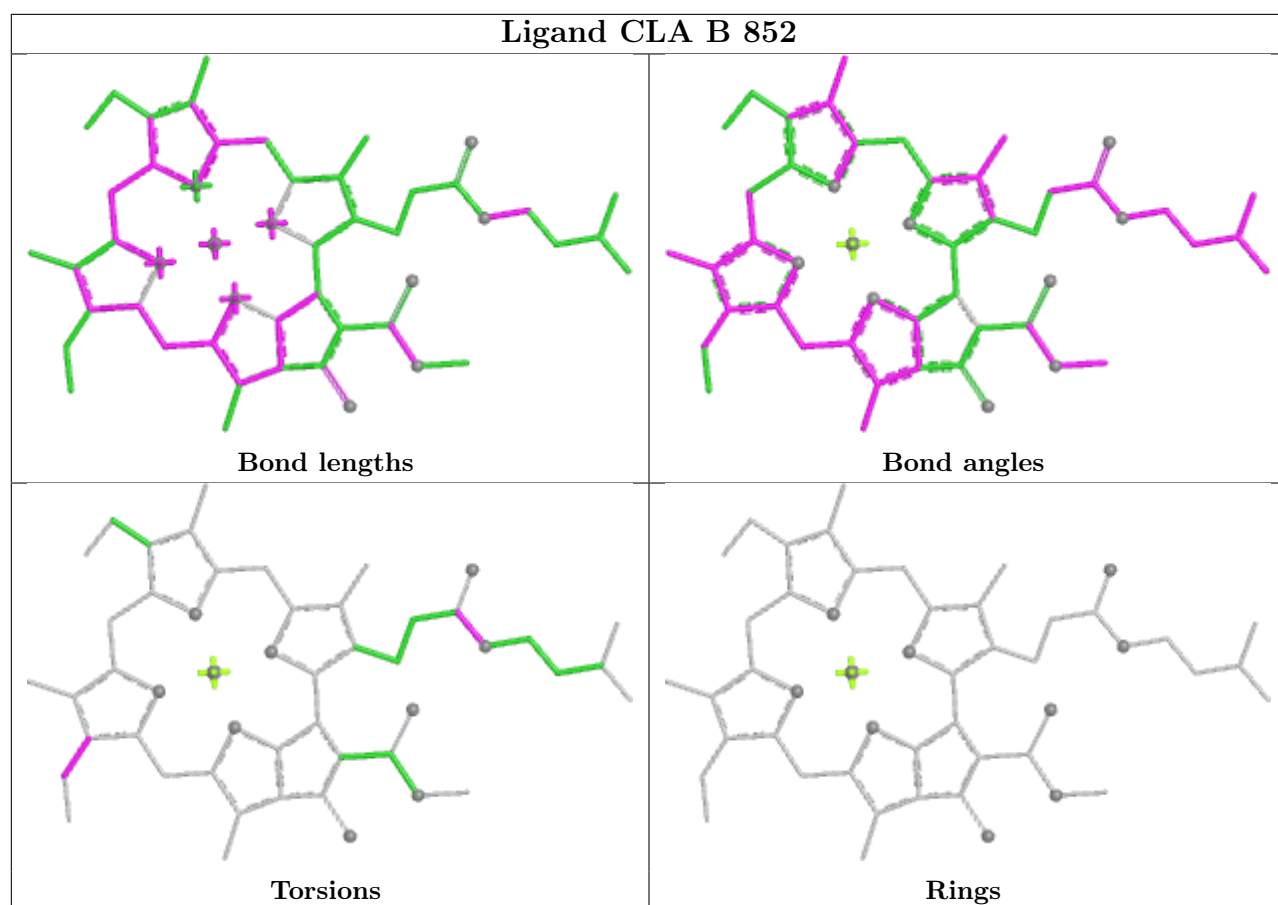
Rings

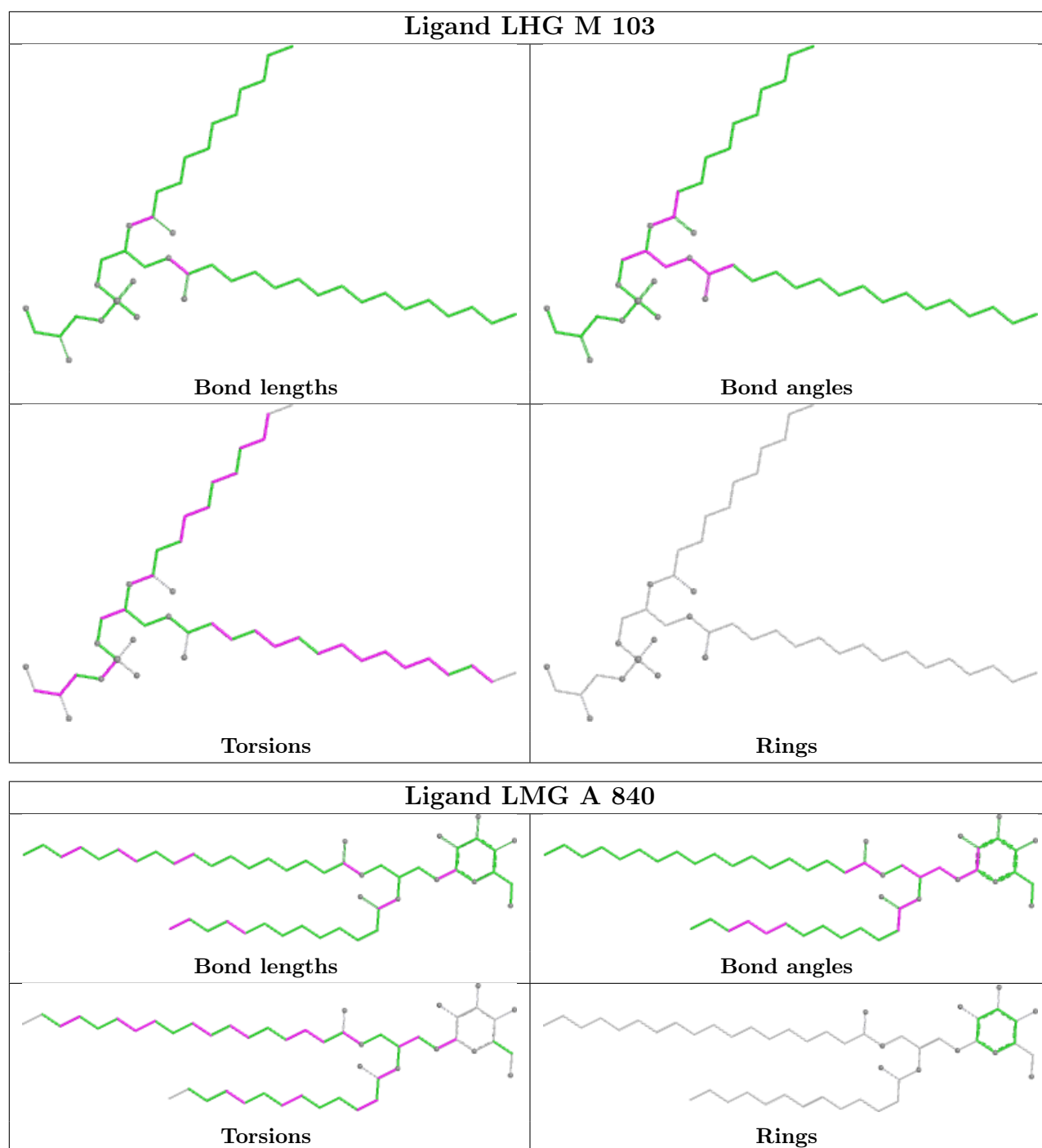
Ligand CLA B 823



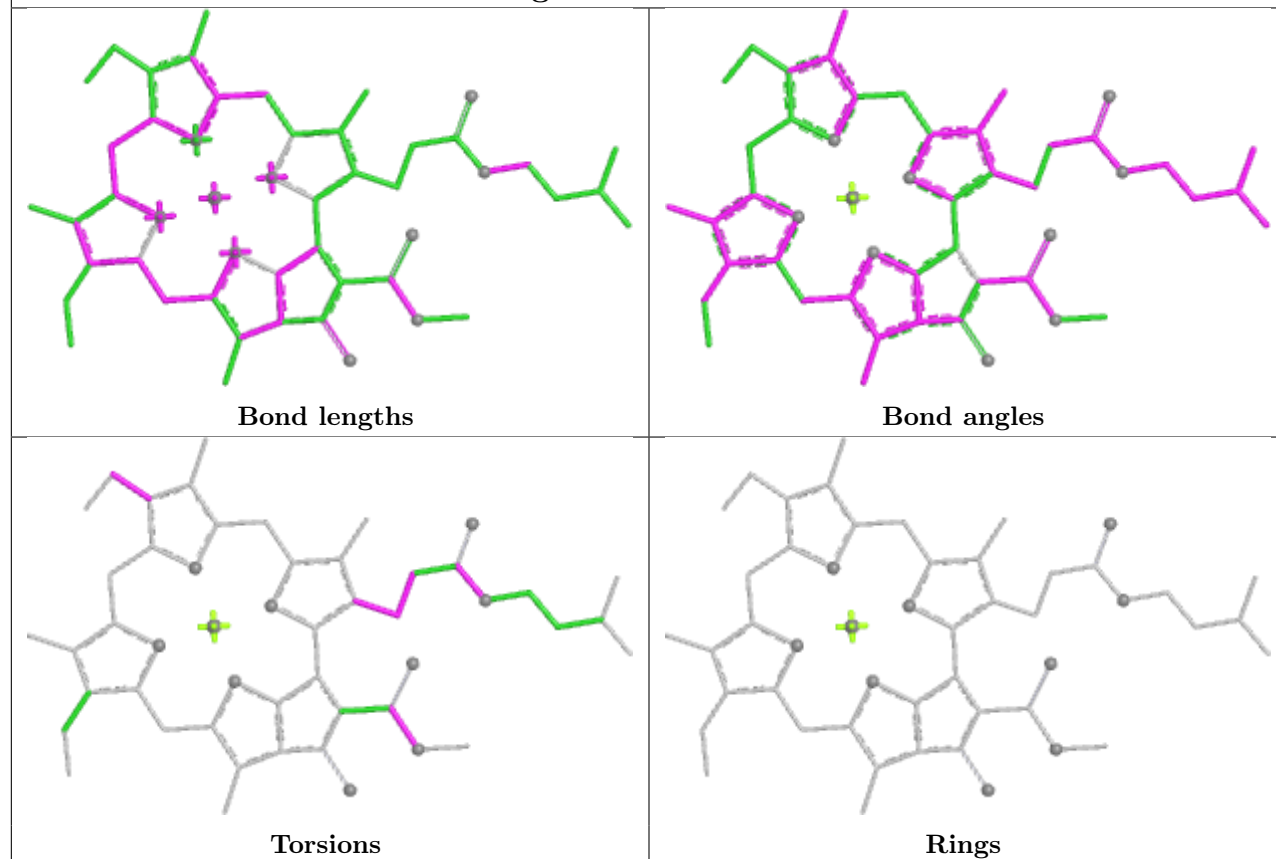
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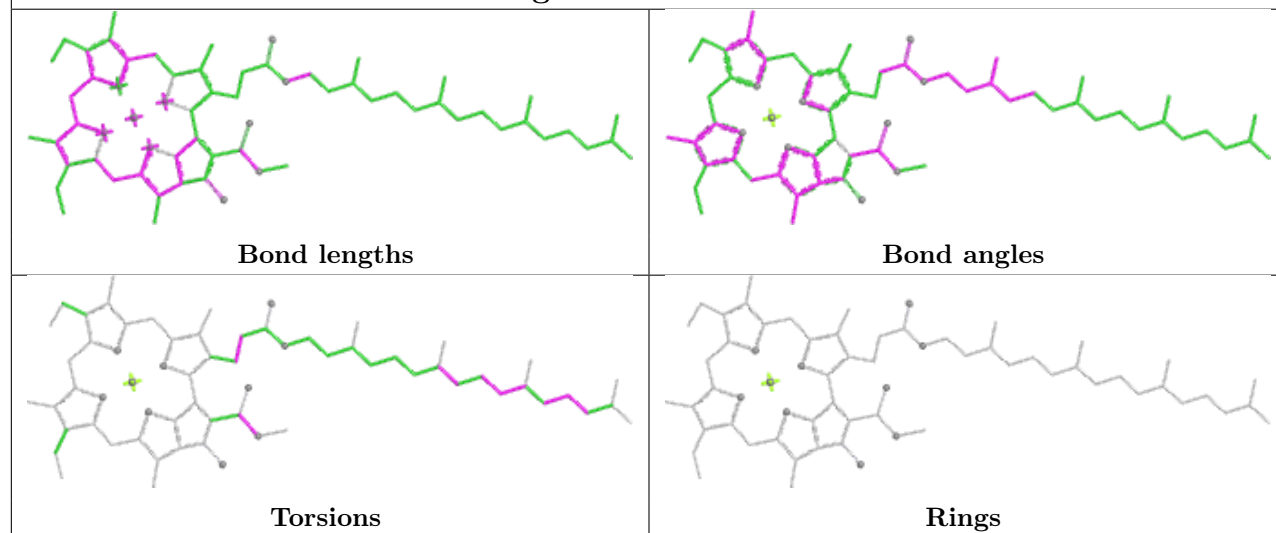




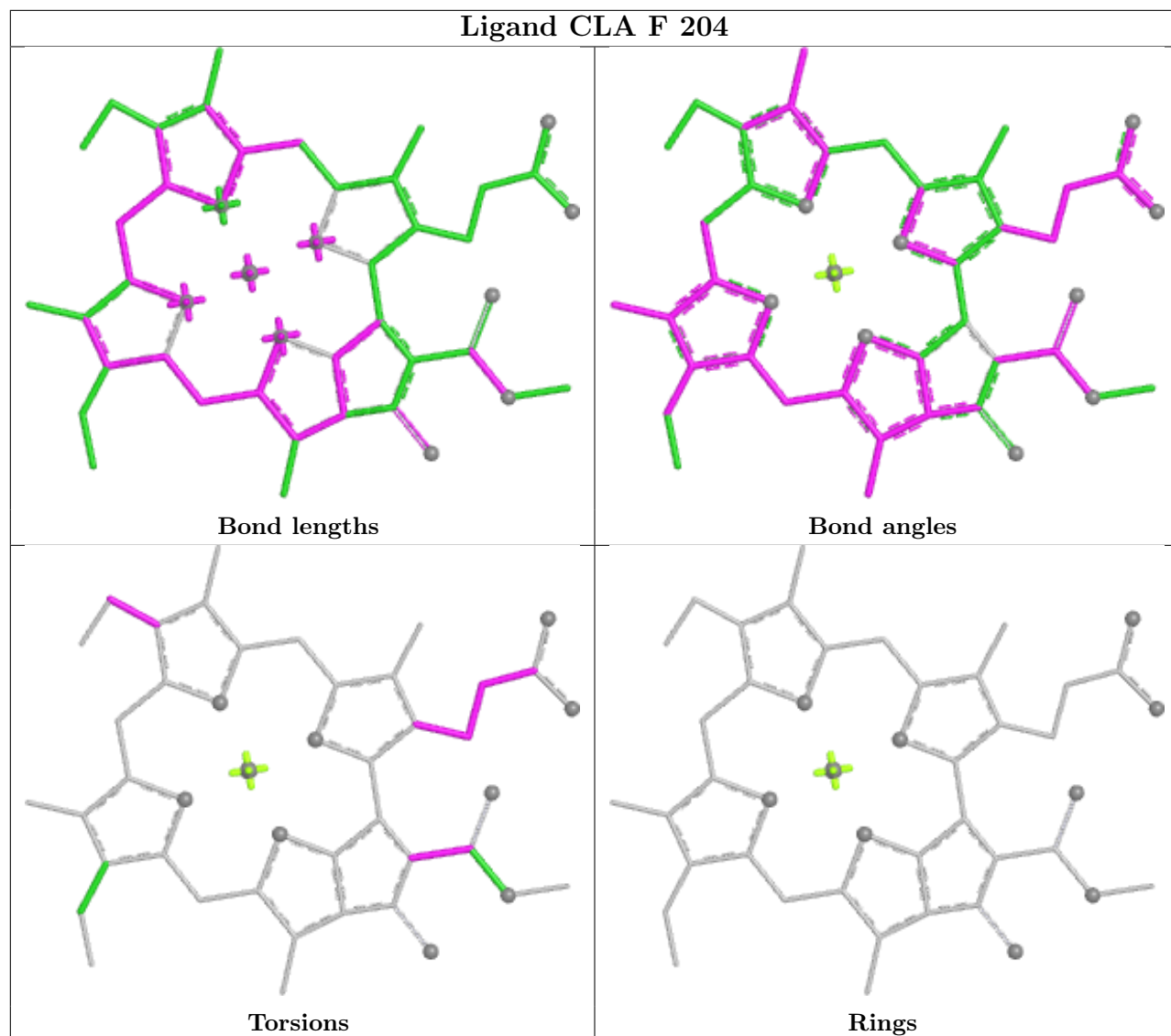
Ligand CLA A 808



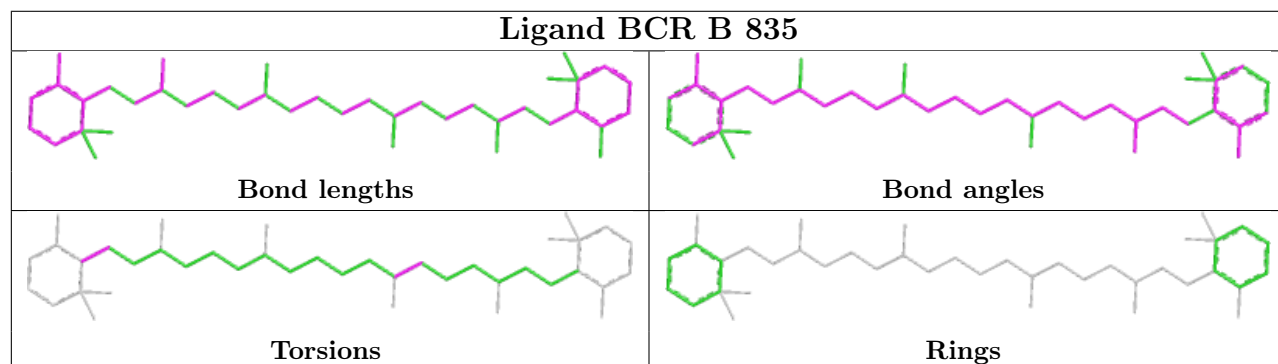
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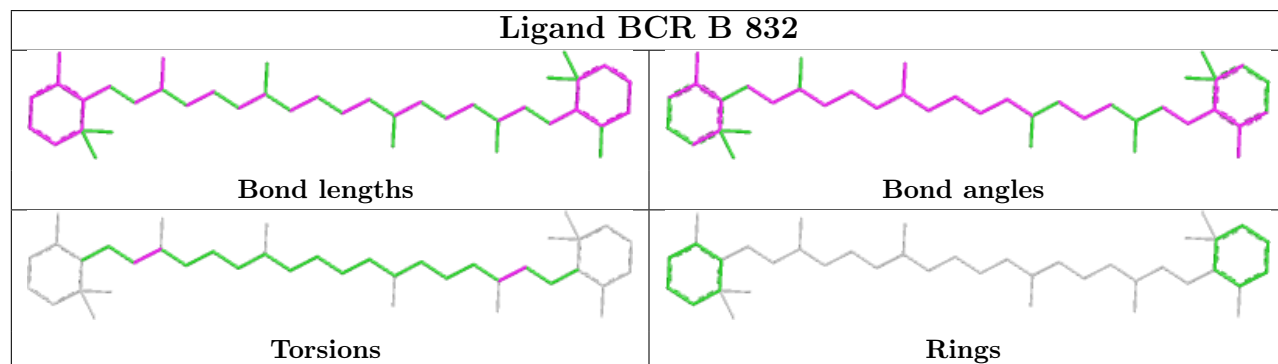
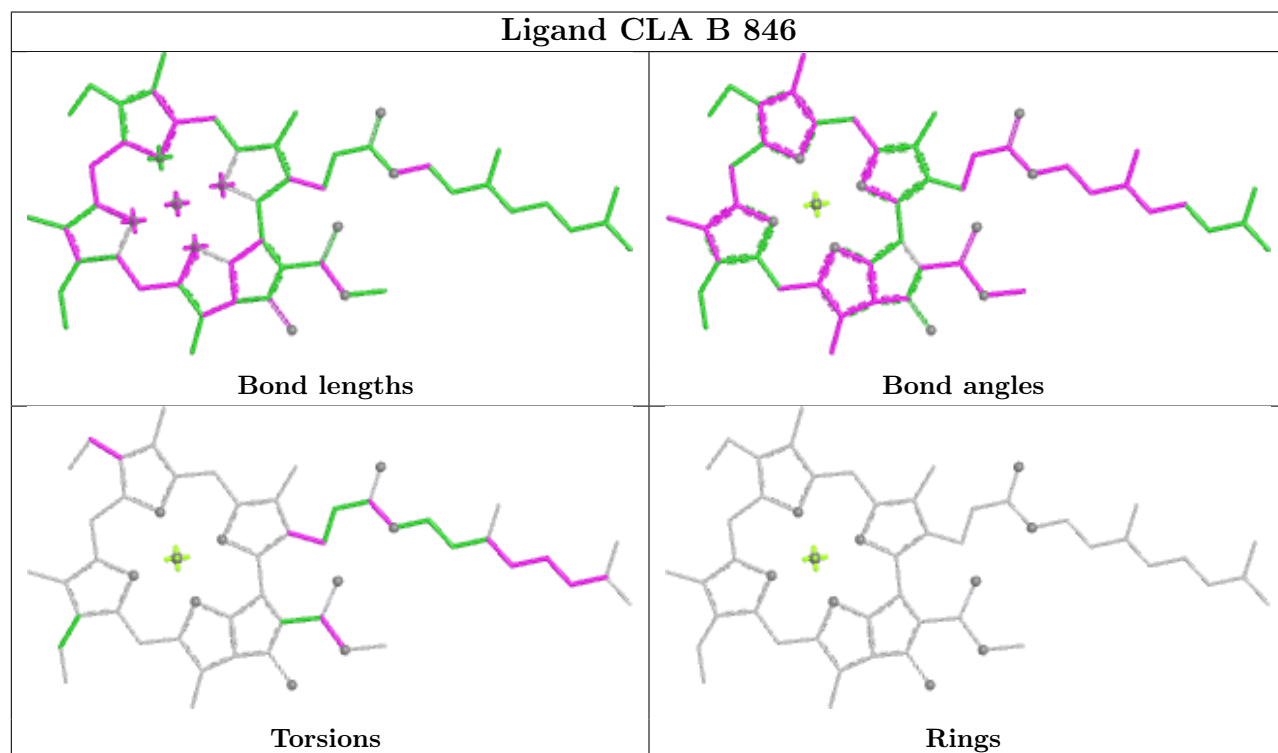
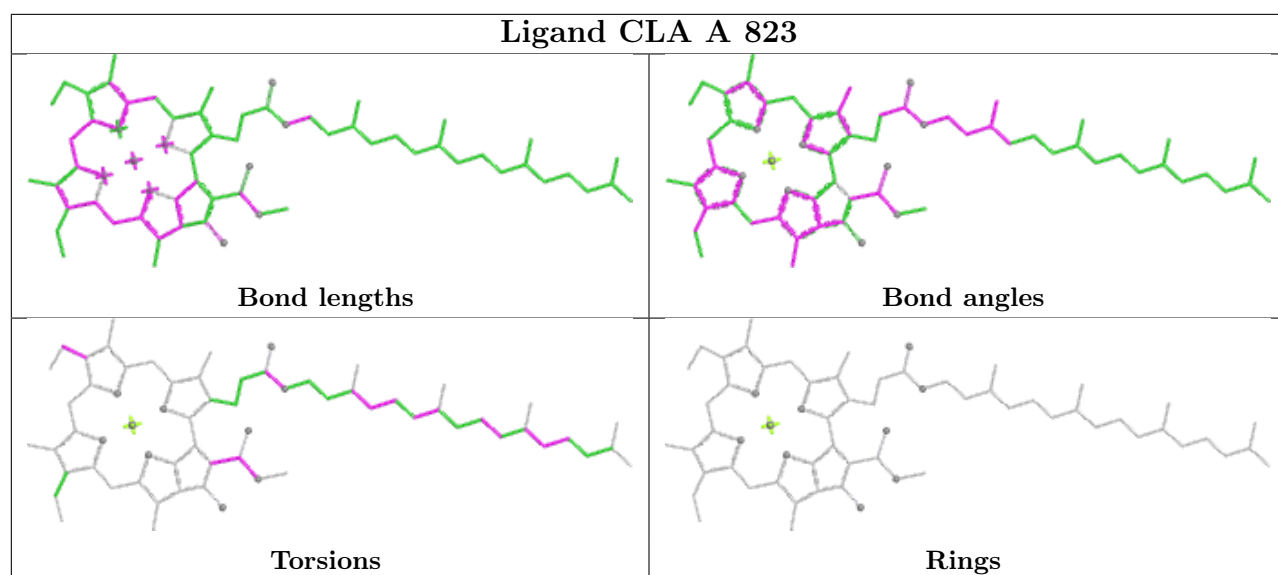


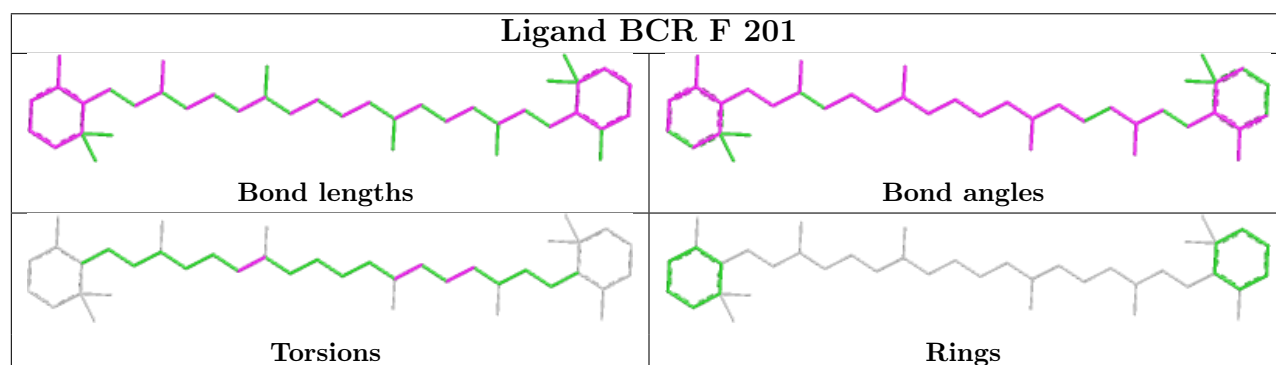
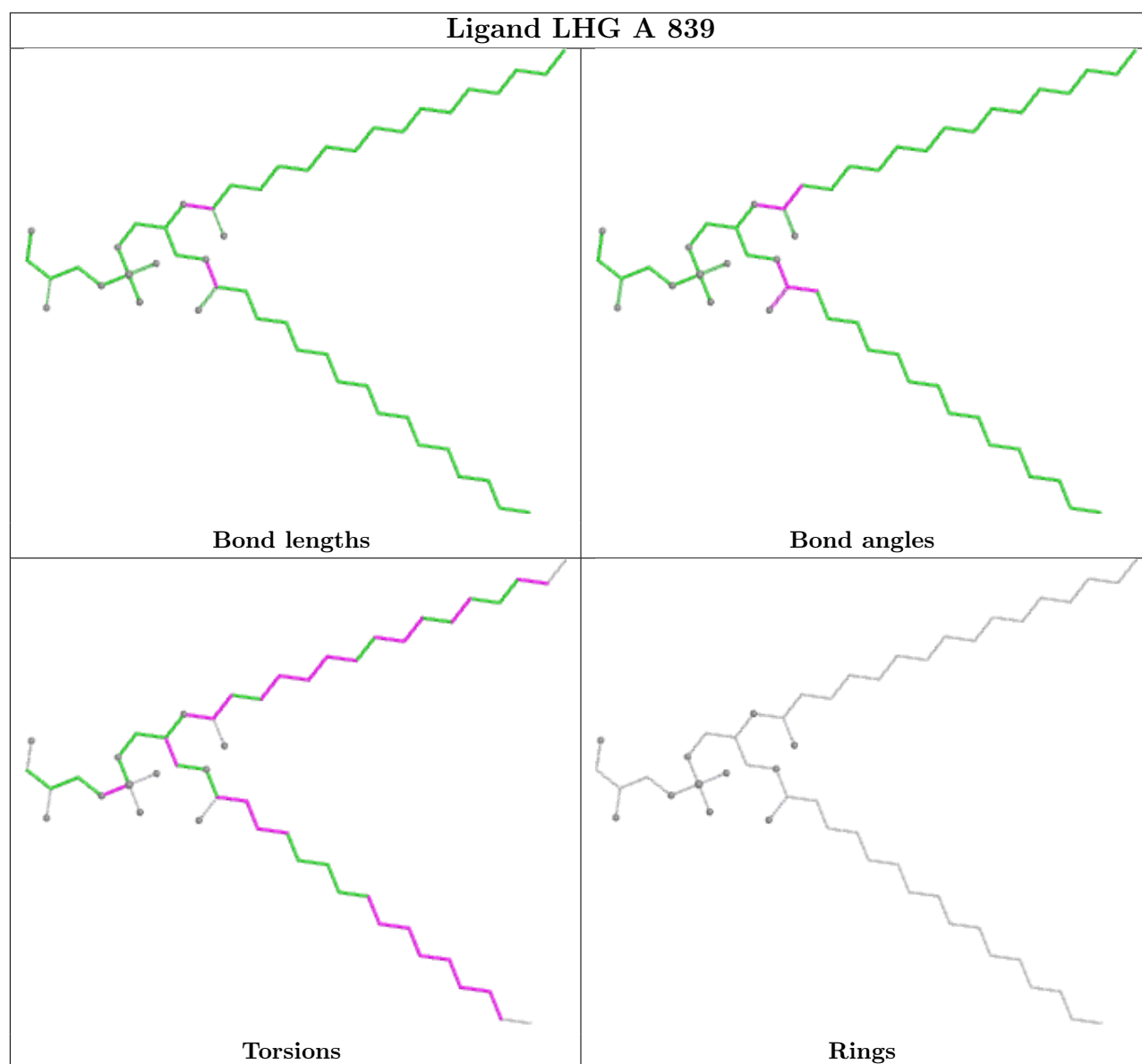
Ligand CLA F 204

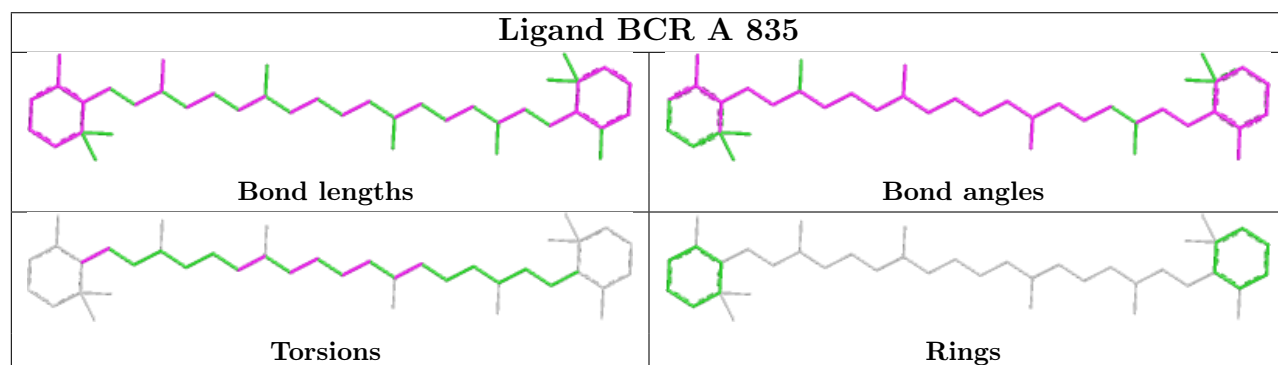
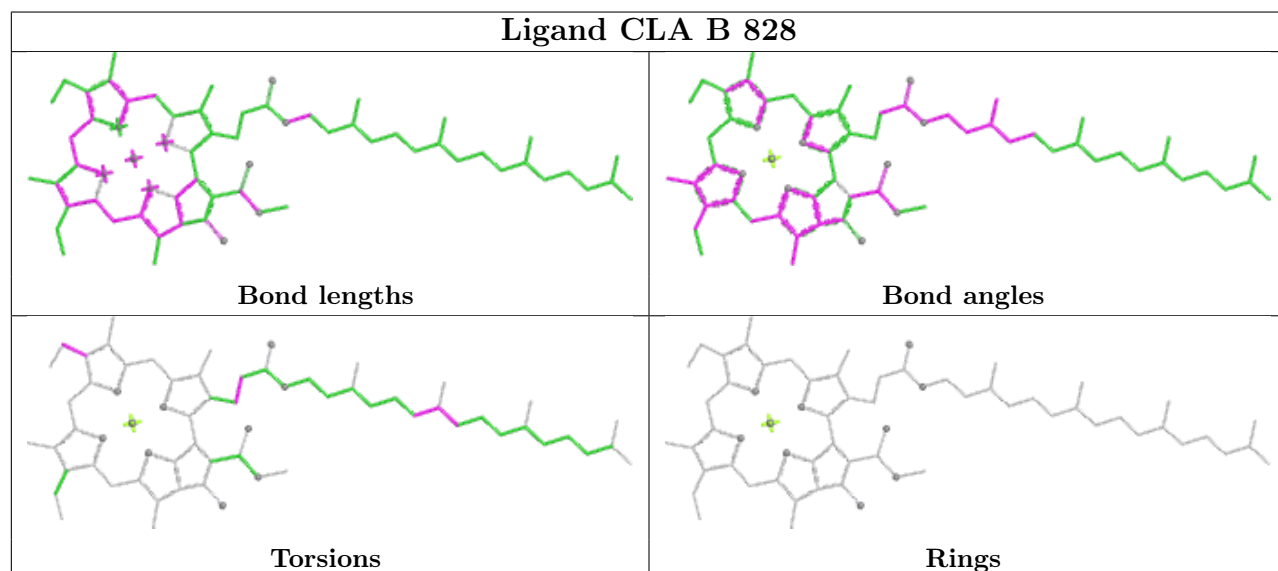
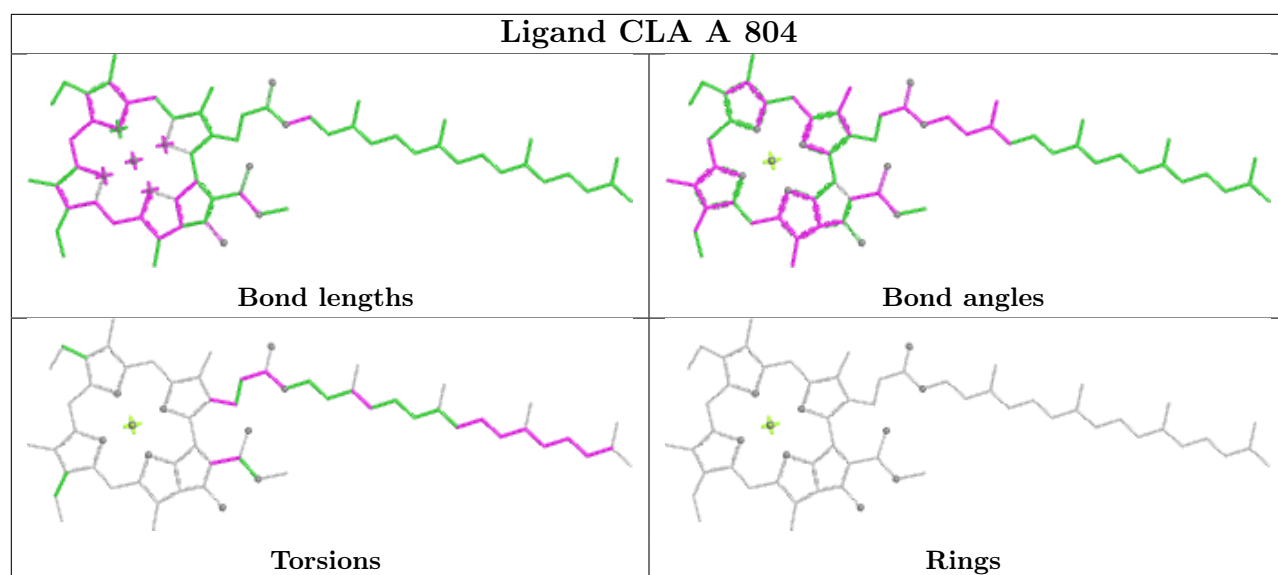


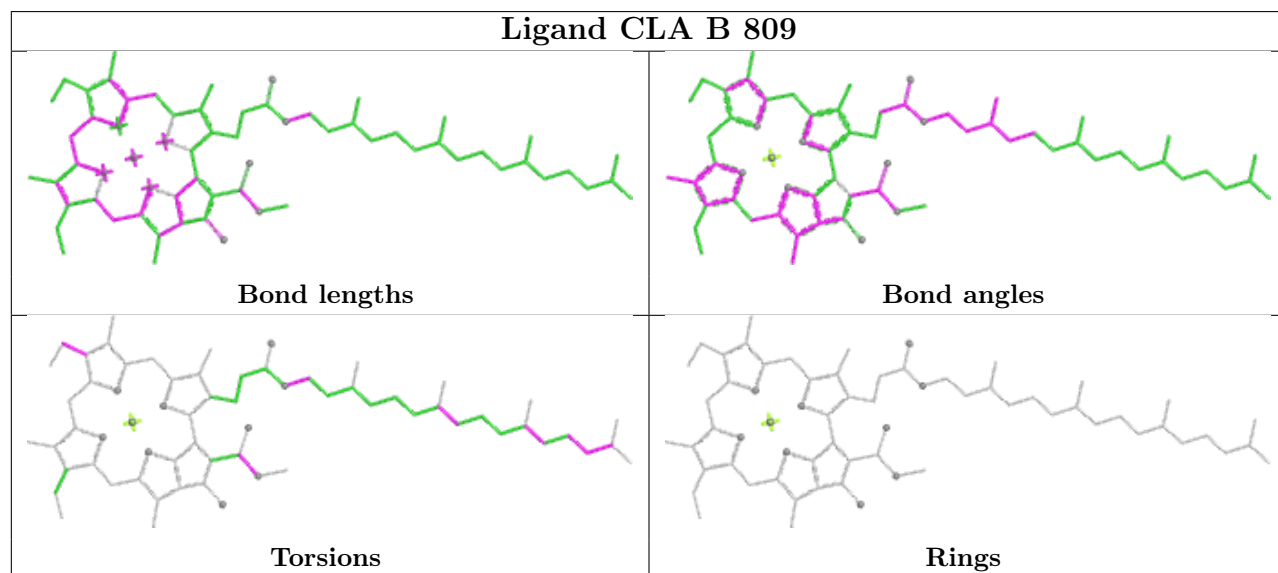
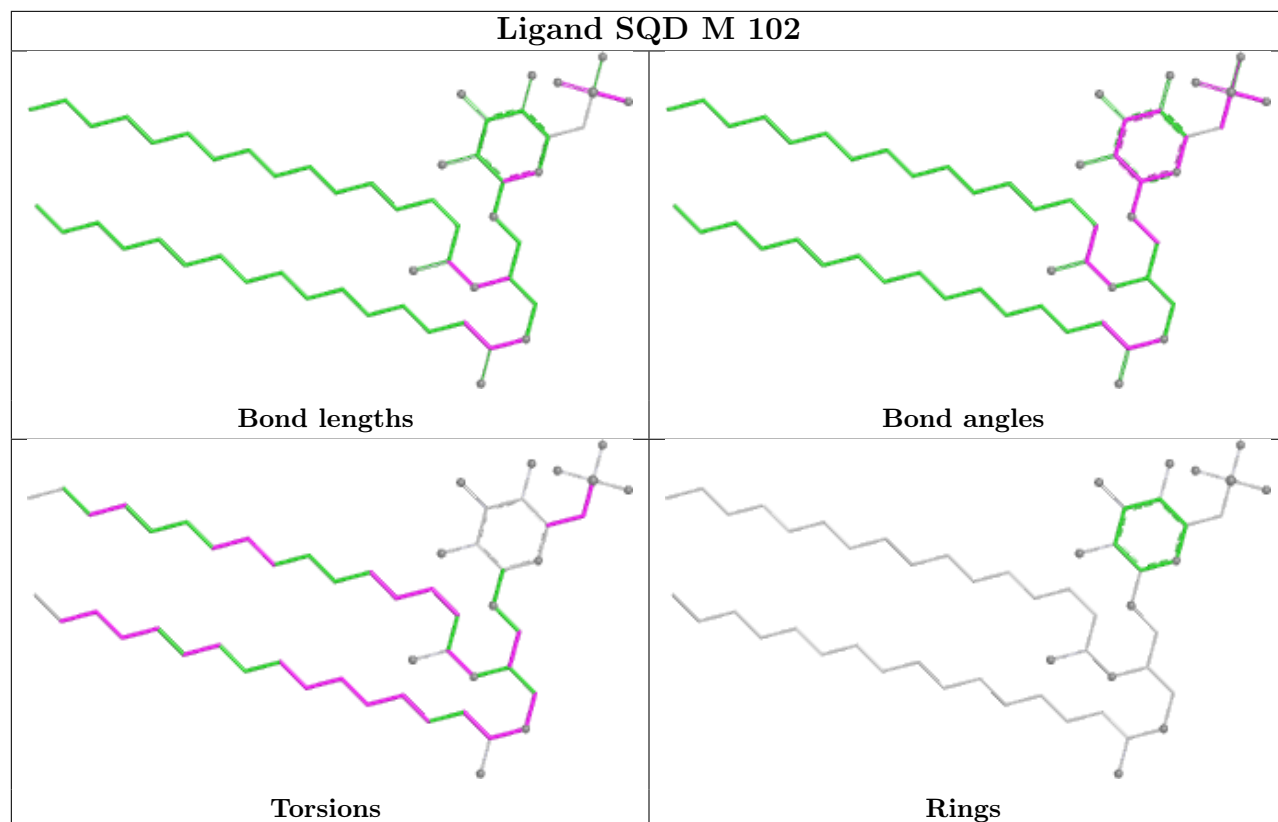
Ligand BCR B 835

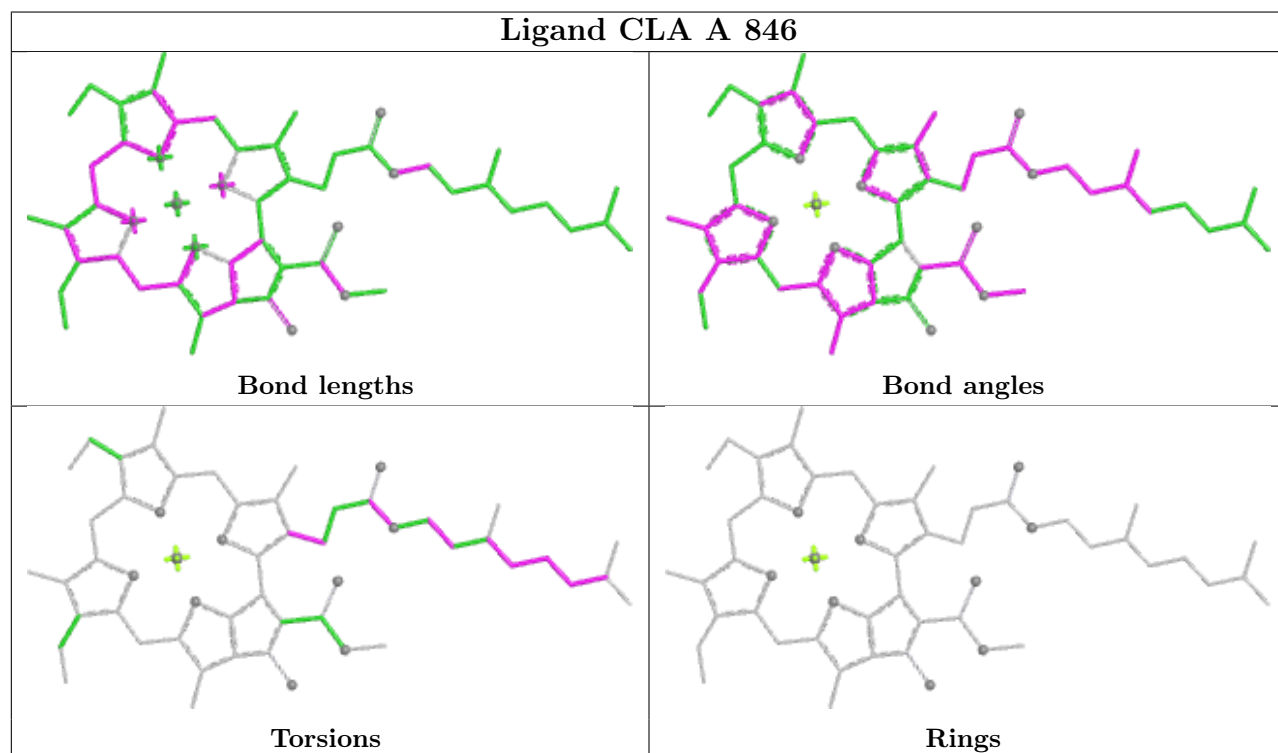
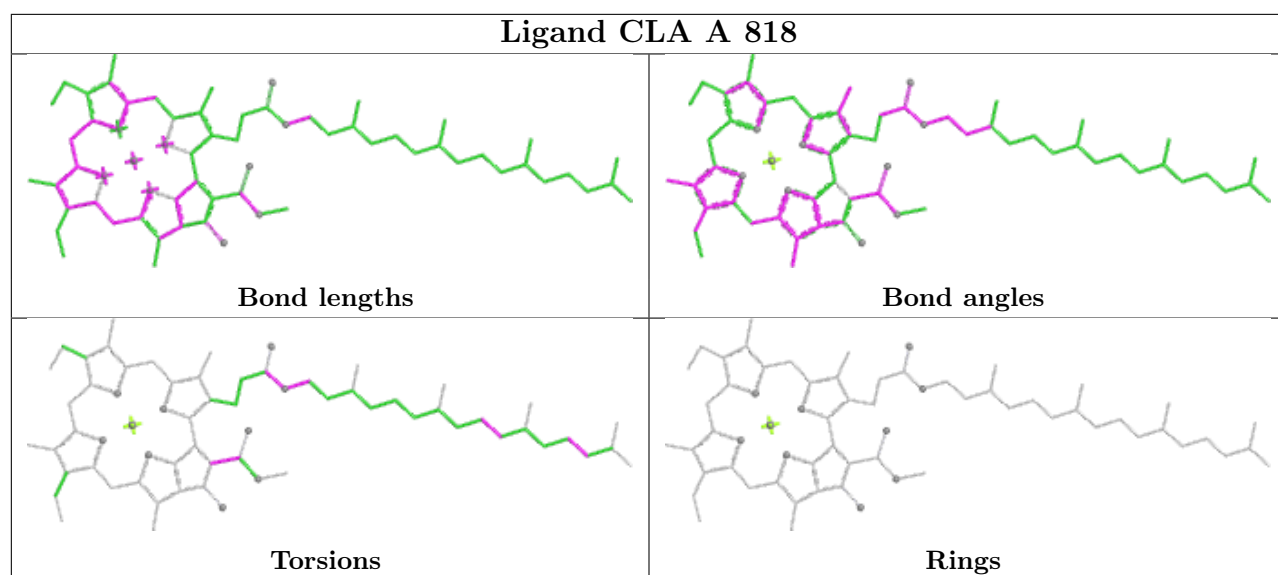




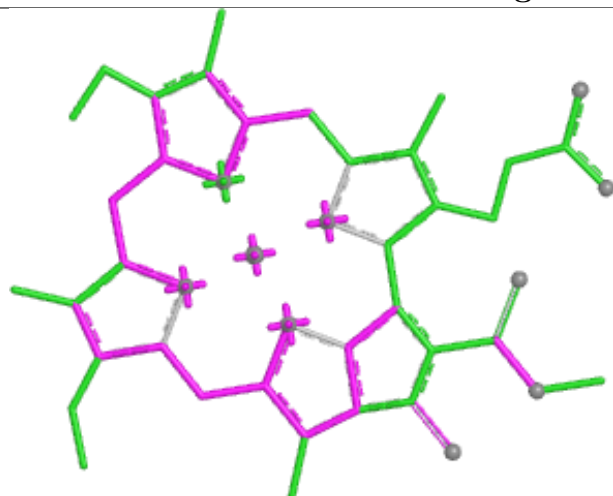




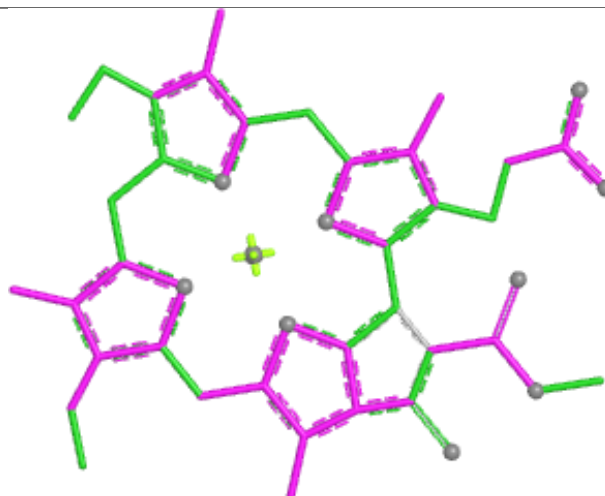




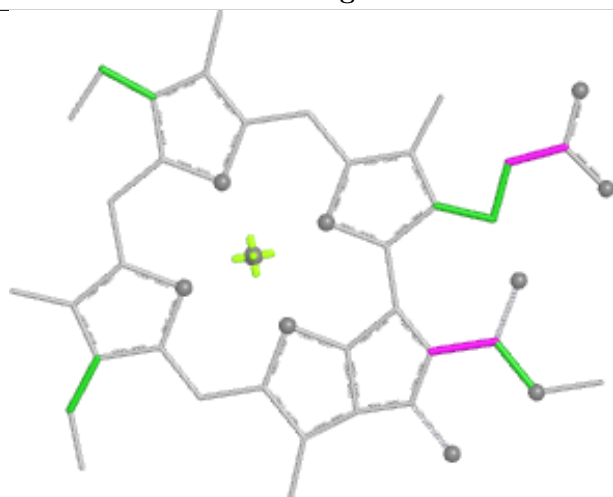
Ligand CLA B 830



Bond lengths



Bond angles

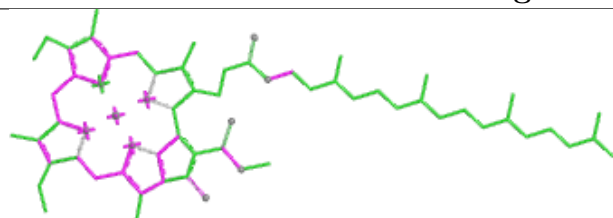


Torsions

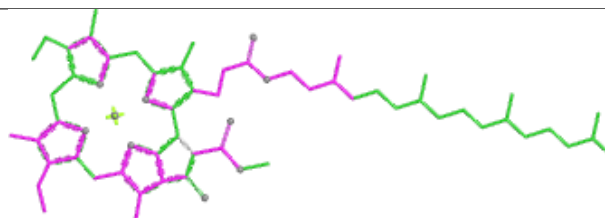


Rings

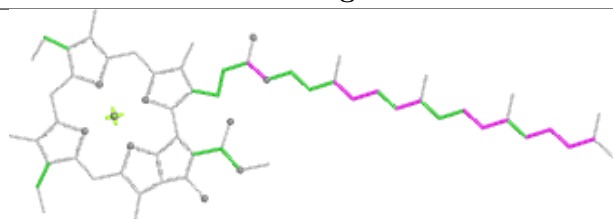
Ligand CLA A 849



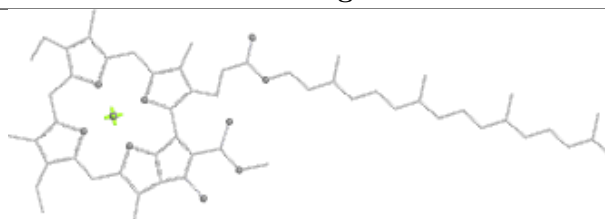
Bond lengths



Bond angles

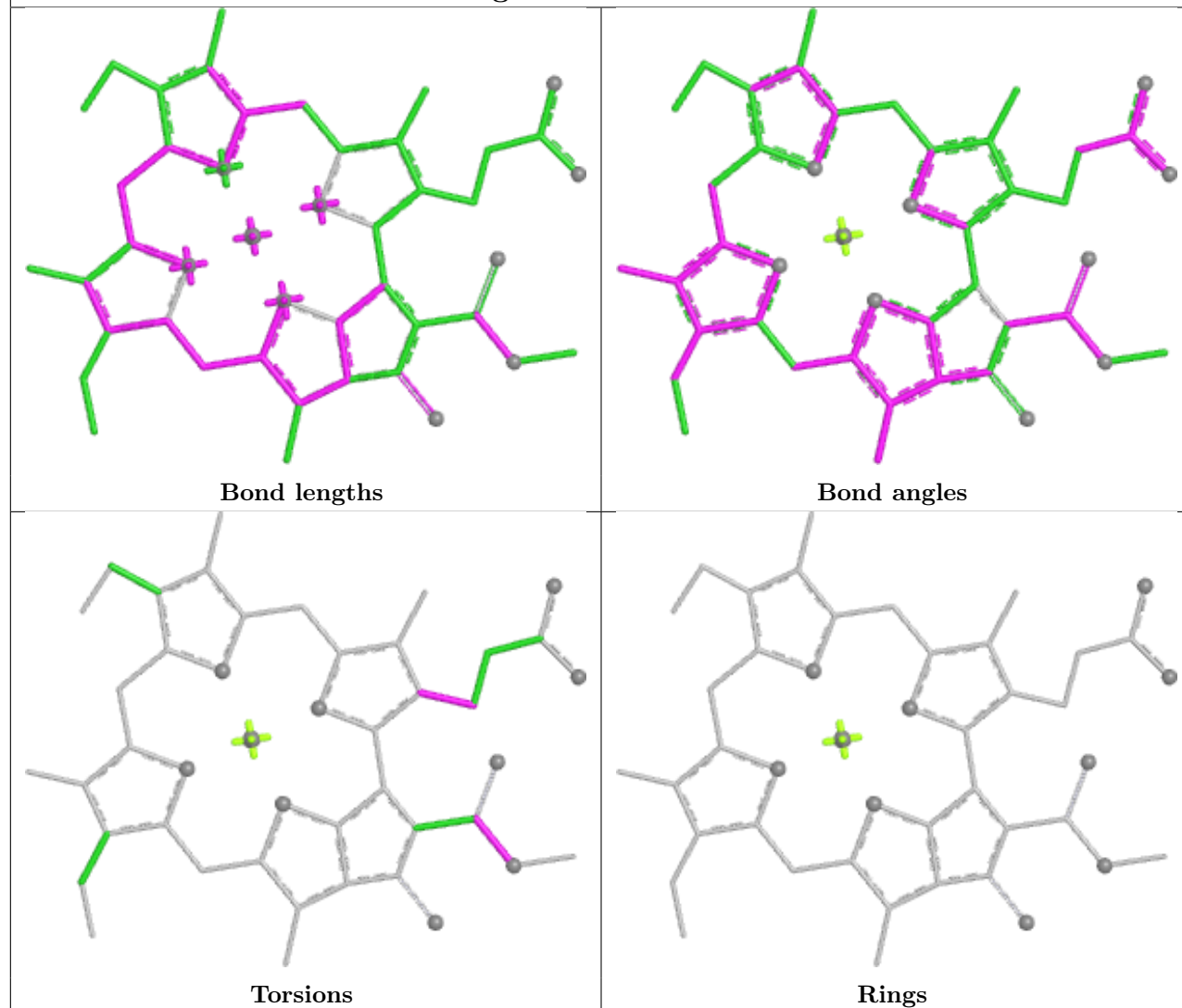


Torsions

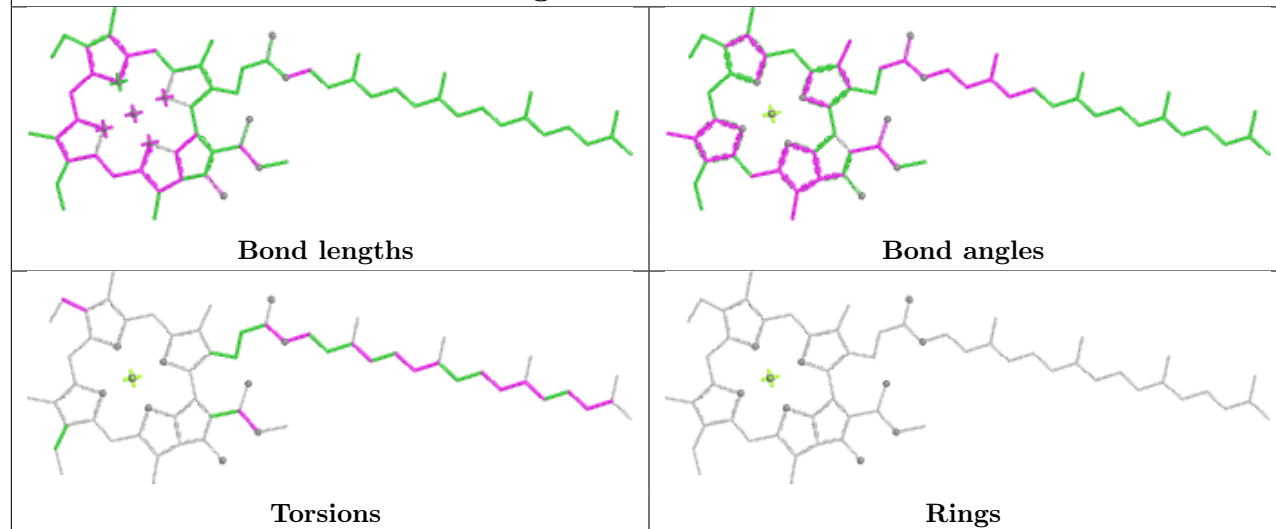


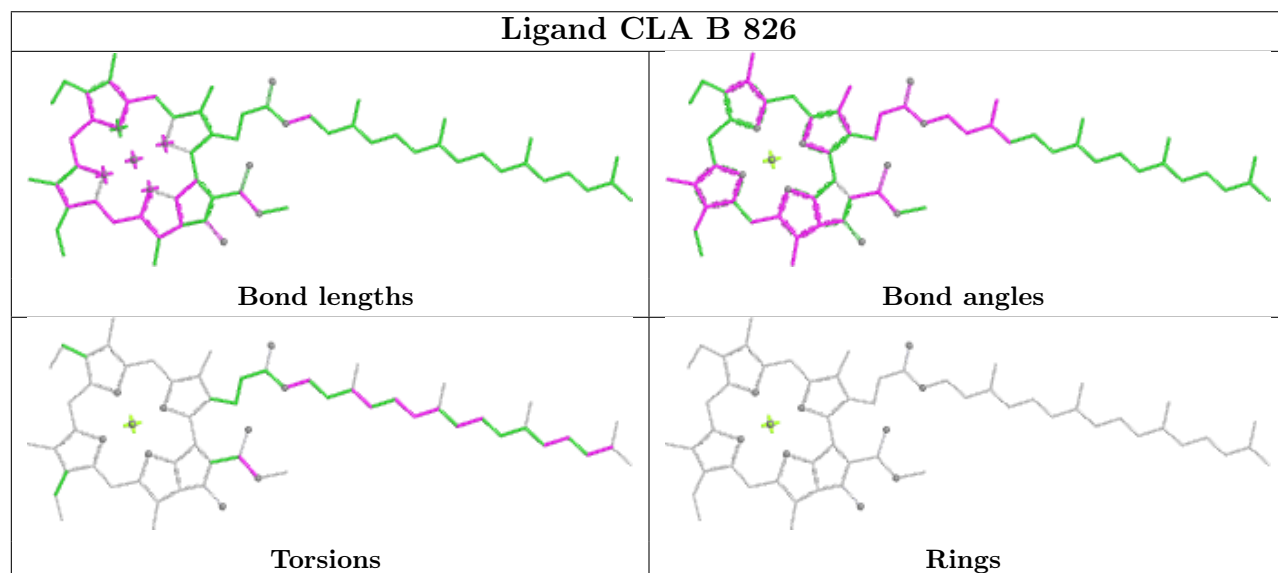
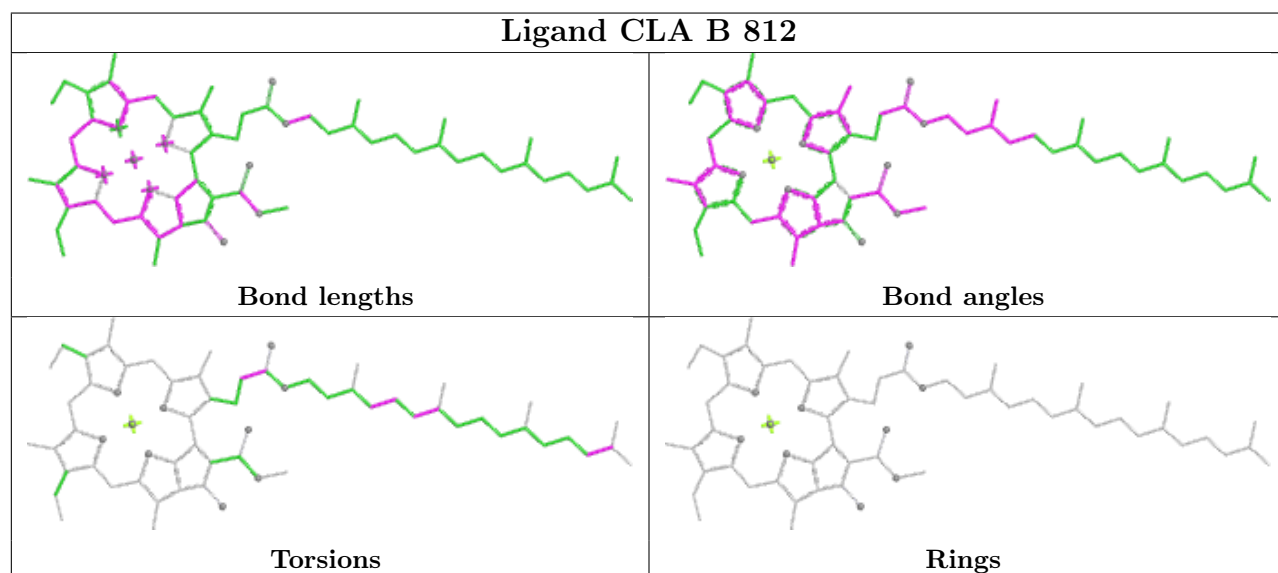
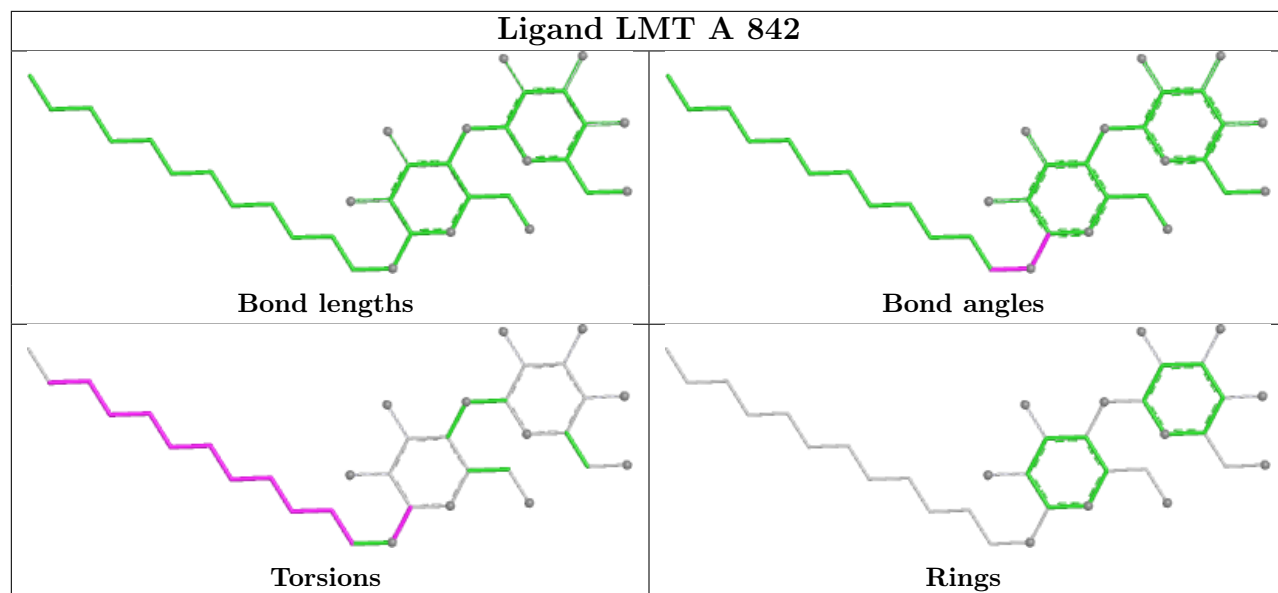
Rings

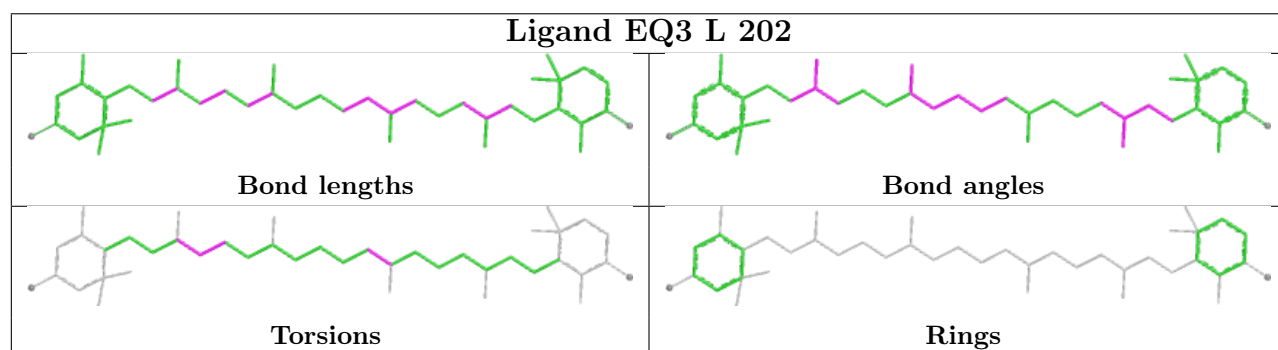
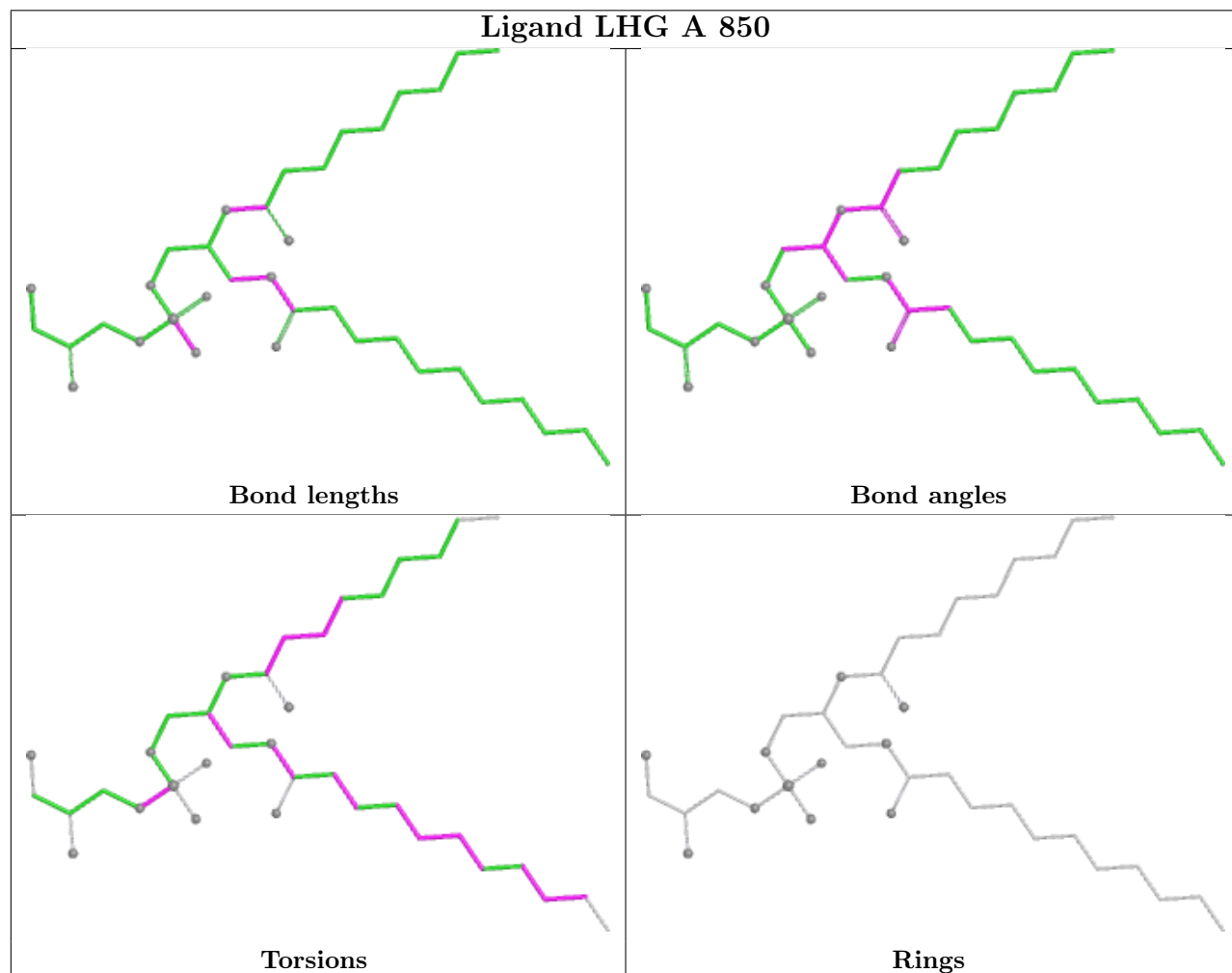
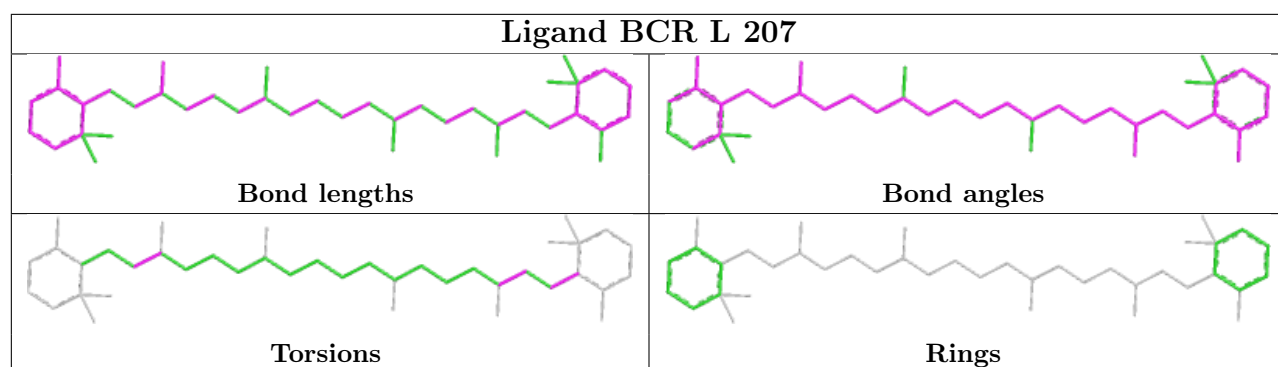
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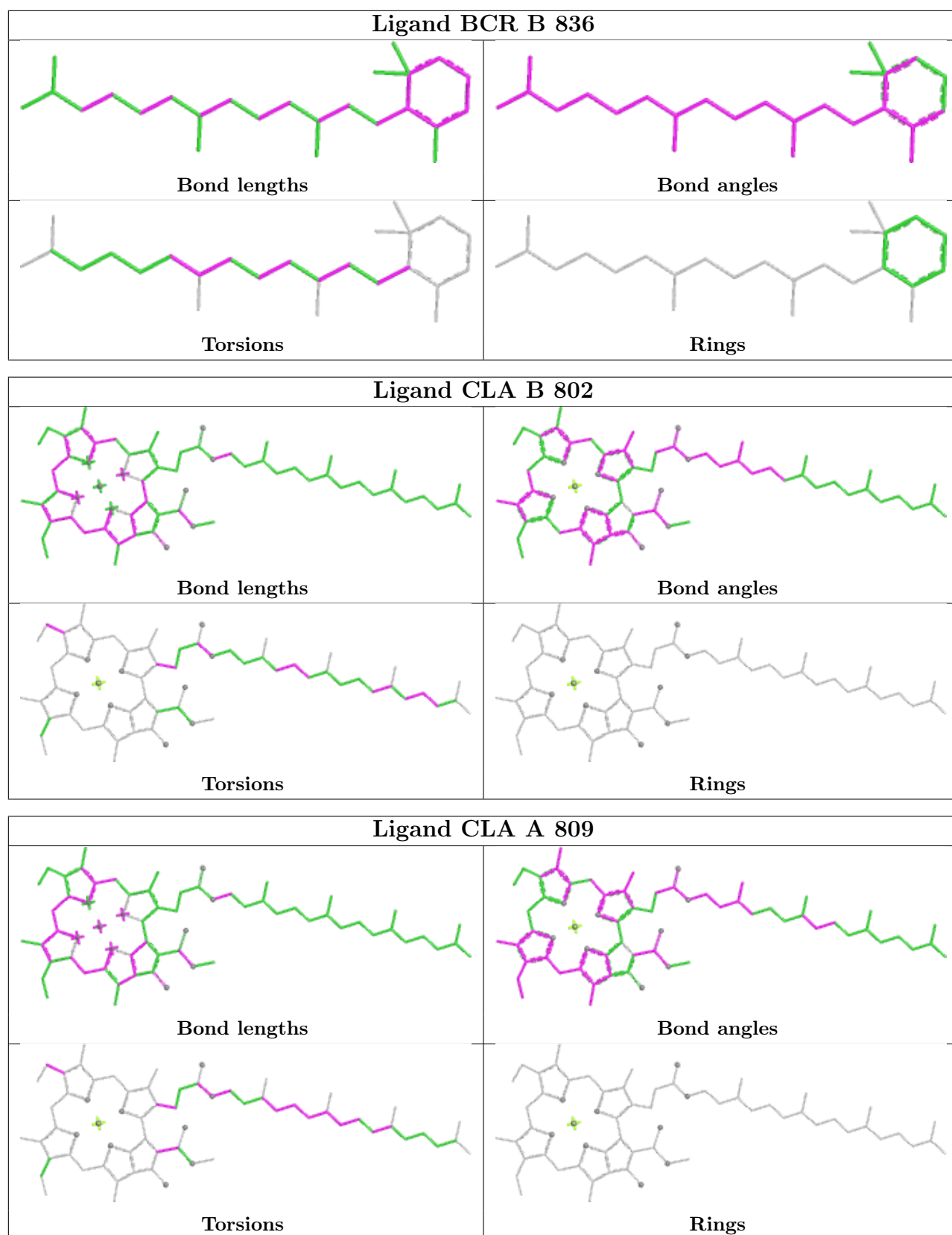


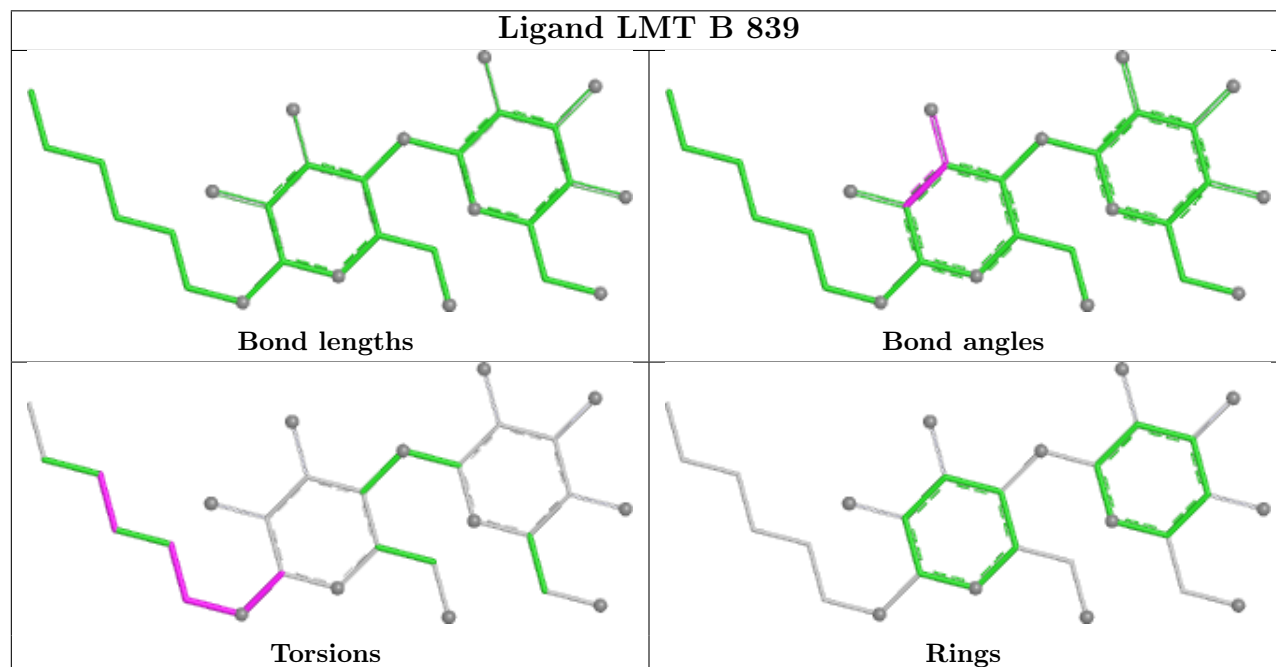
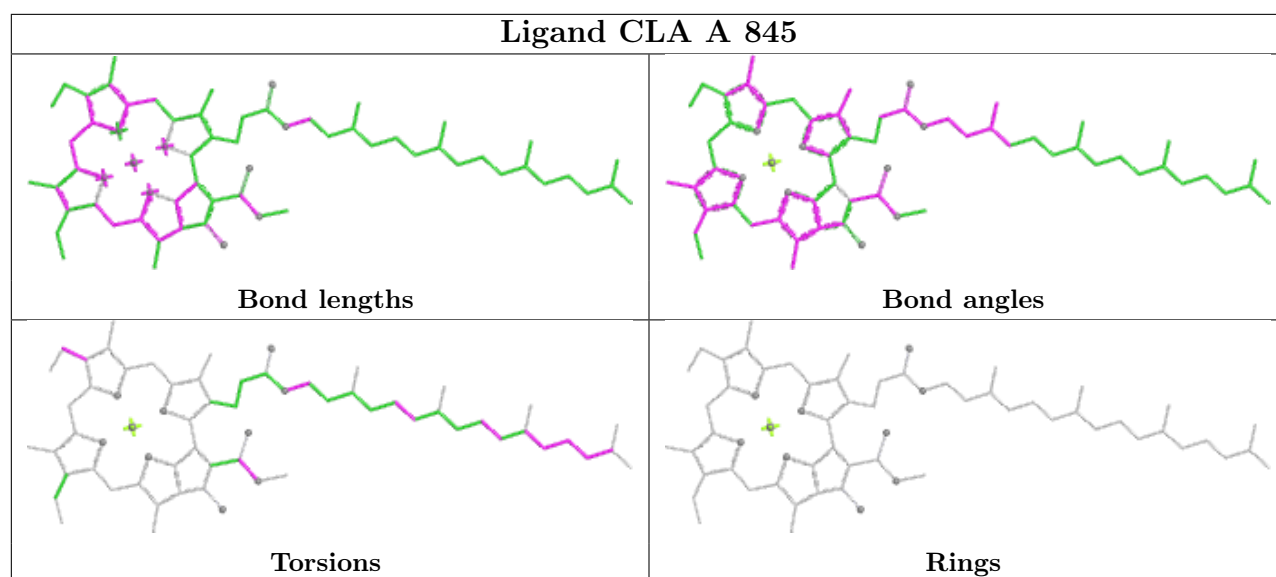
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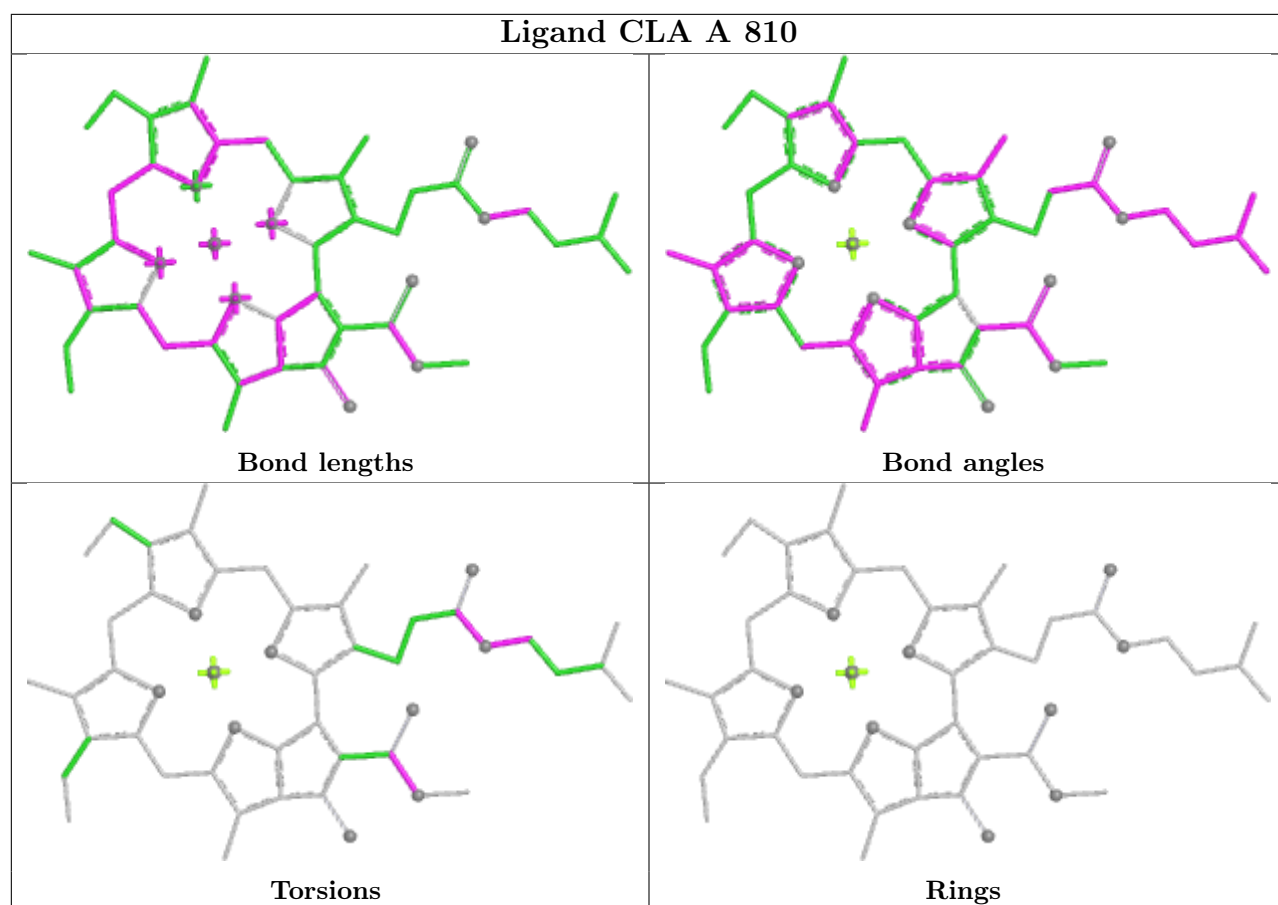




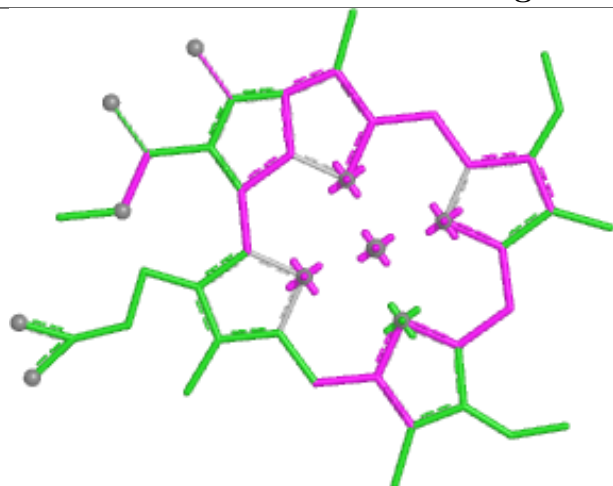




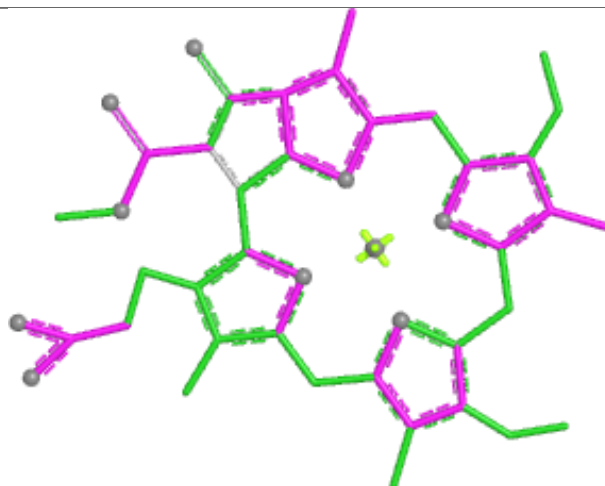




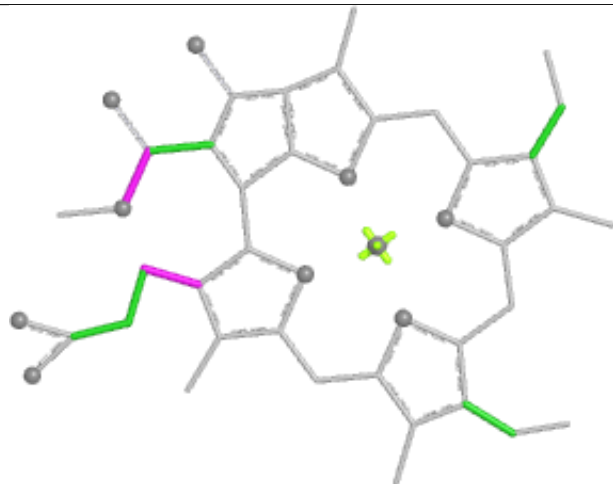
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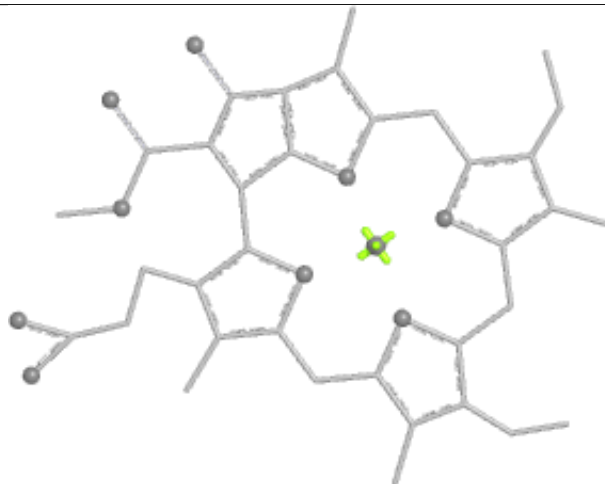
Bond lengths



Bond angles

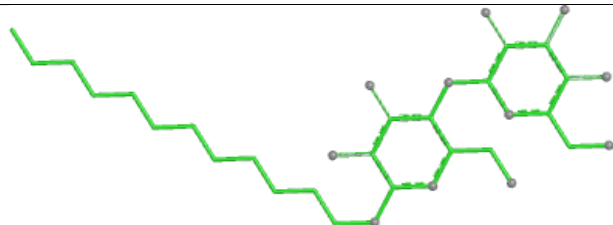


Torsions

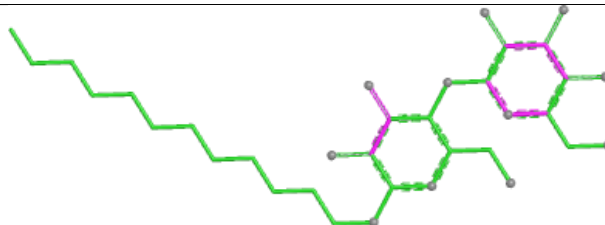


Rings

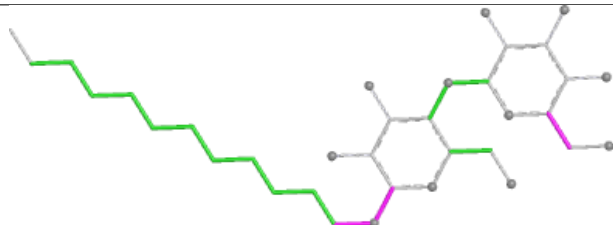
Ligand LMT A 853



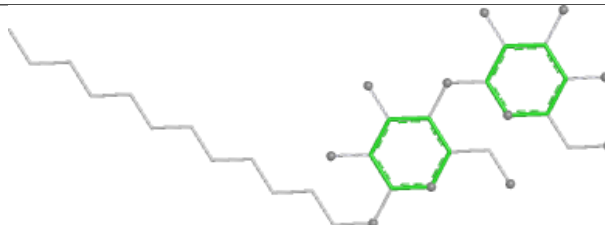
Bond lengths



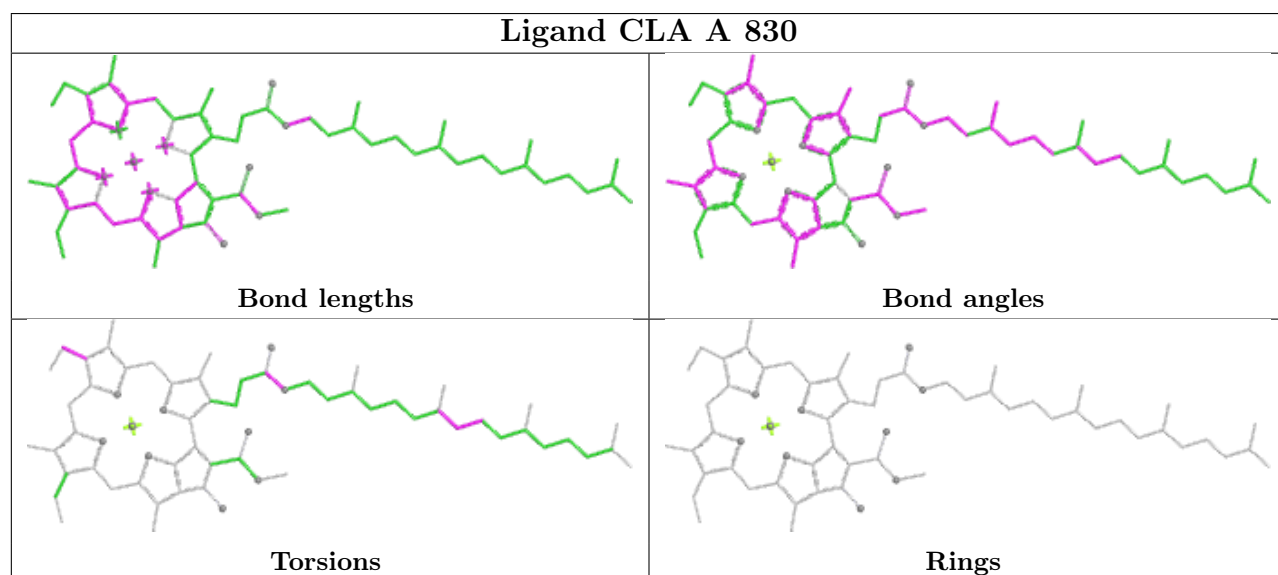
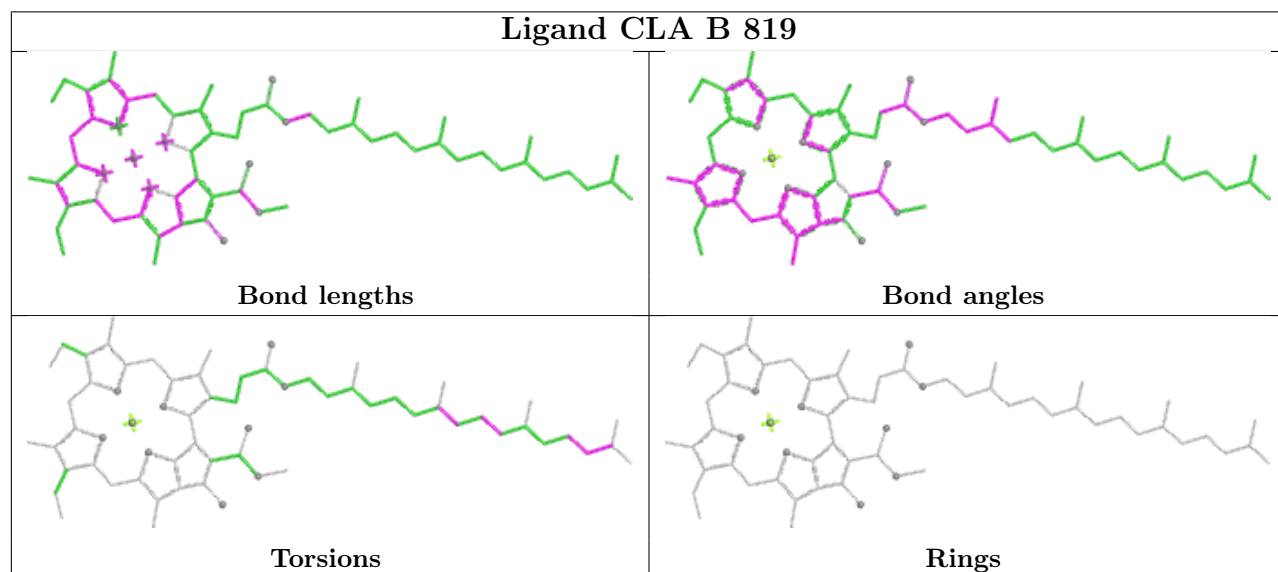
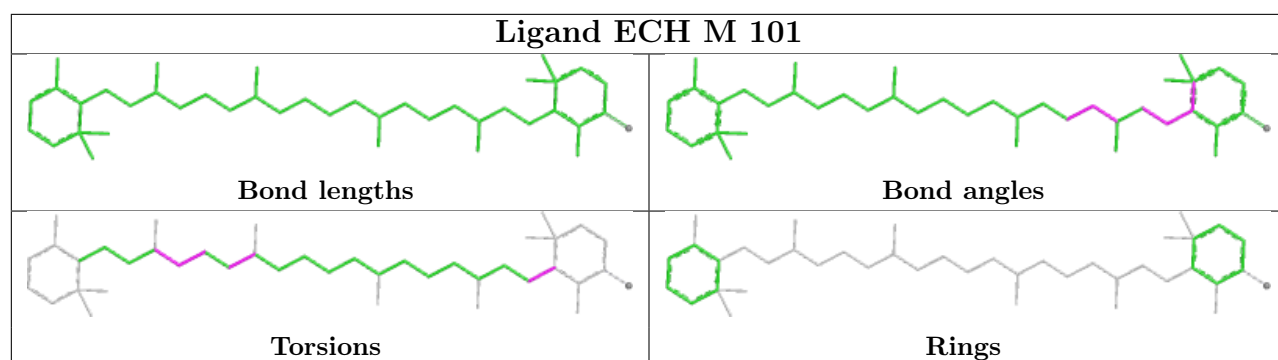
Bond angles

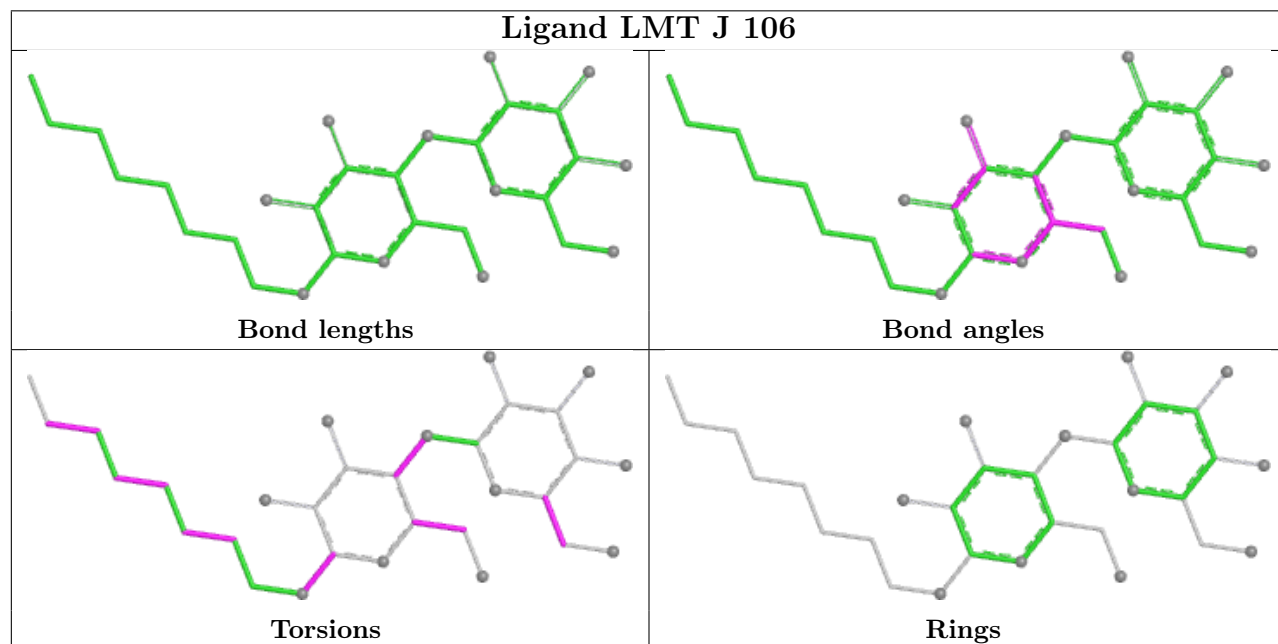
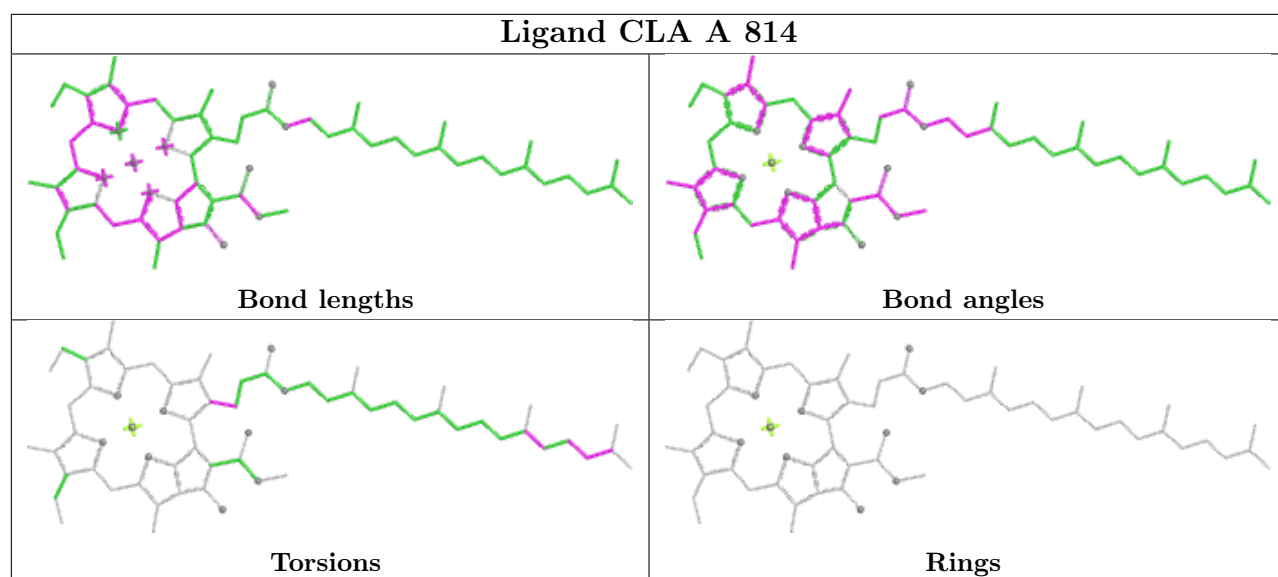


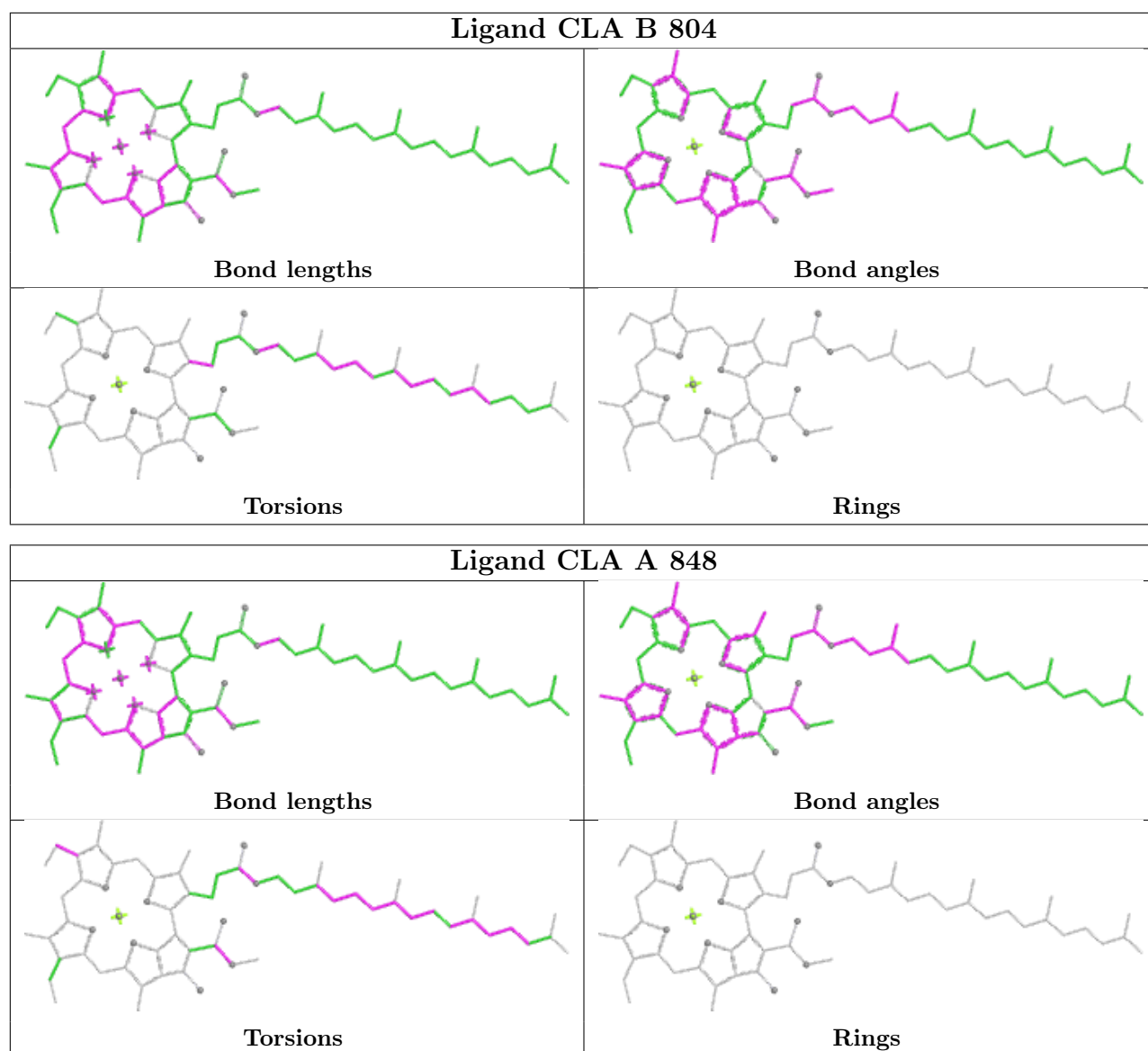
Torsions



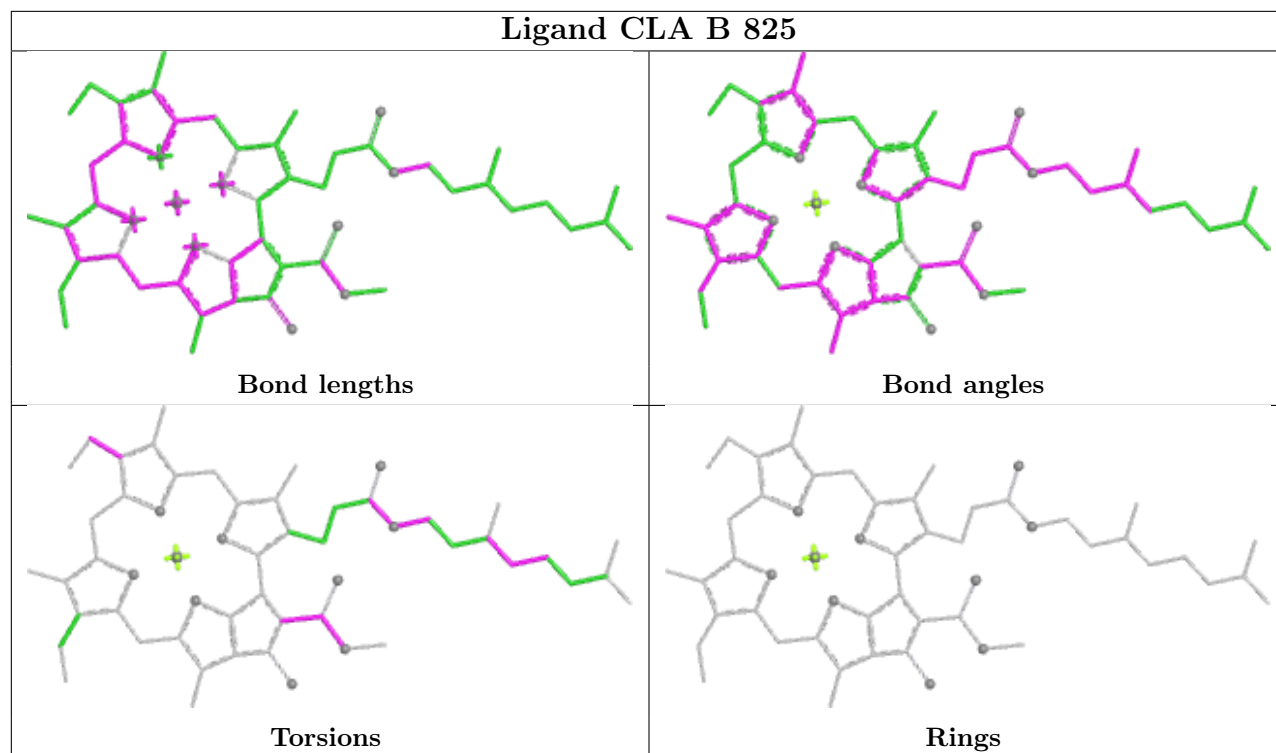
Rings



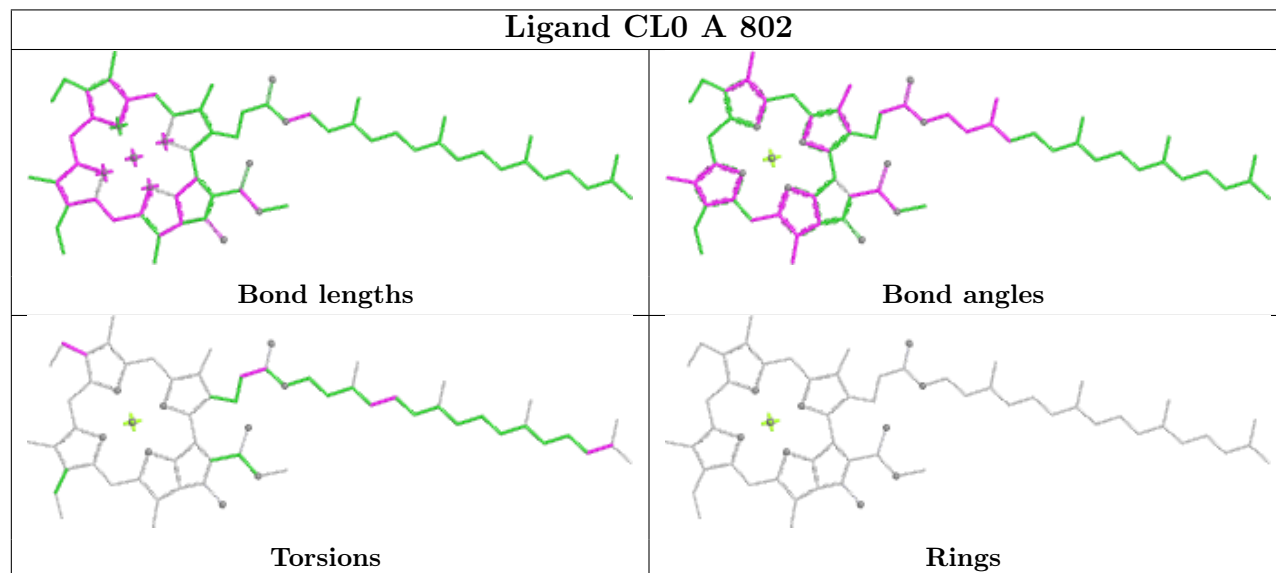


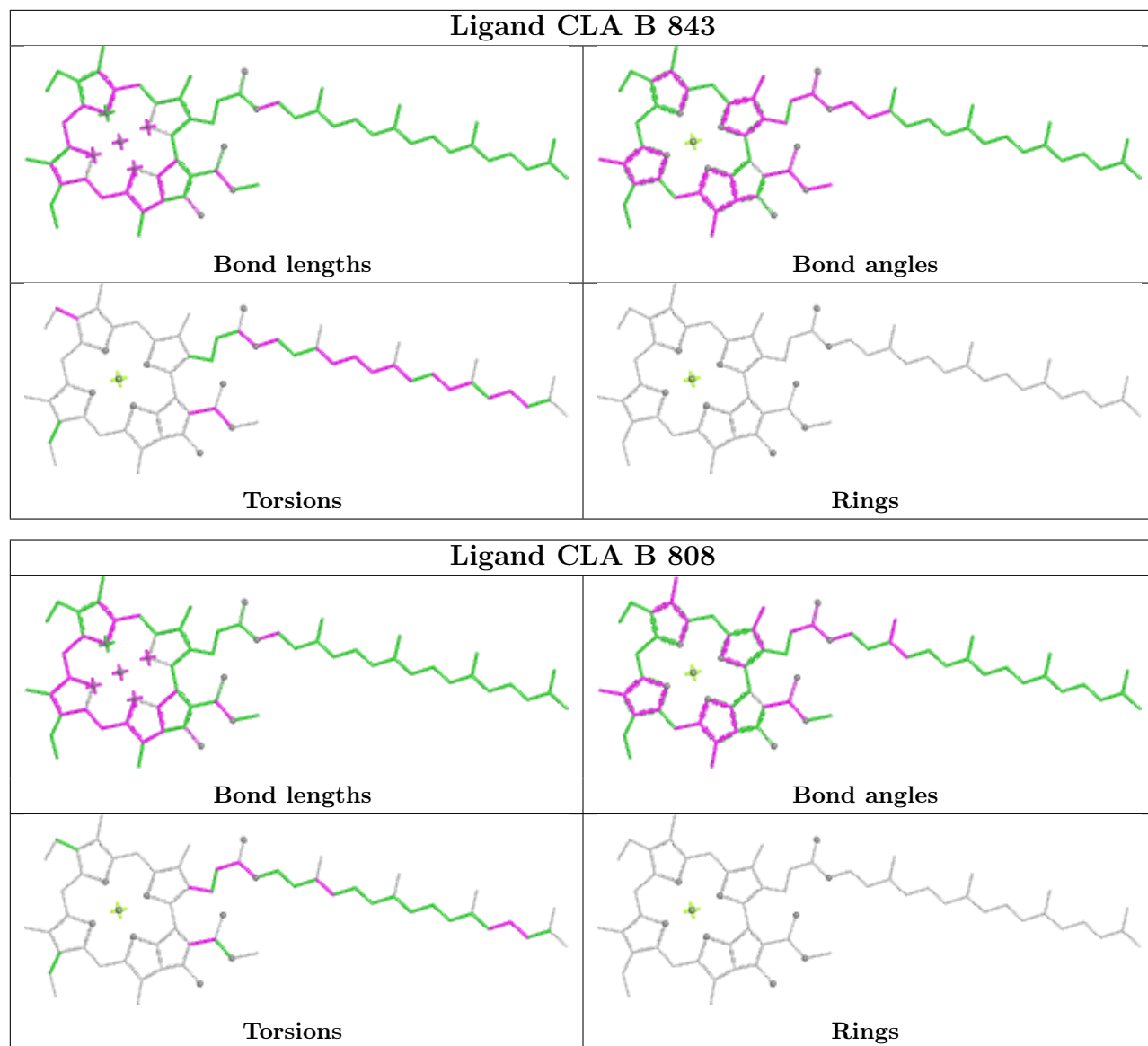


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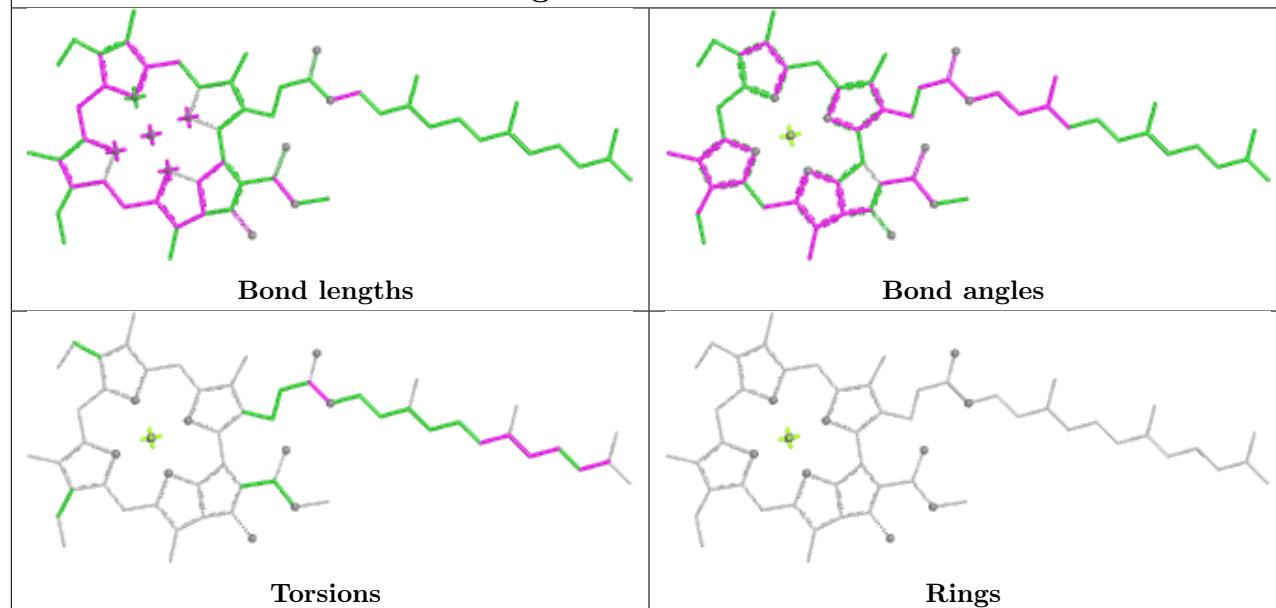


Ligand CL0 A 802

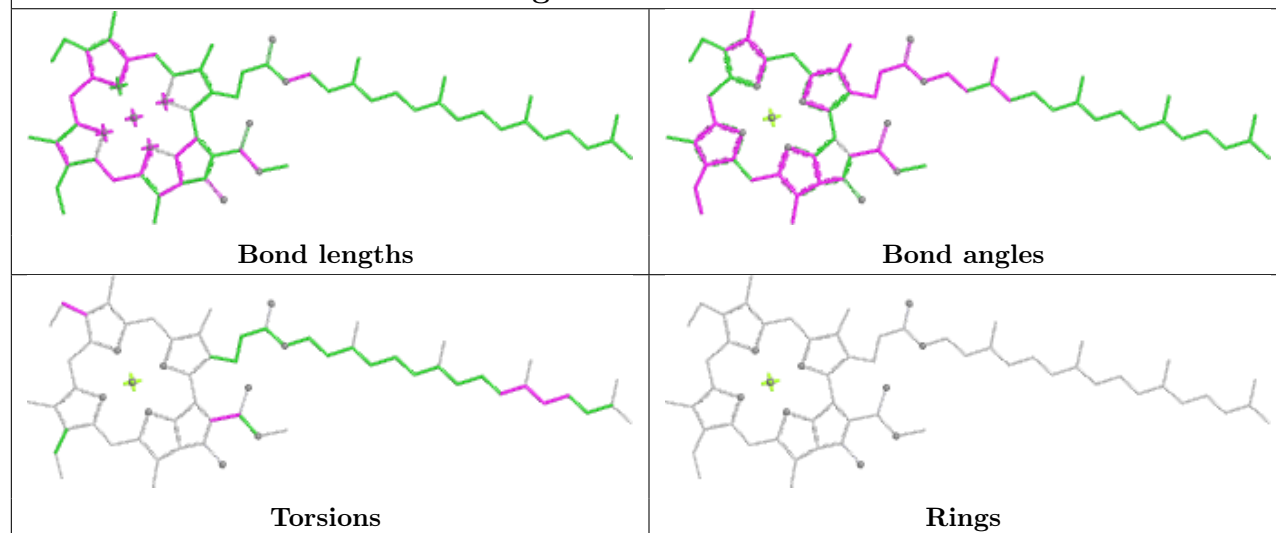


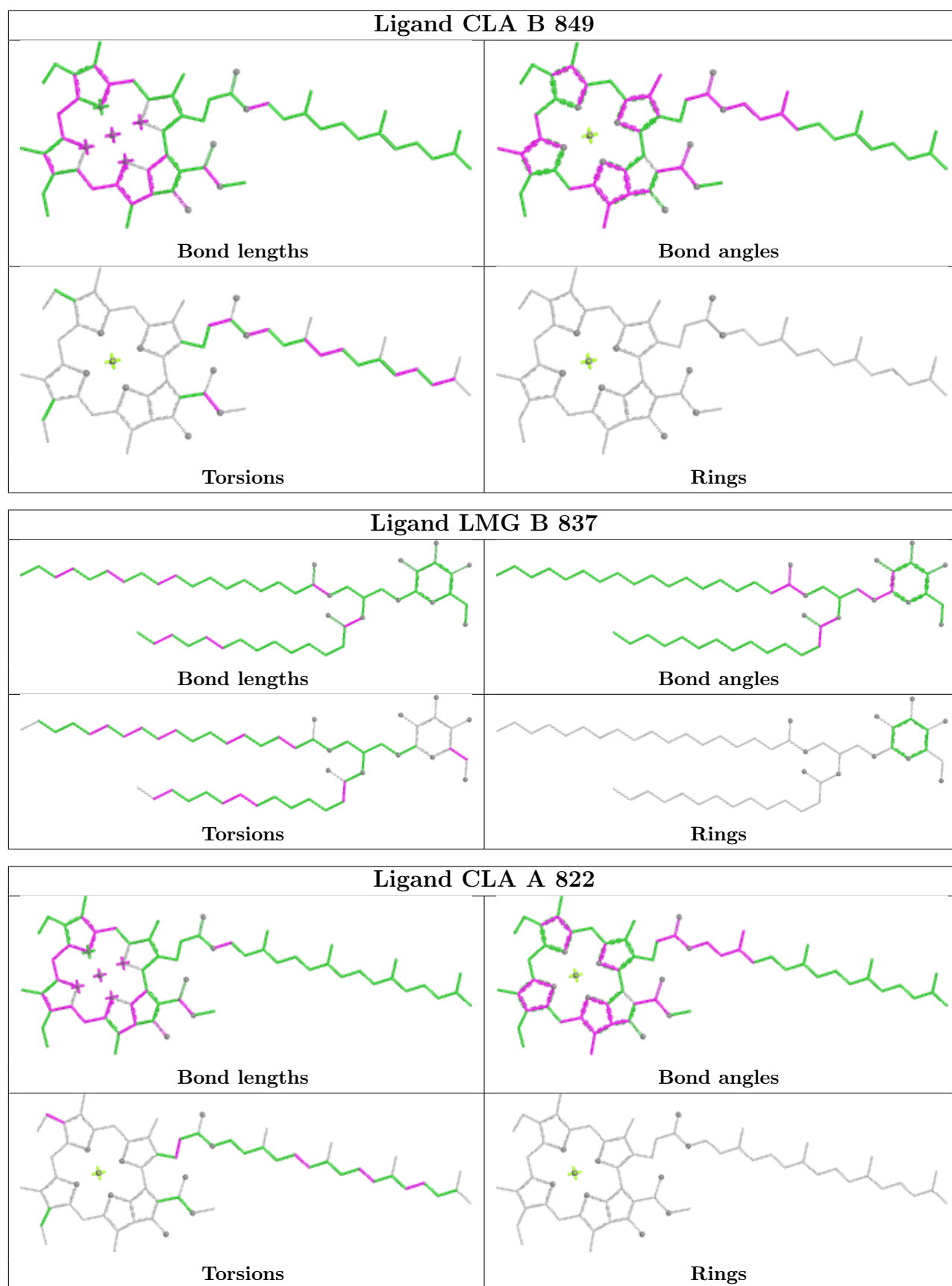


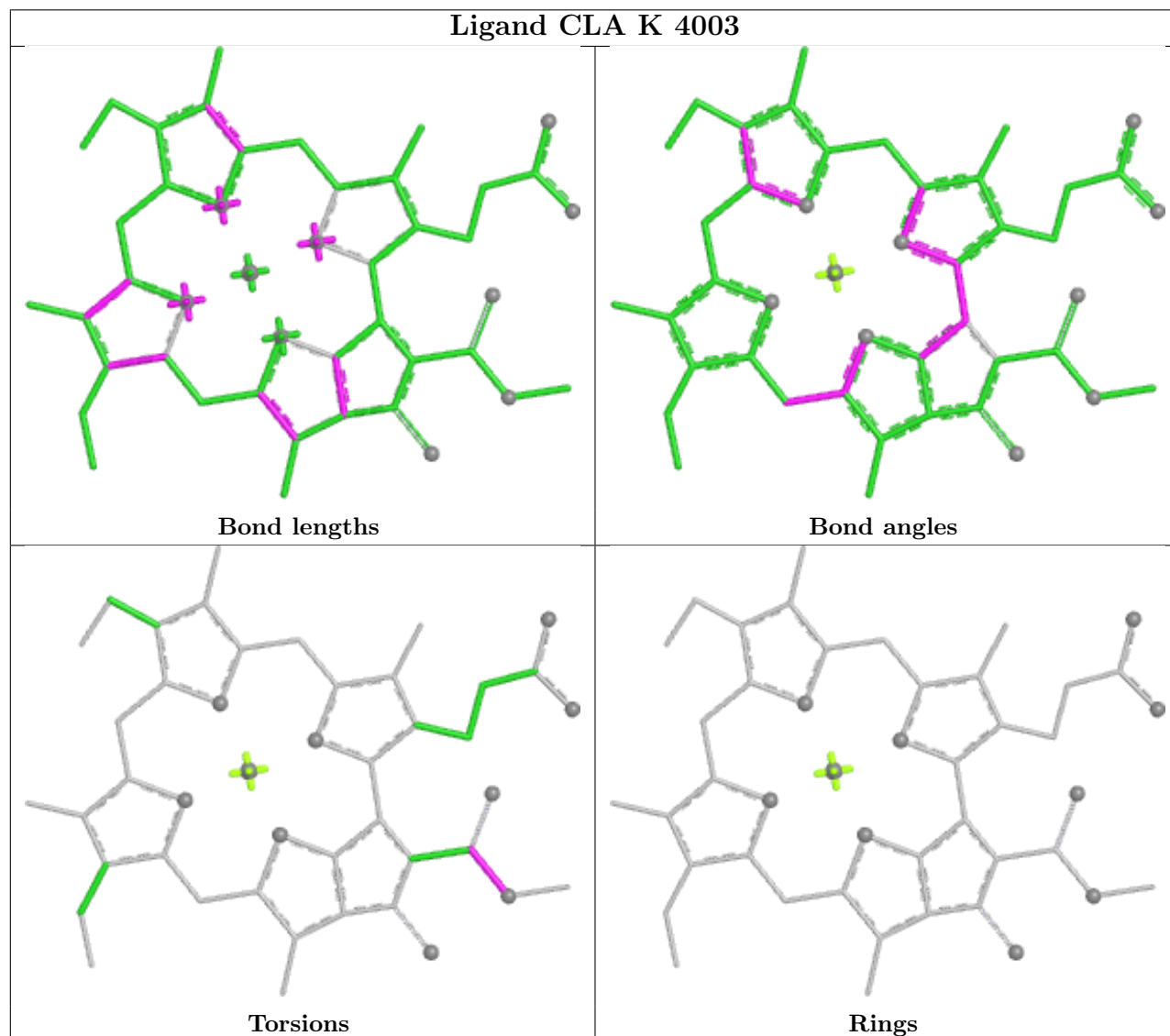
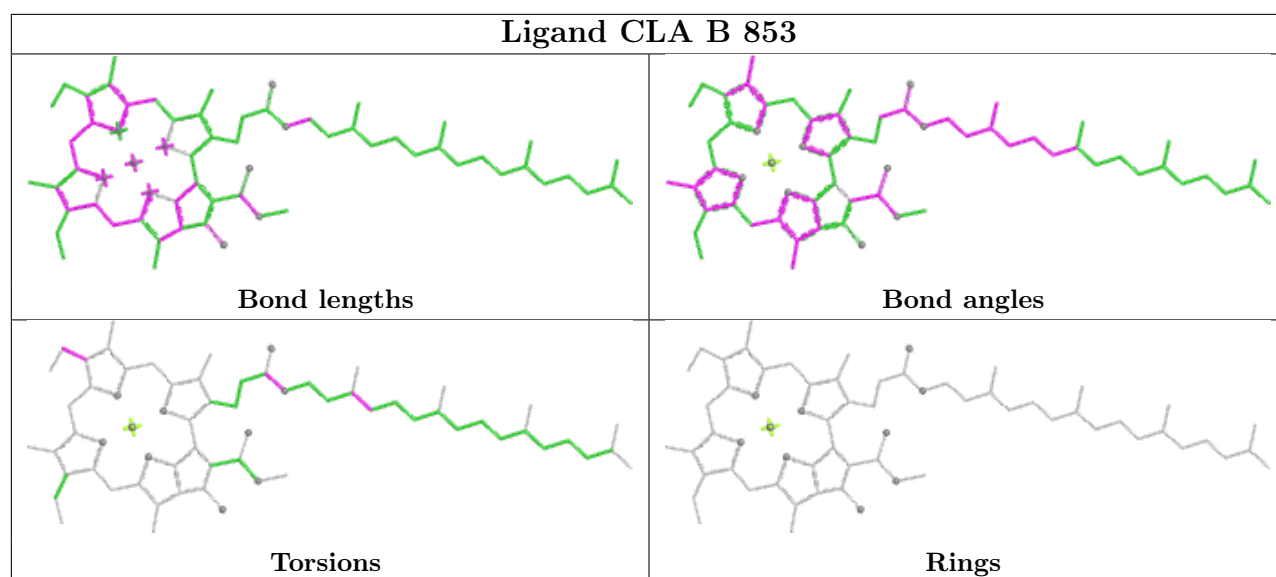
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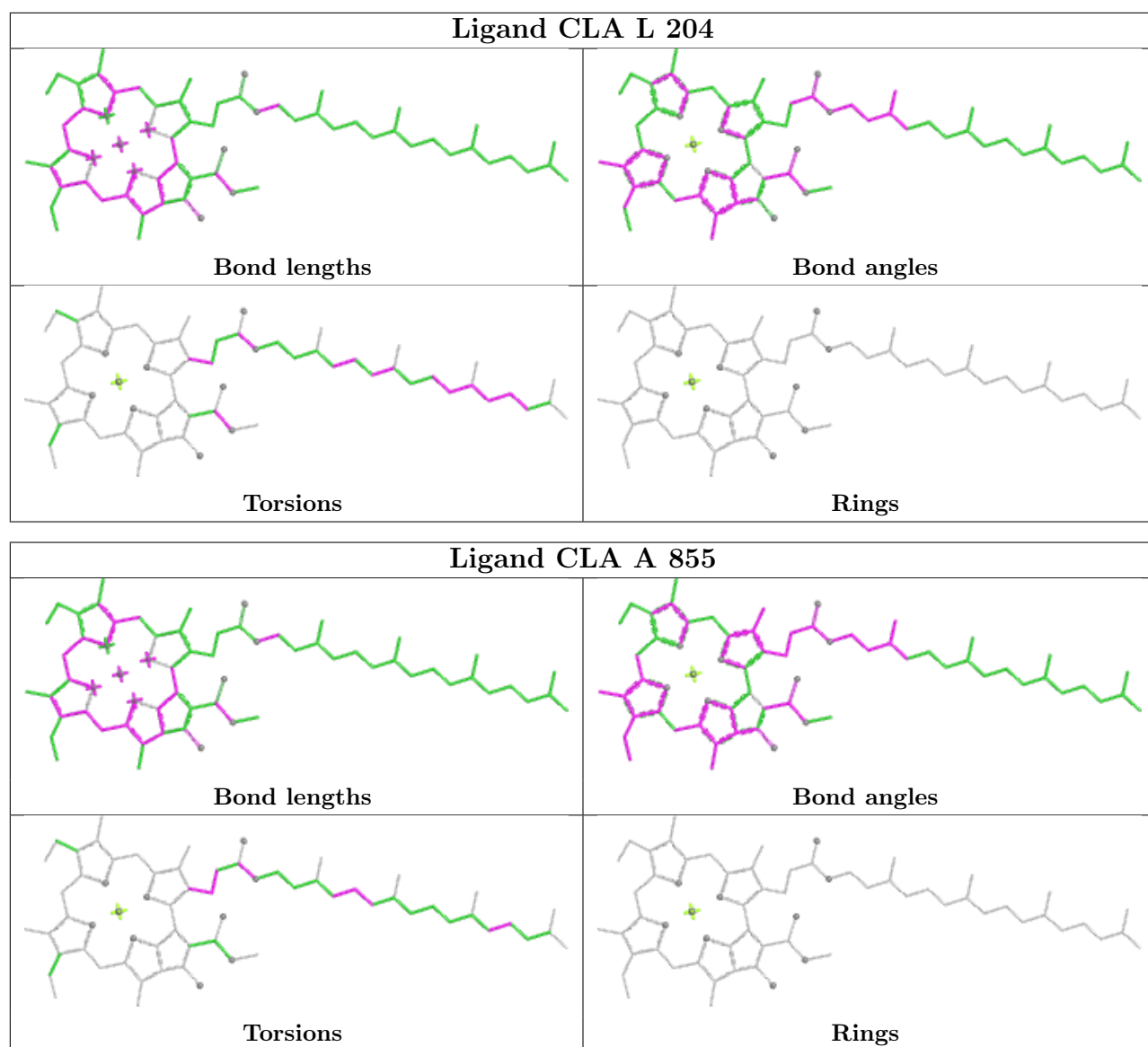


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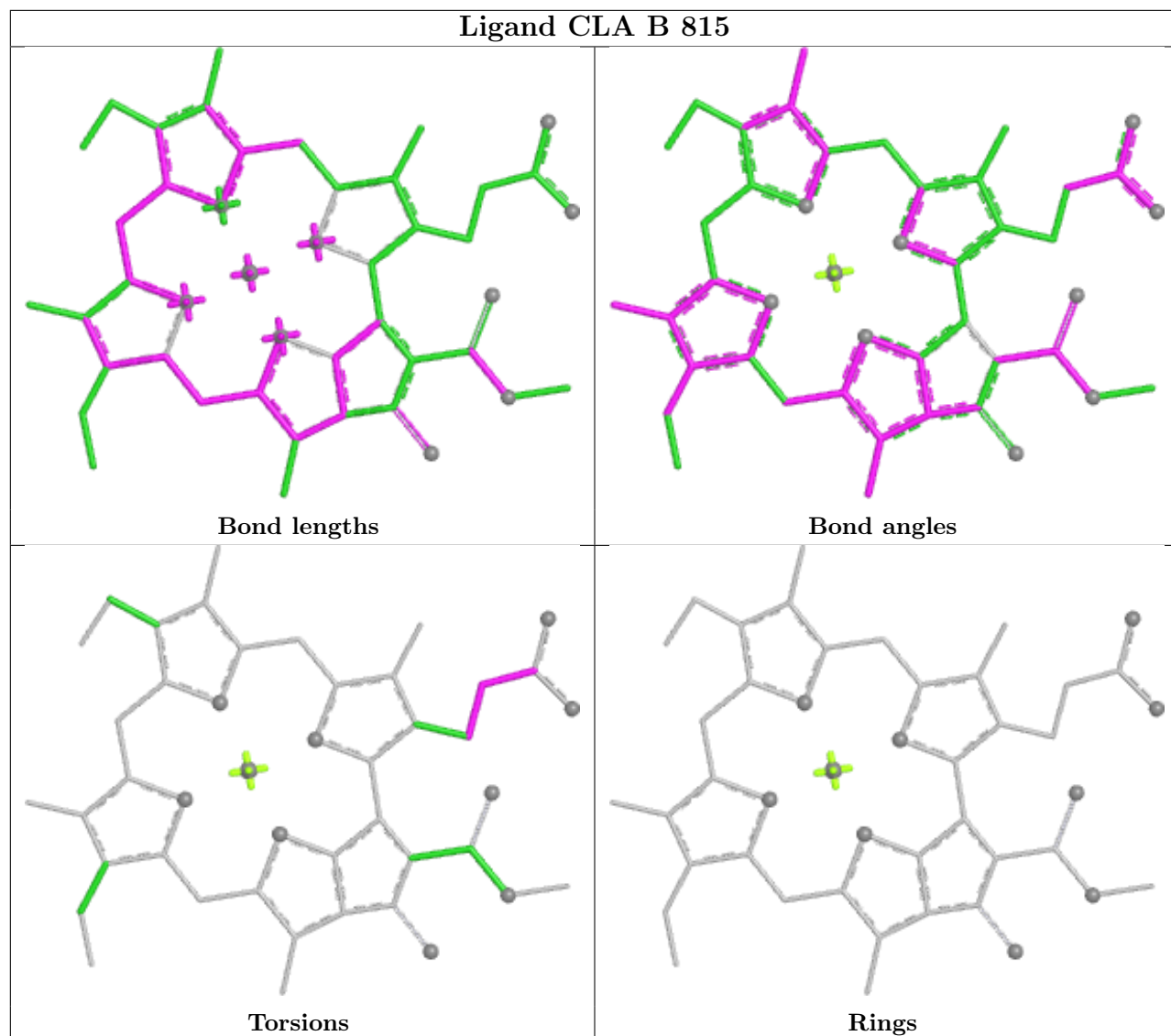




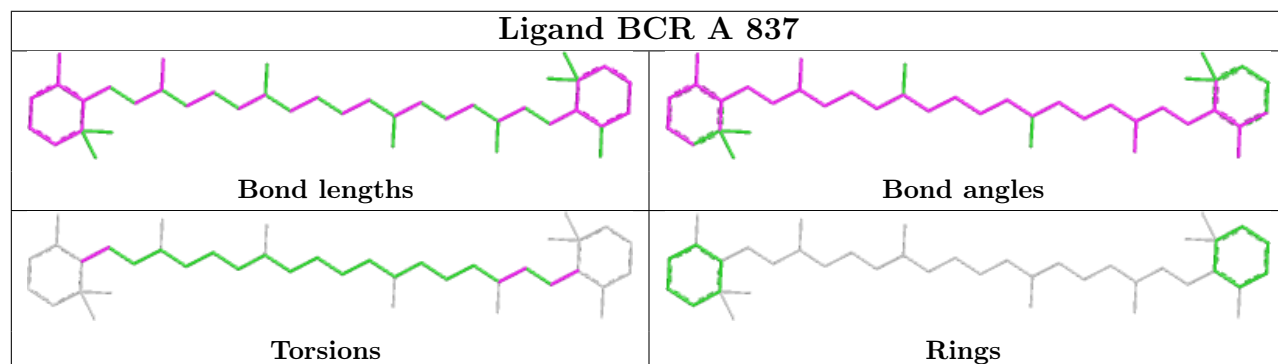


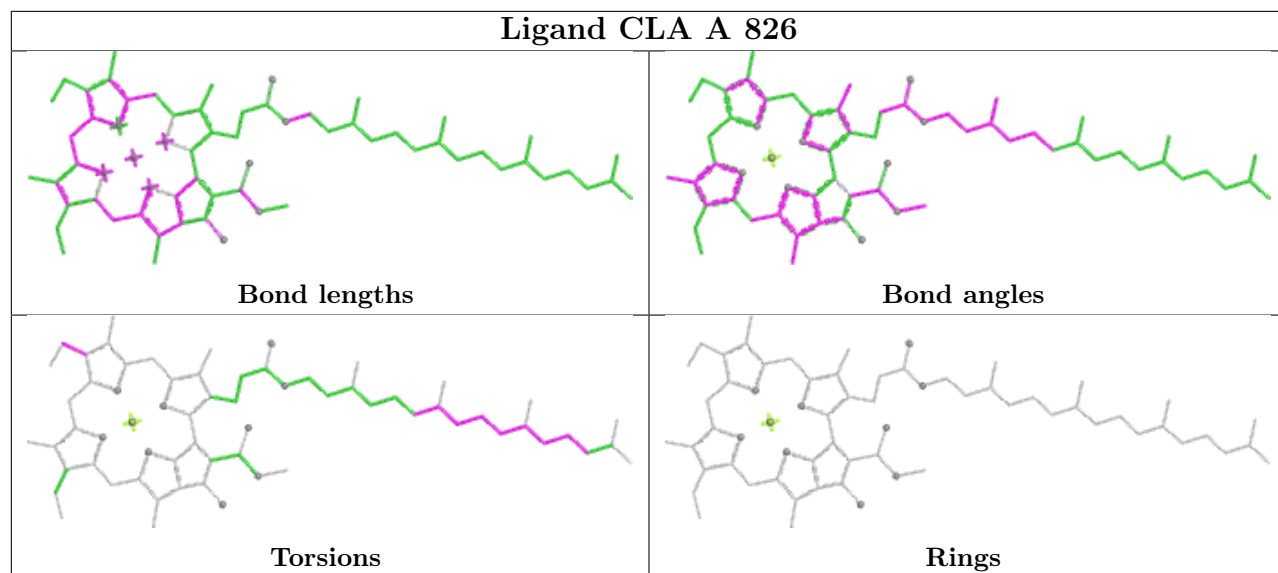
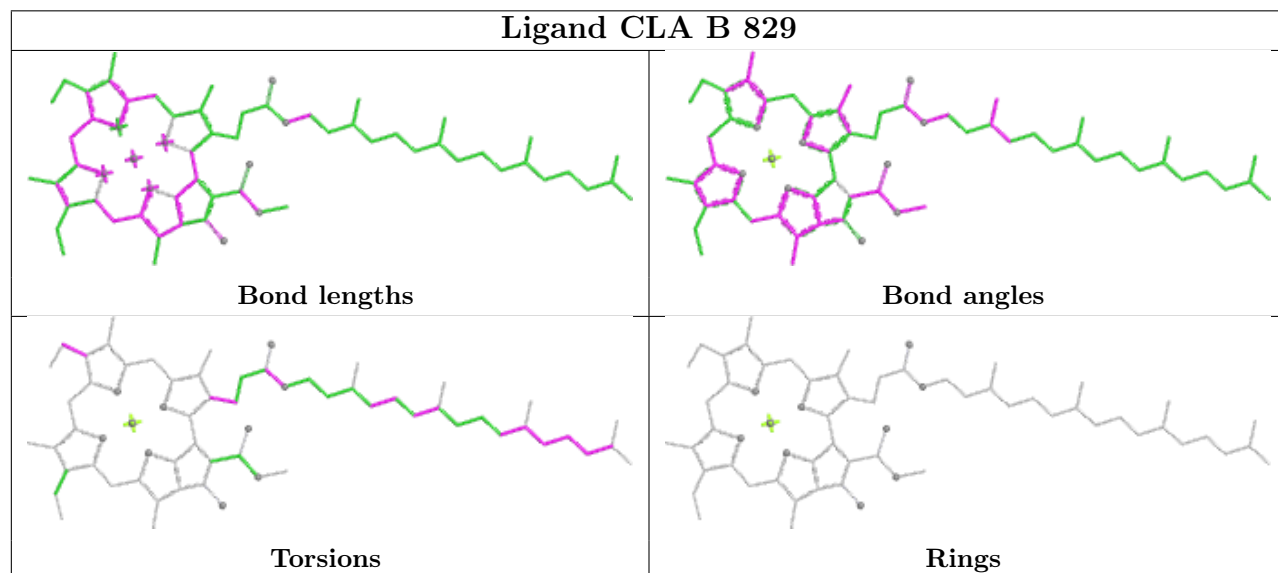
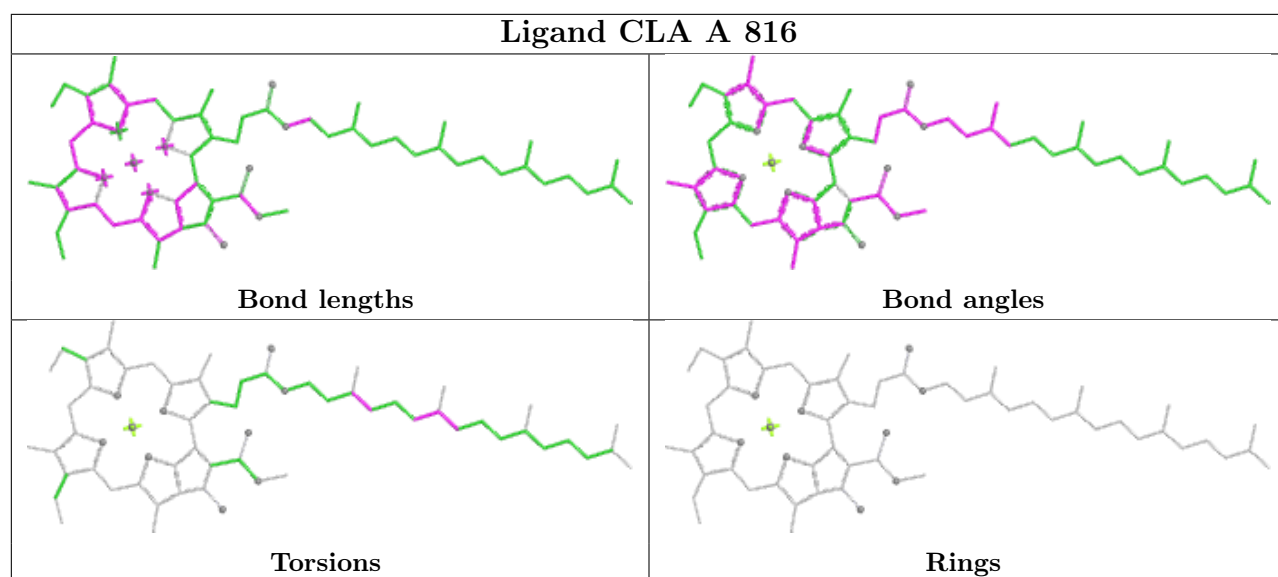


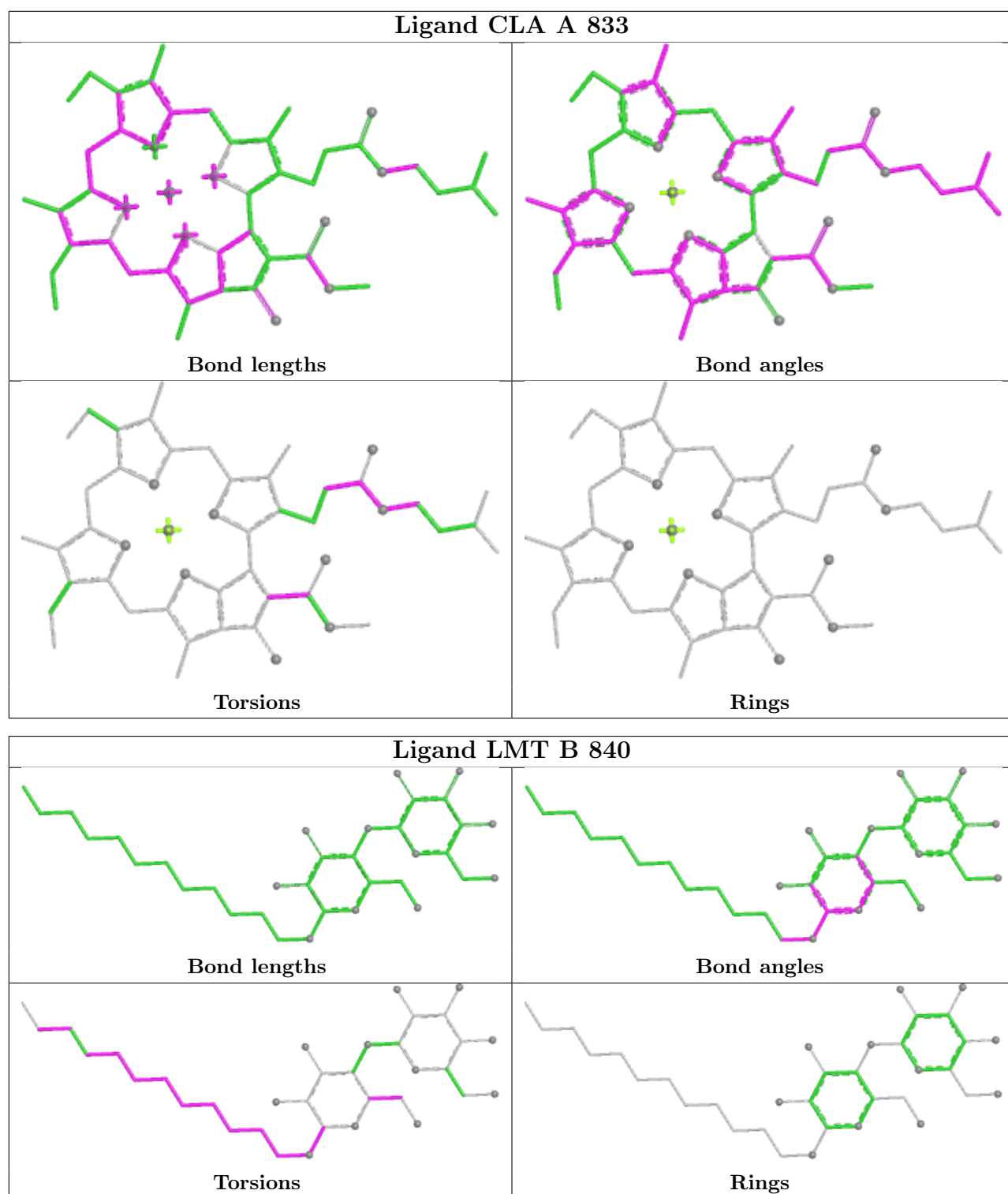
Ligand CLA B 815

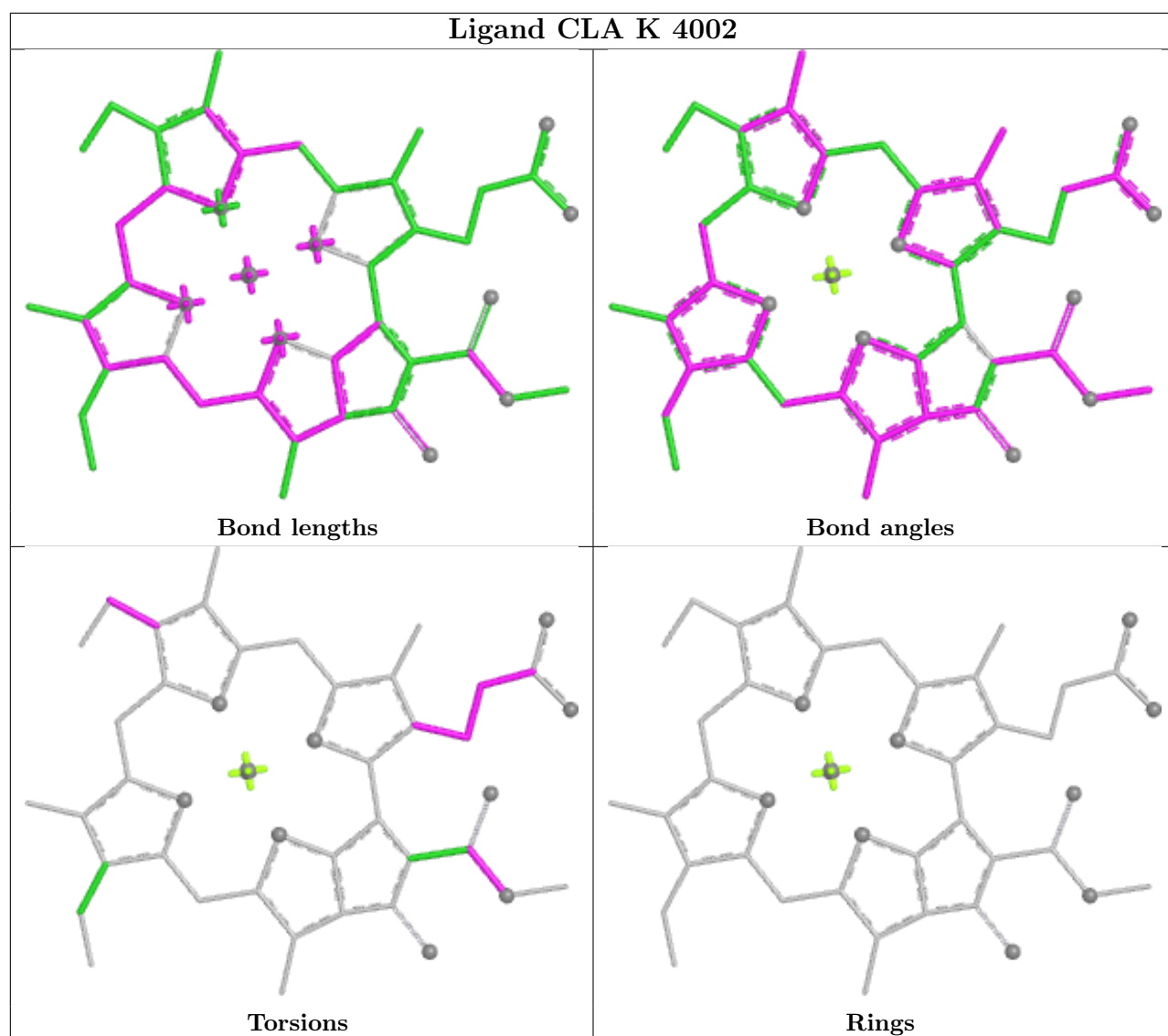


Ligand BCR A 837

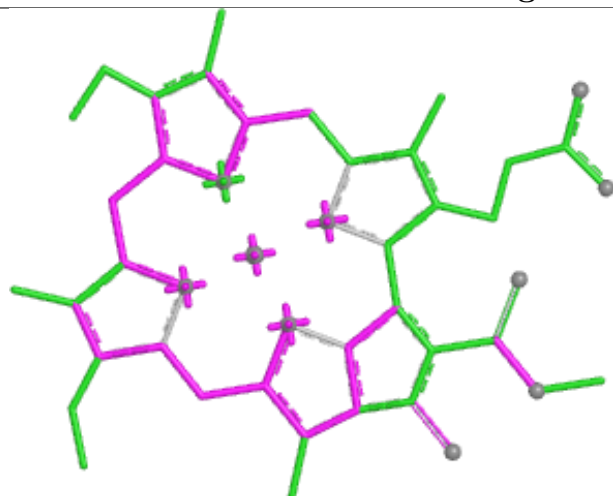




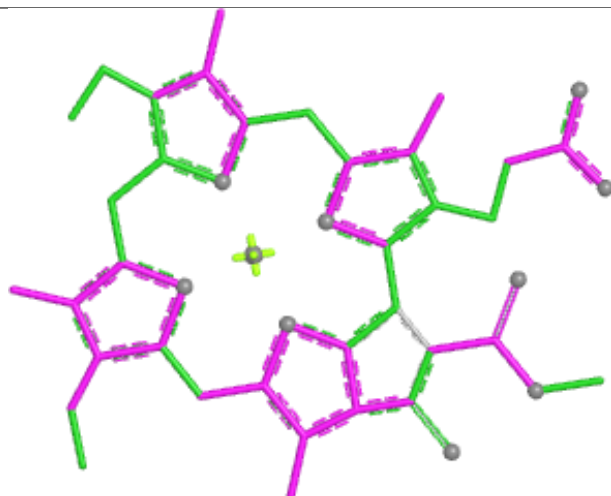




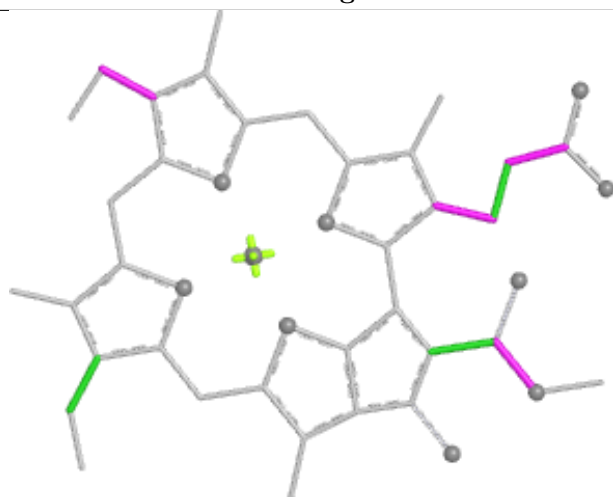
Ligand CLA J 102



Bond lengths



Bond angles

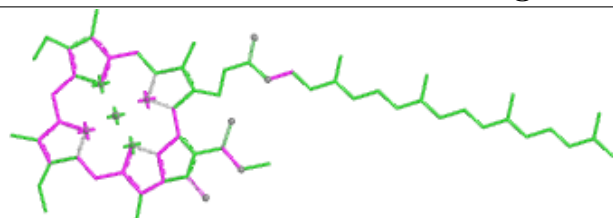


Torsions

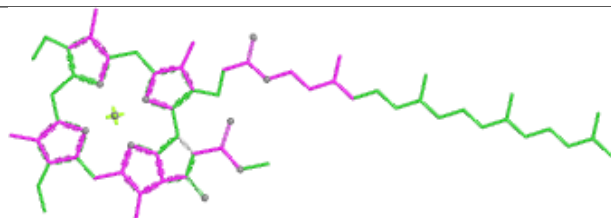


Rings

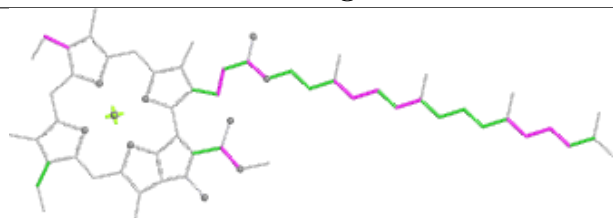
Ligand CLA A 831



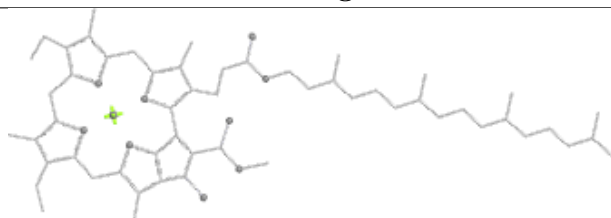
Bond lengths



Bond angles

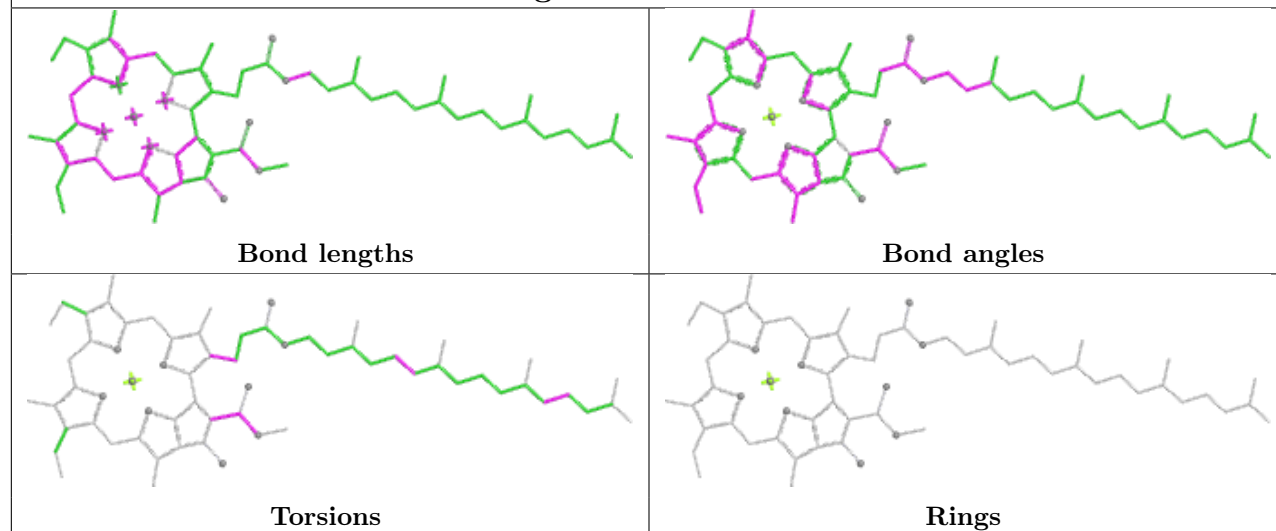


Torsions

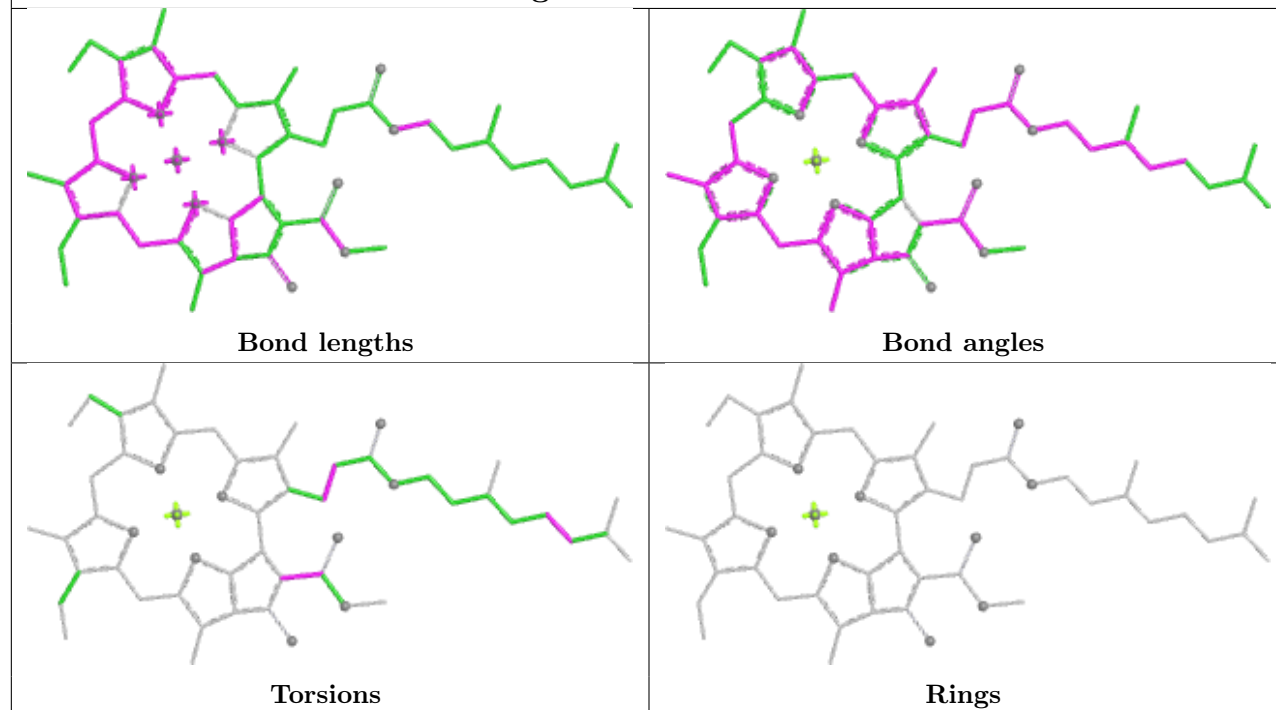


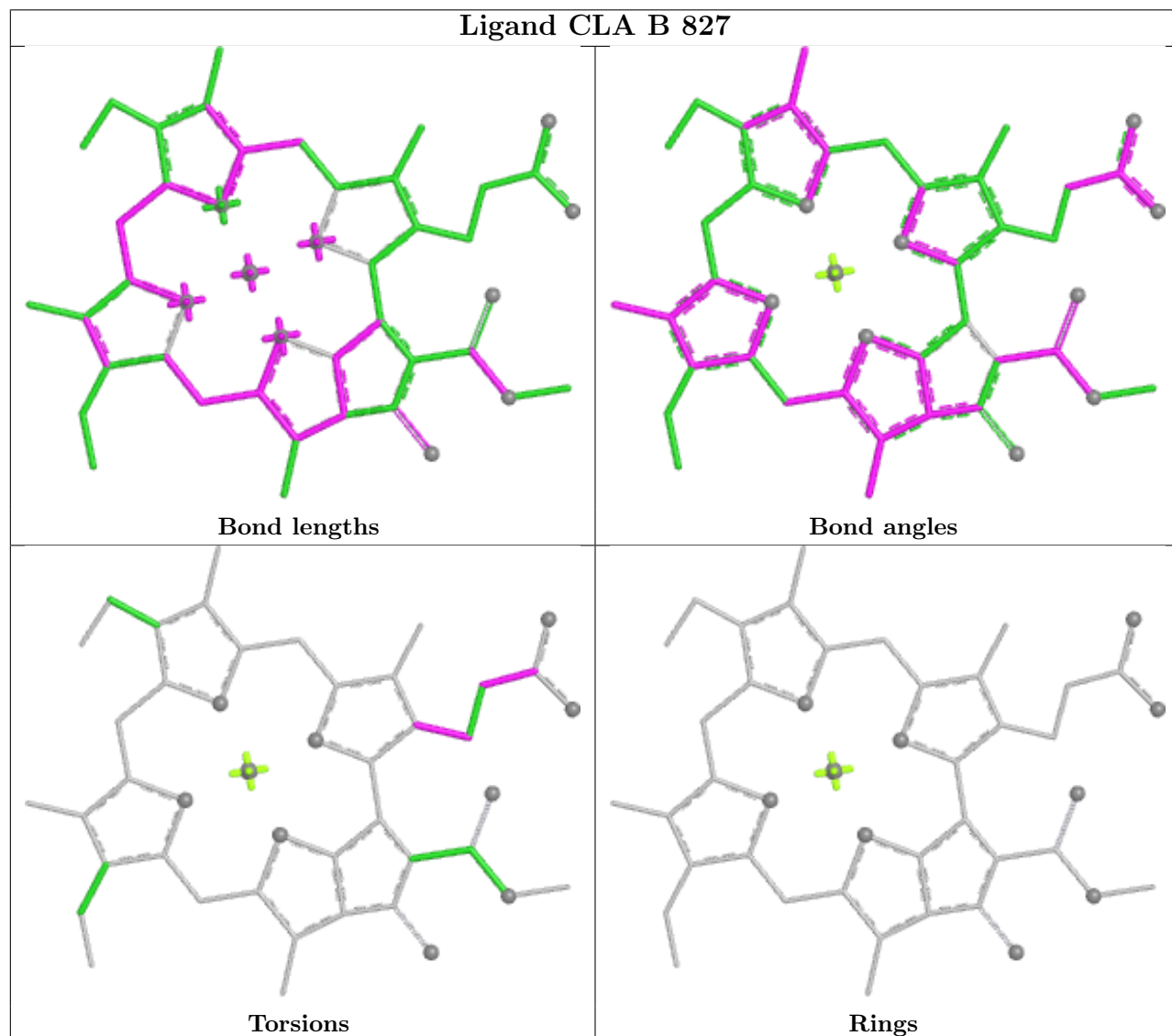
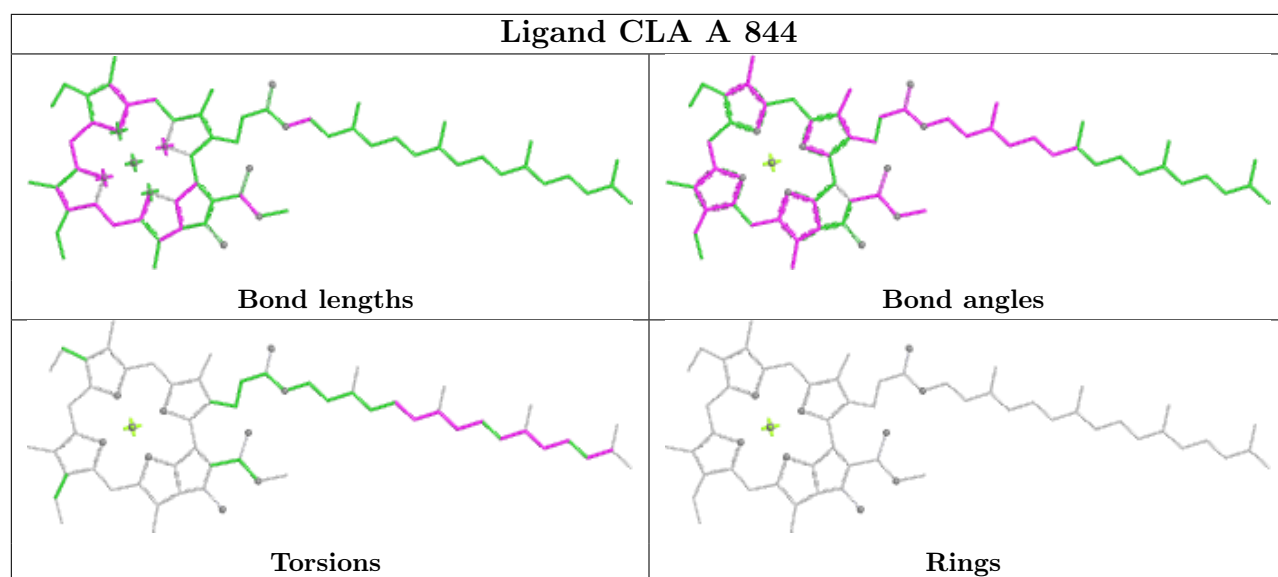
Rings

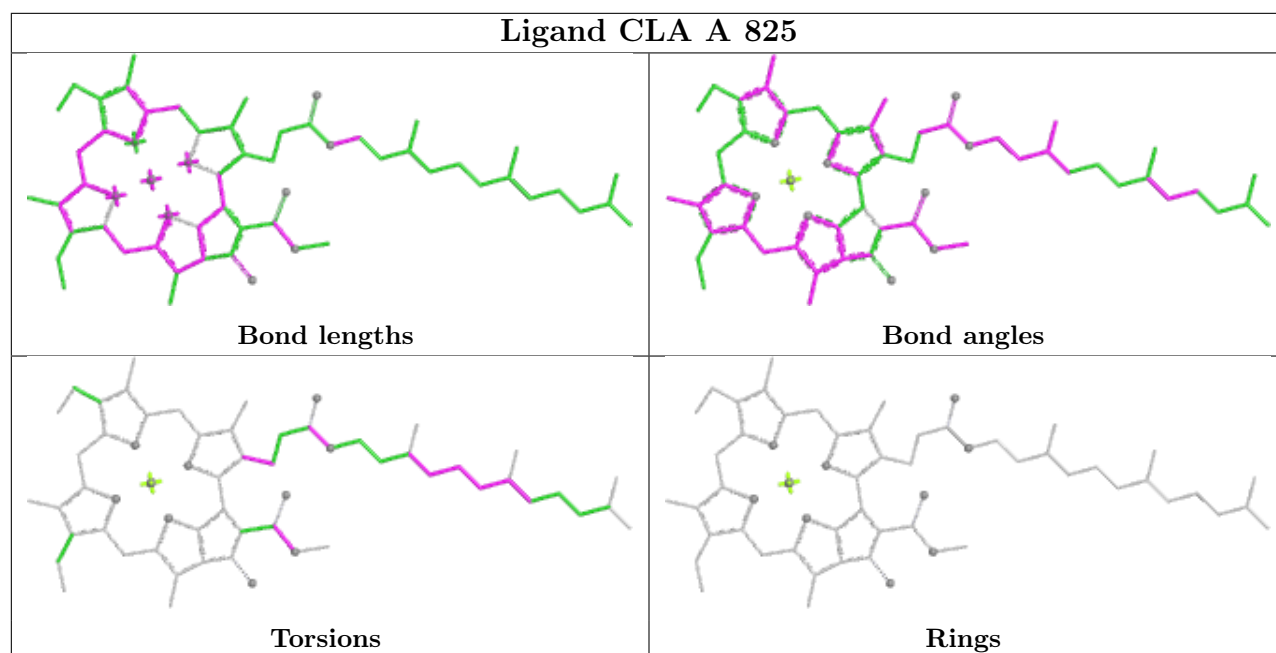
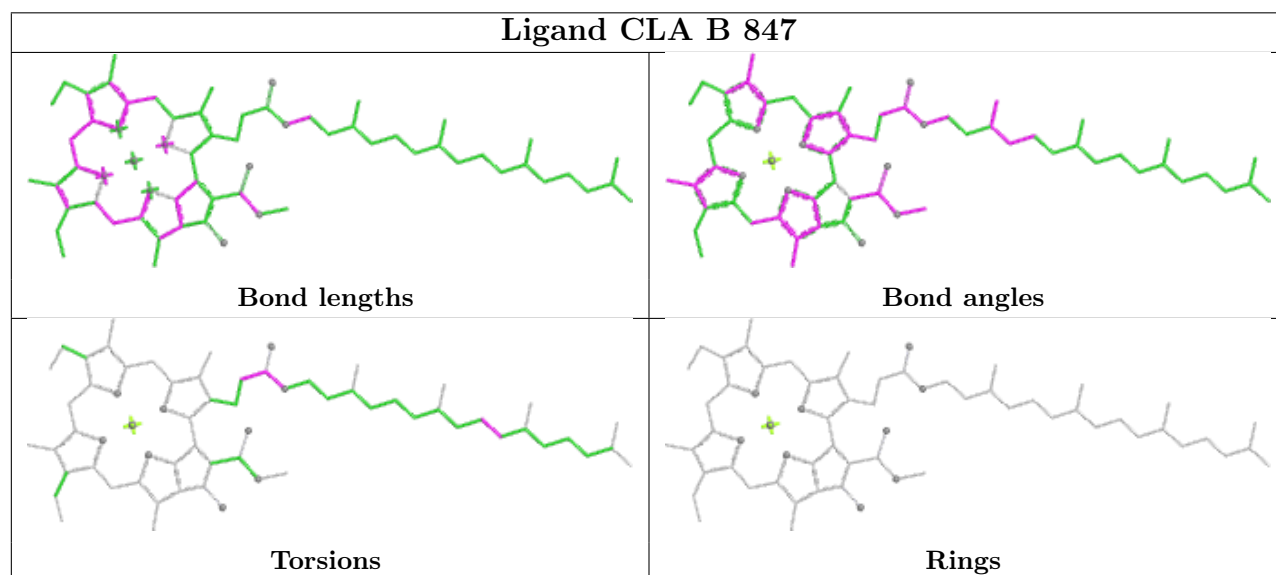
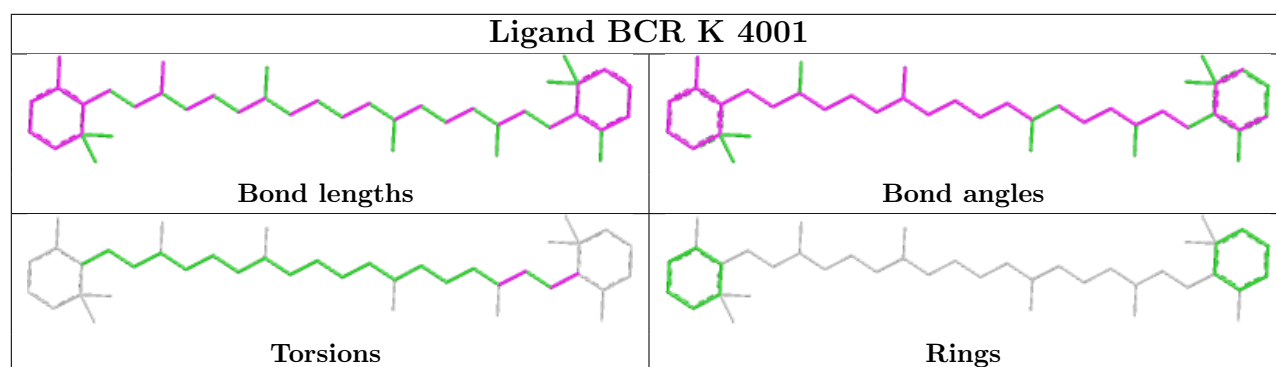
Ligand CLA L 201

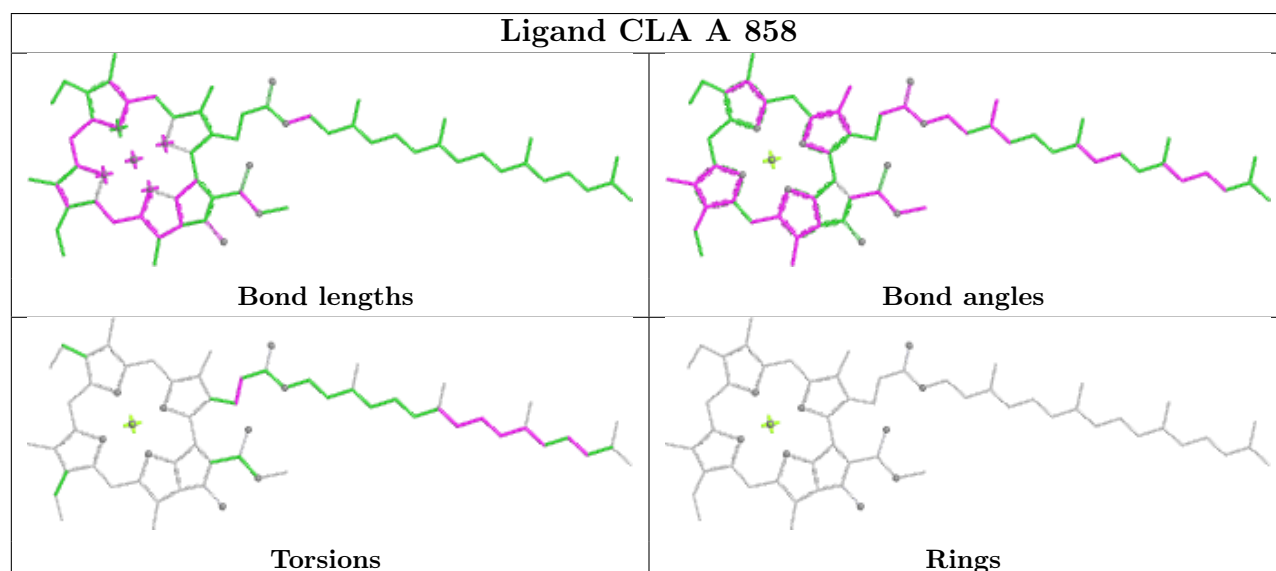
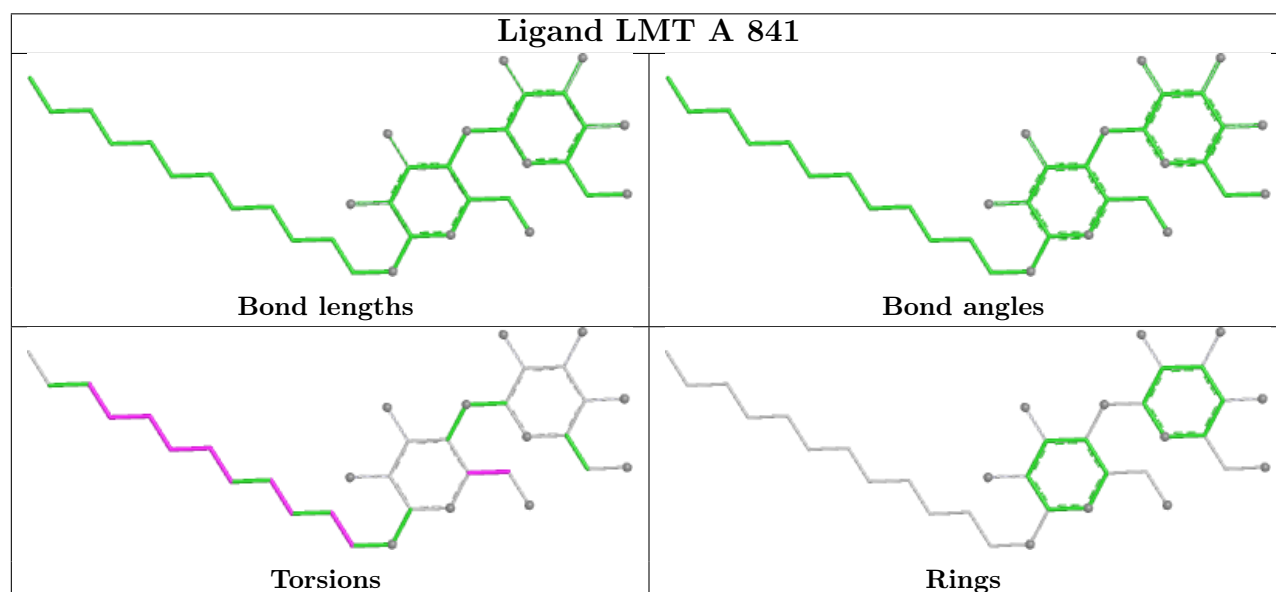
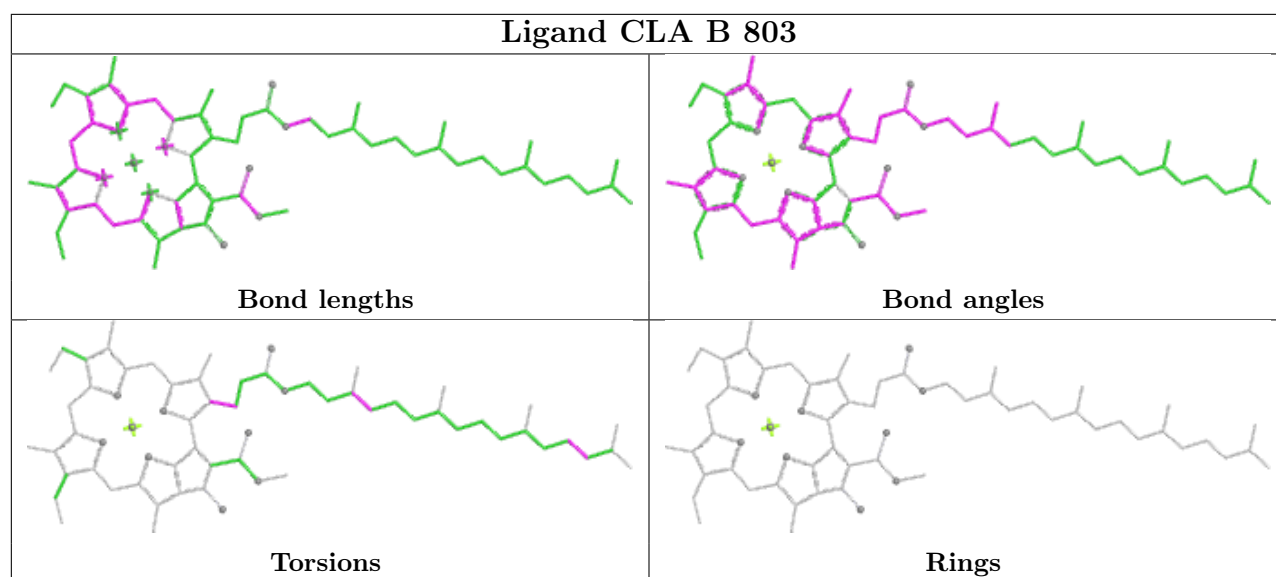


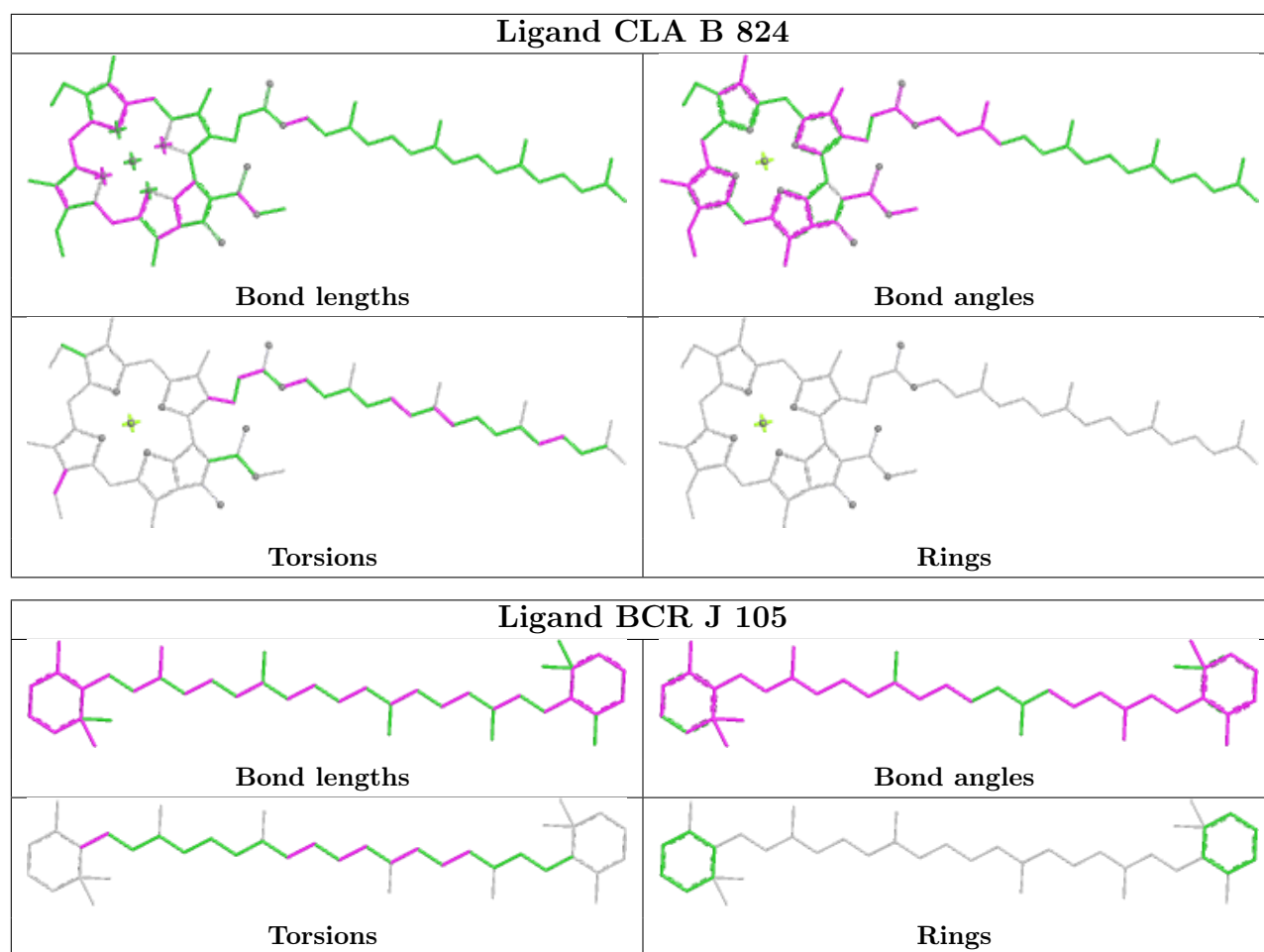
Ligand CLA A 852



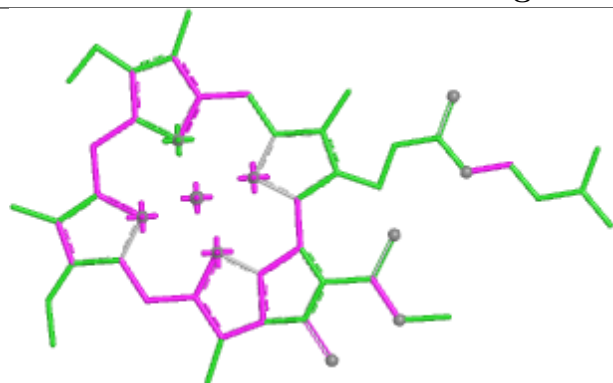




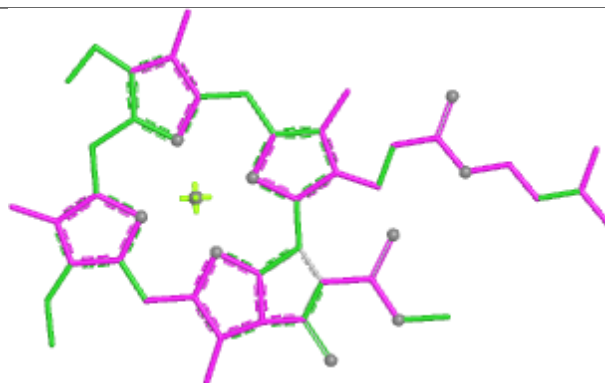




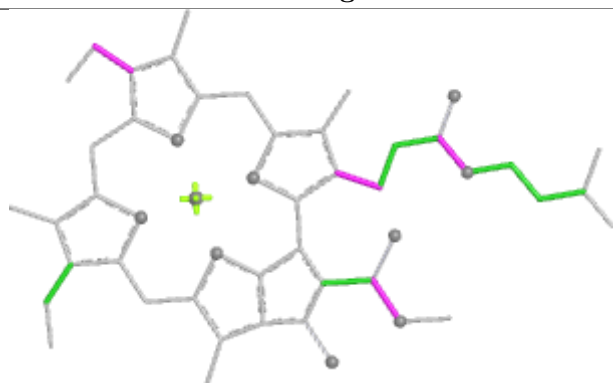
Ligand CLA A 832



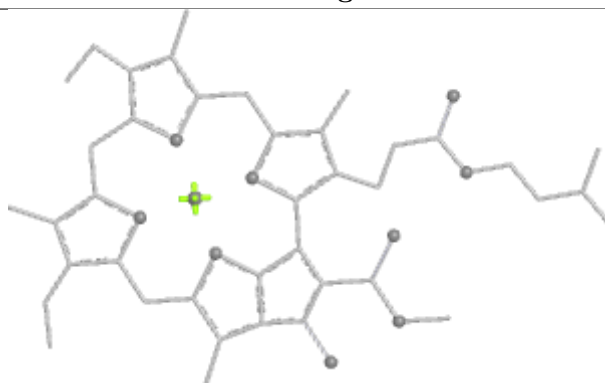
Bond lengths



Bond angles

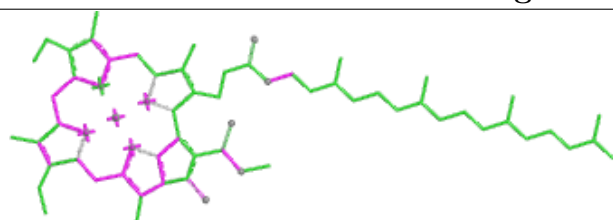


Torsions

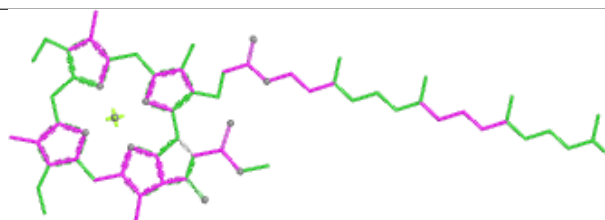


Rings

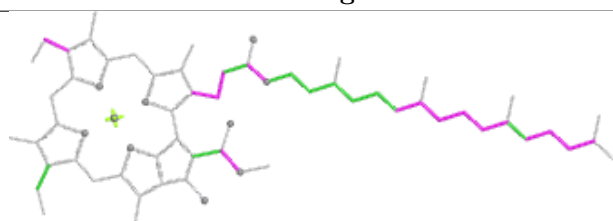
Ligand CLA B 820



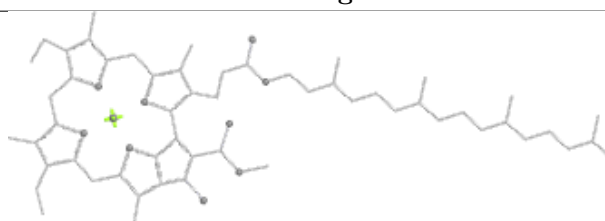
Bond lengths



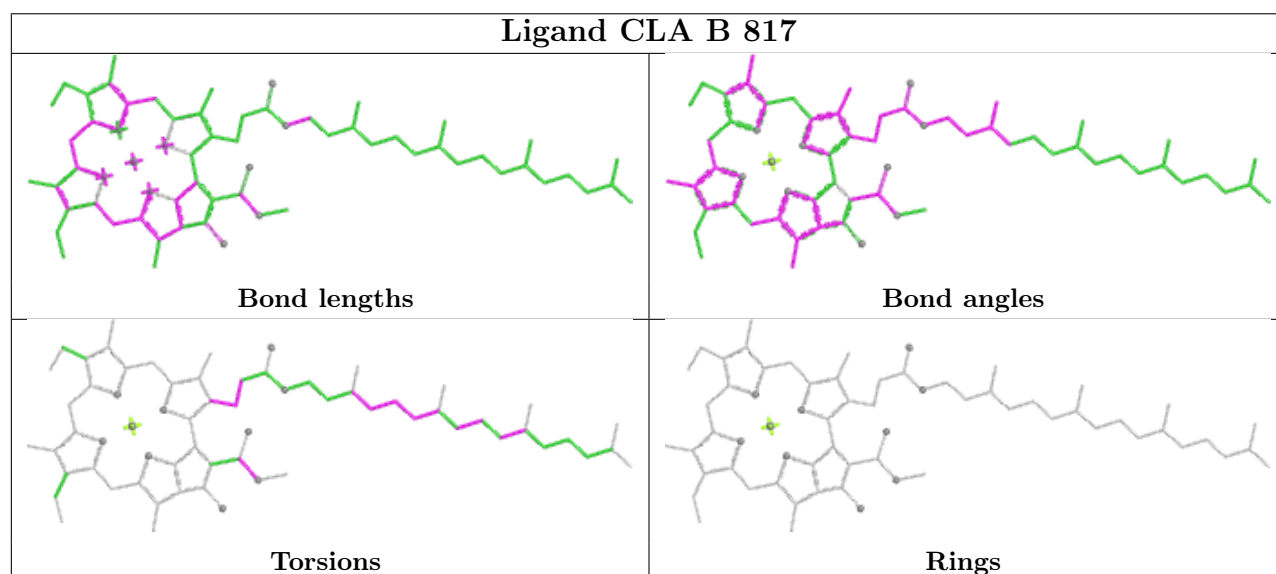
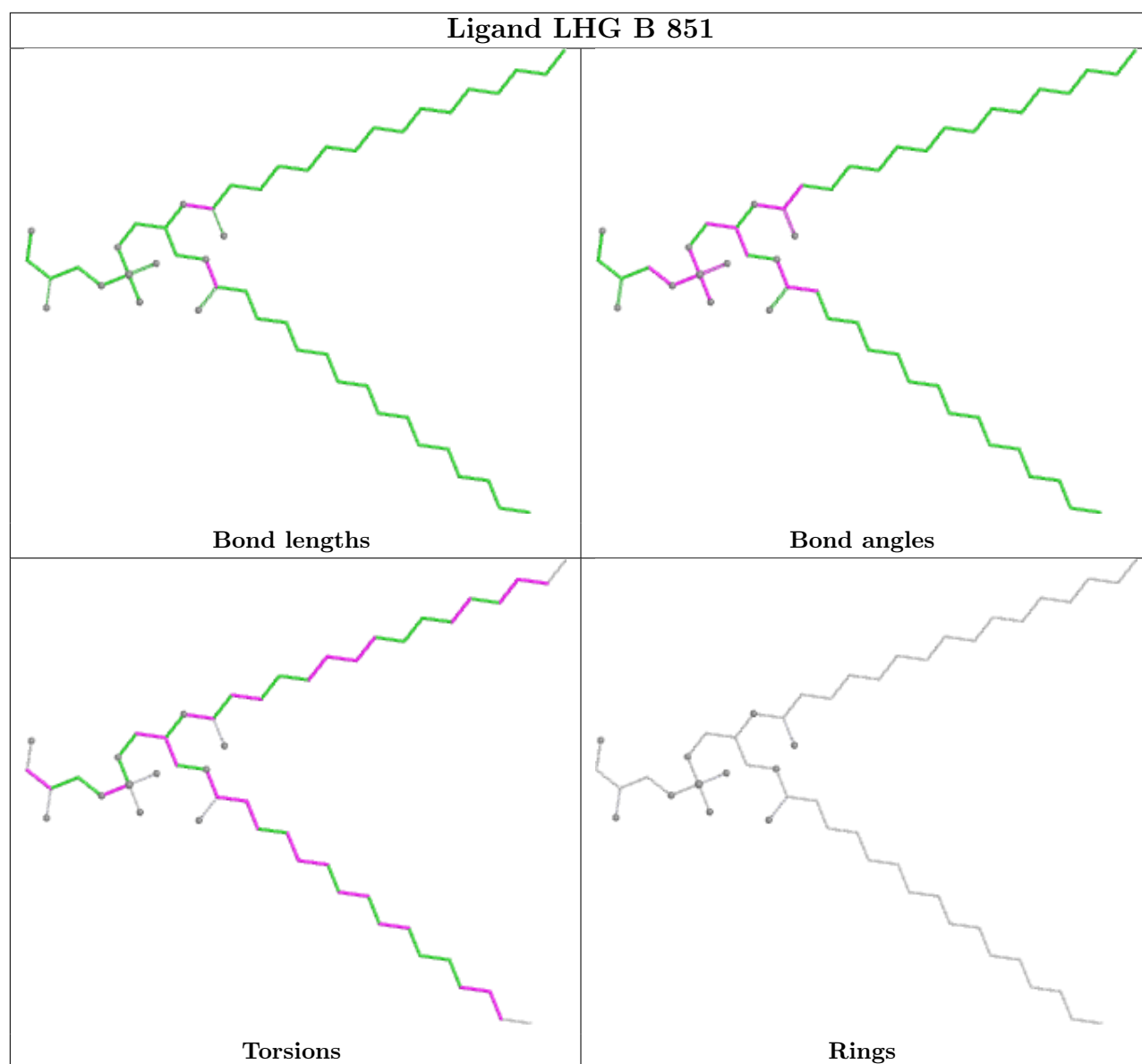
Bond angles

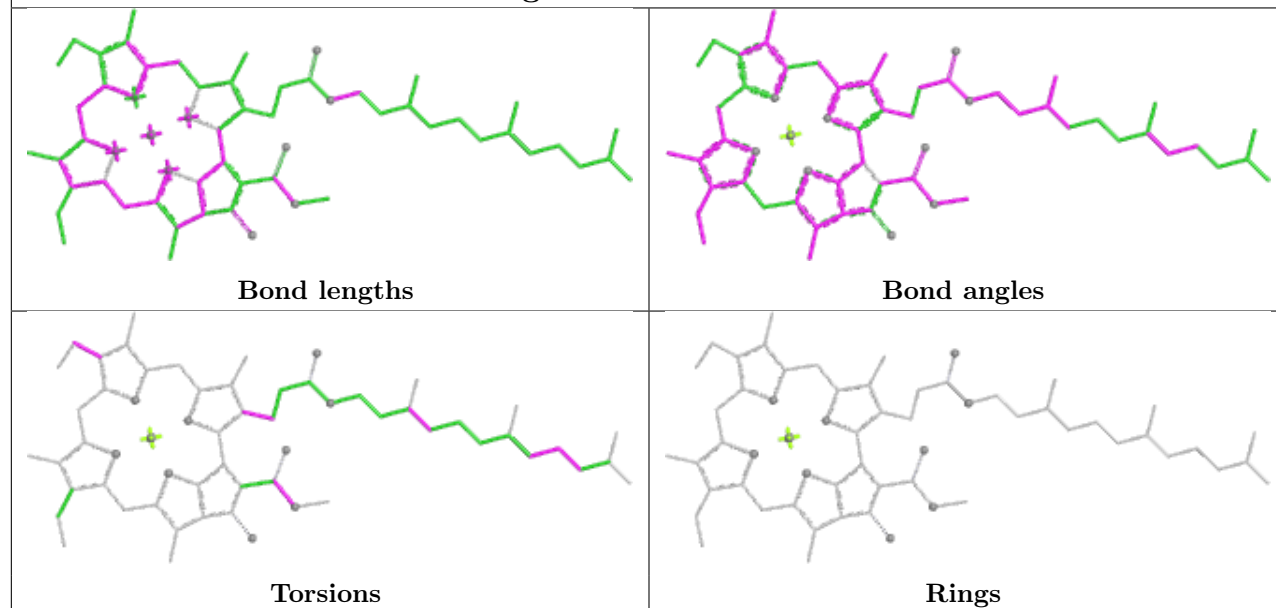
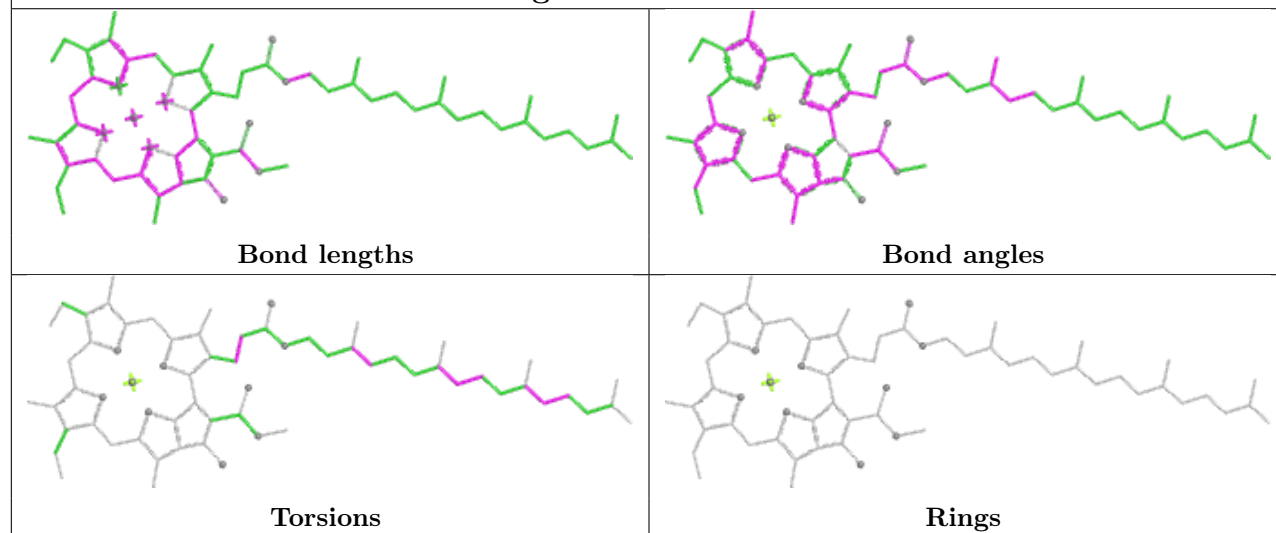


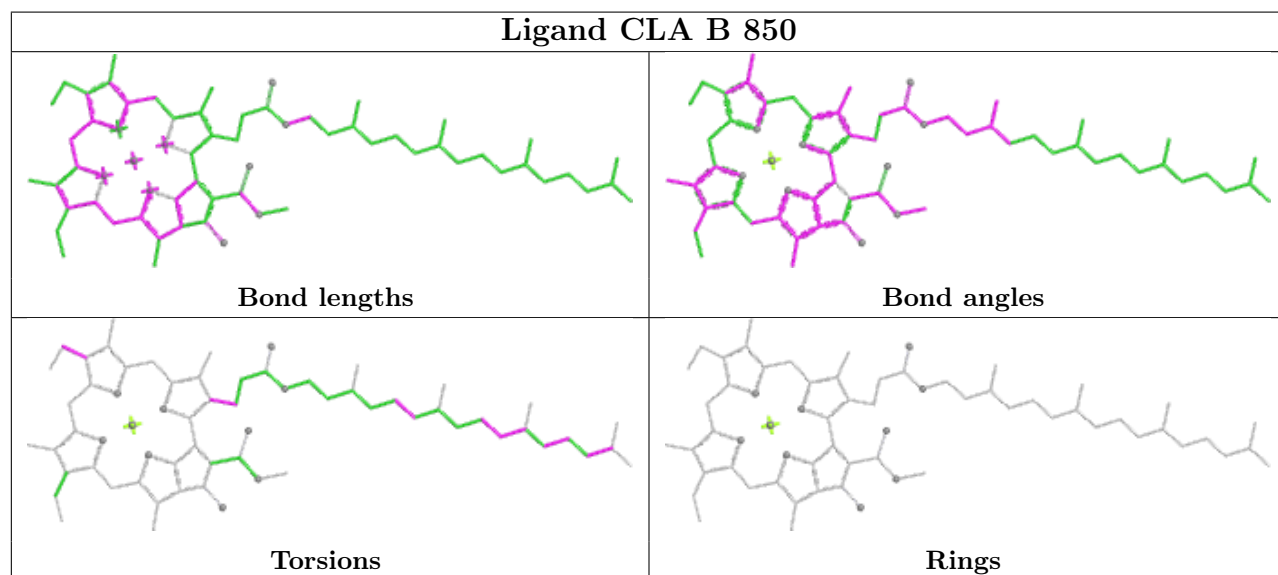
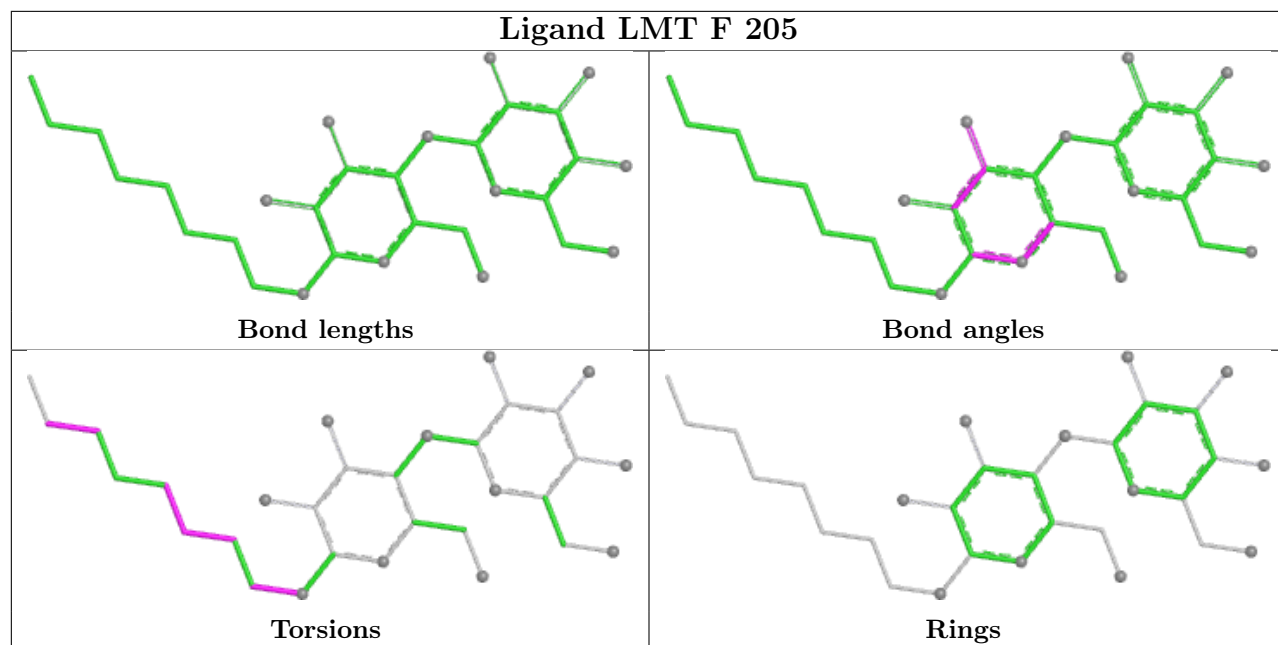
Torsions

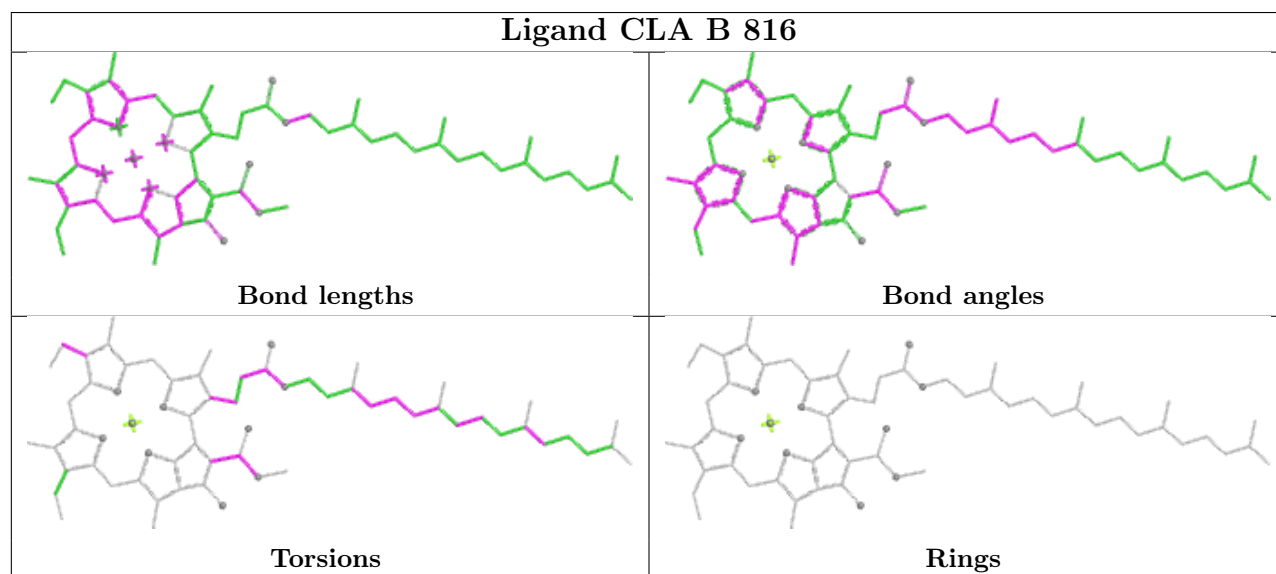
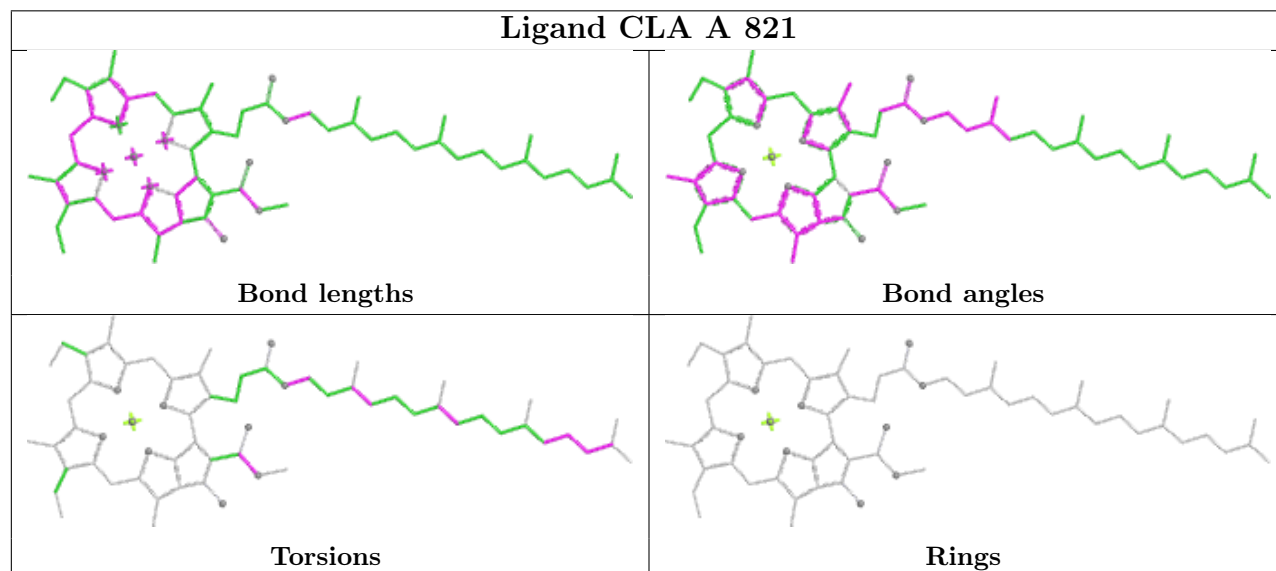
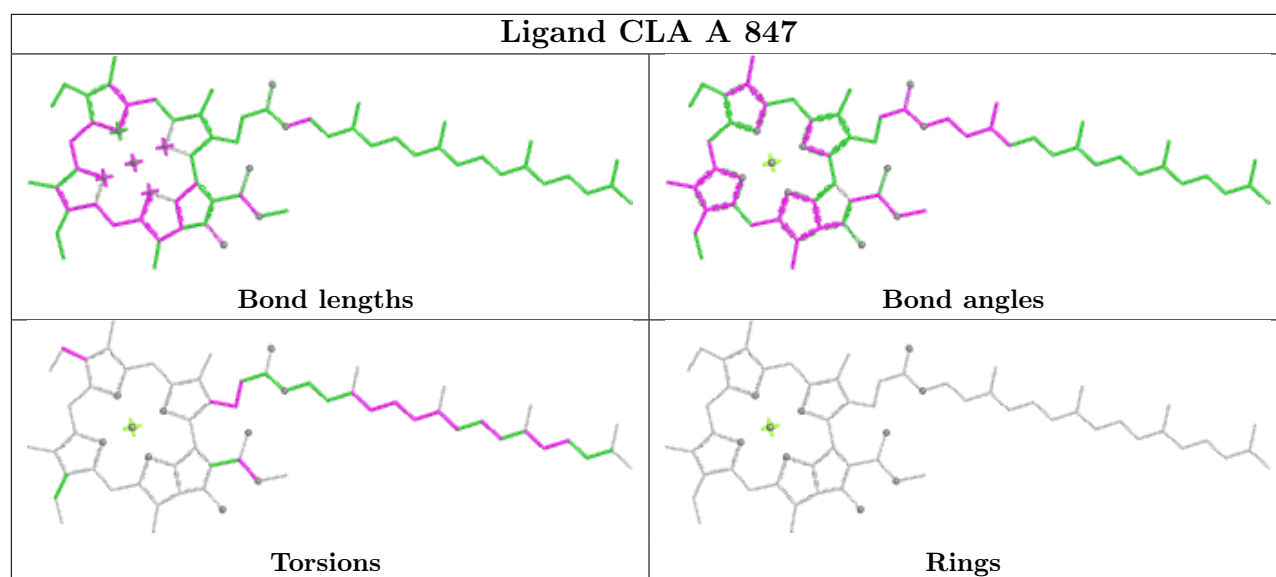


Rings

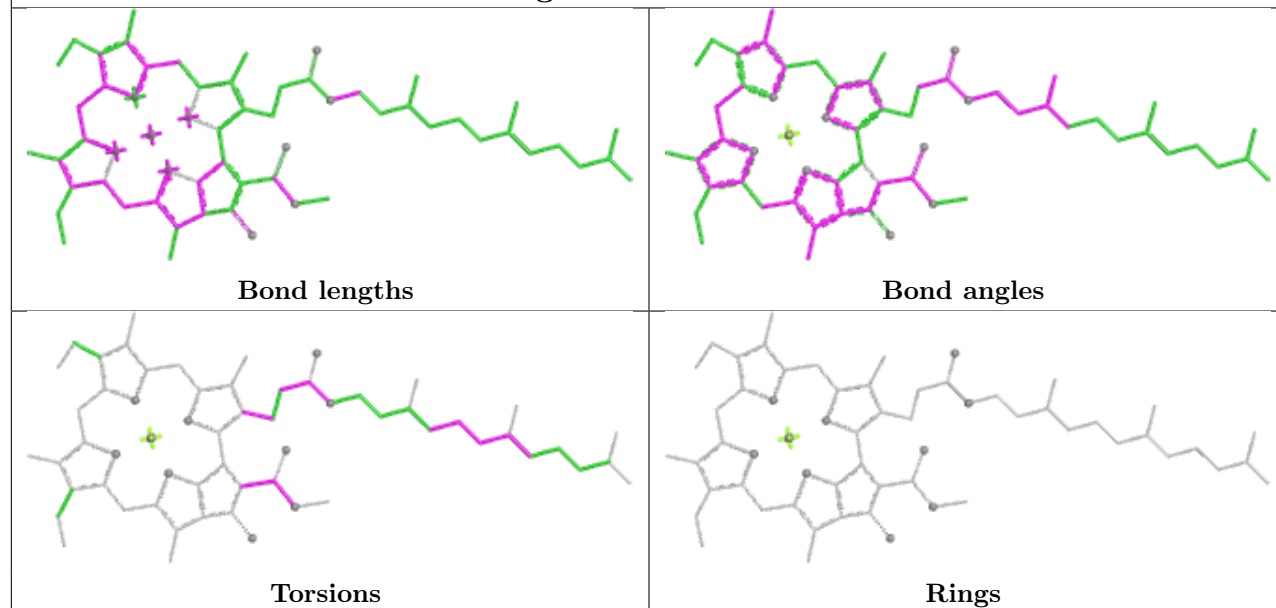


Ligand CLA K 4004**Ligand CLA B 813**

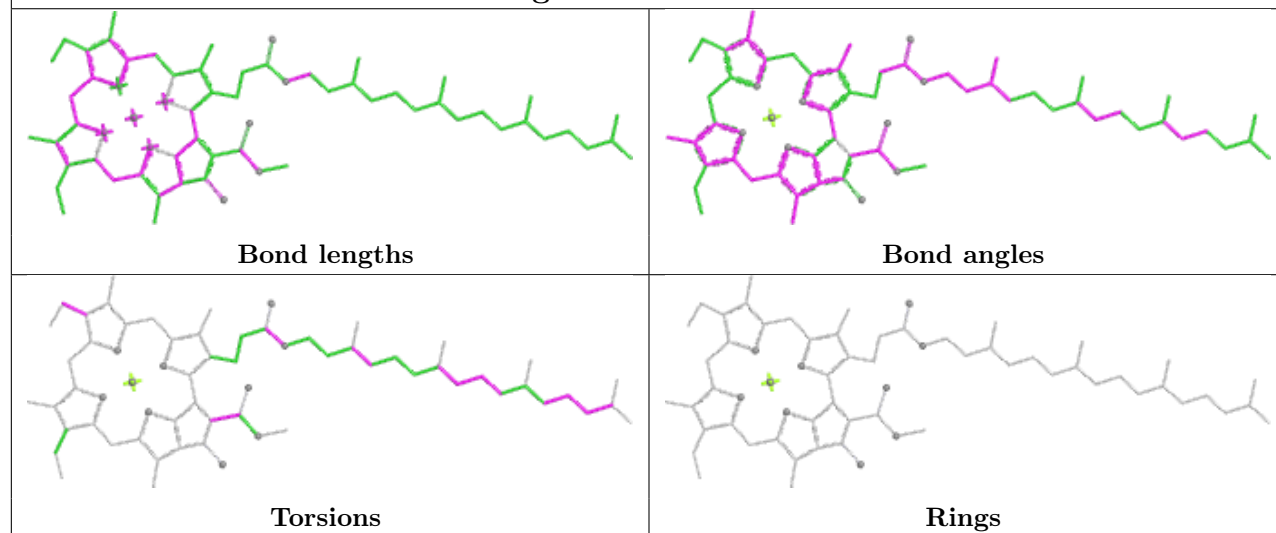


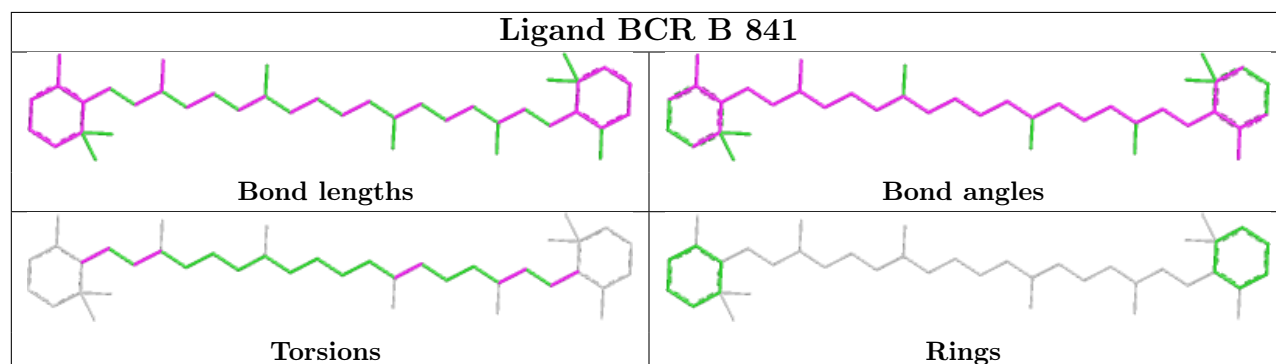
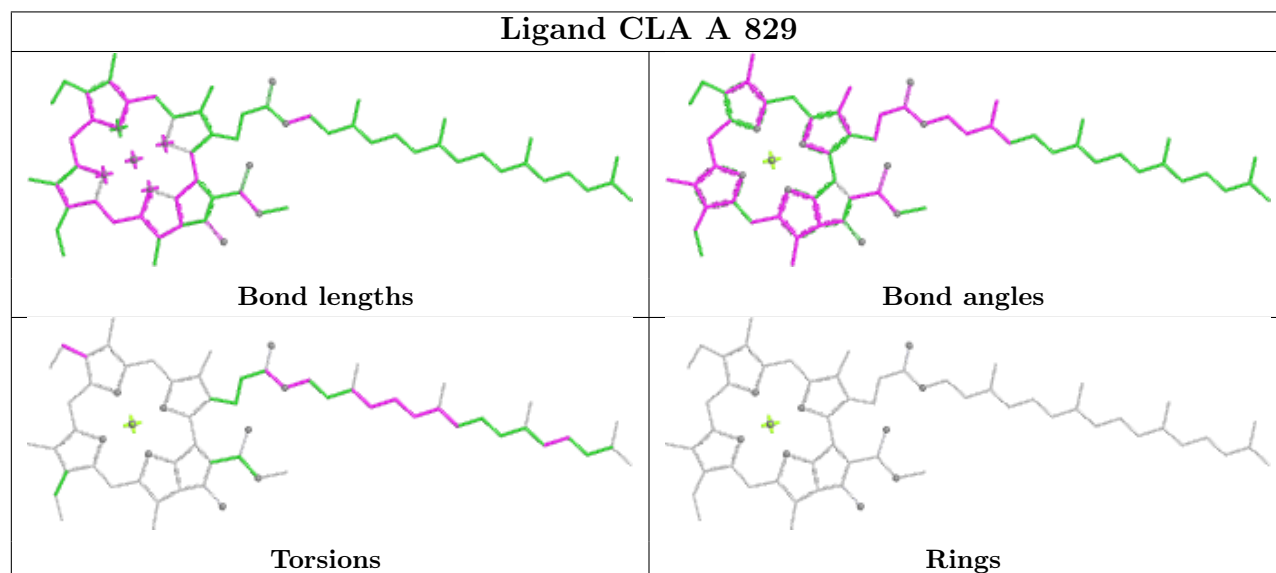
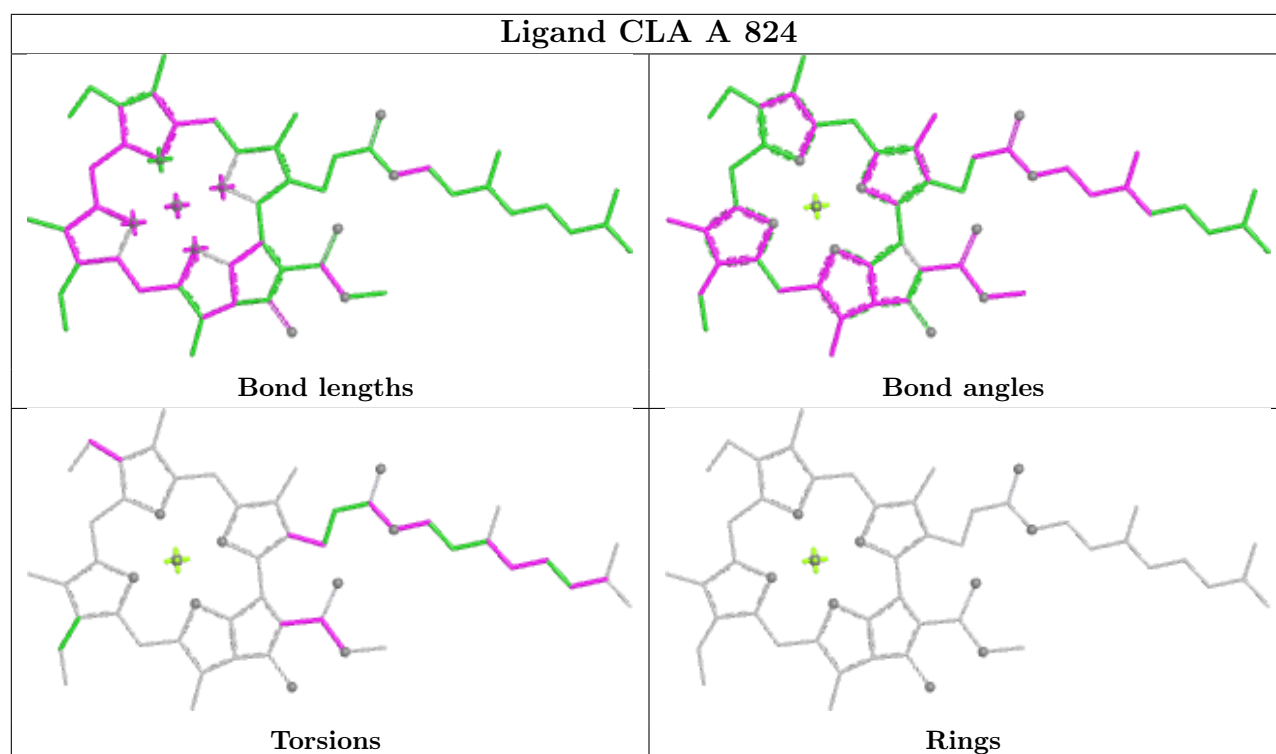


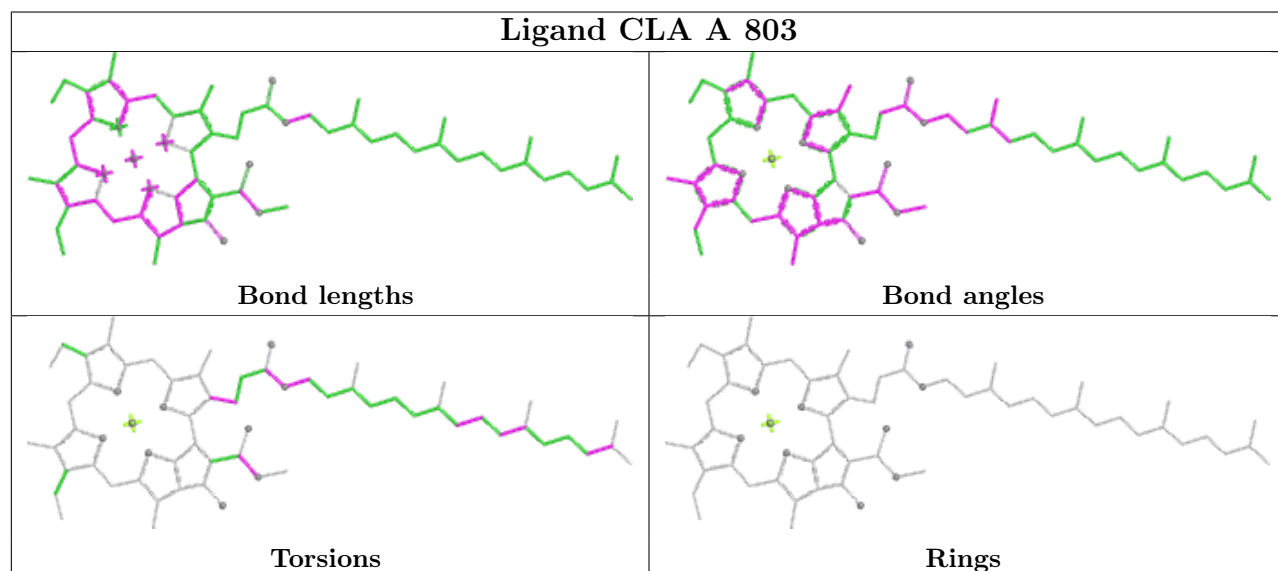
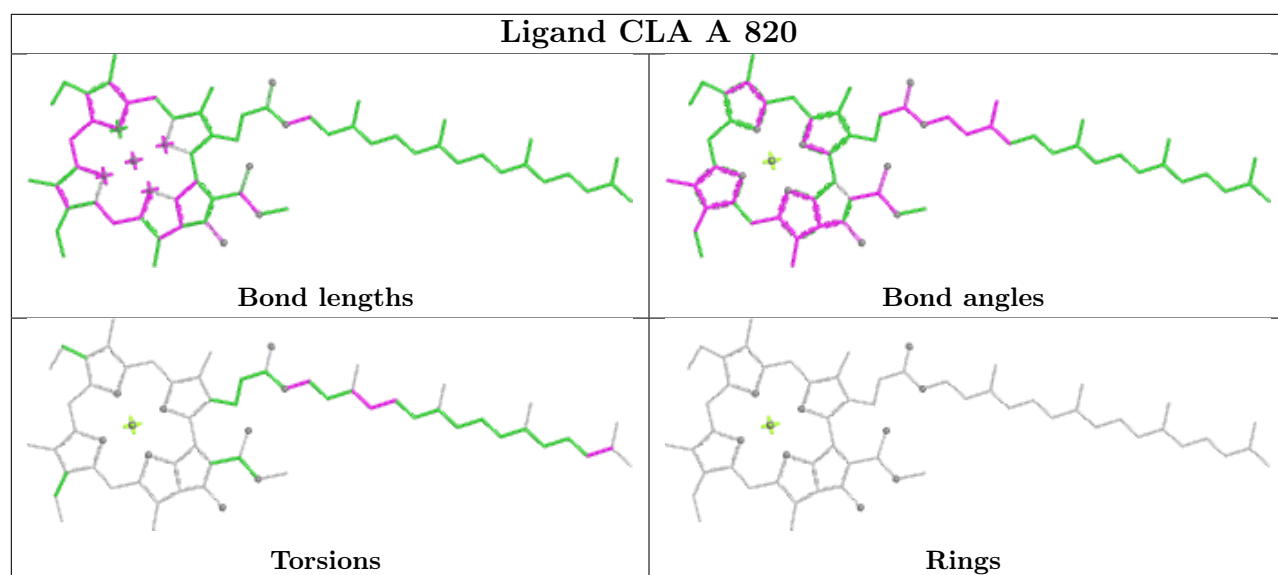
Ligand CLA J 101

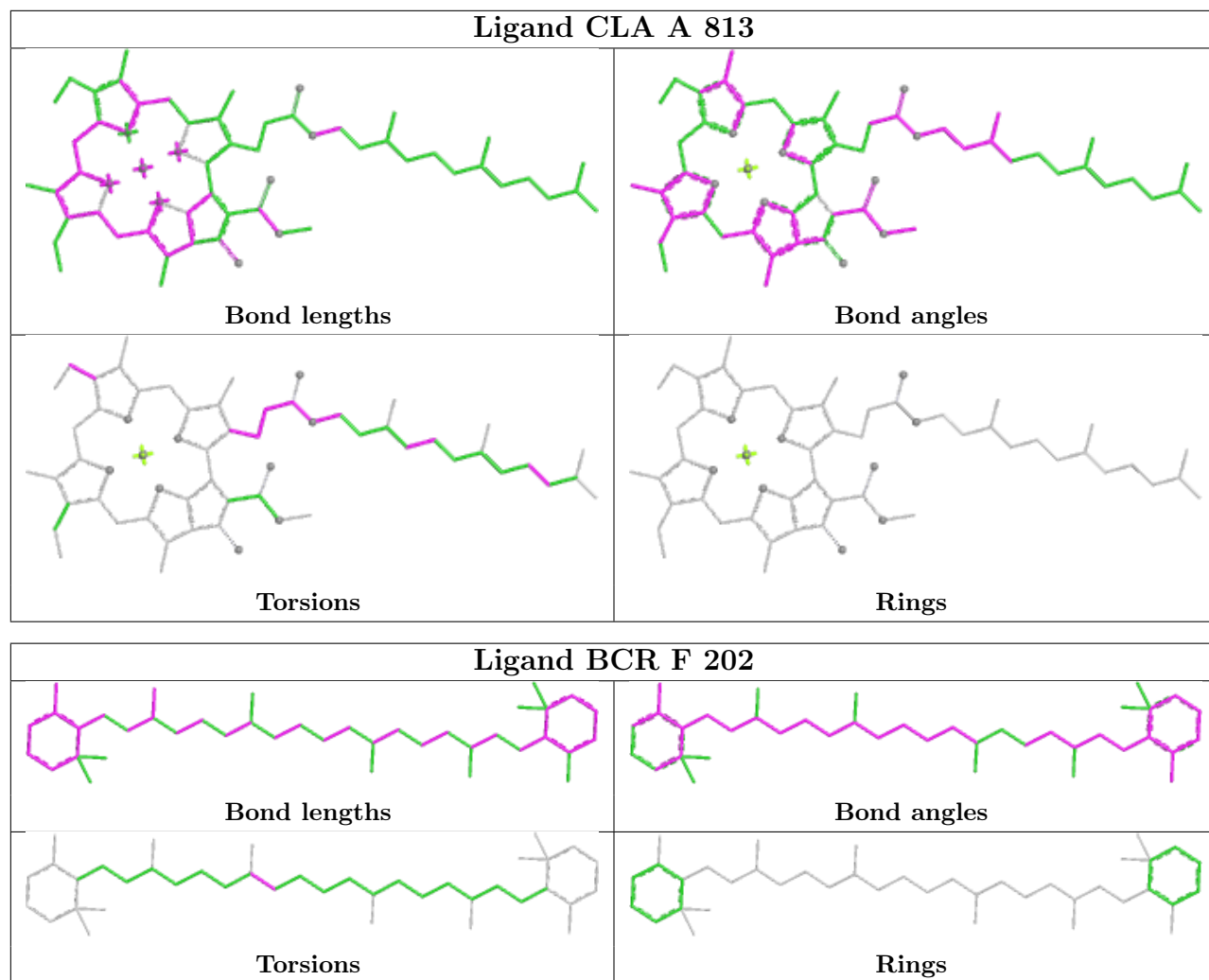


Ligand CLA B 818

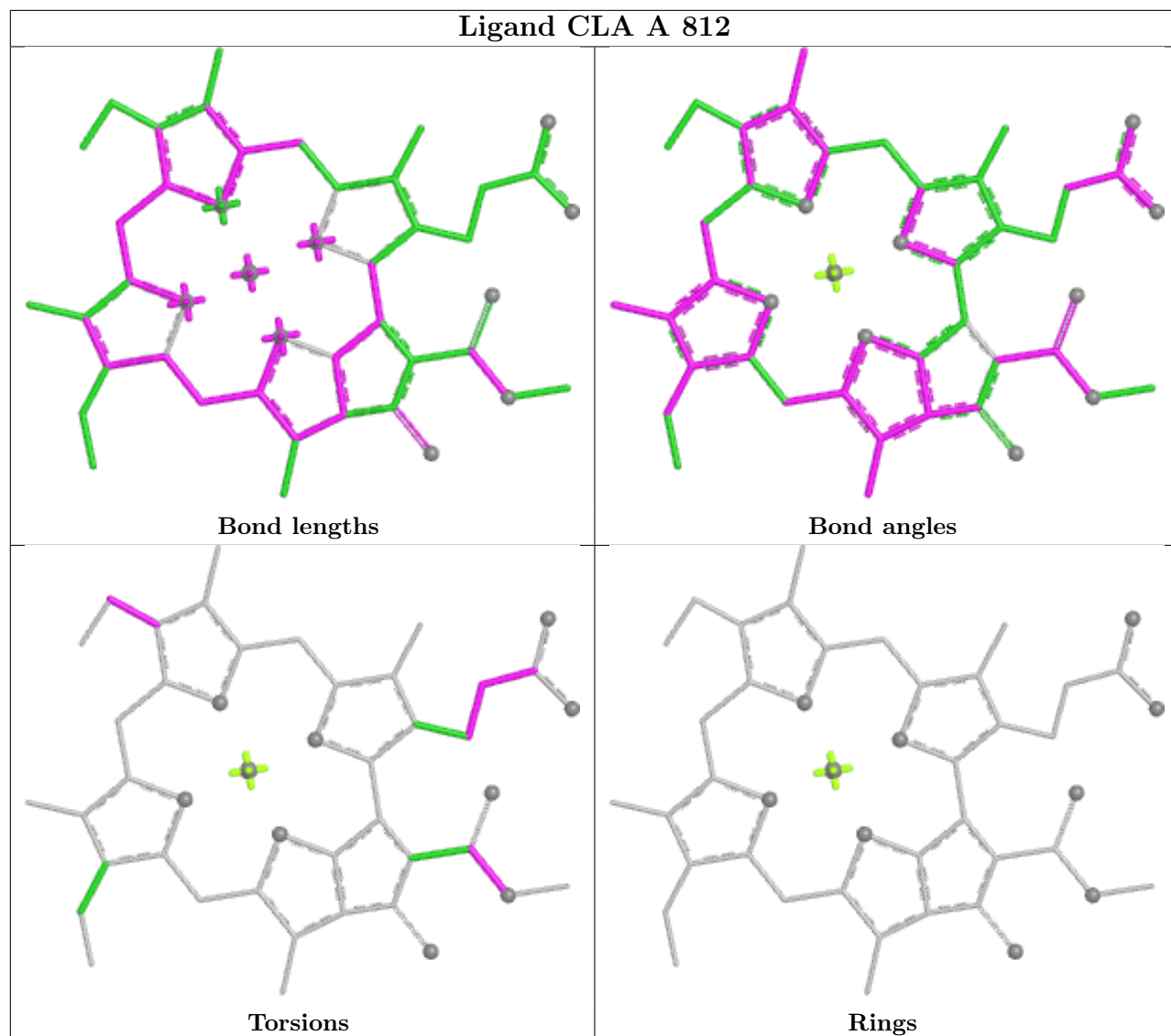




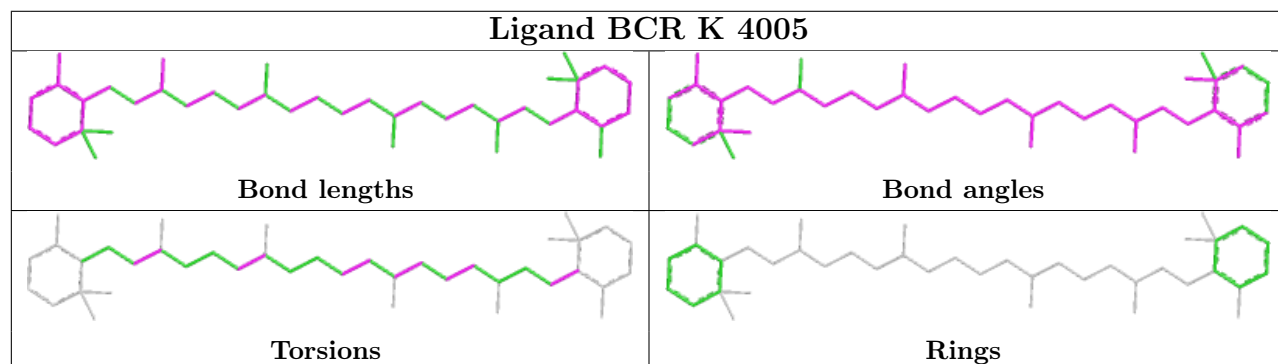


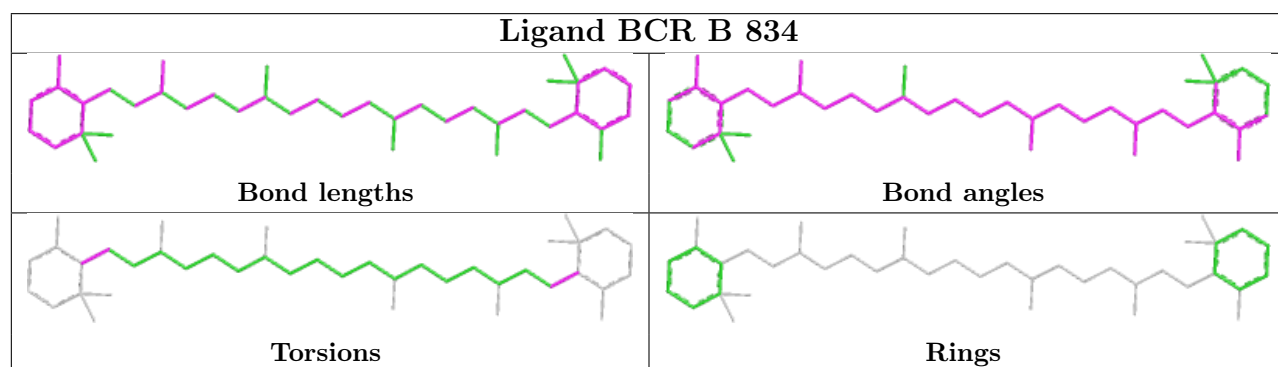
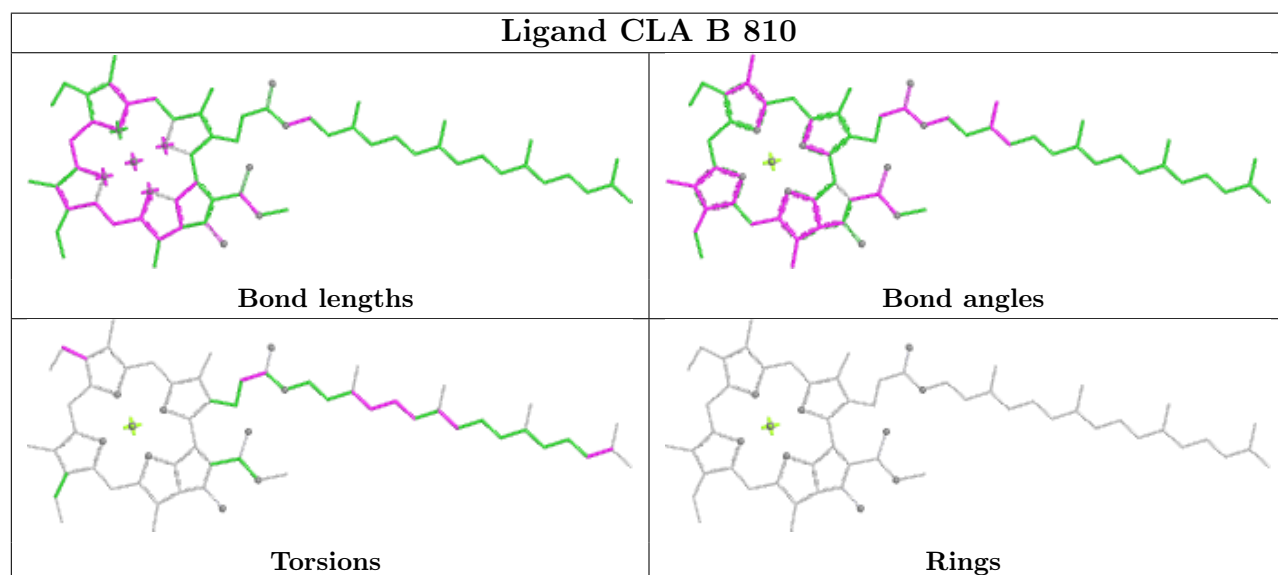
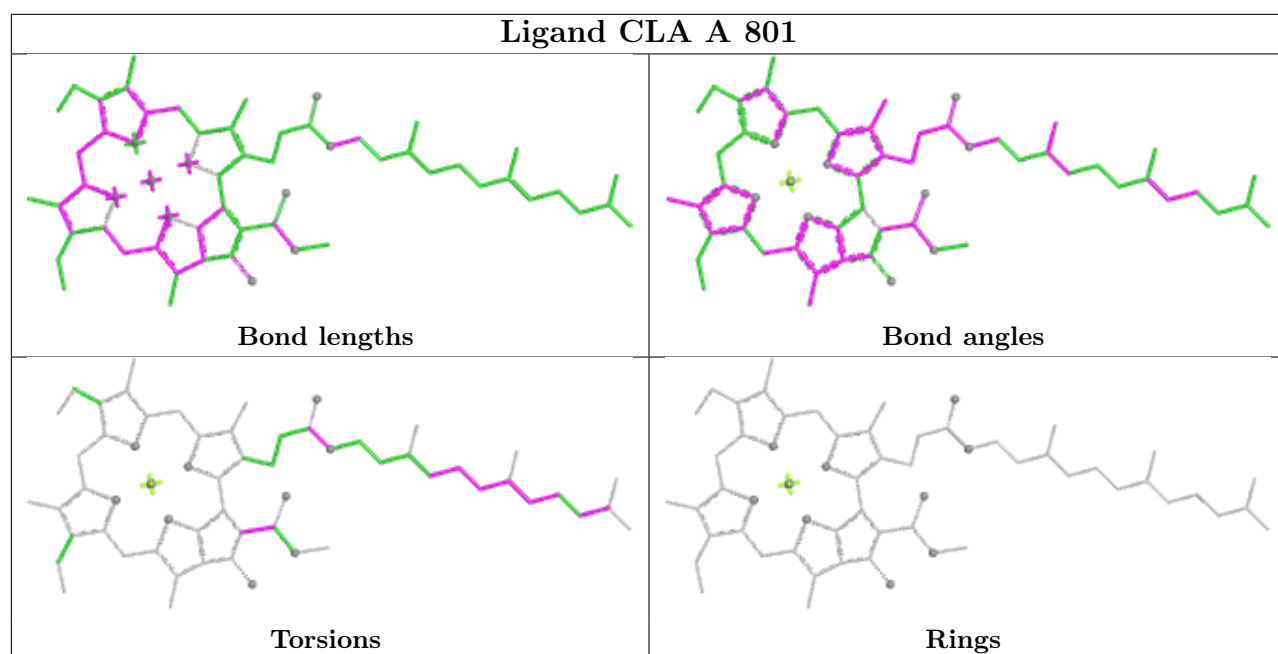


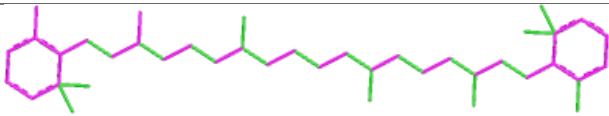
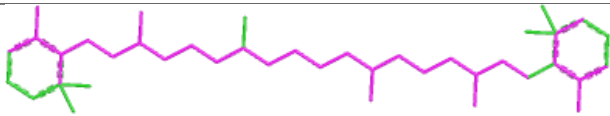
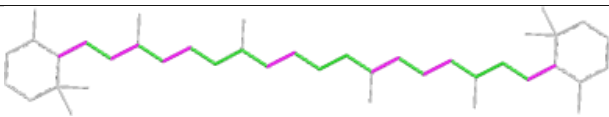
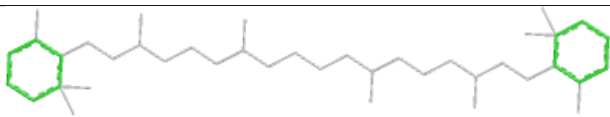
Ligand CLA A 812

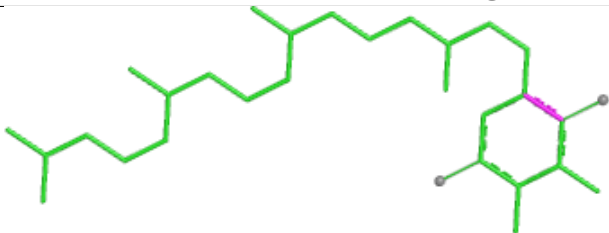
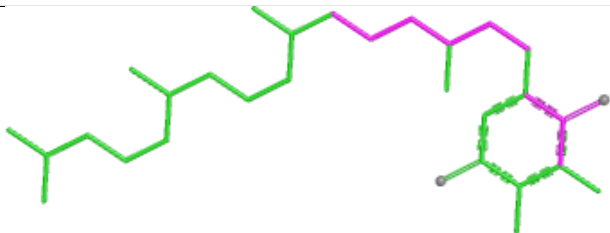
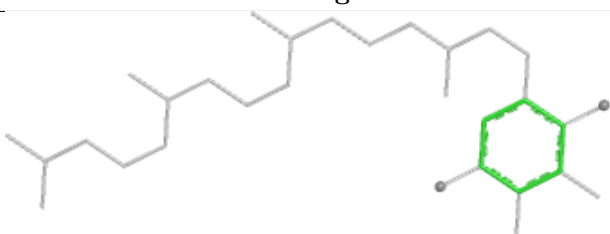


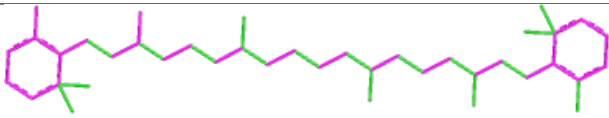
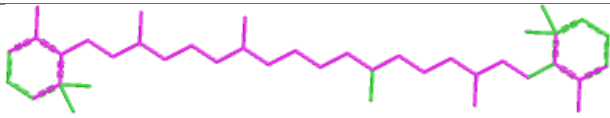
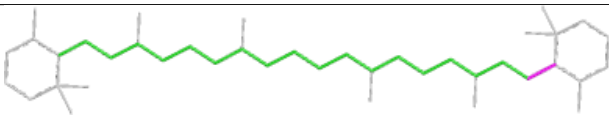
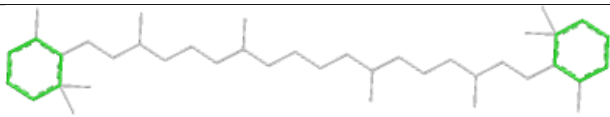
Ligand BCR K 4005

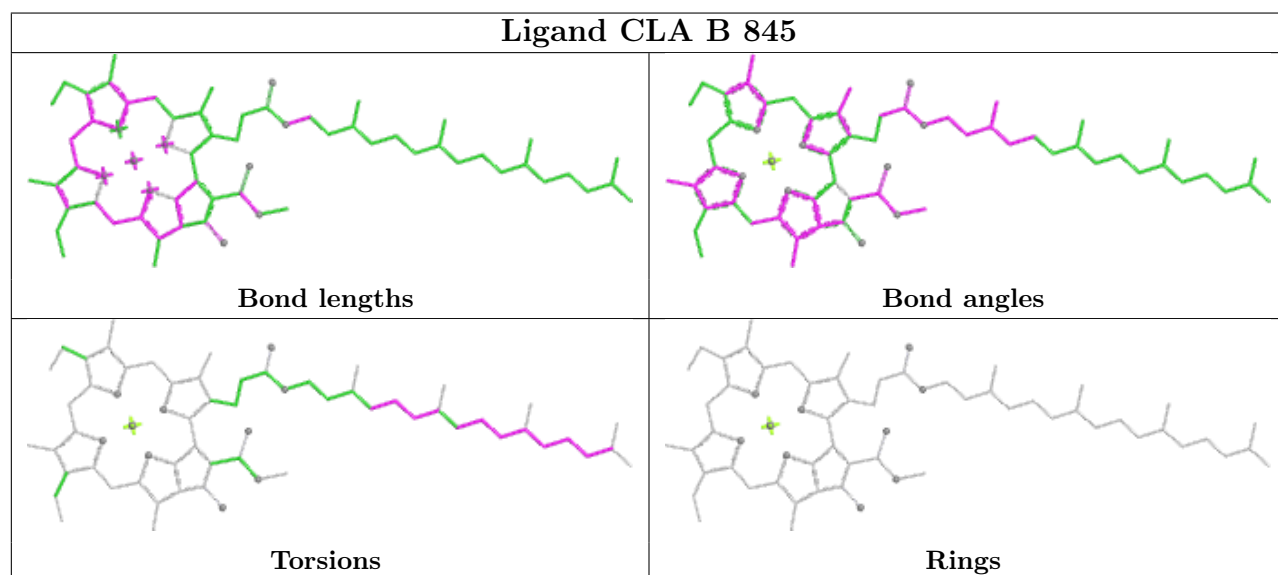
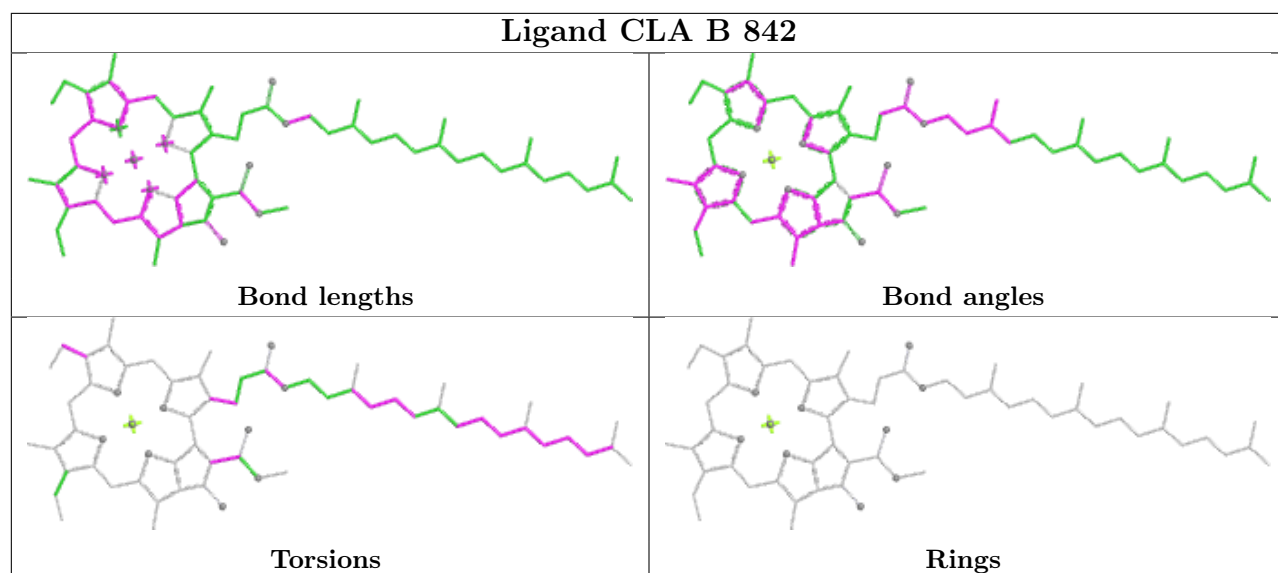
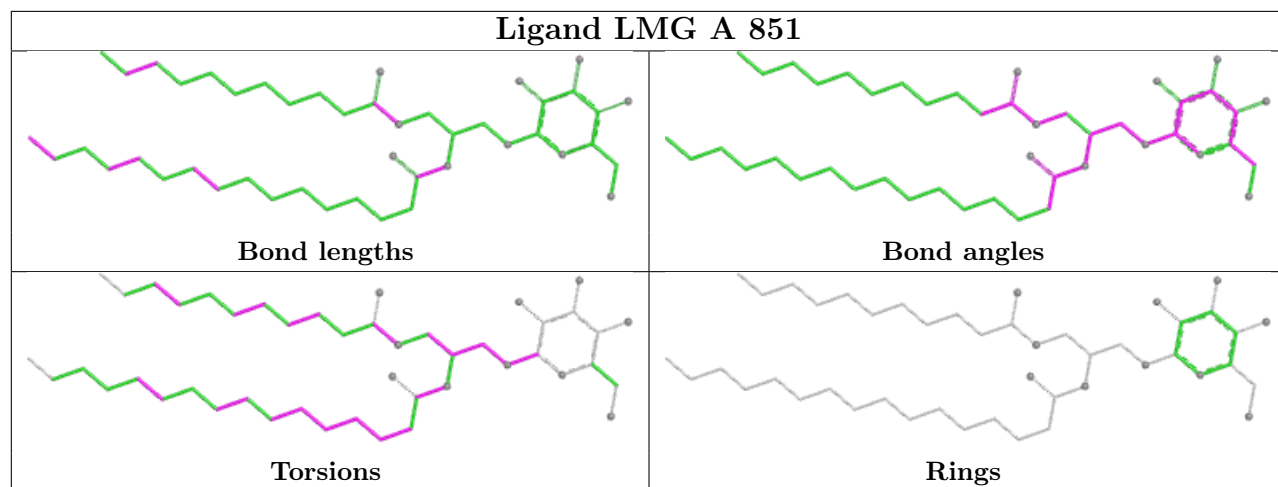


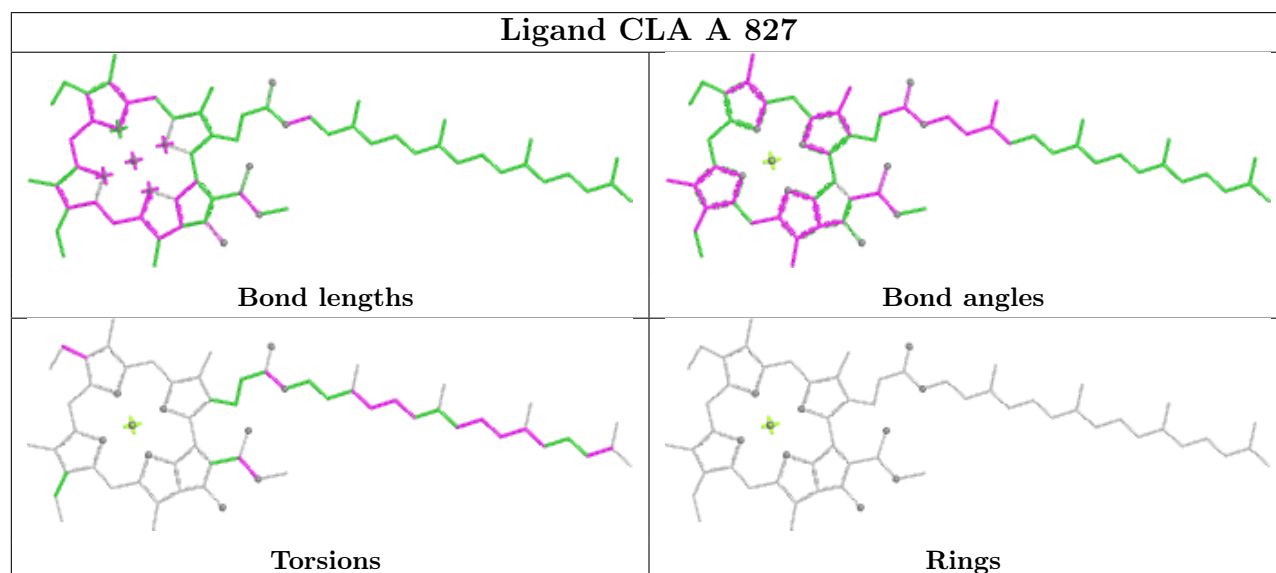
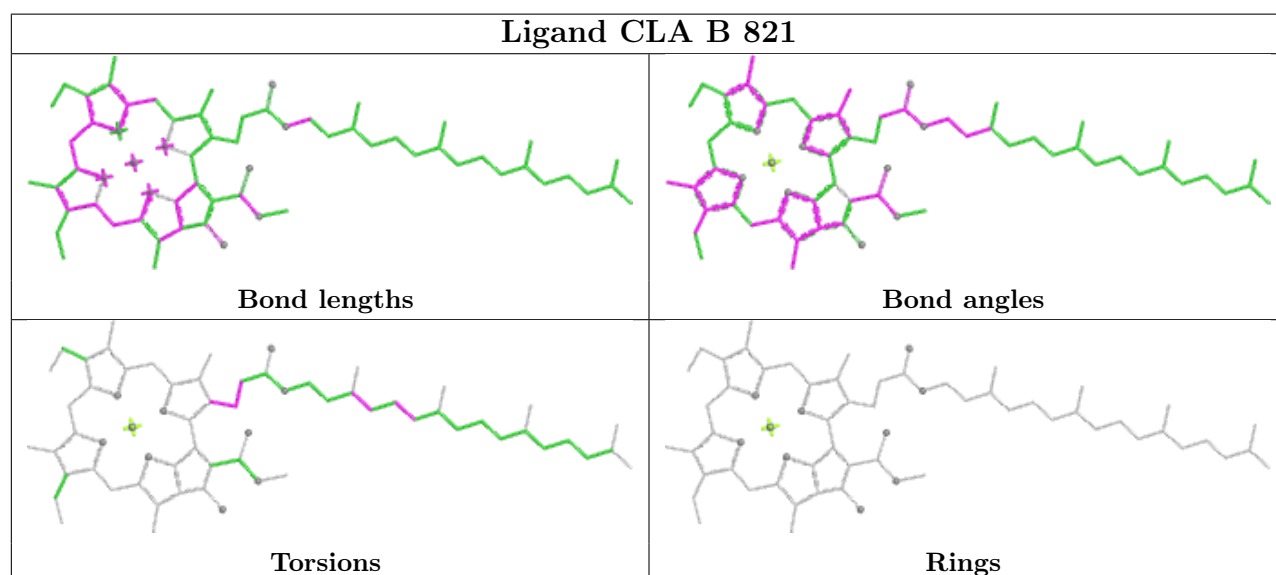
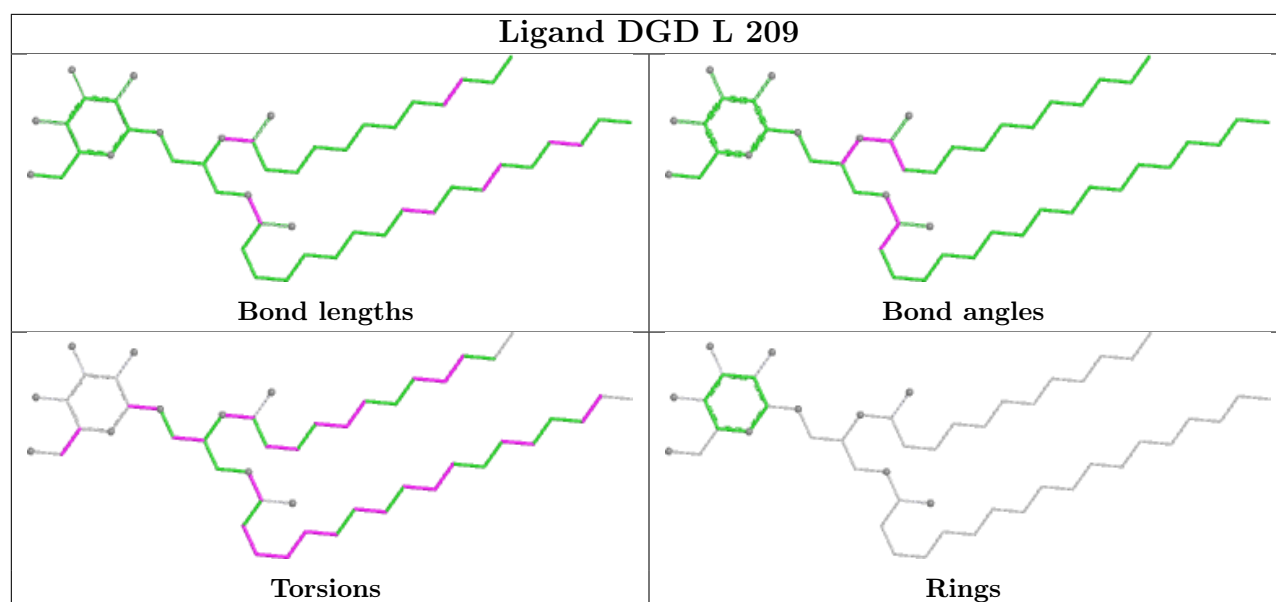


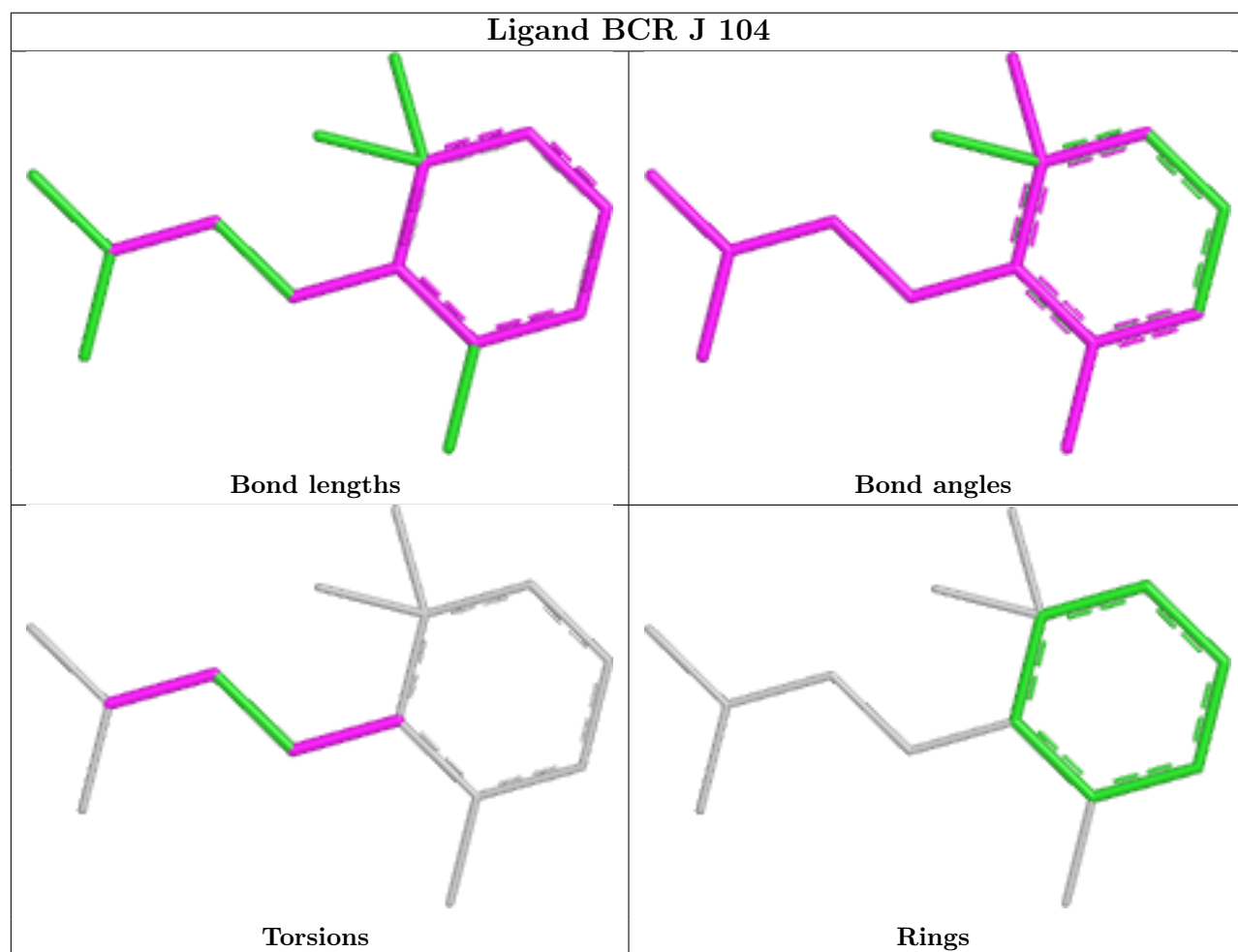
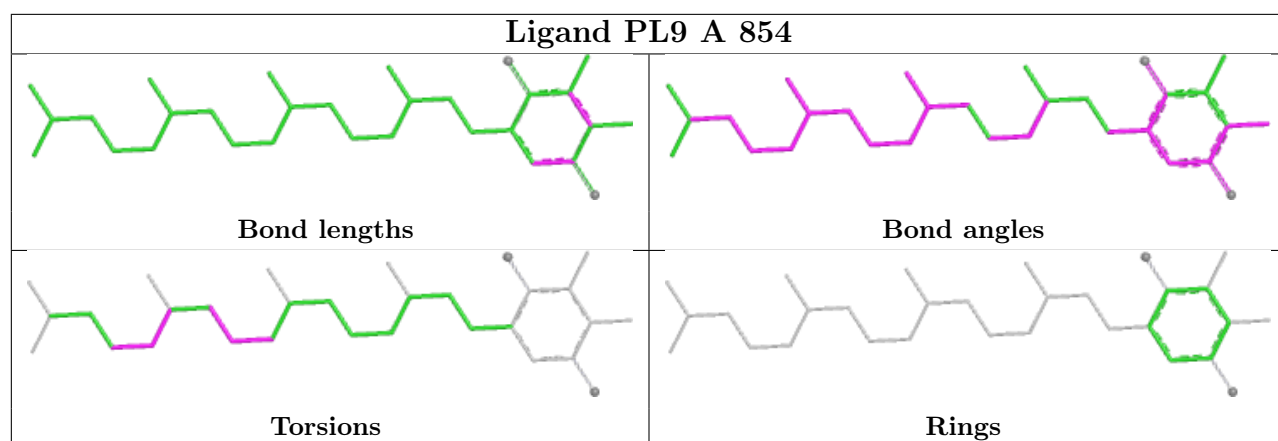
Ligand BCR J 107	
	
Bond lengths	Bond angles
	
Torsions	Rings

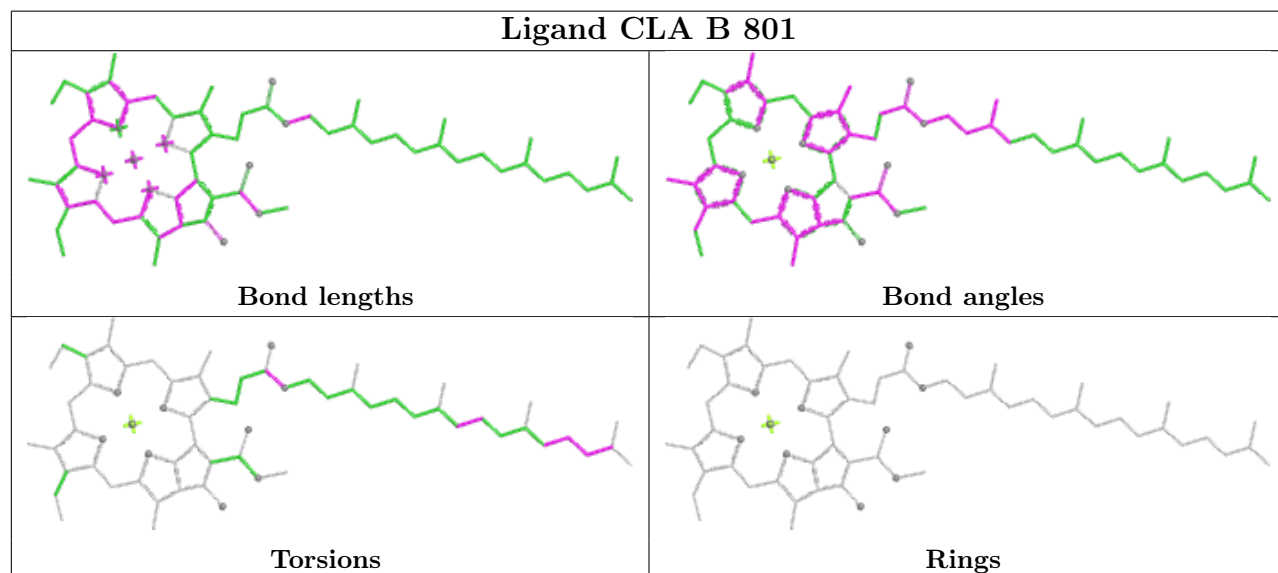
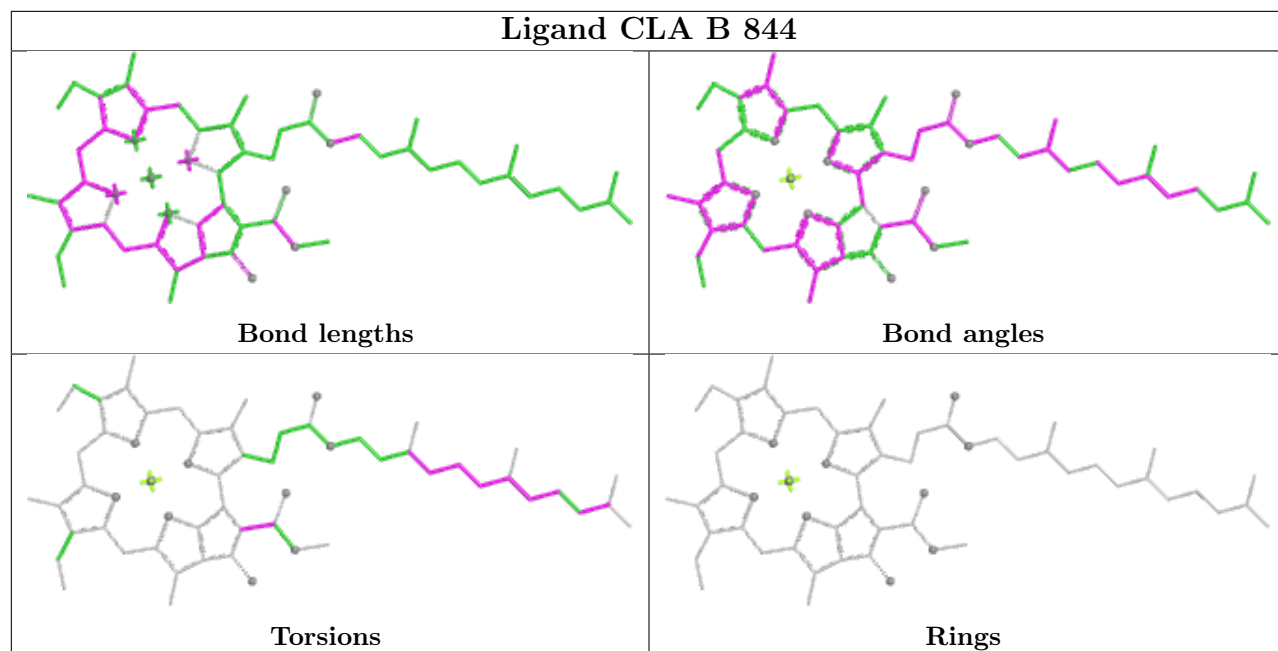
Ligand A1AGD B 831	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 836	
	
Bond lengths	Bond angles
	
Torsions	Rings

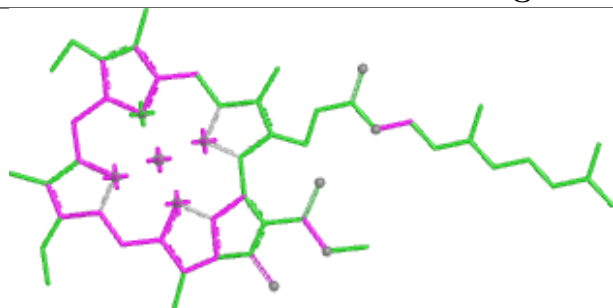




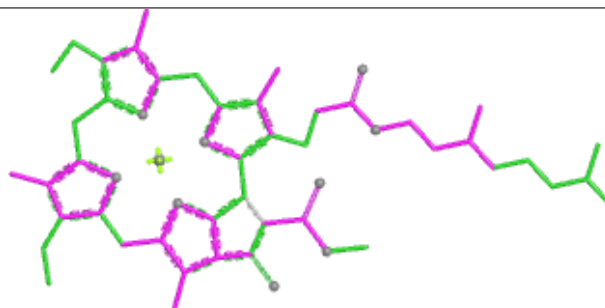




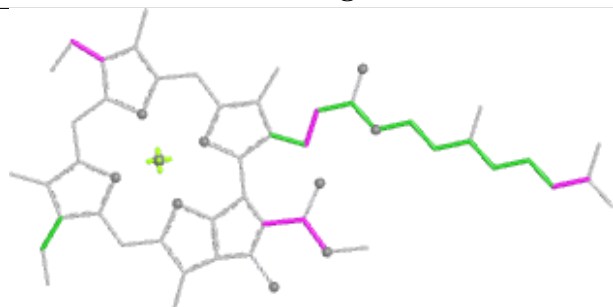
Ligand CLA A 807



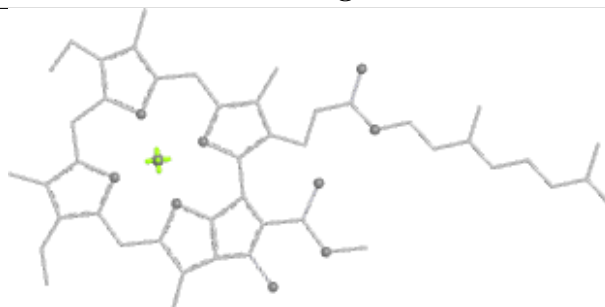
Bond lengths



Bond angles

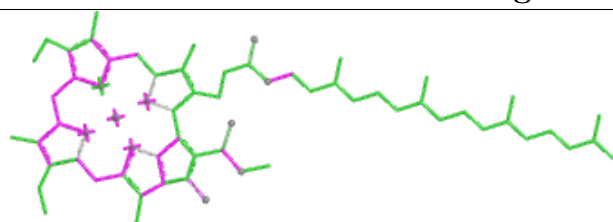


Torsions

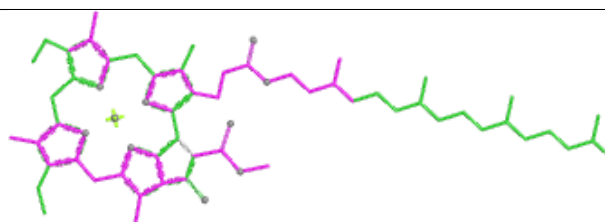


Rings

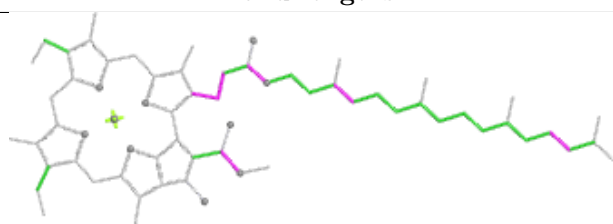
Ligand CLA A 805



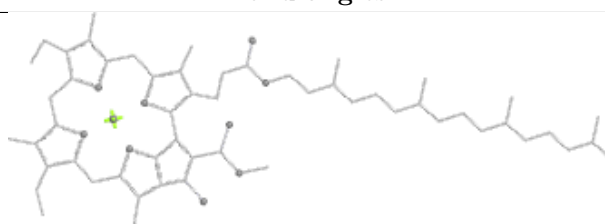
Bond lengths



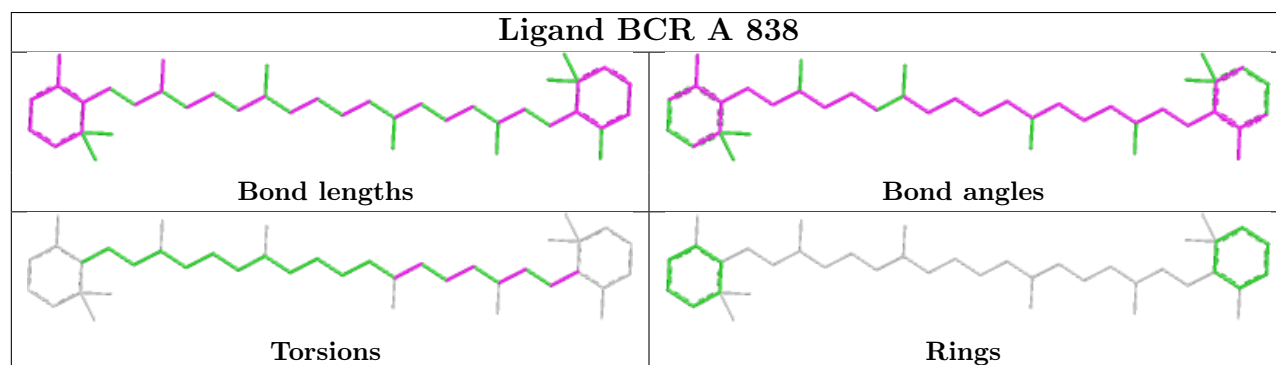
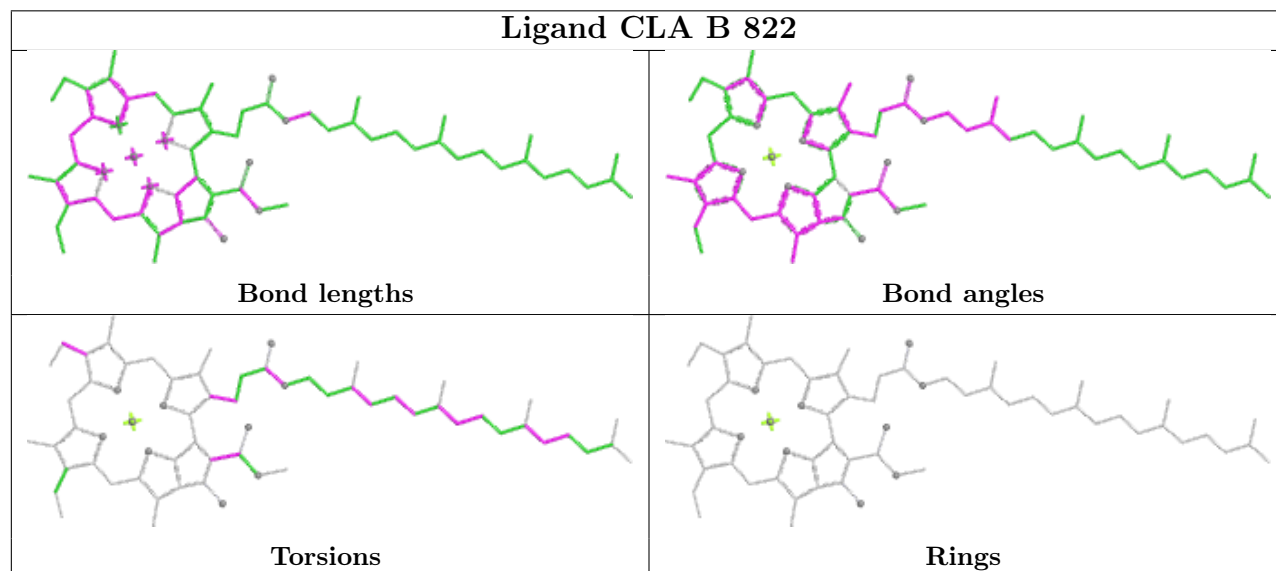
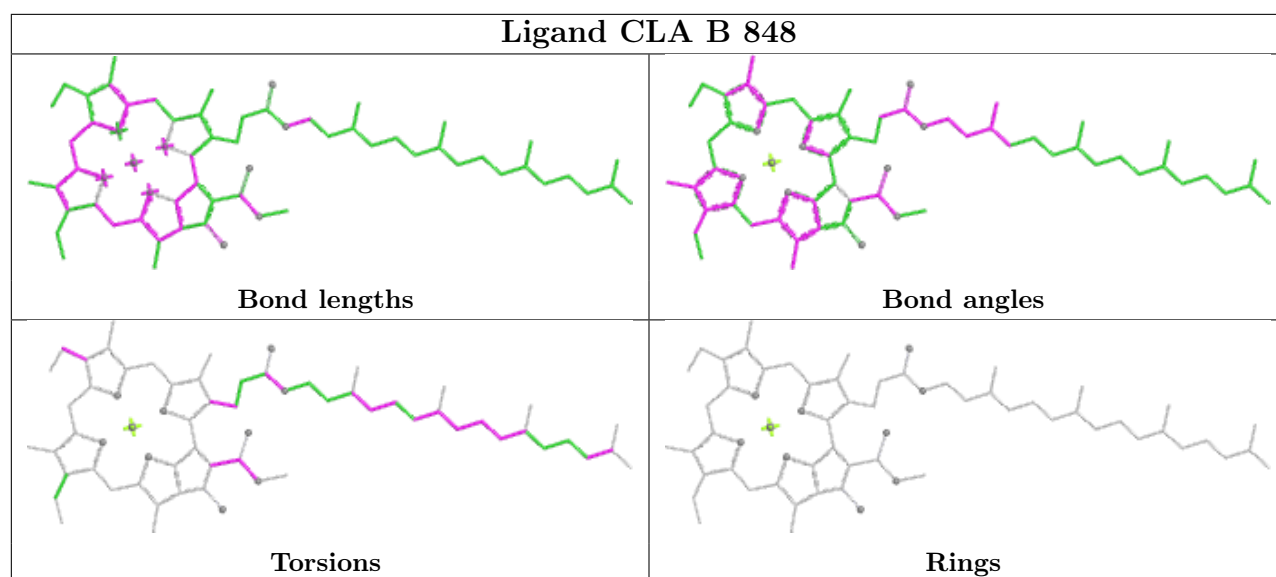
Bond angles

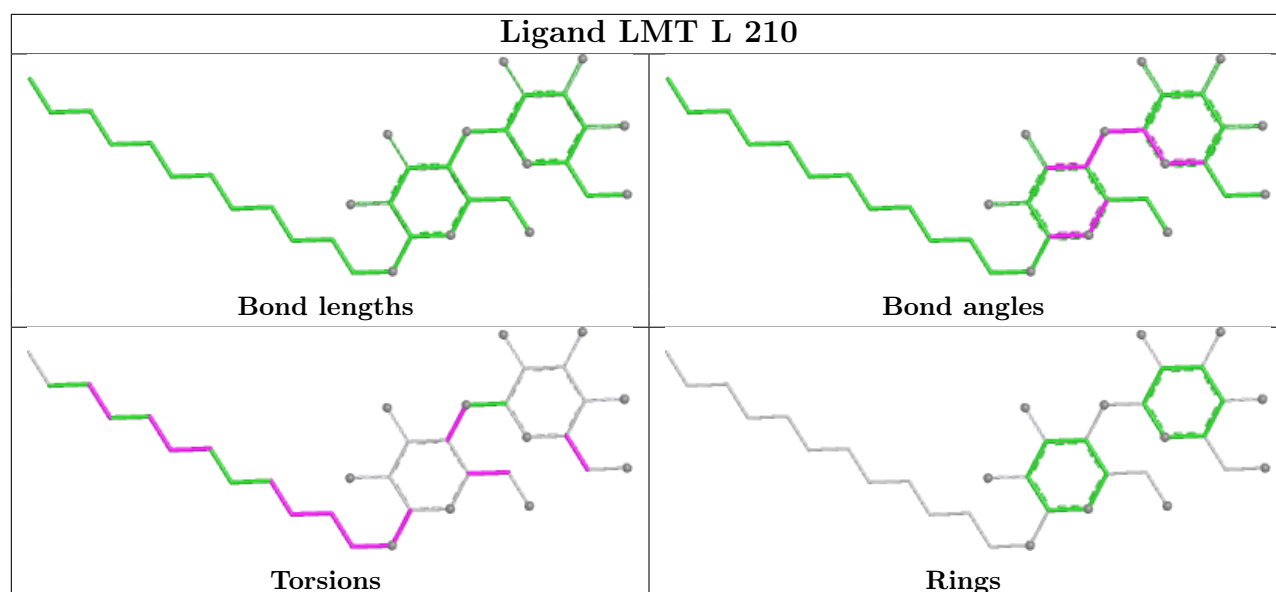
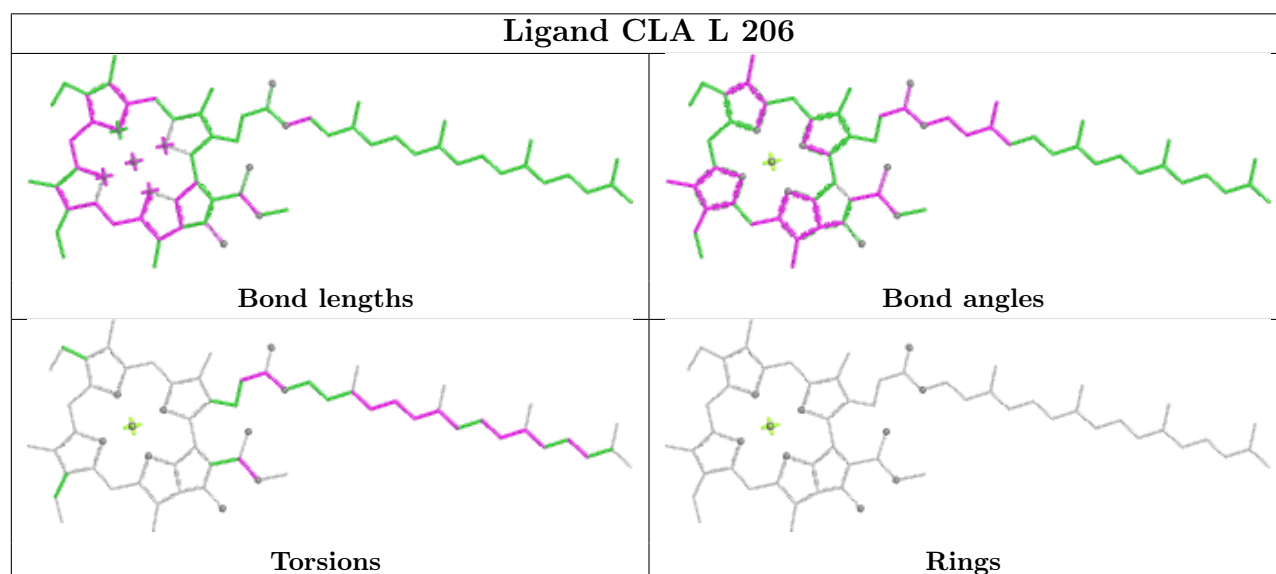
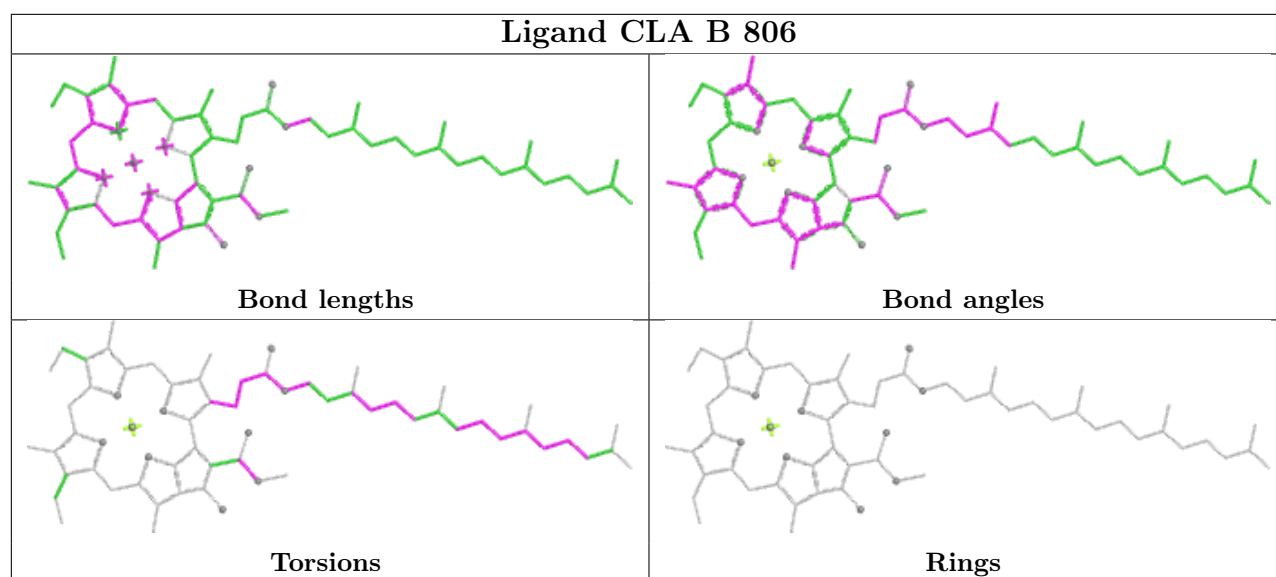


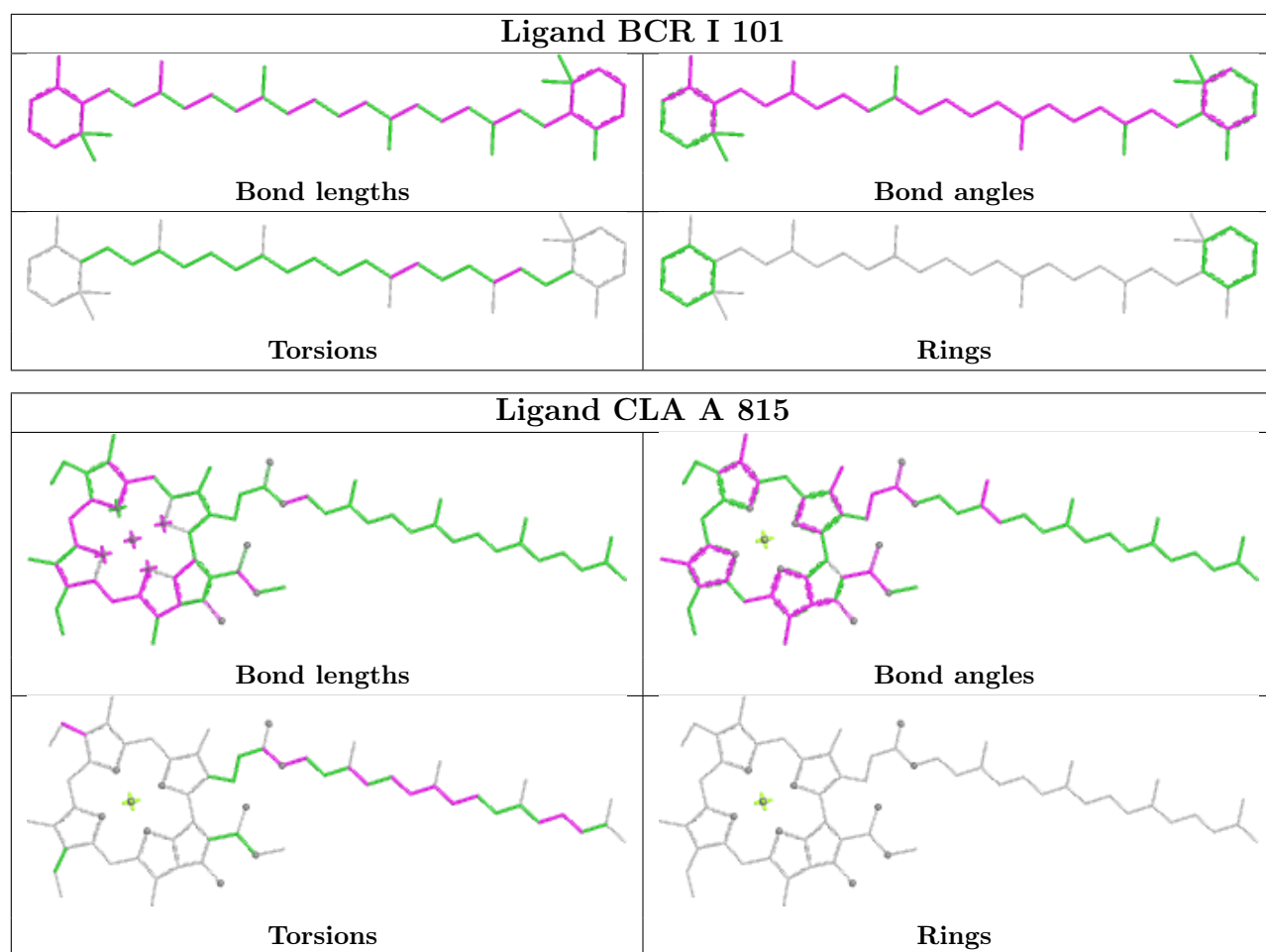
Torsions



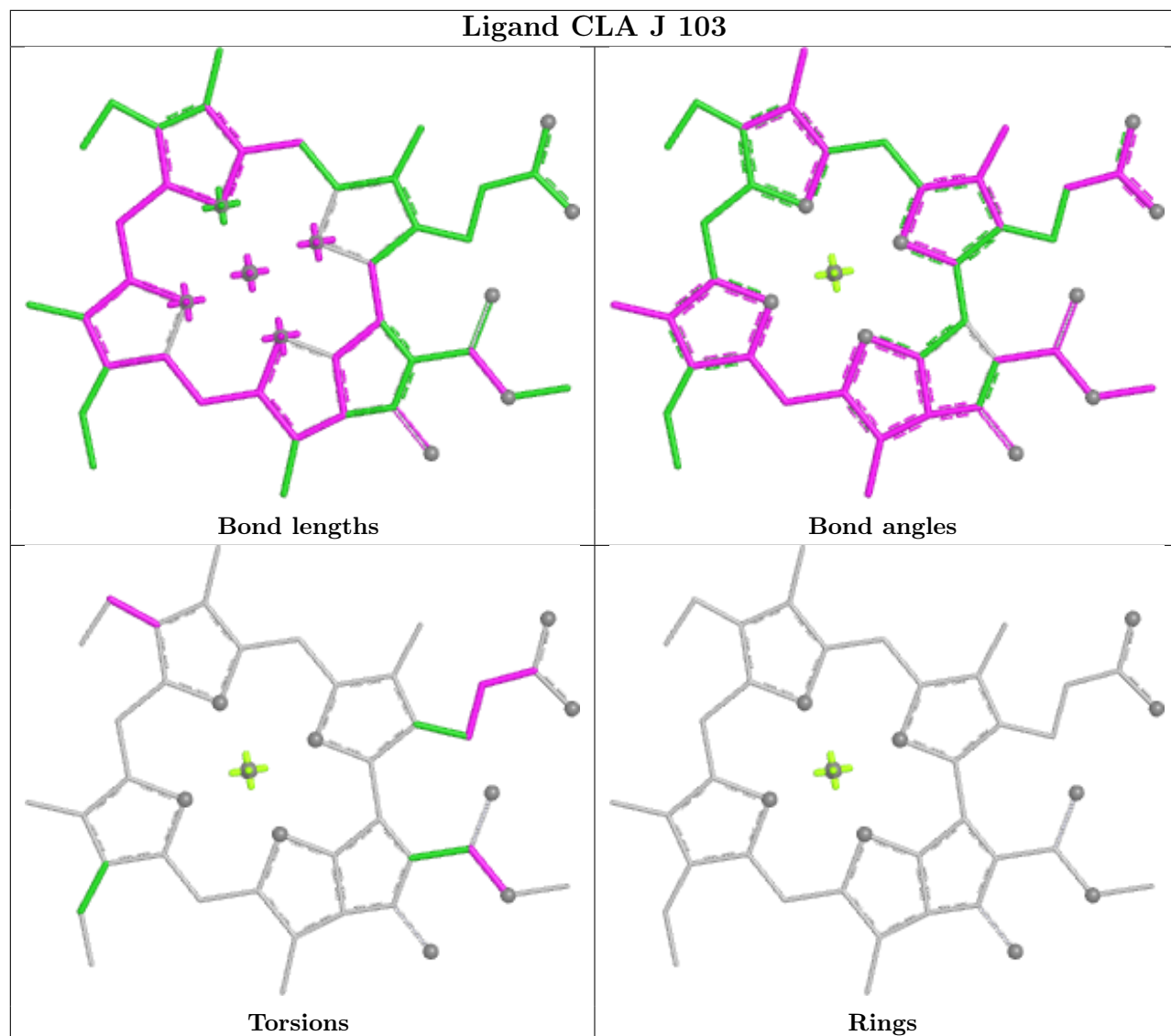
Rings



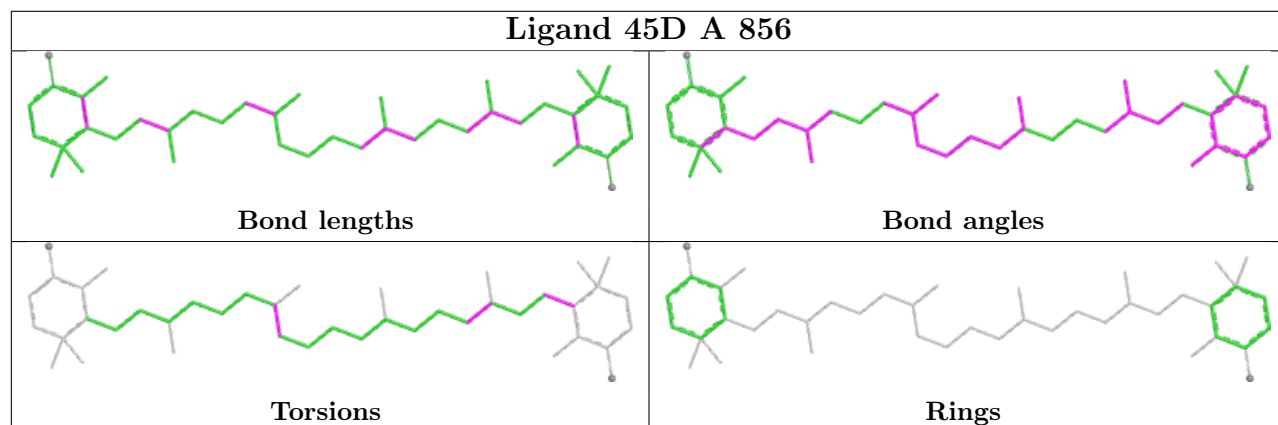


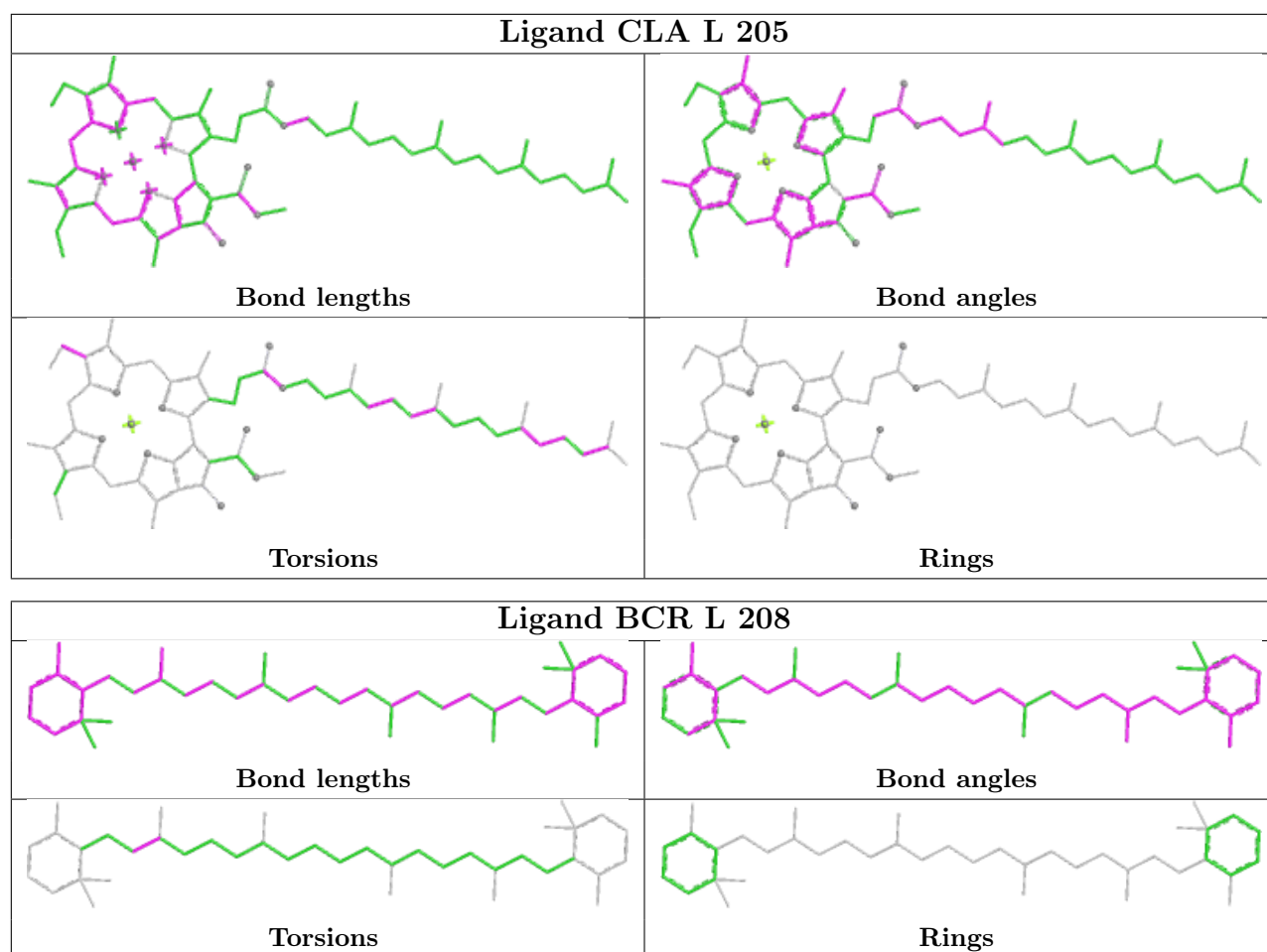


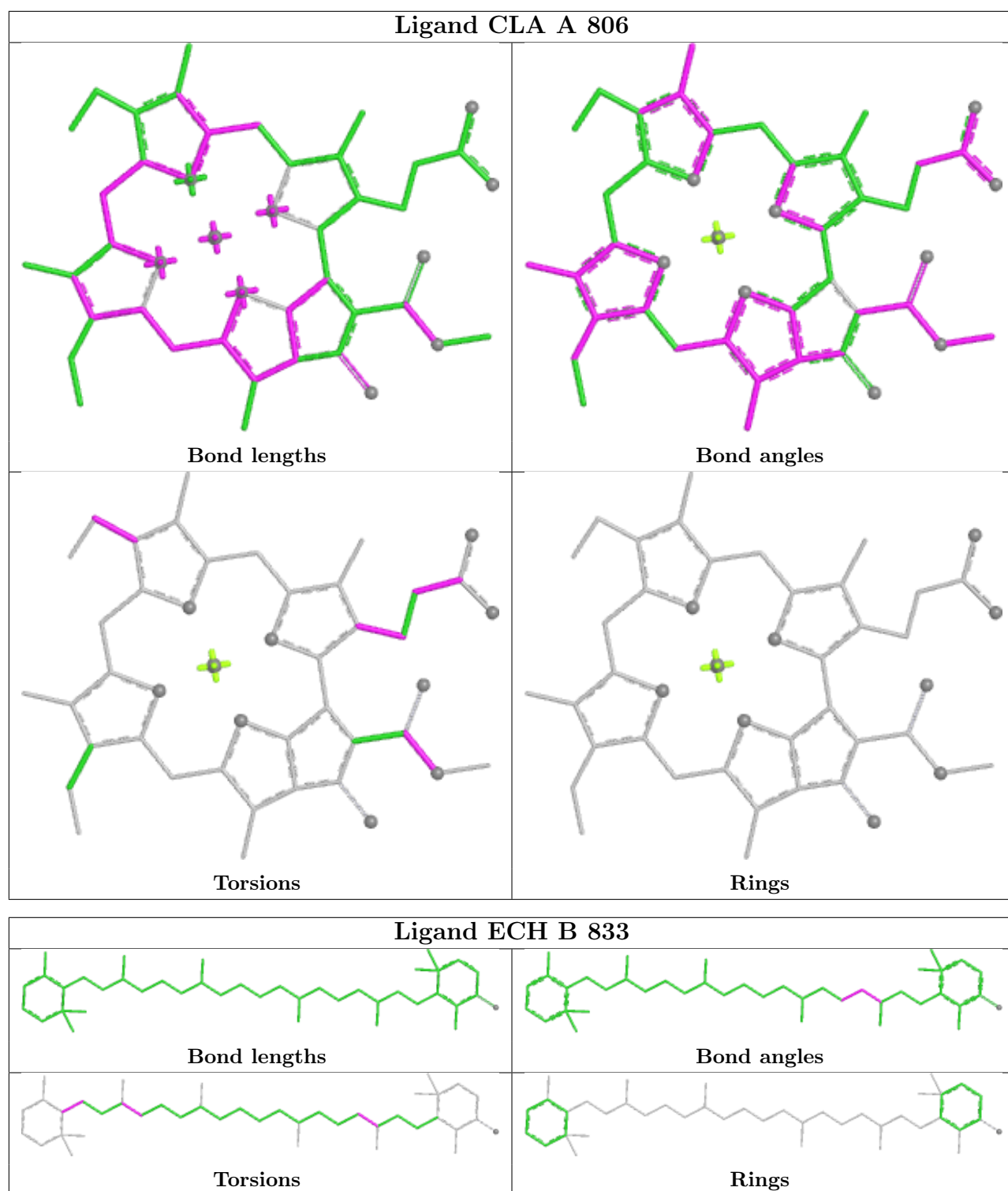
Ligand CLA J 103



Ligand 45D A 856







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

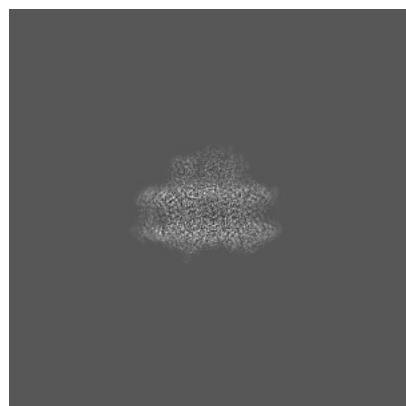
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73077. These allow visual inspection of the internal detail of the map and identification of artifacts.

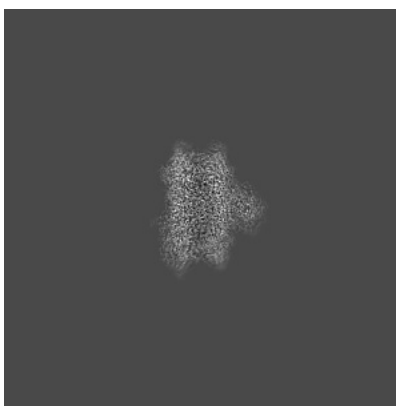
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

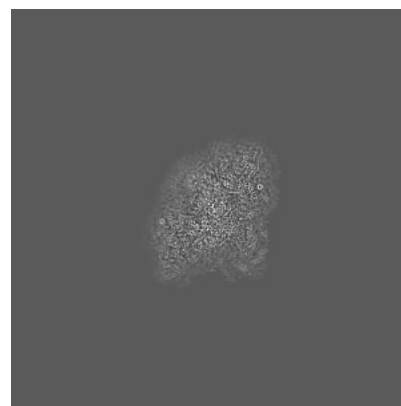
6.1.1 Primary map



X

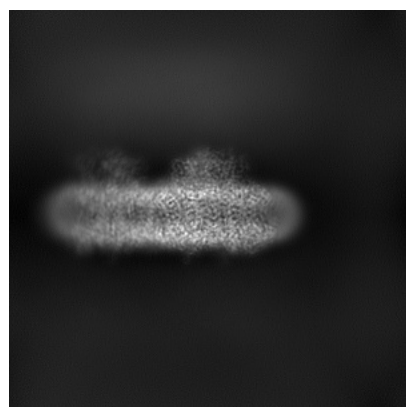


Y

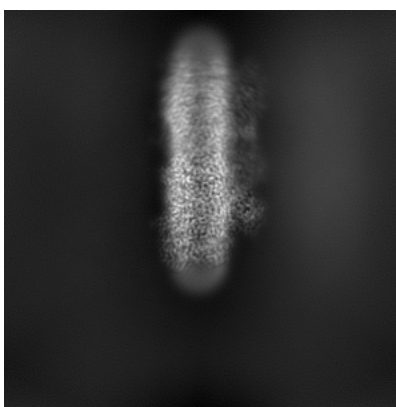


Z

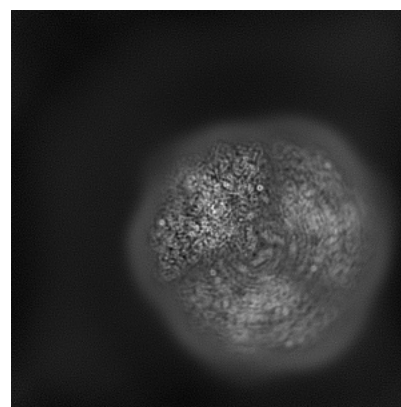
6.1.2 Raw map



X



Y

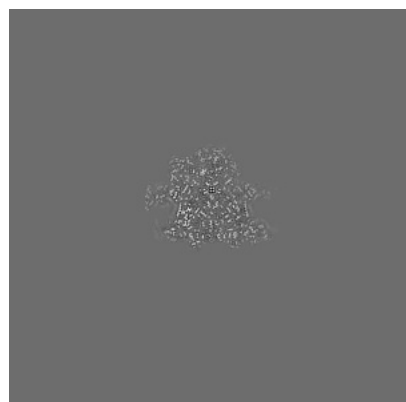


Z

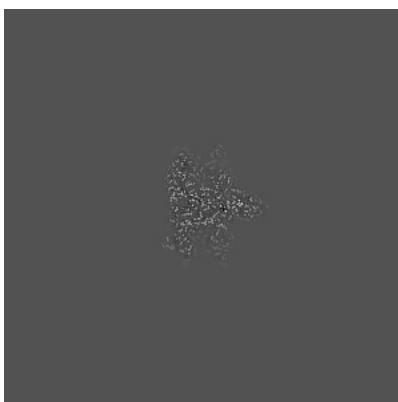
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 210

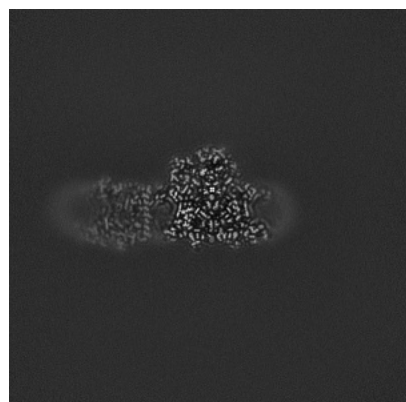


Y Index: 210

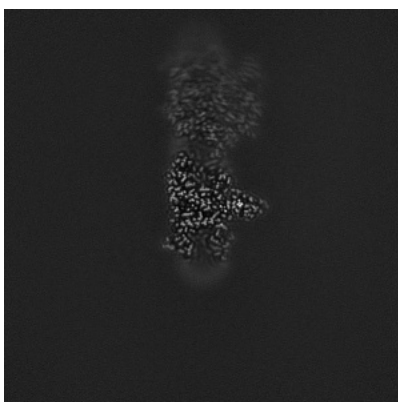


Z Index: 210

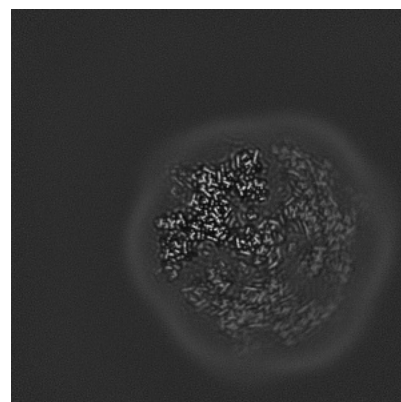
6.2.2 Raw map



X Index: 210



Y Index: 210

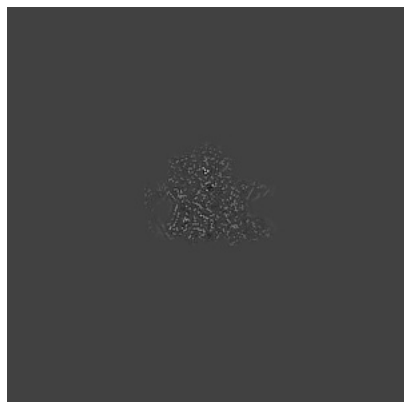


Z Index: 210

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: 213

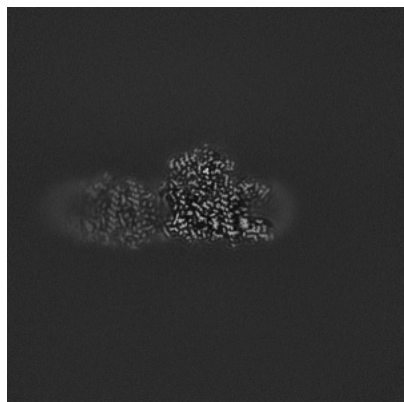


Y Index: 188

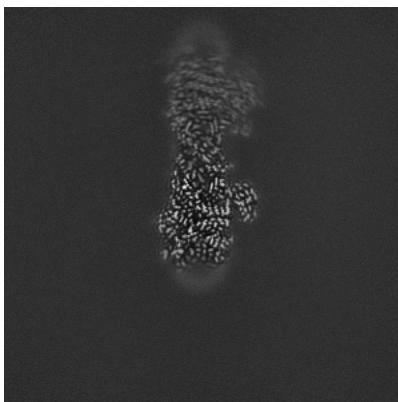


Z Index: 191

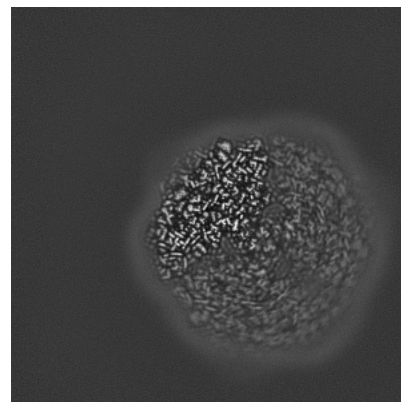
6.3.2 Raw map



X Index: 215



Y Index: 191

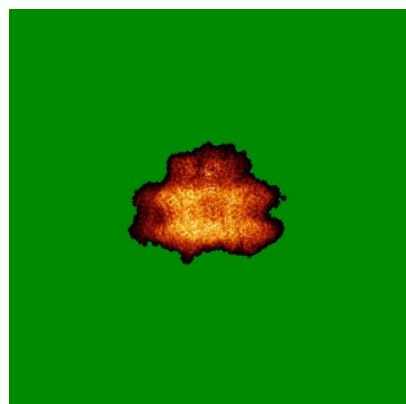


Z Index: 191

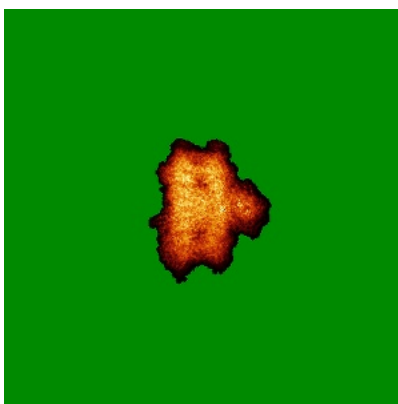
The images above show the largest variance slices of the map in three orthogonal directions.

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

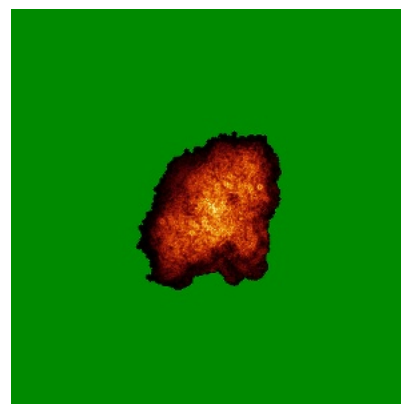
6.4.1 Primary map



X

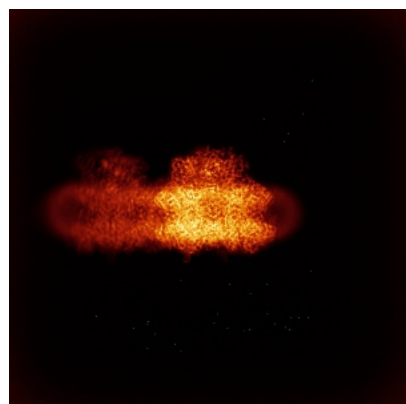


Y

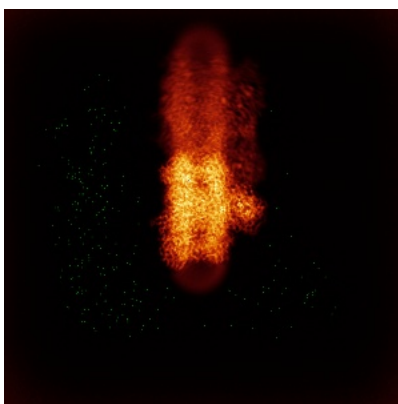


Z

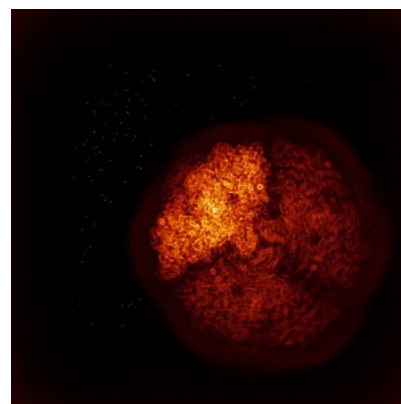
6.4.2 Raw map



X



Y

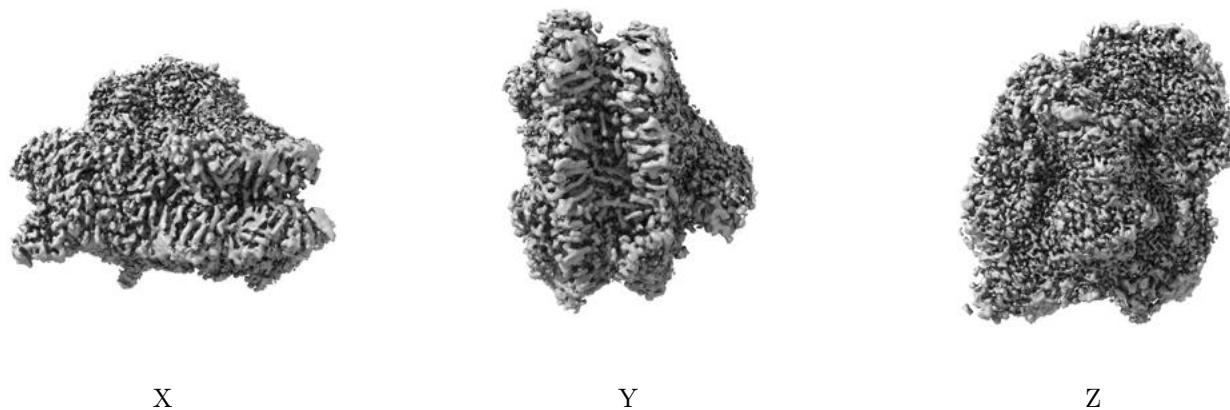


Z

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

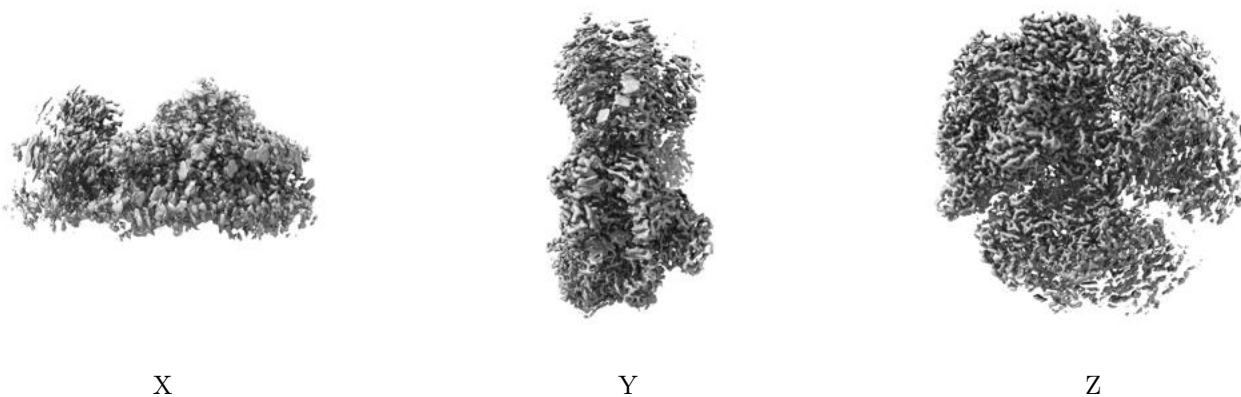
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0353. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

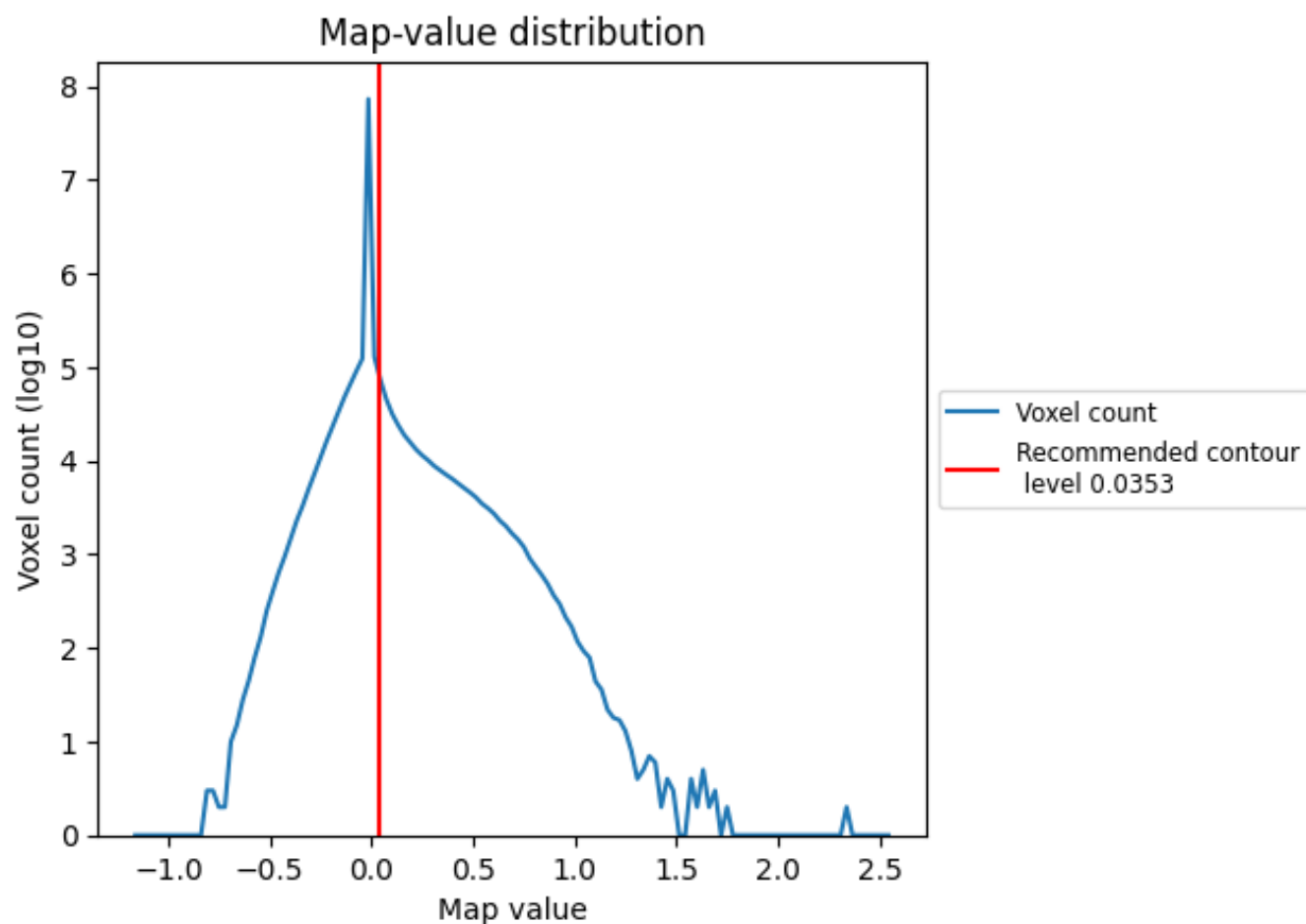
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

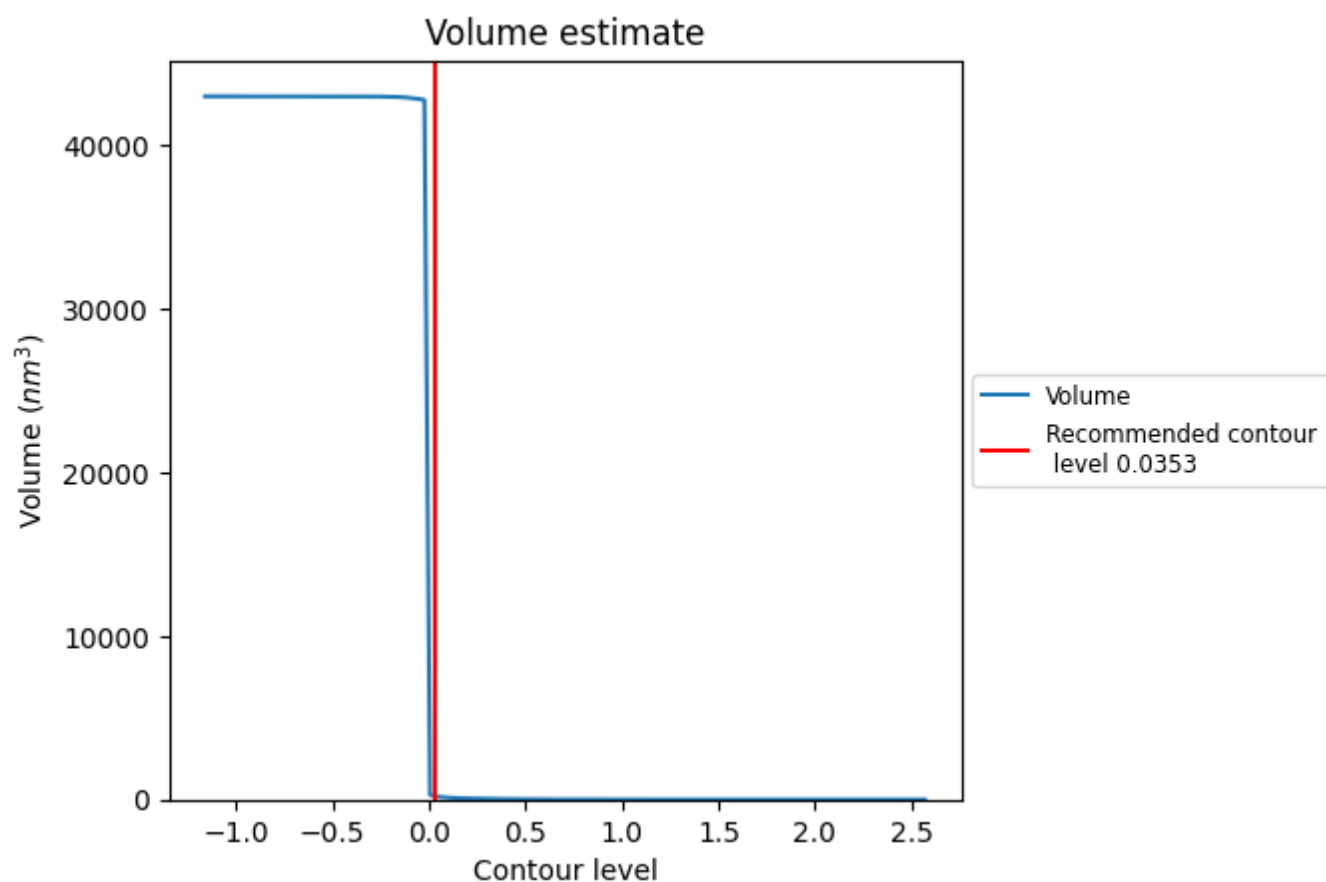
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

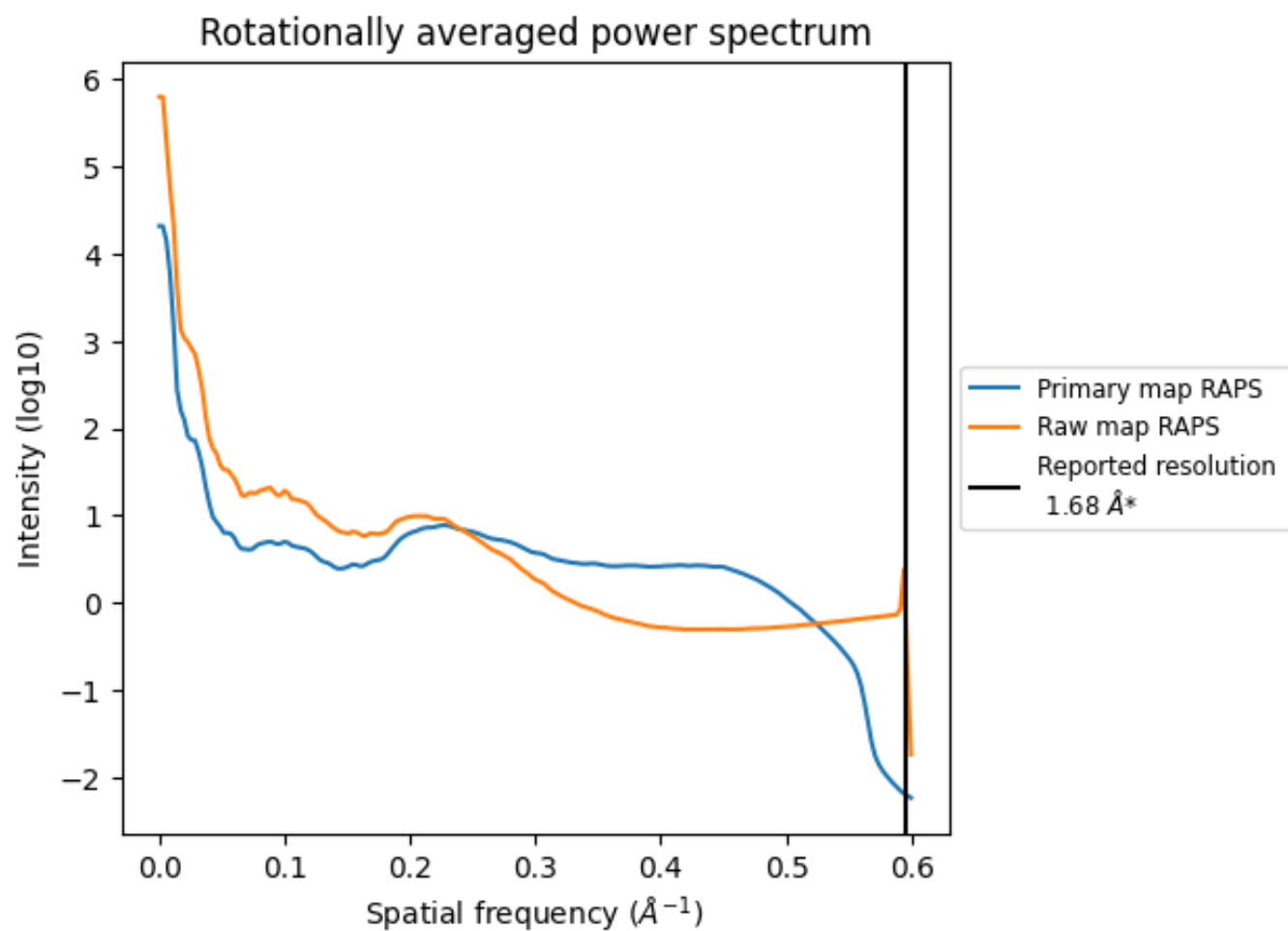
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 203 nm³; this corresponds to an approximate mass of 183 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

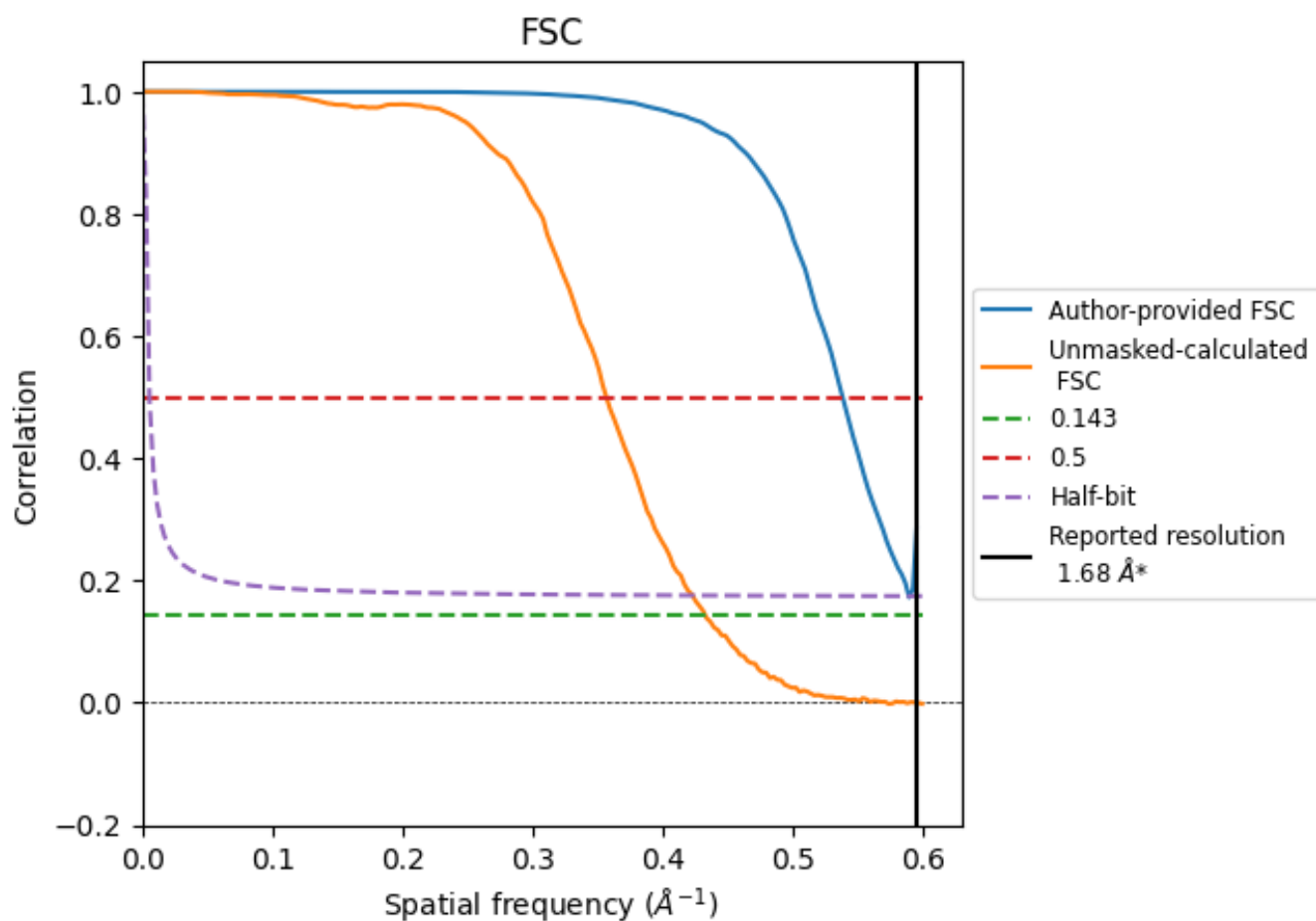


*Reported resolution corresponds to spatial frequency of 0.595 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.595 Å⁻¹

8.2 Resolution estimates [i](#)

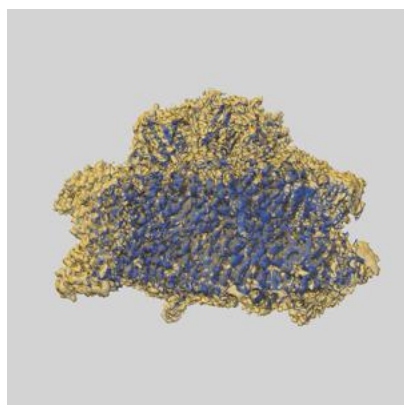
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.68	-	-
Author-provided FSC curve	-	1.86	1.70
Unmasked-calculated*	2.31	2.80	2.36

*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 2.31 differs from the reported value 1.68 by more than 10 %

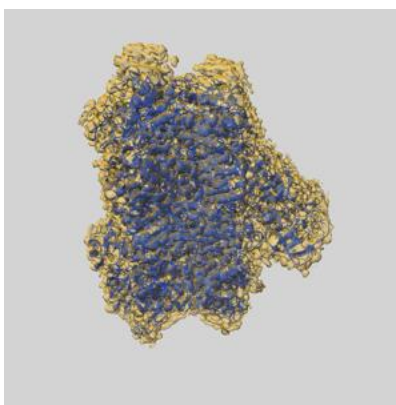
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-73077 and PDB model 9YL7. Per-residue inclusion information can be found in section [3](#) on page [20](#).

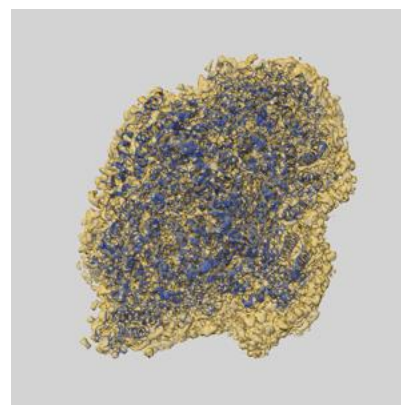
9.1 Map-model overlay [i](#)



X



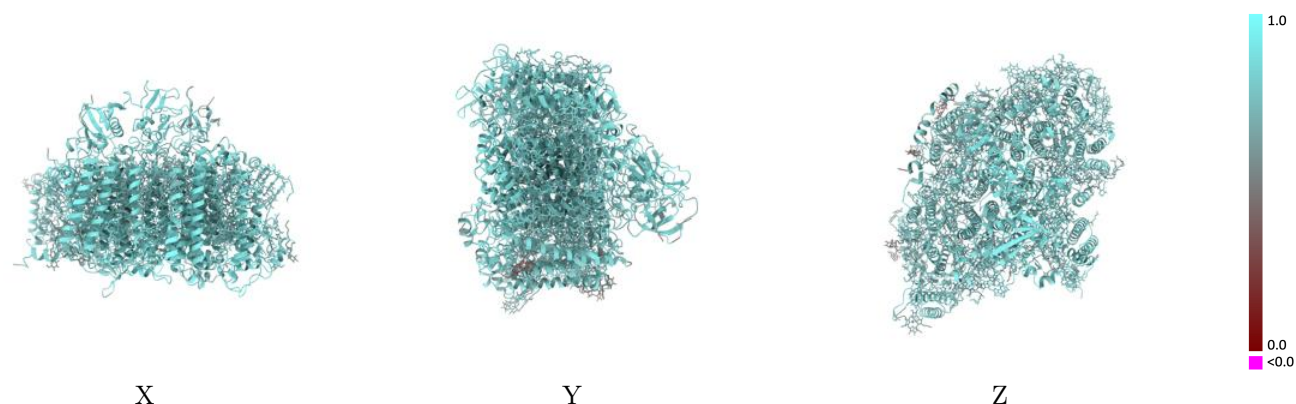
Y



Z

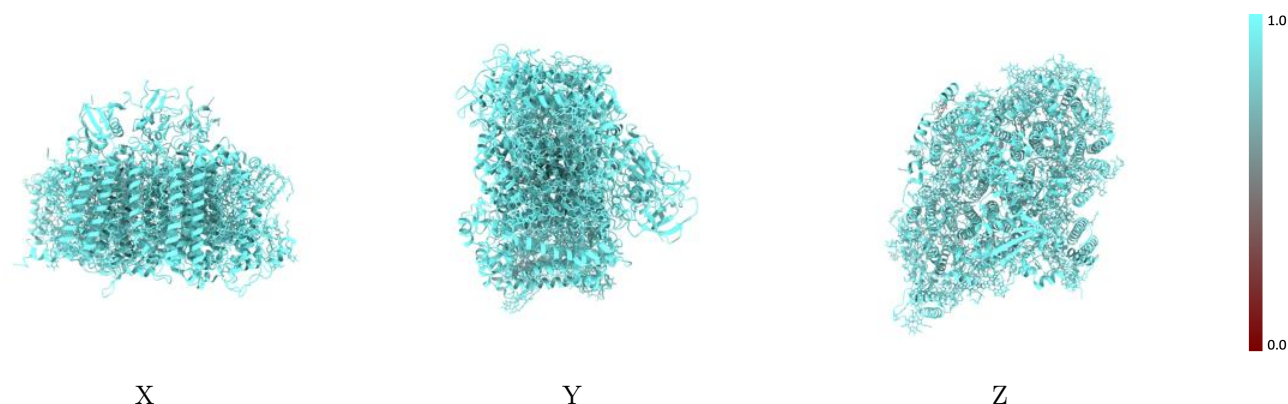
The images above show the 3D surface view of the map at the recommended contour level 0.0353 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



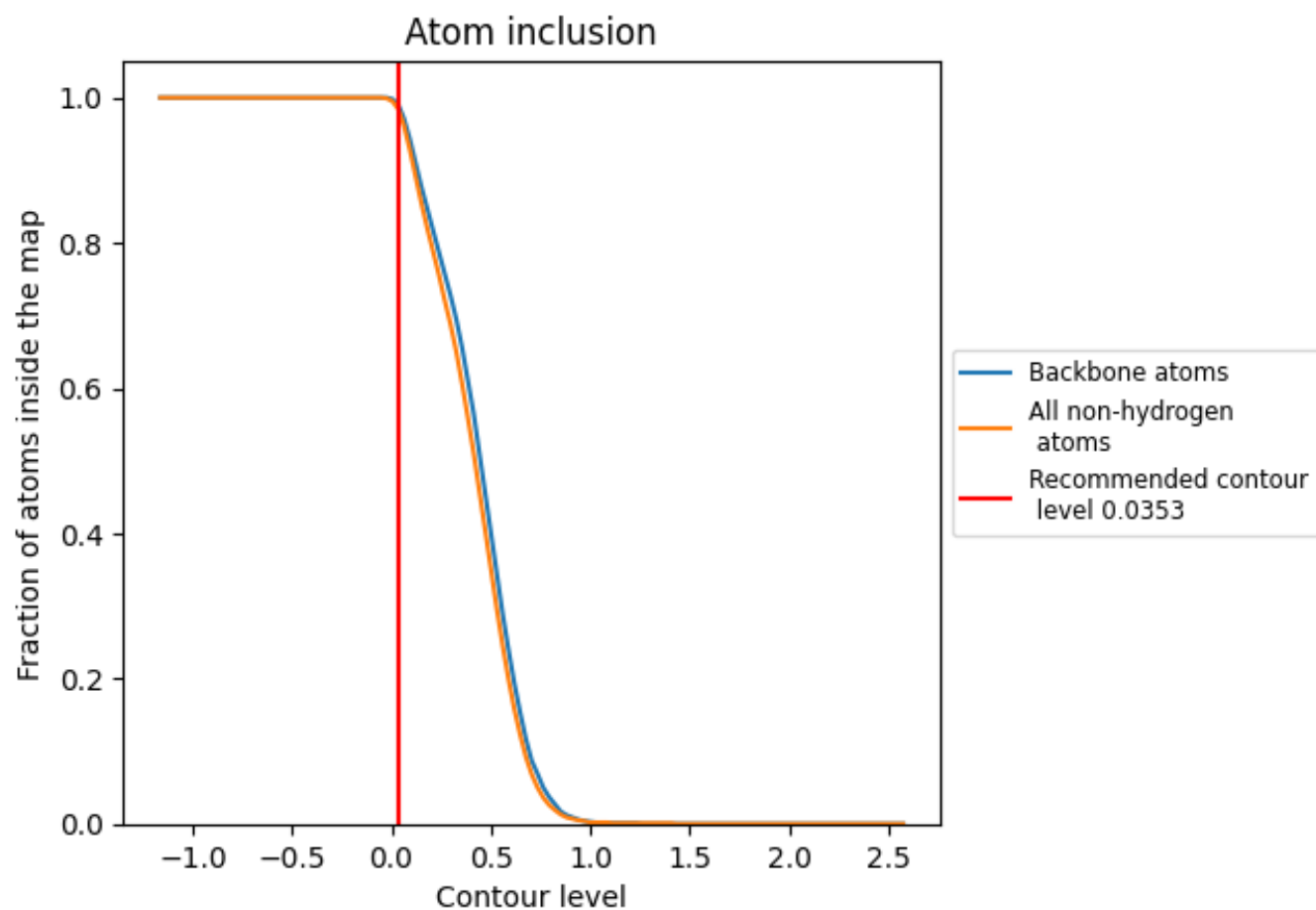
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0353).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 98% 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 (0.0353) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9840	0.7910
A	0.9880	0.8000
B	0.9900	0.8060
C	0.9970	0.8320
D	0.9870	0.7960
E	0.9580	0.7350
F	0.9690	0.7330
I	0.9970	0.8220
J	0.9020	0.6570
K	0.9800	0.7450
L	0.9820	0.7830
M	0.9810	0.7560

1.0

0.0

<0.0