Full wwPDB EM Validation Report

Sep 30, 2026 – 06:44 PM JST

PDB ID	:	6KMX / pdb_00006kmx
EMDB ID	:	EMD-0727
Title	:	Structure of PSI from H. hongdechloris grown under far-red light condition
Authors	:	Kato, K.; Nagao, R.; Shen, J.R.; Miyazaki, N.; Akita, F.
Deposited on	:	2019-08-01
Resolution	:	2.41 Å(reported)
Based on initial model	:	1JB0

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

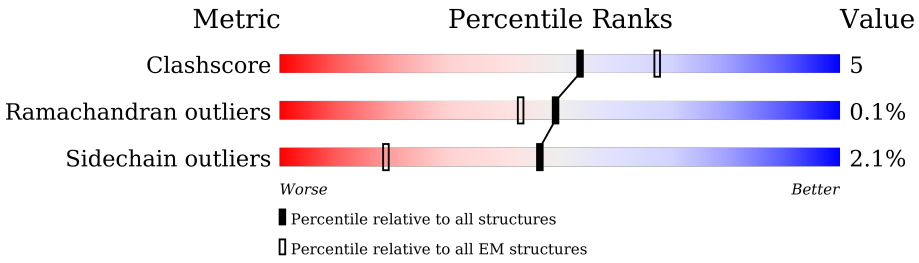
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

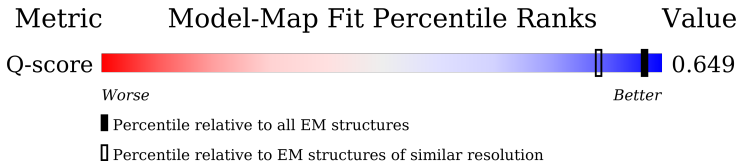
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.41 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	5662 (1.92 - 2.91)

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 <=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	aA	784	8% 81% 10% • 9%
1	bA	784	8% 81% 10% • 9%
1	cA	784	8% 81% 10% • 9%
2	aB	743	13% 86% 11% •

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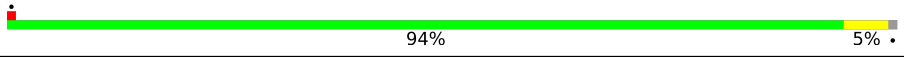
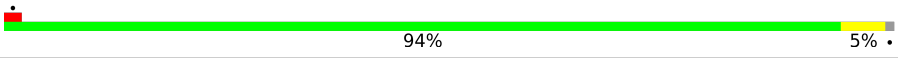
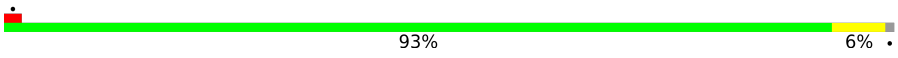
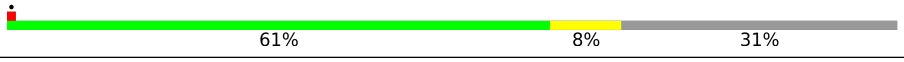
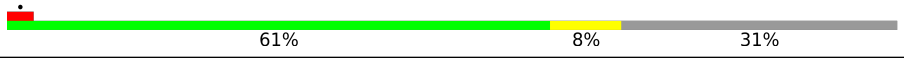
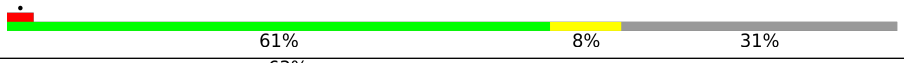
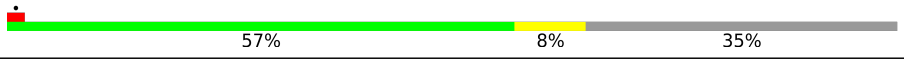
Mol	Chain	Length	Quality of chain
2	bB	743	
2	cB	743	
3	aC	81	
3	bC	81	
3	cC	81	
4	aD	142	
4	bD	142	
4	cD	142	
5	aE	68	
5	bE	68	
5	cE	68	
6	aI	63	
6	bI	63	
6	cI	63	
7	aK	96	
7	bK	96	
7	cK	96	
8	aL	189	
8	bL	189	
8	cL	189	
9	aM	31	
9	bM	31	
9	cM	31	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	F6C	aA	826	X	-	-	-
12	F6C	aA	827	X	-	-	-
12	F6C	aA	830	X	-	-	-
12	F6C	aA	832	X	-	-	-
12	F6C	aA	844	X	-	-	-
12	F6C	aB	824	X	-	-	-
12	F6C	aL	202	X	-	-	-
12	F6C	bA	826	X	-	-	-
12	F6C	bA	827	X	-	-	-
12	F6C	bA	830	X	-	-	-
12	F6C	bA	832	X	-	-	-
12	F6C	bA	844	X	-	-	-
12	F6C	bB	824	X	-	-	-
12	F6C	bL	202	X	-	-	-
12	F6C	cA	826	X	-	-	-
12	F6C	cA	827	X	-	-	-
12	F6C	cA	830	X	-	-	-
12	F6C	cA	832	X	-	-	-
12	F6C	cA	844	X	-	-	-
12	F6C	cB	824	X	-	-	-
12	F6C	cL	202	X	-	-	-

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 65112 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	aA	717	Total	C	N	O	S	0	0
			5669	3724	966	950	29		
1	bA	717	Total	C	N	O	S	0	0
			5669	3724	966	950	29		
1	cA	717	Total	C	N	O	S	0	0
			5669	3724	966	950	29		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	aB	727	Total	C	N	O	S	0	0
			5783	3786	976	996	25		
2	bB	727	Total	C	N	O	S	0	0
			5783	3786	976	996	25		
2	cB	727	Total	C	N	O	S	0	0
			5783	3786	976	996	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	aC	80	Total	C	N	O	S	0	0
			596	366	102	117	11		
3	bC	80	Total	C	N	O	S	0	0
			596	366	102	117	11		
3	cC	80	Total	C	N	O	S	0	0
			596	366	102	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	aD	98	Total	C	N	O	S	0	0
			768	492	130	143	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	bD	98	Total	C	N	O	S	0	0
			768	492	130	143	3		
4	cD	98	Total	C	N	O	S	0	0
			768	492	130	143	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	aE	61	Total	C	N	O	0	0
			499	317	87	95		
5	bE	61	Total	C	N	O	0	0
			499	317	87	95		
5	cE	61	Total	C	N	O	0	0
			499	317	87	95		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	aI	41	Total	C	N	O	S	0	0
			349	247	48	52	2		
6	bI	41	Total	C	N	O	S	0	0
			349	247	48	52	2		
6	cI	41	Total	C	N	O	S	0	0
			349	247	48	52	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	aK	46	Total	C	N	O	S	0	0
			317	206	55	54	2		
7	bK	46	Total	C	N	O	S	0	0
			317	206	55	54	2		
7	cK	46	Total	C	N	O	S	0	0
			317	206	55	54	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	aL	172	Total	C	N	O	S	0	0
			1303	838	223	239	3		
8	bL	172	Total	C	N	O	S	0	0
			1303	838	223	239	3		

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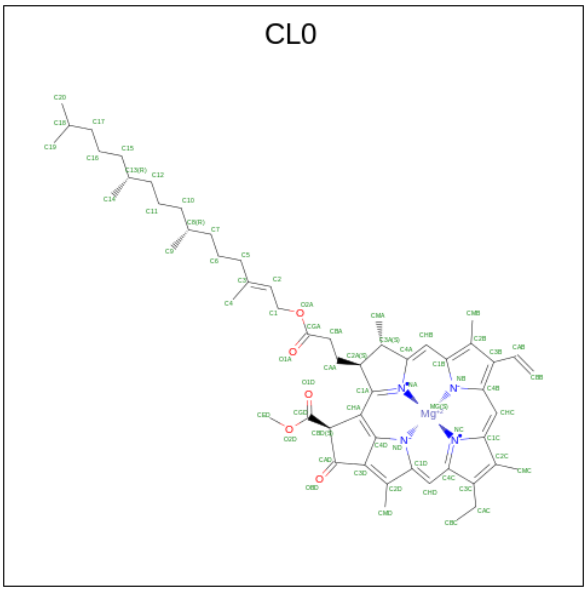
Mol	Chain	Residues	Atoms					AltConf	Trace
8	cL	172	Total	C	N	O	S	0	0
			1303	838	223	239	3		

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

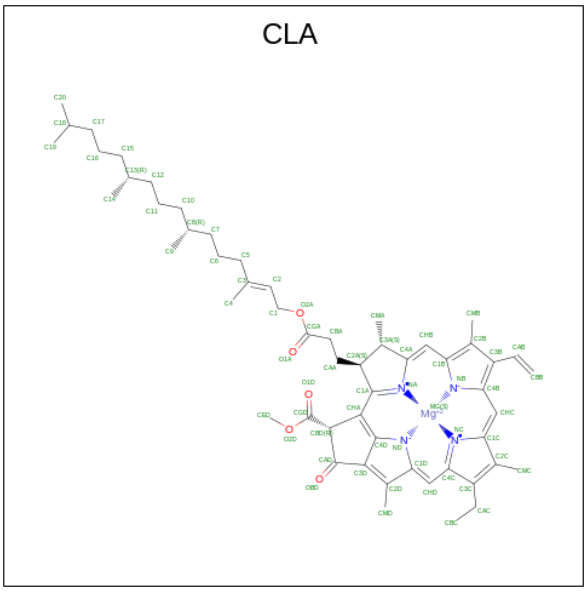
Mol	Chain	Residues	Atoms					AltConf	Trace
9	aM	31	Total	C	N	O	S	0	0
			241	162	36	42	1		
9	bM	31	Total	C	N	O	S	0	0
			241	162	36	42	1		
9	cM	31	Total	C	N	O	S	0	0
			241	162	36	42	1		

- Molecule 10 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
10	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 11 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
11	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
11	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
11	aA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
11	aB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
11	aK	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
11	aK	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	aL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	aL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
11	bA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
11	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
11	bA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
11	bB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	bK	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
11	bK	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
11	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
11	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
11	cB	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
11	cB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	cK	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
11	cK	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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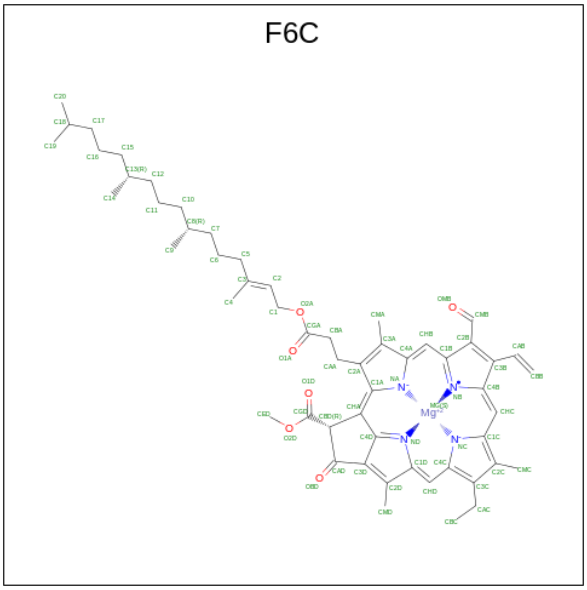
Mol	Chain	Residues	Atoms					AltConf
11	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 12 is Chlorophyll F (CCD ID: F6C) (formula: $C_{55}H_{68}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
12	aA	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
12	aA	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
12	aA	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
12	aA	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
12	aA	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
12	aB	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
12	aL	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
12	bA	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
12	bA	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
12	bA	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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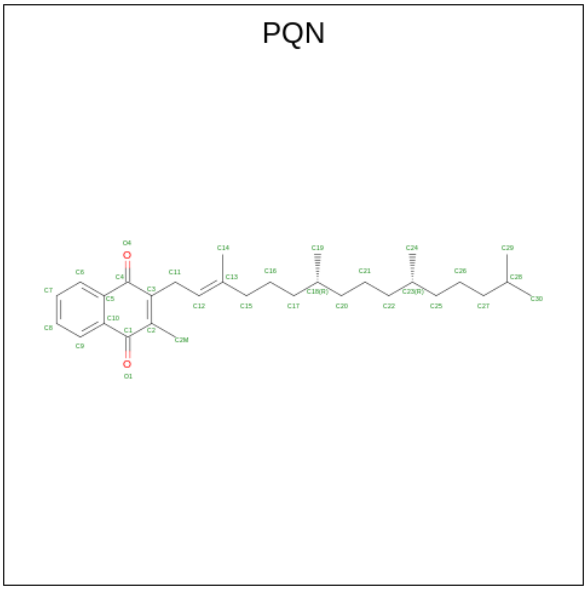
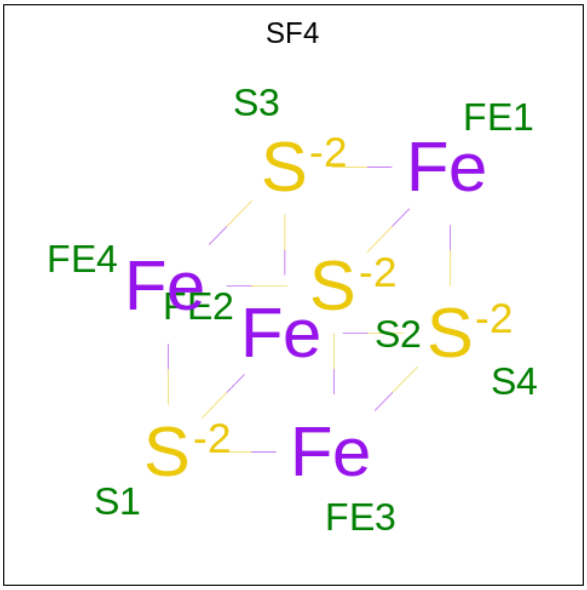
Mol	Chain	Residues	Atoms					AltConf
12	bA	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
12	bA	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
12	bB	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
12	bL	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
12	cA	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
12	cA	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
12	cA	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
12	cA	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
12	cA	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
12	cB	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
12	cL	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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



Mol	Chain	Residues	Atoms	AltConf
13	aA	1	Total C O 33 31 2	0
13	aB	1	Total C O 28 26 2	0
13	bA	1	Total C O 33 31 2	0
13	bB	1	Total C O 28 26 2	0
13	cA	1	Total C O 33 31 2	0
13	cB	1	Total C O 28 26 2	0

- Molecule 14 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
14	aA	1	Total Fe S 8 4 4	0
14	aC	1	Total Fe S 8 4 4	0
14	aC	1	Total Fe S 8 4 4	0
14	bA	1	Total Fe S 8 4 4	0
14	bC	1	Total Fe S 8 4 4	0
14	bC	1	Total Fe S 8 4 4	0

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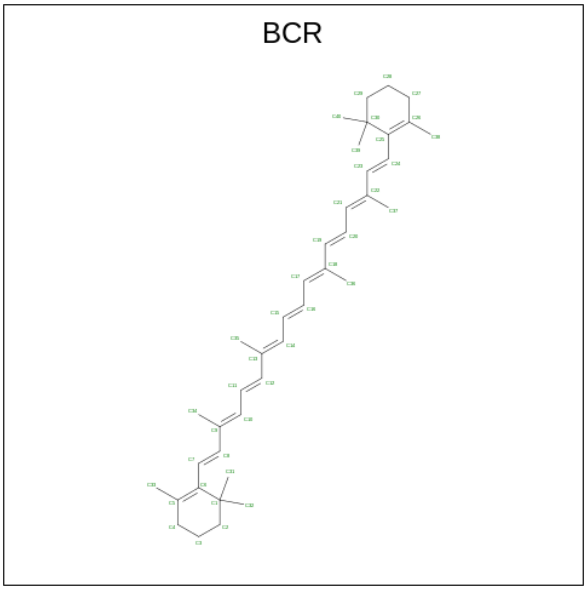
Mol	Chain	Residues	Atoms	AltConf
14	cA	1	Total Fe S 8 4 4	0
14	cC	1	Total Fe S 8 4 4	0
14	cC	1	Total Fe S 8 4 4	0

- Molecule 15 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
15	aA	1	Total C 40 40	0
15	aA	1	Total C 40 40	0
15	aA	1	Total C 40 40	0
15	aA	1	Total C 40 40	0
15	aA	1	Total C 40 40	0
15	aB	1	Total C 40 40	0
15	aB	1	Total C 40 40	0
15	aB	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
15	aB	1	Total C 40 40	0
15	aB	1	Total C 40 40	0
15	aB	1	Total C 40 40	0
15	aI	1	Total C 40 40	0
15	aK	1	Total C 40 40	0
15	aL	1	Total C 40 40	0
15	aL	1	Total C 40 40	0
15	aL	1	Total C 40 40	0
15	aM	1	Total C 40 40	0
15	bA	1	Total C 40 40	0
15	bA	1	Total C 40 40	0
15	bA	1	Total C 40 40	0
15	bA	1	Total C 40 40	0
15	bA	1	Total C 40 40	0
15	bB	1	Total C 40 40	0
15	bB	1	Total C 40 40	0
15	bB	1	Total C 40 40	0
15	bB	1	Total C 40 40	0
15	bB	1	Total C 40 40	0
15	bB	1	Total C 40 40	0
15	bI	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
15	bK	1	Total C 40 40	0
15	bL	1	Total C 40 40	0
15	bL	1	Total C 40 40	0
15	bL	1	Total C 40 40	0
15	bM	1	Total C 40 40	0
15	cA	1	Total C 40 40	0
15	cA	1	Total C 40 40	0
15	cA	1	Total C 40 40	0
15	cA	1	Total C 40 40	0
15	cA	1	Total C 40 40	0
15	cB	1	Total C 40 40	0
15	cB	1	Total C 40 40	0
15	cB	1	Total C 40 40	0
15	cB	1	Total C 40 40	0
15	cB	1	Total C 40 40	0
15	cB	1	Total C 40 40	0
15	cI	1	Total C 40 40	0
15	cK	1	Total C 40 40	0
15	cL	1	Total C 40 40	0
15	cL	1	Total C 40 40	0
15	cL	1	Total C 40 40	0

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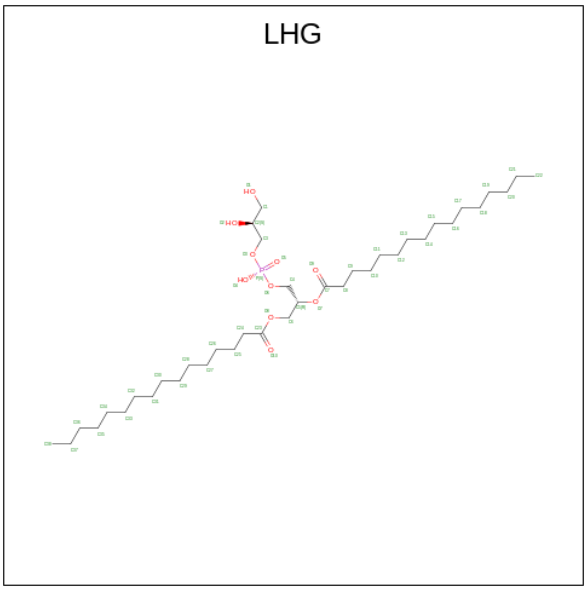
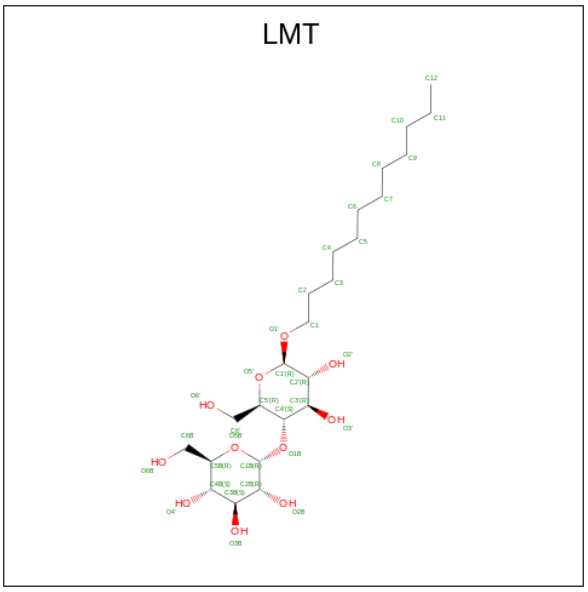
Mol	Chain	Residues	Atoms	AltConf
15	cM	1	Total C 40 40	0

- Molecule 16 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



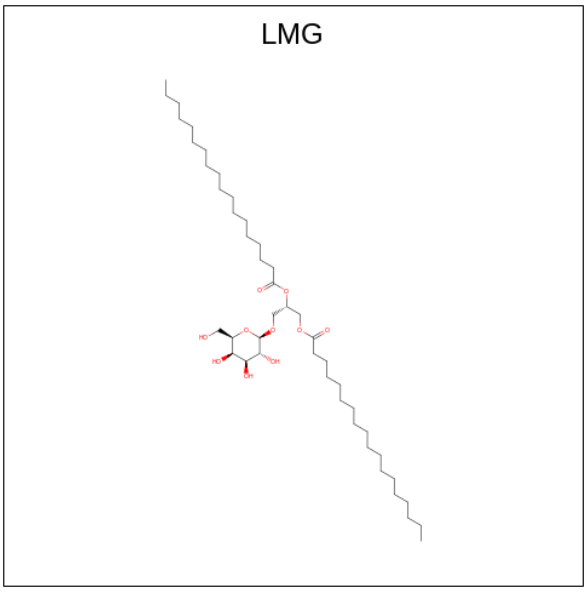
Mol	Chain	Residues	Atoms	AltConf
16	aA	1	Total C O P 49 38 10 1	0
16	bA	1	Total C O P 49 38 10 1	0
16	cA	1	Total C O P 49 38 10 1	0

- Molecule 17 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
17	aA	1	Total	C	O	0
			35	24	11	
17	bA	1	Total	C	O	0
			35	24	11	
17	cA	1	Total	C	O	0
			35	24	11	

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	AltConf
18	aB	1	Total C O 46 36 10	0
18	bB	1	Total C O 46 36 10	0
18	cB	1	Total C O 46 36 10	0

- Molecule 19 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms	AltConf
19	aI	1	Total C 9 9	0
19	aL	4	Total C O 56 52 4	0
19	bI	1	Total C 9 9	0
19	bL	4	Total C O 56 52 4	0
19	cI	2	Total C O 25 23 2	0
19	cL	3	Total C O 40 38 2	0

- Molecule 20 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
20	aL	1	Total Ca 1 1	0
20	bL	1	Total Ca 1 1	0
20	cL	1	Total Ca 1 1	0

- Molecule 21 is water.

Mol	Chain	Residues	Atoms	AltConf
21	aA	72	Total O 72 72	0
21	aB	72	Total O 72 72	0
21	aC	21	Total O 21 21	0

Continued on next page...

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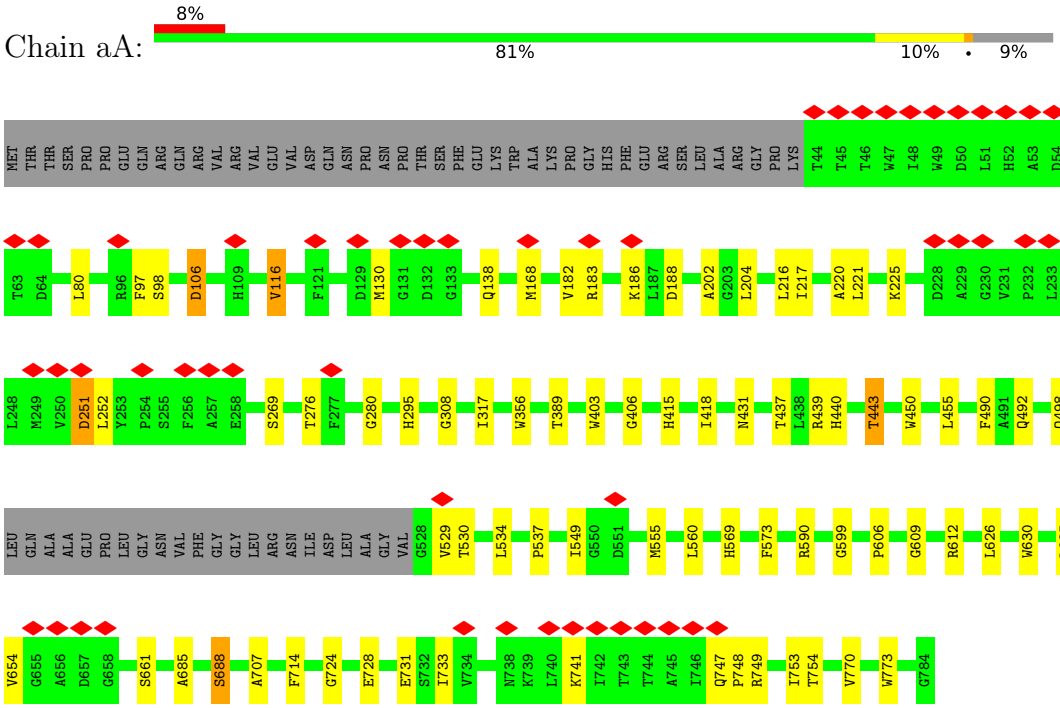
Mol	Chain	Residues	Atoms	AltConf
21	aD	15	Total O 15 15	0
21	aI	5	Total O 5 5	0
21	aK	1	Total O 1 1	0
21	aL	25	Total O 25 25	0
21	aM	1	Total O 1 1	0
21	bA	72	Total O 72 72	0
21	bB	72	Total O 72 72	0
21	bC	20	Total O 20 20	0
21	bD	16	Total O 16 16	0
21	bI	6	Total O 6 6	0
21	bK	1	Total O 1 1	0
21	bL	24	Total O 24 24	0
21	bM	1	Total O 1 1	0
21	cA	72	Total O 72 72	0
21	cB	72	Total O 72 72	0
21	cC	21	Total O 21 21	0
21	cD	15	Total O 15 15	0
21	cI	6	Total O 6 6	0
21	cK	1	Total O 1 1	0
21	cL	24	Total O 24 24	0
21	cM	1	Total O 1 1	0

3 Residue-property plots (i)

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.

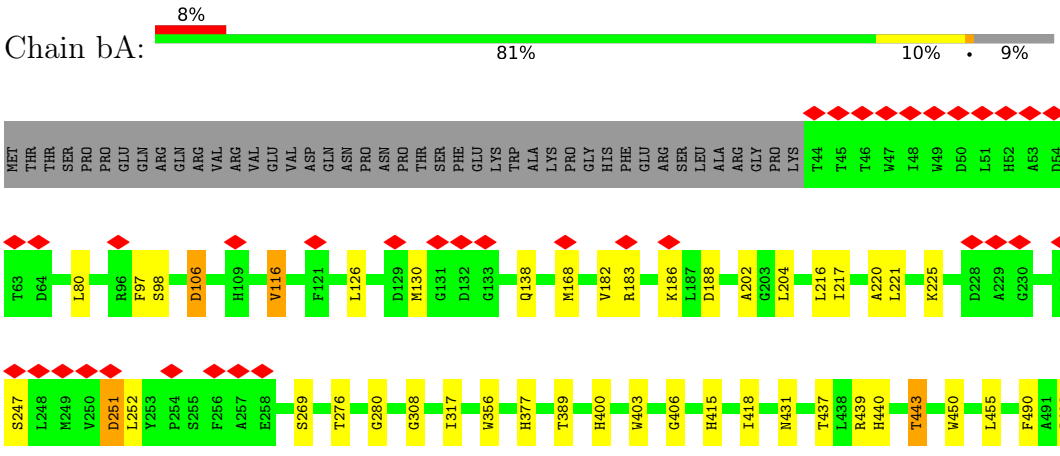
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

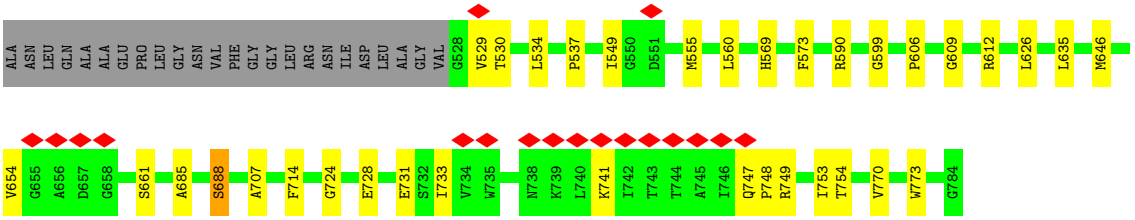
Chain aA:



• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain bA:

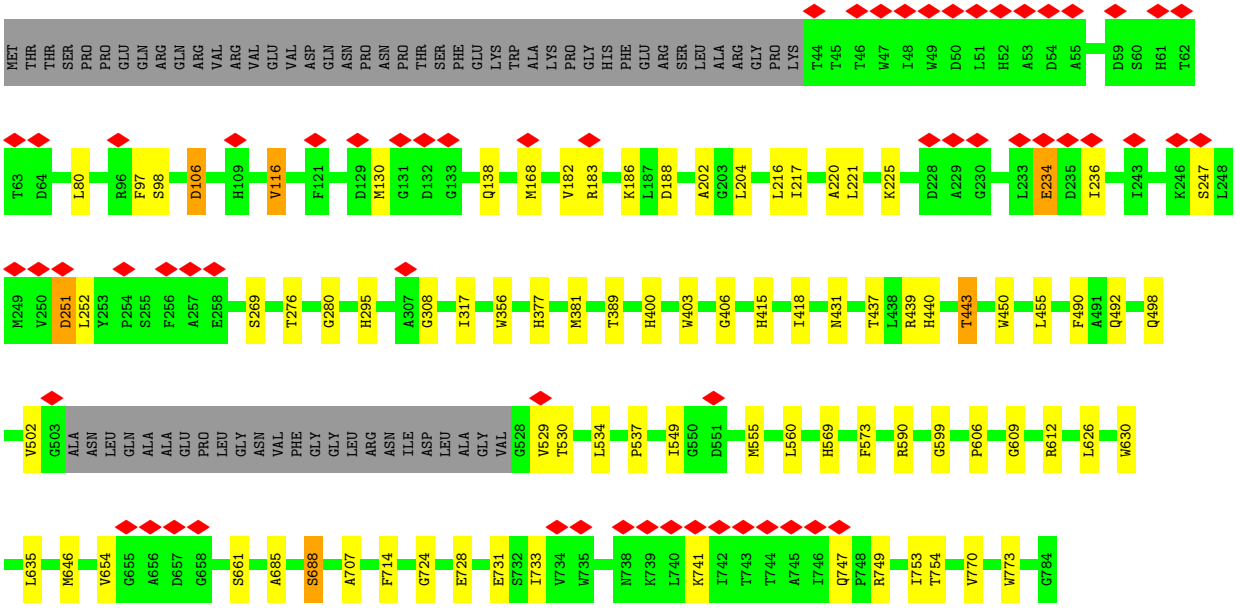




• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain cA:

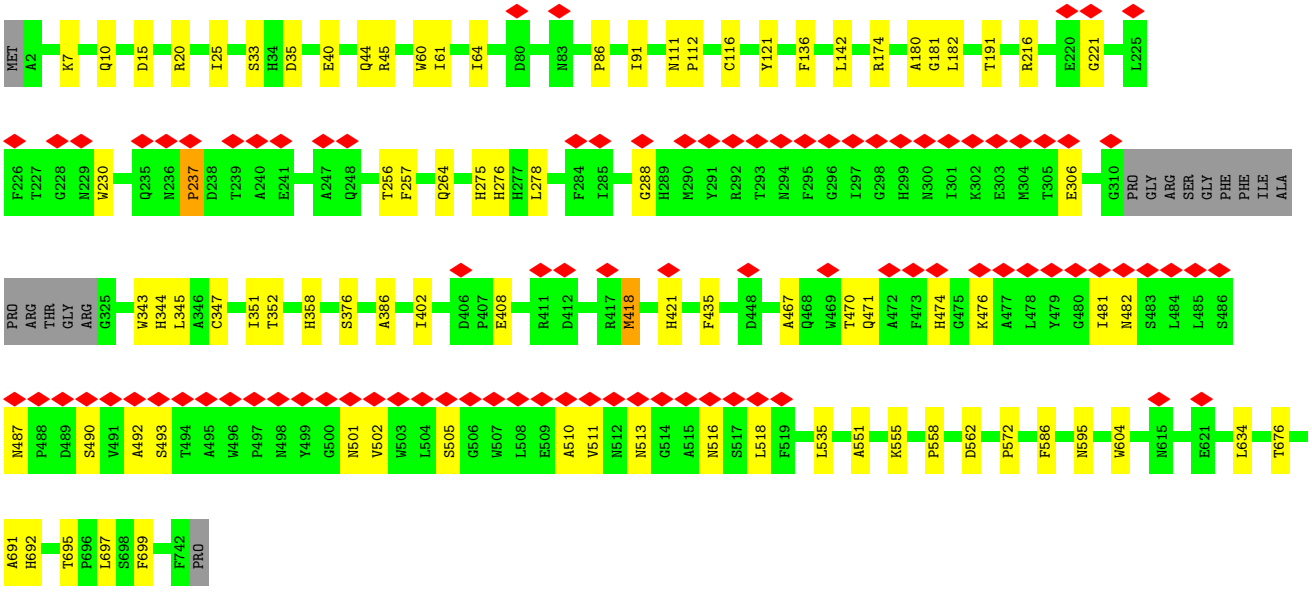




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

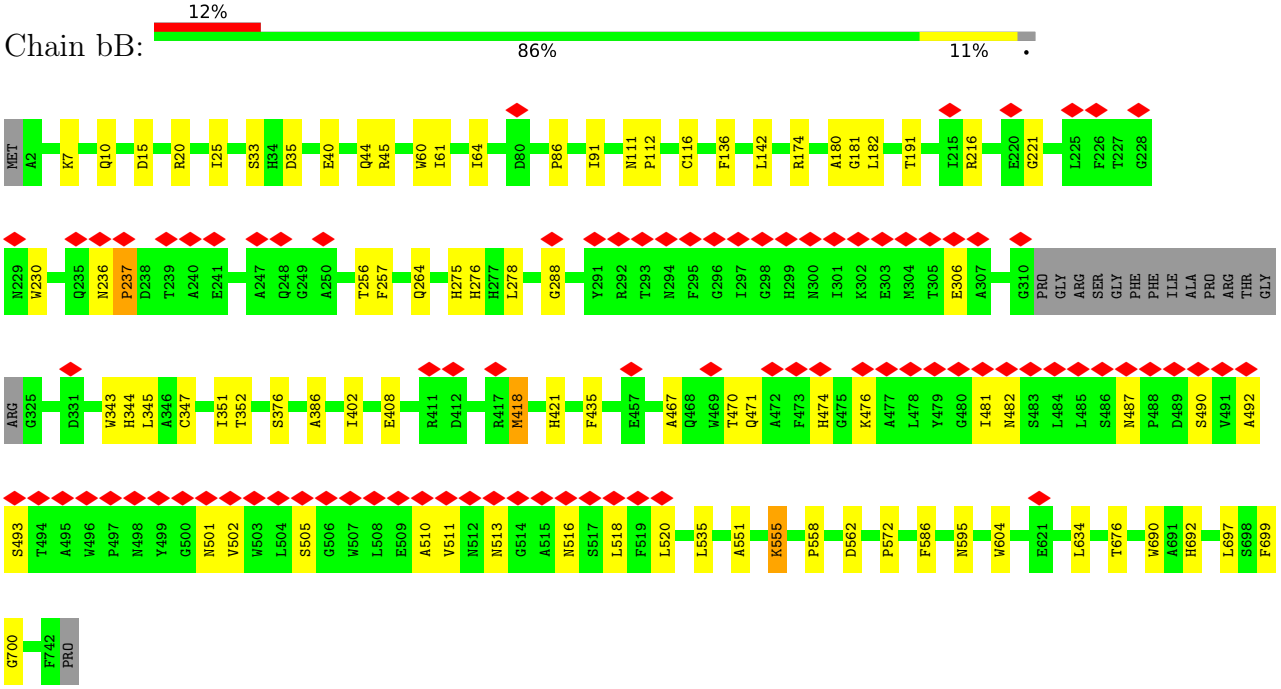
Chain aB:





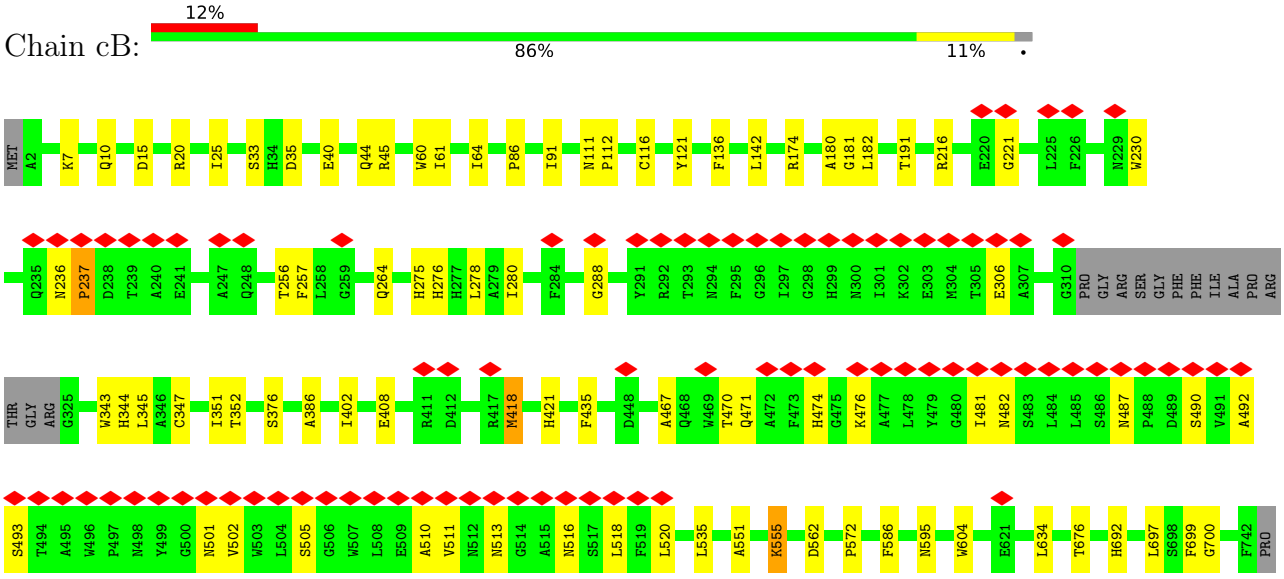
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain bB:



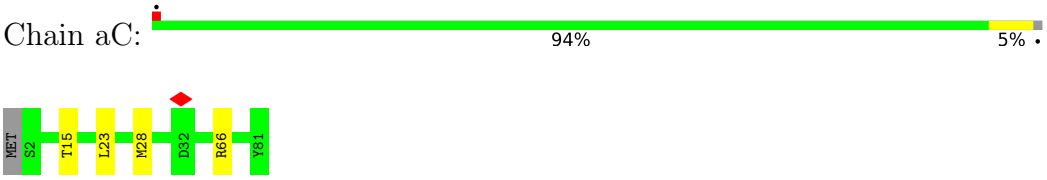
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain cB:



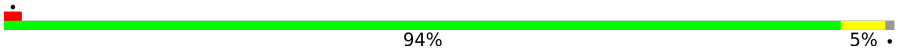
• Molecule 3: Photosystem I iron-sulfur center

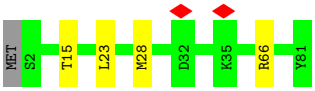
Chain aC:



• Molecule 3: Photosystem I iron-sulfur center

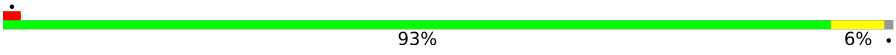
Chain bC:

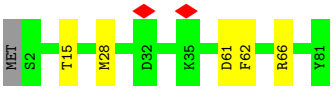




• Molecule 3: Photosystem I iron-sulfur center

Chain cC:

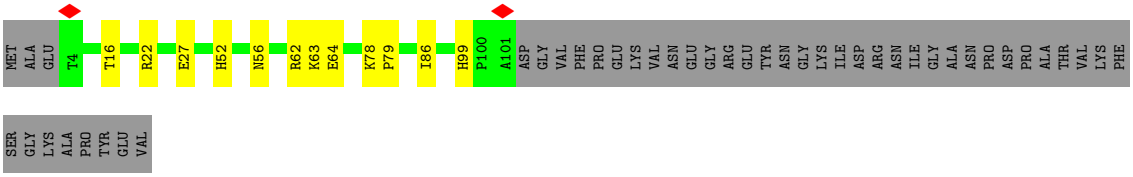




• Molecule 4: Photosystem I reaction center subunit II

Chain aD:

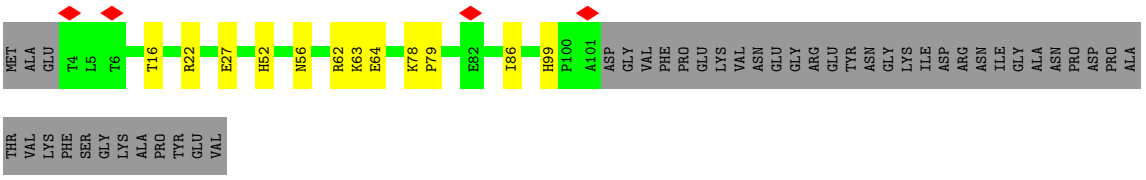




• Molecule 4: Photosystem I reaction center subunit II

Chain bD:

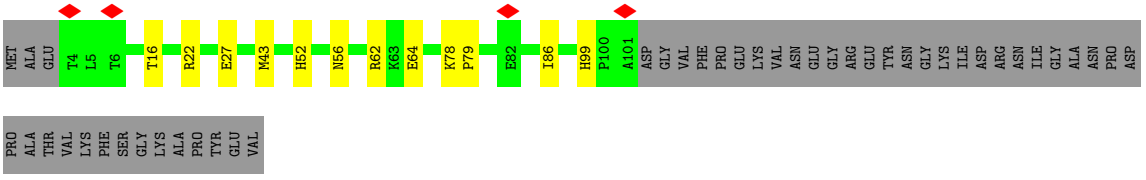




• Molecule 4: Photosystem I reaction center subunit II

Chain cD:

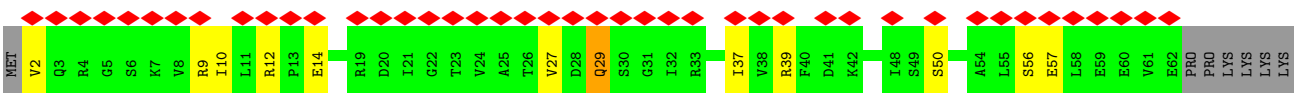




• Molecule 5: Photosystem I reaction center subunit IV

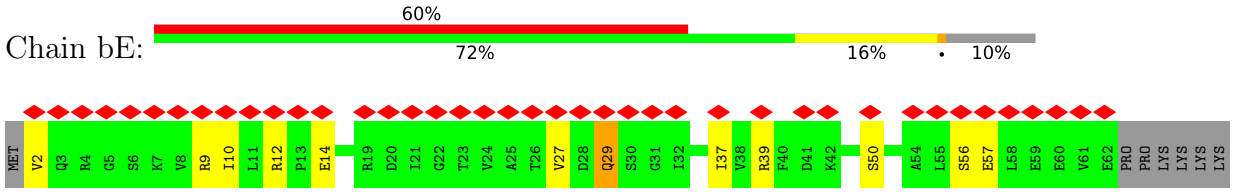
Chain aE:





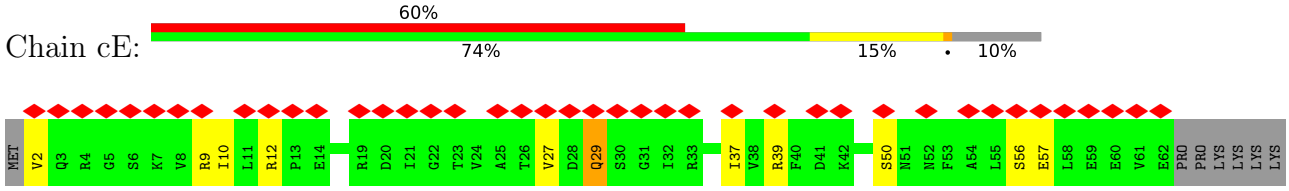
• Molecule 5: Photosystem I reaction center subunit IV

Chain bE:



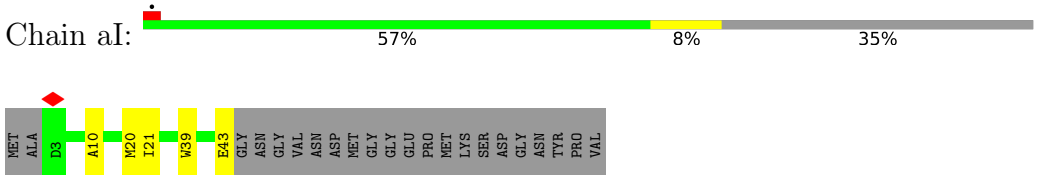
• Molecule 5: Photosystem I reaction center subunit IV

Chain cE:



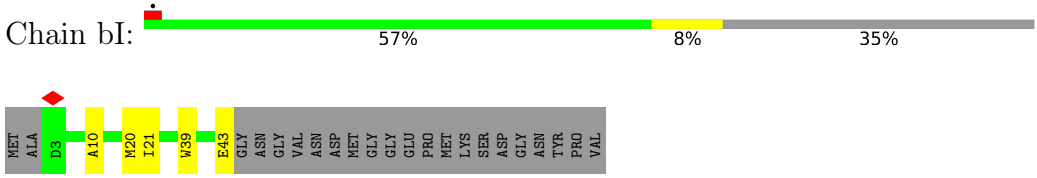
• Molecule 6: Photosystem I reaction center subunit VIII

Chain aI:



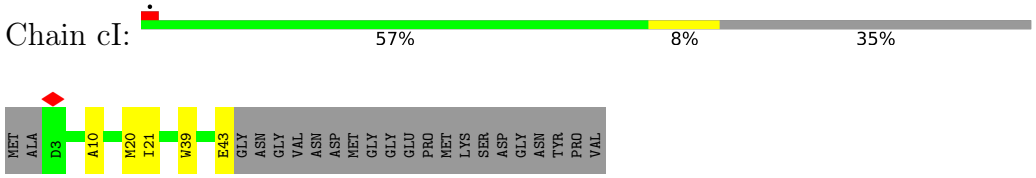
• Molecule 6: Photosystem I reaction center subunit VIII

Chain bI:



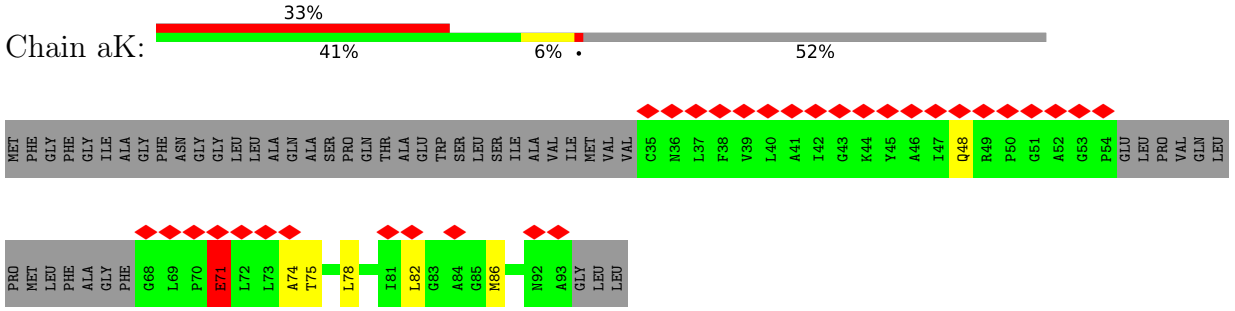
• Molecule 6: Photosystem I reaction center subunit VIII

Chain cI:



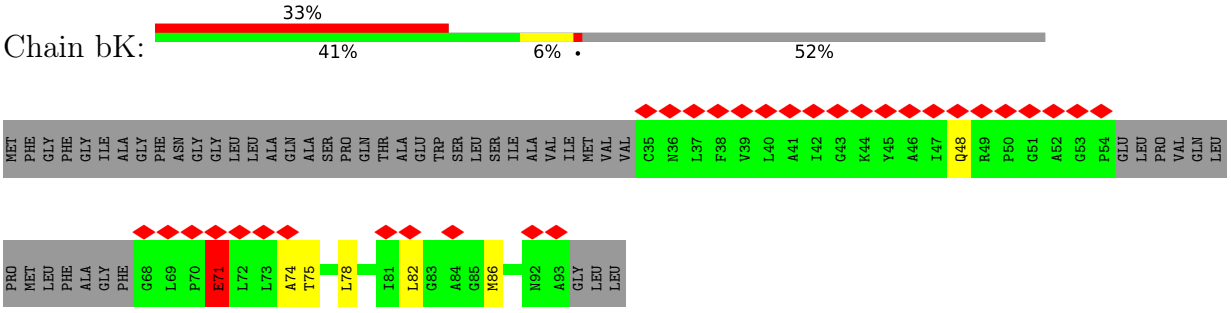
• Molecule 7: Photosystem I reaction center subunit PsaK

Chain aK:



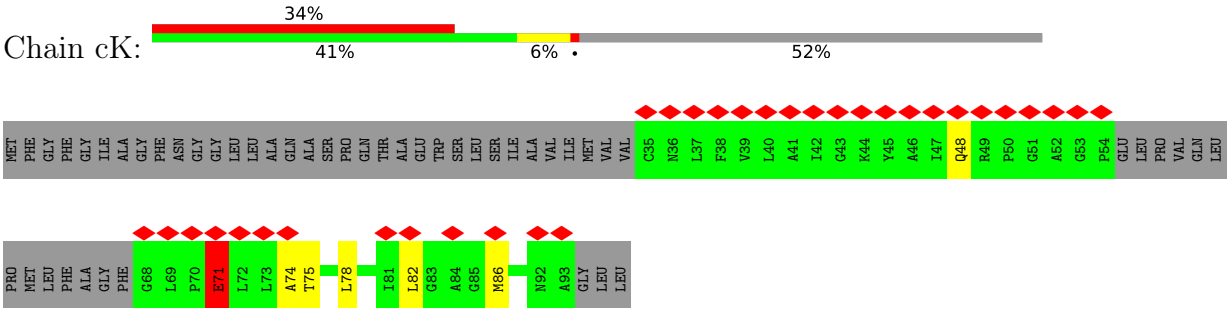
• Molecule 7: Photosystem I reaction center subunit PsaK

Chain bK:



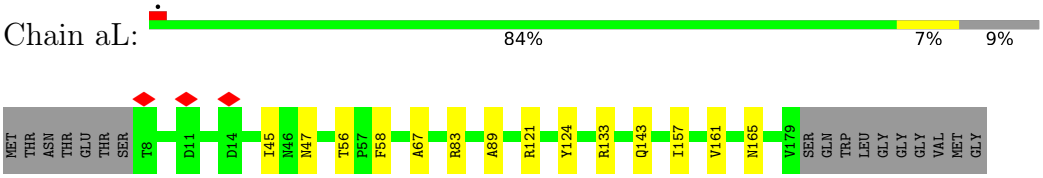
• Molecule 7: Photosystem I reaction center subunit PsaK

Chain cK:



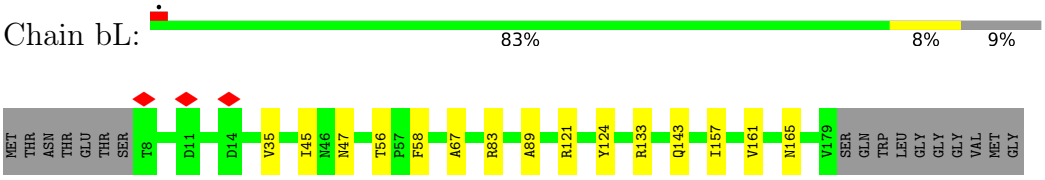
• Molecule 8: Photosystem I reaction center subunit XI

Chain aL:



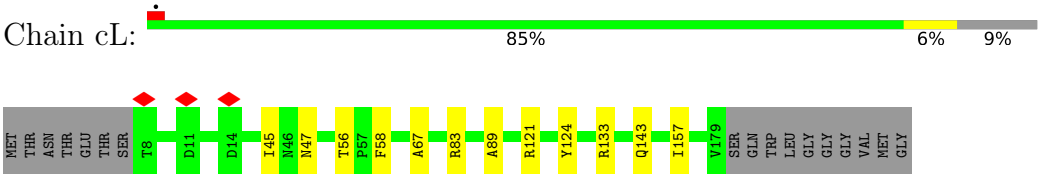
• Molecule 8: Photosystem I reaction center subunit XI

Chain bL:



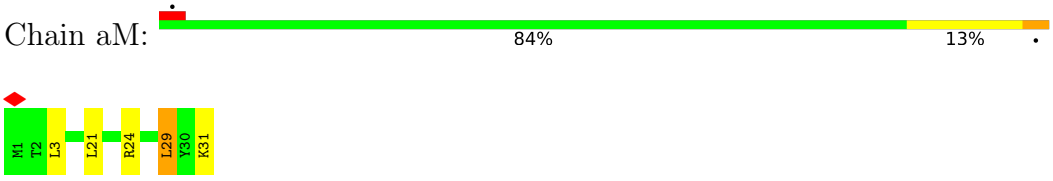
• Molecule 8: Photosystem I reaction center subunit XI

Chain cL:



• Molecule 9: Photosystem I reaction center subunit XII

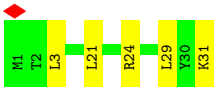
Chain aM:



• Molecule 9: Photosystem I reaction center subunit XII

Chain bM:

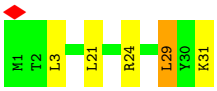




• Molecule 9: Photosystem I reaction center subunit XII

Chain cM:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	311993	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	47	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.915	Depositor
Minimum map value	-0.310	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	313.2, 313.2, 313.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87, 0.87, 0.87	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: F6C, LHG, SF4, LMG, CA, UNL, LMT, CL0, BCR, PQN, CLA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	aA	0.20	0/5868	0.47	3/7993 (0.0%)
1	bA	0.20	0/5868	0.47	3/7993 (0.0%)
1	cA	0.20	0/5868	0.47	2/7993 (0.0%)
2	aB	0.20	0/5993	0.49	1/8185 (0.0%)
2	bB	0.20	0/5993	0.49	1/8185 (0.0%)
2	cB	0.20	0/5993	0.49	1/8185 (0.0%)
3	aC	0.18	0/606	0.49	0/820
3	bC	0.18	0/606	0.49	0/820
3	cC	0.18	0/606	0.49	0/820
4	aD	0.17	0/785	0.43	0/1061
4	bD	0.17	0/785	0.43	0/1061
4	cD	0.17	0/785	0.43	0/1061
5	aE	0.31	0/509	0.71	1/689 (0.1%)
5	bE	0.31	0/509	0.71	1/689 (0.1%)
5	cE	0.31	0/509	0.71	1/689 (0.1%)
6	aI	0.30	0/365	0.64	0/503
6	bI	0.30	0/365	0.64	0/503
6	cI	0.30	0/365	0.64	0/503
7	aK	0.23	0/321	0.71	1/433 (0.2%)
7	bK	0.24	0/321	0.71	1/433 (0.2%)
7	cK	0.24	0/321	0.71	1/433 (0.2%)
8	aL	0.19	0/1334	0.45	0/1819
8	bL	0.19	0/1334	0.45	0/1819
8	cL	0.20	0/1334	0.45	0/1819
9	aM	0.23	0/244	0.61	0/332
9	bM	0.23	0/244	0.60	0/332
9	cM	0.23	0/244	0.60	0/332
All	All	0.21	0/48075	0.50	17/65505 (0.0%)

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	aB	0	1
2	bB	0	1
2	cB	0	1
9	aM	0	1
9	bM	0	1
9	cM	0	1
All	All	0	6

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	cA	234	GLU	CA-CB-CG	7.39	128.89	114.10
1	bA	234	GLU	CA-CB-CG	7.37	128.84	114.10
1	aA	234	GLU	CA-CB-CG	7.35	128.79	114.10
7	aK	71	GLU	CA-CB-CG	6.70	127.49	114.10
7	cK	71	GLU	CA-CB-CG	6.69	127.48	114.10
7	bK	71	GLU	CA-CB-CG	6.67	127.44	114.10
1	bA	106	ASP	CB-CA-C	6.50	119.98	111.01
1	aA	106	ASP	CB-CA-C	6.49	119.96	111.01
1	cA	106	ASP	CB-CA-C	6.47	119.94	111.01
2	bB	482	ASN	N-CA-CB	-5.45	103.86	112.63
2	aB	482	ASN	N-CA-CB	-5.45	103.86	112.63
2	cB	482	ASN	N-CA-CB	-5.43	103.88	112.63
5	aE	29	GLN	CB-CG-CD	5.16	121.37	112.60
5	bE	29	GLN	CB-CG-CD	5.15	121.36	112.60
5	cE	29	GLN	CB-CG-CD	5.14	121.34	112.60
1	aA	234	GLU	CB-CA-C	-5.03	101.02	110.67
1	bA	234	GLU	CB-CA-C	-5.01	101.05	110.67

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	aB	481	ILE	Peptide
9	aM	29	LEU	Peptide
2	bB	481	ILE	Peptide
9	bM	29	LEU	Peptide
2	cB	481	ILE	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
9	cM	29	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	aA	5669	0	5487	49	0
1	bA	5669	0	5487	50	0
1	cA	5669	0	5487	51	0
2	aB	5783	0	5519	59	0
2	bB	5783	0	5519	59	0
2	cB	5783	0	5519	59	0
3	aC	596	0	576	3	0
3	bC	596	0	576	3	0
3	cC	596	0	576	3	0
4	aD	768	0	774	8	0
4	bD	768	0	774	7	0
4	cD	768	0	774	8	0
5	aE	499	0	488	4	0
5	bE	499	0	488	4	0
5	cE	499	0	488	3	0
6	aI	349	0	353	5	0
6	bI	349	0	353	4	0
6	cI	349	0	353	5	0
7	aK	317	0	336	5	0
7	bK	317	0	336	5	0
7	cK	317	0	336	5	0
8	aL	1303	0	1301	14	0
8	bL	1303	0	1301	15	0
8	cL	1303	0	1301	13	0
9	aM	241	0	266	6	0
9	bM	241	0	266	4	0
9	cM	241	0	266	6	0
10	aA	65	0	72	0	0
10	bA	65	0	72	0	0
10	cA	65	0	72	0	0
11	aA	2112	0	1999	48	0
11	aB	2116	0	1932	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	aK	89	0	68	1	0
11	aL	195	0	216	6	0
11	bA	2112	0	1999	46	0
11	bB	2116	0	1932	48	0
11	bK	89	0	68	1	0
11	bL	195	0	216	8	0
11	cA	2112	0	1999	53	0
11	cB	2116	0	1932	54	0
11	cK	89	0	68	1	0
11	cL	195	0	216	5	0
12	aA	305	0	0	0	0
12	aB	58	0	0	1	0
12	aL	66	0	0	0	0
12	bA	305	0	0	0	0
12	bB	58	0	0	0	0
12	bL	66	0	0	0	0
12	cA	305	0	0	0	0
12	cB	58	0	0	1	0
12	cL	66	0	0	0	0
13	aA	33	0	46	0	0
13	aB	28	0	33	3	0
13	bA	33	0	46	1	0
13	bB	28	0	33	2	0
13	cA	33	0	46	1	0
13	cB	28	0	33	1	0
14	aA	8	0	0	0	0
14	aC	16	0	0	0	0
14	bA	8	0	0	0	0
14	bC	16	0	0	0	0
14	cA	8	0	0	0	0
14	cC	16	0	0	0	0
15	aA	200	0	280	16	0
15	aB	240	0	336	9	0
15	aI	40	0	56	2	0
15	aK	40	0	56	2	0
15	aL	120	0	168	7	0
15	aM	40	0	56	0	0
15	bA	200	0	280	18	0
15	bB	240	0	336	7	0
15	bI	40	0	56	0	0
15	bK	40	0	56	2	0
15	bL	120	0	168	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	bM	40	0	56	2	0
15	cA	200	0	280	15	0
15	cB	240	0	336	10	0
15	cI	40	0	56	0	0
15	cK	40	0	56	2	0
15	cL	120	0	168	9	0
15	cM	40	0	56	0	0
16	aA	49	0	74	1	0
16	bA	49	0	74	1	0
16	cA	49	0	74	1	0
17	aA	35	0	46	2	0
17	bA	35	0	46	2	0
17	cA	35	0	46	2	0
18	aB	46	0	65	1	0
18	bB	46	0	65	1	0
18	cB	46	0	65	1	0
19	aI	9	0	0	0	0
19	aL	56	0	0	0	0
19	bI	9	0	0	0	0
19	bL	56	0	0	0	0
19	cI	25	0	0	0	0
19	cL	40	0	0	0	0
20	aL	1	0	0	0	0
20	bL	1	0	0	0	0
20	cL	1	0	0	0	0
21	aA	72	0	0	1	0
21	aB	72	0	0	1	0
21	aC	21	0	0	0	0
21	aD	15	0	0	0	0
21	aI	5	0	0	0	0
21	aK	1	0	0	0	0
21	aL	25	0	0	0	0
21	aM	1	0	0	0	0
21	bA	72	0	0	1	0
21	bB	72	0	0	1	0
21	bC	20	0	0	0	0
21	bD	16	0	0	0	0
21	bI	6	0	0	0	0
21	bK	1	0	0	0	0
21	bL	24	0	0	0	0
21	bM	1	0	0	0	0
21	cA	72	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	cB	72	0	0	1	0
21	cC	21	0	0	0	0
21	cD	15	0	0	0	0
21	cI	6	0	0	0	0
21	cK	1	0	0	0	0
21	cL	24	0	0	0	0
21	cM	1	0	0	0	0
All	All	65112	0	61809	653	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (653) 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)
4:aD:52:HIS:H	4:aD:56:ASN:HD21	1.33	0.76
4:cD:52:HIS:H	4:cD:56:ASN:HD21	1.34	0.76
4:bD:52:HIS:H	4:bD:56:ASN:HD21	1.34	0.75
11:aB:840:CLA:HAC2	15:aB:846:BCR:H21C	1.69	0.73
11:cB:840:CLA:HAC2	15:cB:846:BCR:H21C	1.69	0.73
11:bB:840:CLA:HAC2	15:bB:846:BCR:H21C	1.69	0.72
7:aK:78:LEU:HB2	15:aK:102:BCR:H24C	1.74	0.69
1:bA:707:ALA:HB1	15:bA:851:BCR:H15C	1.75	0.69
7:bK:78:LEU:HB2	15:bK:102:BCR:H24C	1.74	0.69
8:aL:143:GLN:HE22	8:bL:58:PHE:HB3	1.58	0.68
1:aA:707:ALA:HB1	15:aA:851:BCR:H15C	1.75	0.67
2:bB:7:LYS:HD2	9:bM:31:LYS:HB3	1.76	0.67
1:cA:707:ALA:HB1	15:cA:851:BCR:H15C	1.75	0.67
7:cK:78:LEU:HB2	15:cK:102:BCR:H24C	1.74	0.67
11:aA:825:CLA:HAC1	15:aA:849:BCR:HC8	1.79	0.65
11:bA:825:CLA:HAC1	15:bA:849:BCR:HC8	1.79	0.64
11:cA:806:CLA:H72	15:cA:848:BCR:H24C	1.80	0.64
8:bL:143:GLN:HE22	8:cL:58:PHE:HB3	1.62	0.64
11:aA:806:CLA:H72	15:aA:848:BCR:H24C	1.80	0.64
2:cB:25:ILE:HD11	15:cL:207:BCR:H322	1.80	0.63
11:aB:818:CLA:HAA2	11:aB:823:CLA:HAB	1.80	0.63
2:bB:25:ILE:HD11	15:bL:207:BCR:H322	1.80	0.63
11:aA:822:CLA:H2	11:aA:824:CLA:HBC1	1.81	0.63
1:bA:770:VAL:HG22	15:bA:851:BCR:H323	1.81	0.63
11:bA:806:CLA:H72	15:bA:848:BCR:H24C	1.79	0.63
1:bA:502:VAL:HG12	1:bA:534:LEU:HD13	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:cB:818:CLA:HAA2	11:cB:823:CLA:HAB	1.80	0.63
2:cB:7:LYS:HD2	9:cM:31:LYS:HB3	1.81	0.63
2:aB:25:ILE:HD11	15:aL:207:BCR:H322	1.81	0.62
11:bA:822:CLA:H2	11:bA:824:CLA:HBC1	1.81	0.62
11:cA:825:CLA:HAC1	15:cA:849:BCR:HC8	1.79	0.62
11:bB:818:CLA:HAA2	11:bB:823:CLA:HAB	1.80	0.62
1:cA:770:VAL:HG22	15:cA:851:BCR:H323	1.81	0.62
2:aB:7:LYS:HD2	9:aM:31:LYS:HB3	1.81	0.61
1:aA:502:VAL:HG12	1:aA:534:LEU:HD13	1.81	0.61
1:aA:770:VAL:HG22	15:aA:851:BCR:H323	1.81	0.61
11:cA:822:CLA:H2	11:cA:824:CLA:HBC1	1.81	0.61
11:bB:806:CLA:H162	11:bB:827:CLA:HBB2	1.82	0.61
8:aL:58:PHE:HB3	8:cL:143:GLN:HE22	1.64	0.61
1:cA:502:VAL:HG12	1:cA:534:LEU:HD13	1.81	0.61
11:aB:825:CLA:HED1	11:aB:833:CLA:HAB	1.83	0.61
5:aE:10:ILE:HG22	5:aE:12:ARG:H	1.66	0.60
11:bB:825:CLA:HED1	11:bB:833:CLA:HAB	1.83	0.60
2:cB:493:SER:O	2:cB:501:ASN:ND2	2.35	0.60
11:cB:806:CLA:H162	11:cB:827:CLA:HBB2	1.82	0.60
5:cE:10:ILE:HG22	5:cE:12:ARG:H	1.66	0.60
11:aB:806:CLA:H162	11:aB:827:CLA:HBB2	1.82	0.60
2:bB:15:ASP:HB3	2:bB:20:ARG:HB2	1.84	0.60
2:bB:64:ILE:HG23	11:bB:808:CLA:HED2	1.84	0.60
2:bB:351:ILE:HD12	11:bB:817:CLA:H71	1.84	0.60
5:bE:10:ILE:HG22	5:bE:12:ARG:H	1.66	0.60
11:cB:825:CLA:HED1	11:cB:833:CLA:HAB	1.83	0.60
2:aB:15:ASP:HB3	2:aB:20:ARG:HB2	1.84	0.59
2:aB:493:SER:O	2:aB:501:ASN:ND2	2.35	0.59
11:bA:814:CLA:H161	15:bA:848:BCR:H353	1.85	0.59
2:bB:493:SER:O	2:bB:501:ASN:ND2	2.35	0.59
11:aA:814:CLA:H161	15:aA:848:BCR:H353	1.85	0.59
11:bA:820:CLA:H8	11:bA:820:CLA:HAB	1.85	0.59
1:aA:317:ILE:HD13	7:aK:74:ALA:HB2	1.85	0.59
2:aB:510:ALA:O	2:aB:516:ASN:ND2	2.36	0.59
2:cB:15:ASP:HB3	2:cB:20:ARG:HB2	1.84	0.59
2:aB:64:ILE:HG23	11:aB:808:CLA:HED2	1.84	0.59
11:cA:820:CLA:HAB	11:cA:820:CLA:H8	1.85	0.59
11:cB:807:CLA:H43	6:cI:20:MET:HE2	1.85	0.59
11:aA:820:CLA:HAB	11:aA:820:CLA:H8	1.85	0.59
15:aA:851:BCR:H362	11:aB:802:CLA:H52	1.84	0.59
1:cA:490:PHE:HB3	11:cA:838:CLA:H11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:bB:807:CLA:H43	6:bI:20:MET:HE2	1.85	0.58
15:cA:851:BCR:H362	11:cB:802:CLA:H52	1.84	0.58
2:cB:64:ILE:HG23	11:cB:808:CLA:HED2	1.84	0.58
3:aC:23:LEU:O	4:aD:63:LYS:NZ	2.35	0.58
11:cA:833:CLA:H42	8:cL:45:ILE:HD11	1.85	0.58
2:cB:351:ILE:HD12	11:cB:817:CLA:H71	1.84	0.58
1:cA:186:LYS:NZ	1:cA:188:ASP:OD2	2.36	0.58
1:bA:317:ILE:HD13	7:bK:74:ALA:HB2	1.85	0.58
11:bA:833:CLA:H42	8:bL:45:ILE:HD11	1.85	0.58
2:bB:510:ALA:O	2:bB:516:ASN:ND2	2.36	0.58
11:cA:814:CLA:H161	15:cA:848:BCR:H353	1.85	0.58
8:aL:56:THR:HG21	8:cL:143:GLN:HG2	1.85	0.58
11:aB:804:CLA:HBC3	11:aB:828:CLA:H41	1.86	0.58
1:bA:490:PHE:HB3	11:bA:838:CLA:H11	1.85	0.58
2:cB:510:ALA:O	2:cB:516:ASN:ND2	2.36	0.58
2:aB:351:ILE:HD12	11:aB:817:CLA:H71	1.84	0.57
11:cA:820:CLA:H101	11:cA:822:CLA:H142	1.86	0.57
1:aA:490:PHE:HB3	11:aA:838:CLA:H11	1.85	0.57
2:aB:86:PRO:HB2	2:aB:116:CYS:HB3	1.86	0.57
11:aB:807:CLA:H43	6:aI:20:MET:HE2	1.85	0.57
2:bB:276:HIS:HE1	11:bB:816:CLA:ND	2.03	0.57
11:cB:804:CLA:HBC3	11:cB:828:CLA:H41	1.86	0.57
1:cA:317:ILE:HD13	7:cK:74:ALA:HB2	1.85	0.57
2:cB:86:PRO:HB2	2:cB:116:CYS:HB3	1.86	0.57
11:aA:833:CLA:H42	8:aL:45:ILE:HD11	1.85	0.57
2:aB:276:HIS:HE1	11:aB:816:CLA:ND	2.03	0.57
15:bA:851:BCR:H362	11:bB:802:CLA:H52	1.84	0.57
8:aL:143:GLN:HG2	8:bL:56:THR:HG21	1.85	0.57
2:cB:276:HIS:HE1	11:cB:816:CLA:ND	2.03	0.56
11:aA:820:CLA:H101	11:aA:822:CLA:H142	1.87	0.56
11:bA:820:CLA:H101	11:bA:822:CLA:H142	1.87	0.56
8:bL:47:ASN:HB3	11:bL:204:CLA:HAC1	1.88	0.56
1:aA:186:LYS:NZ	1:aA:188:ASP:OD2	2.36	0.56
8:aL:47:ASN:HB3	11:aL:204:CLA:HAC1	1.88	0.56
2:bB:86:PRO:HB2	2:bB:116:CYS:HB3	1.86	0.56
11:bB:804:CLA:HBC3	11:bB:828:CLA:H41	1.86	0.56
1:bA:186:LYS:NZ	1:bA:188:ASP:OD2	2.36	0.56
8:cL:47:ASN:HB3	11:cL:204:CLA:HAC1	1.88	0.56
1:aA:217:ILE:HA	1:aA:221:LEU:HD12	1.87	0.56
1:cA:406:GLY:HA3	1:cA:635:LEU:HD11	1.87	0.56
1:bA:356:TRP:HB3	11:bA:806:CLA:HAC1	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:cA:217:ILE:HA	1:cA:221:LEU:HD12	1.87	0.55
1:bA:217:ILE:HA	1:bA:221:LEU:HD12	1.87	0.55
2:bB:595:ASN:HB2	11:bB:802:CLA:HBC2	1.89	0.55
1:bA:406:GLY:HA3	1:bA:635:LEU:HD11	1.87	0.55
1:aA:356:TRP:HB3	11:aA:806:CLA:HAC1	1.88	0.55
1:aA:406:GLY:HA3	1:aA:635:LEU:HD11	1.87	0.55
2:aB:595:ASN:HB2	11:aB:802:CLA:HBC2	1.89	0.55
1:aA:216:LEU:HA	1:aA:220:ALA:HB3	1.89	0.55
2:cB:595:ASN:HB2	11:cB:802:CLA:HBC2	1.89	0.55
1:cA:225:LYS:HD3	1:cA:252:LEU:HB3	1.90	0.54
1:aA:225:LYS:HD3	1:aA:252:LEU:HB3	1.90	0.54
1:cA:356:TRP:HB3	11:cA:806:CLA:HAC1	1.88	0.54
1:cA:216:LEU:HA	1:cA:220:ALA:HB3	1.89	0.53
2:bB:180:ALA:HB2	2:bB:288:GLY:HA3	1.91	0.53
11:bB:810:CLA:HBD	15:bB:848:BCR:HC7	1.91	0.53
11:cB:810:CLA:HBD	15:cB:848:BCR:HC7	1.90	0.53
1:bA:216:LEU:HA	1:bA:220:ALA:HB3	1.89	0.53
2:aB:237:PRO:HB3	2:aB:256:THR:HG21	1.91	0.53
11:aB:810:CLA:HBD	15:aB:848:BCR:HC7	1.91	0.53
1:bA:225:LYS:HD3	1:bA:252:LEU:HB3	1.90	0.53
2:bB:237:PRO:HB3	2:bB:256:THR:HG21	1.91	0.53
8:bL:143:GLN:HG2	8:cL:56:THR:HG21	1.91	0.53
2:aB:180:ALA:HB2	2:aB:288:GLY:HA3	1.91	0.53
4:cD:86:ILE:HB	4:cD:99:HIS:HB3	1.91	0.53
11:aA:820:CLA:H191	11:aA:822:CLA:H52	1.91	0.53
2:bB:174:ARG:HB2	11:bB:812:CLA:HBC2	1.91	0.52
6:aI:43:GLU:OE1	8:aL:121:ARG:NH2	2.43	0.52
1:cA:443:THR:CG2	4:cD:16:THR:HG21	2.39	0.52
4:bD:86:ILE:HB	4:bD:99:HIS:HB3	1.91	0.52
6:bI:43:GLU:OE1	8:bL:121:ARG:NH2	2.43	0.52
2:cB:180:ALA:HB2	2:cB:288:GLY:HA3	1.90	0.52
11:aA:804:CLA:HBB2	11:aA:812:CLA:H112	1.92	0.52
2:aB:174:ARG:HB2	11:aB:812:CLA:HBC2	1.91	0.52
4:aD:86:ILE:HB	4:aD:99:HIS:HB3	1.91	0.52
11:bA:820:CLA:H191	11:bA:822:CLA:H52	1.91	0.52
6:cI:43:GLU:OE1	8:cL:121:ARG:NH2	2.43	0.52
2:aB:470:THR:O	2:aB:474:HIS:ND1	2.37	0.52
11:cA:820:CLA:H191	11:cA:822:CLA:H52	1.91	0.52
2:cB:237:PRO:HB3	2:cB:256:THR:HG21	1.91	0.52
2:cB:174:ARG:HB2	11:cB:812:CLA:HBC2	1.91	0.52
11:cB:839:CLA:HBB2	13:cB:841:PQN:H141	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:aB:839:CLA:HBB2	13:aB:841:PQN:H141	1.92	0.51
11:bB:839:CLA:HBB2	13:bB:841:PQN:H141	1.92	0.51
2:aB:61:ILE:HG23	2:aB:142:LEU:HD13	1.93	0.51
2:bB:470:THR:O	2:bB:474:HIS:ND1	2.37	0.51
11:cA:821:CLA:H122	11:cA:821:CLA:HBB1	1.93	0.51
2:cB:61:ILE:HG23	2:cB:142:LEU:HD13	1.93	0.51
1:aA:612:ARG:NH1	21:aA:908:HOH:O	2.44	0.51
1:cA:251:ASP:OD1	1:cA:251:ASP:N	2.44	0.51
2:bB:487:ASN:HB3	2:bB:490:SER:HB2	1.93	0.50
2:cB:470:THR:O	2:cB:474:HIS:ND1	2.37	0.50
1:aA:529:VAL:HG13	1:aA:530:THR:HG23	1.94	0.50
1:bA:529:VAL:HG13	1:bA:530:THR:HG23	1.94	0.50
11:bA:804:CLA:HBB2	11:bA:812:CLA:H112	1.92	0.50
11:cA:804:CLA:HBB2	11:cA:812:CLA:H112	1.92	0.50
11:aA:821:CLA:HBB1	11:aA:821:CLA:H122	1.93	0.50
2:aB:487:ASN:HB3	2:aB:490:SER:HB2	1.93	0.50
1:cA:529:VAL:HG13	1:cA:530:THR:HG23	1.94	0.49
2:cB:487:ASN:HB3	2:cB:490:SER:HB2	1.93	0.49
2:bB:45:ARG:HH22	11:bB:804:CLA:HED2	1.77	0.49
1:aA:251:ASP:OD1	1:aA:251:ASP:N	2.44	0.49
1:bA:443:THR:HG22	2:bB:690:TRP:CH2	2.48	0.49
1:cA:747:GLN:OE1	1:cA:749:ARG:NH2	2.46	0.49
11:cA:814:CLA:H41	15:cA:848:BCR:H19C	1.94	0.49
1:bA:251:ASP:OD1	1:bA:251:ASP:N	2.44	0.49
11:bA:821:CLA:HBB1	11:bA:821:CLA:H122	1.93	0.49
2:bB:61:ILE:HG23	2:bB:142:LEU:HD13	1.93	0.49
2:cB:45:ARG:HH22	11:cB:804:CLA:HED2	1.77	0.49
2:cB:111:ASN:HD22	6:cI:10:ALA:H	1.61	0.49
2:cB:692:HIS:O	8:cL:133:ARG:NH2	2.42	0.49
1:aA:443:THR:CG2	4:aD:16:THR:HG21	2.42	0.48
1:bA:747:GLN:OE1	1:bA:749:ARG:NH2	2.46	0.48
7:bK:71:GLU:O	7:bK:75:THR:OG1	2.25	0.48
2:aB:45:ARG:HH22	11:aB:804:CLA:HED2	1.77	0.48
2:cB:471:GLN:HB3	2:cB:476:LYS:HD3	1.96	0.48
2:aB:344:HIS:CG	11:aB:823:CLA:HAA1	2.49	0.48
2:bB:344:HIS:CG	11:bB:823:CLA:HAA1	2.49	0.48
5:cE:39:ARG:HG3	5:cE:50:SER:HB2	1.96	0.48
1:aA:747:GLN:OE1	1:aA:749:ARG:NH2	2.46	0.48
11:aB:816:CLA:H3A	11:aB:816:CLA:HBA2	1.61	0.48
7:bK:86:MET:HG3	11:bK:103:CLA:HAB	1.96	0.48
1:aA:443:THR:HG22	4:aD:16:THR:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:bA:840:CLA:HBA1	11:bA:840:CLA:HBD	1.96	0.48
1:cA:431:ASN:OD1	1:cA:439:ARG:NH2	2.47	0.48
1:bA:443:THR:CG2	4:bD:16:THR:HG21	2.43	0.48
1:bA:612:ARG:NH1	21:bA:907:HOH:O	2.46	0.48
2:bB:111:ASN:HD22	6:bI:10:ALA:H	1.61	0.48
1:aA:555:MET:HE1	1:aA:646:MET:HE1	1.96	0.48
11:aA:814:CLA:H41	15:aA:848:BCR:H19C	1.94	0.48
11:bA:814:CLA:H41	15:bA:848:BCR:H19C	1.94	0.48
1:aA:492:GLN:NE2	1:aA:560:LEU:O	2.42	0.47
7:aK:86:MET:HG3	11:aK:103:CLA:HAB	1.96	0.47
1:bA:431:ASN:OD1	1:bA:439:ARG:NH2	2.47	0.47
1:cA:276:THR:HA	11:cA:818:CLA:HED1	1.96	0.47
2:aB:91:ILE:HB	2:aB:112:PRO:HB2	1.96	0.47
2:aB:136:PHE:HB2	9:aM:3:LEU:HD21	1.96	0.47
2:bB:471:GLN:HB3	2:bB:476:LYS:HD3	1.96	0.47
1:aA:276:THR:HA	11:aA:818:CLA:HED1	1.96	0.47
1:bA:773:TRP:NE1	11:bA:829:CLA:O1A	2.45	0.47
2:aB:471:GLN:HB3	2:aB:476:LYS:HD3	1.96	0.47
2:cB:586:PHE:HZ	18:cB:847:LMG:H362	1.80	0.47
11:aA:840:CLA:HBA1	11:aA:840:CLA:HBD	1.96	0.47
2:bB:275:HIS:HB3	11:bB:816:CLA:HMB1	1.97	0.47
6:aI:39:TRP:HE1	9:aM:31:LYS:HE2	1.79	0.47
1:bA:276:THR:HA	11:bA:818:CLA:HED1	1.96	0.47
2:cB:40:GLU:OE2	2:cB:44:GLN:NE2	2.48	0.47
1:aA:590:ARG:O	1:aA:599:GLY:N	2.45	0.47
2:aB:111:ASN:HD22	6:aI:10:ALA:H	1.61	0.47
2:aB:586:PHE:HZ	18:aB:847:LMG:H362	1.80	0.47
11:cA:840:CLA:HBD	11:cA:840:CLA:HBA1	1.96	0.47
2:cB:344:HIS:CG	11:cB:823:CLA:HAA1	2.49	0.47
11:cB:804:CLA:HAA2	9:cM:29:LEU:HB3	1.97	0.47
5:aE:39:ARG:HG3	5:aE:50:SER:HB2	1.96	0.47
9:aM:21:LEU:HD23	9:aM:24:ARG:HD3	1.97	0.47
1:cA:612:ARG:NH1	21:cA:908:HOH:O	2.46	0.47
2:cB:91:ILE:HB	2:cB:112:PRO:HB2	1.96	0.47
2:cB:136:PHE:HB2	9:cM:3:LEU:HD21	1.96	0.47
2:cB:216:ARG:HD3	2:cB:221:GLY:HA3	1.97	0.47
2:cB:501:ASN:OD1	2:cB:501:ASN:N	2.48	0.47
1:bA:492:GLN:NE2	1:bA:560:LEU:O	2.42	0.47
1:bA:590:ARG:O	1:bA:599:GLY:N	2.45	0.47
2:bB:586:PHE:HZ	18:bB:847:LMG:H362	1.80	0.47
1:cA:492:GLN:NE2	1:cA:560:LEU:O	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:cA:555:MET:HE1	1:cA:646:MET:HE1	1.96	0.47
6:cI:39:TRP:HE1	9:cM:31:LYS:HE2	1.79	0.47
11:aB:804:CLA:HAA2	9:aM:29:LEU:HB3	1.97	0.47
13:bA:845:PQN:H241	13:bA:845:PQN:H262	1.79	0.47
5:bE:39:ARG:HG3	5:bE:50:SER:HB2	1.96	0.47
1:aA:431:ASN:OD1	1:aA:439:ARG:NH2	2.47	0.46
1:bA:555:MET:HE1	1:bA:646:MET:HE1	1.96	0.46
11:cB:821:CLA:H41	11:cB:821:CLA:H62	1.68	0.46
11:cB:829:CLA:HBA2	11:cB:829:CLA:H3A	1.49	0.46
7:cK:86:MET:HG3	11:cK:103:CLA:HAB	1.96	0.46
2:aB:40:GLU:OE2	2:aB:44:GLN:NE2	2.48	0.46
11:aB:806:CLA:H143	11:aB:827:CLA:HBB2	1.97	0.46
11:bA:823:CLA:HBA1	7:bK:48:GLN:HB3	1.97	0.46
1:cA:773:TRP:NE1	11:cA:829:CLA:O1A	2.45	0.46
1:aA:773:TRP:NE1	11:aA:829:CLA:O1A	2.45	0.46
2:aB:275:HIS:HB3	11:aB:816:CLA:HMB1	1.97	0.46
2:bB:40:GLU:OE2	2:bB:44:GLN:NE2	2.48	0.46
2:bB:91:ILE:HB	2:bB:112:PRO:HB2	1.96	0.46
2:cB:257:PHE:HD2	2:cB:502:VAL:HB	1.80	0.46
2:bB:264:GLN:NE2	21:bB:909:HOH:O	2.47	0.46
11:cA:809:CLA:H3A	11:cA:809:CLA:HBA2	1.54	0.46
11:aA:813:CLA:HHC	11:aA:813:CLA:HBB1	1.98	0.46
11:bA:813:CLA:HHC	11:bA:813:CLA:HBB1	1.98	0.46
11:bA:821:CLA:H3A	11:bA:821:CLA:HBA2	1.66	0.46
2:bB:257:PHE:HD2	2:bB:502:VAL:HB	1.80	0.46
2:bB:558:PRO:HB2	5:bE:14:GLU:HG3	1.96	0.46
2:bB:692:HIS:O	8:bL:133:ARG:NH2	2.42	0.46
1:cA:437:THR:HA	1:cA:440:HIS:CE1	2.51	0.46
11:cB:806:CLA:H143	11:cB:827:CLA:HBB2	1.97	0.46
1:bA:724:GLY:O	1:bA:728:GLU:HG3	2.16	0.46
11:bB:806:CLA:H143	11:bB:827:CLA:HBB2	1.97	0.46
11:bB:821:CLA:H41	11:bB:821:CLA:H62	1.69	0.46
11:cA:813:CLA:HHC	11:cA:813:CLA:HBB1	1.98	0.46
2:cB:264:GLN:NE2	21:cB:909:HOH:O	2.47	0.46
2:cB:275:HIS:HB3	11:cB:816:CLA:HMB1	1.97	0.46
9:cM:21:LEU:HD23	9:cM:24:ARG:HD3	1.97	0.46
1:aA:724:GLY:O	1:aA:728:GLU:HG3	2.16	0.46
11:aA:823:CLA:HBA1	7:aK:48:GLN:HB3	1.97	0.46
3:bC:15:THR:HG22	3:bC:28:MET:HG3	1.98	0.46
2:aB:558:PRO:HB2	5:aE:14:GLU:HG3	1.98	0.46
11:bA:833:CLA:HAC2	11:bL:205:CLA:H18	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:bA:839:CLA:H191	11:bL:205:CLA:H71	1.98	0.46
11:bB:804:CLA:HMB2	15:bM:101:BCR:HC21	1.98	0.46
11:bB:819:CLA:HBA2	11:bB:819:CLA:H3A	1.64	0.46
1:aA:130:MET:HE1	1:aA:138:GLN:HB2	1.98	0.46
11:aA:833:CLA:HAC2	11:aL:205:CLA:H18	1.98	0.46
2:aB:692:HIS:O	8:aL:133:ARG:NH2	2.42	0.46
11:bA:809:CLA:HAB	11:bA:829:CLA:H152	1.98	0.46
8:bL:161:VAL:O	8:bL:165:ASN:ND2	2.44	0.46
1:aA:437:THR:HA	1:aA:440:HIS:CE1	2.51	0.45
2:aB:60:TRP:HB2	11:aB:808:CLA:H192	1.98	0.45
4:aD:22:ARG:NH2	4:aD:27:GLU:OE2	2.49	0.45
11:bA:823:CLA:H3A	11:bA:823:CLA:HBA2	1.61	0.45
2:aB:257:PHE:HD2	2:aB:502:VAL:HB	1.80	0.45
2:aB:435:PHE:CD2	11:aB:837:CLA:HAB	2.52	0.45
1:bA:130:MET:HE1	1:bA:138:GLN:HB2	1.98	0.45
2:bB:191:THR:HG21	2:bB:278:LEU:HB2	1.98	0.45
2:bB:216:ARG:HD3	2:bB:221:GLY:HA3	1.97	0.45
11:bB:829:CLA:H3A	11:bB:829:CLA:HBA2	1.49	0.45
2:cB:435:PHE:CD2	11:cB:837:CLA:HAB	2.52	0.45
15:cB:848:BCR:H382	15:cB:848:BCR:H371	1.99	0.45
11:bA:806:CLA:HBA1	11:bA:806:CLA:H3A	1.73	0.45
4:bD:22:ARG:NH2	4:bD:27:GLU:OE2	2.49	0.45
1:cA:450:TRP:HH2	11:cA:839:CLA:H151	1.82	0.45
11:cA:823:CLA:HBA1	7:cK:48:GLN:HB3	1.97	0.45
2:aB:216:ARG:HD3	2:aB:221:GLY:HA3	1.97	0.45
1:bA:437:THR:HA	1:bA:440:HIS:CE1	2.51	0.45
1:cA:724:GLY:O	1:cA:728:GLU:HG3	2.16	0.45
17:cA:853:LMT:H6'2	8:cL:83:ARG:HH11	1.82	0.45
2:cB:492:ALA:HB2	11:cB:834:CLA:HBC3	1.99	0.45
2:aB:181:GLY:HA3	11:aB:812:CLA:HBB1	1.99	0.45
15:bB:848:BCR:H382	15:bB:848:BCR:H371	1.99	0.45
15:cL:207:BCR:H15C	15:cL:207:BCR:H351	1.84	0.45
11:aA:803:CLA:H102	15:aA:851:BCR:H24C	1.99	0.45
15:aB:848:BCR:H371	15:aB:848:BCR:H382	1.99	0.45
1:bA:685:ALA:O	1:bA:688:SER:OG	2.35	0.45
11:cA:840:CLA:H111	11:cA:840:CLA:H193	1.98	0.45
11:aB:806:CLA:H72	11:aB:806:CLA:H111	1.50	0.45
11:cA:809:CLA:HAB	11:cA:829:CLA:H152	1.98	0.45
15:aA:847:BCR:H383	15:aK:102:BCR:H10C	1.99	0.45
3:aC:15:THR:HG22	3:aC:28:MET:HG3	1.98	0.45
8:aL:161:VAL:O	8:aL:165:ASN:ND2	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:bA:202:ALA:HB2	1:bA:308:GLY:HA3	1.99	0.45
11:bA:840:CLA:H111	11:bA:840:CLA:H193	1.98	0.45
9:bM:21:LEU:HD23	9:bM:24:ARG:HD3	1.97	0.45
11:aA:803:CLA:H92	11:aA:803:CLA:H61	1.83	0.45
11:aA:840:CLA:H192	11:aA:840:CLA:H162	1.87	0.45
17:aA:853:LMT:H6'2	8:aL:83:ARG:HH11	1.82	0.45
2:bB:181:GLY:HA3	11:bB:812:CLA:HBB1	1.99	0.45
2:cB:345:LEU:HD21	11:cB:828:CLA:HAB	1.99	0.45
1:aA:280:GLY:N	1:aA:537:PRO:O	2.50	0.45
2:aB:191:THR:HG21	2:aB:278:LEU:HB2	1.98	0.45
15:aL:207:BCR:H20C	15:aL:207:BCR:H361	1.85	0.45
2:bB:345:LEU:HD21	11:bB:828:CLA:HAB	1.99	0.45
1:cA:130:MET:HE1	1:cA:138:GLN:HB2	1.98	0.45
13:cA:845:PQN:H241	13:cA:845:PQN:H262	1.79	0.45
4:cD:22:ARG:NH2	4:cD:27:GLU:OE2	2.49	0.45
11:aB:805:CLA:H192	11:aB:805:CLA:H162	1.85	0.44
1:bA:747:GLN:HA	1:bA:748:PRO:HD3	1.86	0.44
2:bB:435:PHE:CD2	11:bB:837:CLA:HAB	2.52	0.44
3:bC:66:ARG:HA	3:bC:66:ARG:HD2	1.79	0.44
11:cA:839:CLA:H191	11:cL:205:CLA:H71	1.98	0.44
11:aA:809:CLA:HAB	11:aA:829:CLA:H152	1.98	0.44
11:aA:839:CLA:H191	11:aL:205:CLA:H71	1.98	0.44
15:bA:847:BCR:H20C	15:bA:847:BCR:H361	1.86	0.44
2:bB:60:TRP:HB2	11:bB:808:CLA:H192	1.98	0.44
2:bB:555:LYS:HB2	2:bB:555:LYS:HE2	1.77	0.44
1:cA:443:THR:HG22	4:cD:16:THR:HG21	1.99	0.44
11:cA:819:CLA:HBA2	11:cA:819:CLA:H3A	1.72	0.44
15:cA:847:BCR:H383	15:cK:102:BCR:H10C	1.99	0.44
2:cB:699:PHE:O	8:cL:124:TYR:OH	2.29	0.44
1:aA:450:TRP:HH2	11:aA:839:CLA:H151	1.82	0.44
11:aA:840:CLA:H111	11:aA:840:CLA:H193	1.98	0.44
2:aB:345:LEU:HD21	11:aB:828:CLA:HAB	1.99	0.44
11:cA:806:CLA:HBA1	11:cA:806:CLA:H3A	1.73	0.44
1:aA:685:ALA:O	1:aA:688:SER:OG	2.35	0.44
8:aL:67:ALA:HA	15:aL:208:BCR:H16C	2.00	0.44
15:bB:845:BCR:H15C	15:bB:845:BCR:H351	1.85	0.44
2:cB:60:TRP:HB2	11:cB:808:CLA:H192	1.98	0.44
2:aB:264:GLN:NE2	21:aB:909:HOH:O	2.46	0.44
2:aB:347:CYS:HB3	11:aB:823:CLA:H42	2.00	0.44
15:bA:847:BCR:H383	15:bK:102:BCR:H10C	1.99	0.44
2:bB:467:ALA:HB1	11:bB:836:CLA:HBD	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:bB:492:ALA:HB2	11:bB:834:CLA:HBC3	1.98	0.44
11:bB:805:CLA:H192	11:bB:805:CLA:H162	1.85	0.44
11:cA:835:CLA:H61	11:cA:835:CLA:H92	1.86	0.44
2:cB:181:GLY:HA3	11:cB:812:CLA:HBB1	1.99	0.44
1:aA:182:VAL:HG12	1:aA:183:ARG:HG3	1.99	0.44
11:aB:823:CLA:H62	11:aB:823:CLA:H41	1.83	0.44
11:bA:803:CLA:H102	15:bA:851:BCR:H24C	1.99	0.44
2:cB:191:THR:HG21	2:cB:278:LEU:HB2	1.98	0.44
11:cB:806:CLA:H72	11:cB:806:CLA:H111	1.50	0.44
1:bA:182:VAL:HG12	1:bA:183:ARG:HG3	1.99	0.44
1:bA:450:TRP:HH2	11:bA:839:CLA:H151	1.82	0.44
1:cA:685:ALA:O	1:cA:688:SER:OG	2.35	0.44
11:cA:833:CLA:HAC2	11:cL:205:CLA:H18	1.98	0.44
11:bA:822:CLA:H51	11:bA:828:CLA:H61	2.00	0.44
11:cB:805:CLA:H142	11:cB:805:CLA:H111	1.88	0.44
11:aA:809:CLA:H3A	11:aA:809:CLA:HBA2	1.54	0.44
2:aB:492:ALA:HB2	11:aB:834:CLA:HBC3	1.99	0.44
1:bA:280:GLY:N	1:bA:537:PRO:O	2.50	0.44
1:cA:182:VAL:HG12	1:cA:183:ARG:HG3	1.99	0.44
11:cA:803:CLA:H102	15:cA:851:BCR:H24C	1.99	0.43
17:bA:853:LMT:H6'2	8:bL:83:ARG:HH11	1.81	0.43
2:bB:343:TRP:HZ2	11:bB:823:CLA:HBB1	1.83	0.43
4:bD:62:ARG:NH2	4:bD:64:GLU:OE2	2.51	0.43
1:cA:280:GLY:N	1:cA:537:PRO:O	2.50	0.43
2:cB:402:ILE:HD11	2:cB:551:ALA:HB1	2.00	0.43
15:cB:845:BCR:H371	15:cB:845:BCR:H24C	1.81	0.43
3:cC:15:THR:HG22	3:cC:28:MET:HG3	1.98	0.43
2:aB:697:LEU:HB2	15:aL:203:BCR:H282	2.01	0.43
11:bB:816:CLA:H3A	11:bB:816:CLA:HBA2	1.61	0.43
11:cA:831:CLA:H111	16:cA:852:LHG:H192	2.00	0.43
2:cB:467:ALA:HB1	11:cB:836:CLA:HBD	2.00	0.43
11:cB:827:CLA:HBA2	11:cB:827:CLA:H3A	1.64	0.43
8:cL:67:ALA:HA	15:cL:208:BCR:H16C	2.00	0.43
2:aB:467:ALA:HB1	11:aB:836:CLA:HBD	2.00	0.43
11:aB:837:CLA:HMA2	11:aB:838:CLA:HED2	2.01	0.43
11:bB:806:CLA:H72	11:bB:806:CLA:H111	1.50	0.43
15:cA:851:BCR:H403	15:cA:851:BCR:H371	2.01	0.43
2:cB:343:TRP:HZ2	11:cB:823:CLA:HBB1	1.83	0.43
8:cL:157:ILE:HG23	15:cL:208:BCR:H323	2.00	0.43
11:aA:821:CLA:H3A	11:aA:821:CLA:HBA2	1.66	0.43
15:bA:849:BCR:H20C	15:bA:849:BCR:H361	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:bB:699:PHE:O	8:bL:124:TYR:OH	2.29	0.43
3:cC:61:ASP:HA	3:cC:62:PHE:HA	1.89	0.43
1:aA:415:HIS:HA	1:aA:418:ILE:HD12	2.00	0.43
11:aA:822:CLA:H51	11:aA:828:CLA:H61	2.00	0.43
2:aB:182:LEU:HD13	11:aB:812:CLA:HHB	2.00	0.43
2:aB:699:PHE:O	8:aL:124:TYR:OH	2.29	0.43
2:bB:10:GLN:N	2:bB:35:ASP:OD2	2.50	0.43
2:bB:402:ILE:HD11	2:bB:551:ALA:HB1	2.00	0.43
2:cB:182:LEU:HD13	11:cB:812:CLA:HHB	2.01	0.43
11:cB:837:CLA:HMA2	11:cB:838:CLA:HED2	2.01	0.43
1:aA:204:LEU:HD11	11:aA:814:CLA:H42	2.01	0.43
15:bA:851:BCR:H403	15:bA:851:BCR:H371	2.01	0.43
2:bB:136:PHE:HB2	9:bM:3:LEU:HD21	2.00	0.43
8:bL:157:ILE:HG23	15:bL:208:BCR:H323	2.00	0.43
1:cA:202:ALA:HB2	1:cA:308:GLY:HA3	1.99	0.43
2:cB:634:LEU:HD11	11:cB:801:CLA:H72	2.01	0.43
1:aA:202:ALA:HB2	1:aA:308:GLY:HA3	1.99	0.43
8:bL:67:ALA:HA	15:bL:208:BCR:H16C	2.00	0.43
15:bL:203:BCR:H20C	15:bL:203:BCR:H361	1.80	0.43
11:aA:831:CLA:H111	16:aA:852:LHG:H192	2.00	0.43
15:aA:850:BCR:H15C	15:aA:850:BCR:H351	1.87	0.43
2:bB:182:LEU:HD13	11:bB:812:CLA:HHB	2.00	0.43
11:bB:837:CLA:HMA2	11:bB:838:CLA:HED2	2.01	0.43
1:cA:590:ARG:O	1:cA:599:GLY:N	2.45	0.43
2:cB:347:CYS:HB3	11:cB:823:CLA:H42	2.00	0.43
15:cL:208:BCR:H20C	15:cL:208:BCR:H361	1.87	0.43
1:aA:269:SER:HA	11:aA:818:CLA:HAA2	2.01	0.43
2:cB:510:ALA:HB1	2:cB:518:LEU:HD21	2.01	0.43
11:aA:843:CLA:H3A	11:aA:843:CLA:HBA2	1.77	0.42
1:bA:609:GLY:HA2	2:bB:572:PRO:HD3	2.01	0.42
11:bA:831:CLA:H111	16:bA:852:LHG:H192	2.00	0.42
2:bB:347:CYS:HB3	11:bB:823:CLA:H42	2.00	0.42
11:cA:822:CLA:H51	11:cA:828:CLA:H61	2.00	0.42
11:cB:805:CLA:HBA1	11:cB:805:CLA:H3A	1.71	0.42
2:aB:402:ILE:HD11	2:aB:551:ALA:HB1	2.01	0.42
1:bA:80:LEU:HD22	11:bA:806:CLA:H92	2.01	0.42
1:bA:626:LEU:HD22	2:bB:676:THR:HG22	2.01	0.42
2:bB:510:ALA:HB1	2:bB:518:LEU:HD21	2.01	0.42
2:bB:697:LEU:HB2	15:bL:203:BCR:H282	2.01	0.42
6:bI:39:TRP:HE1	9:bM:31:LYS:HE2	1.84	0.42
1:aA:80:LEU:HD22	11:aA:806:CLA:H92	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:aA:403:TRP:CD1	11:aA:829:CLA:HAB	2.54	0.42
2:aB:535:LEU:HD21	11:aB:802:CLA:HBB1	2.01	0.42
13:aB:841:PQN:H172	13:aB:841:PQN:H212	1.76	0.42
2:bB:352:THR:HB	2:bB:386:ALA:HB2	2.01	0.42
15:bB:843:BCR:H20C	15:bB:843:BCR:H361	1.91	0.42
1:cA:403:TRP:CD1	11:cA:829:CLA:HAB	2.54	0.42
1:cA:415:HIS:HA	1:cA:418:ILE:HD12	2.01	0.42
11:cA:806:CLA:H151	15:cA:847:BCR:H323	2.01	0.42
11:cB:816:CLA:H3A	11:cB:816:CLA:HBA2	1.60	0.42
4:cD:62:ARG:NH2	4:cD:64:GLU:OE2	2.51	0.42
3:aC:66:ARG:HD2	3:aC:66:ARG:HA	1.79	0.42
15:bA:851:BCR:H15C	15:bA:851:BCR:H351	1.91	0.42
1:cA:269:SER:HA	11:cA:818:CLA:HAA2	2.01	0.42
1:cA:626:LEU:HD22	2:cB:676:THR:HG22	2.01	0.42
2:cB:10:GLN:N	2:cB:35:ASP:OD2	2.50	0.42
2:cB:471:GLN:NE2	2:cB:520:LEU:O	2.50	0.42
15:cL:208:BCR:H11C	15:cL:208:BCR:H341	1.93	0.42
11:aA:813:CLA:H2	11:aA:813:CLA:H62	1.80	0.42
15:aA:851:BCR:H371	15:aA:851:BCR:H403	2.01	0.42
2:aB:691:ALA:O	2:aB:695:THR:OG1	2.27	0.42
11:bB:816:CLA:H72	11:bB:816:CLA:H111	1.84	0.42
1:aA:609:GLY:HA2	2:aB:572:PRO:HD3	2.01	0.42
1:aA:626:LEU:HD22	2:aB:676:THR:HG22	2.02	0.42
8:aL:157:ILE:HG23	15:aL:208:BCR:H323	2.00	0.42
1:bA:389:THR:HG21	1:bA:549:ILE:HB	2.02	0.42
11:bB:832:CLA:H3A	11:bB:832:CLA:HBA2	1.70	0.42
3:bC:23:LEU:O	4:bD:63:LYS:NZ	2.47	0.42
15:bL:203:BCR:H11C	15:bL:203:BCR:H341	1.92	0.42
1:cA:773:TRP:CG	15:cA:851:BCR:HC22	2.55	0.42
2:cB:697:LEU:HB2	15:cL:203:BCR:H282	2.01	0.42
3:cC:66:ARG:HD2	3:cC:66:ARG:HA	1.79	0.42
11:cL:206:CLA:HBA1	11:cL:206:CLA:H3A	1.76	0.42
11:aA:836:CLA:HBB1	11:aA:838:CLA:HED2	2.02	0.42
2:aB:343:TRP:HZ2	11:aB:823:CLA:HBB1	1.83	0.42
1:bA:773:TRP:CG	15:bA:851:BCR:HC22	2.55	0.42
2:bB:604:TRP:HB2	11:bB:836:CLA:HMC1	2.02	0.42
2:bB:634:LEU:HD11	11:bB:801:CLA:H72	2.01	0.42
15:bM:101:BCR:H20C	15:bM:101:BCR:H361	1.92	0.42
11:cB:832:CLA:HBA2	11:cB:832:CLA:H3A	1.70	0.42
15:aA:847:BCR:H15C	15:aA:847:BCR:H351	1.91	0.42
11:aL:206:CLA:H141	11:aL:206:CLA:H161	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:bA:269:SER:HA	11:bA:818:CLA:HAA2	2.01	0.42
15:bA:847:BCR:H15C	15:bA:847:BCR:H351	1.91	0.42
2:bB:418:MET:HA	2:bB:421:HIS:HB2	2.02	0.42
1:cA:204:LEU:HD11	11:cA:814:CLA:H42	2.01	0.42
1:cA:377:HIS:ND1	11:cA:819:CLA:OBD	2.53	0.42
15:cB:845:BCR:H15C	15:cB:845:BCR:H351	1.85	0.42
11:aA:824:CLA:HBB1	11:aA:825:CLA:H3A	2.01	0.42
2:aB:634:LEU:HD11	11:aB:801:CLA:H72	2.01	0.42
1:bA:204:LEU:HD11	11:bA:814:CLA:H42	2.01	0.42
2:bB:535:LEU:HD21	11:bB:802:CLA:HBB1	2.01	0.42
11:bL:206:CLA:HBA1	11:bL:206:CLA:H3A	1.76	0.42
1:cA:609:GLY:HA2	2:cB:572:PRO:HD3	2.01	0.42
2:aB:10:GLN:N	2:aB:35:ASP:OD2	2.50	0.42
11:aB:805:CLA:HBA1	11:aB:805:CLA:H3A	1.70	0.42
11:aB:808:CLA:H202	11:aB:808:CLA:H162	1.93	0.42
11:aL:205:CLA:H3A	11:aL:205:CLA:HBA2	1.66	0.42
1:bA:400:HIS:HE1	11:bA:829:CLA:ND	2.15	0.42
11:bA:824:CLA:HBB1	11:bA:825:CLA:H3A	2.01	0.42
11:bA:836:CLA:HBB1	11:bA:838:CLA:HED2	2.02	0.42
11:bL:206:CLA:H141	11:bL:206:CLA:H161	1.84	0.42
1:cA:714:PHE:HZ	11:cA:843:CLA:HBC2	1.85	0.42
11:cA:836:CLA:HBB1	11:cA:838:CLA:HED2	2.02	0.42
11:cB:812:CLA:H111	11:cB:812:CLA:H71	1.86	0.42
1:aA:773:TRP:CG	15:aA:851:BCR:HC22	2.55	0.41
11:aA:825:CLA:H143	11:aA:825:CLA:H111	1.93	0.41
11:aB:801:CLA:H62	11:aB:801:CLA:H102	1.88	0.41
11:bA:843:CLA:HBA2	11:bA:843:CLA:H3A	1.77	0.41
2:bB:692:HIS:NE2	2:bB:700:GLY:O	2.36	0.41
4:bD:78:LYS:HD2	4:bD:79:PRO:HA	2.02	0.41
11:cA:824:CLA:HBB1	11:cA:825:CLA:H3A	2.01	0.41
11:aA:806:CLA:H151	15:aA:847:BCR:H323	2.01	0.41
15:aA:849:BCR:H15C	15:aA:849:BCR:H351	1.85	0.41
4:aD:62:ARG:NH2	4:aD:64:GLU:OE2	2.51	0.41
15:aI:101:BCR:H11C	15:aI:101:BCR:H341	1.89	0.41
1:cA:80:LEU:HD22	11:cA:806:CLA:H92	2.01	0.41
15:cA:849:BCR:H20C	15:cA:849:BCR:H361	1.87	0.41
2:cB:535:LEU:HD21	11:cB:802:CLA:HBB1	2.01	0.41
11:cB:823:CLA:H62	11:cB:823:CLA:H41	1.83	0.41
1:aA:630:TRP:HE1	11:aB:803:CLA:C1D	2.34	0.41
11:aA:803:CLA:H91	15:aA:851:BCR:H383	2.03	0.41
2:aB:7:LYS:HE3	2:aB:7:LYS:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:aB:358:HIS:ND1	11:aB:816:CLA:OBD	2.51	0.41
2:aB:510:ALA:HB1	2:aB:518:LEU:HD21	2.01	0.41
2:aB:604:TRP:HB2	11:aB:836:CLA:HMC1	2.01	0.41
11:aB:813:CLA:HBA1	15:aB:844:BCR:H383	2.02	0.41
4:aD:78:LYS:HD2	4:aD:79:PRO:HA	2.02	0.41
6:aI:39:TRP:NE1	9:aM:31:LYS:HE2	2.35	0.41
15:aL:208:BCR:H20C	15:aL:208:BCR:H361	1.87	0.41
1:bA:377:HIS:ND1	11:bA:819:CLA:OBD	2.53	0.41
1:bA:403:TRP:CD1	11:bA:829:CLA:HAB	2.54	0.41
1:bA:415:HIS:HA	1:bA:418:ILE:HD12	2.01	0.41
11:bB:805:CLA:H3A	11:bB:805:CLA:HBA1	1.71	0.41
11:cA:813:CLA:H2	11:cA:813:CLA:H62	1.80	0.41
1:bA:714:PHE:HZ	11:bA:843:CLA:HBC2	1.85	0.41
15:bB:842:BCR:H20C	15:bB:842:BCR:H361	1.90	0.41
1:cA:389:THR:HG21	1:cA:549:ILE:HB	2.02	0.41
11:cA:829:CLA:H3A	11:cA:829:CLA:HBA2	1.80	0.41
2:cB:236:ASN:OD1	2:cB:236:ASN:N	2.54	0.41
2:cB:352:THR:HB	2:cB:386:ALA:HB2	2.01	0.41
2:cB:692:HIS:NE2	2:cB:700:GLY:O	2.36	0.41
5:aE:2:VAL:HG12	5:aE:27:VAL:HG21	2.02	0.41
1:bA:498:GLN:HE22	11:bA:836:CLA:C1A	2.33	0.41
2:bB:7:LYS:HE3	2:bB:7:LYS:HB2	1.86	0.41
13:bB:841:PQN:H212	13:bB:841:PQN:H172	1.76	0.41
1:cA:400:HIS:HE1	11:cA:829:CLA:ND	2.15	0.41
11:cB:815:CLA:H3A	11:cB:815:CLA:HBA2	1.76	0.41
7:cK:71:GLU:O	7:cK:75:THR:OG1	2.25	0.41
1:aA:97:PHE:HB3	1:aA:116:VAL:HG23	2.02	0.41
1:aA:606:PRO:HB3	1:aA:753:ILE:HB	2.02	0.41
1:aA:714:PHE:HZ	11:aA:843:CLA:HBC2	1.85	0.41
15:aB:843:BCR:H11C	15:aB:843:BCR:H341	1.97	0.41
11:bL:204:CLA:H192	11:bL:204:CLA:H162	1.89	0.41
11:bL:206:CLA:H202	11:bL:206:CLA:H162	1.89	0.41
2:cB:418:MET:HA	2:cB:421:HIS:HB2	2.02	0.41
2:cB:604:TRP:HB2	11:cB:836:CLA:HMC1	2.02	0.41
11:cB:801:CLA:H102	11:cB:801:CLA:H62	1.87	0.41
11:cB:808:CLA:O1A	11:cB:826:CLA:HBD	2.21	0.41
11:cB:813:CLA:HBA1	15:cB:844:BCR:H383	2.03	0.41
6:cI:39:TRP:NE1	9:cM:31:LYS:HE2	2.35	0.41
1:aA:569:HIS:CD2	17:aA:853:LMT:H123	2.55	0.41
11:aB:808:CLA:O1A	11:aB:826:CLA:HBD	2.21	0.41
11:aB:815:CLA:H2	11:aB:815:CLA:H62	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:aB:817:CLA:H41	11:aB:817:CLA:H62	1.87	0.41
15:aI:101:BCR:H20C	15:aI:101:BCR:H361	1.91	0.41
1:bA:606:PRO:HB3	1:bA:753:ILE:HB	2.03	0.41
11:cA:807:CLA:H71	11:cA:807:CLA:H112	1.87	0.41
11:cA:839:CLA:H203	11:cA:839:CLA:H162	1.91	0.41
2:cB:230:TRP:HZ3	11:cB:815:CLA:H91	1.86	0.41
11:cB:828:CLA:H61	11:cB:828:CLA:H2	1.86	0.41
15:cL:203:BCR:H20C	15:cL:203:BCR:H361	1.80	0.41
11:cL:205:CLA:H3A	11:cL:205:CLA:HBA2	1.66	0.41
1:aA:389:THR:HG21	1:aA:549:ILE:HB	2.02	0.41
2:aB:352:THR:HB	2:aB:386:ALA:HB2	2.01	0.41
2:aB:418:MET:HA	2:aB:421:HIS:HB2	2.02	0.41
11:aB:801:CLA:H202	11:aB:802:CLA:HHB	2.03	0.41
11:aB:815:CLA:H3A	11:aB:815:CLA:HBA2	1.76	0.41
15:aL:203:BCR:H11C	15:aL:203:BCR:H341	1.92	0.41
11:aL:206:CLA:HBA1	11:aL:206:CLA:H3A	1.77	0.41
1:bA:97:PHE:HB3	1:bA:116:VAL:HG23	2.02	0.41
1:bA:569:HIS:CD2	17:bA:853:LMT:H123	2.56	0.41
11:bA:839:CLA:H203	11:bA:839:CLA:H162	1.91	0.41
2:bB:471:GLN:NE2	2:bB:520:LEU:O	2.50	0.41
11:bB:808:CLA:H202	11:bB:808:CLA:H162	1.93	0.41
11:bB:827:CLA:H3A	11:bB:827:CLA:HBA2	1.64	0.41
1:cA:498:GLN:HE22	11:cA:836:CLA:C1A	2.33	0.41
11:cB:805:CLA:H192	11:cB:805:CLA:H162	1.85	0.41
1:aA:455:LEU:HB3	1:aA:573:PHE:HB2	2.03	0.41
11:aB:827:CLA:H3A	11:aB:827:CLA:HBA2	1.64	0.41
15:aB:845:BCR:H371	15:aB:845:BCR:H24C	1.80	0.41
1:bA:126:LEU:HD11	11:bA:810:CLA:HAC2	2.03	0.41
11:bA:806:CLA:H151	15:bA:847:BCR:H323	2.01	0.41
11:bL:205:CLA:HBA2	11:bL:205:CLA:H3A	1.66	0.41
1:cA:97:PHE:HB3	1:cA:116:VAL:HG23	2.02	0.41
11:cA:820:CLA:HBA2	11:cA:820:CLA:H3A	1.91	0.41
11:cA:843:CLA:H3A	11:cA:843:CLA:HBA2	1.77	0.41
2:cB:555:LYS:HB2	2:cB:555:LYS:HE2	1.77	0.41
11:cB:812:CLA:H203	11:cB:812:CLA:H162	1.91	0.41
15:cB:848:BCR:H20C	15:cB:848:BCR:H361	1.93	0.41
2:aB:230:TRP:HZ3	11:aB:815:CLA:H91	1.86	0.41
1:bA:455:LEU:HB3	1:bA:573:PHE:HB2	2.03	0.41
2:bB:230:TRP:HZ3	11:bB:815:CLA:H91	1.86	0.41
1:cA:606:PRO:HB3	1:cA:753:ILE:HB	2.03	0.41
2:cB:86:PRO:HB3	2:cB:121:TYR:CG	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:aB:841:PQN:H111	13:aB:841:PQN:H2M1	1.93	0.40
15:aB:842:BCR:H351	15:aB:842:BCR:H15C	1.85	0.40
15:bA:849:BCR:H15C	15:bA:849:BCR:H351	1.85	0.40
1:cA:381:MET:HB2	1:cA:381:MET:HE3	1.88	0.40
11:cA:822:CLA:H52	11:cA:822:CLA:H11	1.85	0.40
8:cL:83:ARG:HA	8:cL:89:ALA:HB2	2.03	0.40
1:aA:498:GLN:HE22	11:aA:836:CLA:C1A	2.33	0.40
1:aA:747:GLN:HA	1:aA:748:PRO:HD3	1.86	0.40
2:aB:86:PRO:HB3	2:aB:121:TYR:CG	2.57	0.40
11:aB:832:CLA:H3A	11:aB:832:CLA:HBA2	1.70	0.40
7:aK:71:GLU:O	7:aK:75:THR:OG1	2.25	0.40
11:cA:821:CLA:H3A	11:cA:821:CLA:HBA2	1.66	0.40
11:cB:804:CLA:HBA1	11:cB:804:CLA:HBD	2.04	0.40
4:cD:43:MET:HE3	4:cD:43:MET:HB3	2.01	0.40
11:aA:828:CLA:H41	11:aA:828:CLA:H62	1.91	0.40
11:aA:839:CLA:H203	11:aA:839:CLA:H162	1.91	0.40
2:aB:501:ASN:OD1	2:aB:501:ASN:N	2.48	0.40
11:aB:804:CLA:HBD	11:aB:804:CLA:HBA1	2.04	0.40
12:aB:824:F6C:CHB	11:aB:838:CLA:HAA2	2.51	0.40
11:bA:819:CLA:H3A	11:bA:819:CLA:HBA2	1.71	0.40
11:bA:833:CLA:HBA2	8:bL:35:VAL:HG12	2.04	0.40
11:bB:813:CLA:HBA1	15:bB:844:BCR:H383	2.02	0.40
5:bE:2:VAL:HG12	5:bE:27:VAL:HG21	2.02	0.40
15:bL:207:BCR:H15C	15:bL:207:BCR:H351	1.84	0.40
1:cA:455:LEU:HB3	1:cA:573:PHE:HB2	2.03	0.40
1:cA:569:HIS:CD2	17:cA:853:LMT:H123	2.56	0.40
11:cA:802:CLA:H13	15:cB:846:BCR:H10C	2.03	0.40
11:cA:834:CLA:H122	11:cA:834:CLA:H8	1.87	0.40
15:cA:850:BCR:H20C	15:cA:850:BCR:H361	1.85	0.40
2:cB:280:ILE:HD13	2:cB:280:ILE:HA	1.95	0.40
15:cB:844:BCR:H15C	15:cB:844:BCR:H351	1.91	0.40
4:cD:78:LYS:HD2	4:cD:79:PRO:HA	2.02	0.40
5:cE:2:VAL:HG12	5:cE:27:VAL:HG21	2.02	0.40
15:cL:208:BCR:H371	15:cL:208:BCR:H24C	1.88	0.40
1:aA:295:HIS:HB3	11:aA:819:CLA:HMB1	2.04	0.40
11:aA:802:CLA:H13	15:aB:846:BCR:H10C	2.03	0.40
11:aA:813:CLA:H3A	11:aA:813:CLA:HBA2	1.80	0.40
2:bB:236:ASN:OD1	2:bB:236:ASN:N	2.54	0.40
11:bB:805:CLA:H142	11:bB:805:CLA:H111	1.88	0.40
11:bB:808:CLA:O1A	11:bB:826:CLA:HBD	2.21	0.40
8:bL:83:ARG:HA	8:bL:89:ALA:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:cA:630:TRP:HE1	11:cB:803:CLA:C1D	2.34	0.40
11:cA:803:CLA:H91	15:cA:851:BCR:H383	2.03	0.40
12:cB:824:F6C:CHB	11:cB:838:CLA:HAA2	2.52	0.40
11:cB:837:CLA:H3A	11:cB:837:CLA:HBA2	1.91	0.40
15:cB:842:BCR:H15C	15:cB:842:BCR:H351	1.85	0.40
2:aB:343:TRP:HE1	11:aB:823:CLA:C2B	2.35	0.40
15:aB:845:BCR:H15C	15:aB:845:BCR:H351	1.85	0.40
8:aL:83:ARG:HA	8:aL:89:ALA:HB2	2.03	0.40
11:bA:809:CLA:H3A	11:bA:809:CLA:HBA2	1.53	0.40
15:bA:850:BCR:H11C	15:bA:850:BCR:H341	1.98	0.40
11:bB:801:CLA:H202	11:bB:802:CLA:HHB	2.03	0.40
1:cA:295:HIS:HB3	11:cA:819:CLA:HMB1	2.04	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	aA	713/784 (91%)	696 (98%)	17 (2%)	0	100	100
1	bA	713/784 (91%)	696 (98%)	17 (2%)	0	100	100
1	cA	713/784 (91%)	696 (98%)	17 (2%)	0	100	100
2	aB	723/743 (97%)	696 (96%)	26 (4%)	1 (0%)	48	63
2	bB	723/743 (97%)	696 (96%)	26 (4%)	1 (0%)	48	63
2	cB	723/743 (97%)	696 (96%)	26 (4%)	1 (0%)	48	63
3	aC	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
3	bC	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
3	cC	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
4	aD	96/142 (68%)	94 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	bD	96/142 (68%)	94 (98%)	2 (2%)	0	100	100
4	cD	96/142 (68%)	94 (98%)	2 (2%)	0	100	100
5	aE	59/68 (87%)	54 (92%)	5 (8%)	0	100	100
5	bE	59/68 (87%)	54 (92%)	5 (8%)	0	100	100
5	cE	59/68 (87%)	54 (92%)	5 (8%)	0	100	100
6	aI	39/63 (62%)	36 (92%)	3 (8%)	0	100	100
6	bI	39/63 (62%)	36 (92%)	3 (8%)	0	100	100
6	cI	39/63 (62%)	36 (92%)	3 (8%)	0	100	100
7	aK	42/96 (44%)	40 (95%)	2 (5%)	0	100	100
7	bK	42/96 (44%)	40 (95%)	2 (5%)	0	100	100
7	cK	42/96 (44%)	40 (95%)	2 (5%)	0	100	100
8	aL	170/189 (90%)	169 (99%)	1 (1%)	0	100	100
8	bL	170/189 (90%)	169 (99%)	1 (1%)	0	100	100
8	cL	170/189 (90%)	169 (99%)	1 (1%)	0	100	100
9	aM	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
9	bM	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
9	cM	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
All	All	5847/6591 (89%)	5661 (97%)	183 (3%)	3 (0%)	49	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	aB	237	PRO
2	bB	237	PRO
2	cB	237	PRO

5.3.2 Protein sidechains (i)

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	aA	578/633 (91%)	562 (97%)	16 (3%)	38	58
1	bA	578/633 (91%)	562 (97%)	16 (3%)	38	58
1	cA	578/633 (91%)	562 (97%)	16 (3%)	38	58
2	aB	586/598 (98%)	576 (98%)	10 (2%)	53	73
2	bB	586/598 (98%)	576 (98%)	10 (2%)	53	73
2	cB	586/598 (98%)	576 (98%)	10 (2%)	53	73
3	aC	68/69 (99%)	68 (100%)	0	100	100
3	bC	68/69 (99%)	68 (100%)	0	100	100
3	cC	68/69 (99%)	68 (100%)	0	100	100
4	aD	80/115 (70%)	80 (100%)	0	100	100
4	bD	80/115 (70%)	80 (100%)	0	100	100
4	cD	80/115 (70%)	80 (100%)	0	100	100
5	aE	54/61 (88%)	49 (91%)	5 (9%)	8	13
5	bE	54/61 (88%)	49 (91%)	5 (9%)	8	13
5	cE	54/61 (88%)	49 (91%)	5 (9%)	8	13
6	aI	36/52 (69%)	35 (97%)	1 (3%)	38	58
6	bI	36/52 (69%)	35 (97%)	1 (3%)	38	58
6	cI	36/52 (69%)	35 (97%)	1 (3%)	38	58
7	aK	30/67 (45%)	28 (93%)	2 (7%)	15	24
7	bK	30/67 (45%)	28 (93%)	2 (7%)	15	24
7	cK	30/67 (45%)	28 (93%)	2 (7%)	15	24
8	aL	136/149 (91%)	136 (100%)	0	100	100
8	bL	136/149 (91%)	136 (100%)	0	100	100
8	cL	136/149 (91%)	136 (100%)	0	100	100
9	aM	27/27 (100%)	27 (100%)	0	100	100
9	bM	27/27 (100%)	27 (100%)	0	100	100
9	cM	27/27 (100%)	27 (100%)	0	100	100
All	All	4785/5313 (90%)	4683 (98%)	102 (2%)	46	67

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	aA	98	SER

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Mol	Chain	Res	Type
1	aA	106	ASP
1	aA	116	VAL
1	aA	168	MET
1	aA	234	GLU
1	aA	236	ILE
1	aA	247	SER
1	aA	251	ASP
1	aA	443	THR
1	aA	654	VAL
1	aA	661	SER
1	aA	688	SER
1	aA	731	GLU
1	aA	733	ILE
1	aA	741	LYS
1	aA	754	THR
2	aB	33	SER
2	aB	306	GLU
2	aB	376	SER
2	aB	408	GLU
2	aB	418	MET
2	aB	505	SER
2	aB	511	VAL
2	aB	513	ASN
2	aB	555	LYS
2	aB	562	ASP
5	aE	9	ARG
5	aE	29	GLN
5	aE	37	ILE
5	aE	56	SER
5	aE	57	GLU
6	aI	21	ILE
7	aK	71	GLU
7	aK	82	LEU
1	bA	98	SER
1	bA	106	ASP
1	bA	116	VAL
1	bA	168	MET
1	bA	234	GLU
1	bA	236	ILE
1	bA	247	SER
1	bA	251	ASP
1	bA	443	THR

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Mol	Chain	Res	Type
1	bA	654	VAL
1	bA	661	SER
1	bA	688	SER
1	bA	731	GLU
1	bA	733	ILE
1	bA	741	LYS
1	bA	754	THR
2	bB	33	SER
2	bB	306	GLU
2	bB	376	SER
2	bB	408	GLU
2	bB	418	MET
2	bB	505	SER
2	bB	511	VAL
2	bB	513	ASN
2	bB	555	LYS
2	bB	562	ASP
5	bE	9	ARG
5	bE	29	GLN
5	bE	37	ILE
5	bE	56	SER
5	bE	57	GLU
6	bI	21	ILE
7	bK	71	GLU
7	bK	82	LEU
1	cA	98	SER
1	cA	106	ASP
1	cA	116	VAL
1	cA	168	MET
1	cA	234	GLU
1	cA	236	ILE
1	cA	247	SER
1	cA	251	ASP
1	cA	443	THR
1	cA	654	VAL
1	cA	661	SER
1	cA	688	SER
1	cA	731	GLU
1	cA	733	ILE
1	cA	741	LYS
1	cA	754	THR
2	cB	33	SER

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Mol	Chain	Res	Type
2	cB	306	GLU
2	cB	376	SER
2	cB	408	GLU
2	cB	418	MET
2	cB	505	SER
2	cB	511	VAL
2	cB	513	ASN
2	cB	555	LYS
2	cB	562	ASP
5	cE	9	ARG
5	cE	29	GLN
5	cE	37	ILE
5	cE	56	SER
5	cE	57	GLU
6	cI	21	ILE
7	cK	71	GLU
7	cK	82	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	aA	61	HIS
1	aA	138	GLN
1	aA	224	ASN
1	aA	267	ASN
1	aA	338	ASN
1	aA	540	HIS
1	aA	670	GLN
1	aA	755	GLN
2	aB	41	ASN
2	aB	83	ASN
2	aB	111	ASN
2	aB	132	ASN
2	aB	205	GLN
2	aB	211	ASN
2	aB	262	HIS
2	aB	300	ASN
2	aB	309	GLN
2	aB	340	GLN
2	aB	512	ASN
2	aB	620	ASN
2	aB	713	GLN

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Mol	Chain	Res	Type
3	aC	16	GLN
4	aD	52	HIS
4	aD	56	ASN
6	aI	6	GLN
7	aK	48	GLN
8	aL	25	ASN
8	aL	117	GLN
8	aL	143	GLN
8	aL	178	ASN
1	bA	61	HIS
1	bA	138	GLN
1	bA	224	ASN
1	bA	267	ASN
1	bA	338	ASN
1	bA	540	HIS
1	bA	670	GLN
1	bA	755	GLN
2	bB	41	ASN
2	bB	83	ASN
2	bB	111	ASN
2	bB	133	ASN
2	bB	205	GLN
2	bB	262	HIS
2	bB	300	ASN
2	bB	309	GLN
2	bB	340	GLN
2	bB	512	ASN
2	bB	620	ASN
2	bB	713	GLN
3	bC	16	GLN
4	bD	52	HIS
4	bD	56	ASN
6	bI	6	GLN
7	bK	48	GLN
8	bL	25	ASN
8	bL	117	GLN
8	bL	143	GLN
1	cA	61	HIS
1	cA	138	GLN
1	cA	224	ASN
1	cA	267	ASN
1	cA	338	ASN

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Mol	Chain	Res	Type
1	cA	540	HIS
1	cA	670	GLN
1	cA	755	GLN
2	cB	41	ASN
2	cB	83	ASN
2	cB	111	ASN
2	cB	205	GLN
2	cB	262	HIS
2	cB	300	ASN
2	cB	309	GLN
2	cB	340	GLN
2	cB	512	ASN
2	cB	620	ASN
2	cB	713	GLN
3	cC	16	GLN
4	cD	52	HIS
4	cD	56	ASN
5	cE	51	ASN
6	cI	6	GLN
7	cK	48	GLN
8	cL	25	ASN
8	cL	117	GLN
8	cL	143	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 363 ligands modelled in this entry, 15 are unknown and 3 are monoatomic - leaving 345 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	$\#\|Z\| > 2$
14	SF4	aA	846	2,1	0,12,12	-	-	-		
10	CL0	bA	801	1	69,73,73	1.98	20 (28%)	83,113,113	2.81	32 (38%)
14	SF4	cC	101	3	0,12,12	-	-	-		
11	CLA	cA	834	1	69,73,73	1.99	20 (28%)	83,113,113	2.72	32 (38%)
11	CLA	aB	811	2	49,53,73	2.44	21 (42%)	59,89,113	3.08	24 (40%)
11	CLA	cB	823	2	58,62,73	2.18	21 (36%)	69,99,113	2.97	29 (42%)
11	CLA	cA	835	1	69,73,73	2.00	19 (27%)	83,113,113	2.75	28 (33%)
15	BCR	bL	203	-	41,41,41	1.11	3 (7%)	56,56,56	1.23	6 (10%)
11	CLA	aB	823	2	58,62,73	2.18	21 (36%)	69,99,113	2.97	29 (42%)
17	LMT	aA	853	-	36,36,36	0.40	0	47,47,47	1.37	5 (10%)
11	CLA	bB	817	2	64,68,73	2.09	19 (29%)	77,107,113	2.91	29 (37%)
11	CLA	bB	833	2	49,53,73	2.44	20 (40%)	59,89,113	3.20	27 (45%)
11	CLA	bB	808	2	69,73,73	1.97	20 (28%)	83,113,113	2.70	29 (34%)
11	CLA	cA	840	1	69,73,73	2.02	20 (28%)	83,113,113	2.93	33 (39%)
11	CLA	bA	816	1	49,53,73	2.42	20 (40%)	59,89,113	3.10	24 (40%)
11	CLA	cA	842	-	49,53,73	2.42	21 (42%)	59,89,113	3.18	26 (44%)
14	SF4	cC	102	3	0,12,12	-	-	-		
11	CLA	aB	819	2	51,55,73	2.35	21 (41%)	61,91,113	3.00	28 (45%)
15	BCR	cB	848	-	41,41,41	1.00	2 (4%)	56,56,56	1.42	8 (14%)
15	BCR	cB	843	-	41,41,41	1.05	2 (4%)	56,56,56	1.14	3 (5%)
11	CLA	bA	837	1	49,53,73	2.41	21 (42%)	59,89,113	3.21	26 (44%)
11	CLA	cA	805	1	49,53,73	2.44	21 (42%)	59,89,113	3.19	25 (42%)
11	CLA	aB	838	2	51,55,73	2.33	20 (39%)	61,91,113	3.18	27 (44%)
13	PQN	bB	841	-	29,29,34	1.69	2 (6%)	36,39,45	1.17	4 (11%)
11	CLA	cB	813	2	60,64,73	2.15	21 (35%)	72,102,113	2.85	30 (41%)
14	SF4	aC	102	3	0,12,12	-	-	-		
15	BCR	aB	848	-	41,41,41	0.99	2 (4%)	56,56,56	1.42	8 (14%)
11	CLA	bA	802	21	69,73,73	1.98	20 (28%)	83,113,113	2.89	35 (42%)
16	LHG	cA	852	-	48,48,48	0.61	1 (2%)	51,54,54	1.24	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	F6C	cA	827	21	62,64,74	2.66	26 (41%)	69,102,114	4.10	35 (50%)
11	CLA	bA	813	11,1	58,62,73	2.22	20 (34%)	69,99,113	2.90	27 (39%)
11	CLA	bA	805	1	49,53,73	2.45	21 (42%)	59,89,113	3.20	25 (42%)
11	CLA	cB	816	2	63,67,73	2.15	20 (31%)	75,105,113	2.86	30 (40%)
11	CLA	cA	815	1	49,53,73	2.41	20 (40%)	59,89,113	3.09	26 (44%)
11	CLA	cB	839	21	69,73,73	2.00	19 (27%)	83,113,113	2.61	27 (32%)
11	CLA	bB	813	2	60,64,73	2.15	21 (35%)	72,102,113	2.84	30 (41%)
11	CLA	cA	813	11,1	58,62,73	2.22	20 (34%)	69,99,113	2.90	27 (39%)
14	SF4	aC	101	3	0,12,12	-	-	-		
11	CLA	cA	804	1	49,53,73	2.43	20 (40%)	59,89,113	3.14	26 (44%)
11	CLA	cL	205	8	69,73,73	2.00	20 (28%)	83,113,113	2.70	27 (32%)
11	CLA	bA	812	1	69,73,73	2.06	20 (28%)	83,113,113	2.70	28 (33%)
15	BCR	aI	101	-	41,41,41	1.02	2 (4%)	56,56,56	1.23	6 (10%)
12	F6C	bL	202	2	72,74,74	2.49	28 (38%)	81,114,114	3.51	36 (44%)
11	CLA	cB	837	2	59,63,73	2.19	20 (33%)	71,101,113	2.90	28 (39%)
11	CLA	cA	803	-	60,64,73	2.12	19 (31%)	72,102,113	2.96	30 (41%)
11	CLA	cA	822	21	69,73,73	2.02	19 (27%)	83,113,113	2.59	28 (33%)
15	BCR	bL	207	-	41,41,41	1.05	2 (4%)	56,56,56	1.41	9 (16%)
11	CLA	cA	811	11,1	49,53,73	2.44	20 (40%)	59,89,113	3.13	25 (42%)
11	CLA	cB	805	2	69,73,73	2.01	20 (28%)	83,113,113	2.78	30 (36%)
11	CLA	cA	809	1	49,53,73	2.40	21 (42%)	59,89,113	3.20	27 (45%)
11	CLA	cB	838	2	51,55,73	2.33	20 (39%)	61,91,113	3.19	27 (44%)
11	CLA	aA	840	1	69,73,73	2.02	20 (28%)	83,113,113	2.93	32 (38%)
11	CLA	bA	840	1	69,73,73	2.02	20 (28%)	83,113,113	2.93	33 (39%)
11	CLA	aA	821	1	65,69,73	2.06	21 (32%)	78,108,113	2.72	30 (38%)
11	CLA	aB	817	2	64,68,73	2.08	19 (29%)	77,107,113	2.90	29 (37%)
11	CLA	aA	831	1	69,73,73	1.99	19 (27%)	83,113,113	2.68	29 (34%)
15	BCR	bA	847	-	41,41,41	1.03	2 (4%)	56,56,56	1.35	7 (12%)
11	CLA	bA	838	1	55,59,73	2.24	20 (36%)	66,96,113	3.06	33 (50%)
11	CLA	cA	807	1	69,73,73	2.00	20 (28%)	83,113,113	2.79	32 (38%)
11	CLA	cA	838	1	55,59,73	2.24	20 (36%)	66,96,113	3.05	32 (48%)
15	BCR	bB	846	-	41,41,41	1.05	2 (4%)	56,56,56	1.19	5 (8%)
11	CLA	bB	814	2	49,53,73	2.41	21 (42%)	59,89,113	3.17	27 (45%)
11	CLA	aB	802	21	61,65,73	2.13	20 (32%)	73,103,113	3.05	30 (41%)
11	CLA	aB	815	2	59,63,73	2.18	21 (35%)	71,101,113	2.93	28 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	CLA	aL	206	21	69,73,73	2.01	20 (28%)	83,113,113	2.72	30 (36%)
11	CLA	aA	808	1	55,59,73	2.27	21 (38%)	66,96,113	3.10	27 (40%)
11	CLA	cA	810	1	49,53,73	2.38	20 (40%)	59,89,113	3.07	27 (45%)
15	BCR	cM	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.29	7 (12%)
11	CLA	cB	825	2	69,73,73	2.02	20 (28%)	83,113,113	2.78	29 (34%)
11	CLA	aA	842	-	49,53,73	2.42	21 (42%)	59,89,113	3.18	26 (44%)
11	CLA	cA	814	1	69,73,73	2.03	20 (28%)	83,113,113	2.76	30 (36%)
11	CLA	cA	833	1	69,73,73	2.03	20 (28%)	83,113,113	2.71	27 (32%)
11	CLA	bA	829	1	69,73,73	2.03	21 (30%)	83,113,113	4.59	31 (37%)
12	F6C	aA	844	21	72,74,74	2.47	27 (37%)	81,114,114	3.71	37 (45%)
11	CLA	bB	826	2	65,69,73	2.03	21 (32%)	78,108,113	2.86	30 (38%)
17	LMT	cA	853	-	36,36,36	0.39	0	47,47,47	1.37	5 (10%)
15	BCR	bI	101	-	41,41,41	1.02	2 (4%)	56,56,56	1.23	6 (10%)
11	CLA	cA	802	21	69,73,73	1.99	20 (28%)	83,113,113	2.90	35 (42%)
15	BCR	aB	845	-	41,41,41	1.08	2 (4%)	56,56,56	1.25	5 (8%)
15	BCR	aB	843	-	41,41,41	1.05	2 (4%)	56,56,56	1.14	3 (5%)
11	CLA	cB	834	-	49,53,73	2.44	20 (40%)	59,89,113	3.03	25 (42%)
11	CLA	bB	831	2	60,64,73	2.19	20 (33%)	72,102,113	3.08	31 (43%)
11	CLA	bB	811	2	49,53,73	2.45	20 (40%)	59,89,113	3.09	24 (40%)
11	CLA	cB	840	2	49,53,73	2.37	19 (38%)	59,89,113	3.09	24 (40%)
11	CLA	bA	804	1	49,53,73	2.44	20 (40%)	59,89,113	3.15	25 (42%)
15	BCR	bB	843	-	41,41,41	1.04	2 (4%)	56,56,56	1.15	3 (5%)
11	CLA	cB	804	2	54,58,73	2.29	21 (38%)	65,95,113	3.15	32 (49%)
11	CLA	cB	807	2	65,69,73	2.04	20 (30%)	78,108,113	2.82	29 (37%)
11	CLA	aB	835	-	49,53,73	2.43	21 (42%)	59,89,113	3.14	26 (44%)
11	CLA	cA	828	1	64,68,73	2.06	19 (29%)	77,107,113	2.93	31 (40%)
12	F6C	cA	830	1	72,74,74	2.44	26 (36%)	81,114,114	3.64	35 (43%)
11	CLA	bA	821	1	65,69,73	2.07	21 (32%)	78,108,113	2.72	30 (38%)
14	SF4	cA	846	2,1	0,12,12	-	-	-		
11	CLA	aA	818	1	58,62,73	2.15	20 (34%)	69,99,113	3.07	27 (39%)
11	CLA	aA	823	1	49,53,73	2.36	20 (40%)	59,89,113	3.26	24 (40%)
11	CLA	cA	806	1	69,73,73	2.01	20 (28%)	83,113,113	2.82	31 (37%)
11	CLA	aA	815	1	49,53,73	2.41	20 (40%)	59,89,113	3.09	26 (44%)
11	CLA	aB	804	2	54,58,73	2.28	21 (38%)	65,95,113	3.16	32 (49%)
12	F6C	aL	202	2	72,74,74	2.49	28 (38%)	81,114,114	3.51	36 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	CLA	aA	822	21	69,73,73	2.02	19 (27%)	83,113,113	2.60	27 (32%)
11	CLA	cA	836	1	49,53,73	2.31	19 (38%)	59,89,113	2.99	25 (42%)
11	CLA	bA	803	-	60,64,73	2.12	18 (30%)	72,102,113	2.95	30 (41%)
11	CLA	cB	808	2	69,73,73	1.97	20 (28%)	83,113,113	2.70	29 (34%)
11	CLA	aA	810	1	49,53,73	2.38	21 (42%)	59,89,113	3.08	27 (45%)
11	CLA	aB	829	2	49,53,73	2.38	19 (38%)	59,89,113	3.12	27 (45%)
15	BCR	aB	842	-	41,41,41	1.03	2 (4%)	56,56,56	1.24	4 (7%)
11	CLA	bA	809	1	49,53,73	2.40	21 (42%)	59,89,113	3.20	27 (45%)
11	CLA	bA	835	1	69,73,73	2.00	19 (27%)	83,113,113	2.75	28 (33%)
15	BCR	cL	203	-	41,41,41	1.11	3 (7%)	56,56,56	1.24	6 (10%)
11	CLA	aB	813	2	60,64,73	2.15	21 (35%)	72,102,113	2.85	30 (41%)
15	BCR	aA	848	-	41,41,41	1.08	2 (4%)	56,56,56	1.23	5 (8%)
11	CLA	cB	836	2	55,59,73	2.26	20 (36%)	66,96,113	3.04	29 (43%)
15	BCR	bB	848	-	41,41,41	1.00	2 (4%)	56,56,56	1.42	8 (14%)
11	CLA	cB	802	21	61,65,73	2.13	20 (32%)	73,103,113	3.04	30 (41%)
11	CLA	cB	815	2	59,63,73	2.19	21 (35%)	71,101,113	2.93	28 (39%)
11	CLA	cA	825	1	69,73,73	2.00	20 (28%)	83,113,113	2.66	31 (37%)
15	BCR	cB	845	-	41,41,41	1.08	2 (4%)	56,56,56	1.26	5 (8%)
11	CLA	cL	204	8	69,73,73	2.01	21 (30%)	83,113,113	2.73	26 (31%)
10	CL0	aA	801	1	69,73,73	1.99	20 (28%)	83,113,113	2.82	32 (38%)
11	CLA	bA	823	1	49,53,73	2.36	20 (40%)	59,89,113	3.26	24 (40%)
11	CLA	aB	808	2	69,73,73	1.97	20 (28%)	83,113,113	2.71	29 (34%)
15	BCR	aL	207	-	41,41,41	1.05	2 (4%)	56,56,56	1.41	9 (16%)
11	CLA	bB	838	2	51,55,73	2.33	20 (39%)	61,91,113	3.18	27 (44%)
11	CLA	cB	803	-	65,69,73	2.01	20 (30%)	78,108,113	2.80	26 (33%)
11	CLA	aB	801	2	69,73,73	1.94	20 (28%)	83,113,113	2.85	34 (40%)
12	F6C	cB	824	21	64,66,74	2.58	27 (42%)	71,104,114	4.08	36 (50%)
11	CLA	cB	835	-	49,53,73	2.43	21 (42%)	59,89,113	3.15	26 (44%)
11	CLA	cB	811	2	49,53,73	2.44	20 (40%)	59,89,113	3.09	24 (40%)
11	CLA	aA	839	1	69,73,73	1.99	19 (27%)	83,113,113	2.70	29 (34%)
15	BCR	aB	846	-	41,41,41	1.05	2 (4%)	56,56,56	1.19	5 (8%)
13	PQN	cA	845	-	34,34,34	1.60	2 (5%)	42,45,45	1.11	4 (9%)
11	CLA	aB	812	2	69,73,73	2.04	21 (30%)	83,113,113	2.69	31 (37%)
11	CLA	cA	816	1	49,53,73	2.43	21 (42%)	59,89,113	3.11	24 (40%)
11	CLA	aA	824	-	55,59,73	2.26	19 (34%)	66,96,113	3.02	29 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	CLA	aA	820	1	69,73,73	2.01	19 (27%)	83,113,113	2.70	31 (37%)
11	CLA	aB	810	2	49,53,73	2.40	20 (40%)	59,89,113	3.14	27 (45%)
11	CLA	bB	820	2	49,53,73	2.39	20 (40%)	59,89,113	3.19	25 (42%)
15	BCR	bK	102	-	41,41,41	1.04	2 (4%)	56,56,56	1.31	7 (12%)
14	SF4	bA	846	2,1	0,12,12	-	-	-		
12	F6C	cA	826	21	72,74,74	2.51	24 (33%)	81,114,114	3.53	33 (40%)
15	BCR	cB	842	-	41,41,41	1.03	2 (4%)	56,56,56	1.24	4 (7%)
11	CLA	aB	832	2	49,53,73	2.44	21 (42%)	59,89,113	3.17	26 (44%)
11	CLA	cB	819	2	51,55,73	2.35	21 (41%)	61,91,113	3.00	27 (44%)
11	CLA	aB	809	2	51,55,73	2.28	19 (37%)	61,91,113	3.05	26 (42%)
11	CLA	aA	829	1	69,73,73	2.03	21 (30%)	83,113,113	4.59	31 (37%)
17	LMT	bA	853	-	36,36,36	0.40	0	47,47,47	1.37	5 (10%)
11	CLA	bK	101	7	43,46,73	2.33	17 (39%)	51,79,113	3.30	25 (49%)
11	CLA	aA	802	21	69,73,73	1.99	20 (28%)	83,113,113	2.89	35 (42%)
11	CLA	cA	818	1	58,62,73	2.15	20 (34%)	69,99,113	3.08	27 (39%)
18	LMG	bB	847	-	46,46,55	0.82	1 (2%)	54,54,63	1.37	8 (14%)
11	CLA	bB	819	2	51,55,73	2.35	21 (41%)	61,91,113	3.00	27 (44%)
11	CLA	bB	822	2	49,53,73	2.38	18 (36%)	59,89,113	3.32	25 (42%)
11	CLA	bA	819	1	58,62,73	2.21	19 (32%)	69,99,113	3.00	27 (39%)
12	F6C	bA	832	1	57,59,74	2.74	27 (47%)	63,96,114	4.21	36 (57%)
11	CLA	aA	841	1	54,58,73	2.30	21 (38%)	65,95,113	3.07	29 (44%)
11	CLA	aB	807	2	65,69,73	2.04	20 (30%)	78,108,113	2.83	29 (37%)
11	CLA	cK	103	21	55,59,73	2.27	21 (38%)	66,96,113	3.07	28 (42%)
11	CLA	bB	809	2	51,55,73	2.29	20 (39%)	61,91,113	3.06	26 (42%)
11	CLA	cA	821	1	65,69,73	2.07	21 (32%)	78,108,113	2.72	30 (38%)
11	CLA	cB	832	2	49,53,73	2.45	21 (42%)	59,89,113	3.16	26 (44%)
15	BCR	cB	846	-	41,41,41	1.04	2 (4%)	56,56,56	1.19	5 (8%)
11	CLA	aB	822	2	49,53,73	2.38	18 (36%)	59,89,113	3.32	25 (42%)
11	CLA	aB	814	2	49,53,73	2.40	20 (40%)	59,89,113	3.18	27 (45%)
15	BCR	cA	851	-	41,41,41	1.03	2 (4%)	56,56,56	1.24	8 (14%)
11	CLA	cB	812	2	69,73,73	2.03	21 (30%)	83,113,113	2.67	30 (36%)
11	CLA	bA	807	1	69,73,73	2.00	20 (28%)	83,113,113	2.79	32 (38%)
11	CLA	bB	829	2	49,53,73	2.39	19 (38%)	59,89,113	3.13	27 (45%)
11	CLA	aB	837	2	59,63,73	2.18	20 (33%)	71,101,113	2.89	28 (39%)
11	CLA	bA	831	1	69,73,73	2.00	19 (27%)	83,113,113	2.68	29 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	CLA	bB	804	2	54,58,73	2.29	21 (38%)	65,95,113	3.15	32 (49%)
12	F6C	aA	832	1	57,59,74	2.74	27 (47%)	63,96,114	4.21	36 (57%)
13	PQN	cB	841	-	29,29,34	1.70	2 (6%)	36,39,45	1.18	4 (11%)
15	BCR	aL	208	-	41,41,41	1.04	2 (4%)	56,56,56	1.27	8 (14%)
11	CLA	cA	817	21	53,57,73	2.33	21 (39%)	62,93,113	3.01	26 (41%)
11	CLA	bA	839	1	69,73,73	1.99	19 (27%)	83,113,113	2.71	29 (34%)
11	CLA	aB	827	2	69,73,73	1.98	20 (28%)	83,113,113	2.57	27 (32%)
11	CLA	aA	825	1	69,73,73	2.00	20 (28%)	83,113,113	2.66	31 (37%)
11	CLA	cB	828	2	59,63,73	2.19	18 (30%)	71,101,113	2.78	29 (40%)
11	CLA	aB	826	2	65,69,73	2.03	21 (32%)	78,108,113	2.84	30 (38%)
11	CLA	cA	820	1	69,73,73	2.02	19 (27%)	83,113,113	2.70	31 (37%)
12	F6C	aB	824	21	64,66,74	2.59	27 (42%)	71,104,114	4.08	36 (50%)
15	BCR	cI	103	-	41,41,41	1.02	2 (4%)	56,56,56	1.23	6 (10%)
11	CLA	aA	833	1	69,73,73	2.03	20 (28%)	83,113,113	2.71	27 (32%)
11	CLA	cB	831	2	60,64,73	2.19	20 (33%)	72,102,113	3.09	30 (41%)
11	CLA	bB	828	2	59,63,73	2.19	18 (30%)	71,101,113	2.78	28 (39%)
12	F6C	bA	844	21	72,74,74	2.47	27 (37%)	81,114,114	3.72	37 (45%)
11	CLA	aA	807	1	69,73,73	2.00	20 (28%)	83,113,113	2.78	32 (38%)
11	CLA	bB	836	2	55,59,73	2.27	20 (36%)	66,96,113	3.04	29 (43%)
15	BCR	bA	849	-	41,41,41	1.07	2 (4%)	56,56,56	1.29	6 (10%)
11	CLA	cB	809	2	51,55,73	2.28	20 (39%)	61,91,113	3.05	26 (42%)
11	CLA	bB	815	2	59,63,73	2.18	21 (35%)	71,101,113	2.94	28 (39%)
11	CLA	cB	827	2	69,73,73	1.98	20 (28%)	83,113,113	2.58	27 (32%)
15	BCR	cL	207	-	41,41,41	1.06	2 (4%)	56,56,56	1.40	9 (16%)
11	CLA	cA	824	-	55,59,73	2.25	19 (34%)	66,96,113	3.02	30 (45%)
18	LMG	aB	847	-	46,46,55	0.82	1 (2%)	54,54,63	1.37	8 (14%)
15	BCR	aA	849	-	41,41,41	1.07	2 (4%)	56,56,56	1.29	5 (8%)
11	CLA	cB	822	2	49,53,73	2.37	18 (36%)	59,89,113	3.31	25 (42%)
15	BCR	cA	850	-	41,41,41	1.05	2 (4%)	56,56,56	1.20	3 (5%)
11	CLA	bB	803	-	65,69,73	2.01	20 (30%)	78,108,113	2.80	26 (33%)
11	CLA	bB	805	2	69,73,73	2.01	20 (28%)	83,113,113	2.79	30 (36%)
12	F6C	bB	824	21	64,66,74	2.59	27 (42%)	71,104,114	4.08	36 (50%)
11	CLA	bB	835	-	49,53,73	2.43	21 (42%)	59,89,113	3.15	26 (44%)
11	CLA	cA	812	1	69,73,73	2.05	20 (28%)	83,113,113	2.69	29 (34%)
11	CLA	bB	825	2	69,73,73	2.03	20 (28%)	83,113,113	2.78	29 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	CLA	cB	801	2	69,73,73	1.94	20 (28%)	83,113,113	2.84	34 (40%)
11	CLA	aB	803	-	65,69,73	2.01	20 (30%)	78,108,113	2.80	26 (33%)
11	CLA	bA	818	1	58,62,73	2.15	20 (34%)	69,99,113	3.07	27 (39%)
15	BCR	bA	851	-	41,41,41	1.03	2 (4%)	56,56,56	1.23	8 (14%)
11	CLA	bA	815	1	49,53,73	2.41	20 (40%)	59,89,113	3.09	26 (44%)
14	SF4	bC	102	3	0,12,12	-	-	-		
15	BCR	aL	203	-	41,41,41	1.11	3 (7%)	56,56,56	1.25	6 (10%)
11	CLA	cB	829	2	49,53,73	2.38	19 (38%)	59,89,113	3.14	27 (45%)
11	CLA	bL	206	21	69,73,73	2.00	20 (28%)	83,113,113	2.72	29 (34%)
11	CLA	bB	834	-	49,53,73	2.44	20 (40%)	59,89,113	3.03	25 (42%)
11	CLA	aA	806	1	69,73,73	2.01	20 (28%)	83,113,113	2.82	31 (37%)
12	F6C	bA	826	21	72,74,74	2.51	24 (33%)	81,114,114	3.53	33 (40%)
11	CLA	bB	801	2	69,73,73	1.94	19 (27%)	83,113,113	2.84	34 (40%)
15	BCR	bB	845	-	41,41,41	1.08	2 (4%)	56,56,56	1.25	5 (8%)
15	BCR	bB	844	-	41,41,41	1.03	2 (4%)	56,56,56	1.22	5 (8%)
11	CLA	cB	814	2	49,53,73	2.40	20 (40%)	59,89,113	3.17	27 (45%)
15	BCR	bA	848	-	41,41,41	1.08	2 (4%)	56,56,56	1.23	5 (8%)
11	CLA	aB	833	2	49,53,73	2.44	20 (40%)	59,89,113	3.21	27 (45%)
11	CLA	aA	803	-	60,64,73	2.13	18 (30%)	72,102,113	2.96	30 (41%)
11	CLA	bA	814	1	69,73,73	2.03	21 (30%)	83,113,113	2.77	29 (34%)
11	CLA	bA	843	1	55,59,73	2.27	20 (36%)	66,96,113	2.98	28 (42%)
11	CLA	aA	835	1	69,73,73	2.00	19 (27%)	83,113,113	2.75	28 (33%)
11	CLA	cL	206	21	69,73,73	2.00	20 (28%)	83,113,113	2.72	29 (34%)
15	BCR	aA	851	-	41,41,41	1.03	2 (4%)	56,56,56	1.23	8 (14%)
11	CLA	cA	839	1	69,73,73	1.99	19 (27%)	83,113,113	2.70	29 (34%)
18	LMG	cB	847	-	46,46,55	0.82	1 (2%)	54,54,63	1.37	8 (14%)
11	CLA	aB	840	2	49,53,73	2.37	19 (38%)	59,89,113	3.08	24 (40%)
12	F6C	bA	830	1	72,74,74	2.43	25 (34%)	81,114,114	3.64	35 (43%)
12	F6C	cA	844	21	72,74,74	2.47	27 (37%)	81,114,114	3.73	37 (45%)
11	CLA	cB	818	-	69,73,73	2.01	19 (27%)	83,113,113	2.65	25 (30%)
11	CLA	bB	832	2	49,53,73	2.45	21 (42%)	59,89,113	3.17	26 (44%)
12	F6C	aA	830	1	72,74,74	2.43	26 (36%)	81,114,114	3.65	35 (43%)
11	CLA	bA	833	1	69,73,73	2.03	20 (28%)	83,113,113	2.71	27 (32%)
11	CLA	bL	205	8	69,73,73	2.01	20 (28%)	83,113,113	2.70	27 (32%)
11	CLA	cB	830	2	53,57,73	2.33	21 (39%)	62,93,113	3.04	27 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	CLA	aB	818	-	69,73,73	2.01	19 (27%)	83,113,113	2.65	24 (28%)
14	SF4	bC	101	3	0,12,12	-	-	-		
11	CLA	aA	819	1	58,62,73	2.21	20 (34%)	69,99,113	3.01	28 (40%)
11	CLA	bL	204	8	69,73,73	2.01	21 (30%)	83,113,113	2.74	26 (31%)
11	CLA	aA	813	11,1	58,62,73	2.22	20 (34%)	69,99,113	2.90	27 (39%)
11	CLA	bA	820	1	69,73,73	2.01	19 (27%)	83,113,113	2.71	31 (37%)
11	CLA	cB	821	-	59,63,73	2.23	21 (35%)	71,101,113	2.89	27 (38%)
10	CL0	cA	801	1	69,73,73	1.99	20 (28%)	83,113,113	2.82	32 (38%)
11	CLA	cB	810	2	49,53,73	2.39	20 (40%)	59,89,113	3.13	27 (45%)
11	CLA	aB	830	2	53,57,73	2.33	21 (39%)	62,93,113	3.04	26 (41%)
15	BCR	bB	842	-	41,41,41	1.02	2 (4%)	56,56,56	1.24	4 (7%)
11	CLA	bB	810	2	49,53,73	2.39	20 (40%)	59,89,113	3.13	27 (45%)
11	CLA	aK	103	21	55,59,73	2.27	21 (38%)	66,96,113	3.05	28 (42%)
11	CLA	aB	820	2	49,53,73	2.39	20 (40%)	59,89,113	3.21	25 (42%)
16	LHG	aA	852	-	48,48,48	0.61	1 (2%)	51,54,54	1.24	6 (11%)
11	CLA	cB	833	2	49,53,73	2.44	20 (40%)	59,89,113	3.21	27 (45%)
15	BCR	aA	850	-	41,41,41	1.05	2 (4%)	56,56,56	1.20	4 (7%)
15	BCR	bA	850	-	41,41,41	1.04	2 (4%)	56,56,56	1.19	4 (7%)
11	CLA	aL	205	8	69,73,73	2.01	21 (30%)	83,113,113	2.69	27 (32%)
11	CLA	bB	806	2	69,73,73	1.99	19 (27%)	83,113,113	2.72	28 (33%)
11	CLA	bA	817	21	53,57,73	2.33	21 (39%)	62,93,113	3.02	26 (41%)
11	CLA	cB	817	2	64,68,73	2.08	19 (29%)	77,107,113	2.91	30 (38%)
11	CLA	aA	837	1	49,53,73	2.41	21 (42%)	59,89,113	3.21	26 (44%)
11	CLA	bK	103	21	55,59,73	2.27	21 (38%)	66,96,113	3.07	28 (42%)
11	CLA	bB	802	21	61,65,73	2.13	20 (32%)	73,103,113	3.04	30 (41%)
13	PQN	aB	841	-	29,29,34	1.68	2 (6%)	36,39,45	1.17	4 (11%)
15	BCR	aB	844	-	41,41,41	1.02	2 (4%)	56,56,56	1.22	5 (8%)
11	CLA	aA	805	1	49,53,73	2.44	21 (42%)	59,89,113	3.19	25 (42%)
11	CLA	cB	820	2	49,53,73	2.40	20 (40%)	59,89,113	3.20	25 (42%)
15	BCR	aA	847	-	41,41,41	1.04	2 (4%)	56,56,56	1.34	7 (12%)
11	CLA	aA	838	1	55,59,73	2.25	20 (36%)	66,96,113	3.06	31 (46%)
11	CLA	aB	805	2	69,73,73	2.01	20 (28%)	83,113,113	2.79	30 (36%)
11	CLA	bB	812	2	69,73,73	2.04	20 (28%)	83,113,113	2.68	30 (36%)
16	LHG	bA	852	-	48,48,48	0.60	1 (2%)	51,54,54	1.25	6 (11%)
11	CLA	bB	823	2	58,62,73	2.19	21 (36%)	69,99,113	2.98	29 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	CLA	cA	841	1	54,58,73	2.30	21 (38%)	65,95,113	3.07	29 (44%)
11	CLA	cA	843	1	55,59,73	2.27	20 (36%)	66,96,113	2.99	28 (42%)
15	BCR	cA	847	-	41,41,41	1.03	2 (4%)	56,56,56	1.34	7 (12%)
11	CLA	aA	828	1	64,68,73	2.06	19 (29%)	77,107,113	2.92	31 (40%)
11	CLA	bA	828	1	64,68,73	2.06	19 (29%)	77,107,113	2.93	31 (40%)
15	BCR	cA	848	-	41,41,41	1.08	2 (4%)	56,56,56	1.23	5 (8%)
13	PQN	bA	845	-	34,34,34	1.60	2 (5%)	42,45,45	1.10	4 (9%)
11	CLA	bA	825	1	69,73,73	2.00	20 (28%)	83,113,113	2.67	31 (37%)
11	CLA	bB	837	2	59,63,73	2.19	20 (33%)	71,101,113	2.90	28 (39%)
15	BCR	aK	102	-	41,41,41	1.05	2 (4%)	56,56,56	1.31	8 (14%)
12	F6C	cL	202	2	72,74,74	2.49	28 (38%)	81,114,114	3.51	35 (43%)
11	CLA	bA	806	1	69,73,73	2.01	20 (28%)	83,113,113	2.82	31 (37%)
13	PQN	aA	845	-	34,34,34	1.60	2 (5%)	42,45,45	1.11	4 (9%)
11	CLA	cA	823	1	49,53,73	2.36	20 (40%)	59,89,113	3.26	24 (40%)
11	CLA	aB	806	2	69,73,73	2.00	19 (27%)	83,113,113	2.72	28 (33%)
11	CLA	bA	841	1	54,58,73	2.30	21 (38%)	65,95,113	3.07	29 (44%)
11	CLA	bB	840	2	49,53,73	2.37	19 (38%)	59,89,113	3.08	24 (40%)
11	CLA	bB	807	2	65,69,73	2.04	20 (30%)	78,108,113	2.83	29 (37%)
15	BCR	bM	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.29	8 (14%)
11	CLA	aB	836	2	55,59,73	2.26	19 (34%)	66,96,113	3.05	29 (43%)
15	BCR	cB	844	-	41,41,41	1.03	2 (4%)	56,56,56	1.22	5 (8%)
11	CLA	bB	816	2	63,67,73	2.14	20 (31%)	75,105,113	2.85	30 (40%)
11	CLA	bA	834	1	69,73,73	2.00	20 (28%)	83,113,113	2.72	32 (38%)
11	CLA	bA	824	-	55,59,73	2.26	19 (34%)	66,96,113	3.02	30 (45%)
11	CLA	aA	809	1	49,53,73	2.40	21 (42%)	59,89,113	3.21	27 (45%)
11	CLA	aB	821	-	59,63,73	2.23	21 (35%)	71,101,113	2.90	27 (38%)
11	CLA	aA	834	1	69,73,73	2.00	20 (28%)	83,113,113	2.72	32 (38%)
11	CLA	aL	204	8	69,73,73	2.00	21 (30%)	83,113,113	2.73	25 (30%)
11	CLA	cB	806	2	69,73,73	1.99	19 (27%)	83,113,113	2.71	29 (34%)
11	CLA	aB	828	2	59,63,73	2.19	18 (30%)	71,101,113	2.77	30 (42%)
11	CLA	cA	808	1	55,59,73	2.27	21 (38%)	66,96,113	3.10	27 (40%)
12	F6C	bA	827	21	62,64,74	2.66	26 (41%)	69,102,114	4.11	36 (52%)
11	CLA	cA	837	1	49,53,73	2.42	21 (42%)	59,89,113	3.22	26 (44%)
11	CLA	cB	826	2	65,69,73	2.03	21 (32%)	78,108,113	2.85	30 (38%)
11	CLA	aB	834	-	49,53,73	2.45	20 (40%)	59,89,113	3.03	25 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	CLA	bB	818	-	69,73,73	2.01	19 (27%)	83,113,113	2.65	25 (30%)
15	BCR	aM	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.29	7 (12%)
11	CLA	aA	804	1	49,53,73	2.43	20 (40%)	59,89,113	3.13	26 (44%)
11	CLA	aA	812	1	69,73,73	2.06	21 (30%)	83,113,113	2.69	28 (33%)
11	CLA	aA	814	1	69,73,73	2.03	20 (28%)	83,113,113	2.77	30 (36%)
11	CLA	bB	839	21	69,73,73	2.00	19 (27%)	83,113,113	2.61	27 (32%)
11	CLA	aA	843	1	55,59,73	2.28	20 (36%)	66,96,113	2.98	28 (42%)
11	CLA	bB	821	-	59,63,73	2.23	21 (35%)	71,101,113	2.90	27 (38%)
11	CLA	aB	825	2	69,73,73	2.03	20 (28%)	83,113,113	2.77	29 (34%)
15	BCR	bL	208	-	41,41,41	1.04	2 (4%)	56,56,56	1.26	7 (12%)
15	BCR	cA	849	-	41,41,41	1.08	2 (4%)	56,56,56	1.28	5 (8%)
11	CLA	bB	827	2	69,73,73	1.98	20 (28%)	83,113,113	2.58	26 (31%)
11	CLA	bA	842	-	49,53,73	2.41	21 (42%)	59,89,113	3.17	26 (44%)
11	CLA	aB	831	2	60,64,73	2.19	20 (33%)	72,102,113	3.08	31 (43%)
11	CLA	bA	836	1	49,53,73	2.32	19 (38%)	59,89,113	2.99	25 (42%)
11	CLA	bA	808	1	55,59,73	2.27	21 (38%)	66,96,113	3.10	27 (40%)
12	F6C	aA	827	21	62,64,74	2.66	26 (41%)	69,102,114	4.11	36 (52%)
11	CLA	aA	836	1	49,53,73	2.32	19 (38%)	59,89,113	3.00	25 (42%)
11	CLA	aA	817	21	53,57,73	2.33	21 (39%)	62,93,113	3.02	26 (41%)
11	CLA	aB	839	21	69,73,73	1.99	19 (27%)	83,113,113	2.61	27 (32%)
15	BCR	cK	102	-	41,41,41	1.05	2 (4%)	56,56,56	1.30	8 (14%)
15	BCR	cL	208	-	41,41,41	1.04	2 (4%)	56,56,56	1.27	7 (12%)
12	F6C	aA	826	21	72,74,74	2.51	24 (33%)	81,114,114	3.53	33 (40%)
11	CLA	bB	830	2	53,57,73	2.33	21 (39%)	62,93,113	3.04	26 (41%)
11	CLA	cA	829	1	69,73,73	2.03	21 (30%)	83,113,113	4.59	31 (37%)
11	CLA	bA	810	1	49,53,73	2.38	21 (42%)	59,89,113	3.08	27 (45%)
11	CLA	cK	101	7	43,46,73	2.33	17 (39%)	51,79,113	3.30	25 (49%)
11	CLA	aK	101	7	43,46,73	2.34	17 (39%)	51,79,113	3.30	25 (49%)
11	CLA	bA	822	21	69,73,73	2.02	19 (27%)	83,113,113	2.60	27 (32%)
11	CLA	cA	819	1	58,62,73	2.21	20 (34%)	69,99,113	3.00	28 (40%)
11	CLA	aA	816	1	49,53,73	2.42	21 (42%)	59,89,113	3.11	24 (40%)
12	F6C	cA	832	1	57,59,74	2.74	27 (47%)	63,96,114	4.20	36 (57%)
11	CLA	bA	811	11,1	49,53,73	2.43	20 (40%)	59,89,113	3.12	24 (40%)
11	CLA	cA	831	1	69,73,73	1.99	18 (26%)	83,113,113	2.67	29 (34%)
11	CLA	aA	811	11,1	49,53,73	2.43	20 (40%)	59,89,113	3.11	24 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	CLA	aB	816	2	63,67,73	2.15	20 (31%)	75,105,113	2.86	30 (40%)

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
14	SF4	aA	846	2,1	-	-	0/6/5/5
10	CL0	bA	801	1	-	5/39/115/115	-
14	SF4	cC	101	3	-	-	0/6/5/5
11	CLA	cA	834	1	-	9/39/115/115	-
11	CLA	aB	811	2	-	5/15/91/115	-
11	CLA	cB	823	2	-	9/26/102/115	-
11	CLA	cA	835	1	-	13/39/115/115	-
15	BCR	bL	203	-	-	8/29/63/63	0/2/2/2
11	CLA	aB	823	2	-	9/26/102/115	-
17	LMT	aA	853	-	-	12/21/61/61	0/2/2/2
11	CLA	bB	817	2	-	14/33/109/115	-
11	CLA	bB	833	2	-	5/15/91/115	-
11	CLA	bB	808	2	-	11/39/115/115	-
11	CLA	cA	840	1	-	19/39/115/115	-
11	CLA	bA	816	1	-	5/15/91/115	-
11	CLA	cA	842	-	-	8/15/91/115	-
14	SF4	cC	102	3	-	-	0/6/5/5
11	CLA	aB	819	2	-	9/18/94/115	-
15	BCR	cB	848	-	-	18/29/63/63	0/2/2/2
15	BCR	cB	843	-	-	9/29/63/63	0/2/2/2
11	CLA	bA	837	1	-	6/15/91/115	-
11	CLA	cA	805	1	-	8/15/91/115	-
11	CLA	aB	838	2	-	5/18/94/115	-
13	PQN	bB	841	-	-	2/17/37/43	0/2/2/2
11	CLA	cB	813	2	-	10/29/105/115	-
14	SF4	aC	102	3	-	-	0/6/5/5
15	BCR	aB	848	-	-	18/29/63/63	0/2/2/2
11	CLA	bA	802	21	-	6/39/115/115	-
16	LHG	cA	852	-	-	27/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	F6C	cA	827	21	2/2/8/16	11/29/85/97	-
11	CLA	bA	813	11,1	-	8/26/102/115	-
11	CLA	bA	805	1	-	8/15/91/115	-
11	CLA	cB	816	2	-	12/32/108/115	-
11	CLA	cA	815	1	-	5/15/91/115	-
11	CLA	cB	839	21	-	10/39/115/115	-
11	CLA	bB	813	2	-	10/29/105/115	-
11	CLA	cA	813	11,1	-	8/26/102/115	-
14	SF4	aC	101	3	-	-	0/6/5/5
11	CLA	cA	804	1	-	11/15/91/115	-
11	CLA	cL	205	8	-	15/39/115/115	-
11	CLA	bA	812	1	-	13/39/115/115	-
15	BCR	aI	101	-	-	11/29/63/63	0/2/2/2
12	F6C	bL	202	2	1/1/10/16	16/41/97/97	-
11	CLA	cB	837	2	-	8/27/103/115	-
11	CLA	cA	803	-	-	7/29/105/115	-
11	CLA	cA	822	21	-	19/39/115/115	-
15	BCR	bL	207	-	-	9/29/63/63	0/2/2/2
11	CLA	cA	811	11,1	-	5/15/91/115	-
11	CLA	cB	805	2	-	13/39/115/115	-
11	CLA	cA	809	1	-	8/15/91/115	-
11	CLA	cB	838	2	-	5/18/94/115	-
11	CLA	aA	840	1	-	19/39/115/115	-
11	CLA	bA	840	1	-	19/39/115/115	-
11	CLA	aA	821	1	-	16/35/111/115	-
11	CLA	aB	817	2	-	14/33/109/115	-
11	CLA	aA	831	1	-	12/39/115/115	-
15	BCR	bA	847	-	-	9/29/63/63	0/2/2/2
11	CLA	bA	838	1	-	9/23/99/115	-
11	CLA	cA	807	1	-	18/39/115/115	-
11	CLA	cA	838	1	-	9/23/99/115	-
15	BCR	bB	846	-	-	13/29/63/63	0/2/2/2
11	CLA	bB	814	2	-	6/15/91/115	-
11	CLA	aB	802	21	-	10/30/106/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	aB	815	2	-	13/27/103/115	-
11	CLA	aL	206	21	-	15/39/115/115	-
11	CLA	aA	808	1	-	5/23/99/115	-
11	CLA	cA	810	1	-	4/15/91/115	-
15	BCR	cM	101	-	-	7/29/63/63	0/2/2/2
11	CLA	cB	825	2	-	10/39/115/115	-
11	CLA	aA	842	-	-	8/15/91/115	-
11	CLA	cA	814	1	-	14/39/115/115	-
11	CLA	cA	833	1	-	14/39/115/115	-
11	CLA	bA	829	1	-	12/39/115/115	-
12	F6C	aA	844	21	1/1/10/16	13/41/97/97	-
11	CLA	bB	826	2	-	12/35/111/115	-
17	LMT	cA	853	-	-	12/21/61/61	0/2/2/2
15	BCR	bI	101	-	-	11/29/63/63	0/2/2/2
11	CLA	cA	802	21	-	6/39/115/115	-
15	BCR	aB	845	-	-	9/29/63/63	0/2/2/2
15	BCR	aB	843	-	-	9/29/63/63	0/2/2/2
11	CLA	cB	834	-	-	6/15/91/115	-
11	CLA	bB	831	2	-	7/29/105/115	-
11	CLA	bB	811	2	-	5/15/91/115	-
11	CLA	cB	840	2	-	5/15/91/115	-
11	CLA	bA	804	1	-	11/15/91/115	-
15	BCR	bB	843	-	-	9/29/63/63	0/2/2/2
11	CLA	cB	804	2	-	8/21/97/115	-
11	CLA	cB	807	2	-	3/35/111/115	-
12	F6C	cA	830	1	1/1/10/16	7/41/97/97	-
11	CLA	aB	835	-	-	4/15/91/115	-
11	CLA	cA	828	1	-	12/33/109/115	-
11	CLA	bA	821	1	-	16/35/111/115	-
14	SF4	cA	846	2,1	-	-	0/6/5/5
11	CLA	aA	818	1	-	10/26/102/115	-
11	CLA	aA	823	1	-	9/15/91/115	-
11	CLA	cA	806	1	-	16/39/115/115	-
11	CLA	aA	815	1	-	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	aB	804	2	-	8/21/97/115	-
12	F6C	aL	202	2	1/1/10/16	16/41/97/97	-
11	CLA	aA	822	21	-	19/39/115/115	-
11	CLA	cA	836	1	-	6/15/91/115	-
11	CLA	bA	803	-	-	7/29/105/115	-
11	CLA	cB	808	2	-	10/39/115/115	-
11	CLA	aA	810	1	-	4/15/91/115	-
11	CLA	aB	829	2	-	6/15/91/115	-
15	BCR	aB	842	-	-	15/29/63/63	0/2/2/2
11	CLA	bA	809	1	-	8/15/91/115	-
11	CLA	bA	835	1	-	13/39/115/115	-
15	BCR	cL	203	-	-	8/29/63/63	0/2/2/2
11	CLA	aB	813	2	-	10/29/105/115	-
15	BCR	aA	848	-	-	13/29/63/63	0/2/2/2
11	CLA	cB	836	2	-	10/23/99/115	-
15	BCR	bB	848	-	-	18/29/63/63	0/2/2/2
11	CLA	cB	802	21	-	10/30/106/115	-
11	CLA	cB	815	2	-	13/27/103/115	-
11	CLA	cA	825	1	-	14/39/115/115	-
15	BCR	cB	845	-	-	9/29/63/63	0/2/2/2
11	CLA	cL	204	8	-	5/39/115/115	-
10	CL0	aA	801	1	-	5/39/115/115	-
11	CLA	bA	823	1	-	9/15/91/115	-
11	CLA	aB	808	2	-	11/39/115/115	-
15	BCR	aL	207	-	-	9/29/63/63	0/2/2/2
11	CLA	bB	838	2	-	5/18/94/115	-
11	CLA	cB	803	-	-	7/35/111/115	-
11	CLA	aB	801	2	-	11/39/115/115	-
12	F6C	cB	824	21	1/1/8/16	9/32/88/97	-
11	CLA	cB	835	-	-	4/15/91/115	-
11	CLA	cB	811	2	-	5/15/91/115	-
11	CLA	aA	839	1	-	7/39/115/115	-
15	BCR	aB	846	-	-	13/29/63/63	0/2/2/2
13	PQN	cA	845	-	-	3/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	aB	812	2	-	18/39/115/115	-
11	CLA	cA	816	1	-	5/15/91/115	-
11	CLA	aA	824	-	-	12/23/99/115	-
11	CLA	aA	820	1	-	12/39/115/115	-
11	CLA	aB	810	2	-	7/15/91/115	-
11	CLA	bB	820	2	-	8/15/91/115	-
15	BCR	bK	102	-	-	8/29/63/63	0/2/2/2
14	SF4	bA	846	2,1	-	-	0/6/5/5
12	F6C	cA	826	21	1/1/10/16	11/41/97/97	-
15	BCR	cB	842	-	-	15/29/63/63	0/2/2/2
11	CLA	aB	832	2	-	9/15/91/115	-
11	CLA	cB	819	2	-	9/18/94/115	-
11	CLA	aB	809	2	-	11/18/94/115	-
11	CLA	aA	829	1	-	12/39/115/115	-
17	LMT	bA	853	-	-	12/21/61/61	0/2/2/2
11	CLA	bK	101	7	-	2/6/78/115	-
11	CLA	aA	802	21	-	6/39/115/115	-
11	CLA	cA	818	1	-	10/26/102/115	-
18	LMG	bB	847	-	-	17/41/61/70	0/1/1/1
11	CLA	bB	819	2	-	9/18/94/115	-
11	CLA	bB	822	2	-	8/15/91/115	-
11	CLA	bA	819	1	-	12/26/102/115	-
12	F6C	bA	832	1	1/1/7/16	11/23/79/97	-
11	CLA	aA	841	1	-	6/21/97/115	-
11	CLA	aB	807	2	-	3/35/111/115	-
11	CLA	cK	103	21	-	6/23/99/115	-
11	CLA	bB	809	2	-	11/18/94/115	-
11	CLA	cA	821	1	-	16/35/111/115	-
11	CLA	cB	832	2	-	9/15/91/115	-
15	BCR	cB	846	-	-	13/29/63/63	0/2/2/2
11	CLA	aB	822	2	-	8/15/91/115	-
11	CLA	aB	814	2	-	6/15/91/115	-
15	BCR	cA	851	-	-	20/29/63/63	0/2/2/2
11	CLA	cB	812	2	-	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	bA	807	1	-	18/39/115/115	-
11	CLA	bB	829	2	-	6/15/91/115	-
11	CLA	aB	837	2	-	8/27/103/115	-
11	CLA	bA	831	1	-	12/39/115/115	-
11	CLA	bB	804	2	-	8/21/97/115	-
12	F6C	aA	832	1	1/1/7/16	11/23/79/97	-
13	PQN	cB	841	-	-	2/17/37/43	0/2/2/2
15	BCR	aL	208	-	-	7/29/63/63	0/2/2/2
11	CLA	cA	817	21	-	7/20/96/115	-
11	CLA	bA	839	1	-	7/39/115/115	-
11	CLA	aB	827	2	-	10/39/115/115	-
11	CLA	aA	825	1	-	14/39/115/115	-
11	CLA	cB	828	2	-	7/27/103/115	-
11	CLA	aB	826	2	-	12/35/111/115	-
11	CLA	cA	820	1	-	12/39/115/115	-
12	F6C	aB	824	21	1/1/8/16	9/32/88/97	-
15	BCR	cI	103	-	-	11/29/63/63	0/2/2/2
11	CLA	aA	833	1	-	14/39/115/115	-
11	CLA	cB	831	2	-	7/29/105/115	-
11	CLA	bB	828	2	-	7/27/103/115	-
12	F6C	bA	844	21	1/1/10/16	13/41/97/97	-
11	CLA	aA	807	1	-	18/39/115/115	-
11	CLA	bB	836	2	-	10/23/99/115	-
15	BCR	bA	849	-	-	12/29/63/63	0/2/2/2
11	CLA	cB	809	2	-	11/18/94/115	-
11	CLA	bB	815	2	-	13/27/103/115	-
11	CLA	cB	827	2	-	10/39/115/115	-
15	BCR	cL	207	-	-	9/29/63/63	0/2/2/2
11	CLA	cA	824	-	-	12/23/99/115	-
18	LMG	aB	847	-	-	17/41/61/70	0/1/1/1
15	BCR	aA	849	-	-	12/29/63/63	0/2/2/2
11	CLA	cB	822	2	-	8/15/91/115	-
15	BCR	cA	850	-	-	6/29/63/63	0/2/2/2
11	CLA	bB	803	-	-	7/35/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	bB	805	2	-	13/39/115/115	-
12	F6C	bB	824	21	1/1/8/16	9/32/88/97	-
11	CLA	bB	835	-	-	4/15/91/115	-
11	CLA	cA	812	1	-	13/39/115/115	-
11	CLA	bB	825	2	-	10/39/115/115	-
11	CLA	cB	801	2	-	11/39/115/115	-
11	CLA	aB	803	-	-	7/35/111/115	-
11	CLA	bA	818	1	-	10/26/102/115	-
15	BCR	bA	851	-	-	20/29/63/63	0/2/2/2
11	CLA	bA	815	1	-	5/15/91/115	-
14	SF4	bC	102	3	-	-	0/6/5/5
15	BCR	aL	203	-	-	8/29/63/63	0/2/2/2
11	CLA	cB	829	2	-	6/15/91/115	-
11	CLA	bL	206	21	-	15/39/115/115	-
11	CLA	bB	834	-	-	7/15/91/115	-
11	CLA	aA	806	1	-	16/39/115/115	-
12	F6C	bA	826	21	1/1/10/16	11/41/97/97	-
11	CLA	bB	801	2	-	11/39/115/115	-
15	BCR	bB	845	-	-	9/29/63/63	0/2/2/2
15	BCR	bB	844	-	-	11/29/63/63	0/2/2/2
11	CLA	cB	814	2	-	6/15/91/115	-
15	BCR	bA	848	-	-	13/29/63/63	0/2/2/2
11	CLA	aB	833	2	-	5/15/91/115	-
11	CLA	aA	803	-	-	7/29/105/115	-
11	CLA	bA	814	1	-	14/39/115/115	-
11	CLA	bA	843	1	-	9/23/99/115	-
11	CLA	aA	835	1	-	13/39/115/115	-
11	CLA	cL	206	21	-	15/39/115/115	-
15	BCR	aA	851	-	-	20/29/63/63	0/2/2/2
11	CLA	cA	839	1	-	7/39/115/115	-
18	LMG	cB	847	-	-	17/41/61/70	0/1/1/1
12	F6C	bA	830	1	1/1/10/16	7/41/97/97	-
11	CLA	aB	840	2	-	5/15/91/115	-
12	F6C	cA	844	21	1/1/10/16	13/41/97/97	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	cB	818	-	-	8/39/115/115	-
11	CLA	bB	832	2	-	9/15/91/115	-
12	F6C	aA	830	1	1/1/10/16	7/41/97/97	-
11	CLA	bA	833	1	-	14/39/115/115	-
11	CLA	bL	205	8	-	15/39/115/115	-
11	CLA	cB	830	2	-	9/20/96/115	-
11	CLA	aB	818	-	-	8/39/115/115	-
14	SF4	bC	101	3	-	-	0/6/5/5
11	CLA	aA	819	1	-	12/26/102/115	-
11	CLA	bL	204	8	-	5/39/115/115	-
11	CLA	aA	813	11,1	-	8/26/102/115	-
11	CLA	bA	820	1	-	12/39/115/115	-
11	CLA	cB	821	-	-	10/27/103/115	-
10	CL0	cA	801	1	-	5/39/115/115	-
11	CLA	cB	810	2	-	7/15/91/115	-
11	CLA	aB	830	2	-	9/20/96/115	-
15	BCR	bB	842	-	-	15/29/63/63	0/2/2/2
11	CLA	bB	810	2	-	7/15/91/115	-
11	CLA	aK	103	21	-	6/23/99/115	-
11	CLA	aB	820	2	-	8/15/91/115	-
16	LHG	aA	852	-	-	27/53/53/53	-
11	CLA	cB	833	2	-	5/15/91/115	-
15	BCR	aA	850	-	-	6/29/63/63	0/2/2/2
15	BCR	bA	850	-	-	6/29/63/63	0/2/2/2
11	CLA	aL	205	8	-	15/39/115/115	-
11	CLA	bB	806	2	-	20/39/115/115	-
11	CLA	bA	817	21	-	7/20/96/115	-
11	CLA	cB	817	2	-	14/33/109/115	-
11	CLA	aA	837	1	-	6/15/91/115	-
11	CLA	bK	103	21	-	6/23/99/115	-
11	CLA	bB	802	21	-	10/30/106/115	-
13	PQN	aB	841	-	-	2/17/37/43	0/2/2/2
15	BCR	aB	844	-	-	11/29/63/63	0/2/2/2
11	CLA	aA	805	1	-	8/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	cB	820	2	-	8/15/91/115	-
15	BCR	aA	847	-	-	9/29/63/63	0/2/2/2
11	CLA	aA	838	1	-	9/23/99/115	-
11	CLA	aB	805	2	-	13/39/115/115	-
11	CLA	bB	812	2	-	18/39/115/115	-
16	LHG	bA	852	-	-	27/53/53/53	-
11	CLA	bB	823	2	-	9/26/102/115	-
11	CLA	cA	841	1	-	6/21/97/115	-
11	CLA	cA	843	1	-	9/23/99/115	-
15	BCR	cA	847	-	-	9/29/63/63	0/2/2/2
11	CLA	aA	828	1	-	12/33/109/115	-
11	CLA	bA	828	1	-	12/33/109/115	-
15	BCR	cA	848	-	-	13/29/63/63	0/2/2/2
13	PQN	bA	845	-	-	3/23/43/43	0/2/2/2
11	CLA	bA	825	1	-	14/39/115/115	-
11	CLA	bB	837	2	-	8/27/103/115	-
15	BCR	aK	102	-	-	8/29/63/63	0/2/2/2
12	F6C	cL	202	2	1/1/10/16	16/41/97/97	-
11	CLA	bA	806	1	-	16/39/115/115	-
13	PQN	aA	845	-	-	3/23/43/43	0/2/2/2
11	CLA	cA	823	1	-	9/15/91/115	-
11	CLA	aB	806	2	-	20/39/115/115	-
11	CLA	bA	841	1	-	6/21/97/115	-
11	CLA	bB	840	2	-	5/15/91/115	-
11	CLA	bB	807	2	-	3/35/111/115	-
15	BCR	bM	101	-	-	7/29/63/63	0/2/2/2
11	CLA	aB	836	2	-	10/23/99/115	-
15	BCR	cB	844	-	-	11/29/63/63	0/2/2/2
11	CLA	bB	816	2	-	12/32/108/115	-
11	CLA	bA	834	1	-	9/39/115/115	-
11	CLA	bA	824	-	-	12/23/99/115	-
11	CLA	aA	809	1	-	8/15/91/115	-
11	CLA	aB	821	-	-	10/27/103/115	-
11	CLA	aA	834	1	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	aL	204	8	-	5/39/115/115	-
11	CLA	cB	806	2	-	20/39/115/115	-
11	CLA	aB	828	2	-	7/27/103/115	-
11	CLA	cA	808	1	-	5/23/99/115	-
12	F6C	bA	827	21	2/2/8/16	11/29/85/97	-
11	CLA	cA	837	1	-	6/15/91/115	-
11	CLA	cB	826	2	-	12/35/111/115	-
11	CLA	aB	834	-	-	7/15/91/115	-
11	CLA	bB	818	-	-	8/39/115/115	-
15	BCR	aM	101	-	-	7/29/63/63	0/2/2/2
11	CLA	aA	804	1	-	11/15/91/115	-
11	CLA	aA	812	1	-	13/39/115/115	-
11	CLA	aA	814	1	-	14/39/115/115	-
11	CLA	bB	839	21	-	10/39/115/115	-
11	CLA	aA	843	1	-	9/23/99/115	-
11	CLA	bB	821	-	-	10/27/103/115	-
11	CLA	aB	825	2	-	10/39/115/115	-
15	BCR	bL	208	-	-	7/29/63/63	0/2/2/2
15	BCR	cA	849	-	-	12/29/63/63	0/2/2/2
11	CLA	bB	827	2	-	10/39/115/115	-
11	CLA	bA	842	-	-	8/15/91/115	-
11	CLA	aB	831	2	-	7/29/105/115	-
11	CLA	bA	836	1	-	6/15/91/115	-
11	CLA	bA	808	1	-	5/23/99/115	-
12	F6C	aA	827	21	2/2/8/16	11/29/85/97	-
11	CLA	aA	836	1	-	6/15/91/115	-
11	CLA	aA	817	21	-	7/20/96/115	-
11	CLA	aB	839	21	-	10/39/115/115	-
15	BCR	cK	102	-	-	8/29/63/63	0/2/2/2
15	BCR	cL	208	-	-	7/29/63/63	0/2/2/2
12	F6C	aA	826	21	1/1/10/16	11/41/97/97	-
11	CLA	bB	830	2	-	9/20/96/115	-
11	CLA	cA	829	1	-	12/39/115/115	-
11	CLA	bA	810	1	-	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	cK	101	7	-	2/6/78/115	-
11	CLA	aK	101	7	-	2/6/78/115	-
11	CLA	bA	822	21	-	19/39/115/115	-
11	CLA	cA	819	1	-	12/26/102/115	-
11	CLA	aA	816	1	-	5/15/91/115	-
12	F6C	cA	832	1	1/1/7/16	11/23/79/97	-
11	CLA	bA	811	11,1	-	5/15/91/115	-
11	CLA	cA	831	1	-	12/39/115/115	-
11	CLA	aA	811	11,1	-	5/15/91/115	-
11	CLA	aB	816	2	-	12/32/108/115	-

All (5655) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cA	826	F6C	C2A-C3A	8.12	1.54	1.36
12	bA	826	F6C	C2A-C3A	8.11	1.54	1.36
12	cA	826	F6C	C1A-CHA	8.11	1.50	1.35
12	aA	826	F6C	C2A-C3A	8.09	1.53	1.36
12	bA	826	F6C	C1A-CHA	8.08	1.50	1.35
12	aA	826	F6C	C1A-CHA	8.08	1.50	1.35
12	aL	202	F6C	C2A-C3A	8.03	1.53	1.36
12	bL	202	F6C	C2A-C3A	8.02	1.53	1.36
12	cL	202	F6C	C2A-C3A	8.02	1.53	1.36
12	bL	202	F6C	C1A-CHA	8.01	1.50	1.35
12	cL	202	F6C	C1A-CHA	8.00	1.50	1.35
12	aL	202	F6C	C1A-CHA	7.96	1.50	1.35
12	aA	827	F6C	C1A-CHA	7.71	1.49	1.35
12	cA	830	F6C	C1A-CHA	7.70	1.49	1.35
12	aA	830	F6C	C1A-CHA	7.69	1.49	1.35
12	bA	830	F6C	C1A-CHA	7.69	1.49	1.35
12	cA	827	F6C	C1A-CHA	7.68	1.49	1.35
12	bA	827	F6C	C1A-CHA	7.66	1.49	1.35
12	aB	824	F6C	C1A-CHA	7.62	1.49	1.35
12	aA	832	F6C	C1A-CHA	7.62	1.49	1.35
12	bB	824	F6C	C1A-CHA	7.61	1.49	1.35
12	cB	824	F6C	C1A-CHA	7.61	1.49	1.35
13	cA	845	PQN	C3-C2	7.61	1.49	1.35
13	aA	845	PQN	C3-C2	7.58	1.49	1.35
12	bA	832	F6C	C1A-CHA	7.58	1.49	1.35
13	bA	845	PQN	C3-C2	7.57	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cA	832	F6C	C1A-CHA	7.57	1.49	1.35
12	aA	844	F6C	C1A-CHA	7.57	1.49	1.35
12	cA	844	F6C	C1A-CHA	7.54	1.49	1.35
12	bA	844	F6C	C1A-CHA	7.54	1.49	1.35
13	cB	841	PQN	C3-C2	7.38	1.48	1.35
13	bB	841	PQN	C3-C2	7.35	1.48	1.35
13	aB	841	PQN	C3-C2	7.31	1.48	1.35
12	bA	827	F6C	C1A-NA	-7.28	1.27	1.37
12	aA	827	F6C	C1A-NA	-7.25	1.27	1.37
12	cA	827	F6C	C1A-NA	-7.24	1.27	1.37
12	bA	832	F6C	C2A-C3A	7.21	1.52	1.36
12	cA	832	F6C	C2A-C3A	7.20	1.52	1.36
12	aA	832	F6C	C2A-C3A	7.18	1.52	1.36
12	aA	830	F6C	C2A-C3A	7.13	1.51	1.36
12	cA	830	F6C	C2A-C3A	7.09	1.51	1.36
12	bA	830	F6C	C2A-C3A	7.08	1.51	1.36
12	bA	827	F6C	C2A-C3A	7.06	1.51	1.36
12	aA	827	F6C	C2A-C3A	7.04	1.51	1.36
12	bB	824	F6C	C1A-NA	-7.04	1.28	1.37
12	cA	844	F6C	C1A-NA	-7.03	1.28	1.37
12	cA	844	F6C	C2A-C3A	7.03	1.51	1.36
12	cA	827	F6C	C2A-C3A	7.03	1.51	1.36
12	aA	844	F6C	C1A-NA	-7.01	1.28	1.37
12	bA	844	F6C	C2A-C3A	6.99	1.51	1.36
12	cB	824	F6C	C1A-NA	-6.99	1.28	1.37
12	aA	844	F6C	C2A-C3A	6.99	1.51	1.36
12	aB	824	F6C	C1A-NA	-6.98	1.28	1.37
12	bA	844	F6C	C1A-NA	-6.96	1.28	1.37
12	aB	824	F6C	C2A-C3A	6.94	1.51	1.36
12	cB	824	F6C	C2A-C3A	6.93	1.51	1.36
12	bB	824	F6C	C2A-C3A	6.90	1.51	1.36
12	bA	830	F6C	C1A-NA	-6.82	1.28	1.37
12	aA	832	F6C	C1A-NA	-6.82	1.28	1.37
12	cA	830	F6C	C1A-NA	-6.82	1.28	1.37
12	cA	832	F6C	C1A-NA	-6.80	1.28	1.37
12	aA	830	F6C	C1A-NA	-6.78	1.28	1.37
12	bA	832	F6C	C1A-NA	-6.77	1.28	1.37
12	cL	202	F6C	C1A-NA	-6.41	1.28	1.37
12	aL	202	F6C	C1A-NA	-6.41	1.28	1.37
12	bL	202	F6C	C1A-NA	-6.34	1.29	1.37
12	aA	826	F6C	C1A-NA	-6.29	1.29	1.37
12	bA	826	F6C	C1A-NA	-6.26	1.29	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cA	826	F6C	C1A-NA	-6.22	1.29	1.37
11	bB	825	CLA	C3C-C2C	5.51	1.48	1.36
11	cB	825	CLA	C3C-C2C	5.50	1.48	1.36
11	aB	825	CLA	C3C-C2C	5.49	1.48	1.36
11	bB	811	CLA	C3C-C2C	5.47	1.48	1.36
11	aB	811	CLA	C3C-C2C	5.47	1.48	1.36
11	cB	811	CLA	C3C-C2C	5.47	1.48	1.36
11	bB	821	CLA	C3C-C2C	5.43	1.48	1.36
11	aB	821	CLA	C3C-C2C	5.42	1.48	1.36
11	cB	821	CLA	C3C-C2C	5.41	1.48	1.36
11	cA	816	CLA	C3C-C2C	5.39	1.48	1.36
11	aB	833	CLA	C3C-C2C	5.38	1.48	1.36
11	cB	833	CLA	C3C-C2C	5.38	1.48	1.36
11	aB	832	CLA	C3C-C2C	5.38	1.48	1.36
11	bB	836	CLA	C3C-C2C	5.37	1.48	1.36
11	cB	816	CLA	C3C-C2C	5.37	1.48	1.36
11	bB	832	CLA	C3C-C2C	5.37	1.48	1.36
11	bA	816	CLA	C3C-C2C	5.37	1.48	1.36
11	bB	833	CLA	C3C-C2C	5.36	1.48	1.36
11	aB	836	CLA	C3C-C2C	5.36	1.48	1.36
11	cB	836	CLA	C3C-C2C	5.35	1.48	1.36
11	aA	816	CLA	C3C-C2C	5.35	1.48	1.36
11	cB	834	CLA	C3C-C2C	5.35	1.48	1.36
11	aB	834	CLA	C3C-C2C	5.35	1.48	1.36
11	bB	816	CLA	C3C-C2C	5.34	1.48	1.36
11	cB	835	CLA	C3C-C2C	5.34	1.48	1.36
11	bA	837	CLA	C3C-C2C	5.33	1.48	1.36
11	aB	816	CLA	C3C-C2C	5.33	1.48	1.36
11	cB	830	CLA	C3C-C2C	5.32	1.48	1.36
11	bB	834	CLA	C3C-C2C	5.32	1.48	1.36
11	bB	830	CLA	C3C-C2C	5.32	1.48	1.36
11	aA	842	CLA	C3C-C2C	5.32	1.48	1.36
11	bA	812	CLA	C3C-C2C	5.32	1.48	1.36
11	bA	817	CLA	C3C-C2C	5.32	1.48	1.36
11	cA	842	CLA	C3C-C2C	5.32	1.48	1.36
11	aA	808	CLA	C3C-C2C	5.31	1.48	1.36
11	bA	811	CLA	C3C-C2C	5.31	1.48	1.36
11	aB	838	CLA	C3C-C2C	5.31	1.48	1.36
11	bB	835	CLA	C3C-C2C	5.31	1.48	1.36
11	aB	830	CLA	C3C-C2C	5.31	1.48	1.36
11	bA	841	CLA	C3C-C2C	5.31	1.48	1.36
11	cB	832	CLA	C3C-C2C	5.31	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	cB	838	CLA	C3C-C2C	5.31	1.48	1.36
11	bK	103	CLA	C3C-C2C	5.31	1.48	1.36
11	cA	812	CLA	C3C-C2C	5.31	1.48	1.36
11	aA	817	CLA	C3C-C2C	5.30	1.48	1.36
11	cA	811	CLA	C3C-C2C	5.30	1.48	1.36
11	aK	103	CLA	C3C-C2C	5.30	1.48	1.36
11	cA	804	CLA	C3C-C2C	5.30	1.48	1.36
11	bA	824	CLA	C3C-C2C	5.30	1.48	1.36
11	cA	808	CLA	C3C-C2C	5.30	1.48	1.36
11	bB	814	CLA	C3C-C2C	5.30	1.48	1.36
11	aL	206	CLA	C3C-C2C	5.30	1.48	1.36
11	aA	841	CLA	C3C-C2C	5.29	1.48	1.36
11	aB	835	CLA	C3C-C2C	5.29	1.48	1.36
11	bB	831	CLA	C3C-C2C	5.29	1.48	1.36
11	aA	811	CLA	C3C-C2C	5.29	1.48	1.36
11	cA	837	CLA	C3C-C2C	5.29	1.48	1.36
11	cA	841	CLA	C3C-C2C	5.29	1.48	1.36
11	cK	103	CLA	C3C-C2C	5.29	1.48	1.36
11	bA	842	CLA	C3C-C2C	5.29	1.48	1.36
11	aA	837	CLA	C3C-C2C	5.29	1.48	1.36
11	aA	831	CLA	C3C-C2C	5.29	1.48	1.36
10	aA	801	CL0	C3C-C2C	5.28	1.48	1.36
11	cA	817	CLA	C3C-C2C	5.28	1.48	1.36
10	cA	801	CL0	C3C-C2C	5.28	1.48	1.36
11	aB	831	CLA	C3C-C2C	5.28	1.48	1.36
11	aK	101	CLA	C3C-C2C	5.28	1.48	1.36
11	aA	812	CLA	C3C-C2C	5.28	1.48	1.36
11	bB	838	CLA	C3C-C2C	5.28	1.48	1.36
11	bA	831	CLA	C3C-C2C	5.28	1.47	1.36
11	aA	815	CLA	C3C-C2C	5.28	1.47	1.36
11	cA	815	CLA	C3C-C2C	5.28	1.47	1.36
11	aA	804	CLA	C3C-C2C	5.27	1.47	1.36
11	bK	101	CLA	C3C-C2C	5.27	1.47	1.36
11	bA	808	CLA	C3C-C2C	5.27	1.47	1.36
11	cB	814	CLA	C3C-C2C	5.27	1.47	1.36
11	cK	101	CLA	C3C-C2C	5.27	1.47	1.36
11	aB	814	CLA	C3C-C2C	5.27	1.47	1.36
11	cA	824	CLA	C3C-C2C	5.26	1.47	1.36
11	bB	819	CLA	C3C-C2C	5.26	1.47	1.36
11	cA	839	CLA	C3C-C2C	5.26	1.47	1.36
11	bA	815	CLA	C3C-C2C	5.26	1.47	1.36
11	cB	831	CLA	C3C-C2C	5.26	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aB	840	CLA	C3C-C2C	5.26	1.47	1.36
11	aB	827	CLA	C3C-C2C	5.26	1.47	1.36
11	cA	831	CLA	C3C-C2C	5.26	1.47	1.36
10	bA	801	CL0	C3C-C2C	5.25	1.47	1.36
11	aA	824	CLA	C3C-C2C	5.25	1.47	1.36
11	cB	837	CLA	C3C-C2C	5.25	1.47	1.36
11	bB	818	CLA	C3C-C2C	5.25	1.47	1.36
11	cB	818	CLA	C3C-C2C	5.25	1.47	1.36
11	bL	206	CLA	C3C-C2C	5.25	1.47	1.36
11	aB	804	CLA	C3C-C2C	5.25	1.47	1.36
11	aB	818	CLA	C3C-C2C	5.25	1.47	1.36
11	cB	827	CLA	C3C-C2C	5.25	1.47	1.36
11	bA	804	CLA	C3C-C2C	5.25	1.47	1.36
11	aA	813	CLA	C3C-C2C	5.25	1.47	1.36
11	cB	804	CLA	C3C-C2C	5.25	1.47	1.36
11	cL	205	CLA	C3C-C2C	5.24	1.47	1.36
11	cA	833	CLA	C3C-C2C	5.23	1.47	1.36
11	aA	842	CLA	O2D-CGD	5.23	1.46	1.33
11	aA	805	CLA	C3C-C2C	5.23	1.47	1.36
11	aL	205	CLA	C3C-C2C	5.23	1.47	1.36
11	bB	804	CLA	C3C-C2C	5.23	1.47	1.36
11	cA	829	CLA	C3C-C2C	5.23	1.47	1.36
11	cA	809	CLA	C3C-C2C	5.23	1.47	1.36
11	cB	819	CLA	C3C-C2C	5.23	1.47	1.36
11	aA	833	CLA	C3C-C2C	5.23	1.47	1.36
11	cA	821	CLA	C3C-C2C	5.23	1.47	1.36
11	aB	837	CLA	C3C-C2C	5.23	1.47	1.36
11	cA	805	CLA	C3C-C2C	5.23	1.47	1.36
11	aB	821	CLA	C1D-ND	5.23	1.44	1.37
11	cA	842	CLA	O2D-CGD	5.23	1.46	1.33
11	aA	821	CLA	C3C-C2C	5.22	1.47	1.36
11	cB	840	CLA	C3C-C2C	5.22	1.47	1.36
11	cB	832	CLA	C1D-ND	5.22	1.44	1.37
11	bA	833	CLA	C3C-C2C	5.22	1.47	1.36
11	bB	828	CLA	C3C-C2C	5.22	1.47	1.36
11	bA	839	CLA	C3C-C2C	5.22	1.47	1.36
11	bA	822	CLA	C3C-C2C	5.22	1.47	1.36
11	cL	206	CLA	C3C-C2C	5.22	1.47	1.36
11	aL	204	CLA	C3C-C2C	5.22	1.47	1.36
11	bA	842	CLA	O2D-CGD	5.22	1.45	1.33
11	aB	834	CLA	C1D-ND	5.22	1.44	1.37
11	cA	822	CLA	C3C-C2C	5.22	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aA	839	CLA	C3C-C2C	5.22	1.47	1.36
11	aA	834	CLA	C3C-C2C	5.22	1.47	1.36
11	aB	819	CLA	C3C-C2C	5.22	1.47	1.36
11	bB	827	CLA	C3C-C2C	5.22	1.47	1.36
11	aA	822	CLA	C3C-C2C	5.21	1.47	1.36
11	cA	813	CLA	C3C-C2C	5.21	1.47	1.36
11	aB	828	CLA	C3C-C2C	5.21	1.47	1.36
11	bA	805	CLA	C3C-C2C	5.21	1.47	1.36
11	bA	829	CLA	C3C-C2C	5.21	1.47	1.36
11	bB	837	CLA	C3C-C2C	5.21	1.47	1.36
11	cB	821	CLA	O2D-CGD	5.21	1.45	1.33
11	aB	813	CLA	C3C-C2C	5.21	1.47	1.36
11	bA	834	CLA	C3C-C2C	5.21	1.47	1.36
11	bA	813	CLA	C3C-C2C	5.21	1.47	1.36
11	cB	813	CLA	C3C-C2C	5.21	1.47	1.36
11	bB	840	CLA	C3C-C2C	5.20	1.47	1.36
11	cA	810	CLA	C3C-C2C	5.20	1.47	1.36
11	bL	204	CLA	C3C-C2C	5.20	1.47	1.36
11	cL	204	CLA	C3C-C2C	5.20	1.47	1.36
11	cB	828	CLA	C3C-C2C	5.20	1.47	1.36
11	aA	841	CLA	O2D-CGD	5.20	1.45	1.33
11	bB	813	CLA	C3C-C2C	5.20	1.47	1.36
11	aA	810	CLA	C3C-C2C	5.20	1.47	1.36
11	cB	805	CLA	C3C-C2C	5.20	1.47	1.36
11	bA	821	CLA	C3C-C2C	5.19	1.47	1.36
11	aB	834	CLA	O2D-CGD	5.19	1.45	1.33
11	aA	809	CLA	C3C-C2C	5.19	1.47	1.36
11	aA	829	CLA	C3C-C2C	5.19	1.47	1.36
11	bA	809	CLA	C3C-C2C	5.19	1.47	1.36
11	bB	821	CLA	O2D-CGD	5.19	1.45	1.33
11	cB	831	CLA	C1D-ND	5.19	1.44	1.37
11	bB	805	CLA	C3C-C2C	5.19	1.47	1.36
11	bL	205	CLA	C3C-C2C	5.19	1.47	1.36
11	aB	821	CLA	O2D-CGD	5.19	1.45	1.33
11	aA	812	CLA	C1D-ND	5.19	1.44	1.37
11	bA	810	CLA	C3C-C2C	5.19	1.47	1.36
11	bA	812	CLA	C1D-ND	5.19	1.44	1.37
11	cB	816	CLA	O2D-CGD	5.18	1.45	1.33
11	cA	834	CLA	C3C-C2C	5.18	1.47	1.36
11	cA	840	CLA	C3C-C2C	5.18	1.47	1.36
11	bB	810	CLA	C3C-C2C	5.18	1.47	1.36
11	aB	810	CLA	C3C-C2C	5.18	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bB	831	CLA	C1D-ND	5.18	1.44	1.37
11	bB	839	CLA	C3C-C2C	5.18	1.47	1.36
11	cB	821	CLA	C1D-ND	5.18	1.44	1.37
11	aB	829	CLA	C1D-ND	5.18	1.44	1.37
11	aA	840	CLA	C3C-C2C	5.18	1.47	1.36
11	cA	823	CLA	C3C-C2C	5.17	1.47	1.36
11	aA	814	CLA	C3C-C2C	5.17	1.47	1.36
11	bA	812	CLA	O2D-CGD	5.17	1.45	1.33
11	aB	832	CLA	C1D-ND	5.17	1.44	1.37
11	cA	843	CLA	C3C-C2C	5.17	1.47	1.36
11	bA	843	CLA	C3C-C2C	5.17	1.47	1.36
11	bB	829	CLA	C1D-ND	5.17	1.44	1.37
11	bB	816	CLA	O2D-CGD	5.17	1.45	1.33
11	cA	841	CLA	O2D-CGD	5.17	1.45	1.33
11	aA	823	CLA	C3C-C2C	5.17	1.47	1.36
11	bA	814	CLA	C3C-C2C	5.17	1.47	1.36
11	cB	820	CLA	C3C-C2C	5.17	1.47	1.36
11	bB	834	CLA	C1D-ND	5.17	1.44	1.37
11	cB	835	CLA	C1D-ND	5.17	1.44	1.37
11	cB	839	CLA	C3C-C2C	5.16	1.47	1.36
11	aB	835	CLA	C1D-ND	5.16	1.44	1.37
11	aA	838	CLA	C3C-C2C	5.16	1.47	1.36
11	bB	835	CLA	C1D-ND	5.16	1.44	1.37
11	cA	811	CLA	O2D-CGD	5.16	1.45	1.33
11	bA	841	CLA	O2D-CGD	5.16	1.45	1.33
11	aB	839	CLA	C3C-C2C	5.16	1.47	1.36
11	cA	814	CLA	C3C-C2C	5.16	1.47	1.36
11	aA	843	CLA	C3C-C2C	5.16	1.47	1.36
11	cA	836	CLA	C3C-C2C	5.16	1.47	1.36
11	bA	823	CLA	C3C-C2C	5.16	1.47	1.36
11	bA	811	CLA	O2D-CGD	5.15	1.45	1.33
11	aA	836	CLA	C3C-C2C	5.15	1.47	1.36
11	bA	840	CLA	C3C-C2C	5.15	1.47	1.36
11	aA	811	CLA	O2D-CGD	5.15	1.45	1.33
11	bB	806	CLA	C3C-C2C	5.15	1.47	1.36
11	aB	816	CLA	O2D-CGD	5.15	1.45	1.33
11	cB	810	CLA	C3C-C2C	5.15	1.47	1.36
11	aA	828	CLA	C1D-ND	5.15	1.44	1.37
11	cA	812	CLA	O2D-CGD	5.15	1.45	1.33
11	cB	806	CLA	C3C-C2C	5.15	1.47	1.36
11	cB	815	CLA	O2D-CGD	5.14	1.45	1.33
11	aB	807	CLA	C3C-C2C	5.14	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bB	832	CLA	C1D-ND	5.14	1.44	1.37
11	cB	834	CLA	C1D-ND	5.14	1.44	1.37
11	aB	805	CLA	C3C-C2C	5.14	1.47	1.36
11	aB	817	CLA	C3C-C2C	5.14	1.47	1.36
11	cA	817	CLA	O2D-CGD	5.14	1.45	1.33
11	aA	802	CLA	C3C-C2C	5.14	1.47	1.36
11	bB	826	CLA	C3C-C2C	5.14	1.47	1.36
11	bA	836	CLA	C3C-C2C	5.14	1.47	1.36
11	aB	835	CLA	O2D-CGD	5.14	1.45	1.33
11	bB	834	CLA	O2D-CGD	5.14	1.45	1.33
11	cA	838	CLA	C3C-C2C	5.14	1.47	1.36
11	bB	821	CLA	C1D-ND	5.13	1.44	1.37
11	aA	835	CLA	C3C-C2C	5.13	1.47	1.36
11	cA	835	CLA	C3C-C2C	5.13	1.47	1.36
11	cB	834	CLA	O2D-CGD	5.13	1.45	1.33
11	bB	835	CLA	O2D-CGD	5.13	1.45	1.33
11	bA	838	CLA	C3C-C2C	5.13	1.47	1.36
11	cB	807	CLA	C3C-C2C	5.13	1.47	1.36
11	bB	820	CLA	C3C-C2C	5.13	1.47	1.36
11	bB	817	CLA	C3C-C2C	5.13	1.47	1.36
12	bA	844	F6C	O2D-CGD	5.13	1.45	1.33
11	aB	815	CLA	O2D-CGD	5.12	1.45	1.33
11	aB	820	CLA	C3C-C2C	5.12	1.47	1.36
11	bA	808	CLA	O2D-CGD	5.12	1.45	1.33
11	cA	802	CLA	C3C-C2C	5.12	1.47	1.36
11	bA	835	CLA	C3C-C2C	5.12	1.47	1.36
11	aB	806	CLA	C3C-C2C	5.12	1.47	1.36
12	aA	844	F6C	O2D-CGD	5.12	1.45	1.33
11	bB	807	CLA	C3C-C2C	5.12	1.47	1.36
11	bB	815	CLA	O2D-CGD	5.11	1.45	1.33
11	cA	812	CLA	C1D-ND	5.11	1.44	1.37
11	aA	808	CLA	O2D-CGD	5.11	1.45	1.33
11	bA	817	CLA	O2D-CGD	5.11	1.45	1.33
11	cB	835	CLA	O2D-CGD	5.11	1.45	1.33
11	cA	807	CLA	C3C-C2C	5.11	1.47	1.36
11	aB	831	CLA	C1D-ND	5.11	1.44	1.37
11	aA	804	CLA	O2D-CGD	5.11	1.45	1.33
11	cB	810	CLA	O2D-CGD	5.11	1.45	1.33
11	aB	823	CLA	C3C-C2C	5.11	1.47	1.36
11	aA	812	CLA	O2D-CGD	5.11	1.45	1.33
11	cB	817	CLA	C3C-C2C	5.11	1.47	1.36
11	aB	809	CLA	C3C-C2C	5.11	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	cB	823	CLA	C3C-C2C	5.11	1.47	1.36
11	bA	803	CLA	C3C-C2C	5.11	1.47	1.36
11	aB	802	CLA	C3C-C2C	5.11	1.47	1.36
12	bA	830	F6C	O2D-CGD	5.11	1.45	1.33
11	aB	836	CLA	O2D-CGD	5.11	1.45	1.33
11	cB	829	CLA	C1D-ND	5.10	1.44	1.37
11	bA	803	CLA	O2D-CGD	5.10	1.45	1.33
11	aA	819	CLA	O2D-CGD	5.10	1.45	1.33
11	bB	810	CLA	O2D-CGD	5.10	1.45	1.33
11	cB	809	CLA	C3C-C2C	5.10	1.47	1.36
11	cB	836	CLA	O2D-CGD	5.10	1.45	1.33
11	bB	809	CLA	C3C-C2C	5.10	1.47	1.36
11	cA	829	CLA	O2D-CGD	5.10	1.45	1.33
11	bB	836	CLA	O2D-CGD	5.10	1.45	1.33
12	cA	844	F6C	O2D-CGD	5.10	1.45	1.33
11	aB	820	CLA	O2D-CGD	5.10	1.45	1.33
11	bB	823	CLA	C3C-C2C	5.10	1.47	1.36
11	bA	802	CLA	C3C-C2C	5.10	1.47	1.36
11	cA	828	CLA	C1D-ND	5.10	1.44	1.37
11	bA	804	CLA	O2D-CGD	5.10	1.45	1.33
11	cA	819	CLA	O2D-CGD	5.10	1.45	1.33
11	cA	804	CLA	O2D-CGD	5.10	1.45	1.33
11	aA	807	CLA	C3C-C2C	5.10	1.47	1.36
11	cB	802	CLA	C3C-C2C	5.10	1.47	1.36
11	aA	817	CLA	O2D-CGD	5.10	1.45	1.33
11	cK	103	CLA	C1D-ND	5.10	1.44	1.37
11	cB	820	CLA	O2D-CGD	5.09	1.45	1.33
11	bB	802	CLA	C3C-C2C	5.09	1.47	1.36
11	bA	828	CLA	C1D-ND	5.09	1.44	1.37
11	aB	826	CLA	C3C-C2C	5.09	1.47	1.36
11	bA	807	CLA	C3C-C2C	5.09	1.47	1.36
11	cA	803	CLA	O2D-CGD	5.09	1.45	1.33
11	bA	819	CLA	O2D-CGD	5.09	1.45	1.33
11	cA	808	CLA	O2D-CGD	5.09	1.45	1.33
11	bK	103	CLA	C1D-ND	5.09	1.44	1.37
11	cA	803	CLA	C3C-C2C	5.09	1.47	1.36
11	cB	826	CLA	C3C-C2C	5.09	1.47	1.36
11	aB	829	CLA	O2D-CGD	5.09	1.45	1.33
11	bA	829	CLA	O2D-CGD	5.09	1.45	1.33
12	aA	827	F6C	O2D-CGD	5.09	1.45	1.33
11	aB	839	CLA	O2D-CGD	5.08	1.45	1.33
11	bB	805	CLA	O2D-CGD	5.08	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bB	829	CLA	O2D-CGD	5.08	1.45	1.33
11	aB	808	CLA	C3C-C2C	5.08	1.47	1.36
11	aA	822	CLA	O2D-CGD	5.08	1.45	1.33
11	cB	837	CLA	O2D-CGD	5.08	1.45	1.33
11	cB	822	CLA	C1D-ND	5.08	1.44	1.37
12	cA	827	F6C	O2D-CGD	5.08	1.45	1.33
11	aB	830	CLA	C1D-ND	5.08	1.44	1.37
11	bB	839	CLA	O2D-CGD	5.08	1.45	1.33
11	cB	829	CLA	O2D-CGD	5.08	1.45	1.33
11	cA	822	CLA	O2D-CGD	5.08	1.45	1.33
11	bA	804	CLA	C1D-ND	5.08	1.44	1.37
11	aA	803	CLA	C3C-C2C	5.08	1.47	1.36
11	aK	103	CLA	C1D-ND	5.08	1.44	1.37
11	aB	805	CLA	O2D-CGD	5.08	1.45	1.33
11	cA	813	CLA	O2D-CGD	5.08	1.45	1.33
11	aA	829	CLA	O2D-CGD	5.08	1.45	1.33
12	cA	830	F6C	O2D-CGD	5.08	1.45	1.33
11	aB	822	CLA	O2D-CGD	5.07	1.45	1.33
11	cK	101	CLA	C1D-ND	5.07	1.44	1.37
11	aA	803	CLA	O2D-CGD	5.07	1.45	1.33
12	aA	830	F6C	O2D-CGD	5.07	1.45	1.33
11	cA	823	CLA	O2D-CGD	5.07	1.45	1.33
11	aK	101	CLA	C1D-ND	5.07	1.44	1.37
11	cB	839	CLA	O2D-CGD	5.07	1.45	1.33
11	bB	820	CLA	O2D-CGD	5.07	1.45	1.33
11	bB	822	CLA	C1D-ND	5.07	1.44	1.37
11	aA	843	CLA	O2D-CGD	5.07	1.45	1.33
11	bA	822	CLA	O2D-CGD	5.07	1.45	1.33
11	bB	837	CLA	O2D-CGD	5.07	1.45	1.33
11	aB	810	CLA	O2D-CGD	5.07	1.45	1.33
11	aB	803	CLA	O2D-CGD	5.07	1.45	1.33
11	aA	824	CLA	O2D-CGD	5.07	1.45	1.33
11	aA	833	CLA	O2D-CGD	5.06	1.45	1.33
12	bA	827	F6C	O2D-CGD	5.06	1.45	1.33
11	bB	823	CLA	O2D-CGD	5.06	1.45	1.33
11	bB	812	CLA	C1D-ND	5.06	1.44	1.37
11	cB	827	CLA	O2D-CGD	5.06	1.45	1.33
11	bL	206	CLA	O2D-CGD	5.06	1.45	1.33
11	bB	814	CLA	C1D-ND	5.06	1.44	1.37
11	aB	811	CLA	O2D-CGD	5.06	1.45	1.33
11	bA	828	CLA	C3C-C2C	5.06	1.47	1.36
11	cA	843	CLA	O2D-CGD	5.06	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aA	804	CLA	C1D-ND	5.06	1.44	1.37
11	cA	824	CLA	O2D-CGD	5.05	1.45	1.33
11	cB	830	CLA	C1D-ND	5.05	1.44	1.37
11	bA	824	CLA	O2D-CGD	5.05	1.45	1.33
11	cB	803	CLA	O2D-CGD	5.05	1.45	1.33
11	aB	837	CLA	O2D-CGD	5.05	1.45	1.33
11	aA	813	CLA	O2D-CGD	5.05	1.45	1.33
11	aB	818	CLA	O2D-CGD	5.05	1.45	1.33
11	bB	822	CLA	O2D-CGD	5.05	1.45	1.33
11	cA	816	CLA	O2D-CGD	5.05	1.45	1.33
11	cB	805	CLA	O2D-CGD	5.05	1.45	1.33
11	bB	808	CLA	C3C-C2C	5.05	1.47	1.36
11	bA	823	CLA	O2D-CGD	5.05	1.45	1.33
11	bA	843	CLA	O2D-CGD	5.05	1.45	1.33
11	bA	839	CLA	O2D-CGD	5.05	1.45	1.33
11	cB	811	CLA	O2D-CGD	5.05	1.45	1.33
11	bB	830	CLA	C1D-ND	5.04	1.44	1.37
11	cB	814	CLA	C1D-ND	5.04	1.44	1.37
11	aL	206	CLA	O2D-CGD	5.04	1.45	1.33
11	aB	822	CLA	C1D-ND	5.04	1.44	1.37
11	cA	828	CLA	C3C-C2C	5.04	1.47	1.36
11	aA	805	CLA	O2D-CGD	5.04	1.45	1.33
11	bB	827	CLA	O2D-CGD	5.04	1.45	1.33
11	cB	823	CLA	O2D-CGD	5.04	1.45	1.33
11	bB	832	CLA	O2D-CGD	5.04	1.45	1.33
11	bA	813	CLA	O2D-CGD	5.04	1.45	1.33
11	bA	833	CLA	O2D-CGD	5.04	1.45	1.33
11	aB	811	CLA	C1D-ND	5.04	1.44	1.37
11	bB	833	CLA	C1D-ND	5.04	1.44	1.37
11	aB	823	CLA	O2D-CGD	5.04	1.45	1.33
11	bB	818	CLA	O2D-CGD	5.04	1.45	1.33
11	cB	822	CLA	O2D-CGD	5.04	1.45	1.33
11	bA	819	CLA	C3C-C2C	5.04	1.47	1.36
11	cA	804	CLA	C1D-ND	5.03	1.44	1.37
11	aA	819	CLA	C3C-C2C	5.03	1.47	1.36
11	cA	805	CLA	C1D-ND	5.03	1.44	1.37
11	cB	811	CLA	C1D-ND	5.03	1.44	1.37
11	bB	840	CLA	O2D-CGD	5.03	1.45	1.33
11	cA	820	CLA	C3C-C2C	5.03	1.47	1.36
11	cB	808	CLA	C3C-C2C	5.03	1.47	1.36
11	bB	812	CLA	C3C-C2C	5.03	1.47	1.36
11	bK	101	CLA	C1D-ND	5.03	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aB	832	CLA	O2D-CGD	5.03	1.45	1.33
11	cL	206	CLA	O2D-CGD	5.03	1.45	1.33
11	bB	825	CLA	O2D-CGD	5.03	1.45	1.33
11	aA	820	CLA	C3C-C2C	5.03	1.47	1.36
11	aB	815	CLA	C1D-ND	5.03	1.44	1.37
11	bA	820	CLA	C3C-C2C	5.03	1.47	1.36
11	aA	828	CLA	C3C-C2C	5.03	1.47	1.36
11	cA	805	CLA	O2D-CGD	5.02	1.45	1.33
11	cA	833	CLA	O2D-CGD	5.02	1.45	1.33
11	bA	805	CLA	O2D-CGD	5.02	1.45	1.33
11	aB	812	CLA	C3C-C2C	5.02	1.47	1.36
11	aB	825	CLA	O2D-CGD	5.02	1.45	1.33
11	aA	823	CLA	O2D-CGD	5.02	1.45	1.33
11	cB	832	CLA	O2D-CGD	5.02	1.45	1.33
11	aB	827	CLA	O2D-CGD	5.02	1.45	1.33
11	cB	825	CLA	O2D-CGD	5.02	1.45	1.33
11	bB	803	CLA	O2D-CGD	5.02	1.45	1.33
11	bB	811	CLA	O2D-CGD	5.02	1.45	1.33
11	cA	807	CLA	C1D-ND	5.02	1.44	1.37
12	cA	826	F6C	O2D-CGD	5.01	1.45	1.33
11	cB	807	CLA	O2D-CGD	5.01	1.45	1.33
11	cA	819	CLA	C3C-C2C	5.01	1.47	1.36
11	cB	840	CLA	O2D-CGD	5.01	1.45	1.33
12	aA	826	F6C	O2D-CGD	5.01	1.45	1.33
11	aA	825	CLA	C3C-C2C	5.01	1.47	1.36
11	bA	816	CLA	O2D-CGD	5.01	1.45	1.33
11	bA	805	CLA	C1D-ND	5.01	1.43	1.37
11	bA	825	CLA	C3C-C2C	5.01	1.47	1.36
11	aB	807	CLA	O2D-CGD	5.01	1.45	1.33
11	cA	825	CLA	C3C-C2C	5.01	1.47	1.36
11	bA	815	CLA	C1D-ND	5.01	1.43	1.37
11	bB	807	CLA	O2D-CGD	5.01	1.45	1.33
11	bB	826	CLA	O2D-CGD	5.01	1.45	1.33
11	cB	826	CLA	O2D-CGD	5.00	1.45	1.33
11	cB	825	CLA	C1D-ND	5.00	1.43	1.37
11	bB	830	CLA	O2D-CGD	5.00	1.45	1.33
12	bA	826	F6C	O2D-CGD	5.00	1.45	1.33
11	aB	833	CLA	C1D-ND	5.00	1.43	1.37
11	bB	825	CLA	C1D-ND	5.00	1.43	1.37
11	cB	815	CLA	C1D-ND	5.00	1.43	1.37
11	cB	818	CLA	O2D-CGD	5.00	1.45	1.33
11	bA	807	CLA	C1D-ND	5.00	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aB	812	CLA	C1D-ND	5.00	1.43	1.37
11	cA	811	CLA	C1D-ND	5.00	1.43	1.37
11	bB	811	CLA	C1D-ND	5.00	1.43	1.37
11	aB	814	CLA	C1D-ND	4.99	1.43	1.37
11	aB	803	CLA	C3C-C2C	4.99	1.47	1.36
11	cB	833	CLA	C1D-ND	4.99	1.43	1.37
11	aA	816	CLA	O2D-CGD	4.99	1.45	1.33
11	aB	809	CLA	O2D-CGD	4.99	1.45	1.33
11	cB	830	CLA	O2D-CGD	4.99	1.45	1.33
11	aA	839	CLA	O2D-CGD	4.99	1.45	1.33
11	aB	830	CLA	O2D-CGD	4.99	1.45	1.33
11	cA	837	CLA	C1D-ND	4.99	1.43	1.37
11	cB	820	CLA	C1D-ND	4.99	1.43	1.37
11	aB	826	CLA	O2D-CGD	4.99	1.45	1.33
11	bB	838	CLA	O2D-CGD	4.99	1.45	1.33
11	bA	811	CLA	C1D-ND	4.99	1.43	1.37
11	cB	838	CLA	O2D-CGD	4.98	1.45	1.33
11	cA	815	CLA	C1D-ND	4.98	1.43	1.37
11	aB	838	CLA	O2D-CGD	4.98	1.45	1.33
11	cA	839	CLA	O2D-CGD	4.98	1.45	1.33
11	aB	825	CLA	C1D-ND	4.98	1.43	1.37
11	cB	812	CLA	C1D-ND	4.98	1.43	1.37
11	aB	840	CLA	O2D-CGD	4.98	1.45	1.33
11	bB	809	CLA	O2D-CGD	4.98	1.45	1.33
11	cL	204	CLA	O2D-CGD	4.98	1.45	1.33
11	aA	815	CLA	C1D-ND	4.97	1.43	1.37
11	cA	819	CLA	C1D-ND	4.97	1.43	1.37
11	bB	815	CLA	C1D-ND	4.97	1.43	1.37
11	cB	809	CLA	O2D-CGD	4.97	1.45	1.33
11	bB	817	CLA	O2D-CGD	4.96	1.45	1.33
11	bL	204	CLA	O2D-CGD	4.96	1.45	1.33
11	cB	814	CLA	O2D-CGD	4.96	1.45	1.33
11	cB	812	CLA	C3C-C2C	4.96	1.47	1.36
11	aB	810	CLA	C1D-ND	4.96	1.43	1.37
11	bB	814	CLA	O2D-CGD	4.96	1.45	1.33
11	aA	817	CLA	C1D-ND	4.95	1.43	1.37
11	aB	814	CLA	O2D-CGD	4.95	1.45	1.33
11	cB	803	CLA	C3C-C2C	4.95	1.47	1.36
11	bA	821	CLA	O2D-CGD	4.95	1.45	1.33
11	aA	828	CLA	O2D-CGD	4.95	1.45	1.33
11	bA	828	CLA	O2D-CGD	4.95	1.45	1.33
11	cA	828	CLA	O2D-CGD	4.95	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bB	803	CLA	C3C-C2C	4.95	1.47	1.36
11	aA	807	CLA	C1D-ND	4.95	1.43	1.37
11	aA	816	CLA	C1D-ND	4.95	1.43	1.37
11	cA	821	CLA	O2D-CGD	4.95	1.45	1.33
11	aA	818	CLA	O2D-CGD	4.95	1.45	1.33
11	aB	817	CLA	O2D-CGD	4.95	1.45	1.33
11	cA	806	CLA	O2D-CGD	4.95	1.45	1.33
11	aB	815	CLA	C3C-C2C	4.95	1.47	1.36
11	aA	840	CLA	C1D-ND	4.95	1.43	1.37
11	cA	809	CLA	O2D-CGD	4.94	1.45	1.33
11	aA	809	CLA	O2D-CGD	4.94	1.45	1.33
11	cB	828	CLA	O2D-CGD	4.94	1.45	1.33
11	aA	837	CLA	C1D-ND	4.94	1.43	1.37
11	bA	818	CLA	O2D-CGD	4.94	1.45	1.33
11	aK	103	CLA	O2D-CGD	4.94	1.45	1.33
11	aA	810	CLA	O2D-CGD	4.94	1.45	1.33
11	aA	838	CLA	O2D-CGD	4.94	1.45	1.33
11	aL	204	CLA	O2D-CGD	4.94	1.45	1.33
11	cB	817	CLA	O2D-CGD	4.94	1.45	1.33
11	bA	816	CLA	C1D-ND	4.94	1.43	1.37
11	aB	820	CLA	C1D-ND	4.94	1.43	1.37
11	bA	840	CLA	C1D-ND	4.94	1.43	1.37
11	bA	809	CLA	O2D-CGD	4.94	1.45	1.33
11	bB	820	CLA	C1D-ND	4.94	1.43	1.37
11	cA	818	CLA	O2D-CGD	4.94	1.45	1.33
11	aA	805	CLA	C1D-ND	4.93	1.43	1.37
11	cK	103	CLA	O2D-CGD	4.93	1.45	1.33
11	bB	828	CLA	O2D-CGD	4.93	1.45	1.33
11	bB	810	CLA	C1D-ND	4.93	1.43	1.37
11	cA	838	CLA	O2D-CGD	4.93	1.45	1.33
11	bA	810	CLA	O2D-CGD	4.93	1.45	1.33
11	cA	802	CLA	O2D-CGD	4.93	1.45	1.33
11	bA	817	CLA	C1D-ND	4.93	1.43	1.37
11	aA	843	CLA	C1D-ND	4.93	1.43	1.37
13	cA	845	PQN	C10-C5	4.93	1.48	1.40
11	aA	802	CLA	O2D-CGD	4.93	1.45	1.33
11	bA	802	CLA	O2D-CGD	4.92	1.45	1.33
11	bA	819	CLA	C1D-ND	4.92	1.43	1.37
11	cA	817	CLA	C1D-ND	4.92	1.43	1.37
11	aB	819	CLA	O2D-CGD	4.92	1.45	1.33
11	bK	103	CLA	O2D-CGD	4.92	1.45	1.33
11	aB	806	CLA	C1D-ND	4.92	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bA	843	CLA	C1D-ND	4.92	1.43	1.37
11	bA	806	CLA	O2D-CGD	4.92	1.45	1.33
11	bA	837	CLA	C1D-ND	4.92	1.43	1.37
13	bA	845	PQN	C10-C5	4.92	1.48	1.40
11	bA	807	CLA	O2D-CGD	4.92	1.45	1.33
11	bA	838	CLA	O2D-CGD	4.92	1.45	1.33
11	cA	806	CLA	C1D-ND	4.92	1.43	1.37
13	cB	841	PQN	C10-C5	4.92	1.48	1.40
11	aA	824	CLA	C1D-ND	4.92	1.43	1.37
11	bL	205	CLA	O2D-CGD	4.92	1.45	1.33
11	cA	810	CLA	O2D-CGD	4.91	1.45	1.33
11	aA	821	CLA	O2D-CGD	4.91	1.45	1.33
11	cB	815	CLA	C3C-C2C	4.91	1.47	1.36
11	aA	806	CLA	O2D-CGD	4.91	1.45	1.33
11	aA	811	CLA	C1D-ND	4.91	1.43	1.37
13	aA	845	PQN	C10-C5	4.91	1.48	1.40
11	bA	824	CLA	C1D-ND	4.91	1.43	1.37
11	bB	806	CLA	C1D-ND	4.91	1.43	1.37
11	aA	819	CLA	C1D-ND	4.91	1.43	1.37
11	cL	205	CLA	O2D-CGD	4.91	1.45	1.33
11	bB	836	CLA	C1D-ND	4.91	1.43	1.37
11	bA	820	CLA	C1D-ND	4.91	1.43	1.37
12	cB	824	F6C	O2D-CGD	4.91	1.45	1.33
11	aA	807	CLA	O2D-CGD	4.90	1.45	1.33
11	bA	806	CLA	C1D-ND	4.90	1.43	1.37
11	cB	819	CLA	O2D-CGD	4.90	1.45	1.33
11	bA	835	CLA	C1D-ND	4.90	1.43	1.37
11	bB	815	CLA	C3C-C2C	4.90	1.47	1.36
11	bB	819	CLA	O2D-CGD	4.90	1.45	1.33
11	cA	808	CLA	C1D-ND	4.90	1.43	1.37
11	cB	806	CLA	C1D-ND	4.90	1.43	1.37
11	cB	810	CLA	C1D-ND	4.90	1.43	1.37
12	cA	832	F6C	O2D-CGD	4.90	1.45	1.33
11	cA	843	CLA	C1D-ND	4.90	1.43	1.37
11	bA	829	CLA	C1D-ND	4.90	1.43	1.37
11	aB	828	CLA	O2D-CGD	4.90	1.45	1.33
11	aA	806	CLA	C1D-ND	4.89	1.43	1.37
11	cA	816	CLA	C1D-ND	4.89	1.43	1.37
11	cA	833	CLA	C1D-ND	4.89	1.43	1.37
12	aB	824	F6C	O2D-CGD	4.89	1.45	1.33
11	cA	814	CLA	C1D-ND	4.89	1.43	1.37
11	cA	820	CLA	C1D-ND	4.89	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	cA	840	CLA	C1D-ND	4.89	1.43	1.37
11	cA	807	CLA	O2D-CGD	4.89	1.45	1.33
12	bB	824	F6C	O2D-CGD	4.89	1.45	1.33
13	bB	841	PQN	C10-C5	4.89	1.48	1.40
11	bB	833	CLA	O2D-CGD	4.89	1.45	1.33
11	aA	834	CLA	O2D-CGD	4.89	1.45	1.33
11	bA	805	CLA	CHC-C1C	4.89	1.48	1.38
11	cA	805	CLA	CHC-C1C	4.89	1.48	1.38
11	bA	808	CLA	C1D-ND	4.89	1.43	1.37
11	cB	816	CLA	C1D-ND	4.89	1.43	1.37
11	aA	808	CLA	C1D-ND	4.88	1.43	1.37
11	aB	804	CLA	C1D-ND	4.88	1.43	1.37
11	cA	834	CLA	O2D-CGD	4.88	1.45	1.33
11	cB	804	CLA	C1D-ND	4.88	1.43	1.37
12	bA	832	F6C	O2D-CGD	4.88	1.45	1.33
11	aL	205	CLA	O2D-CGD	4.88	1.45	1.33
11	bB	804	CLA	C1D-ND	4.88	1.43	1.37
11	cA	842	CLA	C1D-ND	4.88	1.43	1.37
11	cA	813	CLA	C1D-ND	4.88	1.43	1.37
11	aB	836	CLA	C1D-ND	4.87	1.43	1.37
12	aA	832	F6C	O2D-CGD	4.87	1.45	1.33
11	aA	818	CLA	C3C-C2C	4.87	1.47	1.36
11	bA	840	CLA	O2D-CGD	4.87	1.45	1.33
11	aA	820	CLA	O2D-CGD	4.87	1.45	1.33
11	cA	835	CLA	C1D-ND	4.87	1.43	1.37
11	cA	825	CLA	C1D-ND	4.87	1.43	1.37
11	bA	809	CLA	C1D-ND	4.87	1.43	1.37
11	aB	833	CLA	O2D-CGD	4.87	1.45	1.33
11	aA	814	CLA	C1D-ND	4.87	1.43	1.37
11	cA	820	CLA	O2D-CGD	4.86	1.45	1.33
11	aA	842	CLA	C1D-ND	4.86	1.43	1.37
11	aB	805	CLA	C1D-ND	4.86	1.43	1.37
11	aA	805	CLA	CHC-C1C	4.86	1.48	1.38
13	aB	841	PQN	C10-C5	4.86	1.48	1.40
11	cA	809	CLA	C1D-ND	4.86	1.43	1.37
11	bA	834	CLA	O2D-CGD	4.86	1.45	1.33
11	aA	825	CLA	C1D-ND	4.86	1.43	1.37
11	bA	820	CLA	O2D-CGD	4.86	1.45	1.33
11	cB	801	CLA	C3C-C2C	4.86	1.47	1.36
11	aA	829	CLA	C1D-ND	4.86	1.43	1.37
11	aA	809	CLA	C1D-ND	4.85	1.43	1.37
11	aB	816	CLA	C1D-ND	4.85	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aA	815	CLA	O2D-CGD	4.85	1.45	1.33
11	aA	835	CLA	C1D-ND	4.85	1.43	1.37
11	cB	813	CLA	O2D-CGD	4.85	1.45	1.33
11	aA	833	CLA	C1D-ND	4.85	1.43	1.37
11	cA	818	CLA	C3C-C2C	4.85	1.47	1.36
11	cA	824	CLA	C1D-ND	4.85	1.43	1.37
11	bB	804	CLA	O2D-CGD	4.85	1.45	1.33
11	cB	833	CLA	O2D-CGD	4.85	1.45	1.33
11	aA	813	CLA	C1D-ND	4.84	1.43	1.37
11	bB	813	CLA	C1D-ND	4.84	1.43	1.37
11	cA	839	CLA	C1D-ND	4.84	1.43	1.37
11	cB	836	CLA	C1D-ND	4.84	1.43	1.37
10	cA	801	CL0	O2D-CGD	4.84	1.45	1.33
11	bA	818	CLA	C3C-C2C	4.84	1.47	1.36
11	bB	801	CLA	C3C-C2C	4.84	1.47	1.36
11	cB	805	CLA	C1D-ND	4.84	1.43	1.37
11	aA	820	CLA	C1D-ND	4.83	1.43	1.37
11	bA	825	CLA	C1D-ND	4.83	1.43	1.37
11	aB	806	CLA	O2D-CGD	4.83	1.45	1.33
11	bA	813	CLA	C1D-ND	4.83	1.43	1.37
11	bA	833	CLA	C1D-ND	4.83	1.43	1.37
10	bA	801	CL0	O2D-CGD	4.83	1.45	1.33
11	cA	815	CLA	O2D-CGD	4.83	1.45	1.33
11	aB	813	CLA	O2D-CGD	4.83	1.45	1.33
11	cA	831	CLA	O2D-CGD	4.83	1.45	1.33
11	bB	805	CLA	C1D-ND	4.83	1.43	1.37
11	cA	829	CLA	C1D-ND	4.83	1.43	1.37
11	bA	814	CLA	O2D-CGD	4.83	1.45	1.33
11	cA	840	CLA	O2D-CGD	4.83	1.45	1.33
11	bA	842	CLA	C1D-ND	4.82	1.43	1.37
11	aA	840	CLA	O2D-CGD	4.82	1.45	1.33
11	bA	815	CLA	O2D-CGD	4.82	1.45	1.33
11	bB	816	CLA	C1D-ND	4.82	1.43	1.37
11	bB	822	CLA	C3C-C2C	4.82	1.47	1.36
11	aB	801	CLA	C3C-C2C	4.81	1.47	1.36
11	bB	806	CLA	O2D-CGD	4.81	1.44	1.33
10	aA	801	CL0	O2D-CGD	4.81	1.44	1.33
11	aA	839	CLA	C1D-ND	4.81	1.43	1.37
11	aB	831	CLA	O2D-CGD	4.81	1.44	1.33
11	cB	804	CLA	O2D-CGD	4.81	1.44	1.33
11	cB	806	CLA	O2D-CGD	4.81	1.44	1.33
11	bA	814	CLA	C1D-ND	4.81	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aB	804	CLA	O2D-CGD	4.81	1.44	1.33
11	bB	813	CLA	O2D-CGD	4.81	1.44	1.33
11	cA	814	CLA	O2D-CGD	4.80	1.44	1.33
11	aA	819	CLA	CHC-C1C	4.80	1.48	1.38
11	aB	822	CLA	C3C-C2C	4.80	1.46	1.36
11	cB	813	CLA	C1D-ND	4.80	1.43	1.37
11	aB	813	CLA	C1D-ND	4.80	1.43	1.37
11	aB	822	CLA	CHC-C1C	4.80	1.48	1.38
11	aA	814	CLA	O2D-CGD	4.80	1.44	1.33
11	bA	839	CLA	C1D-ND	4.80	1.43	1.37
11	aA	831	CLA	O2D-CGD	4.80	1.44	1.33
11	cB	822	CLA	C3C-C2C	4.79	1.46	1.36
11	aB	840	CLA	C1D-ND	4.79	1.43	1.37
11	cA	819	CLA	CHC-C1C	4.79	1.48	1.38
11	bB	840	CLA	C1D-ND	4.79	1.43	1.37
11	cB	831	CLA	O2D-CGD	4.79	1.44	1.33
11	bB	831	CLA	O2D-CGD	4.79	1.44	1.33
11	bA	831	CLA	O2D-CGD	4.78	1.44	1.33
11	bB	816	CLA	CHC-C1C	4.78	1.48	1.38
11	aB	812	CLA	O2D-CGD	4.78	1.44	1.33
11	cB	840	CLA	C1D-ND	4.78	1.43	1.37
11	cB	822	CLA	CHC-C1C	4.77	1.48	1.38
11	bB	822	CLA	CHC-C1C	4.77	1.48	1.38
11	bA	819	CLA	CHC-C1C	4.77	1.48	1.38
11	aB	837	CLA	C1D-ND	4.76	1.43	1.37
11	bB	838	CLA	C1D-ND	4.76	1.43	1.37
11	aA	836	CLA	O2D-CGD	4.76	1.44	1.33
11	cA	836	CLA	O2D-CGD	4.76	1.44	1.33
11	cA	806	CLA	C3C-C2C	4.76	1.46	1.36
11	cB	838	CLA	C1D-ND	4.76	1.43	1.37
11	aA	834	CLA	C1D-ND	4.75	1.43	1.37
11	bA	806	CLA	C3C-C2C	4.75	1.46	1.36
11	aB	816	CLA	CHC-C1C	4.75	1.48	1.38
11	cB	812	CLA	O2D-CGD	4.75	1.44	1.33
11	aL	204	CLA	C1D-ND	4.74	1.43	1.37
11	bB	837	CLA	C1D-ND	4.74	1.43	1.37
11	bB	817	CLA	C1D-ND	4.74	1.43	1.37
11	cA	834	CLA	C1D-ND	4.74	1.43	1.37
11	cB	818	CLA	C1D-ND	4.73	1.43	1.37
11	aA	822	CLA	C1D-ND	4.73	1.43	1.37
11	cB	801	CLA	O2D-CGD	4.73	1.44	1.33
11	bA	836	CLA	O2D-CGD	4.73	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bA	822	CLA	C1D-ND	4.73	1.43	1.37
11	bB	812	CLA	O2D-CGD	4.73	1.44	1.33
11	aA	841	CLA	C1D-ND	4.72	1.43	1.37
11	cL	204	CLA	C1D-ND	4.72	1.43	1.37
11	bB	801	CLA	O2D-CGD	4.72	1.44	1.33
11	bA	825	CLA	O2D-CGD	4.72	1.44	1.33
11	aA	806	CLA	C3C-C2C	4.72	1.46	1.36
11	aB	838	CLA	C1D-ND	4.72	1.43	1.37
11	aA	825	CLA	O2D-CGD	4.72	1.44	1.33
11	bA	818	CLA	CHC-C1C	4.71	1.48	1.38
11	aB	818	CLA	C1D-ND	4.71	1.43	1.37
11	bA	834	CLA	C1D-ND	4.71	1.43	1.37
11	cB	837	CLA	C1D-ND	4.71	1.43	1.37
11	aB	801	CLA	O2D-CGD	4.71	1.44	1.33
11	cB	804	CLA	CHC-C1C	4.71	1.48	1.38
11	bL	204	CLA	C1D-ND	4.70	1.43	1.37
11	aA	810	CLA	C1D-ND	4.70	1.43	1.37
11	cA	825	CLA	O2D-CGD	4.70	1.44	1.33
11	bB	804	CLA	CHC-C1C	4.70	1.48	1.38
11	cA	841	CLA	C1D-ND	4.70	1.43	1.37
11	aB	808	CLA	O2D-CGD	4.69	1.44	1.33
11	bB	833	CLA	CHC-C1C	4.69	1.48	1.38
11	cA	822	CLA	C1D-ND	4.69	1.43	1.37
11	bB	808	CLA	O2D-CGD	4.69	1.44	1.33
11	aB	833	CLA	CHC-C1C	4.69	1.48	1.38
11	cB	816	CLA	CHC-C1C	4.69	1.48	1.38
11	cB	839	CLA	CHC-C1C	4.69	1.48	1.38
11	aB	837	CLA	CHC-C1C	4.69	1.48	1.38
11	cB	808	CLA	O2D-CGD	4.68	1.44	1.33
11	bA	841	CLA	C1D-ND	4.68	1.43	1.37
11	cA	810	CLA	C1D-ND	4.68	1.43	1.37
11	cB	832	CLA	CHC-C1C	4.68	1.48	1.38
11	bA	810	CLA	C1D-ND	4.68	1.43	1.37
11	bA	837	CLA	O2D-CGD	4.67	1.44	1.33
11	bB	818	CLA	C1D-ND	4.67	1.43	1.37
11	cB	829	CLA	C3C-C2C	4.67	1.46	1.36
11	aA	823	CLA	C1D-ND	4.66	1.43	1.37
11	cA	823	CLA	C1D-ND	4.66	1.43	1.37
11	cA	818	CLA	CHC-C1C	4.66	1.48	1.38
11	cB	817	CLA	C1D-ND	4.66	1.43	1.37
11	bA	823	CLA	C1D-ND	4.65	1.43	1.37
11	bL	206	CLA	C1D-ND	4.65	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aA	838	CLA	C1D-ND	4.65	1.43	1.37
11	aA	818	CLA	CHC-C1C	4.65	1.48	1.38
11	bB	839	CLA	CHC-C1C	4.65	1.48	1.38
11	cA	821	CLA	C1D-ND	4.65	1.43	1.37
11	bB	829	CLA	C3C-C2C	4.65	1.46	1.36
11	cB	837	CLA	CHC-C1C	4.65	1.48	1.38
11	aB	836	CLA	CHC-C1C	4.65	1.48	1.38
11	bA	804	CLA	CHC-C1C	4.65	1.48	1.38
11	aB	832	CLA	CHC-C1C	4.64	1.48	1.38
11	bB	832	CLA	CHC-C1C	4.64	1.48	1.38
11	cA	837	CLA	O2D-CGD	4.64	1.44	1.33
11	cB	833	CLA	CHC-C1C	4.64	1.48	1.38
11	bA	838	CLA	C1D-ND	4.64	1.43	1.37
11	cB	828	CLA	C1B-NB	-4.64	1.32	1.37
11	aB	817	CLA	O2A-CGA	4.64	1.46	1.33
11	bB	837	CLA	CHC-C1C	4.64	1.47	1.38
11	aA	816	CLA	CHC-C1C	4.64	1.47	1.38
11	cB	802	CLA	CHC-C1C	4.64	1.47	1.38
11	aA	837	CLA	O2D-CGD	4.64	1.44	1.33
11	cA	804	CLA	CHC-C1C	4.63	1.47	1.38
11	aB	804	CLA	CHC-C1C	4.63	1.47	1.38
11	cA	816	CLA	CHC-C1C	4.63	1.47	1.38
11	bB	801	CLA	C1D-ND	4.63	1.43	1.37
11	aB	817	CLA	C1D-ND	4.63	1.43	1.37
11	bB	836	CLA	CHC-C1C	4.63	1.47	1.38
11	cA	838	CLA	C1D-ND	4.63	1.43	1.37
11	aB	829	CLA	C3C-C2C	4.63	1.46	1.36
11	aB	802	CLA	CHC-C1C	4.62	1.47	1.38
11	aA	804	CLA	CHC-C1C	4.62	1.47	1.38
11	cA	803	CLA	CHC-C1C	4.62	1.47	1.38
11	bB	828	CLA	C1D-ND	4.62	1.43	1.37
11	bB	817	CLA	O2A-CGA	4.62	1.46	1.33
11	bB	818	CLA	CHC-C1C	4.62	1.47	1.38
11	bK	101	CLA	CHC-C1C	4.62	1.47	1.38
11	aB	802	CLA	O2D-CGD	4.62	1.44	1.33
11	bB	819	CLA	CHC-C1C	4.61	1.47	1.38
11	bB	828	CLA	C1B-NB	-4.61	1.32	1.37
11	cB	818	CLA	CHC-C1C	4.61	1.47	1.38
11	cB	817	CLA	O2A-CGA	4.61	1.46	1.33
11	cB	836	CLA	CHC-C1C	4.61	1.47	1.38
12	cL	202	F6C	O2D-CGD	4.61	1.44	1.33
11	bB	829	CLA	CHD-C1D	4.61	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bB	802	CLA	O2D-CGD	4.61	1.44	1.33
11	cB	828	CLA	C1D-ND	4.61	1.43	1.37
11	aB	839	CLA	CHC-C1C	4.60	1.47	1.38
11	aK	101	CLA	CHC-C1C	4.60	1.47	1.38
11	cA	842	CLA	CHC-C1C	4.60	1.47	1.38
11	cB	829	CLA	CHD-C1D	4.60	1.47	1.38
11	aA	803	CLA	CHC-C1C	4.60	1.47	1.38
11	aB	819	CLA	CHC-C1C	4.60	1.47	1.38
11	aA	837	CLA	CHC-C1C	4.60	1.47	1.38
11	bA	816	CLA	CHC-C1C	4.60	1.47	1.38
11	aL	205	CLA	C1D-ND	4.60	1.43	1.37
11	bB	802	CLA	CHC-C1C	4.60	1.47	1.38
11	cA	835	CLA	O2D-CGD	4.59	1.44	1.33
11	bB	815	CLA	CHC-C1C	4.59	1.47	1.38
11	aB	818	CLA	CHC-C1C	4.59	1.47	1.38
11	bA	821	CLA	C1D-ND	4.59	1.43	1.37
11	bA	803	CLA	CHC-C1C	4.59	1.47	1.38
11	bA	835	CLA	O2D-CGD	4.59	1.44	1.33
12	aL	202	F6C	O2D-CGD	4.59	1.44	1.33
12	bL	202	F6C	O2D-CGD	4.59	1.44	1.33
11	cA	837	CLA	CHC-C1C	4.59	1.47	1.38
11	aB	815	CLA	CHC-C1C	4.58	1.47	1.38
11	bA	842	CLA	CHC-C1C	4.58	1.47	1.38
11	aB	828	CLA	C1D-ND	4.58	1.43	1.37
11	cK	101	CLA	CHC-C1C	4.58	1.47	1.38
11	cB	801	CLA	C1D-ND	4.58	1.43	1.37
11	cL	206	CLA	C1D-ND	4.58	1.43	1.37
11	aB	801	CLA	C1D-ND	4.58	1.43	1.37
11	bA	812	CLA	CHC-C1C	4.58	1.47	1.38
11	aA	835	CLA	O2D-CGD	4.57	1.44	1.33
11	bA	837	CLA	CHC-C1C	4.57	1.47	1.38
11	cB	819	CLA	CHC-C1C	4.57	1.47	1.38
11	cB	815	CLA	CHC-C1C	4.57	1.47	1.38
11	cA	811	CLA	CHC-C1C	4.57	1.47	1.38
11	cB	802	CLA	O2D-CGD	4.57	1.44	1.33
11	aB	828	CLA	C1B-NB	-4.57	1.32	1.37
11	cA	808	CLA	CHC-C1C	4.57	1.47	1.38
11	aA	842	CLA	CHC-C1C	4.56	1.47	1.38
11	bB	819	CLA	C1D-ND	4.56	1.43	1.37
11	aB	811	CLA	CHC-C1C	4.56	1.47	1.38
11	aA	808	CLA	CHC-C1C	4.56	1.47	1.38
11	aB	806	CLA	CHC-C1C	4.56	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	cB	811	CLA	CHC-C1C	4.56	1.47	1.38
11	aB	829	CLA	CHD-C1D	4.56	1.47	1.38
11	bL	205	CLA	C1D-ND	4.55	1.43	1.37
11	cB	819	CLA	C1D-ND	4.55	1.43	1.37
11	cA	841	CLA	CHC-C1C	4.55	1.47	1.38
11	bB	811	CLA	CHC-C1C	4.55	1.47	1.38
11	cL	205	CLA	C1D-ND	4.55	1.43	1.37
11	cA	828	CLA	CHC-C1C	4.55	1.47	1.38
11	bA	841	CLA	CHC-C1C	4.55	1.47	1.38
11	bA	808	CLA	CHC-C1C	4.55	1.47	1.38
11	aB	819	CLA	C1D-ND	4.55	1.43	1.37
11	aA	821	CLA	C1D-ND	4.55	1.43	1.37
11	aA	812	CLA	CHC-C1C	4.54	1.47	1.38
11	aA	811	CLA	CHC-C1C	4.54	1.47	1.38
11	bA	811	CLA	CHC-C1C	4.54	1.47	1.38
11	aB	812	CLA	CHD-C1D	4.54	1.47	1.38
11	aB	830	CLA	CHC-C1C	4.54	1.47	1.38
11	aL	205	CLA	CHC-C1C	4.54	1.47	1.38
11	aL	206	CLA	C1D-ND	4.53	1.43	1.37
11	cB	823	CLA	C1D-ND	4.53	1.43	1.37
11	bL	205	CLA	CHC-C1C	4.53	1.47	1.38
11	aA	828	CLA	CHC-C1C	4.53	1.47	1.38
11	cB	812	CLA	CHD-C1D	4.53	1.47	1.38
11	cB	806	CLA	CHC-C1C	4.53	1.47	1.38
11	bB	832	CLA	O2A-CGA	4.52	1.45	1.30
11	aA	841	CLA	CHC-C1C	4.52	1.47	1.38
11	cA	812	CLA	CHC-C1C	4.52	1.47	1.38
11	cB	832	CLA	O2A-CGA	4.52	1.45	1.30
11	cB	823	CLA	CHC-C1C	4.52	1.47	1.38
11	bB	829	CLA	O2A-CGA	4.52	1.45	1.30
11	bA	833	CLA	CHC-C1C	4.52	1.47	1.38
11	bB	830	CLA	CHC-C1C	4.52	1.47	1.38
11	bB	812	CLA	CHD-C1D	4.51	1.47	1.38
11	bA	814	CLA	CHC-C1C	4.51	1.47	1.38
11	aA	803	CLA	C1B-NB	-4.51	1.32	1.37
11	cL	205	CLA	CHC-C1C	4.51	1.47	1.38
11	aA	802	CLA	C1D-ND	4.51	1.43	1.37
11	bA	804	CLA	O2A-CGA	4.51	1.45	1.30
11	bA	828	CLA	CHC-C1C	4.51	1.47	1.38
11	bB	823	CLA	CHC-C1C	4.51	1.47	1.38
11	cA	814	CLA	CHC-C1C	4.51	1.47	1.38
11	cB	820	CLA	CHC-C1C	4.51	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	cB	840	CLA	O2A-CGA	4.51	1.45	1.30
11	bB	806	CLA	CHC-C1C	4.50	1.47	1.38
11	aA	818	CLA	C1D-ND	4.50	1.43	1.37
11	aB	823	CLA	C1D-ND	4.50	1.43	1.37
11	bA	811	CLA	O2A-CGA	4.50	1.45	1.30
11	cB	820	CLA	O2A-CGA	4.50	1.45	1.30
11	aB	833	CLA	O2A-CGA	4.50	1.45	1.30
11	aB	832	CLA	O2A-CGA	4.50	1.45	1.30
11	bA	816	CLA	O2A-CGA	4.50	1.45	1.30
11	bB	823	CLA	C1D-ND	4.50	1.43	1.37
11	aB	823	CLA	CHC-C1C	4.50	1.47	1.38
11	bB	834	CLA	O2A-CGA	4.50	1.45	1.30
11	aA	804	CLA	O2A-CGA	4.50	1.45	1.30
11	cA	818	CLA	C1D-ND	4.50	1.43	1.37
11	bA	822	CLA	CHC-C1C	4.49	1.47	1.38
11	bB	820	CLA	O2A-CGA	4.49	1.45	1.30
11	aA	814	CLA	CHC-C1C	4.49	1.47	1.38
11	aA	842	CLA	O2A-CGA	4.49	1.45	1.30
11	bB	840	CLA	O2A-CGA	4.49	1.45	1.30
11	bB	825	CLA	CHC-C1C	4.49	1.47	1.38
11	cA	804	CLA	O2A-CGA	4.49	1.45	1.30
11	bA	818	CLA	C1D-ND	4.49	1.43	1.37
11	bA	831	CLA	C1B-NB	-4.49	1.32	1.37
11	aB	829	CLA	O2A-CGA	4.49	1.45	1.30
11	aB	834	CLA	O2A-CGA	4.49	1.45	1.30
11	aA	811	CLA	O2A-CGA	4.49	1.45	1.30
11	bA	805	CLA	O2A-CGA	4.48	1.45	1.30
11	aB	814	CLA	O2A-CGA	4.48	1.45	1.30
11	aA	822	CLA	CHC-C1C	4.48	1.47	1.38
11	cA	805	CLA	O2A-CGA	4.48	1.45	1.30
11	aB	820	CLA	O2A-CGA	4.48	1.45	1.30
11	bA	809	CLA	O2A-CGA	4.48	1.45	1.30
11	cB	829	CLA	O2A-CGA	4.48	1.45	1.30
11	aA	815	CLA	O2A-CGA	4.48	1.45	1.30
11	cA	809	CLA	CHC-C1C	4.48	1.47	1.38
11	cB	830	CLA	CHC-C1C	4.48	1.47	1.38
11	bB	802	CLA	C1D-ND	4.48	1.43	1.37
11	aB	840	CLA	O2A-CGA	4.48	1.45	1.30
11	cB	833	CLA	O2A-CGA	4.48	1.45	1.30
11	cA	811	CLA	O2A-CGA	4.48	1.45	1.30
11	bB	831	CLA	CHC-C1C	4.48	1.47	1.38
11	cA	815	CLA	O2A-CGA	4.48	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aB	802	CLA	C1D-ND	4.48	1.43	1.37
11	cA	809	CLA	O2A-CGA	4.48	1.45	1.30
11	bA	842	CLA	O2A-CGA	4.48	1.45	1.30
11	aA	835	CLA	CHC-C1C	4.48	1.47	1.38
11	bB	820	CLA	CHC-C1C	4.48	1.47	1.38
11	aA	809	CLA	O2A-CGA	4.48	1.45	1.30
12	cA	844	F6C	CHC-C4B	4.47	1.47	1.38
11	aB	825	CLA	CHC-C1C	4.47	1.47	1.38
11	cA	842	CLA	O2A-CGA	4.47	1.45	1.30
11	aA	813	CLA	CHC-C1C	4.47	1.47	1.38
11	cB	814	CLA	O2A-CGA	4.47	1.45	1.30
11	aA	807	CLA	CHC-C1C	4.47	1.47	1.38
11	bB	814	CLA	O2A-CGA	4.47	1.45	1.30
11	bA	809	CLA	CHC-C1C	4.47	1.47	1.38
11	aA	816	CLA	O2A-CGA	4.47	1.45	1.30
11	bB	811	CLA	O2A-CGA	4.47	1.45	1.30
11	aA	809	CLA	CHC-C1C	4.47	1.47	1.38
11	bA	835	CLA	CHC-C1C	4.47	1.47	1.38
11	aA	833	CLA	CHC-C1C	4.47	1.47	1.38
11	bB	833	CLA	O2A-CGA	4.47	1.45	1.30
11	cB	807	CLA	C1D-ND	4.47	1.43	1.37
11	aA	824	CLA	CHC-C1C	4.47	1.47	1.38
11	cB	834	CLA	O2A-CGA	4.46	1.45	1.30
11	bB	826	CLA	CHC-C1C	4.46	1.47	1.38
11	aB	807	CLA	C1D-ND	4.46	1.43	1.37
11	aB	835	CLA	O2A-CGA	4.46	1.45	1.30
11	bB	810	CLA	O2A-CGA	4.46	1.45	1.30
12	bA	844	F6C	CHC-C4B	4.46	1.47	1.38
11	bL	206	CLA	CHC-C1C	4.46	1.47	1.38
11	bA	815	CLA	O2A-CGA	4.46	1.45	1.30
11	cA	816	CLA	O2A-CGA	4.46	1.45	1.30
11	cB	831	CLA	CHC-C1C	4.46	1.47	1.38
11	aA	805	CLA	O2A-CGA	4.46	1.45	1.30
11	aA	810	CLA	CHC-C1C	4.46	1.47	1.38
11	bB	834	CLA	CHD-C1D	4.46	1.47	1.38
11	cA	810	CLA	CHC-C1C	4.46	1.47	1.38
11	bA	840	CLA	CHC-C1C	4.46	1.47	1.38
11	aB	820	CLA	CHC-C1C	4.46	1.47	1.38
11	cK	103	CLA	CHC-C1C	4.46	1.47	1.38
11	bB	835	CLA	O2A-CGA	4.46	1.45	1.30
11	aL	206	CLA	CHC-C1C	4.46	1.47	1.38
11	cA	807	CLA	CHC-C1C	4.46	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	cB	810	CLA	O2A-CGA	4.46	1.45	1.30
11	cB	826	CLA	CHC-C1C	4.45	1.47	1.38
11	aB	831	CLA	CHC-C1C	4.45	1.47	1.38
11	bA	824	CLA	CHC-C1C	4.45	1.47	1.38
11	cB	834	CLA	CHD-C1D	4.45	1.47	1.38
11	cA	833	CLA	CHC-C1C	4.45	1.47	1.38
11	cB	802	CLA	C1D-ND	4.45	1.43	1.37
11	aB	826	CLA	CHC-C1C	4.45	1.47	1.38
11	bA	836	CLA	O2A-CGA	4.45	1.45	1.30
11	cA	822	CLA	CHC-C1C	4.45	1.47	1.38
11	bA	813	CLA	CHC-C1C	4.45	1.47	1.38
11	aB	811	CLA	O2A-CGA	4.44	1.45	1.30
11	cA	813	CLA	CHC-C1C	4.44	1.47	1.38
12	aA	844	F6C	CHC-C4B	4.44	1.47	1.38
11	cA	824	CLA	CHC-C1C	4.44	1.47	1.38
11	bB	821	CLA	CHC-C1C	4.44	1.47	1.38
11	aA	837	CLA	O2A-CGA	4.44	1.45	1.30
11	cA	810	CLA	O2A-CGA	4.44	1.45	1.30
11	aB	835	CLA	CHC-C1C	4.44	1.47	1.38
11	bA	829	CLA	CHC-C1C	4.44	1.47	1.38
11	cA	835	CLA	CHC-C1C	4.44	1.47	1.38
11	cB	825	CLA	CHC-C1C	4.44	1.47	1.38
11	cB	835	CLA	O2A-CGA	4.44	1.45	1.30
11	cA	836	CLA	O2A-CGA	4.44	1.45	1.30
11	aB	821	CLA	CHC-C1C	4.44	1.47	1.38
11	cB	811	CLA	O2A-CGA	4.43	1.45	1.30
11	aK	103	CLA	CHC-C1C	4.43	1.47	1.38
11	cL	206	CLA	CHC-C1C	4.43	1.47	1.38
11	bA	810	CLA	CHC-C1C	4.43	1.47	1.38
11	bB	827	CLA	CHC-C1C	4.43	1.47	1.38
11	aA	836	CLA	O2A-CGA	4.43	1.45	1.30
11	aA	843	CLA	CHC-C1C	4.43	1.47	1.38
11	bA	803	CLA	C1B-NB	-4.43	1.32	1.37
11	cA	803	CLA	C1B-NB	-4.43	1.32	1.37
12	cL	202	F6C	O2A-CGA	4.43	1.46	1.33
11	bA	802	CLA	C1D-ND	4.43	1.43	1.37
11	cA	843	CLA	CHC-C1C	4.43	1.47	1.38
12	aL	202	F6C	O2A-CGA	4.43	1.46	1.33
11	aB	810	CLA	O2A-CGA	4.43	1.45	1.30
11	bA	837	CLA	O2A-CGA	4.42	1.45	1.30
11	cA	829	CLA	CHC-C1C	4.42	1.47	1.38
11	cA	837	CLA	O2A-CGA	4.42	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aA	831	CLA	C1B-NB	-4.42	1.32	1.37
11	bA	807	CLA	CHC-C1C	4.42	1.47	1.38
11	bK	103	CLA	CHC-C1C	4.42	1.47	1.38
11	aB	834	CLA	CHD-C1D	4.42	1.47	1.38
11	cA	840	CLA	CHC-C1C	4.42	1.47	1.38
11	cB	835	CLA	CHC-C1C	4.42	1.47	1.38
11	bB	828	CLA	CHD-C1D	4.42	1.47	1.38
11	aA	810	CLA	O2A-CGA	4.42	1.45	1.30
11	cA	802	CLA	C1D-ND	4.42	1.43	1.37
11	cB	822	CLA	O2A-CGA	4.42	1.45	1.30
12	bL	202	F6C	O2A-CGA	4.42	1.46	1.33
11	cB	821	CLA	CHC-C1C	4.41	1.47	1.38
11	bL	204	CLA	CHC-C1C	4.41	1.47	1.38
11	bA	810	CLA	O2A-CGA	4.41	1.45	1.30
11	bB	807	CLA	C1D-ND	4.41	1.43	1.37
11	bA	843	CLA	CHC-C1C	4.41	1.47	1.38
11	bA	823	CLA	CHC-C1C	4.41	1.47	1.38
11	cA	831	CLA	C1B-NB	-4.41	1.32	1.37
11	aA	823	CLA	CHC-C1C	4.41	1.47	1.38
11	cA	821	CLA	CHC-C1C	4.41	1.47	1.38
11	aL	204	CLA	CHC-C1C	4.40	1.47	1.38
11	cA	823	CLA	CHC-C1C	4.40	1.47	1.38
11	cB	805	CLA	CHC-C1C	4.40	1.47	1.38
11	bB	822	CLA	O2A-CGA	4.40	1.45	1.30
11	bA	831	CLA	C1D-ND	4.40	1.43	1.37
11	bB	838	CLA	CHC-C1C	4.40	1.47	1.38
11	aB	822	CLA	O2A-CGA	4.40	1.45	1.30
11	aA	840	CLA	CHC-C1C	4.40	1.47	1.38
11	aA	838	CLA	CHC-C1C	4.40	1.47	1.38
11	aA	806	CLA	CHC-C1C	4.39	1.47	1.38
11	bB	835	CLA	CHC-C1C	4.39	1.47	1.38
11	aB	828	CLA	CHD-C1D	4.39	1.46	1.38
11	aB	827	CLA	CHC-C1C	4.39	1.47	1.38
11	cB	827	CLA	CHC-C1C	4.39	1.47	1.38
11	aB	838	CLA	CHC-C1C	4.39	1.47	1.38
11	aA	829	CLA	CHC-C1C	4.39	1.47	1.38
11	bA	821	CLA	CHC-C1C	4.38	1.47	1.38
11	aB	805	CLA	CHC-C1C	4.38	1.47	1.38
11	bA	838	CLA	CHC-C1C	4.38	1.47	1.38
11	aA	834	CLA	CHC-C1C	4.38	1.47	1.38
11	cA	806	CLA	CHC-C1C	4.37	1.47	1.38
11	aA	812	CLA	CHD-C1D	4.37	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bA	834	CLA	CHC-C1C	4.37	1.47	1.38
11	cB	838	CLA	CHC-C1C	4.37	1.47	1.38
11	bB	805	CLA	CHC-C1C	4.37	1.47	1.38
11	aA	821	CLA	CHC-C1C	4.37	1.47	1.38
11	aB	802	CLA	O2A-CGA	4.37	1.46	1.33
11	cB	839	CLA	C1D-ND	4.37	1.43	1.37
11	bB	802	CLA	O2A-CGA	4.36	1.46	1.33
11	bB	839	CLA	C1D-ND	4.36	1.43	1.37
11	aA	806	CLA	CHD-C1D	4.36	1.46	1.38
11	cB	801	CLA	CHC-C1C	4.36	1.47	1.38
11	cB	802	CLA	O2A-CGA	4.36	1.46	1.33
11	cB	831	CLA	CHD-C1D	4.36	1.46	1.38
11	bB	834	CLA	CHC-C1C	4.36	1.47	1.38
11	bA	806	CLA	CHD-C1D	4.35	1.46	1.38
11	aB	808	CLA	CHC-C1C	4.35	1.47	1.38
11	cL	204	CLA	CHC-C1C	4.35	1.47	1.38
11	bB	831	CLA	CHD-C1D	4.35	1.46	1.38
11	aA	839	CLA	CHC-C1C	4.35	1.47	1.38
11	bA	806	CLA	CHC-C1C	4.35	1.47	1.38
11	cA	838	CLA	CHC-C1C	4.35	1.47	1.38
11	cB	828	CLA	CHD-C1D	4.35	1.46	1.38
11	bA	823	CLA	O2A-CGA	4.35	1.45	1.30
12	bA	827	F6C	CHC-C4B	4.34	1.47	1.38
11	cA	817	CLA	CHC-C1C	4.34	1.47	1.38
11	cA	823	CLA	O2A-CGA	4.34	1.45	1.30
11	cB	813	CLA	CHC-C1C	4.34	1.47	1.38
11	aB	808	CLA	C1B-NB	-4.34	1.32	1.37
11	bA	815	CLA	CHD-C1D	4.34	1.46	1.38
11	bB	812	CLA	CHC-C1C	4.34	1.47	1.38
11	cA	834	CLA	CHC-C1C	4.34	1.47	1.38
11	cB	810	CLA	CHC-C1C	4.34	1.47	1.38
11	aB	835	CLA	CHD-C1D	4.34	1.46	1.38
11	cB	834	CLA	CHC-C1C	4.34	1.47	1.38
11	cA	806	CLA	CHD-C1D	4.34	1.46	1.38
11	aB	810	CLA	CHC-C1C	4.33	1.47	1.38
11	bB	814	CLA	CHC-C1C	4.33	1.47	1.38
11	bA	812	CLA	CHD-C1D	4.33	1.46	1.38
11	bA	839	CLA	CHC-C1C	4.33	1.47	1.38
11	bA	817	CLA	CHD-C1D	4.33	1.46	1.38
11	bA	817	CLA	CHC-C1C	4.33	1.47	1.38
11	cB	835	CLA	CHD-C1D	4.33	1.46	1.38
12	aA	827	F6C	CHC-C4B	4.33	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aB	831	CLA	CHD-C1D	4.33	1.46	1.38
11	aA	802	CLA	CHD-C1D	4.33	1.46	1.38
11	aB	801	CLA	CHC-C1C	4.33	1.47	1.38
11	cA	817	CLA	CHD-C1D	4.33	1.46	1.38
11	cA	825	CLA	CHC-C1C	4.32	1.47	1.38
11	aA	817	CLA	CHC-C1C	4.32	1.47	1.38
11	aA	831	CLA	C1D-ND	4.32	1.43	1.37
10	cA	801	CL0	CHC-C1C	4.32	1.47	1.38
11	aA	825	CLA	CHC-C1C	4.32	1.47	1.38
11	aB	812	CLA	CHC-C1C	4.32	1.47	1.38
11	aB	814	CLA	CHC-C1C	4.32	1.47	1.38
11	aB	834	CLA	CHC-C1C	4.32	1.47	1.38
11	cA	802	CLA	CHD-C1D	4.32	1.46	1.38
11	bB	832	CLA	CHD-C1D	4.32	1.46	1.38
11	bB	835	CLA	CHD-C1D	4.32	1.46	1.38
11	cA	839	CLA	CHC-C1C	4.32	1.47	1.38
11	aA	823	CLA	O2A-CGA	4.32	1.45	1.30
11	bB	801	CLA	CHC-C1C	4.31	1.47	1.38
11	aA	815	CLA	CHD-C1D	4.31	1.46	1.38
11	aB	814	CLA	CHD-C1D	4.31	1.46	1.38
11	bB	810	CLA	CHC-C1C	4.31	1.47	1.38
11	aB	817	CLA	CHC-C1C	4.31	1.47	1.38
11	aB	839	CLA	C1D-ND	4.31	1.43	1.37
11	bA	814	CLA	CHD-C1D	4.31	1.46	1.38
11	cA	812	CLA	CHD-C1D	4.31	1.46	1.38
11	cB	817	CLA	CHC-C1C	4.31	1.47	1.38
11	bB	817	CLA	CHC-C1C	4.31	1.47	1.38
12	aL	202	F6C	CHC-C4B	4.31	1.47	1.38
10	aA	801	CL0	CHC-C1C	4.31	1.47	1.38
11	cB	812	CLA	CHC-C1C	4.30	1.47	1.38
11	bB	808	CLA	CHC-C1C	4.30	1.47	1.38
12	bL	202	F6C	CHC-C4B	4.30	1.47	1.38
11	cA	815	CLA	CHD-C1D	4.30	1.46	1.38
10	bA	801	CL0	CHC-C1C	4.30	1.47	1.38
11	cB	808	CLA	CHC-C1C	4.30	1.47	1.38
11	aB	832	CLA	CHD-C1D	4.30	1.46	1.38
11	aB	813	CLA	CHC-C1C	4.30	1.47	1.38
11	cA	811	CLA	CHD-C1D	4.30	1.46	1.38
11	cA	840	CLA	O2A-CGA	4.30	1.45	1.33
11	bA	825	CLA	CHC-C1C	4.30	1.47	1.38
11	aA	817	CLA	CHD-C1D	4.30	1.46	1.38
11	cA	831	CLA	C1D-ND	4.30	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bB	813	CLA	CHC-C1C	4.30	1.47	1.38
11	cA	802	CLA	C1B-NB	-4.30	1.32	1.37
12	aA	826	F6C	CHC-C4B	4.30	1.47	1.38
11	aA	840	CLA	O2A-CGA	4.30	1.45	1.33
11	cB	814	CLA	CHD-C1D	4.29	1.46	1.38
11	bB	809	CLA	C1D-ND	4.29	1.43	1.37
11	cB	814	CLA	CHC-C1C	4.29	1.47	1.38
11	bA	802	CLA	CHD-C1D	4.29	1.46	1.38
11	aB	809	CLA	C1D-ND	4.29	1.43	1.37
11	aA	811	CLA	CHD-C1D	4.29	1.46	1.38
11	aB	830	CLA	CHD-C1D	4.29	1.46	1.38
11	bB	811	CLA	CHD-C1D	4.29	1.46	1.38
11	bB	830	CLA	CHD-C1D	4.29	1.46	1.38
12	cA	832	F6C	O2A-CGA	4.28	1.45	1.33
11	cB	811	CLA	CHD-C1D	4.28	1.46	1.38
12	cL	202	F6C	CHC-C4B	4.28	1.47	1.38
11	bA	811	CLA	CHD-C1D	4.28	1.46	1.38
11	cA	804	CLA	CHD-C1D	4.28	1.46	1.38
11	bA	825	CLA	CHD-C1D	4.28	1.46	1.38
11	cA	820	CLA	CHD-C1D	4.28	1.46	1.38
11	bA	840	CLA	O2A-CGA	4.28	1.45	1.33
11	cA	825	CLA	CHD-C1D	4.28	1.46	1.38
12	cA	827	F6C	CHC-C4B	4.28	1.47	1.38
11	bB	810	CLA	CHD-C1D	4.28	1.46	1.38
11	cB	810	CLA	CHD-C1D	4.28	1.46	1.38
11	bB	808	CLA	C1B-NB	-4.28	1.32	1.37
11	bA	802	CLA	C1B-NB	-4.27	1.32	1.37
12	aB	824	F6C	O2A-CGA	4.27	1.45	1.33
11	bB	807	CLA	CHC-C1C	4.27	1.47	1.38
11	bA	804	CLA	CHD-C1D	4.27	1.46	1.38
11	bB	809	CLA	CHC-C1C	4.27	1.47	1.38
11	aA	820	CLA	CHD-C1D	4.27	1.46	1.38
11	aA	835	CLA	O2A-CGA	4.27	1.45	1.33
11	cB	808	CLA	C1B-NB	-4.27	1.32	1.37
11	aA	815	CLA	CHC-C1C	4.27	1.47	1.38
11	cA	814	CLA	CHD-C1D	4.27	1.46	1.38
11	aA	814	CLA	CHD-C1D	4.27	1.46	1.38
11	cB	809	CLA	CHC-C1C	4.27	1.47	1.38
12	bA	832	F6C	O2A-CGA	4.27	1.45	1.33
11	cK	101	CLA	CHD-C1D	4.26	1.46	1.38
12	aA	832	F6C	O2A-CGA	4.26	1.45	1.33
11	bB	813	CLA	O2A-CGA	4.26	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bA	835	CLA	O2A-CGA	4.26	1.45	1.33
11	cB	813	CLA	O2A-CGA	4.26	1.45	1.33
11	cB	830	CLA	CHD-C1D	4.26	1.46	1.38
11	cB	832	CLA	CHD-C1D	4.26	1.46	1.38
11	aB	811	CLA	CHD-C1D	4.26	1.46	1.38
11	bB	821	CLA	CHD-C1D	4.26	1.46	1.38
11	bA	820	CLA	CHD-C1D	4.26	1.46	1.38
11	cA	815	CLA	CHC-C1C	4.26	1.47	1.38
11	cB	821	CLA	CHD-C1D	4.26	1.46	1.38
11	aK	101	CLA	CHD-C1D	4.26	1.46	1.38
11	bK	101	CLA	CHD-C1D	4.26	1.46	1.38
11	aA	825	CLA	CHD-C1D	4.26	1.46	1.38
11	cB	826	CLA	C1D-ND	4.25	1.43	1.37
11	bB	814	CLA	CHD-C1D	4.25	1.46	1.38
11	aB	821	CLA	CHD-C1D	4.25	1.46	1.38
12	cB	824	F6C	O2A-CGA	4.25	1.45	1.33
12	cA	826	F6C	CHC-C4B	4.25	1.47	1.38
11	cA	820	CLA	CHC-C1C	4.25	1.47	1.38
11	cA	824	CLA	CHD-C1D	4.25	1.46	1.38
11	aA	802	CLA	C1B-NB	-4.25	1.32	1.37
11	aA	836	CLA	C1D-ND	4.25	1.43	1.37
11	bB	823	CLA	O2A-CGA	4.25	1.45	1.33
11	bB	827	CLA	O2A-CGA	4.25	1.45	1.33
11	aB	827	CLA	O2A-CGA	4.25	1.45	1.33
11	aB	813	CLA	O2A-CGA	4.25	1.45	1.33
11	cB	823	CLA	O2A-CGA	4.25	1.45	1.33
11	cB	804	CLA	O2A-CGA	4.24	1.45	1.33
11	aA	822	CLA	O2A-CGA	4.24	1.45	1.33
12	bB	824	F6C	O2A-CGA	4.24	1.45	1.33
11	aB	805	CLA	CHD-C1D	4.24	1.46	1.38
11	aA	820	CLA	CHC-C1C	4.24	1.47	1.38
11	cB	827	CLA	O2A-CGA	4.24	1.45	1.33
11	aB	810	CLA	CHD-C1D	4.24	1.46	1.38
11	aA	843	CLA	O2A-CGA	4.24	1.45	1.33
12	bA	826	F6C	CHC-C4B	4.24	1.47	1.38
11	cA	822	CLA	O2A-CGA	4.24	1.45	1.33
11	bB	830	CLA	O2A-CGA	4.24	1.45	1.33
11	cA	835	CLA	O2A-CGA	4.24	1.45	1.33
11	aA	817	CLA	O2A-CGA	4.23	1.45	1.33
11	aB	807	CLA	CHC-C1C	4.23	1.47	1.38
11	aB	809	CLA	CHC-C1C	4.23	1.47	1.38
11	bA	820	CLA	CHC-C1C	4.23	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aA	804	CLA	CHD-C1D	4.23	1.46	1.38
11	bB	836	CLA	O2A-CGA	4.23	1.45	1.33
11	bB	826	CLA	C1D-ND	4.23	1.43	1.37
11	bA	836	CLA	C1D-ND	4.23	1.43	1.37
11	aA	820	CLA	O2A-CGA	4.23	1.45	1.33
11	cB	836	CLA	O2A-CGA	4.23	1.45	1.33
11	aB	826	CLA	C1D-ND	4.23	1.43	1.37
11	bB	816	CLA	CHD-C1D	4.23	1.46	1.38
11	aB	804	CLA	O2A-CGA	4.23	1.45	1.33
11	bB	804	CLA	O2A-CGA	4.22	1.45	1.33
11	aB	833	CLA	CHD-C1D	4.22	1.46	1.38
11	cB	833	CLA	CHD-C1D	4.22	1.46	1.38
11	aA	824	CLA	CHD-C1D	4.22	1.46	1.38
11	aB	830	CLA	O2A-CGA	4.22	1.45	1.33
11	cA	843	CLA	O2A-CGA	4.22	1.45	1.33
11	aB	816	CLA	CHD-C1D	4.22	1.46	1.38
11	cA	816	CLA	CHD-C1D	4.22	1.46	1.38
11	aB	823	CLA	O2A-CGA	4.22	1.45	1.33
11	bA	820	CLA	O2A-CGA	4.22	1.45	1.33
11	bA	815	CLA	CHC-C1C	4.21	1.47	1.38
11	cB	830	CLA	O2A-CGA	4.21	1.45	1.33
11	bA	817	CLA	O2A-CGA	4.21	1.45	1.33
12	cB	824	F6C	CHD-C1D	4.21	1.47	1.38
11	bB	825	CLA	O2A-CGA	4.21	1.45	1.33
11	aB	836	CLA	O2A-CGA	4.21	1.45	1.33
11	cA	803	CLA	O2A-CGA	4.21	1.45	1.33
11	cB	807	CLA	CHC-C1C	4.21	1.47	1.38
11	aB	813	CLA	CHD-C1D	4.20	1.46	1.38
11	bA	822	CLA	O2A-CGA	4.20	1.45	1.33
11	bA	843	CLA	O2A-CGA	4.20	1.45	1.33
11	cA	817	CLA	O2A-CGA	4.20	1.45	1.33
11	aA	822	CLA	CHD-C1D	4.20	1.46	1.38
11	aA	812	CLA	O2A-CGA	4.20	1.45	1.33
11	cA	836	CLA	C1D-ND	4.20	1.42	1.37
11	cB	803	CLA	O2A-CGA	4.20	1.45	1.33
12	bB	824	F6C	CHD-C1D	4.20	1.47	1.38
12	aB	824	F6C	CHD-C1D	4.20	1.47	1.38
11	cA	820	CLA	O2A-CGA	4.20	1.45	1.33
11	cA	833	CLA	CHD-C1D	4.20	1.46	1.38
11	cB	813	CLA	CHD-C1D	4.20	1.46	1.38
11	bB	808	CLA	C1D-ND	4.19	1.42	1.37
11	bA	822	CLA	CHD-C1D	4.19	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	cA	829	CLA	CHD-C1D	4.19	1.46	1.38
11	bA	833	CLA	CHD-C1D	4.19	1.46	1.38
12	bA	826	F6C	O2A-CGA	4.19	1.45	1.33
11	bB	833	CLA	CHD-C1D	4.19	1.46	1.38
11	bA	824	CLA	CHD-C1D	4.19	1.46	1.38
11	cB	809	CLA	C1D-ND	4.19	1.42	1.37
11	aB	825	CLA	O2A-CGA	4.19	1.45	1.33
12	aA	830	F6C	CHC-C4B	4.19	1.47	1.38
12	aA	826	F6C	O2A-CGA	4.19	1.45	1.33
11	aA	803	CLA	O2A-CGA	4.19	1.45	1.33
11	bB	803	CLA	O2A-CGA	4.18	1.45	1.33
11	bB	821	CLA	O2A-CGA	4.18	1.45	1.33
11	aA	805	CLA	CHD-C1D	4.18	1.46	1.38
10	cA	801	CL0	C1D-ND	4.18	1.42	1.37
11	cA	819	CLA	O2A-CGA	4.18	1.45	1.33
12	aA	830	F6C	O2A-CGA	4.18	1.45	1.33
11	bA	824	CLA	O2A-CGA	4.18	1.45	1.33
11	cB	825	CLA	O2A-CGA	4.18	1.45	1.33
11	aA	833	CLA	CHD-C1D	4.18	1.46	1.38
11	cB	821	CLA	O2A-CGA	4.18	1.45	1.33
12	cA	830	F6C	CHC-C4B	4.18	1.47	1.38
11	cA	802	CLA	CHC-C1C	4.18	1.47	1.38
11	cB	816	CLA	CHD-C1D	4.18	1.46	1.38
12	cA	826	F6C	O2A-CGA	4.18	1.45	1.33
12	cA	830	F6C	O2A-CGA	4.17	1.45	1.33
11	bA	803	CLA	O2A-CGA	4.17	1.45	1.33
11	cB	815	CLA	O2A-CGA	4.17	1.45	1.33
11	cB	805	CLA	CHD-C1D	4.17	1.46	1.38
11	cB	806	CLA	O2A-CGA	4.17	1.45	1.33
11	cA	822	CLA	CHD-C1D	4.17	1.46	1.38
11	aA	824	CLA	O2A-CGA	4.17	1.45	1.33
11	cA	812	CLA	O2A-CGA	4.17	1.45	1.33
11	bB	805	CLA	CHD-C1D	4.17	1.46	1.38
12	bA	830	F6C	CHC-C4B	4.17	1.47	1.38
11	bA	828	CLA	O2A-CGA	4.17	1.45	1.33
11	cB	837	CLA	CHD-C1D	4.17	1.46	1.38
11	aA	819	CLA	O2A-CGA	4.17	1.45	1.33
11	bA	812	CLA	O2A-CGA	4.17	1.45	1.33
11	bB	815	CLA	O2A-CGA	4.17	1.45	1.33
11	bA	819	CLA	O2A-CGA	4.17	1.45	1.33
12	bA	826	F6C	C3B-C2B	4.17	1.48	1.39
11	cA	824	CLA	O2A-CGA	4.17	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aB	815	CLA	O2A-CGA	4.17	1.45	1.33
11	aA	816	CLA	CHD-C1D	4.17	1.46	1.38
10	aA	801	CL0	C1D-ND	4.16	1.42	1.37
11	cB	837	CLA	O2A-CGA	4.16	1.45	1.33
11	bA	816	CLA	CHD-C1D	4.16	1.46	1.38
11	aB	821	CLA	O2A-CGA	4.16	1.45	1.33
11	cA	831	CLA	CHC-C1C	4.16	1.47	1.38
11	bB	813	CLA	CHD-C1D	4.16	1.46	1.38
11	aA	835	CLA	CHD-C1D	4.16	1.46	1.38
11	bA	805	CLA	CHD-C1D	4.16	1.46	1.38
11	bA	831	CLA	CHC-C1C	4.16	1.47	1.38
12	cA	826	F6C	C3B-C2B	4.16	1.48	1.39
11	bK	103	CLA	O2A-CGA	4.15	1.45	1.33
11	bA	835	CLA	CHD-C1D	4.15	1.46	1.38
11	aB	837	CLA	O2A-CGA	4.15	1.45	1.33
11	cB	831	CLA	O2A-CGA	4.15	1.45	1.33
11	cA	805	CLA	CHD-C1D	4.15	1.46	1.38
11	bB	840	CLA	CHC-C1C	4.15	1.47	1.38
11	cA	828	CLA	O2A-CGA	4.15	1.45	1.33
11	aB	806	CLA	O2A-CGA	4.15	1.45	1.33
11	aB	831	CLA	O2A-CGA	4.15	1.45	1.33
11	cK	103	CLA	O2A-CGA	4.15	1.45	1.33
11	cB	808	CLA	C1D-ND	4.15	1.42	1.37
11	aB	803	CLA	O2A-CGA	4.15	1.45	1.33
12	aA	826	F6C	C3B-C2B	4.15	1.48	1.39
11	bB	837	CLA	O2A-CGA	4.15	1.45	1.33
11	bA	821	CLA	O2A-CGA	4.15	1.45	1.33
11	cA	809	CLA	CHD-C1D	4.15	1.46	1.38
11	aA	831	CLA	CHC-C1C	4.15	1.46	1.38
11	aA	833	CLA	O2A-CGA	4.15	1.45	1.33
11	bA	837	CLA	CHD-C1D	4.15	1.46	1.38
11	aB	808	CLA	C1D-ND	4.15	1.42	1.37
11	aA	829	CLA	CHD-C1D	4.15	1.46	1.38
11	bB	807	CLA	O2A-CGA	4.15	1.45	1.33
11	aA	828	CLA	O2A-CGA	4.14	1.45	1.33
11	bB	806	CLA	O2A-CGA	4.14	1.45	1.33
11	cB	819	CLA	O2A-CGA	4.14	1.45	1.33
11	bA	809	CLA	CHD-C1D	4.14	1.46	1.38
11	bA	833	CLA	O2A-CGA	4.14	1.45	1.33
11	cA	821	CLA	O2A-CGA	4.14	1.45	1.33
11	cA	837	CLA	CHD-C1D	4.14	1.46	1.38
11	aB	819	CLA	O2A-CGA	4.14	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aA	802	CLA	CHC-C1C	4.14	1.46	1.38
11	bB	819	CLA	O2A-CGA	4.14	1.45	1.33
11	aA	839	CLA	CHD-C1D	4.14	1.46	1.38
11	bA	829	CLA	CHD-C1D	4.14	1.46	1.38
11	aA	809	CLA	CHD-C1D	4.14	1.46	1.38
11	bB	831	CLA	O2A-CGA	4.14	1.45	1.33
11	cB	808	CLA	O2A-CGA	4.14	1.45	1.33
12	cA	832	F6C	CHC-C4B	4.13	1.46	1.38
11	bA	834	CLA	CHD-C1D	4.13	1.46	1.38
11	aB	826	CLA	O2A-CGA	4.13	1.45	1.33
11	cB	807	CLA	O2A-CGA	4.13	1.45	1.33
11	bB	809	CLA	C1B-NB	-4.13	1.32	1.37
12	bA	830	F6C	O2A-CGA	4.13	1.45	1.33
11	aB	807	CLA	O2A-CGA	4.13	1.45	1.33
11	bB	837	CLA	CHD-C1D	4.13	1.46	1.38
11	aB	808	CLA	O2A-CGA	4.13	1.45	1.33
10	bA	801	CL0	C1D-ND	4.13	1.42	1.37
12	bA	832	F6C	CHC-C4B	4.13	1.46	1.38
11	aK	103	CLA	O2A-CGA	4.12	1.45	1.33
11	bB	808	CLA	O2A-CGA	4.12	1.45	1.33
11	bB	818	CLA	O2A-CGA	4.12	1.45	1.33
11	bA	839	CLA	CHD-C1D	4.12	1.46	1.38
11	cA	835	CLA	CHD-C1D	4.12	1.46	1.38
12	cA	827	F6C	O2A-CGA	4.12	1.45	1.33
11	cA	833	CLA	O2A-CGA	4.12	1.45	1.33
11	cB	828	CLA	CHC-C1C	4.12	1.46	1.38
11	cB	809	CLA	C1B-NB	-4.12	1.32	1.37
11	cA	829	CLA	O2A-CGA	4.12	1.45	1.33
11	cB	818	CLA	O2A-CGA	4.12	1.45	1.33
11	cB	826	CLA	O2A-CGA	4.12	1.45	1.33
12	aA	844	F6C	O2A-CGA	4.12	1.45	1.33
11	aL	205	CLA	O2A-CGA	4.12	1.45	1.33
11	aA	834	CLA	CHD-C1D	4.12	1.46	1.38
11	aA	825	CLA	O2A-CGA	4.12	1.45	1.33
11	aA	836	CLA	CHC-C1C	4.12	1.46	1.38
11	bB	838	CLA	O2A-CGA	4.12	1.45	1.33
11	aB	837	CLA	CHD-C1D	4.12	1.46	1.38
12	bA	844	F6C	O2A-CGA	4.11	1.45	1.33
11	bB	815	CLA	CHD-C1D	4.11	1.46	1.38
11	bB	828	CLA	CHC-C1C	4.11	1.46	1.38
11	bA	817	CLA	C1B-NB	-4.11	1.32	1.37
11	cA	839	CLA	CHD-C1D	4.11	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bA	827	F6C	O2A-CGA	4.11	1.45	1.33
12	aA	832	F6C	CHC-C4B	4.11	1.46	1.38
11	bB	816	CLA	O2A-CGA	4.11	1.45	1.33
11	aB	818	CLA	O2A-CGA	4.11	1.45	1.33
11	aA	829	CLA	O2A-CGA	4.11	1.45	1.33
11	bA	840	CLA	CHD-C1D	4.11	1.46	1.38
11	cA	813	CLA	O2A-CGA	4.11	1.45	1.33
11	cA	825	CLA	O2A-CGA	4.11	1.45	1.33
11	aA	837	CLA	CHD-C1D	4.11	1.46	1.38
11	aA	821	CLA	O2A-CGA	4.11	1.45	1.33
11	bA	825	CLA	O2A-CGA	4.11	1.45	1.33
11	bA	815	CLA	C1B-NB	-4.11	1.32	1.37
11	aB	816	CLA	O2A-CGA	4.11	1.45	1.33
11	bA	802	CLA	CHC-C1C	4.10	1.46	1.38
11	bA	829	CLA	O2A-CGA	4.10	1.45	1.33
11	bA	836	CLA	CHC-C1C	4.10	1.46	1.38
11	bB	826	CLA	O2A-CGA	4.10	1.45	1.33
11	cA	831	CLA	O2A-CGA	4.10	1.45	1.33
11	aA	813	CLA	O2A-CGA	4.10	1.45	1.33
11	cA	843	CLA	CHD-C1D	4.10	1.46	1.38
12	aL	202	F6C	C1D-ND	4.10	1.43	1.37
11	cK	103	CLA	CHD-C1D	4.10	1.46	1.38
11	cA	840	CLA	CHD-C1D	4.10	1.46	1.38
11	cB	840	CLA	CHC-C1C	4.10	1.46	1.38
11	bA	813	CLA	O2A-CGA	4.10	1.45	1.33
11	aA	807	CLA	O2A-CGA	4.10	1.45	1.33
11	aA	817	CLA	C1B-NB	-4.09	1.32	1.37
11	cA	820	CLA	C1B-NB	-4.09	1.32	1.37
11	bL	205	CLA	O2A-CGA	4.09	1.45	1.33
11	aA	818	CLA	O2A-CGA	4.09	1.45	1.33
11	aB	809	CLA	C1B-NB	-4.09	1.32	1.37
11	aB	823	CLA	CHD-C1D	4.09	1.46	1.38
11	cB	840	CLA	CHD-C1D	4.09	1.46	1.38
11	aA	831	CLA	O2A-CGA	4.09	1.45	1.33
12	aA	832	F6C	CHD-C1D	4.09	1.46	1.38
11	aA	808	CLA	CHD-C1D	4.09	1.46	1.38
11	aA	807	CLA	CHD-C1D	4.09	1.46	1.38
12	bA	832	F6C	CHD-C1D	4.09	1.46	1.38
11	aB	802	CLA	CHD-C1D	4.09	1.46	1.38
11	cA	836	CLA	CHC-C1C	4.09	1.46	1.38
11	cB	815	CLA	CHD-C1D	4.09	1.46	1.38
11	cB	838	CLA	O2A-CGA	4.09	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bA	807	CLA	O2A-CGA	4.09	1.45	1.33
11	aB	815	CLA	CHD-C1D	4.09	1.46	1.38
11	aB	840	CLA	CHC-C1C	4.09	1.46	1.38
11	bA	843	CLA	CHD-C1D	4.09	1.46	1.38
11	aB	838	CLA	O2A-CGA	4.09	1.45	1.33
11	cB	802	CLA	CHD-C1D	4.09	1.46	1.38
10	aA	801	CL0	O2A-CGA	4.08	1.45	1.33
11	cL	205	CLA	O2A-CGA	4.08	1.45	1.33
11	cA	818	CLA	O2A-CGA	4.08	1.45	1.33
11	cB	816	CLA	O2A-CGA	4.08	1.45	1.33
10	cA	801	CL0	O2A-CGA	4.08	1.45	1.33
12	aA	827	F6C	O2A-CGA	4.08	1.45	1.33
11	cB	827	CLA	C1B-NB	-4.08	1.32	1.37
11	bA	818	CLA	O2A-CGA	4.08	1.45	1.33
11	cA	834	CLA	CHD-C1D	4.08	1.46	1.38
11	bA	808	CLA	CHD-C1D	4.08	1.46	1.38
11	bA	831	CLA	O2A-CGA	4.08	1.45	1.33
11	aA	840	CLA	CHD-C1D	4.08	1.46	1.38
11	bB	840	CLA	CHD-C1D	4.08	1.46	1.38
11	cA	807	CLA	CHD-C1D	4.08	1.46	1.38
11	aA	842	CLA	CHD-C1D	4.08	1.46	1.38
11	cA	842	CLA	CHD-C1D	4.08	1.46	1.38
12	cA	844	F6C	O2A-CGA	4.08	1.45	1.33
11	bB	840	CLA	C1B-NB	-4.07	1.32	1.37
11	aA	841	CLA	O2A-CGA	4.07	1.45	1.33
11	bA	841	CLA	CHD-C1D	4.07	1.46	1.38
11	cB	817	CLA	C1B-NB	-4.07	1.32	1.37
12	cA	844	F6C	CHD-C1D	4.07	1.46	1.38
11	aK	103	CLA	CHD-C1D	4.07	1.46	1.38
11	bA	841	CLA	O2A-CGA	4.07	1.45	1.33
12	cA	832	F6C	CHD-C1D	4.07	1.46	1.38
11	aA	841	CLA	CHD-C1D	4.07	1.46	1.38
11	cB	840	CLA	C1B-NB	-4.07	1.32	1.37
11	aB	829	CLA	CHD-C4C	4.07	1.48	1.39
11	bB	819	CLA	CHD-C1D	4.07	1.46	1.38
11	bK	103	CLA	CHD-C1D	4.07	1.46	1.38
11	cA	815	CLA	C1B-NB	-4.07	1.32	1.37
12	aA	844	F6C	C3B-C2B	4.07	1.48	1.39
12	cA	844	F6C	C3B-C2B	4.07	1.48	1.39
11	aA	838	CLA	C1B-NB	-4.07	1.32	1.37
11	aA	815	CLA	C1B-NB	-4.06	1.32	1.37
11	aB	803	CLA	CHC-C1C	4.06	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bA	820	CLA	C1B-NB	-4.06	1.32	1.37
12	cL	202	F6C	C1D-ND	4.06	1.43	1.37
11	bB	803	CLA	CHC-C1C	4.06	1.46	1.38
12	bA	844	F6C	C3B-C2B	4.06	1.48	1.39
11	cB	819	CLA	CHD-C1D	4.06	1.46	1.38
11	cB	829	CLA	CHD-C4C	4.06	1.48	1.39
11	cA	807	CLA	O2A-CGA	4.06	1.45	1.33
11	bA	814	CLA	O2A-CGA	4.06	1.45	1.33
12	bL	202	F6C	C1D-ND	4.06	1.43	1.37
11	aB	817	CLA	C1B-NB	-4.06	1.32	1.37
11	aA	843	CLA	CHD-C1D	4.06	1.46	1.38
11	aB	840	CLA	CHD-C1D	4.06	1.46	1.38
11	cA	808	CLA	CHD-C1D	4.06	1.46	1.38
11	aB	819	CLA	CHD-C1D	4.06	1.46	1.38
10	bA	801	CL0	O2A-CGA	4.06	1.45	1.33
11	cB	839	CLA	O2A-CGA	4.06	1.45	1.33
11	bB	823	CLA	CHD-C1D	4.06	1.46	1.38
11	cA	841	CLA	O2A-CGA	4.06	1.45	1.33
11	aA	820	CLA	C1B-NB	-4.06	1.32	1.37
11	cA	814	CLA	O2A-CGA	4.06	1.45	1.33
11	bA	813	CLA	CHD-C1D	4.05	1.46	1.38
11	bA	807	CLA	CHD-C1D	4.05	1.46	1.38
11	cA	817	CLA	C1B-NB	-4.05	1.32	1.37
11	aB	839	CLA	O2A-CGA	4.05	1.45	1.33
12	aA	844	F6C	CHD-C1D	4.05	1.46	1.38
11	bB	839	CLA	O2A-CGA	4.05	1.45	1.33
11	aB	828	CLA	CHC-C1C	4.05	1.46	1.38
11	cA	813	CLA	CHD-C1D	4.05	1.46	1.38
11	bB	829	CLA	CHD-C4C	4.05	1.48	1.39
11	aB	827	CLA	C1B-NB	-4.05	1.32	1.37
11	bA	842	CLA	CHD-C1D	4.05	1.46	1.38
11	bB	809	CLA	O2A-CGA	4.05	1.45	1.33
12	bA	844	F6C	CHD-C1D	4.05	1.46	1.38
11	cL	205	CLA	CHD-C1D	4.05	1.46	1.38
11	cB	803	CLA	CHC-C1C	4.05	1.46	1.38
11	cA	808	CLA	O2A-CGA	4.05	1.45	1.33
12	bB	824	F6C	CHD-C4C	4.05	1.48	1.39
11	cB	809	CLA	O2A-CGA	4.04	1.45	1.33
11	bB	817	CLA	C1B-NB	-4.04	1.32	1.37
11	bB	817	CLA	CHD-C1D	4.04	1.46	1.38
12	aB	824	F6C	CHC-C4B	4.04	1.46	1.38
11	aA	814	CLA	O2A-CGA	4.04	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bA	838	CLA	C1B-NB	-4.04	1.32	1.37
11	aB	809	CLA	O2A-CGA	4.04	1.45	1.33
11	cL	204	CLA	O2A-CGA	4.04	1.45	1.33
11	aA	808	CLA	O2A-CGA	4.04	1.45	1.33
11	cA	841	CLA	CHD-C1D	4.04	1.46	1.38
11	aL	204	CLA	O2A-CGA	4.03	1.45	1.33
11	bL	204	CLA	CHD-C1D	4.03	1.46	1.38
11	aL	205	CLA	CHD-C1D	4.03	1.46	1.38
11	aA	810	CLA	CHD-C1D	4.03	1.46	1.38
11	bB	802	CLA	CHD-C1D	4.03	1.46	1.38
11	bB	827	CLA	C1B-NB	-4.03	1.32	1.37
12	aB	824	F6C	CHD-C4C	4.03	1.48	1.39
11	bL	205	CLA	CHD-C1D	4.03	1.46	1.38
11	aB	832	CLA	CHD-C4C	4.03	1.48	1.39
12	bL	202	F6C	C3B-C2B	4.03	1.48	1.39
11	aB	833	CLA	CHD-C4C	4.03	1.48	1.39
11	bA	808	CLA	O2A-CGA	4.02	1.45	1.33
11	cA	810	CLA	CHD-C1D	4.02	1.46	1.38
11	bA	831	CLA	CHD-C1D	4.02	1.46	1.38
11	bB	802	CLA	C1B-NB	-4.02	1.32	1.37
11	aA	813	CLA	CHD-C1D	4.02	1.46	1.38
11	bA	806	CLA	O2A-CGA	4.02	1.45	1.33
11	cA	806	CLA	O2A-CGA	4.02	1.45	1.33
11	cB	832	CLA	CHD-C4C	4.02	1.48	1.39
11	cB	823	CLA	CHD-C1D	4.02	1.46	1.38
11	aB	836	CLA	CHD-C1D	4.02	1.46	1.38
11	cL	206	CLA	CHD-C1D	4.01	1.46	1.38
11	bA	819	CLA	CHD-C1D	4.01	1.46	1.38
11	cB	834	CLA	C1B-NB	-4.01	1.32	1.37
11	bL	204	CLA	O2A-CGA	4.01	1.45	1.33
11	cB	804	CLA	CHD-C1D	4.01	1.46	1.38
11	bA	810	CLA	CHD-C1D	4.01	1.46	1.38
11	bB	833	CLA	CHD-C4C	4.01	1.48	1.39
11	aB	817	CLA	CHD-C1D	4.01	1.46	1.38
11	aL	206	CLA	CHD-C1D	4.01	1.46	1.38
12	aA	832	F6C	C1D-ND	4.01	1.43	1.37
11	aA	812	CLA	CHD-C4C	4.01	1.48	1.39
11	bA	824	CLA	C1B-NB	-4.01	1.32	1.37
12	cA	830	F6C	C3B-C2B	4.01	1.48	1.39
11	aB	816	CLA	CHD-C4C	4.01	1.48	1.39
11	aA	836	CLA	C1B-NB	-4.01	1.32	1.37
11	cB	838	CLA	CHD-C1D	4.01	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	cL	204	CLA	CHD-C1D	4.00	1.46	1.38
11	cB	833	CLA	CHD-C4C	4.00	1.48	1.39
11	aB	804	CLA	CHD-C1D	4.00	1.46	1.38
11	cB	817	CLA	CHD-C1D	4.00	1.46	1.38
12	bB	824	F6C	CHC-C4B	4.00	1.46	1.38
11	cB	820	CLA	CHD-C1D	4.00	1.46	1.38
11	bA	834	CLA	O2A-CGA	4.00	1.45	1.33
11	aB	802	CLA	C1B-NB	-4.00	1.32	1.37
11	aB	820	CLA	CHD-C1D	4.00	1.46	1.38
11	bB	818	CLA	CHD-C1D	4.00	1.46	1.38
11	cB	802	CLA	C1B-NB	-4.00	1.32	1.37
11	aA	834	CLA	O2A-CGA	4.00	1.45	1.33
12	aA	827	F6C	C1D-ND	4.00	1.43	1.37
11	cB	816	CLA	CHD-C4C	3.99	1.48	1.39
11	aB	840	CLA	C1B-NB	-3.99	1.32	1.37
11	aB	818	CLA	CHD-C1D	3.99	1.46	1.38
11	bB	820	CLA	CHD-C1D	3.99	1.46	1.38
11	bL	206	CLA	CHD-C1D	3.99	1.46	1.38
12	cB	824	F6C	CHC-C4B	3.99	1.46	1.38
11	bB	832	CLA	CHD-C4C	3.99	1.48	1.39
11	cA	806	CLA	CHD-C4C	3.99	1.48	1.39
11	cA	838	CLA	O2A-CGA	3.99	1.45	1.33
11	bA	838	CLA	CHD-C1D	3.99	1.46	1.38
11	aB	834	CLA	CHD-C4C	3.99	1.48	1.39
11	aA	806	CLA	O2A-CGA	3.99	1.45	1.33
11	aA	831	CLA	CHD-C1D	3.98	1.46	1.38
12	cB	824	F6C	CHD-C4C	3.98	1.48	1.39
11	aA	811	CLA	CHD-C4C	3.98	1.48	1.39
12	cL	202	F6C	C3B-C2B	3.98	1.48	1.39
11	aL	204	CLA	CHD-C1D	3.98	1.46	1.38
11	bA	813	CLA	C1B-NB	-3.98	1.32	1.37
11	cA	838	CLA	C1B-NB	-3.98	1.32	1.37
12	aL	202	F6C	C3B-C2B	3.98	1.48	1.39
11	cA	819	CLA	CHD-C1D	3.98	1.46	1.38
11	bA	806	CLA	CHD-C4C	3.98	1.48	1.39
11	bB	836	CLA	CHD-C1D	3.98	1.46	1.38
12	bA	832	F6C	CHD-C4C	3.98	1.48	1.39
11	cA	831	CLA	CHD-C1D	3.98	1.46	1.38
11	cA	812	CLA	CHD-C4C	3.98	1.48	1.39
11	bB	809	CLA	CHD-C1D	3.98	1.46	1.38
11	cA	821	CLA	CHD-C1D	3.98	1.46	1.38
11	aB	826	CLA	C1B-NB	-3.98	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aA	806	CLA	CHD-C4C	3.98	1.48	1.39
11	aA	838	CLA	O2A-CGA	3.97	1.45	1.33
11	aB	812	CLA	O2A-CGA	3.97	1.45	1.33
11	cB	812	CLA	O2A-CGA	3.97	1.45	1.33
11	bB	838	CLA	CHD-C1D	3.97	1.46	1.38
11	bA	812	CLA	CHD-C4C	3.97	1.48	1.39
11	cB	836	CLA	CHD-C1D	3.97	1.46	1.38
11	cA	811	CLA	CHD-C4C	3.97	1.48	1.39
11	bB	834	CLA	CHD-C4C	3.97	1.48	1.39
11	bB	804	CLA	CHD-C1D	3.97	1.46	1.38
11	bB	816	CLA	CHD-C4C	3.97	1.48	1.39
11	aA	838	CLA	CHD-C1D	3.97	1.46	1.38
11	cB	818	CLA	CHD-C1D	3.97	1.46	1.38
12	cA	827	F6C	CHD-C1D	3.96	1.46	1.38
11	aB	834	CLA	C1B-NB	-3.96	1.32	1.37
11	aA	802	CLA	C3D-C2D	3.96	1.49	1.39
11	cA	834	CLA	O2A-CGA	3.96	1.44	1.33
11	bB	826	CLA	C1B-NB	-3.96	1.32	1.37
11	aA	819	CLA	CHD-C1D	3.96	1.46	1.38
11	cB	834	CLA	CHD-C4C	3.96	1.48	1.39
11	aB	835	CLA	CHD-C4C	3.96	1.48	1.39
11	bB	835	CLA	CHD-C4C	3.96	1.48	1.39
11	aB	838	CLA	CHD-C1D	3.96	1.46	1.38
11	bA	836	CLA	C1B-NB	-3.96	1.32	1.37
11	bB	812	CLA	O2A-CGA	3.96	1.44	1.33
11	bA	821	CLA	CHD-C1D	3.96	1.46	1.38
11	bA	804	CLA	CHD-C4C	3.96	1.48	1.39
11	bA	811	CLA	CHD-C4C	3.96	1.48	1.39
11	cB	801	CLA	O2A-CGA	3.96	1.44	1.33
12	bA	827	F6C	C1D-ND	3.96	1.43	1.37
11	cA	836	CLA	C1B-NB	-3.96	1.32	1.37
12	aA	827	F6C	CHD-C1D	3.96	1.46	1.38
12	bA	830	F6C	C3B-C2B	3.96	1.48	1.39
12	cA	832	F6C	CHD-C4C	3.95	1.48	1.39
11	cB	809	CLA	CHD-C1D	3.95	1.46	1.38
12	aB	824	F6C	C3D-C2D	3.95	1.49	1.39
12	cA	827	F6C	C1D-ND	3.95	1.43	1.37
11	aA	802	CLA	O2A-CGA	3.95	1.44	1.33
11	aB	806	CLA	CHD-C1D	3.95	1.46	1.38
12	aA	830	F6C	C3B-C2B	3.95	1.48	1.39
11	aA	823	CLA	C3D-C2D	3.95	1.49	1.39
12	bB	824	F6C	C3D-C2D	3.95	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aA	804	CLA	CHD-C4C	3.95	1.48	1.39
11	bB	801	CLA	O2A-CGA	3.95	1.44	1.33
11	cL	204	CLA	C1B-NB	-3.95	1.32	1.37
11	aA	821	CLA	CHD-C1D	3.95	1.46	1.38
11	aA	843	CLA	C1B-NB	-3.95	1.32	1.37
11	cB	826	CLA	C1B-NB	-3.94	1.32	1.37
11	cB	805	CLA	CHD-C4C	3.94	1.48	1.39
12	cB	824	F6C	C3D-C2D	3.94	1.49	1.39
12	cA	844	F6C	C1D-ND	3.94	1.43	1.37
11	cA	804	CLA	CHD-C4C	3.94	1.48	1.39
12	cA	827	F6C	C3B-C2B	3.94	1.48	1.39
12	bA	832	F6C	C1D-ND	3.94	1.43	1.37
11	bB	839	CLA	CHD-C1D	3.94	1.46	1.38
11	bA	802	CLA	C3D-C2D	3.94	1.49	1.39
11	cB	803	CLA	C1B-NB	-3.94	1.32	1.37
11	bA	838	CLA	O2A-CGA	3.94	1.44	1.33
11	bA	802	CLA	O2A-CGA	3.94	1.44	1.33
11	aA	824	CLA	C1B-NB	-3.94	1.32	1.37
11	bB	803	CLA	C1B-NB	-3.94	1.32	1.37
11	cK	101	CLA	CHD-C4C	3.94	1.48	1.39
11	aA	813	CLA	C1B-NB	-3.94	1.32	1.37
11	aK	101	CLA	CHD-C4C	3.94	1.48	1.39
12	cA	832	F6C	C1D-ND	3.94	1.43	1.37
11	cA	802	CLA	O2A-CGA	3.94	1.44	1.33
11	bB	831	CLA	CHD-C4C	3.94	1.48	1.39
11	cA	802	CLA	C3D-C2D	3.94	1.49	1.39
11	cB	818	CLA	C1B-NB	-3.93	1.32	1.37
11	aB	809	CLA	CHD-C1D	3.93	1.46	1.38
11	bA	823	CLA	C3D-C2D	3.93	1.49	1.39
11	aB	810	CLA	C1B-NB	-3.93	1.32	1.37
11	cA	823	CLA	C3D-C2D	3.93	1.49	1.39
11	cA	824	CLA	C1B-NB	-3.93	1.32	1.37
11	cA	820	CLA	CHD-C4C	3.93	1.48	1.39
11	aB	801	CLA	O2A-CGA	3.93	1.44	1.33
11	aB	808	CLA	CHD-C1D	3.93	1.46	1.38
12	bA	844	F6C	C1D-ND	3.93	1.43	1.37
11	bB	805	CLA	CHD-C4C	3.93	1.48	1.39
11	bK	101	CLA	CHD-C4C	3.93	1.48	1.39
11	cB	839	CLA	CHD-C1D	3.93	1.46	1.38
11	cB	810	CLA	C1B-NB	-3.93	1.33	1.37
11	cB	835	CLA	CHD-C4C	3.93	1.48	1.39
12	bA	827	F6C	CHD-C1D	3.93	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	cA	838	CLA	CHD-C1D	3.93	1.46	1.38
11	aA	820	CLA	CHD-C4C	3.93	1.48	1.39
12	aA	832	F6C	CHD-C4C	3.92	1.48	1.39
11	aB	839	CLA	CHD-C1D	3.92	1.46	1.38
11	bB	830	CLA	CHD-C4C	3.92	1.48	1.39
12	cA	844	F6C	CHD-C4C	3.92	1.48	1.39
11	cB	806	CLA	CHD-C1D	3.92	1.46	1.38
11	cA	817	CLA	CHD-C4C	3.92	1.48	1.39
11	bA	820	CLA	CHD-C4C	3.92	1.48	1.39
11	aA	817	CLA	CHD-C4C	3.91	1.48	1.39
11	cB	830	CLA	CHD-C4C	3.91	1.48	1.39
11	cB	828	CLA	CHD-C4C	3.91	1.48	1.39
11	aB	839	CLA	C1B-NB	-3.91	1.33	1.37
11	bB	834	CLA	C1B-NB	-3.91	1.33	1.37
12	bA	844	F6C	CHD-C4C	3.91	1.48	1.39
11	aL	206	CLA	O2A-CGA	3.91	1.44	1.33
11	aB	831	CLA	CHD-C4C	3.91	1.48	1.39
11	bA	817	CLA	CHD-C4C	3.91	1.48	1.39
11	bB	806	CLA	CHD-C1D	3.91	1.46	1.38
11	aA	841	CLA	C3D-C2D	3.91	1.49	1.39
11	bB	810	CLA	C1B-NB	-3.91	1.33	1.37
11	aA	836	CLA	CHD-C1D	3.91	1.46	1.38
12	aA	827	F6C	C3B-C2B	3.91	1.48	1.39
11	bA	805	CLA	CHD-C4C	3.91	1.48	1.39
11	aB	810	CLA	CHD-C4C	3.91	1.48	1.39
11	bA	814	CLA	CHD-C4C	3.91	1.48	1.39
11	cA	836	CLA	CHD-C1D	3.91	1.46	1.38
11	bA	841	CLA	C3D-C2D	3.91	1.49	1.39
12	aA	844	F6C	C1D-ND	3.90	1.43	1.37
12	bA	827	F6C	C3B-C2B	3.90	1.48	1.39
11	bA	803	CLA	C3D-C2D	3.90	1.49	1.39
11	aA	805	CLA	CHD-C4C	3.90	1.48	1.39
12	cB	824	F6C	C1D-ND	3.90	1.43	1.37
11	bB	827	CLA	CHD-C1D	3.90	1.46	1.38
11	aB	820	CLA	CHD-C4C	3.90	1.48	1.39
11	bL	206	CLA	O2A-CGA	3.90	1.44	1.33
11	cA	841	CLA	C3D-C2D	3.90	1.49	1.39
11	bB	820	CLA	CHD-C4C	3.90	1.48	1.39
11	aA	803	CLA	C3D-C2D	3.90	1.49	1.39
11	cB	831	CLA	CHD-C4C	3.90	1.48	1.39
11	aB	814	CLA	CHD-C4C	3.89	1.48	1.39
11	cA	814	CLA	CHD-C4C	3.89	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	cL	206	CLA	O2A-CGA	3.89	1.44	1.33
11	cA	809	CLA	CHD-C4C	3.89	1.48	1.39
11	cB	820	CLA	CHD-C4C	3.89	1.48	1.39
11	cB	827	CLA	CHD-C1D	3.89	1.45	1.38
11	aA	809	CLA	CHD-C4C	3.89	1.48	1.39
11	aA	815	CLA	CHD-C4C	3.89	1.48	1.39
11	aB	830	CLA	CHD-C4C	3.89	1.48	1.39
11	bA	836	CLA	CHD-C1D	3.89	1.45	1.38
12	aA	826	F6C	C1D-ND	3.89	1.43	1.37
11	bB	808	CLA	CHD-C1D	3.89	1.45	1.38
11	aA	831	CLA	C3D-C2D	3.89	1.49	1.39
11	bA	839	CLA	CHD-C4C	3.89	1.48	1.39
11	cB	810	CLA	CHD-C4C	3.89	1.48	1.39
11	bA	842	CLA	CHD-C4C	3.89	1.48	1.39
11	cB	805	CLA	O2A-CGA	3.89	1.44	1.33
11	bB	814	CLA	CHD-C4C	3.89	1.48	1.39
11	bA	833	CLA	C1B-NB	-3.89	1.33	1.37
11	bB	828	CLA	CHD-C4C	3.89	1.48	1.39
11	cA	805	CLA	CHD-C4C	3.89	1.48	1.39
11	cB	825	CLA	CHD-C1D	3.89	1.45	1.38
11	aB	812	CLA	CHD-C4C	3.89	1.48	1.39
11	bL	204	CLA	C1B-NB	-3.88	1.33	1.37
12	cL	202	F6C	CHD-C1D	3.88	1.46	1.38
11	aA	833	CLA	CHD-C4C	3.88	1.48	1.39
11	cB	817	CLA	CHD-C4C	3.88	1.48	1.39
12	aA	844	F6C	CHD-C4C	3.88	1.48	1.39
12	aL	202	F6C	CHD-C1D	3.88	1.46	1.38
11	bA	815	CLA	CHD-C4C	3.88	1.48	1.39
11	aB	818	CLA	C1B-NB	-3.88	1.33	1.37
11	cA	803	CLA	C3D-C2D	3.88	1.49	1.39
11	aB	828	CLA	CHD-C4C	3.88	1.48	1.39
11	cA	842	CLA	CHD-C4C	3.88	1.48	1.39
11	bA	825	CLA	C1B-NB	-3.88	1.33	1.37
11	cA	813	CLA	C1B-NB	-3.88	1.33	1.37
11	aA	808	CLA	CHD-C4C	3.88	1.48	1.39
11	aB	803	CLA	C3D-C2D	3.88	1.49	1.39
12	bA	830	F6C	C3D-C2D	3.88	1.49	1.39
12	cA	830	F6C	C3D-C2D	3.88	1.49	1.39
11	bB	825	CLA	CHD-C1D	3.88	1.45	1.38
11	aB	838	CLA	CHD-C4C	3.88	1.48	1.39
12	bA	826	F6C	C1D-ND	3.88	1.43	1.37
11	aA	839	CLA	CHD-C4C	3.88	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bA	824	CLA	CHD-C4C	3.88	1.48	1.39
11	cA	815	CLA	CHD-C4C	3.88	1.48	1.39
11	bA	831	CLA	C3D-C2D	3.88	1.49	1.39
12	cA	827	F6C	C3D-C2D	3.88	1.49	1.39
11	cB	812	CLA	CHD-C4C	3.87	1.48	1.39
11	bA	806	CLA	C1B-NB	-3.87	1.33	1.37
11	aA	816	CLA	CHD-C4C	3.87	1.48	1.39
11	bB	805	CLA	O2A-CGA	3.87	1.44	1.33
11	aA	842	CLA	CHD-C4C	3.87	1.48	1.39
11	aA	833	CLA	C1B-NB	-3.87	1.33	1.37
11	aB	811	CLA	CHD-C4C	3.87	1.48	1.39
11	cB	808	CLA	CHD-C1D	3.87	1.45	1.38
11	cA	843	CLA	C1B-NB	-3.87	1.33	1.37
11	cA	840	CLA	CHD-C4C	3.87	1.48	1.39
11	bA	833	CLA	CHD-C4C	3.87	1.48	1.39
12	aB	824	F6C	C1D-ND	3.87	1.43	1.37
11	bA	809	CLA	CHD-C4C	3.87	1.48	1.39
11	aB	817	CLA	CHD-C4C	3.87	1.48	1.39
11	cA	831	CLA	C3D-C2D	3.87	1.49	1.39
11	aA	829	CLA	CHD-C4C	3.87	1.48	1.39
11	cB	814	CLA	CHD-C4C	3.87	1.48	1.39
11	cB	837	CLA	CHD-C4C	3.87	1.48	1.39
12	aA	830	F6C	C3D-C2D	3.87	1.49	1.39
11	cB	803	CLA	C3D-C2D	3.87	1.49	1.39
11	aB	807	CLA	CHD-C1D	3.87	1.45	1.38
11	aB	805	CLA	CHD-C4C	3.87	1.48	1.39
11	bB	810	CLA	CHD-C4C	3.87	1.48	1.39
11	bB	839	CLA	C1B-NB	-3.87	1.33	1.37
12	cA	826	F6C	CHD-C1D	3.86	1.46	1.38
11	cA	808	CLA	CHD-C4C	3.86	1.48	1.39
12	bA	827	F6C	C3D-C2D	3.86	1.49	1.39
12	cA	827	F6C	CHD-C4C	3.86	1.48	1.39
11	bB	829	CLA	OBD-CAD	3.86	1.29	1.22
11	cA	825	CLA	C1B-NB	-3.86	1.33	1.37
11	bA	829	CLA	CHD-C4C	3.86	1.48	1.39
12	bA	827	F6C	CHD-C4C	3.86	1.48	1.39
12	aA	827	F6C	C3D-C2D	3.86	1.49	1.39
11	cA	833	CLA	C1B-NB	-3.86	1.33	1.37
11	bA	839	CLA	O2A-CGA	3.86	1.44	1.33
11	aA	814	CLA	CHD-C4C	3.86	1.48	1.39
12	cA	826	F6C	C1D-ND	3.86	1.43	1.37
11	cA	839	CLA	O2A-CGA	3.86	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bB	812	CLA	CHD-C4C	3.86	1.48	1.39
11	aB	805	CLA	O2A-CGA	3.86	1.44	1.33
11	bA	816	CLA	CHD-C4C	3.86	1.48	1.39
11	cB	839	CLA	C1B-NB	-3.85	1.33	1.37
11	aB	803	CLA	C1B-NB	-3.85	1.33	1.37
11	bB	803	CLA	C1D-ND	3.85	1.42	1.37
11	bB	838	CLA	CHD-C4C	3.85	1.48	1.39
11	cA	839	CLA	CHD-C4C	3.85	1.48	1.39
11	bB	818	CLA	C1B-NB	-3.85	1.33	1.37
11	aA	839	CLA	O2A-CGA	3.85	1.44	1.33
11	bA	808	CLA	CHD-C4C	3.85	1.48	1.39
11	bB	821	CLA	CHD-C4C	3.85	1.48	1.39
11	cB	807	CLA	C1B-NB	-3.85	1.33	1.37
11	cB	838	CLA	CHD-C4C	3.85	1.48	1.39
11	aA	840	CLA	CHD-C4C	3.85	1.48	1.39
11	bB	811	CLA	CHD-C4C	3.85	1.48	1.39
11	cB	811	CLA	CHD-C4C	3.85	1.48	1.39
11	bB	837	CLA	CHD-C4C	3.85	1.48	1.39
11	aA	824	CLA	CHD-C4C	3.85	1.48	1.39
11	bB	817	CLA	CHD-C4C	3.85	1.48	1.39
11	bB	807	CLA	C1B-NB	-3.85	1.33	1.37
12	bB	824	F6C	C1D-ND	3.85	1.43	1.37
11	aB	825	CLA	CHD-C1D	3.85	1.45	1.38
11	aA	805	CLA	C3D-C2D	3.85	1.49	1.39
11	bA	805	CLA	C3D-C2D	3.85	1.49	1.39
11	aA	825	CLA	C1B-NB	-3.84	1.33	1.37
12	aA	826	F6C	CHD-C1D	3.84	1.46	1.38
11	bA	840	CLA	CHD-C4C	3.84	1.48	1.39
11	bL	205	CLA	C3D-C2D	3.84	1.49	1.39
11	cB	803	CLA	C1D-ND	3.84	1.42	1.37
12	aA	844	F6C	C3D-C2D	3.84	1.49	1.39
11	bB	828	CLA	O2A-CGA	3.84	1.44	1.33
11	cA	811	CLA	C1B-NB	-3.84	1.33	1.37
12	cA	844	F6C	C3D-C2D	3.84	1.49	1.39
11	aB	827	CLA	CHD-C1D	3.84	1.45	1.38
11	cA	805	CLA	C3D-C2D	3.84	1.49	1.39
11	bA	819	CLA	CHC-C4B	3.84	1.48	1.39
11	bB	829	CLA	C3D-C2D	3.84	1.49	1.39
11	aA	841	CLA	CHD-C4C	3.84	1.48	1.39
11	aA	819	CLA	CHC-C4B	3.84	1.48	1.39
11	cA	829	CLA	C1B-NB	-3.84	1.33	1.37
11	aB	828	CLA	O2A-CGA	3.84	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	cA	833	CLA	CHD-C4C	3.83	1.48	1.39
11	cA	807	CLA	CHD-C4C	3.83	1.48	1.39
11	cA	824	CLA	CHD-C4C	3.83	1.48	1.39
12	bL	202	F6C	CHD-C1D	3.83	1.46	1.38
11	bA	825	CLA	CHD-C4C	3.83	1.48	1.39
11	bA	829	CLA	C1B-NB	-3.83	1.33	1.37
12	bA	830	F6C	CHB-C1B	3.83	1.48	1.39
11	aB	809	CLA	C3D-C2D	3.83	1.49	1.39
11	aL	205	CLA	C3D-C2D	3.83	1.49	1.39
11	aB	837	CLA	CHD-C4C	3.83	1.48	1.39
11	aB	829	CLA	CHC-C1C	3.83	1.46	1.38
11	cA	816	CLA	CHD-C4C	3.83	1.48	1.39
11	cB	807	CLA	CHD-C1D	3.83	1.45	1.38
11	cA	819	CLA	CHC-C4B	3.83	1.48	1.39
12	aA	830	F6C	CHB-C1B	3.83	1.48	1.39
11	bA	837	CLA	CHD-C4C	3.82	1.48	1.39
11	bK	103	CLA	CHD-C4C	3.82	1.48	1.39
11	bB	814	CLA	C3D-C2D	3.82	1.49	1.39
11	aA	811	CLA	C1B-NB	-3.82	1.33	1.37
12	aA	830	F6C	CHD-C1D	3.82	1.46	1.38
11	bA	841	CLA	CHD-C4C	3.82	1.48	1.39
11	aA	825	CLA	CHD-C4C	3.82	1.48	1.39
12	bA	826	F6C	CHD-C1D	3.82	1.46	1.38
11	bB	807	CLA	CHD-C1D	3.82	1.45	1.38
11	aB	821	CLA	CHD-C4C	3.82	1.48	1.39
11	cA	802	CLA	CHD-C4C	3.82	1.48	1.39
11	aA	817	CLA	C3D-C2D	3.82	1.49	1.39
11	bA	835	CLA	C3D-C2D	3.82	1.49	1.39
12	aA	827	F6C	CHD-C4C	3.82	1.48	1.39
11	aB	829	CLA	C3D-C2D	3.82	1.49	1.39
11	bB	822	CLA	CHD-C1D	3.82	1.45	1.38
11	aB	812	CLA	C3D-C2D	3.82	1.49	1.39
11	aB	801	CLA	CHD-C1D	3.82	1.45	1.38
11	bA	807	CLA	CHD-C4C	3.82	1.47	1.39
11	aA	835	CLA	C3D-C2D	3.82	1.49	1.39
11	aB	814	CLA	C3D-C2D	3.82	1.49	1.39
10	cA	801	CL0	CHD-C1D	3.82	1.45	1.38
12	bA	844	F6C	C3D-C2D	3.82	1.49	1.39
11	bA	835	CLA	CHD-C4C	3.82	1.47	1.39
11	bA	821	CLA	C1B-NB	-3.82	1.33	1.37
11	aB	802	CLA	C3D-C2D	3.82	1.49	1.39
12	bA	830	F6C	CHD-C1D	3.82	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	cA	829	CLA	CHD-C4C	3.82	1.47	1.39
11	cA	841	CLA	CHD-C4C	3.82	1.47	1.39
11	aA	807	CLA	CHD-C4C	3.81	1.47	1.39
11	cB	829	CLA	CHC-C1C	3.81	1.46	1.38
11	cB	829	CLA	C3D-C2D	3.81	1.49	1.39
11	cL	205	CLA	C3D-C2D	3.81	1.49	1.39
11	bL	205	CLA	C1B-NB	-3.81	1.33	1.37
11	cB	828	CLA	O2A-CGA	3.81	1.44	1.33
11	aA	813	CLA	CHD-C4C	3.81	1.47	1.39
11	aB	803	CLA	C1D-ND	3.81	1.42	1.37
11	bB	803	CLA	C3D-C2D	3.81	1.49	1.39
11	aA	804	CLA	OBD-CAD	3.81	1.29	1.22
11	bA	815	CLA	C3D-C2D	3.81	1.49	1.39
11	cA	835	CLA	CHD-C4C	3.81	1.47	1.39
11	cA	837	CLA	CHD-C4C	3.81	1.47	1.39
11	aA	806	CLA	C1B-NB	-3.81	1.33	1.37
11	cB	821	CLA	CHD-C4C	3.81	1.47	1.39
11	aB	807	CLA	C1B-NB	-3.81	1.33	1.37
11	aB	805	CLA	C3D-C2D	3.81	1.49	1.39
11	cA	806	CLA	C1B-NB	-3.81	1.33	1.37
11	bB	809	CLA	C3D-C2D	3.81	1.49	1.39
11	bA	843	CLA	C1B-NB	-3.81	1.33	1.37
12	cA	830	F6C	CHD-C1D	3.81	1.46	1.38
11	bB	812	CLA	C3D-C2D	3.80	1.49	1.39
11	cA	825	CLA	CHD-C4C	3.80	1.47	1.39
11	bB	829	CLA	CHC-C1C	3.80	1.46	1.38
11	aB	830	CLA	C3D-C2D	3.80	1.49	1.39
11	bA	805	CLA	CHC-C4B	3.80	1.47	1.39
11	aB	805	CLA	C1B-NB	-3.80	1.33	1.37
11	aA	835	CLA	CHD-C4C	3.80	1.47	1.39
11	aB	829	CLA	OBD-CAD	3.80	1.29	1.22
11	cA	817	CLA	C3D-C2D	3.80	1.49	1.39
11	aA	829	CLA	C1B-NB	-3.80	1.33	1.37
11	cB	801	CLA	CHD-C1D	3.80	1.45	1.38
11	cA	835	CLA	C3D-C2D	3.80	1.49	1.39
11	cB	812	CLA	C3D-C2D	3.80	1.49	1.39
11	bB	830	CLA	C3D-C2D	3.80	1.49	1.39
11	bA	810	CLA	CHB-C1B	3.80	1.47	1.39
11	aA	802	CLA	CHD-C4C	3.80	1.47	1.39
11	bB	802	CLA	C3D-C2D	3.80	1.49	1.39
11	aB	833	CLA	OBD-CAD	3.80	1.29	1.22
11	cB	833	CLA	OBD-CAD	3.80	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aA	815	CLA	C3D-C2D	3.80	1.49	1.39
11	bB	805	CLA	C3D-C2D	3.80	1.49	1.39
11	cB	829	CLA	OBD-CAD	3.80	1.29	1.22
12	cA	826	F6C	C3D-C2D	3.80	1.49	1.39
11	aL	204	CLA	C1B-NB	-3.80	1.33	1.37
11	cA	822	CLA	C1B-NB	-3.80	1.33	1.37
11	bA	817	CLA	C3D-C2D	3.80	1.49	1.39
11	aA	837	CLA	CHD-C4C	3.80	1.47	1.39
11	cB	830	CLA	C3D-C2D	3.80	1.49	1.39
11	cB	816	CLA	C1B-NB	-3.80	1.33	1.37
11	cB	830	CLA	C1B-NB	-3.80	1.33	1.37
11	aB	822	CLA	CHD-C1D	3.79	1.45	1.38
11	bB	816	CLA	C3D-C2D	3.79	1.49	1.39
11	bA	805	CLA	OBD-CAD	3.79	1.29	1.22
11	bB	816	CLA	C1B-NB	-3.79	1.33	1.37
11	cA	811	CLA	C3D-C2D	3.79	1.49	1.39
12	bB	824	F6C	C3B-C2B	3.79	1.48	1.39
11	cA	812	CLA	C3D-C2D	3.79	1.49	1.39
11	cB	805	CLA	C3D-C2D	3.79	1.49	1.39
11	cB	802	CLA	C3D-C2D	3.79	1.49	1.39
11	aB	819	CLA	C1B-NB	-3.79	1.33	1.37
11	bA	823	CLA	OBD-CAD	3.79	1.29	1.22
11	cB	836	CLA	CHC-C4B	3.79	1.47	1.39
11	bB	819	CLA	OBD-CAD	3.79	1.29	1.22
12	cA	830	F6C	CHB-C1B	3.79	1.47	1.39
11	bB	801	CLA	CHD-C1D	3.79	1.45	1.38
11	bA	804	CLA	C3D-C2D	3.79	1.49	1.39
11	aB	835	CLA	C3D-C2D	3.79	1.49	1.39
11	aB	823	CLA	C1B-NB	-3.79	1.33	1.37
11	aB	827	CLA	C1D-ND	3.79	1.42	1.37
11	bA	804	CLA	OBD-CAD	3.79	1.29	1.22
11	cA	815	CLA	C3D-C2D	3.79	1.49	1.39
11	cB	805	CLA	C1B-NB	-3.79	1.33	1.37
11	cB	823	CLA	C1B-NB	-3.79	1.33	1.37
11	aB	821	CLA	OBD-CAD	3.79	1.29	1.22
11	bB	807	CLA	CHD-C4C	3.79	1.47	1.39
11	cB	835	CLA	C3D-C2D	3.79	1.49	1.39
12	aA	826	F6C	C3D-C2D	3.79	1.49	1.39
11	bB	836	CLA	CHC-C4B	3.79	1.47	1.39
10	bA	801	CL0	CHD-C1D	3.79	1.45	1.38
12	bA	826	F6C	C3D-C2D	3.78	1.49	1.39
11	cA	804	CLA	C3D-C2D	3.78	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	cB	821	CLA	OBD-CAD	3.78	1.29	1.22
11	bL	206	CLA	C3D-C2D	3.78	1.49	1.39
11	cB	814	CLA	C3D-C2D	3.78	1.49	1.39
11	bA	802	CLA	CHD-C4C	3.78	1.47	1.39
11	bB	835	CLA	OBD-CAD	3.78	1.29	1.22
11	cB	822	CLA	CHD-C1D	3.78	1.45	1.38
12	cA	832	F6C	C3D-C2D	3.78	1.49	1.39
11	cA	822	CLA	CHD-C4C	3.78	1.47	1.39
11	cB	811	CLA	C3D-C2D	3.78	1.49	1.39
12	aB	824	F6C	C3B-C2B	3.78	1.48	1.39
11	cK	101	CLA	C3D-C2D	3.78	1.49	1.39
11	aK	103	CLA	CHD-C4C	3.78	1.47	1.39
11	aK	101	CLA	C3D-C2D	3.78	1.49	1.39
11	cL	205	CLA	CHD-C4C	3.78	1.47	1.39
11	cL	206	CLA	C3D-C2D	3.78	1.49	1.39
10	cA	801	CL0	C1B-NB	-3.78	1.33	1.37
11	aB	807	CLA	CHD-C4C	3.78	1.47	1.39
12	bA	826	F6C	C3C-C2C	3.78	1.48	1.38
11	cA	834	CLA	CHD-C4C	3.78	1.47	1.39
11	bB	821	CLA	C3D-C2D	3.78	1.49	1.39
11	bB	819	CLA	CHD-C4C	3.78	1.47	1.39
11	aB	816	CLA	C3D-C2D	3.78	1.49	1.39
11	bB	835	CLA	C3D-C2D	3.78	1.49	1.39
11	cK	103	CLA	CHD-C4C	3.78	1.47	1.39
11	cA	805	CLA	CHC-C4B	3.78	1.47	1.39
11	cB	816	CLA	C3D-C2D	3.78	1.49	1.39
11	aA	810	CLA	CHB-C1B	3.78	1.47	1.39
11	aA	822	CLA	C1B-NB	-3.77	1.33	1.37
11	aB	818	CLA	CHD-C4C	3.77	1.47	1.39
11	bB	833	CLA	OBD-CAD	3.77	1.29	1.22
11	aA	819	CLA	C1B-NB	-3.77	1.33	1.37
11	cA	840	CLA	C1B-NB	-3.77	1.33	1.37
11	bA	812	CLA	C3D-C2D	3.77	1.49	1.39
11	cB	832	CLA	C3D-C2D	3.77	1.49	1.39
11	aA	805	CLA	CHC-C4B	3.77	1.47	1.39
11	aA	820	CLA	C3D-C2D	3.77	1.49	1.39
11	bK	101	CLA	C3D-C2D	3.77	1.49	1.39
11	aA	822	CLA	CHD-C4C	3.77	1.47	1.39
11	aB	834	CLA	C3D-C2D	3.77	1.49	1.39
11	cB	809	CLA	C3D-C2D	3.77	1.49	1.39
11	cB	819	CLA	CHD-C4C	3.77	1.47	1.39
11	cB	818	CLA	C3D-C2D	3.77	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	cB	807	CLA	CHD-C4C	3.77	1.47	1.39
11	bA	811	CLA	C1B-NB	-3.77	1.33	1.37
11	aB	819	CLA	CHD-C4C	3.77	1.47	1.39
11	bA	834	CLA	CHD-C4C	3.77	1.47	1.39
11	aA	821	CLA	C1B-NB	-3.77	1.33	1.37
11	aA	843	CLA	CHD-C4C	3.77	1.47	1.39
10	aA	801	CL0	CHD-C1D	3.77	1.45	1.38
12	cB	824	F6C	C3B-C2B	3.77	1.47	1.39
11	bB	834	CLA	C3D-C2D	3.77	1.49	1.39
11	cA	843	CLA	CHD-C4C	3.77	1.47	1.39
11	aA	805	CLA	OBD-CAD	3.77	1.29	1.22
11	cA	823	CLA	C1B-NB	-3.77	1.33	1.37
12	aA	832	F6C	C3D-C2D	3.77	1.49	1.39
11	bA	813	CLA	CHD-C4C	3.77	1.47	1.39
11	aB	836	CLA	CHC-C4B	3.77	1.47	1.39
11	bB	821	CLA	OBD-CAD	3.77	1.29	1.22
11	aL	206	CLA	C3D-C2D	3.77	1.49	1.39
11	bB	820	CLA	OBD-CAD	3.77	1.29	1.22
11	cB	837	CLA	C3D-C2D	3.76	1.49	1.39
11	bL	205	CLA	CHD-C4C	3.76	1.47	1.39
11	bB	840	CLA	CHD-C4C	3.76	1.47	1.39
11	cA	818	CLA	C1B-NB	-3.76	1.33	1.37
11	cB	827	CLA	C1D-ND	3.76	1.42	1.37
11	aB	819	CLA	OBD-CAD	3.76	1.29	1.22
11	bB	832	CLA	OBD-CAD	3.76	1.29	1.22
11	aA	833	CLA	C3D-C2D	3.76	1.49	1.39
11	bA	822	CLA	C1B-NB	-3.76	1.33	1.37
11	bB	802	CLA	CHD-C4C	3.76	1.47	1.39
11	cA	823	CLA	OBD-CAD	3.76	1.29	1.22
11	cA	838	CLA	CHD-C4C	3.76	1.47	1.39
11	aA	839	CLA	C1B-NB	-3.76	1.33	1.37
11	bA	811	CLA	C3D-C2D	3.76	1.49	1.39
11	aA	823	CLA	OBD-CAD	3.76	1.29	1.22
11	cB	820	CLA	OBD-CAD	3.76	1.29	1.22
11	aL	205	CLA	CHD-C4C	3.76	1.47	1.39
11	cA	833	CLA	C3D-C2D	3.76	1.49	1.39
11	cB	806	CLA	CHD-C4C	3.76	1.47	1.39
11	aA	811	CLA	C3D-C2D	3.76	1.49	1.39
11	aA	812	CLA	C3D-C2D	3.76	1.49	1.39
11	bB	832	CLA	C3D-C2D	3.76	1.49	1.39
11	cB	834	CLA	C3D-C2D	3.76	1.49	1.39
11	aA	834	CLA	CHD-C4C	3.76	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aA	816	CLA	C1B-NB	-3.76	1.33	1.37
11	aB	806	CLA	CHD-C4C	3.76	1.47	1.39
11	bB	811	CLA	C3D-C2D	3.76	1.49	1.39
11	cB	819	CLA	OBD-CAD	3.76	1.29	1.22
11	bA	820	CLA	C3D-C2D	3.76	1.49	1.39
11	bB	818	CLA	C3D-C2D	3.76	1.49	1.39
11	aB	813	CLA	CHD-C4C	3.76	1.47	1.39
12	cA	827	F6C	CHB-C1B	3.76	1.47	1.39
11	cB	840	CLA	CHD-C4C	3.75	1.47	1.39
11	aB	832	CLA	C3D-C2D	3.75	1.49	1.39
12	bA	832	F6C	C3D-C2D	3.75	1.49	1.39
11	bB	823	CLA	C1B-NB	-3.75	1.33	1.37
11	aA	804	CLA	C3D-C2D	3.75	1.49	1.39
11	bA	806	CLA	C3D-C2D	3.75	1.49	1.39
11	aB	811	CLA	C3D-C2D	3.75	1.49	1.39
11	cA	820	CLA	C3D-C2D	3.75	1.49	1.39
11	cB	829	CLA	C1B-NB	-3.75	1.33	1.37
11	cL	205	CLA	C1B-NB	-3.75	1.33	1.37
11	bA	843	CLA	CHD-C4C	3.75	1.47	1.39
11	bB	805	CLA	C1B-NB	-3.75	1.33	1.37
11	bB	806	CLA	CHD-C4C	3.75	1.47	1.39
11	cB	835	CLA	OBD-CAD	3.75	1.28	1.22
11	aB	840	CLA	CHD-C4C	3.75	1.47	1.39
11	aB	827	CLA	C3D-C2D	3.75	1.49	1.39
11	cB	821	CLA	C3D-C2D	3.75	1.49	1.39
11	bB	823	CLA	CHD-C4C	3.75	1.47	1.39
11	aL	205	CLA	C1B-NB	-3.75	1.33	1.37
11	cB	823	CLA	CHD-C4C	3.75	1.47	1.39
11	bB	818	CLA	CHD-C4C	3.75	1.47	1.39
11	bB	827	CLA	C3D-C2D	3.75	1.49	1.39
11	bL	204	CLA	C3D-C2D	3.75	1.49	1.39
11	cA	804	CLA	OBD-CAD	3.75	1.28	1.22
11	cL	204	CLA	C3D-C2D	3.75	1.49	1.39
11	bA	819	CLA	C1B-NB	-3.75	1.33	1.37
11	aB	839	CLA	CHC-C4B	3.75	1.47	1.39
11	bB	839	CLA	CHC-C4B	3.75	1.47	1.39
11	aB	837	CLA	C3D-C2D	3.75	1.49	1.39
11	cA	816	CLA	C1B-NB	-3.75	1.33	1.37
11	aB	821	CLA	C3D-C2D	3.75	1.49	1.39
11	bB	827	CLA	C1D-ND	3.75	1.42	1.37
11	aL	204	CLA	C3D-C2D	3.75	1.49	1.39
11	cA	822	CLA	C3D-C2D	3.74	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aA	818	CLA	C1B-NB	-3.74	1.33	1.37
12	bA	827	F6C	CHB-C1B	3.74	1.47	1.39
11	cA	810	CLA	CHB-C1B	3.74	1.47	1.39
11	bA	808	CLA	OBD-CAD	3.74	1.28	1.22
12	cA	826	F6C	C3C-C2C	3.74	1.48	1.38
11	aB	832	CLA	OBD-CAD	3.74	1.28	1.22
11	cB	832	CLA	OBD-CAD	3.74	1.28	1.22
11	aA	822	CLA	C3D-C2D	3.74	1.49	1.39
11	bA	822	CLA	C3D-C2D	3.74	1.49	1.39
11	cB	813	CLA	CHD-C4C	3.74	1.47	1.39
11	cL	206	CLA	CHD-C4C	3.74	1.47	1.39
11	cA	819	CLA	C1B-NB	-3.74	1.33	1.37
11	bA	838	CLA	CHD-C4C	3.74	1.47	1.39
11	aB	818	CLA	C3D-C2D	3.74	1.49	1.39
12	aA	832	F6C	CHB-C1B	3.74	1.47	1.39
11	cA	805	CLA	OBD-CAD	3.74	1.28	1.22
11	bA	822	CLA	CHD-C4C	3.74	1.47	1.39
11	bA	816	CLA	C1B-NB	-3.74	1.33	1.37
12	bA	832	F6C	CHB-C1B	3.74	1.47	1.39
11	aA	823	CLA	C1B-NB	-3.74	1.33	1.37
11	aA	817	CLA	OBD-CAD	3.74	1.28	1.22
11	cB	818	CLA	CHD-C4C	3.74	1.47	1.39
11	aA	843	CLA	C3D-C2D	3.74	1.49	1.39
12	aA	826	F6C	C3C-C2C	3.74	1.48	1.38
11	cA	839	CLA	C1B-NB	-3.74	1.33	1.37
11	cA	842	CLA	OBD-CAD	3.74	1.28	1.22
11	aB	830	CLA	C1B-NB	-3.74	1.33	1.37
11	cB	827	CLA	C3D-C2D	3.74	1.49	1.39
11	cA	813	CLA	CHD-C4C	3.74	1.47	1.39
11	bB	837	CLA	C3D-C2D	3.74	1.49	1.39
11	aA	803	CLA	C1D-ND	3.73	1.42	1.37
11	aB	810	CLA	C3D-C2D	3.73	1.49	1.39
11	bB	815	CLA	OBD-CAD	3.73	1.28	1.22
11	bB	834	CLA	OBD-CAD	3.73	1.28	1.22
11	bB	818	CLA	OBD-CAD	3.73	1.28	1.22
11	bB	813	CLA	CHD-C4C	3.73	1.47	1.39
11	bA	814	CLA	C3D-C2D	3.73	1.49	1.39
12	aA	826	F6C	CHB-C1B	3.73	1.47	1.39
11	cB	834	CLA	OBD-CAD	3.73	1.28	1.22
11	cA	831	CLA	CHD-C4C	3.73	1.47	1.39
11	aB	816	CLA	C1B-NB	-3.73	1.33	1.37
11	cB	819	CLA	C1B-NB	-3.73	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bA	817	CLA	OBD-CAD	3.73	1.28	1.22
11	bA	833	CLA	C3D-C2D	3.73	1.49	1.39
11	cA	806	CLA	C3D-C2D	3.73	1.49	1.39
11	aL	206	CLA	CHD-C4C	3.73	1.47	1.39
11	cL	204	CLA	CHD-C4C	3.73	1.47	1.39
11	aA	838	CLA	CHD-C4C	3.73	1.47	1.39
12	cA	832	F6C	CHB-C1B	3.73	1.47	1.39
11	aA	814	CLA	C3D-C2D	3.73	1.49	1.39
12	aA	827	F6C	CHB-C1B	3.73	1.47	1.39
11	aB	815	CLA	C3D-C2D	3.73	1.49	1.39
11	cA	818	CLA	CHC-C4B	3.73	1.47	1.39
11	bB	825	CLA	CHD-C4C	3.73	1.47	1.39
11	aA	814	CLA	OBD-CAD	3.73	1.28	1.22
11	aB	835	CLA	OBD-CAD	3.73	1.28	1.22
11	cA	823	CLA	CHD-C1D	3.73	1.45	1.38
11	bB	811	CLA	OBD-CAD	3.73	1.28	1.22
12	cL	202	F6C	C3D-C2D	3.73	1.49	1.39
11	cA	841	CLA	OBD-CAD	3.73	1.28	1.22
11	cA	843	CLA	C3D-C2D	3.72	1.49	1.39
10	bA	801	CL0	C1B-NB	-3.72	1.33	1.37
11	aA	813	CLA	CHC-C4B	3.72	1.47	1.39
11	bB	815	CLA	C3D-C2D	3.72	1.49	1.39
11	cB	802	CLA	CHD-C4C	3.72	1.47	1.39
11	aB	815	CLA	OBD-CAD	3.72	1.28	1.22
11	aA	808	CLA	C3D-C2D	3.72	1.49	1.39
11	bA	818	CLA	C1B-NB	-3.72	1.33	1.37
11	cA	817	CLA	OBD-CAD	3.72	1.28	1.22
11	bB	836	CLA	CHD-C4C	3.72	1.47	1.39
11	bA	843	CLA	C3D-C2D	3.72	1.49	1.39
11	aB	825	CLA	CHD-C4C	3.72	1.47	1.39
11	bB	815	CLA	CHD-C4C	3.72	1.47	1.39
11	aB	820	CLA	OBD-CAD	3.72	1.28	1.22
11	bA	823	CLA	CHD-C1D	3.72	1.45	1.38
11	bA	818	CLA	C3D-C2D	3.72	1.49	1.39
11	bB	819	CLA	C1B-NB	-3.72	1.33	1.37
11	cA	821	CLA	C1B-NB	-3.72	1.33	1.37
11	aB	815	CLA	CHD-C4C	3.72	1.47	1.39
11	cB	815	CLA	CHD-C4C	3.72	1.47	1.39
11	bA	828	CLA	CHD-C1D	3.72	1.45	1.38
11	cA	837	CLA	C3D-C2D	3.72	1.49	1.39
11	bA	842	CLA	OBD-CAD	3.72	1.28	1.22
11	aB	801	CLA	CHB-C1B	3.72	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	cB	833	CLA	CHC-C4B	3.72	1.47	1.39
11	bA	813	CLA	CHC-C4B	3.72	1.47	1.39
11	cB	801	CLA	CHB-C1B	3.72	1.47	1.39
11	cA	808	CLA	OBD-CAD	3.72	1.28	1.22
11	bB	830	CLA	C1B-NB	-3.72	1.33	1.37
11	aA	810	CLA	OBD-CAD	3.72	1.28	1.22
11	aB	802	CLA	CHD-C4C	3.72	1.47	1.39
11	cA	828	CLA	CHD-C1D	3.72	1.45	1.38
11	cB	810	CLA	C3D-C2D	3.71	1.49	1.39
11	aA	818	CLA	C3D-C2D	3.71	1.49	1.39
11	bA	836	CLA	C3D-C2D	3.71	1.49	1.39
12	bA	832	F6C	C3B-C2B	3.71	1.47	1.39
11	bL	206	CLA	CHD-C4C	3.71	1.47	1.39
11	bA	825	CLA	C3D-C2D	3.71	1.49	1.39
11	aA	823	CLA	CHD-C1D	3.71	1.45	1.38
11	aA	831	CLA	CHD-C4C	3.71	1.47	1.39
11	aL	204	CLA	CHD-C4C	3.71	1.47	1.39
11	cA	816	CLA	C3D-C2D	3.71	1.49	1.39
11	aA	806	CLA	C3D-C2D	3.71	1.49	1.39
11	bB	804	CLA	CHD-C4C	3.71	1.47	1.39
11	aB	829	CLA	C1B-NB	-3.71	1.33	1.37
11	bA	805	CLA	C1B-NB	-3.71	1.33	1.37
11	cA	819	CLA	CHD-C4C	3.71	1.47	1.39
12	aA	844	F6C	CHC-C1C	3.71	1.47	1.39
11	aA	842	CLA	OBD-CAD	3.71	1.28	1.22
11	aB	812	CLA	C1B-NB	-3.71	1.33	1.37
11	bA	810	CLA	CHD-C4C	3.71	1.47	1.39
11	bA	808	CLA	C3D-C2D	3.71	1.49	1.39
11	cA	809	CLA	C3D-C2D	3.71	1.49	1.39
11	cA	810	CLA	OBD-CAD	3.71	1.28	1.22
11	aA	839	CLA	C3D-C2D	3.71	1.49	1.39
11	cA	814	CLA	C3D-C2D	3.71	1.49	1.39
11	cB	815	CLA	C3D-C2D	3.71	1.49	1.39
12	bA	826	F6C	CHB-C1B	3.71	1.47	1.39
11	cB	836	CLA	CHD-C4C	3.71	1.47	1.39
11	bB	810	CLA	C3D-C2D	3.71	1.49	1.39
11	cB	817	CLA	C3D-C2D	3.71	1.49	1.39
11	cB	839	CLA	CHC-C4B	3.71	1.47	1.39
11	bB	820	CLA	C3D-C2D	3.71	1.49	1.39
11	cA	813	CLA	C3D-C2D	3.71	1.49	1.39
11	bB	831	CLA	OBD-CAD	3.71	1.28	1.22
12	cA	826	F6C	CHB-C1B	3.71	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	cA	836	CLA	C3D-C2D	3.71	1.49	1.39
11	bA	813	CLA	OBD-CAD	3.71	1.28	1.22
11	aA	809	CLA	C3D-C2D	3.71	1.49	1.39
11	aA	808	CLA	OBD-CAD	3.70	1.28	1.22
11	cB	815	CLA	OBD-CAD	3.70	1.28	1.22
11	aB	823	CLA	CHD-C4C	3.70	1.47	1.39
12	cA	832	F6C	C3B-C2B	3.70	1.47	1.39
11	aA	828	CLA	CHD-C1D	3.70	1.45	1.38
11	aA	825	CLA	C3D-C2D	3.70	1.49	1.39
11	cA	818	CLA	C3D-C2D	3.70	1.49	1.39
12	aA	832	F6C	C3B-C2B	3.70	1.47	1.39
11	cB	811	CLA	OBD-CAD	3.70	1.28	1.22
11	bB	831	CLA	C3D-C2D	3.70	1.49	1.39
11	cA	808	CLA	C3D-C2D	3.70	1.49	1.39
11	bA	810	CLA	OBD-CAD	3.70	1.28	1.22
11	aA	842	CLA	C3D-C2D	3.70	1.49	1.39
11	bB	817	CLA	C3D-C2D	3.70	1.49	1.39
11	aB	831	CLA	OBD-CAD	3.70	1.28	1.22
11	cB	820	CLA	C3D-C2D	3.70	1.49	1.39
11	aA	818	CLA	CHC-C4B	3.70	1.47	1.39
11	aB	836	CLA	CHD-C4C	3.70	1.47	1.39
11	aA	813	CLA	C3D-C2D	3.70	1.49	1.39
11	bA	821	CLA	OBD-CAD	3.70	1.28	1.22
12	bL	202	F6C	C3D-C2D	3.70	1.49	1.39
11	bA	816	CLA	C3D-C2D	3.70	1.49	1.39
12	aL	202	F6C	C3D-C2D	3.70	1.49	1.39
11	aA	842	CLA	CHC-C4B	3.70	1.47	1.39
11	aA	836	CLA	OBD-CAD	3.70	1.28	1.22
11	bA	811	CLA	OBD-CAD	3.70	1.28	1.22
11	aB	818	CLA	OBD-CAD	3.70	1.28	1.22
11	bB	829	CLA	C1B-NB	-3.70	1.33	1.37
11	bB	838	CLA	C3D-C2D	3.70	1.49	1.39
11	cB	838	CLA	C3D-C2D	3.70	1.49	1.39
12	cA	827	F6C	CHC-C1C	3.70	1.47	1.39
11	cB	838	CLA	C1B-NB	-3.70	1.33	1.37
11	cA	839	CLA	C3D-C2D	3.70	1.49	1.39
11	bA	839	CLA	C3D-C2D	3.70	1.49	1.39
11	cA	813	CLA	OBD-CAD	3.70	1.28	1.22
11	bA	821	CLA	CHD-C4C	3.70	1.47	1.39
11	cB	831	CLA	OBD-CAD	3.70	1.28	1.22
11	cA	842	CLA	C3D-C2D	3.70	1.49	1.39
11	aB	804	CLA	OBD-CAD	3.69	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bA	837	CLA	C3D-C2D	3.69	1.49	1.39
11	cA	840	CLA	C3D-C2D	3.69	1.49	1.39
11	cB	831	CLA	C3D-C2D	3.69	1.49	1.39
11	aB	838	CLA	C3D-C2D	3.69	1.49	1.39
10	aA	801	CL0	C1B-NB	-3.69	1.33	1.37
11	cA	813	CLA	CHC-C4B	3.69	1.47	1.39
11	aA	812	CLA	OBD-CAD	3.69	1.28	1.22
11	aB	834	CLA	OBD-CAD	3.69	1.28	1.22
11	aB	817	CLA	C3D-C2D	3.69	1.49	1.39
11	bA	831	CLA	CHD-C4C	3.69	1.47	1.39
11	bA	835	CLA	OBD-CAD	3.69	1.28	1.22
11	aA	819	CLA	CHD-C4C	3.69	1.47	1.39
10	cA	801	CL0	C3D-C2D	3.69	1.49	1.39
12	bA	826	F6C	CHD-C4C	3.69	1.47	1.39
10	aA	801	CL0	C3D-C2D	3.69	1.49	1.39
11	aA	819	CLA	C3D-C2D	3.69	1.49	1.39
11	aA	837	CLA	OBD-CAD	3.69	1.28	1.22
11	aA	840	CLA	C1B-NB	-3.69	1.33	1.37
11	cB	813	CLA	C3D-C2D	3.69	1.49	1.39
11	cB	804	CLA	CHD-C4C	3.69	1.47	1.39
12	bA	830	F6C	OBD-CAD	3.69	1.28	1.22
12	aA	827	F6C	CHC-C1C	3.69	1.47	1.39
11	aA	840	CLA	C3D-C2D	3.69	1.49	1.39
11	cB	822	CLA	C3D-C2D	3.69	1.49	1.39
11	aA	841	CLA	OBD-CAD	3.69	1.28	1.22
11	cB	825	CLA	CHD-C4C	3.68	1.47	1.39
11	aA	816	CLA	C3D-C2D	3.68	1.49	1.39
11	aB	833	CLA	CHC-C4B	3.68	1.47	1.39
11	bA	823	CLA	C1B-NB	-3.68	1.33	1.37
11	bA	839	CLA	C1B-NB	-3.68	1.33	1.37
11	bB	801	CLA	CHB-C1B	3.68	1.47	1.39
11	bB	833	CLA	CHC-C4B	3.68	1.47	1.39
11	aB	816	CLA	OBD-CAD	3.68	1.28	1.22
11	bB	833	CLA	C3D-C2D	3.68	1.49	1.39
11	cB	828	CLA	OBD-CAD	3.68	1.28	1.22
11	aB	820	CLA	C3D-C2D	3.68	1.49	1.39
11	aB	811	CLA	OBD-CAD	3.68	1.28	1.22
11	cA	806	CLA	OBD-CAD	3.68	1.28	1.22
11	bA	841	CLA	OBD-CAD	3.68	1.28	1.22
11	aA	836	CLA	C3D-C2D	3.68	1.49	1.39
11	aB	804	CLA	CHD-C4C	3.68	1.47	1.39
11	bK	103	CLA	C3D-C2D	3.68	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	cA	814	CLA	OBD-CAD	3.68	1.28	1.22
11	cA	837	CLA	OBD-CAD	3.68	1.28	1.22
11	cA	825	CLA	C3D-C2D	3.68	1.49	1.39
11	cA	810	CLA	CHD-C4C	3.68	1.47	1.39
11	aB	819	CLA	C3D-C2D	3.68	1.49	1.39
11	bA	840	CLA	C3D-C2D	3.68	1.49	1.39
11	bA	819	CLA	CHD-C4C	3.68	1.47	1.39
11	cA	821	CLA	CHD-C4C	3.68	1.47	1.39
11	aB	822	CLA	C3D-C2D	3.68	1.49	1.39
11	aB	837	CLA	C1B-NB	-3.68	1.33	1.37
11	cB	833	CLA	C3D-C2D	3.68	1.49	1.39
11	bA	842	CLA	CHC-C4B	3.68	1.47	1.39
11	aA	816	CLA	CHC-C4B	3.68	1.47	1.39
11	bL	204	CLA	CHD-C4C	3.68	1.47	1.39
11	bA	813	CLA	C3D-C2D	3.68	1.49	1.39
11	cA	803	CLA	C1D-ND	3.68	1.42	1.37
11	aA	821	CLA	OBD-CAD	3.68	1.28	1.22
11	aA	807	CLA	C1B-NB	-3.68	1.33	1.37
11	bB	804	CLA	OBD-CAD	3.67	1.28	1.22
12	cA	844	F6C	OBD-CAD	3.67	1.28	1.22
11	bA	818	CLA	CHC-C4B	3.67	1.47	1.39
11	bA	812	CLA	OBD-CAD	3.67	1.28	1.22
11	cA	821	CLA	OBD-CAD	3.67	1.28	1.22
11	aB	833	CLA	C3D-C2D	3.67	1.49	1.39
11	bA	829	CLA	C3D-C2D	3.67	1.49	1.39
11	bA	806	CLA	OBD-CAD	3.67	1.28	1.22
11	cK	101	CLA	CHC-C4B	3.67	1.47	1.39
12	cA	844	F6C	CHC-C1C	3.67	1.47	1.39
11	aB	831	CLA	C3D-C2D	3.67	1.49	1.39
11	cB	816	CLA	OBD-CAD	3.67	1.28	1.22
12	aL	202	F6C	CHD-C4C	3.67	1.47	1.39
11	cA	842	CLA	CHC-C4B	3.67	1.47	1.39
11	bA	803	CLA	C1D-ND	3.67	1.42	1.37
12	bA	844	F6C	CHB-C1B	3.67	1.47	1.39
11	aA	823	CLA	CHD-C4C	3.67	1.47	1.39
11	aB	813	CLA	C3D-C2D	3.67	1.49	1.39
11	cA	837	CLA	C1B-NB	-3.67	1.33	1.37
11	aA	810	CLA	CHD-C4C	3.67	1.47	1.39
11	aA	837	CLA	C3D-C2D	3.67	1.49	1.39
11	cB	819	CLA	C3D-C2D	3.67	1.49	1.39
11	bB	822	CLA	C3D-C2D	3.67	1.49	1.39
11	bA	836	CLA	OBD-CAD	3.67	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aA	826	F6C	OBD-CAD	3.67	1.28	1.22
11	aA	842	CLA	C1B-NB	-3.67	1.33	1.37
10	aA	801	CL0	CHD-C4C	3.67	1.47	1.39
12	cA	826	F6C	OBD-CAD	3.67	1.28	1.22
10	cA	801	CL0	CHD-C4C	3.67	1.47	1.39
11	aA	806	CLA	OBD-CAD	3.67	1.28	1.22
11	bA	814	CLA	OBD-CAD	3.67	1.28	1.22
11	cL	206	CLA	OBD-CAD	3.67	1.28	1.22
11	aA	829	CLA	C3D-C2D	3.67	1.49	1.39
11	bA	842	CLA	C3D-C2D	3.67	1.49	1.39
11	aK	103	CLA	C3D-C2D	3.67	1.49	1.39
12	aA	826	F6C	CHD-C4C	3.67	1.47	1.39
11	aA	837	CLA	C1B-NB	-3.67	1.33	1.37
11	bB	812	CLA	C1B-NB	-3.67	1.33	1.37
12	bL	202	F6C	CHD-C4C	3.67	1.47	1.39
11	aA	821	CLA	CHD-C4C	3.66	1.47	1.39
11	bA	816	CLA	CHC-C4B	3.66	1.47	1.39
12	aA	830	F6C	CHD-C4C	3.66	1.47	1.39
11	bA	809	CLA	C3D-C2D	3.66	1.49	1.39
11	bB	819	CLA	C3D-C2D	3.66	1.49	1.39
11	bA	809	CLA	C1B-NB	-3.66	1.33	1.37
11	cA	807	CLA	C1B-NB	-3.66	1.33	1.37
11	aA	813	CLA	OBD-CAD	3.66	1.28	1.22
11	bB	816	CLA	OBD-CAD	3.66	1.28	1.22
11	cA	840	CLA	CHC-C4B	3.66	1.47	1.39
11	bB	837	CLA	C1B-NB	-3.66	1.33	1.37
11	cB	840	CLA	C3D-C2D	3.66	1.49	1.39
11	bA	837	CLA	OBD-CAD	3.66	1.28	1.22
11	bB	828	CLA	OBD-CAD	3.66	1.28	1.22
11	cA	812	CLA	OBD-CAD	3.66	1.28	1.22
11	cB	813	CLA	C1B-NB	-3.66	1.33	1.37
11	cA	807	CLA	C3D-C2D	3.66	1.49	1.39
11	bB	813	CLA	C1B-NB	-3.66	1.33	1.37
11	cA	829	CLA	C3D-C2D	3.66	1.49	1.39
11	bA	807	CLA	C1B-NB	-3.66	1.33	1.37
12	aA	844	F6C	OBD-CAD	3.66	1.28	1.22
11	aA	811	CLA	OBD-CAD	3.66	1.28	1.22
12	cA	826	F6C	CHD-C4C	3.66	1.47	1.39
11	bB	825	CLA	CHC-C4B	3.66	1.47	1.39
11	bB	838	CLA	C1B-NB	-3.66	1.33	1.37
11	cA	822	CLA	OBD-CAD	3.66	1.28	1.22
11	cK	103	CLA	C3D-C2D	3.66	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bB	809	CLA	CHD-C4C	3.66	1.47	1.39
11	aB	806	CLA	C1B-NB	-3.66	1.33	1.37
11	aB	840	CLA	C3D-C2D	3.66	1.49	1.39
11	aB	804	CLA	CHC-C4B	3.66	1.47	1.39
11	cA	803	CLA	OBD-CAD	3.66	1.28	1.22
11	aB	823	CLA	C3D-C2D	3.66	1.49	1.39
11	bA	819	CLA	C3D-C2D	3.66	1.49	1.39
11	cA	811	CLA	OBD-CAD	3.65	1.28	1.22
11	cA	821	CLA	CHB-C1B	3.65	1.47	1.39
11	aB	838	CLA	C1B-NB	-3.65	1.33	1.37
11	cK	103	CLA	OBD-CAD	3.65	1.28	1.22
12	cA	844	F6C	CHB-C1B	3.65	1.47	1.39
11	aB	801	CLA	OBD-CAD	3.65	1.28	1.22
11	bB	807	CLA	C3D-C2D	3.65	1.49	1.39
11	aB	825	CLA	CHB-C1B	3.65	1.47	1.39
11	aA	822	CLA	OBD-CAD	3.65	1.28	1.22
11	bB	840	CLA	C3D-C2D	3.65	1.49	1.39
11	cB	809	CLA	CHD-C4C	3.65	1.47	1.39
11	bB	803	CLA	CHD-C1D	3.65	1.45	1.38
11	cA	829	CLA	OBD-CAD	3.65	1.28	1.22
11	aB	818	CLA	CHC-C4B	3.65	1.47	1.39
11	bA	804	CLA	CHC-C4B	3.65	1.47	1.39
11	cA	816	CLA	CHC-C4B	3.65	1.47	1.39
11	bA	843	CLA	OBD-CAD	3.65	1.28	1.22
12	bA	844	F6C	OBD-CAD	3.65	1.28	1.22
11	aL	206	CLA	C1B-NB	-3.65	1.33	1.37
11	cB	815	CLA	CHC-C4B	3.65	1.47	1.39
12	cL	202	F6C	CHD-C4C	3.65	1.47	1.39
12	bA	826	F6C	OBD-CAD	3.65	1.28	1.22
11	aB	825	CLA	CHC-C4B	3.65	1.47	1.39
11	aB	820	CLA	C1B-NB	-3.65	1.33	1.37
11	bB	813	CLA	C3D-C2D	3.65	1.49	1.39
11	cA	809	CLA	OBD-CAD	3.65	1.28	1.22
11	bB	804	CLA	C3D-C2D	3.65	1.49	1.39
11	aB	840	CLA	OBD-CAD	3.65	1.28	1.22
11	cB	812	CLA	C1B-NB	-3.65	1.33	1.37
10	bA	801	CL0	CHD-C4C	3.65	1.47	1.39
11	bB	823	CLA	C3D-C2D	3.65	1.49	1.39
11	aB	813	CLA	C1B-NB	-3.65	1.33	1.37
11	bB	803	CLA	C4B-NB	-3.65	1.33	1.37
11	cB	803	CLA	C4B-NB	-3.64	1.33	1.37
11	bA	809	CLA	OBD-CAD	3.64	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	cA	842	CLA	C1B-NB	-3.64	1.33	1.37
11	cB	837	CLA	C1B-NB	-3.64	1.33	1.37
11	aA	829	CLA	OBD-CAD	3.64	1.28	1.22
11	cB	818	CLA	OBD-CAD	3.64	1.28	1.22
11	bA	825	CLA	OBD-CAD	3.64	1.28	1.22
11	bA	842	CLA	C1B-NB	-3.64	1.33	1.37
11	bA	807	CLA	C3D-C2D	3.64	1.49	1.39
11	aB	807	CLA	C3D-C2D	3.64	1.49	1.39
12	bA	827	F6C	CHC-C1C	3.64	1.47	1.39
12	bA	844	F6C	CHC-C1C	3.64	1.47	1.39
11	bA	823	CLA	CHD-C4C	3.64	1.47	1.39
11	aA	840	CLA	CHC-C4B	3.64	1.47	1.39
11	aK	101	CLA	CHC-C4B	3.64	1.47	1.39
11	aB	803	CLA	CHD-C1D	3.64	1.45	1.38
12	bA	826	F6C	CHC-C1C	3.64	1.47	1.39
11	cB	825	CLA	C3D-C2D	3.64	1.49	1.39
11	cB	804	CLA	CHC-C4B	3.64	1.47	1.39
11	aB	809	CLA	CHD-C4C	3.64	1.47	1.39
11	cB	823	CLA	C3D-C2D	3.64	1.49	1.39
11	bA	821	CLA	CHB-C1B	3.64	1.47	1.39
11	bB	803	CLA	OBD-CAD	3.64	1.28	1.22
11	aB	804	CLA	C3D-C2D	3.64	1.49	1.39
12	cA	830	F6C	CHD-C4C	3.64	1.47	1.39
11	aA	803	CLA	OBD-CAD	3.64	1.28	1.22
11	bB	825	CLA	CHB-C1B	3.64	1.47	1.39
10	bA	801	CL0	C3D-C2D	3.63	1.49	1.39
11	cB	816	CLA	CHC-C4B	3.63	1.47	1.39
11	cB	825	CLA	CHC-C4B	3.63	1.47	1.39
11	aA	835	CLA	OBD-CAD	3.63	1.28	1.22
11	bB	804	CLA	CHC-C4B	3.63	1.47	1.39
11	cB	825	CLA	CHB-C1B	3.63	1.47	1.39
11	cA	804	CLA	CHC-C4B	3.63	1.47	1.39
11	bA	840	CLA	CHC-C4B	3.63	1.47	1.39
11	cA	819	CLA	C3D-C2D	3.63	1.49	1.39
11	aL	205	CLA	OBD-CAD	3.63	1.28	1.22
11	aA	804	CLA	CHC-C4B	3.63	1.47	1.39
11	aA	807	CLA	C3D-C2D	3.63	1.49	1.39
11	cB	832	CLA	CHC-C4B	3.63	1.47	1.39
11	bK	103	CLA	C1B-NB	-3.63	1.33	1.37
11	cA	835	CLA	C1B-NB	-3.63	1.33	1.37
11	cA	834	CLA	C1B-NB	-3.63	1.33	1.37
12	cA	827	F6C	OBD-CAD	3.63	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aB	825	CLA	C3D-C2D	3.63	1.49	1.39
11	cB	836	CLA	C3D-C2D	3.63	1.49	1.39
11	cL	205	CLA	OBD-CAD	3.63	1.28	1.22
12	aA	830	F6C	OBD-CAD	3.63	1.28	1.22
11	aB	831	CLA	C1B-NB	-3.63	1.33	1.37
11	cA	814	CLA	C1B-NB	-3.63	1.33	1.37
11	cA	843	CLA	OBD-CAD	3.63	1.28	1.22
12	cA	830	F6C	OBD-CAD	3.63	1.28	1.22
11	aB	803	CLA	OBD-CAD	3.63	1.28	1.22
11	cB	803	CLA	OBD-CAD	3.63	1.28	1.22
11	aK	103	CLA	OBD-CAD	3.63	1.28	1.22
11	bB	840	CLA	OBD-CAD	3.63	1.28	1.22
11	cA	803	CLA	CHD-C4C	3.63	1.47	1.39
11	bA	822	CLA	OBD-CAD	3.63	1.28	1.22
11	cB	822	CLA	CHC-C4B	3.63	1.47	1.39
11	bB	837	CLA	CHC-C4B	3.62	1.47	1.39
11	aB	822	CLA	OBD-CAD	3.62	1.28	1.22
11	aB	828	CLA	OBD-CAD	3.62	1.28	1.22
11	aB	839	CLA	CHD-C4C	3.62	1.47	1.39
11	bB	817	CLA	OBD-CAD	3.62	1.28	1.22
11	cA	836	CLA	OBD-CAD	3.62	1.28	1.22
11	aB	832	CLA	CHC-C4B	3.62	1.47	1.39
11	bB	818	CLA	CHC-C4B	3.62	1.47	1.39
12	bA	830	F6C	CHD-C4C	3.62	1.47	1.39
11	cB	837	CLA	CHC-C4B	3.62	1.47	1.39
11	aA	809	CLA	OBD-CAD	3.62	1.28	1.22
11	bL	205	CLA	OBD-CAD	3.62	1.28	1.22
11	bB	814	CLA	C1B-NB	-3.62	1.33	1.37
11	cB	821	CLA	CHB-C1B	3.62	1.47	1.39
11	bA	840	CLA	C1B-NB	-3.62	1.33	1.37
11	aB	836	CLA	C3D-C2D	3.62	1.49	1.39
11	aB	816	CLA	CHC-C4B	3.62	1.47	1.39
11	bB	815	CLA	CHC-C4B	3.62	1.47	1.39
11	cA	823	CLA	CHD-C4C	3.62	1.47	1.39
11	aB	815	CLA	CHC-C4B	3.62	1.47	1.39
11	bA	829	CLA	OBD-CAD	3.62	1.28	1.22
11	aK	103	CLA	C1B-NB	-3.62	1.33	1.37
11	bA	818	CLA	CHD-C1D	3.62	1.45	1.38
11	cB	820	CLA	C1B-NB	-3.62	1.33	1.37
11	cA	821	CLA	C3D-C2D	3.62	1.49	1.39
11	cA	815	CLA	OBD-CAD	3.61	1.28	1.22
11	bB	821	CLA	CHB-C1B	3.61	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bB	836	CLA	C3D-C2D	3.61	1.49	1.39
11	cA	820	CLA	OBD-CAD	3.61	1.28	1.22
11	aL	206	CLA	OBD-CAD	3.61	1.28	1.22
11	cA	835	CLA	OBD-CAD	3.61	1.28	1.22
11	bB	826	CLA	CHD-C1D	3.61	1.45	1.38
11	cB	817	CLA	OBD-CAD	3.61	1.28	1.22
11	bB	825	CLA	C3D-C2D	3.61	1.49	1.39
11	cB	804	CLA	C3D-C2D	3.61	1.49	1.39
11	cB	804	CLA	OBD-CAD	3.61	1.28	1.22
11	cB	803	CLA	CHD-C1D	3.61	1.45	1.38
11	cB	826	CLA	CHD-C1D	3.61	1.45	1.38
11	bB	835	CLA	CHB-C1B	3.61	1.47	1.39
11	aA	825	CLA	OBD-CAD	3.61	1.28	1.22
11	bL	204	CLA	OBD-CAD	3.61	1.28	1.22
11	bA	834	CLA	C1B-NB	-3.61	1.33	1.37
11	cA	841	CLA	C1B-NB	-3.61	1.33	1.37
11	bB	822	CLA	CHC-C4B	3.61	1.47	1.39
12	cA	826	F6C	CHC-C1C	3.61	1.47	1.39
11	bA	804	CLA	CHB-C1B	3.61	1.47	1.39
11	bK	101	CLA	CHC-C4B	3.61	1.47	1.39
11	bA	807	CLA	CHB-C1B	3.61	1.47	1.39
11	aA	843	CLA	OBD-CAD	3.61	1.28	1.22
11	cA	816	CLA	OBD-CAD	3.61	1.28	1.22
11	bA	803	CLA	CHD-C4C	3.61	1.47	1.39
11	cB	807	CLA	C3D-C2D	3.61	1.49	1.39
11	cB	806	CLA	C1B-NB	-3.60	1.33	1.37
11	cA	825	CLA	OBD-CAD	3.60	1.28	1.22
11	cA	841	CLA	CHC-C4B	3.60	1.47	1.39
11	cB	811	CLA	CHC-C4B	3.60	1.47	1.39
11	aA	804	CLA	CHB-C1B	3.60	1.47	1.39
11	cA	822	CLA	CHB-C1B	3.60	1.47	1.39
11	bB	832	CLA	CHC-C4B	3.60	1.47	1.39
11	bA	814	CLA	C1B-NB	-3.60	1.33	1.37
11	aB	821	CLA	CHB-C1B	3.60	1.47	1.39
11	aB	820	CLA	CHB-C1B	3.60	1.47	1.39
11	aB	822	CLA	CHD-C4C	3.60	1.47	1.39
11	cB	822	CLA	CHD-C4C	3.60	1.47	1.39
11	cB	818	CLA	CHC-C4B	3.60	1.47	1.39
11	cB	803	CLA	CHD-C4C	3.60	1.47	1.39
11	aL	206	CLA	CHB-C1B	3.60	1.47	1.39
11	aA	821	CLA	CHB-C1B	3.60	1.47	1.39
12	aA	826	F6C	CHC-C1C	3.60	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bB	806	CLA	C3D-C2D	3.60	1.49	1.39
10	aA	801	CL0	OBD-CAD	3.60	1.28	1.22
10	bA	801	CL0	OBD-CAD	3.60	1.28	1.22
11	cL	204	CLA	OBD-CAD	3.60	1.28	1.22
11	aB	806	CLA	C3D-C2D	3.60	1.48	1.39
11	cA	837	CLA	CHC-C4B	3.60	1.47	1.39
11	aB	803	CLA	C4B-NB	-3.60	1.33	1.37
11	cB	835	CLA	CHB-C1B	3.60	1.47	1.39
11	aA	820	CLA	OBD-CAD	3.60	1.28	1.22
11	bL	206	CLA	OBD-CAD	3.60	1.28	1.22
11	aB	837	CLA	CHC-C4B	3.60	1.47	1.39
11	cA	804	CLA	CHB-C1B	3.60	1.47	1.39
11	aA	818	CLA	CHD-C1D	3.60	1.45	1.38
11	cB	808	CLA	OBD-CAD	3.60	1.28	1.22
11	bB	826	CLA	OBD-CAD	3.60	1.28	1.22
12	aA	844	F6C	CHB-C1B	3.60	1.47	1.39
11	aA	828	CLA	CHB-C1B	3.60	1.47	1.39
11	bA	815	CLA	OBD-CAD	3.60	1.28	1.22
11	cB	840	CLA	OBD-CAD	3.60	1.28	1.22
11	bB	839	CLA	CHD-C4C	3.60	1.47	1.39
11	bA	837	CLA	CHC-C4B	3.60	1.47	1.39
11	aA	841	CLA	CHC-C4B	3.60	1.47	1.39
11	aB	826	CLA	CHD-C1D	3.59	1.45	1.38
11	bK	103	CLA	OBD-CAD	3.59	1.28	1.22
11	aB	811	CLA	CHC-C4B	3.59	1.47	1.39
11	bB	806	CLA	CHC-C4B	3.59	1.47	1.39
11	bA	837	CLA	C1B-NB	-3.59	1.33	1.37
11	aA	821	CLA	C3D-C2D	3.59	1.48	1.39
12	bA	827	F6C	OBD-CAD	3.59	1.28	1.22
11	aB	822	CLA	CHC-C4B	3.59	1.47	1.39
11	bB	819	CLA	CHB-C1B	3.59	1.47	1.39
11	aB	814	CLA	C1B-NB	-3.59	1.33	1.37
11	bA	803	CLA	OBD-CAD	3.59	1.28	1.22
11	aA	837	CLA	CHC-C4B	3.59	1.47	1.39
11	cA	807	CLA	CHB-C1B	3.59	1.47	1.39
11	cB	819	CLA	CHC-C4B	3.59	1.47	1.39
11	aA	834	CLA	C1B-NB	-3.59	1.33	1.37
11	bB	811	CLA	C1B-NB	-3.59	1.33	1.37
12	aA	827	F6C	OBD-CAD	3.59	1.28	1.22
11	bA	841	CLA	CHC-C4B	3.59	1.47	1.39
11	cA	805	CLA	C1B-NB	-3.59	1.33	1.37
11	bB	822	CLA	OBD-CAD	3.59	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aB	835	CLA	CHB-C1B	3.59	1.47	1.39
11	aA	839	CLA	CHB-C1B	3.59	1.47	1.39
11	bB	822	CLA	CHD-C4C	3.59	1.47	1.39
11	bB	808	CLA	C3D-C2D	3.59	1.48	1.39
11	bB	811	CLA	CHC-C4B	3.59	1.47	1.39
11	bK	103	CLA	CHC-C4B	3.59	1.47	1.39
11	cB	839	CLA	CHD-C4C	3.59	1.47	1.39
11	aA	807	CLA	CHB-C1B	3.59	1.47	1.39
11	cA	818	CLA	CHD-C1D	3.59	1.45	1.38
11	bB	816	CLA	CHC-C4B	3.59	1.47	1.39
11	bB	820	CLA	CHB-C1B	3.59	1.47	1.39
11	bB	801	CLA	OBD-CAD	3.59	1.28	1.22
11	bL	206	CLA	C1B-NB	-3.58	1.33	1.37
11	cB	808	CLA	C3D-C2D	3.58	1.48	1.39
11	cB	815	CLA	C1B-NB	-3.58	1.33	1.37
11	cB	806	CLA	C3D-C2D	3.58	1.48	1.39
11	aA	803	CLA	CHD-C4C	3.58	1.47	1.39
11	aA	822	CLA	CHB-C1B	3.58	1.47	1.39
11	cB	807	CLA	CHB-C1B	3.58	1.47	1.39
11	aK	101	CLA	C1B-NB	-3.58	1.33	1.37
11	aB	808	CLA	OBD-CAD	3.58	1.28	1.22
11	bB	802	CLA	CHC-C4B	3.58	1.47	1.39
11	bA	822	CLA	CHB-C1B	3.58	1.47	1.39
11	cK	103	CLA	C1B-NB	-3.58	1.33	1.37
12	cA	832	F6C	CHC-C1C	3.58	1.47	1.39
11	aB	807	CLA	CHB-C1B	3.58	1.47	1.39
11	aB	808	CLA	C3D-C2D	3.58	1.48	1.39
12	cB	824	F6C	CHB-C1B	3.58	1.47	1.39
11	bB	806	CLA	C1B-NB	-3.58	1.33	1.37
11	cB	814	CLA	C1B-NB	-3.58	1.33	1.37
11	bA	824	CLA	C3D-C2D	3.58	1.48	1.39
11	bL	206	CLA	CHB-C1B	3.58	1.47	1.39
11	cL	204	CLA	CHB-C1B	3.58	1.47	1.39
11	cA	828	CLA	CHB-C1B	3.58	1.47	1.39
11	cA	809	CLA	C1B-NB	-3.58	1.33	1.37
11	bA	821	CLA	C3D-C2D	3.57	1.48	1.39
11	aA	821	CLA	CHC-C4B	3.57	1.47	1.39
11	aB	821	CLA	CHC-C4B	3.57	1.47	1.39
11	bB	821	CLA	CHC-C4B	3.57	1.47	1.39
11	cB	806	CLA	CHC-C4B	3.57	1.47	1.39
11	cB	820	CLA	CHB-C1B	3.57	1.47	1.39
12	aB	824	F6C	CHB-C1B	3.57	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aA	815	CLA	OBD-CAD	3.57	1.28	1.22
11	bB	838	CLA	CHC-C4B	3.57	1.47	1.39
11	cB	821	CLA	CHC-C4B	3.57	1.47	1.39
11	bB	840	CLA	CHB-C1B	3.57	1.47	1.39
11	cB	801	CLA	OBD-CAD	3.57	1.28	1.22
11	bB	820	CLA	C1B-NB	-3.57	1.33	1.37
11	cB	828	CLA	CHB-C1B	3.57	1.47	1.39
11	cA	831	CLA	OBD-CAD	3.57	1.28	1.22
11	aA	824	CLA	C3D-C2D	3.57	1.48	1.39
11	aB	838	CLA	CHC-C4B	3.57	1.47	1.39
11	bB	803	CLA	CHD-C4C	3.57	1.47	1.39
11	aL	204	CLA	OBD-CAD	3.57	1.28	1.22
11	bA	828	CLA	CHB-C1B	3.57	1.47	1.39
11	aA	805	CLA	C1B-NB	-3.57	1.33	1.37
11	aA	834	CLA	C3D-C2D	3.57	1.48	1.39
11	bA	828	CLA	C3D-C2D	3.57	1.48	1.39
11	aB	826	CLA	OBD-CAD	3.57	1.28	1.22
11	bB	819	CLA	CHC-C4B	3.57	1.47	1.39
11	cB	804	CLA	C1B-NB	-3.57	1.33	1.37
11	aB	817	CLA	OBD-CAD	3.57	1.28	1.22
11	bA	834	CLA	OBD-CAD	3.57	1.28	1.22
11	bB	808	CLA	OBD-CAD	3.57	1.28	1.22
11	aB	840	CLA	CHB-C1B	3.57	1.47	1.39
11	aA	823	CLA	CHB-C1B	3.57	1.47	1.39
11	bB	823	CLA	OBD-CAD	3.57	1.28	1.22
11	aB	819	CLA	CHB-C1B	3.57	1.47	1.39
11	aA	814	CLA	C1B-NB	-3.57	1.33	1.37
12	bA	832	F6C	CHC-C1C	3.57	1.47	1.39
11	cA	839	CLA	CHB-C1B	3.57	1.47	1.39
12	bB	824	F6C	CHB-C1B	3.57	1.47	1.39
11	cB	819	CLA	CHB-C1B	3.56	1.47	1.39
11	cA	818	CLA	OBD-CAD	3.56	1.28	1.22
11	cA	834	CLA	C3D-C2D	3.56	1.48	1.39
11	bB	830	CLA	CHC-C4B	3.56	1.47	1.39
11	cB	826	CLA	CHD-C4C	3.56	1.47	1.39
11	bA	841	CLA	C1B-NB	-3.56	1.33	1.37
11	aK	103	CLA	CHC-C4B	3.56	1.47	1.39
11	aA	808	CLA	C1B-NB	-3.56	1.33	1.37
11	cA	821	CLA	CHC-C4B	3.56	1.47	1.39
11	bA	836	CLA	CHD-C4C	3.56	1.47	1.39
10	cA	801	CL0	OBD-CAD	3.56	1.28	1.22
11	bA	810	CLA	C3D-C2D	3.56	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	cA	823	CLA	CHB-C1B	3.56	1.47	1.39
11	cL	206	CLA	CHB-C1B	3.56	1.47	1.39
11	bA	818	CLA	OBD-CAD	3.56	1.28	1.22
12	aA	832	F6C	CHC-C1C	3.56	1.47	1.39
11	bB	815	CLA	C1B-NB	-3.56	1.33	1.37
10	aA	801	CL0	CHB-C1B	3.56	1.47	1.39
11	cB	822	CLA	OBD-CAD	3.56	1.28	1.22
11	bA	834	CLA	C3D-C2D	3.56	1.48	1.39
11	aA	831	CLA	OBD-CAD	3.56	1.28	1.22
11	cB	823	CLA	OBD-CAD	3.56	1.28	1.22
11	cB	826	CLA	OBD-CAD	3.56	1.28	1.22
11	aA	835	CLA	C1B-NB	-3.56	1.33	1.37
12	cA	830	F6C	CHC-C1C	3.55	1.47	1.39
11	cA	828	CLA	C1B-NB	-3.55	1.33	1.37
11	cB	827	CLA	CHD-C4C	3.55	1.47	1.39
11	aB	825	CLA	C1B-NB	-3.55	1.33	1.37
11	aB	836	CLA	C1B-NB	-3.55	1.33	1.37
11	bA	821	CLA	CHC-C4B	3.55	1.47	1.39
11	cB	840	CLA	CHB-C1B	3.55	1.47	1.39
11	bB	826	CLA	CHD-C4C	3.55	1.47	1.39
11	aB	813	CLA	OBD-CAD	3.55	1.28	1.22
11	bA	843	CLA	CHC-C4B	3.55	1.47	1.39
11	aB	803	CLA	CHD-C4C	3.55	1.47	1.39
10	cA	801	CL0	CHB-C1B	3.55	1.47	1.39
11	cA	843	CLA	CHC-C4B	3.55	1.47	1.39
11	cA	824	CLA	C3D-C2D	3.55	1.48	1.39
11	cB	812	CLA	CHB-C1B	3.55	1.47	1.39
11	cA	828	CLA	C3D-C2D	3.55	1.48	1.39
11	bK	103	CLA	CHB-C1B	3.55	1.47	1.39
11	cB	811	CLA	C1B-NB	-3.55	1.33	1.37
11	bK	101	CLA	C1B-NB	-3.55	1.33	1.37
11	aB	806	CLA	CHC-C4B	3.55	1.47	1.39
11	bA	816	CLA	OBD-CAD	3.55	1.28	1.22
12	aB	824	F6C	OBD-CAD	3.55	1.28	1.22
11	aA	810	CLA	C3D-C2D	3.55	1.48	1.39
11	aB	819	CLA	CHC-C4B	3.55	1.47	1.39
11	bB	827	CLA	CHD-C4C	3.54	1.47	1.39
11	bA	839	CLA	CHB-C1B	3.54	1.47	1.39
11	aB	823	CLA	OBD-CAD	3.54	1.28	1.22
11	aB	815	CLA	C1B-NB	-3.54	1.33	1.37
11	bA	823	CLA	CHB-C1B	3.54	1.47	1.39
12	bA	830	F6C	CHC-C1C	3.54	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bB	804	CLA	C1B-NB	-3.54	1.33	1.37
11	cB	831	CLA	CHC-C4B	3.54	1.47	1.39
11	bA	840	CLA	OBD-CAD	3.54	1.28	1.22
11	cK	101	CLA	C1B-NB	-3.54	1.33	1.37
11	aA	809	CLA	C1B-NB	-3.54	1.33	1.37
11	aA	840	CLA	OBD-CAD	3.54	1.28	1.22
11	bA	835	CLA	C1B-NB	-3.54	1.33	1.37
11	bB	807	CLA	CHB-C1B	3.54	1.47	1.39
11	aA	834	CLA	OBD-CAD	3.54	1.28	1.22
11	bL	204	CLA	CHB-C1B	3.54	1.47	1.39
11	cA	810	CLA	C3D-C2D	3.54	1.48	1.39
10	bA	801	CL0	CHB-C1B	3.54	1.47	1.39
11	cB	806	CLA	CHB-C1B	3.54	1.47	1.39
11	cK	103	CLA	CHC-C4B	3.54	1.47	1.39
11	cB	838	CLA	CHC-C4B	3.54	1.47	1.39
11	cB	836	CLA	C1B-NB	-3.54	1.33	1.37
11	aA	810	CLA	CHC-C4B	3.54	1.47	1.39
11	cB	822	CLA	CHB-C1B	3.54	1.47	1.39
11	aA	824	CLA	OBD-CAD	3.54	1.28	1.22
11	bB	831	CLA	C1B-NB	-3.54	1.33	1.37
11	aA	816	CLA	OBD-CAD	3.54	1.28	1.22
11	cL	206	CLA	C1B-NB	-3.54	1.33	1.37
11	bB	825	CLA	C1B-NB	-3.54	1.33	1.37
11	aB	831	CLA	CHC-C4B	3.53	1.47	1.39
11	aA	803	CLA	CHC-C4B	3.53	1.47	1.39
11	aK	103	CLA	CHB-C1B	3.53	1.47	1.39
11	aA	834	CLA	CHB-C1B	3.53	1.47	1.39
11	cA	834	CLA	OBD-CAD	3.53	1.28	1.22
11	bA	820	CLA	OBD-CAD	3.53	1.28	1.22
11	cB	825	CLA	C1B-NB	-3.53	1.33	1.37
11	aA	828	CLA	CHD-C4C	3.53	1.47	1.39
11	cA	828	CLA	CHD-C4C	3.53	1.47	1.39
11	aA	838	CLA	CHB-C1B	3.53	1.47	1.39
11	aA	843	CLA	CHC-C4B	3.53	1.47	1.39
11	aB	806	CLA	CHB-C1B	3.53	1.47	1.39
11	aA	818	CLA	CHD-C4C	3.53	1.47	1.39
11	aA	838	CLA	C3D-C2D	3.53	1.48	1.39
11	bB	828	CLA	CHB-C1B	3.53	1.47	1.39
11	bB	829	CLA	CHB-C1B	3.53	1.47	1.39
11	bA	812	CLA	C1B-NB	-3.53	1.33	1.37
11	bB	826	CLA	C3D-C2D	3.53	1.48	1.39
11	aA	818	CLA	OBD-CAD	3.53	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aA	830	F6C	CHC-C1C	3.53	1.47	1.39
11	aA	836	CLA	CHD-C4C	3.52	1.47	1.39
11	bB	822	CLA	CHB-C1B	3.52	1.47	1.39
11	aA	828	CLA	C3D-C2D	3.52	1.48	1.39
11	cA	838	CLA	C3D-C2D	3.52	1.48	1.39
11	aB	822	CLA	CHB-C1B	3.52	1.47	1.39
11	aL	204	CLA	CHB-C1B	3.52	1.47	1.39
11	bB	830	CLA	OBD-CAD	3.52	1.28	1.22
11	bB	812	CLA	C4B-NB	-3.52	1.33	1.37
11	bA	810	CLA	CHC-C4B	3.52	1.47	1.39
11	cA	810	CLA	CHC-C4B	3.52	1.47	1.39
11	cB	830	CLA	CHC-C4B	3.52	1.47	1.39
11	aA	812	CLA	C1B-NB	-3.52	1.33	1.37
11	aB	804	CLA	C1B-NB	-3.52	1.33	1.37
11	cA	838	CLA	CHB-C1B	3.52	1.47	1.39
11	aB	810	CLA	CHB-C1B	3.52	1.47	1.39
11	aB	826	CLA	CHD-C4C	3.52	1.47	1.39
11	cA	818	CLA	CHD-C4C	3.52	1.47	1.39
11	cK	103	CLA	CHB-C1B	3.52	1.47	1.39
11	aB	812	CLA	CHB-C1B	3.52	1.47	1.39
11	cA	810	CLA	C1B-NB	-3.52	1.33	1.37
11	cB	831	CLA	C1B-NB	-3.52	1.33	1.37
11	aB	829	CLA	CHB-C1B	3.52	1.47	1.39
11	aB	811	CLA	C1B-NB	-3.52	1.33	1.37
11	cA	836	CLA	CHD-C4C	3.52	1.47	1.39
11	cA	834	CLA	CHB-C1B	3.52	1.47	1.39
11	aB	804	CLA	CHB-C1B	3.52	1.47	1.39
11	bB	831	CLA	CHC-C4B	3.52	1.47	1.39
11	cB	810	CLA	CHB-C1B	3.52	1.47	1.39
11	cB	826	CLA	C3D-C2D	3.51	1.48	1.39
11	aB	828	CLA	CHB-C1B	3.51	1.47	1.39
11	aB	809	CLA	CHB-C1B	3.51	1.47	1.39
11	cB	830	CLA	OBD-CAD	3.51	1.28	1.22
11	bB	823	CLA	CHC-C4B	3.51	1.47	1.39
11	bL	205	CLA	CHC-C4B	3.51	1.47	1.39
11	aB	802	CLA	CHC-C4B	3.51	1.47	1.39
11	bB	812	CLA	CHB-C1B	3.51	1.47	1.39
10	bA	801	CL0	C4B-NB	-3.51	1.33	1.37
11	aB	827	CLA	CHD-C4C	3.51	1.47	1.39
11	aB	820	CLA	CHC-C4B	3.51	1.47	1.39
11	aA	841	CLA	C1B-NB	-3.51	1.33	1.37
11	bB	835	CLA	C1B-NB	-3.51	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aB	830	CLA	CHC-C4B	3.51	1.47	1.39
11	aB	810	CLA	OBD-CAD	3.51	1.28	1.22
11	aB	830	CLA	OBD-CAD	3.51	1.28	1.22
11	bB	813	CLA	OBD-CAD	3.51	1.28	1.22
11	bA	831	CLA	OBD-CAD	3.51	1.28	1.22
11	bA	838	CLA	CHB-C1B	3.51	1.47	1.39
11	cB	829	CLA	CHB-C1B	3.51	1.47	1.39
11	cB	804	CLA	CHB-C1B	3.51	1.47	1.39
11	cA	808	CLA	C1B-NB	-3.51	1.33	1.37
11	aB	839	CLA	CHB-C1B	3.51	1.47	1.39
11	bB	806	CLA	CHB-C1B	3.51	1.47	1.39
11	cA	803	CLA	CHC-C4B	3.51	1.47	1.39
11	bA	828	CLA	C1B-NB	-3.51	1.33	1.37
11	bA	803	CLA	CHC-C4B	3.51	1.47	1.39
11	aB	812	CLA	C4B-NB	-3.50	1.33	1.37
11	bB	833	CLA	C1B-NB	-3.50	1.33	1.37
11	cA	822	CLA	CHC-C4B	3.50	1.47	1.39
11	bA	828	CLA	CHD-C4C	3.50	1.47	1.39
11	cL	205	CLA	CHC-C4B	3.50	1.47	1.39
11	aB	821	CLA	C1B-NB	-3.50	1.33	1.37
11	cB	823	CLA	CHC-C4B	3.50	1.47	1.39
11	cA	840	CLA	OBD-CAD	3.50	1.28	1.22
11	bA	822	CLA	CHC-C4B	3.50	1.47	1.39
11	cB	812	CLA	C4B-NB	-3.50	1.33	1.37
11	aA	818	CLA	CHB-C1B	3.50	1.47	1.39
11	bA	809	CLA	CHC-C4B	3.50	1.47	1.39
11	bB	838	CLA	CHB-C1B	3.50	1.47	1.39
11	bA	808	CLA	C1B-NB	-3.50	1.33	1.37
11	bB	836	CLA	C1B-NB	-3.50	1.33	1.37
11	aA	836	CLA	CHB-C1B	3.50	1.47	1.39
11	bA	818	CLA	CHD-C4C	3.50	1.47	1.39
11	cA	838	CLA	C4B-NB	-3.50	1.33	1.37
11	cB	834	CLA	CHB-C1B	3.50	1.47	1.39
11	aA	810	CLA	C1B-NB	-3.50	1.33	1.37
11	cB	833	CLA	C1B-NB	-3.50	1.33	1.37
11	aA	809	CLA	CHC-C4B	3.49	1.47	1.39
11	bA	836	CLA	CHB-C1B	3.49	1.47	1.39
11	cK	101	CLA	CHB-C1B	3.49	1.47	1.39
11	aA	833	CLA	CHB-C1B	3.49	1.47	1.39
11	bB	811	CLA	CHB-C1B	3.49	1.47	1.39
11	cB	802	CLA	CHC-C4B	3.49	1.47	1.39
11	aB	833	CLA	C1B-NB	-3.49	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bK	101	CLA	CHB-C1B	3.49	1.47	1.39
12	cB	824	F6C	OBD-CAD	3.49	1.28	1.22
11	bB	812	CLA	OBD-CAD	3.49	1.28	1.22
11	bB	839	CLA	CHB-C1B	3.49	1.47	1.39
11	aK	101	CLA	CHB-C1B	3.49	1.47	1.39
11	aB	826	CLA	C3D-C2D	3.49	1.48	1.39
11	cA	838	CLA	CHC-C4B	3.49	1.47	1.39
11	bB	809	CLA	CHB-C1B	3.49	1.47	1.39
11	bA	838	CLA	C3D-C2D	3.49	1.48	1.39
11	cB	813	CLA	OBD-CAD	3.49	1.28	1.22
11	aA	828	CLA	C1B-NB	-3.49	1.33	1.37
11	bB	832	CLA	CHB-C1B	3.49	1.47	1.39
11	bA	824	CLA	OBD-CAD	3.49	1.28	1.22
11	bB	821	CLA	C1B-NB	-3.48	1.33	1.37
11	aB	834	CLA	CHB-C1B	3.48	1.47	1.39
11	cA	812	CLA	CHC-C4B	3.48	1.47	1.39
11	cA	824	CLA	OBD-CAD	3.48	1.28	1.22
11	bA	828	CLA	CHC-C4B	3.48	1.47	1.39
11	cA	818	CLA	CHB-C1B	3.48	1.47	1.39
11	cB	802	CLA	OBD-CAD	3.48	1.28	1.22
11	cB	835	CLA	C1B-NB	-3.48	1.33	1.37
11	bB	837	CLA	CHB-C1B	3.48	1.47	1.39
11	cB	801	CLA	C3D-C2D	3.48	1.48	1.39
11	aA	807	CLA	OBD-CAD	3.48	1.28	1.22
11	bB	826	CLA	CHB-C1B	3.48	1.47	1.39
11	cB	811	CLA	CHB-C1B	3.48	1.47	1.39
11	cB	812	CLA	OBD-CAD	3.48	1.28	1.22
12	bB	824	F6C	OBD-CAD	3.48	1.28	1.22
11	cB	809	CLA	CHB-C1B	3.48	1.47	1.39
11	aB	835	CLA	C1B-NB	-3.48	1.33	1.37
11	bB	822	CLA	C1B-NB	-3.48	1.33	1.37
11	aA	813	CLA	CHB-C1B	3.48	1.47	1.39
11	cB	839	CLA	CHB-C1B	3.48	1.47	1.39
11	bA	834	CLA	CHB-C1B	3.48	1.47	1.39
11	aL	205	CLA	CHC-C4B	3.48	1.47	1.39
11	cL	206	CLA	CHC-C4B	3.48	1.47	1.39
11	cB	826	CLA	CHC-C4B	3.48	1.47	1.39
11	bA	838	CLA	CHC-C4B	3.47	1.47	1.39
11	bB	804	CLA	CHB-C1B	3.47	1.47	1.39
11	cB	820	CLA	CHC-C4B	3.47	1.47	1.39
11	cB	810	CLA	OBD-CAD	3.47	1.28	1.22
11	bA	807	CLA	CHC-C4B	3.47	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aA	822	CLA	CHC-C4B	3.47	1.47	1.39
11	cA	833	CLA	CHC-C4B	3.47	1.47	1.39
11	bA	818	CLA	CHB-C1B	3.47	1.47	1.39
11	bB	810	CLA	CHB-C1B	3.47	1.47	1.39
10	cA	801	CL0	C4B-NB	-3.47	1.33	1.37
11	aB	814	CLA	OBD-CAD	3.47	1.28	1.22
11	bA	808	CLA	CHC-C4B	3.47	1.47	1.39
11	cA	809	CLA	CHC-C4B	3.47	1.47	1.39
11	aA	811	CLA	CHC-C4B	3.47	1.47	1.39
11	aA	838	CLA	CHC-C4B	3.47	1.47	1.39
11	bA	833	CLA	CHB-C1B	3.47	1.47	1.39
11	bA	804	CLA	C1B-NB	-3.47	1.33	1.37
11	bB	834	CLA	CHB-C1B	3.46	1.47	1.39
11	cA	833	CLA	CHB-C1B	3.46	1.47	1.39
11	cB	837	CLA	CHB-C1B	3.46	1.47	1.39
11	aB	826	CLA	CHB-C1B	3.46	1.47	1.39
11	aB	837	CLA	CHB-C1B	3.46	1.47	1.39
11	aB	823	CLA	CHC-C4B	3.46	1.47	1.39
11	cB	814	CLA	OBD-CAD	3.46	1.28	1.22
11	cA	836	CLA	CHB-C1B	3.46	1.47	1.39
11	aA	843	CLA	CHB-C1B	3.46	1.47	1.39
11	bB	801	CLA	C1B-NB	-3.46	1.33	1.37
12	cB	824	F6C	CHC-C1C	3.46	1.47	1.39
12	bB	824	F6C	CHC-C1C	3.46	1.47	1.39
11	bB	810	CLA	OBD-CAD	3.46	1.28	1.22
11	cB	813	CLA	CHB-C1B	3.46	1.47	1.39
11	aB	827	CLA	CHC-C4B	3.46	1.47	1.39
11	aB	812	CLA	OBD-CAD	3.46	1.28	1.22
11	cA	843	CLA	CHB-C1B	3.46	1.47	1.39
12	cL	202	F6C	CHB-C1B	3.46	1.47	1.39
11	aB	836	CLA	CHB-C1B	3.46	1.47	1.39
11	bA	841	CLA	CHB-C1B	3.46	1.47	1.39
11	bA	839	CLA	CHC-C4B	3.45	1.47	1.39
11	bA	802	CLA	C4B-NB	-3.45	1.33	1.37
11	aB	811	CLA	CHB-C1B	3.45	1.47	1.39
12	aL	202	F6C	CHB-C1B	3.45	1.47	1.39
11	bA	813	CLA	CHB-C1B	3.45	1.47	1.39
11	bA	843	CLA	CHB-C1B	3.45	1.47	1.39
11	bA	810	CLA	C1B-NB	-3.45	1.33	1.37
11	aL	206	CLA	CHC-C4B	3.45	1.47	1.39
12	aB	824	F6C	CHC-C1C	3.45	1.47	1.39
11	cA	812	CLA	C1B-NB	-3.45	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bB	808	CLA	CHD-C4C	3.45	1.47	1.39
11	cB	832	CLA	CHB-C1B	3.45	1.47	1.39
11	bB	801	CLA	C3D-C2D	3.45	1.48	1.39
11	cB	838	CLA	CHB-C1B	3.45	1.47	1.39
11	cB	827	CLA	OBD-CAD	3.45	1.28	1.22
12	bL	202	F6C	CHB-C1B	3.45	1.47	1.39
10	aA	801	CL0	C4B-NB	-3.45	1.33	1.37
11	aA	837	CLA	CHB-C1B	3.45	1.47	1.39
11	cA	841	CLA	CHB-C1B	3.45	1.47	1.39
11	aB	801	CLA	C3D-C2D	3.45	1.48	1.39
11	cA	811	CLA	CHB-C1B	3.45	1.47	1.39
11	bB	823	CLA	CHB-C1B	3.45	1.47	1.39
11	aA	828	CLA	CHC-C4B	3.45	1.47	1.39
11	cA	814	CLA	CHC-C4B	3.45	1.47	1.39
11	cA	813	CLA	CHB-C1B	3.45	1.47	1.39
11	cB	832	CLA	C1B-NB	-3.45	1.33	1.37
11	cA	839	CLA	CHC-C4B	3.45	1.47	1.39
11	bA	806	CLA	CHC-C4B	3.44	1.47	1.39
11	bB	832	CLA	C1B-NB	-3.44	1.33	1.37
11	bA	807	CLA	OBD-CAD	3.44	1.28	1.22
11	cB	808	CLA	CHD-C4C	3.44	1.47	1.39
11	bB	835	CLA	CHC-C4B	3.44	1.47	1.39
11	aA	811	CLA	CHB-C1B	3.44	1.47	1.39
11	aB	826	CLA	CHC-C4B	3.44	1.47	1.39
11	bL	206	CLA	CHC-C4B	3.44	1.47	1.39
11	aA	806	CLA	CHC-C4B	3.44	1.47	1.39
11	bB	820	CLA	CHC-C4B	3.44	1.47	1.39
11	aA	808	CLA	CHC-C4B	3.44	1.47	1.39
11	aA	812	CLA	CHC-C4B	3.44	1.47	1.39
11	bA	811	CLA	CHC-C4B	3.44	1.47	1.39
11	bA	835	CLA	CHC-C4B	3.44	1.47	1.39
11	cA	816	CLA	CHB-C1B	3.44	1.47	1.39
12	cA	830	F6C	C1D-ND	3.44	1.42	1.37
11	bL	205	CLA	CHB-C1B	3.44	1.47	1.39
11	cA	823	CLA	CHC-C4B	3.44	1.47	1.39
11	cA	807	CLA	CHC-C4B	3.44	1.47	1.39
11	aA	807	CLA	CHC-C4B	3.44	1.47	1.39
11	bB	826	CLA	CHC-C4B	3.44	1.47	1.39
11	aA	802	CLA	C4B-NB	-3.44	1.33	1.37
11	aB	801	CLA	C1B-NB	-3.44	1.33	1.37
11	aA	841	CLA	CHB-C1B	3.44	1.47	1.39
11	bB	836	CLA	CHB-C1B	3.43	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	cB	839	CLA	OBD-CAD	3.43	1.28	1.22
11	bB	839	CLA	OBD-CAD	3.43	1.28	1.22
11	cB	826	CLA	CHB-C1B	3.43	1.47	1.39
11	cA	835	CLA	CHC-C4B	3.43	1.47	1.39
11	aB	802	CLA	OBD-CAD	3.43	1.28	1.22
11	aB	808	CLA	CHD-C4C	3.43	1.47	1.39
11	aA	814	CLA	CHC-C4B	3.43	1.47	1.39
11	bA	814	CLA	CHC-C4B	3.43	1.47	1.39
11	aA	838	CLA	C4B-NB	-3.43	1.33	1.37
11	bB	813	CLA	CHB-C1B	3.43	1.47	1.39
11	aA	804	CLA	C1B-NB	-3.43	1.33	1.37
11	cB	801	CLA	CHD-C4C	3.43	1.47	1.39
11	bA	833	CLA	CHC-C4B	3.43	1.47	1.39
11	bB	815	CLA	CHB-C1B	3.43	1.47	1.39
11	aA	823	CLA	CHC-C4B	3.43	1.47	1.39
11	aA	833	CLA	CHC-C4B	3.43	1.47	1.39
11	aB	835	CLA	CHC-C4B	3.43	1.47	1.39
11	cA	837	CLA	CHB-C1B	3.43	1.47	1.39
11	aB	839	CLA	OBD-CAD	3.43	1.28	1.22
11	cA	828	CLA	CHC-C4B	3.43	1.47	1.39
11	cL	204	CLA	CHC-C4B	3.43	1.47	1.39
11	bA	838	CLA	C4B-NB	-3.43	1.33	1.37
11	bA	812	CLA	CHC-C4B	3.43	1.47	1.39
11	bB	814	CLA	OBD-CAD	3.42	1.28	1.22
11	cA	802	CLA	C4B-NB	-3.42	1.33	1.37
11	aB	838	CLA	CHB-C1B	3.42	1.47	1.39
11	bB	827	CLA	CHC-C4B	3.42	1.47	1.39
12	bB	824	F6C	C3C-C2C	3.42	1.48	1.38
11	cB	836	CLA	CHB-C1B	3.42	1.47	1.39
11	cA	808	CLA	CHC-C4B	3.42	1.47	1.39
11	aB	813	CLA	CHB-C1B	3.42	1.47	1.39
11	bA	831	CLA	CHB-C1B	3.42	1.47	1.39
11	aB	832	CLA	CHB-C1B	3.42	1.47	1.39
11	cB	835	CLA	CHC-C4B	3.42	1.47	1.39
11	bB	801	CLA	CHD-C4C	3.42	1.47	1.39
11	aB	827	CLA	OBD-CAD	3.42	1.28	1.22
11	cA	814	CLA	CHB-C1B	3.42	1.47	1.39
11	cA	811	CLA	CHC-C4B	3.42	1.47	1.39
11	bA	837	CLA	CHB-C1B	3.42	1.47	1.39
11	bA	811	CLA	CHB-C1B	3.42	1.47	1.39
11	cB	814	CLA	CHC-C4B	3.42	1.47	1.39
11	cB	827	CLA	CHC-C4B	3.42	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aA	835	CLA	CHC-C4B	3.42	1.47	1.39
11	aA	839	CLA	CHC-C4B	3.42	1.47	1.39
11	bA	823	CLA	CHC-C4B	3.41	1.47	1.39
11	aL	205	CLA	CHB-C1B	3.41	1.47	1.39
11	cA	806	CLA	CHC-C4B	3.41	1.47	1.39
11	aB	817	CLA	C4B-NB	-3.41	1.33	1.37
11	bA	838	CLA	OBD-CAD	3.41	1.28	1.22
11	cL	205	CLA	CHB-C1B	3.41	1.47	1.39
11	bB	802	CLA	OBD-CAD	3.41	1.28	1.22
11	cA	831	CLA	CHB-C1B	3.41	1.47	1.39
11	aB	828	CLA	C4B-NB	-3.41	1.33	1.37
11	cB	823	CLA	CHB-C1B	3.41	1.47	1.39
12	bL	202	F6C	CHC-C1C	3.41	1.47	1.39
11	aA	803	CLA	C4B-NB	-3.41	1.33	1.37
11	bB	814	CLA	CHC-C4B	3.41	1.47	1.39
11	cA	807	CLA	OBD-CAD	3.41	1.28	1.22
11	cB	815	CLA	CHB-C1B	3.41	1.47	1.39
11	cB	822	CLA	C1B-NB	-3.41	1.33	1.37
11	aA	816	CLA	CHB-C1B	3.41	1.47	1.39
12	aB	824	F6C	C3C-C2C	3.41	1.47	1.38
11	cA	829	CLA	CHC-C4B	3.41	1.47	1.39
11	aA	808	CLA	CHB-C1B	3.41	1.47	1.39
12	aA	830	F6C	C1D-ND	3.41	1.42	1.37
11	aB	817	CLA	CHB-C1B	3.41	1.47	1.39
12	bA	832	F6C	C3C-C2C	3.41	1.47	1.38
11	aB	815	CLA	CHB-C1B	3.41	1.47	1.39
11	cB	828	CLA	C4B-NB	-3.41	1.33	1.37
12	bA	830	F6C	C1D-ND	3.40	1.42	1.37
11	bB	838	CLA	OBD-CAD	3.40	1.28	1.22
11	aA	814	CLA	CHB-C1B	3.40	1.47	1.39
12	cB	824	F6C	C3C-C2C	3.40	1.47	1.38
11	bB	817	CLA	CHB-C1B	3.40	1.47	1.39
11	cB	838	CLA	OBD-CAD	3.40	1.28	1.22
11	cB	817	CLA	CHB-C1B	3.40	1.47	1.39
11	cA	804	CLA	C1B-NB	-3.40	1.33	1.37
11	cB	821	CLA	C1B-NB	-3.40	1.33	1.37
11	bB	830	CLA	CHB-C1B	3.40	1.47	1.39
11	bA	803	CLA	CHD-C1D	3.40	1.45	1.38
11	aA	829	CLA	CHC-C4B	3.40	1.47	1.39
11	aB	801	CLA	CHD-C4C	3.40	1.47	1.39
11	bA	816	CLA	CHB-C1B	3.40	1.47	1.39
11	aB	822	CLA	C1B-NB	-3.40	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aB	823	CLA	CHB-C1B	3.40	1.47	1.39
11	bB	805	CLA	CHC-C4B	3.39	1.47	1.39
11	bB	828	CLA	C4B-NB	-3.39	1.33	1.37
11	bA	814	CLA	CHB-C1B	3.39	1.47	1.39
11	bA	817	CLA	CHB-C1B	3.39	1.47	1.39
11	bL	204	CLA	CHC-C4B	3.39	1.47	1.39
11	aA	803	CLA	CHD-C1D	3.39	1.45	1.38
11	bA	829	CLA	CHC-C4B	3.39	1.47	1.39
11	aA	819	CLA	CHB-C1B	3.39	1.47	1.39
11	cB	830	CLA	CHB-C1B	3.39	1.47	1.39
12	bA	827	F6C	C3C-C2C	3.39	1.47	1.38
11	cA	808	CLA	CHB-C1B	3.39	1.47	1.39
11	aB	838	CLA	OBD-CAD	3.39	1.28	1.22
11	aA	831	CLA	CHB-C1B	3.39	1.47	1.39
11	bB	801	CLA	CHC-C4B	3.39	1.47	1.39
11	cB	833	CLA	CHB-C1B	3.38	1.47	1.39
11	bA	819	CLA	CHB-C1B	3.38	1.47	1.39
12	cL	202	F6C	CHC-C1C	3.38	1.47	1.39
11	bB	827	CLA	OBD-CAD	3.38	1.28	1.22
11	cA	825	CLA	CHC-C4B	3.38	1.47	1.39
11	cA	803	CLA	CHD-C1D	3.38	1.45	1.38
11	aA	817	CLA	CHB-C1B	3.38	1.47	1.39
11	aA	813	CLA	C3B-C4B	3.38	1.50	1.42
11	aA	825	CLA	CHC-C4B	3.38	1.47	1.39
11	aB	828	CLA	C3D-C2D	3.38	1.48	1.39
12	aA	844	F6C	C3C-C2C	3.38	1.47	1.38
11	aB	805	CLA	CHC-C4B	3.38	1.47	1.39
12	bA	844	F6C	C3C-C2C	3.38	1.47	1.38
11	cB	801	CLA	C1B-NB	-3.38	1.33	1.37
10	aA	801	CL0	CHC-C4B	3.38	1.47	1.39
11	cB	809	CLA	C4B-NB	-3.38	1.33	1.37
11	aB	814	CLA	CHC-C4B	3.38	1.47	1.39
11	aB	818	CLA	CHB-C1B	3.37	1.47	1.39
11	aL	204	CLA	CHC-C4B	3.37	1.47	1.39
11	cA	813	CLA	C3B-C4B	3.37	1.50	1.42
11	cB	818	CLA	CHB-C1B	3.37	1.47	1.39
11	cB	827	CLA	CHB-C1B	3.37	1.47	1.39
11	bB	833	CLA	CHB-C1B	3.37	1.47	1.39
10	cA	801	CL0	CHC-C4B	3.37	1.47	1.39
11	bB	827	CLA	CHB-C1B	3.37	1.47	1.39
11	aA	829	CLA	CHB-C1B	3.37	1.47	1.39
12	cA	832	F6C	C3C-C2C	3.37	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aA	833	CLA	OBD-CAD	3.37	1.28	1.22
11	cA	819	CLA	OBD-CAD	3.37	1.28	1.22
11	bA	825	CLA	CHB-C1B	3.37	1.47	1.39
11	bA	825	CLA	CHC-C4B	3.37	1.47	1.39
12	cA	844	F6C	C3C-C2C	3.37	1.47	1.38
11	aB	827	CLA	CHB-C1B	3.37	1.47	1.39
12	aA	827	F6C	C3C-C2C	3.37	1.47	1.38
11	aB	832	CLA	C1B-NB	-3.37	1.33	1.37
11	aA	824	CLA	CHB-C1B	3.37	1.47	1.39
11	cA	819	CLA	CHB-C1B	3.37	1.47	1.39
12	cA	827	F6C	C3C-C2C	3.37	1.47	1.38
11	aA	819	CLA	OBD-CAD	3.36	1.28	1.22
11	cA	817	CLA	CHB-C1B	3.36	1.47	1.39
11	cB	812	CLA	CHC-C4B	3.36	1.47	1.39
11	aB	807	CLA	C4B-NB	-3.36	1.33	1.37
11	cB	801	CLA	CHC-C4B	3.36	1.46	1.39
11	aA	838	CLA	OBD-CAD	3.36	1.28	1.22
11	aB	801	CLA	CHC-C4B	3.36	1.46	1.39
11	cB	828	CLA	C3D-C2D	3.36	1.48	1.39
11	bA	813	CLA	C3B-C4B	3.36	1.50	1.42
11	bB	818	CLA	CHB-C1B	3.36	1.46	1.39
11	cA	825	CLA	CHB-C1B	3.36	1.46	1.39
11	bA	833	CLA	OBD-CAD	3.36	1.28	1.22
11	cA	829	CLA	CHB-C1B	3.36	1.46	1.39
12	aA	832	F6C	C3C-C2C	3.36	1.47	1.38
11	bA	829	CLA	C4B-NB	-3.36	1.33	1.37
11	cA	838	CLA	OBD-CAD	3.36	1.28	1.22
11	aB	833	CLA	CHB-C1B	3.36	1.46	1.39
11	bA	829	CLA	CHB-C1B	3.36	1.46	1.39
11	bA	834	CLA	CHC-C4B	3.36	1.46	1.39
12	aL	202	F6C	CHC-C1C	3.36	1.46	1.39
11	bB	809	CLA	C4B-NB	-3.36	1.33	1.37
11	cA	815	CLA	CHB-C1B	3.35	1.46	1.39
11	aB	830	CLA	CHB-C1B	3.35	1.46	1.39
11	bA	819	CLA	OBD-CAD	3.35	1.28	1.22
11	aA	825	CLA	CHB-C1B	3.35	1.46	1.39
11	aA	809	CLA	C4B-NB	-3.35	1.33	1.37
11	aA	834	CLA	CHC-C4B	3.35	1.46	1.39
11	bA	808	CLA	CHB-C1B	3.35	1.46	1.39
11	bA	803	CLA	C4B-NB	-3.35	1.33	1.37
11	cA	803	CLA	C4B-NB	-3.35	1.33	1.37
11	cA	831	CLA	C4B-NB	-3.35	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aB	840	CLA	CHC-C4B	3.35	1.46	1.39
11	cA	833	CLA	OBD-CAD	3.35	1.28	1.22
11	aA	815	CLA	CHB-C1B	3.35	1.46	1.39
11	aB	812	CLA	CHC-C4B	3.35	1.46	1.39
11	aB	813	CLA	CHC-C4B	3.35	1.46	1.39
11	bB	812	CLA	CHC-C4B	3.35	1.46	1.39
11	cA	834	CLA	CHC-C4B	3.35	1.46	1.39
12	bL	202	F6C	C3C-C2C	3.34	1.47	1.38
12	aA	832	F6C	OBD-CAD	3.34	1.28	1.22
11	aB	809	CLA	C4B-NB	-3.34	1.33	1.37
11	aA	824	CLA	CHC-C4B	3.34	1.46	1.39
12	aL	202	F6C	C3C-C2C	3.34	1.47	1.38
11	cA	824	CLA	CHB-C1B	3.34	1.46	1.39
11	cA	842	CLA	CHB-C1B	3.34	1.46	1.39
11	cL	204	CLA	C4B-NB	-3.34	1.33	1.37
11	bB	807	CLA	C4B-NB	-3.34	1.33	1.37
11	bA	824	CLA	CHB-C1B	3.34	1.46	1.39
11	cB	813	CLA	CHC-C4B	3.34	1.46	1.39
10	bA	801	CL0	CHC-C4B	3.34	1.46	1.39
11	cB	805	CLA	C4B-NB	-3.34	1.33	1.37
11	cB	805	CLA	CHC-C4B	3.34	1.46	1.39
11	aA	840	CLA	CHB-C1B	3.34	1.46	1.39
11	aB	814	CLA	CHB-C1B	3.34	1.46	1.39
11	bA	828	CLA	C4B-NB	-3.33	1.33	1.37
11	aA	812	CLA	CHB-C1B	3.33	1.46	1.39
11	cB	807	CLA	CHC-C4B	3.33	1.46	1.39
11	aA	829	CLA	C4B-NB	-3.33	1.33	1.37
11	cA	815	CLA	C4B-NB	-3.33	1.33	1.37
11	bA	840	CLA	CHB-C1B	3.33	1.46	1.39
11	cA	829	CLA	C4B-NB	-3.33	1.33	1.37
12	cA	830	F6C	C3C-C2C	3.33	1.47	1.38
11	bB	814	CLA	CHB-C1B	3.33	1.46	1.39
11	bB	805	CLA	C4B-NB	-3.33	1.33	1.37
11	bB	817	CLA	C4B-NB	-3.33	1.33	1.37
11	bB	828	CLA	C3D-C2D	3.33	1.48	1.39
11	bA	824	CLA	CHC-C4B	3.33	1.46	1.39
11	cA	809	CLA	C4B-NB	-3.33	1.33	1.37
11	cA	833	CLA	C4B-NB	-3.33	1.33	1.37
11	aB	831	CLA	CHB-C1B	3.33	1.46	1.39
11	cA	805	CLA	CHB-C1B	3.33	1.46	1.39
11	cA	824	CLA	CHC-C4B	3.33	1.46	1.39
12	bA	830	F6C	C3C-C2C	3.33	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	cB	814	CLA	CHB-C1B	3.33	1.46	1.39
11	bA	812	CLA	CHB-C1B	3.33	1.46	1.39
11	bB	807	CLA	CHC-C4B	3.32	1.46	1.39
11	aB	827	CLA	C4B-NB	-3.32	1.33	1.37
11	bA	831	CLA	C4B-NB	-3.32	1.33	1.37
11	bA	809	CLA	C4B-NB	-3.32	1.33	1.37
11	bA	842	CLA	CHB-C1B	3.32	1.46	1.39
12	cA	832	F6C	OBD-CAD	3.32	1.28	1.22
12	cL	202	F6C	C3C-C2C	3.32	1.47	1.38
11	cB	807	CLA	C4B-NB	-3.32	1.33	1.37
11	cB	807	CLA	OBD-CAD	3.32	1.28	1.22
11	bB	827	CLA	C4B-NB	-3.32	1.33	1.37
11	bB	807	CLA	OBD-CAD	3.32	1.28	1.22
11	bA	815	CLA	CHB-C1B	3.32	1.46	1.39
11	cB	840	CLA	CHC-C4B	3.32	1.46	1.39
11	aA	815	CLA	C4B-NB	-3.32	1.33	1.37
12	aA	830	F6C	C3C-C2C	3.32	1.47	1.38
11	aB	807	CLA	CHC-C4B	3.32	1.46	1.39
11	cA	840	CLA	CHB-C1B	3.32	1.46	1.39
11	cA	812	CLA	CHB-C1B	3.31	1.46	1.39
11	cB	837	CLA	OBD-CAD	3.31	1.28	1.22
11	cB	808	CLA	CHC-C4B	3.31	1.46	1.39
11	bB	806	CLA	C4B-NB	-3.31	1.33	1.37
11	bA	809	CLA	CHB-C1B	3.31	1.46	1.39
12	bA	832	F6C	OBD-CAD	3.31	1.28	1.22
11	bB	834	CLA	CHC-C4B	3.31	1.46	1.39
11	cB	831	CLA	CHB-C1B	3.31	1.46	1.39
11	cB	834	CLA	CHC-C4B	3.31	1.46	1.39
11	bB	839	CLA	C3D-C2D	3.30	1.48	1.39
11	bL	204	CLA	C4B-NB	-3.30	1.33	1.37
11	cB	817	CLA	C4B-NB	-3.30	1.33	1.37
11	aB	808	CLA	CHC-C4B	3.30	1.46	1.39
11	bA	815	CLA	C4B-NB	-3.30	1.33	1.37
11	bA	833	CLA	C4B-NB	-3.30	1.33	1.37
11	bA	805	CLA	CHB-C1B	3.30	1.46	1.39
11	aA	842	CLA	CHB-C1B	3.30	1.46	1.39
11	bB	831	CLA	CHB-C1B	3.30	1.46	1.39
11	aB	805	CLA	C4B-NB	-3.29	1.33	1.37
11	cB	817	CLA	CHC-C4B	3.29	1.46	1.39
11	bB	808	CLA	CHC-C4B	3.29	1.46	1.39
11	cA	817	CLA	CHC-C4B	3.29	1.46	1.39
11	aA	831	CLA	C4B-NB	-3.29	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bB	817	CLA	CHC-C4B	3.29	1.46	1.39
11	aB	837	CLA	OBD-CAD	3.29	1.28	1.22
11	bB	837	CLA	OBD-CAD	3.29	1.28	1.22
11	aB	834	CLA	CHC-C4B	3.29	1.46	1.39
11	cB	839	CLA	C3D-C2D	3.28	1.48	1.39
11	cB	827	CLA	C4B-NB	-3.28	1.33	1.37
11	aA	828	CLA	OBD-CAD	3.28	1.28	1.22
11	aL	204	CLA	C4B-NB	-3.28	1.33	1.37
11	aB	817	CLA	CHC-C4B	3.28	1.46	1.39
11	bB	840	CLA	CHC-C4B	3.28	1.46	1.39
11	bB	813	CLA	CHC-C4B	3.28	1.46	1.39
12	cA	844	F6C	C4A-NA	-3.28	1.33	1.37
11	aA	809	CLA	CHB-C1B	3.28	1.46	1.39
11	cA	809	CLA	CHB-C1B	3.28	1.46	1.39
11	bB	810	CLA	CHC-C4B	3.28	1.46	1.39
11	aB	807	CLA	OBD-CAD	3.28	1.28	1.22
11	aA	835	CLA	CHB-C1B	3.28	1.46	1.39
11	aB	806	CLA	C4B-NB	-3.28	1.33	1.37
11	bA	814	CLA	C4B-NB	-3.28	1.33	1.37
11	bA	835	CLA	CHB-C1B	3.28	1.46	1.39
11	cA	820	CLA	CHB-C1B	3.28	1.46	1.39
11	aB	808	CLA	CHB-C1B	3.28	1.46	1.39
11	bA	817	CLA	CHC-C4B	3.27	1.46	1.39
11	aA	814	CLA	C4B-NB	-3.27	1.33	1.37
11	cA	814	CLA	C4B-NB	-3.27	1.33	1.37
11	cA	835	CLA	CHB-C1B	3.27	1.46	1.39
12	bA	844	F6C	C4A-NA	-3.27	1.33	1.37
11	aB	839	CLA	C3D-C2D	3.27	1.48	1.39
12	aA	844	F6C	C4A-NA	-3.26	1.33	1.37
11	aA	820	CLA	CHB-C1B	3.26	1.46	1.39
11	aB	816	CLA	CHB-C1B	3.26	1.46	1.39
11	aA	805	CLA	CHB-C1B	3.26	1.46	1.39
11	cB	825	CLA	OBD-CAD	3.26	1.28	1.22
11	bA	837	CLA	C4B-NB	-3.26	1.33	1.37
11	cB	816	CLA	CHB-C1B	3.26	1.46	1.39
11	aB	810	CLA	CHC-C4B	3.25	1.46	1.39
11	aA	828	CLA	C4B-NB	-3.25	1.33	1.37
11	aA	833	CLA	C4B-NB	-3.25	1.33	1.37
12	aB	824	F6C	C4A-NA	-3.25	1.33	1.37
11	aA	817	CLA	CHC-C4B	3.25	1.46	1.39
11	bA	820	CLA	CHB-C1B	3.25	1.46	1.39
11	bB	825	CLA	OBD-CAD	3.25	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	cA	837	CLA	C4B-NB	-3.25	1.33	1.37
11	bA	834	CLA	C4B-NB	-3.25	1.33	1.37
11	cB	810	CLA	CHC-C4B	3.25	1.46	1.39
11	cB	808	CLA	C4B-NB	-3.25	1.33	1.37
11	cB	806	CLA	C4B-NB	-3.24	1.33	1.37
11	bA	828	CLA	OBD-CAD	3.24	1.28	1.22
11	bB	808	CLA	C4B-NB	-3.24	1.33	1.37
12	bB	824	F6C	C4A-NA	-3.24	1.33	1.37
11	aA	837	CLA	C4B-NB	-3.24	1.33	1.37
12	cB	824	F6C	C4A-NA	-3.24	1.33	1.37
11	cB	808	CLA	CHB-C1B	3.23	1.46	1.39
11	aB	813	CLA	C4B-NB	-3.23	1.33	1.37
11	cA	828	CLA	C4B-NB	-3.23	1.33	1.37
11	bA	802	CLA	CHB-C1B	3.23	1.46	1.39
11	aB	808	CLA	C4B-NB	-3.23	1.33	1.37
12	cA	832	F6C	C4A-NA	-3.23	1.33	1.37
11	bB	808	CLA	CHB-C1B	3.23	1.46	1.39
11	aB	805	CLA	CHB-C1B	3.23	1.46	1.39
11	cA	825	CLA	C4B-NB	-3.22	1.33	1.37
11	cB	813	CLA	C4B-NB	-3.22	1.33	1.37
11	bB	816	CLA	CHB-C1B	3.22	1.46	1.39
12	bA	832	F6C	C4A-NA	-3.22	1.33	1.37
11	aA	835	CLA	C4B-NB	-3.22	1.33	1.37
11	aA	820	CLA	CHC-C4B	3.22	1.46	1.39
11	cB	826	CLA	C4B-NB	-3.22	1.33	1.37
11	aB	825	CLA	OBD-CAD	3.22	1.28	1.22
12	cL	202	F6C	OBD-CAD	3.21	1.28	1.22
11	aA	836	CLA	CHC-C4B	3.21	1.46	1.39
12	bL	202	F6C	OBD-CAD	3.21	1.28	1.22
11	cA	836	CLA	CHC-C4B	3.21	1.46	1.39
11	cB	805	CLA	CHB-C1B	3.21	1.46	1.39
11	bB	801	CLA	C4B-NB	-3.21	1.33	1.37
11	aA	840	CLA	C3B-C4B	3.20	1.50	1.42
11	bA	820	CLA	CHC-C4B	3.20	1.46	1.39
11	aA	836	CLA	C4B-NB	-3.20	1.33	1.37
11	bA	840	CLA	C3B-C4B	3.20	1.50	1.42
11	cA	802	CLA	CHB-C1B	3.20	1.46	1.39
11	aB	826	CLA	C4B-NB	-3.20	1.33	1.37
11	cA	815	CLA	CHC-C4B	3.19	1.46	1.39
11	cA	834	CLA	C4B-NB	-3.19	1.33	1.37
11	aA	802	CLA	CHB-C1B	3.19	1.46	1.39
11	cA	828	CLA	OBD-CAD	3.19	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	cA	817	CLA	C4B-NB	-3.19	1.33	1.37
11	bB	805	CLA	CHB-C1B	3.19	1.46	1.39
11	aA	825	CLA	C4B-NB	-3.19	1.33	1.37
11	cA	820	CLA	CHC-C4B	3.19	1.46	1.39
11	bA	802	CLA	CHC-C4B	3.19	1.46	1.39
11	bA	815	CLA	CHC-C4B	3.19	1.46	1.39
11	cL	206	CLA	C4B-NB	-3.19	1.33	1.37
11	aB	802	CLA	C4B-NB	-3.18	1.33	1.37
11	bA	836	CLA	C4B-NB	-3.18	1.33	1.37
11	bB	826	CLA	C4B-NB	-3.18	1.33	1.37
11	cA	808	CLA	C4B-NB	-3.18	1.33	1.37
11	bA	836	CLA	CHC-C4B	3.18	1.46	1.39
11	aB	825	CLA	C4B-NB	-3.18	1.33	1.37
11	bA	835	CLA	C4B-NB	-3.18	1.33	1.37
11	cB	801	CLA	C4B-NB	-3.18	1.33	1.37
11	aA	815	CLA	CHC-C4B	3.18	1.46	1.39
11	bB	813	CLA	C4B-NB	-3.18	1.33	1.37
11	aB	809	CLA	CHC-C4B	3.18	1.46	1.39
11	cA	836	CLA	C4B-NB	-3.18	1.33	1.37
11	cA	802	CLA	OBD-CAD	3.17	1.27	1.22
12	cA	830	F6C	C4A-NA	-3.17	1.33	1.37
11	cA	840	CLA	C3B-C4B	3.17	1.50	1.42
11	bA	824	CLA	C4B-NB	-3.17	1.33	1.37
11	bB	802	CLA	C4B-NB	-3.17	1.33	1.37
11	aA	824	CLA	C4B-NB	-3.17	1.33	1.37
12	aL	202	F6C	OBD-CAD	3.17	1.27	1.22
11	bB	809	CLA	CHC-C4B	3.17	1.46	1.39
12	aA	832	F6C	C4A-NA	-3.17	1.33	1.37
11	aL	206	CLA	C4B-NB	-3.17	1.33	1.37
11	bA	831	CLA	CHC-C4B	3.17	1.46	1.39
11	bA	825	CLA	C4B-NB	-3.16	1.33	1.37
11	cA	835	CLA	C4B-NB	-3.16	1.33	1.37
11	bB	825	CLA	C4B-NB	-3.16	1.33	1.37
11	cB	802	CLA	C4B-NB	-3.16	1.33	1.37
11	cA	831	CLA	CHC-C4B	3.16	1.46	1.39
11	aA	802	CLA	OBD-CAD	3.15	1.27	1.22
11	cB	809	CLA	CHC-C4B	3.15	1.46	1.39
11	aB	828	CLA	CHC-C4B	3.15	1.46	1.39
11	cB	822	CLA	C4B-NB	-3.15	1.33	1.37
11	aA	831	CLA	CHC-C4B	3.15	1.46	1.39
11	cB	825	CLA	C4B-NB	-3.15	1.33	1.37
11	cB	806	CLA	OBD-CAD	3.15	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bA	802	CLA	OBD-CAD	3.15	1.27	1.22
11	aA	834	CLA	C4B-NB	-3.15	1.33	1.37
11	aB	801	CLA	C4B-NB	-3.15	1.33	1.37
11	aA	808	CLA	C4B-NB	-3.14	1.33	1.37
11	cB	828	CLA	CHC-C4B	3.13	1.46	1.39
11	bA	816	CLA	C3B-C4B	3.13	1.50	1.42
11	aA	816	CLA	C3B-C4B	3.13	1.50	1.42
11	aB	822	CLA	C4B-NB	-3.13	1.33	1.37
11	bB	819	CLA	C4B-NB	-3.12	1.33	1.37
11	bL	205	CLA	C4B-NB	-3.12	1.33	1.37
11	aA	802	CLA	CHC-C4B	3.12	1.46	1.39
11	aB	806	CLA	OBD-CAD	3.12	1.27	1.22
11	aL	205	CLA	C4B-NB	-3.12	1.33	1.37
11	bB	839	CLA	C4B-NB	-3.12	1.33	1.37
11	cA	802	CLA	CHC-C4B	3.12	1.46	1.39
11	cL	205	CLA	C4B-NB	-3.12	1.34	1.37
15	bL	203	BCR	C1-C6	-3.11	1.49	1.53
15	aL	203	BCR	C1-C6	-3.11	1.49	1.53
11	bL	206	CLA	C4B-NB	-3.10	1.34	1.37
11	cA	820	CLA	C4B-NB	-3.10	1.34	1.37
11	cA	816	CLA	C3B-C4B	3.10	1.50	1.42
11	bB	828	CLA	CHC-C4B	3.10	1.46	1.39
11	bB	822	CLA	C4B-NB	-3.10	1.34	1.37
11	bB	802	CLA	CHB-C1B	3.10	1.46	1.39
11	bA	808	CLA	C4B-NB	-3.09	1.34	1.37
11	bB	804	CLA	C4B-NB	-3.09	1.34	1.37
11	bB	806	CLA	OBD-CAD	3.09	1.27	1.22
11	bB	836	CLA	C4B-NB	-3.09	1.34	1.37
15	cL	203	BCR	C1-C6	-3.09	1.49	1.53
11	cB	804	CLA	C4B-NB	-3.09	1.34	1.37
11	bA	817	CLA	C4B-NB	-3.09	1.34	1.37
11	aA	819	CLA	C3B-C4B	3.09	1.50	1.42
11	aK	103	CLA	C4B-NB	-3.09	1.34	1.37
11	cB	803	CLA	CHC-C4B	3.09	1.46	1.39
11	cA	824	CLA	C4B-NB	-3.08	1.34	1.37
11	cB	831	CLA	C4B-NB	-3.08	1.34	1.37
11	bB	803	CLA	CHB-C1B	3.08	1.46	1.39
11	cB	802	CLA	CHB-C1B	3.08	1.46	1.39
11	aB	803	CLA	CHC-C4B	3.08	1.46	1.39
12	aA	830	F6C	C4A-NA	-3.08	1.34	1.37
11	cB	803	CLA	CHB-C1B	3.08	1.46	1.39
11	bB	811	CLA	C4B-NB	-3.08	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aB	804	CLA	C4B-NB	-3.07	1.34	1.37
11	aB	839	CLA	C4B-NB	-3.07	1.34	1.37
11	aA	823	CLA	C4B-NB	-3.07	1.34	1.37
11	cA	812	CLA	C4B-NB	-3.07	1.34	1.37
11	bA	819	CLA	C3B-C4B	3.07	1.49	1.42
11	bB	814	CLA	C4B-NB	-3.07	1.34	1.37
11	cB	816	CLA	C4B-NB	-3.07	1.34	1.37
11	aB	802	CLA	CHB-C1B	3.07	1.46	1.39
11	aB	836	CLA	C4B-NB	-3.07	1.34	1.37
11	bB	803	CLA	CHC-C4B	3.07	1.46	1.39
11	aB	803	CLA	CHB-C1B	3.07	1.46	1.39
11	bB	830	CLA	C4B-NB	-3.07	1.34	1.37
11	cA	819	CLA	C3B-C4B	3.07	1.49	1.42
11	aB	831	CLA	C4B-NB	-3.07	1.34	1.37
12	bA	830	F6C	C4A-NA	-3.07	1.34	1.37
11	aA	820	CLA	C4B-NB	-3.07	1.34	1.37
11	bA	807	CLA	C4B-NB	-3.07	1.34	1.37
11	aB	816	CLA	C4B-NB	-3.06	1.34	1.37
11	cB	837	CLA	C4B-NB	-3.06	1.34	1.37
11	aB	830	CLA	C4B-NB	-3.06	1.34	1.37
11	bA	819	CLA	C4B-NB	-3.06	1.34	1.37
11	cB	839	CLA	C4B-NB	-3.06	1.34	1.37
11	cB	836	CLA	C4B-NB	-3.05	1.34	1.37
11	cB	819	CLA	C4B-NB	-3.05	1.34	1.37
11	bA	806	CLA	C3B-C4B	3.05	1.49	1.42
11	aB	840	CLA	C4B-NB	-3.05	1.34	1.37
11	aB	819	CLA	C4B-NB	-3.05	1.34	1.37
11	aA	812	CLA	C4B-NB	-3.05	1.34	1.37
11	aA	817	CLA	C4B-NB	-3.05	1.34	1.37
11	bK	103	CLA	C4B-NB	-3.05	1.34	1.37
15	aB	842	BCR	C1-C6	-3.05	1.49	1.53
11	bA	820	CLA	C4B-NB	-3.05	1.34	1.37
11	cB	814	CLA	C4B-NB	-3.05	1.34	1.37
11	cB	833	CLA	C3B-C4B	3.05	1.49	1.42
11	aA	839	CLA	C4B-NB	-3.05	1.34	1.37
11	cA	807	CLA	C4B-NB	-3.05	1.34	1.37
11	bA	823	CLA	C4B-NB	-3.04	1.34	1.37
11	bA	839	CLA	C4B-NB	-3.04	1.34	1.37
11	cA	823	CLA	C4B-NB	-3.04	1.34	1.37
11	cA	806	CLA	C3B-C4B	3.04	1.49	1.42
11	aB	833	CLA	C3B-C4B	3.04	1.49	1.42
11	aA	806	CLA	C3B-C4B	3.04	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aA	805	CLA	C3B-C4B	3.04	1.49	1.42
11	cA	839	CLA	C4B-NB	-3.04	1.34	1.37
11	bB	840	CLA	C4B-NB	-3.03	1.34	1.37
11	bB	833	CLA	C3B-C4B	3.03	1.49	1.42
15	bA	848	BCR	C30-C25	-3.03	1.49	1.53
11	bA	841	CLA	C4B-NB	-3.03	1.34	1.37
11	bB	816	CLA	C4B-NB	-3.02	1.34	1.37
15	cB	842	BCR	C1-C6	-3.02	1.49	1.53
11	bB	801	CLA	C1B-C2B	3.02	1.50	1.43
11	cB	801	CLA	C1B-C2B	3.02	1.50	1.43
11	cA	810	CLA	C4B-NB	-3.02	1.34	1.37
11	bA	810	CLA	C4B-NB	-3.02	1.34	1.37
11	cB	811	CLA	C4B-NB	-3.02	1.34	1.37
15	cA	848	BCR	C30-C25	-3.02	1.49	1.53
12	aL	202	F6C	C1A-C2A	3.01	1.52	1.45
11	aA	841	CLA	C4B-NB	-3.01	1.34	1.37
11	aA	807	CLA	C4B-NB	-3.01	1.34	1.37
11	bA	805	CLA	C3B-C4B	3.01	1.49	1.42
11	cB	838	CLA	C3B-C4B	3.01	1.49	1.42
11	bB	831	CLA	C4B-NB	-3.01	1.34	1.37
11	bB	838	CLA	C3B-C4B	3.01	1.49	1.42
12	aA	827	F6C	C4A-NA	-3.01	1.34	1.37
11	bB	810	CLA	C4B-NB	-3.00	1.34	1.37
11	cA	805	CLA	C3B-C4B	3.00	1.49	1.42
11	aA	803	CLA	CHB-C1B	3.00	1.46	1.39
11	aA	819	CLA	C4B-NB	-3.00	1.34	1.37
11	aB	811	CLA	C4B-NB	-3.00	1.34	1.37
11	bB	829	CLA	C4B-NB	-3.00	1.34	1.37
11	cB	810	CLA	C4B-NB	-3.00	1.34	1.37
11	bB	837	CLA	C4B-NB	-3.00	1.34	1.37
15	aA	848	BCR	C30-C25	-3.00	1.49	1.53
11	bA	806	CLA	C4B-NB	-3.00	1.34	1.37
11	cA	803	CLA	CHB-C1B	3.00	1.46	1.39
11	bA	842	CLA	C3B-C4B	3.00	1.49	1.42
15	aK	102	BCR	C1-C6	-3.00	1.49	1.53
11	aB	838	CLA	C3B-C4B	3.00	1.49	1.42
11	aB	801	CLA	C1B-C2B	2.99	1.50	1.43
11	cA	806	CLA	C4B-NB	-2.99	1.34	1.37
11	bA	811	CLA	C4B-NB	-2.99	1.34	1.37
11	cA	841	CLA	C4B-NB	-2.99	1.34	1.37
11	aB	814	CLA	C4B-NB	-2.99	1.34	1.37
11	cA	842	CLA	C3B-C4B	2.99	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aB	829	CLA	C4B-NB	-2.98	1.34	1.37
11	cB	829	CLA	C4B-NB	-2.98	1.34	1.37
11	aB	820	CLA	C4B-NB	-2.98	1.34	1.37
15	bK	102	BCR	C1-C6	-2.98	1.49	1.53
11	cK	103	CLA	C4B-NB	-2.98	1.34	1.37
11	bA	803	CLA	CHB-C1B	2.98	1.46	1.39
11	aA	811	CLA	C4B-NB	-2.98	1.34	1.37
11	bA	843	CLA	C4B-NB	-2.98	1.34	1.37
11	cB	840	CLA	C4B-NB	-2.97	1.34	1.37
11	aA	806	CLA	C4B-NB	-2.97	1.34	1.37
11	aA	842	CLA	C3B-C4B	2.97	1.49	1.42
11	aA	810	CLA	C4B-NB	-2.97	1.34	1.37
11	cB	830	CLA	C4B-NB	-2.97	1.34	1.37
15	bB	842	BCR	C1-C6	-2.97	1.49	1.53
11	aB	810	CLA	C4B-NB	-2.97	1.34	1.37
11	cB	820	CLA	C4B-NB	-2.97	1.34	1.37
12	bL	202	F6C	C1A-C2A	2.96	1.52	1.45
11	bA	812	CLA	C4B-NB	-2.96	1.34	1.37
11	cB	829	CLA	CHC-C4B	2.96	1.46	1.39
11	aB	837	CLA	C4B-NB	-2.96	1.34	1.37
11	cA	819	CLA	C4B-NB	-2.96	1.34	1.37
11	aA	822	CLA	C4B-NB	-2.96	1.34	1.37
15	cK	102	BCR	C1-C6	-2.96	1.49	1.53
11	bA	822	CLA	C4B-NB	-2.96	1.34	1.37
11	cA	822	CLA	C4B-NB	-2.96	1.34	1.37
11	bB	836	CLA	C3B-C4B	2.96	1.49	1.42
11	cK	101	CLA	C4B-NB	-2.95	1.34	1.37
11	cA	818	CLA	C4B-NB	-2.95	1.34	1.37
11	cB	815	CLA	C4B-NB	-2.95	1.34	1.37
12	bA	827	F6C	C4A-NA	-2.95	1.34	1.37
11	bB	820	CLA	C4B-NB	-2.95	1.34	1.37
11	aB	815	CLA	C4B-NB	-2.95	1.34	1.37
11	cA	811	CLA	C4B-NB	-2.95	1.34	1.37
11	aA	818	CLA	C4B-NB	-2.94	1.34	1.37
11	cB	838	CLA	C4B-NB	-2.94	1.34	1.37
11	aB	829	CLA	CHC-C4B	2.94	1.46	1.39
12	cL	202	F6C	C1A-C2A	2.94	1.51	1.45
11	bK	101	CLA	C3B-C4B	2.94	1.49	1.42
11	cB	818	CLA	C3B-C4B	2.93	1.49	1.42
11	aA	839	CLA	OBD-CAD	2.93	1.27	1.22
11	aA	806	CLA	CHB-C1B	2.93	1.46	1.39
11	aB	836	CLA	C3B-C4B	2.93	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bA	839	CLA	OBD-CAD	2.93	1.27	1.22
11	bA	821	CLA	C3B-C4B	2.93	1.49	1.42
11	aB	814	CLA	C3B-C4B	2.93	1.49	1.42
11	cA	839	CLA	OBD-CAD	2.92	1.27	1.22
11	bA	818	CLA	C4B-NB	-2.92	1.34	1.37
11	cA	806	CLA	CHB-C1B	2.92	1.46	1.39
11	cB	836	CLA	OBD-CAD	2.92	1.27	1.22
11	cB	816	CLA	C3B-C4B	2.92	1.49	1.42
11	aA	821	CLA	C3B-C4B	2.92	1.49	1.42
11	bA	806	CLA	CHB-C1B	2.91	1.45	1.39
11	bB	816	CLA	C3B-C4B	2.91	1.49	1.42
11	bB	829	CLA	CHC-C4B	2.91	1.45	1.39
11	cA	821	CLA	C3B-C4B	2.91	1.49	1.42
15	bB	846	BCR	C30-C25	-2.91	1.49	1.53
15	cB	846	BCR	C30-C25	-2.91	1.49	1.53
11	cB	836	CLA	C3B-C4B	2.91	1.49	1.42
12	cA	827	F6C	C4A-NA	-2.91	1.34	1.37
15	cB	843	BCR	C1-C6	-2.90	1.49	1.53
11	aK	101	CLA	C3B-C4B	2.90	1.49	1.42
11	aK	101	CLA	C4B-NB	-2.90	1.34	1.37
15	bB	845	BCR	C30-C25	-2.90	1.49	1.53
11	aA	843	CLA	C4B-NB	-2.90	1.34	1.37
11	cK	101	CLA	C3B-C4B	2.90	1.49	1.42
11	cB	832	CLA	C4B-NB	-2.90	1.34	1.37
11	bB	811	CLA	C3B-C4B	2.90	1.49	1.42
11	cB	821	CLA	C3B-C4B	2.90	1.49	1.42
11	aB	821	CLA	C3B-C4B	2.90	1.49	1.42
11	aB	832	CLA	C4B-NB	-2.89	1.34	1.37
11	cB	814	CLA	C3B-C4B	2.89	1.49	1.42
11	cA	843	CLA	C4B-NB	-2.89	1.34	1.37
11	aB	818	CLA	C3B-C4B	2.89	1.49	1.42
11	bB	814	CLA	C3B-C4B	2.89	1.49	1.42
11	bB	818	CLA	C3B-C4B	2.89	1.49	1.42
11	bA	843	CLA	C3B-C4B	2.89	1.49	1.42
11	aA	843	CLA	C3B-C4B	2.89	1.49	1.42
11	bB	821	CLA	C3B-C4B	2.89	1.49	1.42
11	bB	823	CLA	C4B-NB	-2.88	1.34	1.37
15	cB	845	BCR	C30-C25	-2.88	1.49	1.53
11	bK	101	CLA	C4B-NB	-2.88	1.34	1.37
11	bB	836	CLA	OBD-CAD	2.88	1.27	1.22
11	cB	833	CLA	C4B-NB	-2.88	1.34	1.37
11	bA	805	CLA	C4B-NB	-2.88	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	cB	835	CLA	C4B-NB	-2.88	1.34	1.37
11	aB	833	CLA	C4B-NB	-2.88	1.34	1.37
11	bB	833	CLA	C4B-NB	-2.88	1.34	1.37
11	aB	816	CLA	C3B-C4B	2.88	1.49	1.42
15	aB	845	BCR	C30-C25	-2.87	1.49	1.53
11	aB	821	CLA	C4B-NB	-2.87	1.34	1.37
11	aB	823	CLA	C4B-NB	-2.87	1.34	1.37
11	aB	809	CLA	OBD-CAD	2.87	1.27	1.22
11	bB	838	CLA	C4B-NB	-2.87	1.34	1.37
11	bB	832	CLA	C3B-C4B	2.87	1.49	1.42
11	aB	805	CLA	OBD-CAD	2.87	1.27	1.22
15	bB	843	BCR	C1-C6	-2.87	1.49	1.53
11	aA	805	CLA	C4B-NB	-2.87	1.34	1.37
11	cA	843	CLA	C3B-C4B	2.87	1.49	1.42
11	bA	804	CLA	C4B-NB	-2.87	1.34	1.37
11	bB	815	CLA	C4B-NB	-2.87	1.34	1.37
11	cB	805	CLA	OBD-CAD	2.86	1.27	1.22
15	aA	850	BCR	C1-C6	-2.86	1.49	1.53
15	aB	843	BCR	C1-C6	-2.86	1.49	1.53
11	cB	832	CLA	C3B-C4B	2.86	1.49	1.42
15	aA	848	BCR	C1-C6	-2.86	1.49	1.53
11	cA	804	CLA	C4B-NB	-2.86	1.34	1.37
11	bB	832	CLA	C4B-NB	-2.86	1.34	1.37
15	aB	846	BCR	C30-C25	-2.86	1.49	1.53
11	bB	835	CLA	C4B-NB	-2.86	1.34	1.37
11	cB	811	CLA	C3B-C4B	2.86	1.49	1.42
11	aK	101	CLA	OBD-CAD	2.86	1.28	1.23
11	bB	809	CLA	OBD-CAD	2.85	1.27	1.22
11	bB	821	CLA	C4B-NB	-2.85	1.34	1.37
11	cA	842	CLA	C4B-NB	-2.85	1.34	1.37
11	bK	101	CLA	OBD-CAD	2.85	1.28	1.23
11	aB	832	CLA	C3B-C4B	2.85	1.49	1.42
11	aB	838	CLA	C4B-NB	-2.85	1.34	1.37
10	cA	801	CL0	C1B-C2B	2.84	1.50	1.43
11	bB	839	CLA	C3B-C4B	2.84	1.49	1.42
11	cA	841	CLA	C3B-C4B	2.84	1.49	1.42
11	cB	823	CLA	C4B-NB	-2.84	1.34	1.37
11	aA	818	CLA	C3B-C4B	2.84	1.49	1.42
11	bA	841	CLA	C3B-C4B	2.84	1.49	1.42
12	aA	826	F6C	C4A-NA	-2.84	1.34	1.37
11	cB	809	CLA	OBD-CAD	2.84	1.27	1.22
11	bA	842	CLA	C4B-NB	-2.84	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bB	822	CLA	C3B-C4B	2.83	1.49	1.42
11	cA	805	CLA	C4B-NB	-2.83	1.34	1.37
15	bA	848	BCR	C1-C6	-2.83	1.49	1.53
11	aB	836	CLA	OBD-CAD	2.83	1.27	1.22
11	bA	818	CLA	C3B-C4B	2.83	1.49	1.42
15	cA	848	BCR	C1-C6	-2.83	1.49	1.53
15	cA	850	BCR	C1-C6	-2.83	1.49	1.53
11	aB	811	CLA	C3B-C4B	2.83	1.49	1.42
11	cA	818	CLA	C3B-C4B	2.83	1.49	1.42
11	bB	834	CLA	C4B-NB	-2.83	1.34	1.37
11	bB	805	CLA	OBD-CAD	2.82	1.27	1.22
15	bA	850	BCR	C1-C6	-2.82	1.49	1.53
11	cK	101	CLA	OBD-CAD	2.82	1.28	1.23
15	cB	844	BCR	C1-C6	-2.82	1.49	1.53
11	aB	834	CLA	C4B-NB	-2.82	1.34	1.37
11	aA	842	CLA	C4B-NB	-2.82	1.34	1.37
11	bB	831	CLA	C3B-C4B	2.81	1.49	1.42
11	aB	830	CLA	C3B-C4B	2.81	1.49	1.42
11	cB	839	CLA	C3B-C4B	2.81	1.49	1.42
11	aA	841	CLA	C3B-C4B	2.81	1.49	1.42
11	aB	839	CLA	C3B-C4B	2.81	1.49	1.42
11	bA	821	CLA	C4B-NB	-2.81	1.34	1.37
11	aA	804	CLA	C4B-NB	-2.80	1.34	1.37
11	cA	821	CLA	C4B-NB	-2.80	1.34	1.37
11	bB	830	CLA	C3B-C4B	2.80	1.49	1.42
11	aB	822	CLA	C3B-C4B	2.80	1.49	1.42
11	cB	821	CLA	C4B-NB	-2.80	1.34	1.37
11	aA	804	CLA	C3B-C4B	2.80	1.49	1.42
11	aA	812	CLA	C3B-C4B	2.80	1.49	1.42
10	bA	801	CL0	C1B-C2B	2.80	1.49	1.43
11	cA	804	CLA	C3B-C4B	2.80	1.49	1.42
11	cB	815	CLA	C3B-C4B	2.80	1.49	1.42
10	aA	801	CL0	C1B-C2B	2.80	1.49	1.43
11	cB	822	CLA	C3B-C4B	2.79	1.49	1.42
11	aB	831	CLA	C3B-C4B	2.79	1.49	1.42
11	aB	834	CLA	C4D-CHA	2.79	1.48	1.38
11	aB	835	CLA	C4B-NB	-2.79	1.34	1.37
12	cA	826	F6C	C4A-NA	-2.79	1.34	1.37
12	aA	826	F6C	C4A-C3A	2.79	1.50	1.45
12	aA	826	F6C	C1A-C2A	2.79	1.51	1.45
11	cB	818	CLA	C4B-NB	-2.79	1.34	1.37
11	cA	840	CLA	C4B-NB	-2.79	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bA	840	CLA	C4B-NB	-2.79	1.34	1.37
11	bB	834	CLA	C4D-CHA	2.79	1.48	1.38
11	aB	818	CLA	C4B-NB	-2.79	1.34	1.37
11	aB	815	CLA	C3B-C4B	2.78	1.49	1.42
11	cB	831	CLA	C3B-C4B	2.78	1.49	1.42
11	aA	821	CLA	C4B-NB	-2.78	1.34	1.37
11	aK	103	CLA	C3B-C4B	2.78	1.49	1.42
15	bB	844	BCR	C1-C6	-2.78	1.49	1.53
11	aB	821	CLA	C4D-CHA	2.77	1.48	1.38
11	cB	834	CLA	C4D-CHA	2.77	1.48	1.38
11	cB	829	CLA	C4D-CHA	2.77	1.48	1.38
12	cA	826	F6C	C1A-C2A	2.77	1.51	1.45
11	bB	818	CLA	C4B-NB	-2.77	1.34	1.37
11	cA	812	CLA	C3B-C4B	2.77	1.49	1.42
11	cB	829	CLA	C1B-C2B	2.77	1.49	1.43
12	bA	826	F6C	C1A-C2A	2.77	1.51	1.45
11	bK	103	CLA	C3B-C4B	2.77	1.49	1.42
11	bA	804	CLA	C3B-C4B	2.77	1.49	1.42
15	aB	844	BCR	C1-C6	-2.77	1.50	1.53
11	cB	834	CLA	C4B-NB	-2.76	1.34	1.37
12	bA	826	F6C	C4A-C3A	2.76	1.50	1.45
11	bB	815	CLA	C3B-C4B	2.76	1.49	1.42
11	cB	830	CLA	C3B-C4B	2.76	1.49	1.42
11	aB	829	CLA	C1B-C2B	2.76	1.49	1.43
11	aB	830	CLA	C4D-CHA	2.76	1.48	1.38
11	cB	815	CLA	C4D-CHA	2.76	1.48	1.38
11	bA	816	CLA	C4B-NB	-2.76	1.34	1.37
11	cK	103	CLA	C3B-C4B	2.76	1.49	1.42
11	bA	805	CLA	C4D-CHA	2.76	1.48	1.38
11	cB	837	CLA	C3B-C4B	2.76	1.49	1.42
11	cB	830	CLA	C4D-CHA	2.76	1.48	1.38
11	bA	812	CLA	C3B-C4B	2.75	1.49	1.42
11	aA	816	CLA	C4B-NB	-2.75	1.34	1.37
11	bB	829	CLA	C1B-C2B	2.75	1.49	1.43
11	aA	805	CLA	C4D-CHA	2.75	1.48	1.38
11	cA	814	CLA	C3B-C4B	2.75	1.49	1.42
15	aA	849	BCR	C1-C6	-2.75	1.50	1.53
15	aL	208	BCR	C30-C25	-2.75	1.50	1.53
11	bB	830	CLA	C4D-CHA	2.75	1.48	1.38
12	bA	827	F6C	C4B-NB	-2.74	1.33	1.37
11	aB	815	CLA	C4D-CHA	2.74	1.48	1.38
11	bB	829	CLA	C4D-CHA	2.74	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bB	815	CLA	C4D-CHA	2.74	1.48	1.38
11	bA	803	CLA	C3B-C4B	2.74	1.49	1.42
12	cA	826	F6C	C4A-C3A	2.74	1.50	1.45
11	aB	829	CLA	C4D-CHA	2.74	1.48	1.38
11	cB	802	CLA	C3B-C4B	2.74	1.49	1.42
11	cB	821	CLA	C4D-CHA	2.73	1.48	1.38
11	aA	814	CLA	C3B-C4B	2.73	1.49	1.42
11	cA	809	CLA	C4D-CHA	2.73	1.48	1.38
11	cA	805	CLA	C4D-CHA	2.73	1.48	1.38
12	bL	202	F6C	C1C-NC	-2.73	1.34	1.37
11	aA	803	CLA	C3B-C4B	2.73	1.49	1.42
11	bB	821	CLA	C4D-CHA	2.73	1.48	1.38
12	aL	202	F6C	C1C-NC	-2.73	1.34	1.37
11	bB	837	CLA	C3B-C4B	2.73	1.49	1.42
12	cA	827	F6C	C4B-NB	-2.72	1.33	1.37
11	cA	816	CLA	C4B-NB	-2.72	1.34	1.37
11	bA	815	CLA	C4D-CHA	2.72	1.48	1.38
11	aB	837	CLA	C3B-C4B	2.72	1.49	1.42
11	aA	817	CLA	C4D-CHA	2.72	1.48	1.38
15	cA	849	BCR	C1-C6	-2.72	1.50	1.53
12	cL	202	F6C	C1C-NC	-2.72	1.34	1.37
12	aL	202	F6C	C4A-C3A	2.72	1.50	1.45
11	bA	837	CLA	C3B-C4B	2.72	1.49	1.42
11	aB	814	CLA	C4D-CHA	2.72	1.48	1.38
12	bA	826	F6C	C4A-NA	-2.72	1.34	1.37
12	aA	827	F6C	C4B-NB	-2.72	1.33	1.37
15	bL	208	BCR	C30-C25	-2.72	1.50	1.53
11	cA	837	CLA	C3B-C4B	2.72	1.49	1.42
11	bA	809	CLA	C4D-CHA	2.72	1.48	1.38
11	cB	814	CLA	C4D-CHA	2.72	1.48	1.38
11	bB	832	CLA	C4D-CHA	2.71	1.48	1.38
11	bA	823	CLA	C4D-CHA	2.71	1.48	1.38
11	bA	814	CLA	C3B-C4B	2.71	1.49	1.42
11	aA	840	CLA	C4B-NB	-2.71	1.34	1.37
11	bA	816	CLA	C4D-CHA	2.71	1.48	1.38
11	aB	832	CLA	C4D-CHA	2.71	1.48	1.38
11	bA	821	CLA	C4D-CHA	2.71	1.48	1.38
11	aB	802	CLA	C3B-C4B	2.71	1.49	1.42
12	bA	826	F6C	CMB-C2B	2.71	1.50	1.45
11	aA	821	CLA	C4D-CHA	2.71	1.48	1.38
11	cA	823	CLA	C4D-CHA	2.71	1.48	1.38
11	bB	813	CLA	C1B-C2B	2.71	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bA	812	CLA	C4D-CHA	2.71	1.48	1.38
11	cB	832	CLA	C4D-CHA	2.70	1.48	1.38
11	cB	831	CLA	C4D-CHA	2.70	1.48	1.38
11	aA	823	CLA	C4D-CHA	2.70	1.48	1.38
12	aA	826	F6C	CMB-C2B	2.70	1.50	1.45
11	cB	804	CLA	C3B-C4B	2.70	1.49	1.42
12	cA	826	F6C	CMB-C2B	2.70	1.50	1.45
11	bA	817	CLA	C4D-CHA	2.70	1.48	1.38
11	bB	831	CLA	C4D-CHA	2.70	1.48	1.38
11	aA	809	CLA	C4D-CHA	2.70	1.48	1.38
11	bB	814	CLA	C4D-CHA	2.70	1.48	1.38
11	aA	837	CLA	C3B-C4B	2.70	1.49	1.42
11	bB	804	CLA	C3B-C4B	2.70	1.49	1.42
11	cB	835	CLA	C3B-C4B	2.70	1.49	1.42
11	aA	815	CLA	C4D-CHA	2.70	1.48	1.38
11	cA	812	CLA	C4D-CHA	2.70	1.48	1.38
11	bB	802	CLA	C3B-C4B	2.70	1.49	1.42
11	bB	823	CLA	C4D-CHA	2.70	1.48	1.38
11	cA	808	CLA	C3B-C4B	2.70	1.49	1.42
11	aB	819	CLA	C3B-C4B	2.70	1.49	1.42
11	cA	839	CLA	C3B-C4B	2.70	1.49	1.42
11	bB	835	CLA	C4D-CHA	2.70	1.48	1.38
11	cA	821	CLA	C4D-CHA	2.70	1.48	1.38
11	aB	823	CLA	C4D-CHA	2.70	1.48	1.38
11	aA	812	CLA	C4D-CHA	2.69	1.48	1.38
11	bB	812	CLA	C4C-C3C	2.69	1.49	1.45
11	cB	819	CLA	C3B-C4B	2.69	1.49	1.42
12	aA	826	F6C	C4B-NB	-2.69	1.33	1.37
11	aB	831	CLA	C4D-CHA	2.69	1.48	1.38
15	bA	849	BCR	C1-C6	-2.69	1.50	1.53
11	aB	804	CLA	C3B-C4B	2.69	1.49	1.42
11	cA	817	CLA	C4D-CHA	2.69	1.48	1.38
12	bA	830	F6C	C4B-NB	-2.69	1.33	1.37
15	bI	101	BCR	C1-C6	-2.69	1.50	1.53
11	cB	811	CLA	C4D-CHA	2.69	1.48	1.38
11	aB	811	CLA	C4D-CHA	2.69	1.48	1.38
11	cB	823	CLA	C4D-CHA	2.69	1.48	1.38
15	aI	101	BCR	C1-C6	-2.69	1.50	1.53
11	cA	815	CLA	C4D-CHA	2.69	1.48	1.38
11	cB	813	CLA	C1B-C2B	2.69	1.49	1.43
11	bB	811	CLA	C4D-CHA	2.69	1.48	1.38
11	bB	812	CLA	C4D-CHA	2.69	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	cB	825	CLA	C4D-CHA	2.69	1.48	1.38
11	bB	835	CLA	C3B-C4B	2.69	1.49	1.42
12	aL	202	F6C	C4B-NB	-2.69	1.33	1.37
11	aB	813	CLA	C1B-C2B	2.69	1.49	1.43
11	cA	803	CLA	C3B-C4B	2.69	1.49	1.42
11	cA	831	CLA	C4D-CHA	2.68	1.47	1.38
11	aB	820	CLA	C4D-CHA	2.68	1.47	1.38
12	bL	202	F6C	C4B-NB	-2.68	1.33	1.37
11	cA	825	CLA	C4D-CHA	2.68	1.47	1.38
11	aB	825	CLA	C3B-C4B	2.68	1.49	1.42
11	aA	807	CLA	C4D-CHA	2.68	1.47	1.38
11	cB	812	CLA	C4D-CHA	2.68	1.47	1.38
11	bA	831	CLA	C4D-CHA	2.68	1.47	1.38
11	bA	841	CLA	C4D-CHA	2.68	1.47	1.38
11	bK	103	CLA	C4D-CHA	2.68	1.47	1.38
11	cK	103	CLA	C4D-CHA	2.68	1.47	1.38
11	aK	103	CLA	C4D-CHA	2.68	1.47	1.38
11	aB	812	CLA	C4C-C3C	2.68	1.49	1.45
12	cA	826	F6C	C4B-NB	-2.68	1.33	1.37
11	aA	839	CLA	C3B-C4B	2.68	1.49	1.42
11	aB	812	CLA	C4D-CHA	2.68	1.47	1.38
11	cB	819	CLA	C4D-CHA	2.68	1.47	1.38
11	aA	825	CLA	C4D-CHA	2.68	1.47	1.38
11	cB	835	CLA	C4D-CHA	2.68	1.47	1.38
15	cI	103	BCR	C1-C6	-2.68	1.50	1.53
11	bL	204	CLA	C4D-CHA	2.68	1.47	1.38
11	aL	205	CLA	C3B-C4B	2.68	1.49	1.42
11	cA	807	CLA	C4D-CHA	2.68	1.47	1.38
11	aA	819	CLA	C4D-CHA	2.68	1.47	1.38
11	aB	835	CLA	C4D-CHA	2.68	1.47	1.38
12	bL	202	F6C	C4A-C3A	2.68	1.50	1.45
11	cA	819	CLA	C4D-CHA	2.68	1.47	1.38
11	cA	825	CLA	C3B-C4B	2.67	1.49	1.42
11	aA	831	CLA	C4D-CHA	2.67	1.47	1.38
15	cL	208	BCR	C30-C25	-2.67	1.50	1.53
11	bA	825	CLA	C4D-CHA	2.67	1.47	1.38
11	cA	841	CLA	C4D-CHA	2.67	1.47	1.38
11	aB	835	CLA	C3B-C4B	2.67	1.49	1.42
11	bB	819	CLA	C3B-C4B	2.67	1.49	1.42
11	bA	807	CLA	C4D-CHA	2.67	1.47	1.38
11	cA	834	CLA	C1B-C2B	2.67	1.49	1.43
11	cA	816	CLA	C4D-CHA	2.67	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aA	816	CLA	C4D-CHA	2.67	1.47	1.38
11	aB	819	CLA	C4D-CHA	2.67	1.47	1.38
11	aA	841	CLA	C4D-CHA	2.67	1.47	1.38
11	bB	820	CLA	C4D-CHA	2.67	1.47	1.38
11	cB	825	CLA	C3B-C4B	2.67	1.49	1.42
11	bA	811	CLA	C4D-CHA	2.67	1.47	1.38
11	bA	811	CLA	C3B-C4B	2.67	1.49	1.42
11	bB	825	CLA	C4D-CHA	2.67	1.47	1.38
11	aA	808	CLA	C3B-C4B	2.67	1.49	1.42
12	cB	824	F6C	C4B-NB	-2.67	1.33	1.37
11	aB	834	CLA	C3B-C4B	2.66	1.49	1.42
11	bA	808	CLA	C3B-C4B	2.66	1.49	1.42
11	cA	824	CLA	C3B-C4B	2.66	1.49	1.42
11	cB	835	CLA	C1B-C2B	2.66	1.49	1.43
11	cA	842	CLA	C4D-CHA	2.66	1.47	1.38
11	bA	825	CLA	C3B-C4B	2.66	1.49	1.42
11	aA	824	CLA	C3B-C4B	2.66	1.49	1.42
11	bA	839	CLA	C3B-C4B	2.66	1.49	1.42
12	aL	202	F6C	CMB-C2B	2.66	1.50	1.45
11	bB	819	CLA	C4D-CHA	2.66	1.47	1.38
11	cL	204	CLA	C4D-CHA	2.66	1.47	1.38
11	aB	803	CLA	C1C-NC	-2.66	1.33	1.37
11	aA	811	CLA	C4D-CHA	2.66	1.47	1.38
11	bA	819	CLA	C4D-CHA	2.66	1.47	1.38
12	cL	202	F6C	C4A-C3A	2.66	1.50	1.45
11	aB	825	CLA	C4D-CHA	2.66	1.47	1.38
11	aL	204	CLA	C4D-CHA	2.66	1.47	1.38
11	cB	803	CLA	C1C-NC	-2.66	1.33	1.37
11	aA	825	CLA	C3B-C4B	2.66	1.49	1.42
11	aA	811	CLA	C3B-C4B	2.66	1.49	1.42
11	aB	829	CLA	C4C-C3C	2.66	1.49	1.45
12	bL	202	F6C	CMB-C2B	2.66	1.50	1.45
11	bA	824	CLA	C3B-C4B	2.66	1.49	1.42
11	bA	828	CLA	C3B-C4B	2.66	1.49	1.42
11	bA	804	CLA	C4D-CHA	2.66	1.47	1.38
11	cA	813	CLA	C4D-CHA	2.66	1.47	1.38
11	cB	820	CLA	C4D-CHA	2.65	1.47	1.38
12	bA	832	F6C	C4B-NB	-2.65	1.33	1.37
11	bL	205	CLA	C3B-C4B	2.65	1.49	1.42
11	aA	804	CLA	C4D-CHA	2.65	1.47	1.38
11	aB	823	CLA	C3B-C4B	2.65	1.49	1.42
11	cA	820	CLA	C4D-CHA	2.65	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aB	816	CLA	C4D-CHA	2.65	1.47	1.38
11	bB	816	CLA	C4D-CHA	2.65	1.47	1.38
11	cA	806	CLA	C4D-CHA	2.65	1.47	1.38
11	aA	828	CLA	C4D-CHA	2.65	1.47	1.38
11	aA	813	CLA	C4D-CHA	2.65	1.47	1.38
11	bA	834	CLA	C1B-C2B	2.65	1.49	1.43
11	bB	825	CLA	C3B-C4B	2.65	1.49	1.42
11	bB	836	CLA	C4D-CHA	2.65	1.47	1.38
11	bB	820	CLA	C3B-C4B	2.65	1.49	1.42
11	cA	804	CLA	C4D-CHA	2.65	1.47	1.38
11	bA	828	CLA	C4D-CHA	2.65	1.47	1.38
11	aA	806	CLA	C4D-CHA	2.64	1.47	1.38
11	bA	820	CLA	C4D-CHA	2.64	1.47	1.38
11	cB	836	CLA	C4D-CHA	2.64	1.47	1.38
11	cB	816	CLA	C4D-CHA	2.64	1.47	1.38
11	cA	811	CLA	C3B-C4B	2.64	1.49	1.42
11	bA	813	CLA	C4D-CHA	2.64	1.47	1.38
12	cA	830	F6C	C4B-NB	-2.64	1.33	1.37
11	aA	813	CLA	C4B-NB	-2.64	1.34	1.37
11	aB	835	CLA	C1B-C2B	2.64	1.49	1.43
12	aA	827	F6C	CMB-C2B	2.64	1.50	1.45
11	cA	811	CLA	C4D-CHA	2.64	1.47	1.38
11	aB	820	CLA	C3B-C4B	2.64	1.48	1.42
12	aB	824	F6C	C4B-NB	-2.64	1.33	1.37
11	aA	820	CLA	C4D-CHA	2.64	1.47	1.38
11	cL	205	CLA	C3B-C4B	2.64	1.48	1.42
11	bA	822	CLA	C4D-CHA	2.64	1.47	1.38
11	aA	842	CLA	C4D-CHA	2.64	1.47	1.38
11	cA	835	CLA	C4D-CHA	2.64	1.47	1.38
11	cA	828	CLA	C3B-C4B	2.64	1.48	1.42
11	cA	822	CLA	C4D-CHA	2.64	1.47	1.38
12	bB	824	F6C	C4B-NB	-2.64	1.33	1.37
11	aB	813	CLA	C4D-CHA	2.64	1.47	1.38
11	aA	828	CLA	C3B-C4B	2.63	1.48	1.42
11	cB	813	CLA	C4D-CHA	2.63	1.47	1.38
12	cL	202	F6C	CMB-C2B	2.63	1.50	1.45
11	cB	812	CLA	C4C-C3C	2.63	1.49	1.45
11	cA	828	CLA	C4D-CHA	2.63	1.47	1.38
15	aM	101	BCR	C1-C6	-2.63	1.50	1.53
11	bB	806	CLA	C4D-CHA	2.63	1.47	1.38
11	bB	813	CLA	C4D-CHA	2.63	1.47	1.38
11	bB	840	CLA	C4D-CHA	2.63	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bM	101	BCR	C1-C6	-2.63	1.50	1.53
12	cA	832	F6C	C4B-NB	-2.63	1.33	1.37
11	bA	806	CLA	C4D-CHA	2.63	1.47	1.38
11	aA	822	CLA	C4D-CHA	2.63	1.47	1.38
11	aB	825	CLA	C1B-C2B	2.63	1.49	1.43
11	bB	834	CLA	C4C-C3C	2.63	1.49	1.45
11	cB	834	CLA	C3B-C4B	2.63	1.48	1.42
11	bA	835	CLA	C4D-CHA	2.63	1.47	1.38
11	cB	840	CLA	C4D-CHA	2.63	1.47	1.38
11	bA	842	CLA	C4D-CHA	2.63	1.47	1.38
11	aA	843	CLA	C4D-CHA	2.63	1.47	1.38
11	bB	823	CLA	C3B-C4B	2.63	1.48	1.42
11	bA	818	CLA	C4D-CHA	2.63	1.47	1.38
11	bB	805	CLA	C4D-CHA	2.62	1.47	1.38
11	cB	820	CLA	C3B-C4B	2.62	1.48	1.42
11	aB	836	CLA	C4D-CHA	2.62	1.47	1.38
11	bA	810	CLA	C4D-CHA	2.62	1.47	1.38
11	cB	823	CLA	C1B-C2B	2.62	1.49	1.43
11	cB	805	CLA	C4D-CHA	2.62	1.47	1.38
11	bB	825	CLA	C1B-C2B	2.62	1.49	1.43
11	cA	813	CLA	C4B-NB	-2.62	1.34	1.37
11	cA	810	CLA	C1B-C2B	2.62	1.49	1.43
11	cA	828	CLA	C1B-C2B	2.62	1.49	1.43
12	aA	832	F6C	C4B-NB	-2.62	1.33	1.37
11	cA	843	CLA	C4D-CHA	2.62	1.47	1.38
12	aA	830	F6C	C4B-NB	-2.62	1.33	1.37
11	bA	828	CLA	C1B-C2B	2.62	1.49	1.43
11	bA	843	CLA	C4D-CHA	2.62	1.47	1.38
11	cL	205	CLA	C4D-CHA	2.62	1.47	1.38
11	aB	804	CLA	C4D-CHA	2.61	1.47	1.38
12	cA	827	F6C	CMB-C2B	2.61	1.50	1.45
11	cB	804	CLA	C4D-CHA	2.61	1.47	1.38
11	aB	837	CLA	C4D-CHA	2.61	1.47	1.38
11	bB	806	CLA	C3B-C4B	2.61	1.48	1.42
12	bA	827	F6C	CMB-C2B	2.61	1.50	1.45
11	cA	810	CLA	C4D-CHA	2.61	1.47	1.38
11	cA	807	CLA	C3B-C4B	2.61	1.48	1.42
11	bB	829	CLA	C4C-C3C	2.61	1.49	1.45
11	aB	840	CLA	C4D-CHA	2.61	1.47	1.38
11	aB	805	CLA	C4D-CHA	2.61	1.47	1.38
11	cB	806	CLA	C4D-CHA	2.61	1.47	1.38
11	aA	834	CLA	C1B-C2B	2.61	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bB	834	CLA	C3B-C4B	2.61	1.48	1.42
11	aA	810	CLA	C4D-CHA	2.61	1.47	1.38
12	cA	827	F6C	C4A-C3A	2.61	1.50	1.45
11	aB	806	CLA	C3B-C4B	2.61	1.48	1.42
11	aA	810	CLA	C1B-C2B	2.61	1.49	1.43
11	aB	822	CLA	C4D-CHA	2.61	1.47	1.38
12	aA	827	F6C	C4A-C3A	2.61	1.50	1.45
11	aB	806	CLA	C4D-CHA	2.61	1.47	1.38
12	bA	826	F6C	C4B-NB	-2.61	1.33	1.37
12	cL	202	F6C	C4B-NB	-2.61	1.33	1.37
11	cB	825	CLA	C1B-C2B	2.61	1.49	1.43
11	bA	813	CLA	C4B-NB	-2.61	1.34	1.37
11	cA	818	CLA	C4D-CHA	2.61	1.47	1.38
11	bB	804	CLA	C4D-CHA	2.61	1.47	1.38
11	aA	835	CLA	C4D-CHA	2.60	1.47	1.38
11	bA	807	CLA	C3B-C4B	2.60	1.48	1.42
11	bB	837	CLA	C4D-CHA	2.60	1.47	1.38
11	bB	823	CLA	C1B-C2B	2.60	1.49	1.43
11	bB	828	CLA	C4D-CHA	2.60	1.47	1.38
11	aA	823	CLA	C3B-C4B	2.60	1.48	1.42
11	aL	205	CLA	C4D-CHA	2.60	1.47	1.38
11	bA	833	CLA	C3B-C4B	2.60	1.48	1.42
11	cA	823	CLA	C3B-C4B	2.60	1.48	1.42
11	bA	823	CLA	C3B-C4B	2.60	1.48	1.42
11	cB	837	CLA	C4D-CHA	2.60	1.47	1.38
11	bL	205	CLA	C4D-CHA	2.60	1.47	1.38
15	cB	845	BCR	C1-C6	-2.60	1.50	1.53
11	cB	810	CLA	C4D-CHA	2.60	1.47	1.38
11	aB	823	CLA	C1B-C2B	2.60	1.49	1.43
11	aA	828	CLA	C1B-C2B	2.60	1.49	1.43
11	bA	836	CLA	C4D-CHA	2.60	1.47	1.38
11	cA	805	CLA	C1C-C2C	2.59	1.49	1.44
11	cB	834	CLA	C4C-C3C	2.59	1.49	1.45
11	bB	822	CLA	C4D-CHA	2.59	1.47	1.38
11	aB	804	CLA	C1B-C2B	2.59	1.49	1.43
11	cB	820	CLA	C1B-C2B	2.59	1.49	1.43
11	aB	828	CLA	C4D-CHA	2.59	1.47	1.38
11	cB	828	CLA	C4D-CHA	2.59	1.47	1.38
11	bB	835	CLA	C1B-C2B	2.59	1.49	1.43
11	aB	810	CLA	C4D-CHA	2.59	1.47	1.38
11	aA	821	CLA	C1B-C2B	2.59	1.49	1.43
11	cB	823	CLA	C3B-C4B	2.59	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bB	803	CLA	C1C-NC	-2.59	1.33	1.37
11	bA	824	CLA	C4D-CHA	2.59	1.47	1.38
11	cB	806	CLA	C3B-C4B	2.59	1.48	1.42
11	aA	829	CLA	C4D-CHA	2.59	1.47	1.38
11	aA	824	CLA	C4D-CHA	2.59	1.47	1.38
11	bA	805	CLA	C1C-C2C	2.59	1.49	1.44
11	bB	821	CLA	C1B-C2B	2.59	1.49	1.43
11	cB	822	CLA	C4D-CHA	2.59	1.47	1.38
11	cA	836	CLA	C4D-CHA	2.58	1.47	1.38
12	bA	844	F6C	C3B-C4B	2.58	1.50	1.44
15	aB	845	BCR	C1-C6	-2.58	1.50	1.53
11	bB	820	CLA	C1B-C2B	2.58	1.49	1.43
12	bA	827	F6C	C4A-C3A	2.58	1.50	1.45
11	aA	833	CLA	C3B-C4B	2.58	1.48	1.42
11	cA	834	CLA	C3B-C4B	2.58	1.48	1.42
11	aA	818	CLA	C4D-CHA	2.58	1.47	1.38
15	bL	207	BCR	C1-C6	-2.58	1.50	1.53
11	bA	829	CLA	C1B-C2B	2.58	1.49	1.43
11	bA	829	CLA	C4D-CHA	2.58	1.47	1.38
11	aA	807	CLA	C3B-C4B	2.58	1.48	1.42
11	aB	826	CLA	C3B-C4B	2.58	1.48	1.42
11	bA	804	CLA	C1B-C2B	2.58	1.49	1.43
11	aA	838	CLA	C4D-CHA	2.58	1.47	1.38
11	cB	829	CLA	C4C-C3C	2.58	1.49	1.45
11	cA	823	CLA	C1B-C2B	2.58	1.49	1.43
15	cM	101	BCR	C1-C6	-2.58	1.50	1.53
11	aA	805	CLA	C1C-C2C	2.58	1.49	1.44
11	bB	810	CLA	C4D-CHA	2.58	1.47	1.38
11	aB	805	CLA	C3B-C4B	2.57	1.48	1.42
11	cB	833	CLA	C4D-CHA	2.57	1.47	1.38
11	aB	808	CLA	C4D-CHA	2.57	1.47	1.38
11	cA	829	CLA	C4D-CHA	2.57	1.47	1.38
11	bA	821	CLA	C1B-C2B	2.57	1.49	1.43
11	bB	805	CLA	C3B-C4B	2.57	1.48	1.42
11	cB	804	CLA	C1B-C2B	2.57	1.49	1.43
12	aA	844	F6C	C3B-C4B	2.57	1.50	1.44
11	bB	804	CLA	C1B-C2B	2.57	1.49	1.43
11	aA	836	CLA	C4D-CHA	2.57	1.47	1.38
11	aB	834	CLA	C4C-C3C	2.57	1.49	1.45
11	bA	838	CLA	C4D-CHA	2.57	1.47	1.38
11	cA	824	CLA	C4D-CHA	2.57	1.47	1.38
11	cA	839	CLA	C4D-CHA	2.57	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aB	839	CLA	C3D-C4D	-2.57	1.38	1.44
11	cB	808	CLA	C4D-CHA	2.57	1.47	1.38
11	aB	833	CLA	C4D-CHA	2.57	1.47	1.38
11	bA	839	CLA	C4D-CHA	2.57	1.47	1.38
11	aA	823	CLA	C1B-C2B	2.57	1.49	1.43
11	aA	804	CLA	C1B-C2B	2.57	1.49	1.43
11	cA	837	CLA	C4D-CHA	2.57	1.47	1.38
11	bB	839	CLA	C3D-C4D	-2.57	1.38	1.44
11	aA	807	CLA	C1B-C2B	2.57	1.49	1.43
11	aA	829	CLA	C1B-C2B	2.57	1.49	1.43
11	bA	807	CLA	C1B-C2B	2.57	1.49	1.43
11	cA	829	CLA	C1B-C2B	2.57	1.49	1.43
11	bB	828	CLA	C4C-C3C	2.57	1.49	1.45
11	aB	821	CLA	C1B-C2B	2.57	1.49	1.43
11	aA	837	CLA	C4D-CHA	2.57	1.47	1.38
11	cA	804	CLA	C1B-C2B	2.57	1.49	1.43
11	aB	804	CLA	C1C-C2C	2.56	1.49	1.44
11	bB	833	CLA	C4D-CHA	2.56	1.47	1.38
11	bB	826	CLA	C3B-C4B	2.56	1.48	1.42
11	bB	808	CLA	C4D-CHA	2.56	1.47	1.38
11	cA	838	CLA	C4D-CHA	2.56	1.47	1.38
15	aA	851	BCR	C30-C25	-2.56	1.50	1.53
11	cA	821	CLA	C1B-C2B	2.56	1.49	1.43
11	aA	840	CLA	C4D-CHA	2.56	1.47	1.38
12	cA	844	F6C	C3B-C4B	2.56	1.50	1.44
11	aA	808	CLA	C4D-CHA	2.56	1.47	1.38
11	bB	826	CLA	C4D-CHA	2.56	1.47	1.38
11	cB	805	CLA	C3B-C4B	2.56	1.48	1.42
11	aA	808	CLA	C1B-C2B	2.56	1.49	1.43
11	aB	826	CLA	C4D-CHA	2.56	1.47	1.38
11	bA	840	CLA	C4D-CHA	2.56	1.47	1.38
11	cB	821	CLA	C1B-C2B	2.56	1.49	1.43
15	bB	845	BCR	C1-C6	-2.56	1.50	1.53
11	cB	826	CLA	C3B-C4B	2.56	1.48	1.42
11	aB	820	CLA	C1B-C2B	2.56	1.49	1.43
11	cA	833	CLA	C3B-C4B	2.56	1.48	1.42
12	bA	830	F6C	C4A-C3A	2.56	1.50	1.45
12	cA	830	F6C	C4A-C3A	2.56	1.50	1.45
11	bB	804	CLA	C1C-C2C	2.56	1.49	1.44
11	aL	206	CLA	C4D-CHA	2.56	1.47	1.38
11	bA	823	CLA	C1B-C2B	2.56	1.49	1.43
11	bA	837	CLA	C4D-CHA	2.55	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aA	833	CLA	C4D-CHA	2.55	1.47	1.38
11	cL	206	CLA	C4D-CHA	2.55	1.47	1.38
15	aL	207	BCR	C1-C6	-2.55	1.50	1.53
11	bA	822	CLA	C3B-C4B	2.55	1.48	1.42
12	cL	202	F6C	C4A-NA	-2.55	1.34	1.37
11	aB	818	CLA	C4D-CHA	2.55	1.47	1.38
11	cA	808	CLA	C4D-CHA	2.55	1.47	1.38
15	cL	207	BCR	C1-C6	-2.55	1.50	1.53
11	cA	835	CLA	C3B-C4B	2.55	1.48	1.42
15	cA	847	BCR	C1-C6	-2.55	1.50	1.53
11	cB	826	CLA	C4D-CHA	2.55	1.47	1.38
11	aA	835	CLA	C3B-C4B	2.55	1.48	1.42
11	bA	810	CLA	C1B-C2B	2.55	1.49	1.43
12	aL	202	F6C	C4A-NA	-2.55	1.34	1.37
15	cA	851	BCR	C30-C25	-2.55	1.50	1.53
12	aA	830	F6C	CMB-C2B	2.55	1.50	1.45
11	aA	822	CLA	C3B-C4B	2.55	1.48	1.42
11	bA	834	CLA	C3B-C4B	2.55	1.48	1.42
11	cA	810	CLA	C3B-C4B	2.55	1.48	1.42
11	bA	834	CLA	C4D-CHA	2.55	1.47	1.38
11	bB	827	CLA	C4D-CHA	2.55	1.47	1.38
11	aA	834	CLA	C4D-CHA	2.55	1.47	1.38
11	aA	839	CLA	C4D-CHA	2.54	1.47	1.38
11	cA	833	CLA	C4D-CHA	2.54	1.47	1.38
11	bA	808	CLA	C1B-C2B	2.54	1.49	1.43
11	cA	807	CLA	C1B-C2B	2.54	1.49	1.43
11	bB	818	CLA	C4D-CHA	2.54	1.47	1.38
11	bL	206	CLA	C4D-CHA	2.54	1.47	1.38
15	bA	851	BCR	C30-C25	-2.54	1.50	1.53
11	bA	810	CLA	C3B-C4B	2.54	1.48	1.42
11	cA	834	CLA	C4D-CHA	2.54	1.47	1.38
11	cB	832	CLA	C1B-C2B	2.54	1.49	1.43
12	aA	830	F6C	C4A-C3A	2.54	1.50	1.45
11	bB	836	CLA	C4C-C3C	2.54	1.49	1.45
11	aA	834	CLA	C3B-C4B	2.54	1.48	1.42
11	cB	839	CLA	C3D-C4D	-2.54	1.38	1.44
11	bA	833	CLA	C4D-CHA	2.54	1.47	1.38
11	cA	808	CLA	C1B-C2B	2.54	1.49	1.43
11	aB	838	CLA	C4D-CHA	2.54	1.47	1.38
11	aB	828	CLA	C3D-C4D	-2.54	1.38	1.44
11	aL	206	CLA	C1B-C2B	2.54	1.49	1.43
15	aA	847	BCR	C1-C6	-2.54	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aK	103	CLA	C1B-C2B	2.54	1.49	1.43
11	cB	828	CLA	C3D-C4D	-2.54	1.38	1.44
11	cB	838	CLA	C4D-CHA	2.54	1.47	1.38
11	bA	835	CLA	C3B-C4B	2.54	1.48	1.42
11	bA	808	CLA	C4D-CHA	2.53	1.47	1.38
15	bA	847	BCR	C1-C6	-2.53	1.50	1.53
11	cA	822	CLA	C3B-C4B	2.53	1.48	1.42
12	aA	844	F6C	CMB-C2B	2.53	1.50	1.45
12	cA	844	F6C	CMB-C2B	2.53	1.50	1.45
11	cA	840	CLA	C4D-CHA	2.53	1.47	1.38
11	bL	206	CLA	C1B-C2B	2.53	1.49	1.43
11	aB	832	CLA	C1B-C2B	2.53	1.49	1.43
11	aL	206	CLA	C3B-C4B	2.53	1.48	1.42
11	aB	827	CLA	C4D-CHA	2.53	1.47	1.38
11	cA	809	CLA	C3B-C4B	2.53	1.48	1.42
11	aB	803	CLA	C4D-CHA	2.53	1.47	1.38
12	aA	826	F6C	C1C-C2C	2.53	1.49	1.43
11	cB	802	CLA	C4D-CHA	2.53	1.47	1.38
11	bB	838	CLA	C4D-CHA	2.53	1.47	1.38
11	cB	818	CLA	C4D-CHA	2.53	1.47	1.38
11	cB	804	CLA	C1C-C2C	2.53	1.49	1.44
12	bA	830	F6C	CMB-C2B	2.53	1.50	1.45
11	cB	836	CLA	C4C-C3C	2.53	1.49	1.45
11	aA	841	CLA	C1B-C2B	2.53	1.49	1.43
11	aA	810	CLA	C3B-C4B	2.53	1.48	1.42
11	bB	803	CLA	C4D-CHA	2.52	1.47	1.38
11	cB	827	CLA	C4D-CHA	2.52	1.47	1.38
11	bB	828	CLA	C3D-C4D	-2.52	1.38	1.44
11	cB	803	CLA	C4D-CHA	2.52	1.47	1.38
11	bB	813	CLA	C3B-C4B	2.52	1.48	1.42
11	bL	204	CLA	C1B-C2B	2.52	1.49	1.43
12	bA	844	F6C	CMB-C2B	2.52	1.50	1.45
11	aB	819	CLA	C1B-C2B	2.52	1.49	1.43
11	aA	803	CLA	C4D-CHA	2.52	1.47	1.38
11	aB	828	CLA	C4C-C3C	2.52	1.49	1.45
11	aB	836	CLA	C4C-C3C	2.52	1.49	1.45
11	cB	817	CLA	C4D-CHA	2.52	1.47	1.38
11	cA	837	CLA	C1B-C2B	2.52	1.49	1.43
11	cB	822	CLA	C1B-C2B	2.52	1.49	1.43
11	cA	820	CLA	C3B-C4B	2.52	1.48	1.42
11	cA	841	CLA	C1B-C2B	2.52	1.49	1.43
11	bB	802	CLA	C4D-CHA	2.52	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bA	803	CLA	C4D-CHA	2.52	1.47	1.38
11	aA	809	CLA	C3B-C4B	2.51	1.48	1.42
11	bB	808	CLA	C3B-C4B	2.51	1.48	1.42
11	bK	103	CLA	C1B-C2B	2.51	1.49	1.43
11	bA	820	CLA	C3B-C4B	2.51	1.48	1.42
11	bA	812	CLA	C1B-C2B	2.51	1.49	1.43
11	cA	803	CLA	C4D-CHA	2.51	1.47	1.38
11	bB	832	CLA	C1B-C2B	2.51	1.49	1.43
11	aB	808	CLA	C3B-C4B	2.51	1.48	1.42
11	aB	802	CLA	C4D-CHA	2.51	1.47	1.38
11	bB	807	CLA	C4D-CHA	2.51	1.47	1.38
11	aA	815	CLA	C3B-C4B	2.51	1.48	1.42
11	bA	812	CLA	C4C-C3C	2.51	1.49	1.45
11	aL	204	CLA	C1B-C2B	2.51	1.49	1.43
11	cL	206	CLA	C1B-C2B	2.51	1.49	1.43
11	bL	206	CLA	C3B-C4B	2.51	1.48	1.42
11	bA	809	CLA	C3B-C4B	2.51	1.48	1.42
11	cB	807	CLA	C4D-CHA	2.51	1.47	1.38
11	cA	802	CLA	C4D-CHA	2.51	1.47	1.38
11	cK	103	CLA	C1B-C2B	2.51	1.49	1.43
15	cL	207	BCR	C30-C25	-2.50	1.50	1.53
11	cA	812	CLA	C4C-C3C	2.50	1.49	1.45
11	cL	204	CLA	C3B-C4B	2.50	1.48	1.42
11	bB	822	CLA	C1B-C2B	2.50	1.49	1.43
11	aB	807	CLA	C4D-CHA	2.50	1.47	1.38
11	aB	817	CLA	C4D-CHA	2.50	1.47	1.38
11	bB	819	CLA	C1B-C2B	2.50	1.49	1.43
11	cB	808	CLA	C3B-C4B	2.50	1.48	1.42
11	bL	204	CLA	C3B-C4B	2.50	1.48	1.42
11	cL	204	CLA	C1B-C2B	2.50	1.49	1.43
11	cB	828	CLA	C4C-C3C	2.50	1.49	1.45
11	bA	837	CLA	C1B-C2B	2.50	1.49	1.43
11	cA	809	CLA	C1B-C2B	2.50	1.49	1.43
11	cB	819	CLA	C1B-C2B	2.50	1.49	1.43
11	cL	206	CLA	C3B-C4B	2.50	1.48	1.42
11	aA	818	CLA	C1B-C2B	2.50	1.49	1.43
11	bA	809	CLA	C1B-C2B	2.50	1.49	1.43
11	cB	813	CLA	C3B-C4B	2.49	1.48	1.42
11	aL	204	CLA	C3B-C4B	2.49	1.48	1.42
11	aA	837	CLA	C1B-C2B	2.49	1.49	1.43
12	cA	826	F6C	C1C-C2C	2.49	1.49	1.43
11	bA	829	CLA	C3B-C4B	2.49	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bK	101	CLA	C1B-C2B	2.49	1.49	1.43
11	aA	820	CLA	C3B-C4B	2.49	1.48	1.42
11	cB	832	CLA	C4C-C3C	2.49	1.49	1.45
12	bA	826	F6C	C1C-C2C	2.49	1.49	1.43
11	aA	809	CLA	C1B-C2B	2.49	1.49	1.43
11	cB	803	CLA	C1B-C2B	2.49	1.49	1.43
10	aA	801	CL0	C4D-CHA	2.49	1.47	1.38
11	aB	839	CLA	C4D-CHA	2.49	1.47	1.38
11	aA	814	CLA	C4D-CHA	2.49	1.47	1.38
11	cA	814	CLA	C4D-CHA	2.49	1.47	1.38
11	bB	817	CLA	C4D-CHA	2.49	1.47	1.38
11	bB	803	CLA	C1B-C2B	2.48	1.49	1.43
11	cB	812	CLA	C1B-C2B	2.48	1.49	1.43
11	bB	811	CLA	C4C-C3C	2.48	1.49	1.45
11	aA	829	CLA	C3B-C4B	2.48	1.48	1.42
11	aK	101	CLA	C1B-C2B	2.48	1.49	1.43
11	aB	814	CLA	C4C-C3C	2.48	1.49	1.45
11	bB	840	CLA	C3B-C4B	2.48	1.48	1.42
12	bL	202	F6C	C4A-NA	-2.48	1.34	1.37
12	cA	830	F6C	CMB-C2B	2.48	1.50	1.45
10	cA	801	CL0	C4D-CHA	2.48	1.47	1.38
11	bB	814	CLA	C4C-C3C	2.48	1.49	1.45
11	bA	814	CLA	C4D-CHA	2.48	1.47	1.38
11	aA	802	CLA	C4D-CHA	2.48	1.47	1.38
11	cA	815	CLA	C3B-C4B	2.48	1.48	1.42
11	bA	841	CLA	C1B-C2B	2.48	1.49	1.43
11	aB	840	CLA	C3B-C4B	2.48	1.48	1.42
11	aB	813	CLA	C3B-C4B	2.48	1.48	1.42
11	aA	812	CLA	C4C-C3C	2.48	1.49	1.45
11	cK	101	CLA	C1B-C2B	2.48	1.49	1.43
11	bA	802	CLA	C4D-CHA	2.48	1.47	1.38
11	aB	822	CLA	C1B-C2B	2.48	1.49	1.43
11	aB	803	CLA	C1B-C2B	2.47	1.49	1.43
10	bA	801	CL0	C4D-CHA	2.47	1.47	1.38
11	bB	839	CLA	C4D-CHA	2.47	1.47	1.38
11	cA	829	CLA	C3B-C4B	2.47	1.48	1.42
11	aB	821	CLA	C4C-C3C	2.47	1.49	1.45
11	bA	818	CLA	C1B-C2B	2.47	1.49	1.43
11	cB	811	CLA	C1B-C2B	2.47	1.49	1.43
11	cB	814	CLA	C4C-C3C	2.47	1.49	1.45
11	bB	812	CLA	C1B-C2B	2.47	1.49	1.43
11	aB	810	CLA	C3B-C4B	2.47	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aB	811	CLA	C1B-C2B	2.47	1.49	1.43
15	aL	207	BCR	C30-C25	-2.47	1.50	1.53
11	cB	839	CLA	C4D-CHA	2.47	1.47	1.38
11	cB	839	CLA	C1C-C2C	2.47	1.49	1.44
15	bL	207	BCR	C30-C25	-2.46	1.50	1.53
11	aB	814	CLA	C1B-C2B	2.46	1.49	1.43
11	cB	807	CLA	C3B-C4B	2.46	1.48	1.42
11	aB	812	CLA	C1B-C2B	2.46	1.49	1.43
11	bB	811	CLA	C1B-C2B	2.46	1.49	1.43
11	bB	807	CLA	C1B-C2B	2.46	1.49	1.43
11	bB	814	CLA	C1B-C2B	2.46	1.49	1.43
11	cB	807	CLA	C1B-C2B	2.46	1.49	1.43
15	aA	849	BCR	C30-C25	-2.46	1.50	1.53
11	cB	827	CLA	C3B-C4B	2.46	1.48	1.42
11	bA	815	CLA	C3B-C4B	2.46	1.48	1.42
11	cB	814	CLA	C1B-C2B	2.46	1.49	1.43
11	bA	819	CLA	C1C-C2C	2.46	1.49	1.44
11	bA	814	CLA	C1B-C2B	2.46	1.49	1.43
11	cA	838	CLA	C3B-C2B	2.45	1.49	1.41
11	aK	103	CLA	C4C-C3C	2.45	1.49	1.45
11	bB	827	CLA	C3B-C4B	2.45	1.48	1.42
11	aA	812	CLA	C1B-C2B	2.45	1.49	1.43
11	cA	818	CLA	C1B-C2B	2.45	1.49	1.43
12	aA	826	F6C	C2B-C1B	2.45	1.49	1.44
11	cB	810	CLA	C3B-C4B	2.45	1.48	1.42
11	bB	810	CLA	C3B-C4B	2.45	1.48	1.42
11	bB	807	CLA	C3B-C4B	2.45	1.48	1.42
11	aA	818	CLA	C1C-C2C	2.45	1.49	1.44
11	bA	815	CLA	C1B-C2B	2.45	1.49	1.43
11	aB	807	CLA	C3B-C4B	2.45	1.48	1.42
12	bA	832	F6C	C4A-C3A	2.45	1.50	1.45
11	aB	827	CLA	C3B-C4B	2.45	1.48	1.42
11	cA	818	CLA	C1C-C2C	2.45	1.49	1.44
11	aB	839	CLA	C1C-C2C	2.45	1.49	1.44
11	aA	838	CLA	C3B-C2B	2.44	1.49	1.41
11	bB	832	CLA	C4C-C3C	2.44	1.49	1.45
11	bB	807	CLA	C3D-C4D	-2.44	1.38	1.44
11	cA	812	CLA	C1B-C2B	2.44	1.49	1.43
11	bA	838	CLA	C3B-C2B	2.44	1.49	1.41
15	cA	849	BCR	C30-C25	-2.44	1.50	1.53
11	bA	818	CLA	C1C-C2C	2.44	1.49	1.44
11	bB	815	CLA	C1C-C2C	2.44	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cA	832	F6C	C4A-C3A	2.44	1.50	1.45
15	bA	849	BCR	C30-C25	-2.44	1.50	1.53
11	aB	838	CLA	C1B-C2B	2.44	1.49	1.43
11	cA	837	CLA	C1C-C2C	2.44	1.49	1.44
11	cA	819	CLA	C1C-C2C	2.44	1.49	1.44
11	cB	840	CLA	C3B-C4B	2.44	1.48	1.42
11	bB	812	CLA	C3B-C4B	2.44	1.48	1.42
11	bB	836	CLA	C3D-C4D	-2.44	1.38	1.44
11	cB	819	CLA	C1C-C2C	2.43	1.49	1.44
11	cA	821	CLA	C4C-C3C	2.43	1.49	1.45
11	bA	824	CLA	C3D-C4D	-2.43	1.38	1.44
11	bB	831	CLA	C1B-C2B	2.43	1.49	1.43
11	bB	821	CLA	C4C-C3C	2.43	1.49	1.45
11	aA	814	CLA	C1B-C2B	2.43	1.49	1.43
11	bB	802	CLA	C1C-C2C	2.43	1.49	1.44
11	aB	801	CLA	C4D-CHA	2.43	1.47	1.38
11	aB	812	CLA	C3B-C4B	2.43	1.48	1.42
11	cB	801	CLA	C4D-CHA	2.43	1.47	1.38
11	aB	831	CLA	C1B-C2B	2.43	1.49	1.43
11	cB	831	CLA	C1B-C2B	2.43	1.49	1.43
15	cB	848	BCR	C1-C6	-2.43	1.50	1.53
15	bB	848	BCR	C1-C6	-2.43	1.50	1.53
11	aB	815	CLA	C1C-C2C	2.43	1.49	1.44
11	aA	838	CLA	C3B-C4B	2.43	1.48	1.42
11	bB	839	CLA	C1C-C2C	2.43	1.49	1.44
11	aA	842	CLA	C1C-C2C	2.43	1.49	1.44
11	cK	103	CLA	C4C-C3C	2.43	1.49	1.45
12	bA	826	F6C	C2B-C1B	2.42	1.49	1.44
11	cA	818	CLA	C3B-C2B	2.42	1.49	1.41
12	cA	827	F6C	C1C-C2C	2.42	1.49	1.43
11	bB	837	CLA	C1B-C2B	2.42	1.49	1.43
11	bA	804	CLA	C1C-C2C	2.42	1.49	1.44
11	cA	838	CLA	C3B-C4B	2.42	1.48	1.42
11	cA	814	CLA	C1B-C2B	2.42	1.49	1.43
12	aA	832	F6C	C4A-C3A	2.42	1.50	1.45
11	cB	815	CLA	C1C-C2C	2.42	1.49	1.44
11	aA	818	CLA	C3B-C2B	2.42	1.49	1.41
11	aA	838	CLA	C3D-C4D	-2.42	1.38	1.44
11	bA	842	CLA	C1C-C2C	2.42	1.49	1.44
11	aA	821	CLA	C4C-C3C	2.42	1.49	1.45
11	cB	821	CLA	C4C-C3C	2.42	1.49	1.45
11	aB	807	CLA	C1B-C2B	2.42	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aB	807	CLA	C3D-C4D	-2.42	1.38	1.44
11	aB	836	CLA	C3D-C4D	-2.42	1.38	1.44
11	cA	835	CLA	C1B-C2B	2.42	1.49	1.43
11	aA	815	CLA	C1B-C2B	2.42	1.49	1.43
11	aB	811	CLA	C4C-C3C	2.42	1.49	1.45
11	cB	833	CLA	C1B-C2B	2.42	1.48	1.43
11	bB	835	CLA	C4C-C3C	2.42	1.49	1.45
15	aB	848	BCR	C1-C6	-2.42	1.50	1.53
11	aL	204	CLA	C3B-C2B	2.41	1.49	1.41
11	aB	832	CLA	C4C-C3C	2.41	1.49	1.45
11	bB	815	CLA	C1B-C2B	2.41	1.48	1.43
11	bB	801	CLA	C4D-CHA	2.41	1.47	1.38
11	bB	809	CLA	C4D-CHA	2.41	1.47	1.38
11	cB	811	CLA	C4C-C3C	2.41	1.49	1.45
11	cB	838	CLA	C1B-C2B	2.41	1.48	1.43
11	cA	804	CLA	C1C-C2C	2.41	1.49	1.44
11	aB	815	CLA	C1B-C2B	2.41	1.48	1.43
11	aA	837	CLA	C1C-C2C	2.41	1.49	1.44
12	aA	827	F6C	C1C-C2C	2.41	1.48	1.43
11	bB	837	CLA	C1C-C2C	2.41	1.49	1.44
15	cA	850	BCR	C30-C25	-2.41	1.50	1.53
11	aB	809	CLA	C4D-CHA	2.41	1.47	1.38
11	bA	821	CLA	C4C-C3C	2.41	1.49	1.45
11	bB	806	CLA	C1B-C2B	2.41	1.48	1.43
12	cA	826	F6C	C2B-C1B	2.41	1.49	1.44
11	aB	833	CLA	C1B-C2B	2.41	1.48	1.43
11	bB	838	CLA	C1B-C2B	2.41	1.48	1.43
11	cB	837	CLA	C1C-C2C	2.41	1.49	1.44
12	cA	830	F6C	C2B-C1B	2.40	1.49	1.44
11	cB	835	CLA	C4C-C3C	2.40	1.49	1.45
11	cB	815	CLA	C1B-C2B	2.40	1.48	1.43
11	cA	815	CLA	C1B-C2B	2.40	1.48	1.43
11	bA	817	CLA	C3B-C4B	2.40	1.48	1.42
11	cB	836	CLA	C3D-C4D	-2.40	1.38	1.44
11	bA	818	CLA	C3B-C2B	2.40	1.49	1.41
11	bB	833	CLA	C1B-C2B	2.40	1.48	1.43
15	bL	203	BCR	C30-C25	-2.40	1.50	1.53
11	aB	837	CLA	C1C-C2C	2.40	1.49	1.44
15	cL	203	BCR	C30-C25	-2.40	1.50	1.53
12	aL	202	F6C	C1C-C2C	2.40	1.48	1.43
11	bB	819	CLA	C1C-C2C	2.40	1.49	1.44
11	bL	204	CLA	C3B-C2B	2.40	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bL	202	F6C	C1C-C2C	2.40	1.48	1.43
11	aB	806	CLA	C1B-C2B	2.40	1.48	1.43
11	cA	824	CLA	C3D-C4D	-2.40	1.38	1.44
11	cB	805	CLA	C1B-C2B	2.40	1.48	1.43
15	cB	843	BCR	C30-C25	-2.40	1.50	1.53
11	aA	804	CLA	C1C-C2C	2.40	1.49	1.44
11	aA	819	CLA	C1C-C2C	2.40	1.49	1.44
11	cB	809	CLA	C4D-CHA	2.40	1.46	1.38
11	bA	838	CLA	C3B-C4B	2.40	1.48	1.42
12	bA	827	F6C	C1C-C2C	2.40	1.48	1.43
11	cL	204	CLA	C3B-C2B	2.40	1.49	1.41
11	cB	807	CLA	C3D-C4D	-2.40	1.38	1.44
11	bK	103	CLA	C4C-C3C	2.40	1.49	1.45
12	bB	824	F6C	CHB-C4A	-2.40	1.33	1.38
11	aB	809	CLA	C3D-C4D	-2.40	1.38	1.44
12	aA	830	F6C	C1C-C2C	2.39	1.48	1.43
11	aA	824	CLA	C3D-C4D	-2.39	1.38	1.44
11	aA	817	CLA	C3B-C4B	2.39	1.48	1.42
11	aA	835	CLA	C1B-C2B	2.39	1.48	1.43
12	cB	824	F6C	CHB-C4A	-2.39	1.33	1.38
11	cA	817	CLA	C3B-C4B	2.39	1.48	1.42
11	bB	809	CLA	C3D-C4D	-2.39	1.38	1.44
12	cL	202	F6C	C1C-C2C	2.39	1.48	1.43
11	cA	831	CLA	C3B-C4B	2.39	1.48	1.42
11	cB	817	CLA	C3B-C4B	2.39	1.48	1.42
11	bB	830	CLA	C4C-C3C	2.39	1.49	1.45
11	bA	835	CLA	C1B-C2B	2.39	1.48	1.43
11	aB	803	CLA	C4C-C3C	2.39	1.49	1.45
11	aA	831	CLA	C3B-C4B	2.39	1.48	1.42
11	aB	819	CLA	C1C-C2C	2.39	1.49	1.44
11	cK	101	CLA	C4C-C3C	2.39	1.49	1.45
11	aB	830	CLA	C4C-C3C	2.39	1.49	1.45
12	aA	844	F6C	C1C-NC	-2.39	1.34	1.37
11	aB	835	CLA	C4C-C3C	2.39	1.49	1.45
11	cB	802	CLA	C1C-C2C	2.39	1.49	1.44
11	cA	838	CLA	C3D-C4D	-2.39	1.38	1.44
12	bA	830	F6C	C1C-C2C	2.38	1.48	1.43
11	cB	823	CLA	C1C-C2C	2.38	1.49	1.44
15	aB	843	BCR	C30-C25	-2.38	1.50	1.53
12	aA	830	F6C	C2B-C1B	2.38	1.49	1.44
11	cB	812	CLA	C3B-C4B	2.38	1.48	1.42
11	cB	803	CLA	C4C-C3C	2.38	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bA	851	BCR	C1-C6	-2.38	1.50	1.53
11	bB	803	CLA	C4C-C3C	2.38	1.49	1.45
11	aB	802	CLA	C1C-C2C	2.38	1.49	1.44
11	bB	823	CLA	C1C-C2C	2.38	1.49	1.44
12	cA	830	F6C	C1A-C2A	2.38	1.50	1.45
11	bA	837	CLA	C1C-C2C	2.38	1.49	1.44
11	bA	803	CLA	C3B-C2B	2.38	1.49	1.41
15	aA	850	BCR	C30-C25	-2.38	1.50	1.53
11	aB	823	CLA	C1C-C2C	2.38	1.49	1.44
11	bA	808	CLA	C1C-C2C	2.38	1.49	1.44
15	aL	203	BCR	C30-C25	-2.37	1.50	1.53
12	cA	844	F6C	CHB-C4A	-2.37	1.33	1.38
11	bA	838	CLA	C3D-C4D	-2.37	1.38	1.44
12	aA	832	F6C	CHB-C4A	-2.37	1.33	1.38
11	cB	806	CLA	C1B-C2B	2.37	1.48	1.43
11	bB	805	CLA	C3D-C4D	-2.37	1.38	1.44
11	cA	803	CLA	C3B-C2B	2.37	1.49	1.41
15	bA	850	BCR	C30-C25	-2.37	1.50	1.53
11	aB	817	CLA	C3B-C4B	2.37	1.48	1.42
15	cA	851	BCR	C1-C6	-2.37	1.50	1.53
15	aA	851	BCR	C1-C6	-2.37	1.50	1.53
11	bA	839	CLA	C1B-C2B	2.37	1.48	1.43
11	aB	837	CLA	C1B-C2B	2.37	1.48	1.43
12	cA	830	F6C	C1C-C2C	2.37	1.48	1.43
11	cA	833	CLA	C3D-C4D	-2.37	1.38	1.44
11	bA	815	CLA	C4C-C3C	2.37	1.49	1.45
11	cB	807	CLA	C4C-C3C	2.37	1.49	1.45
12	aA	830	F6C	C1A-C2A	2.37	1.50	1.45
11	cB	810	CLA	C1B-C2B	2.37	1.48	1.43
11	aA	803	CLA	C3B-C2B	2.37	1.49	1.41
11	cB	809	CLA	C3D-C4D	-2.37	1.38	1.44
11	cB	838	CLA	C4C-C3C	2.37	1.49	1.45
11	cA	837	CLA	C3B-C2B	2.37	1.49	1.41
12	aA	844	F6C	C4B-NB	-2.37	1.34	1.37
11	aB	805	CLA	C1B-C2B	2.36	1.48	1.43
11	aA	810	CLA	C1C-C2C	2.36	1.49	1.44
11	aB	831	CLA	C4C-C3C	2.36	1.49	1.45
11	cA	839	CLA	C4C-C3C	2.36	1.49	1.45
11	aA	841	CLA	C1C-C2C	2.36	1.49	1.44
12	cA	844	F6C	C1C-C2C	2.36	1.48	1.43
11	bB	817	CLA	C3B-C4B	2.36	1.48	1.42
11	cB	830	CLA	C4C-C3C	2.36	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bA	830	F6C	C1A-C2A	2.36	1.50	1.45
11	cA	810	CLA	C1C-C2C	2.36	1.49	1.44
12	bA	830	F6C	C2B-C1B	2.36	1.49	1.44
11	aB	805	CLA	C3D-C4D	-2.36	1.38	1.44
12	cA	844	F6C	C1C-NC	-2.36	1.34	1.37
11	aB	827	CLA	C1B-C2B	2.36	1.48	1.43
11	bA	831	CLA	C3B-C4B	2.36	1.48	1.42
11	aA	833	CLA	C3D-C4D	-2.36	1.38	1.44
12	aB	824	F6C	CHB-C4A	-2.36	1.33	1.38
11	cA	802	CLA	C3D-C4D	-2.36	1.38	1.44
12	bA	826	F6C	CHB-C4A	-2.36	1.33	1.38
11	cA	842	CLA	C1C-C2C	2.35	1.49	1.44
11	bB	827	CLA	C1B-C2B	2.35	1.48	1.43
12	cA	844	F6C	C4B-NB	-2.35	1.34	1.37
11	aA	839	CLA	C4C-C3C	2.35	1.49	1.45
11	aK	101	CLA	C4C-C3C	2.35	1.49	1.45
12	bA	844	F6C	CHB-C4A	-2.35	1.33	1.38
11	cB	840	CLA	C3D-C4D	-2.35	1.38	1.44
11	aA	808	CLA	C1C-C2C	2.35	1.49	1.44
11	cB	837	CLA	C1B-C2B	2.35	1.48	1.43
11	bA	841	CLA	C4C-C3C	2.35	1.49	1.45
11	bB	805	CLA	C1B-C2B	2.35	1.48	1.43
11	cA	831	CLA	C4C-C3C	2.35	1.49	1.45
11	aA	839	CLA	C1B-C2B	2.35	1.48	1.43
11	aA	843	CLA	C1B-C2B	2.35	1.48	1.43
11	cB	827	CLA	C1B-C2B	2.35	1.48	1.43
11	bA	829	CLA	C3B-C2B	2.35	1.49	1.41
11	bA	839	CLA	C4C-C3C	2.35	1.49	1.45
11	cA	839	CLA	C1B-C2B	2.35	1.48	1.43
11	aA	802	CLA	C3D-C4D	-2.35	1.38	1.44
11	cA	820	CLA	C4C-C3C	2.35	1.49	1.45
12	bA	844	F6C	C1C-C2C	2.35	1.48	1.43
11	aA	838	CLA	C1C-C2C	2.35	1.49	1.44
11	cA	838	CLA	C1C-C2C	2.35	1.49	1.44
12	aA	844	F6C	CHB-C4A	-2.35	1.33	1.38
11	aA	820	CLA	C4C-C3C	2.35	1.49	1.45
11	bA	831	CLA	C4C-C3C	2.35	1.49	1.45
11	cA	816	CLA	C4C-C3C	2.35	1.49	1.45
11	aA	837	CLA	C3B-C2B	2.35	1.49	1.41
15	bB	843	BCR	C30-C25	-2.34	1.50	1.53
12	aA	827	F6C	C1C-NC	-2.34	1.34	1.37
11	bK	101	CLA	C4C-C3C	2.34	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	cL	205	CLA	C1B-C2B	2.34	1.48	1.43
11	bA	838	CLA	C1B-C2B	2.34	1.48	1.43
11	bA	829	CLA	C4C-C3C	2.34	1.49	1.45
12	bA	827	F6C	C2B-C1B	2.34	1.49	1.44
12	aA	826	F6C	CHB-C4A	-2.34	1.33	1.38
12	cA	832	F6C	C1A-C2A	2.34	1.50	1.45
11	bL	205	CLA	C1B-C2B	2.34	1.48	1.43
12	bA	832	F6C	CHB-C4A	-2.34	1.33	1.38
11	bB	838	CLA	C4C-C3C	2.34	1.49	1.45
11	cB	831	CLA	C4C-C3C	2.34	1.49	1.45
11	aA	829	CLA	C3B-C2B	2.34	1.49	1.41
11	cB	806	CLA	C3D-C4D	-2.34	1.38	1.44
11	bA	838	CLA	C1C-C2C	2.34	1.49	1.44
11	cA	838	CLA	C1B-C2B	2.34	1.48	1.43
11	cA	822	CLA	C1C-C2C	2.34	1.49	1.44
11	aB	809	CLA	C3B-C4B	2.34	1.48	1.42
11	cA	843	CLA	C1B-C2B	2.34	1.48	1.43
11	aB	807	CLA	C4C-C3C	2.34	1.49	1.45
11	bA	834	CLA	C3D-C4D	-2.34	1.38	1.44
11	bB	806	CLA	C3D-C4D	-2.34	1.38	1.44
11	cA	829	CLA	C4C-C3C	2.34	1.49	1.45
11	aA	838	CLA	C1B-C2B	2.34	1.48	1.43
11	aA	816	CLA	C4C-C3C	2.34	1.49	1.45
11	aA	831	CLA	C4C-C3C	2.34	1.49	1.45
11	bB	807	CLA	C4C-C3C	2.34	1.49	1.45
11	bB	811	CLA	C1C-C2C	2.34	1.49	1.44
11	bB	825	CLA	C3D-C4D	-2.34	1.38	1.44
12	cA	827	F6C	C2B-C1B	2.33	1.49	1.44
11	bA	808	CLA	C4C-C3C	2.33	1.49	1.45
11	bA	820	CLA	C4C-C3C	2.33	1.49	1.45
11	cA	811	CLA	C4C-C3C	2.33	1.49	1.45
11	bA	837	CLA	C3B-C2B	2.33	1.49	1.41
12	aA	832	F6C	C1A-C2A	2.33	1.50	1.45
11	bA	810	CLA	C1C-C2C	2.33	1.49	1.44
11	cA	829	CLA	C3B-C2B	2.33	1.49	1.41
11	aB	810	CLA	C1B-C2B	2.33	1.48	1.43
11	cA	817	CLA	C4C-C3C	2.33	1.49	1.45
11	cA	841	CLA	C1C-C2C	2.33	1.49	1.44
11	bA	806	CLA	C1B-C2B	2.33	1.48	1.43
11	bB	810	CLA	C1B-C2B	2.33	1.48	1.43
11	bA	822	CLA	C1C-C2C	2.33	1.49	1.44
11	cA	808	CLA	C1C-C2C	2.33	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aL	205	CLA	C1B-C2B	2.33	1.48	1.43
12	aA	844	F6C	C1C-C2C	2.33	1.48	1.43
12	bA	844	F6C	C4B-NB	-2.33	1.34	1.37
11	bA	841	CLA	C1C-C2C	2.33	1.49	1.44
11	cA	841	CLA	C4C-C3C	2.33	1.49	1.45
11	cB	825	CLA	C3B-C2B	2.33	1.49	1.41
11	cB	833	CLA	C1C-C2C	2.33	1.49	1.44
10	cA	801	CL0	C3B-C4B	2.33	1.48	1.42
11	cA	808	CLA	C4C-C3C	2.33	1.49	1.45
11	aA	822	CLA	C1C-C2C	2.33	1.49	1.44
11	cA	815	CLA	C4C-C3C	2.33	1.49	1.45
12	cA	832	F6C	CHB-C4A	-2.33	1.33	1.38
10	bA	801	CL0	C3B-C4B	2.32	1.48	1.42
11	aA	841	CLA	C4C-C3C	2.32	1.49	1.45
11	cB	833	CLA	C4C-C3C	2.32	1.49	1.45
11	cA	839	CLA	C3D-C4D	-2.32	1.38	1.44
11	bA	809	CLA	C1C-C2C	2.32	1.49	1.44
11	cB	821	CLA	C1C-C2C	2.32	1.49	1.44
11	aB	826	CLA	C1B-C2B	2.32	1.48	1.43
11	cA	811	CLA	C1B-C2B	2.32	1.48	1.43
11	aA	819	CLA	C3D-C4D	-2.32	1.38	1.44
12	cA	827	F6C	C1C-NC	-2.32	1.34	1.37
11	bB	810	CLA	C3D-C4D	-2.32	1.38	1.44
11	bA	816	CLA	C4C-C3C	2.32	1.49	1.45
11	bA	843	CLA	C3D-C4D	-2.32	1.38	1.44
11	cB	805	CLA	C3D-C4D	-2.32	1.38	1.44
11	aA	815	CLA	C4C-C3C	2.32	1.49	1.45
11	cB	809	CLA	C3B-C4B	2.32	1.48	1.42
11	aA	805	CLA	C1B-C2B	2.32	1.48	1.43
12	aA	844	F6C	C4A-C3A	2.32	1.49	1.45
11	aB	810	CLA	C3D-C4D	-2.32	1.38	1.44
11	bA	817	CLA	C4C-C3C	2.32	1.49	1.45
11	aA	825	CLA	C4C-C3C	2.32	1.49	1.45
11	bA	810	CLA	C4C-C3C	2.32	1.49	1.45
11	bA	843	CLA	C1B-C2B	2.32	1.48	1.43
15	aI	101	BCR	C30-C25	-2.32	1.50	1.53
12	aA	826	F6C	C1C-NC	-2.32	1.34	1.37
11	aB	840	CLA	C3D-C4D	-2.32	1.38	1.44
12	bA	832	F6C	C1A-C2A	2.32	1.50	1.45
11	cA	819	CLA	C3D-C4D	-2.32	1.38	1.44
12	cA	844	F6C	C4A-C3A	2.31	1.49	1.45
11	bB	833	CLA	C4C-C3C	2.31	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aA	822	CLA	C1B-C2B	2.31	1.48	1.43
11	aA	811	CLA	C1B-C2B	2.31	1.48	1.43
11	bB	825	CLA	C3B-C2B	2.31	1.49	1.41
11	bA	811	CLA	C4C-C3C	2.31	1.49	1.45
11	aA	834	CLA	C3D-C4D	-2.31	1.39	1.44
11	bB	837	CLA	C3D-C4D	-2.31	1.39	1.44
11	cA	843	CLA	C3D-C4D	-2.31	1.39	1.44
11	aB	825	CLA	C3B-C2B	2.31	1.49	1.41
11	bA	813	CLA	C4C-C3C	2.31	1.49	1.45
11	bA	802	CLA	C3D-C4D	-2.31	1.39	1.44
11	aA	810	CLA	C4C-C3C	2.31	1.49	1.45
11	bA	802	CLA	C4C-C3C	2.31	1.49	1.45
11	bA	814	CLA	C3D-C4D	-2.31	1.39	1.44
11	cA	840	CLA	C1B-C2B	2.31	1.48	1.43
11	bA	802	CLA	C1B-C2B	2.31	1.48	1.43
11	bB	840	CLA	C3D-C4D	-2.31	1.39	1.44
11	cA	814	CLA	C3D-C4D	-2.31	1.39	1.44
11	cA	833	CLA	C3B-C2B	2.31	1.49	1.41
11	cA	806	CLA	C1B-C2B	2.31	1.48	1.43
11	aB	801	CLA	C3B-C4B	2.31	1.48	1.42
15	bL	203	BCR	C33-C5	-2.31	1.47	1.50
11	aB	821	CLA	C1C-C2C	2.31	1.49	1.44
11	cB	836	CLA	C1C-C2C	2.31	1.49	1.44
11	aB	805	CLA	C4C-C3C	2.31	1.49	1.45
11	aA	811	CLA	C4C-C3C	2.31	1.49	1.45
12	cA	826	F6C	CHB-C4A	-2.30	1.33	1.38
11	aB	806	CLA	C3D-C4D	-2.30	1.39	1.44
11	cA	814	CLA	C4C-C3C	2.30	1.49	1.45
11	bA	840	CLA	C1B-C2B	2.30	1.48	1.43
11	aB	816	CLA	C4C-C3C	2.30	1.49	1.45
11	bB	821	CLA	C1C-C2C	2.30	1.49	1.44
12	cB	824	F6C	C4C-C3C	2.30	1.49	1.44
11	cA	833	CLA	C1B-C2B	2.30	1.48	1.43
11	aA	833	CLA	C3B-C2B	2.30	1.49	1.41
11	cB	808	CLA	C1B-C2B	2.30	1.48	1.43
11	cA	828	CLA	C3D-C4D	-2.30	1.39	1.44
12	cA	827	F6C	CHB-C4A	-2.30	1.33	1.38
11	bA	828	CLA	C3D-C4D	-2.30	1.39	1.44
11	bB	826	CLA	C1B-C2B	2.30	1.48	1.43
11	cA	802	CLA	C1B-C2B	2.30	1.48	1.43
11	bB	804	CLA	C3B-C2B	2.30	1.49	1.41
11	bA	810	CLA	C3D-C4D	-2.30	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bB	801	CLA	C3B-C4B	2.30	1.48	1.42
11	bB	831	CLA	C4C-C3C	2.30	1.49	1.45
11	cB	826	CLA	C1B-C2B	2.30	1.48	1.43
11	bB	809	CLA	C3B-C4B	2.30	1.48	1.42
11	cA	813	CLA	C4C-C3C	2.30	1.49	1.45
11	cA	825	CLA	C4C-C3C	2.30	1.49	1.45
11	aA	840	CLA	C3D-C4D	-2.30	1.39	1.44
11	bA	811	CLA	C1B-C2B	2.30	1.48	1.43
11	bA	822	CLA	C1B-C2B	2.30	1.48	1.43
11	aA	809	CLA	C1C-C2C	2.30	1.49	1.44
11	aA	814	CLA	C3D-C4D	-2.30	1.39	1.44
11	cB	828	CLA	C3B-C4B	2.30	1.48	1.42
11	aA	808	CLA	C4C-C3C	2.30	1.49	1.45
11	aA	811	CLA	C1C-C2C	2.30	1.49	1.44
11	bA	814	CLA	C4C-C3C	2.30	1.49	1.45
11	cA	809	CLA	C1C-C2C	2.30	1.49	1.44
11	aA	839	CLA	C3D-C4D	-2.30	1.39	1.44
11	cA	813	CLA	C1C-C2C	2.30	1.49	1.44
11	aB	838	CLA	C4C-C3C	2.30	1.49	1.45
11	cB	825	CLA	C3D-C4D	-2.30	1.39	1.44
11	cA	834	CLA	C3D-C4D	-2.30	1.39	1.44
11	aA	828	CLA	C1C-NC	-2.30	1.34	1.37
11	aB	811	CLA	C1C-C2C	2.30	1.49	1.44
11	cB	801	CLA	C3B-C4B	2.30	1.48	1.42
11	bA	833	CLA	C3B-C2B	2.30	1.49	1.41
11	bB	838	CLA	C3D-C4D	-2.30	1.39	1.44
11	aK	101	CLA	C1C-C2C	2.30	1.49	1.44
11	bA	840	CLA	C3D-C4D	-2.30	1.39	1.44
11	cA	840	CLA	C3D-C4D	-2.30	1.39	1.44
11	aB	833	CLA	C1C-C2C	2.29	1.49	1.44
11	bB	803	CLA	C3B-C4B	2.29	1.48	1.42
11	bA	815	CLA	C3B-C2B	2.29	1.49	1.41
11	bA	833	CLA	C3D-C4D	-2.29	1.39	1.44
11	bA	821	CLA	C1C-C2C	2.29	1.49	1.44
11	bA	805	CLA	C1B-C2B	2.29	1.48	1.43
11	aB	828	CLA	C3B-C4B	2.29	1.48	1.42
11	aB	812	CLA	C3D-C4D	-2.29	1.39	1.44
11	bA	839	CLA	C3D-C4D	-2.29	1.39	1.44
11	cA	828	CLA	C3B-C2B	2.29	1.49	1.41
11	cA	806	CLA	C3D-C4D	-2.29	1.39	1.44
12	cA	844	F6C	C1A-C2A	2.29	1.50	1.45
12	bA	844	F6C	C4A-C3A	2.29	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aA	806	CLA	C4C-C3C	2.29	1.49	1.45
11	bA	825	CLA	C4C-C3C	2.29	1.49	1.45
12	aA	844	F6C	C1A-C2A	2.29	1.50	1.45
11	cB	812	CLA	C3D-C4D	-2.29	1.39	1.44
12	bA	844	F6C	C1C-NC	-2.29	1.35	1.37
11	aA	842	CLA	C1B-C2B	2.29	1.48	1.43
11	aB	825	CLA	C3D-C4D	-2.29	1.39	1.44
10	aA	801	CL0	C3B-C2B	2.29	1.48	1.41
11	aA	806	CLA	C1B-C2B	2.29	1.48	1.43
11	aA	816	CLA	C1B-C2B	2.29	1.48	1.43
11	aA	828	CLA	C3D-C4D	-2.29	1.39	1.44
11	bB	812	CLA	C3D-C4D	-2.29	1.39	1.44
11	cA	810	CLA	C4C-C3C	2.29	1.49	1.45
12	aB	824	F6C	C4C-C3C	2.29	1.49	1.44
11	aB	826	CLA	C1C-C2C	2.28	1.49	1.44
11	cB	811	CLA	C1C-C2C	2.28	1.49	1.44
11	aA	829	CLA	C4C-C3C	2.28	1.49	1.45
11	aA	828	CLA	C3B-C2B	2.28	1.48	1.41
11	cA	828	CLA	C1C-NC	-2.28	1.34	1.37
10	cA	801	CL0	C3D-C4D	-2.28	1.39	1.44
11	aA	802	CLA	C1B-C2B	2.28	1.48	1.43
12	bB	824	F6C	C1D-C2D	2.28	1.49	1.44
11	cA	815	CLA	C3B-C2B	2.28	1.48	1.41
11	aA	814	CLA	C4C-C3C	2.28	1.49	1.45
11	cB	802	CLA	C3B-C2B	2.28	1.48	1.41
11	cB	825	CLA	C4C-C3C	2.28	1.49	1.45
12	aA	827	F6C	C2B-C1B	2.28	1.49	1.44
10	cA	801	CL0	C3B-C2B	2.28	1.48	1.41
12	bA	832	F6C	CMB-C2B	2.28	1.50	1.45
11	bB	828	CLA	C3B-C4B	2.28	1.48	1.42
11	cB	810	CLA	C3D-C4D	-2.28	1.39	1.44
11	aA	817	CLA	C4C-C3C	2.28	1.49	1.45
11	aA	833	CLA	C1B-C2B	2.28	1.48	1.43
11	aA	813	CLA	C4C-C3C	2.28	1.49	1.45
11	cK	101	CLA	C1C-C2C	2.28	1.49	1.44
11	cA	835	CLA	C3D-C4D	-2.28	1.39	1.44
11	cB	837	CLA	C3D-C4D	-2.28	1.39	1.44
11	cB	836	CLA	C1B-C2B	2.28	1.48	1.43
10	aA	801	CL0	C3B-C4B	2.28	1.48	1.42
11	aA	840	CLA	C1B-C2B	2.28	1.48	1.43
11	cB	804	CLA	C3B-C2B	2.28	1.48	1.41
11	aB	836	CLA	C1B-C2B	2.28	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aA	825	CLA	C1B-C2B	2.28	1.48	1.43
11	aL	206	CLA	C3D-C4D	-2.28	1.39	1.44
11	bA	813	CLA	C1C-C2C	2.28	1.49	1.44
11	cA	805	CLA	C1B-C2B	2.28	1.48	1.43
11	aA	843	CLA	C3D-C4D	-2.28	1.39	1.44
11	cB	828	CLA	C3B-C2B	2.28	1.48	1.41
11	bB	808	CLA	C1B-C2B	2.28	1.48	1.43
10	bA	801	CL0	C1C-C2C	2.28	1.49	1.44
11	aA	806	CLA	C3D-C4D	-2.28	1.39	1.44
11	cA	825	CLA	C1B-C2B	2.28	1.48	1.43
11	aB	837	CLA	C3D-C4D	-2.28	1.39	1.44
11	bL	206	CLA	C3D-C4D	-2.28	1.39	1.44
11	aB	833	CLA	C4C-C3C	2.28	1.49	1.45
12	bA	827	F6C	C1C-NC	-2.28	1.35	1.37
11	bB	826	CLA	C1C-C2C	2.27	1.49	1.44
11	bB	833	CLA	C1C-C2C	2.27	1.49	1.44
11	bB	828	CLA	C3B-C2B	2.27	1.48	1.41
12	bB	824	F6C	C4C-C3C	2.27	1.49	1.44
12	cA	826	F6C	C1C-NC	-2.27	1.35	1.37
11	bB	825	CLA	C4C-C3C	2.27	1.49	1.45
12	cL	202	F6C	C2B-C1B	2.27	1.49	1.44
10	bA	801	CL0	C3B-C2B	2.27	1.48	1.41
11	bL	205	CLA	C1C-C2C	2.27	1.49	1.44
12	cA	832	F6C	CMB-C2B	2.27	1.50	1.45
11	bB	802	CLA	C1B-C2B	2.27	1.48	1.43
11	bA	819	CLA	C3D-C4D	-2.27	1.39	1.44
11	bB	805	CLA	C4C-C3C	2.27	1.49	1.45
11	cB	805	CLA	C4C-C3C	2.27	1.49	1.45
11	cA	822	CLA	C1B-C2B	2.27	1.48	1.43
11	bB	802	CLA	C3B-C2B	2.27	1.48	1.41
12	aA	832	F6C	CMB-C2B	2.27	1.50	1.45
11	aA	815	CLA	C3B-C2B	2.27	1.48	1.41
15	cB	844	BCR	C30-C25	-2.27	1.50	1.53
11	aB	802	CLA	C3B-C2B	2.27	1.48	1.41
11	bB	805	CLA	C3B-C2B	2.27	1.48	1.41
11	cB	817	CLA	C3D-C4D	-2.27	1.39	1.44
11	bA	835	CLA	C3D-C4D	-2.27	1.39	1.44
11	cB	816	CLA	C4C-C3C	2.27	1.48	1.45
11	cA	816	CLA	C1B-C2B	2.27	1.48	1.43
15	aB	844	BCR	C30-C25	-2.27	1.50	1.53
15	aL	203	BCR	C33-C5	-2.27	1.47	1.50
11	bA	842	CLA	C1B-C2B	2.27	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bB	836	CLA	C1C-C2C	2.27	1.49	1.44
15	bB	844	BCR	C30-C25	-2.27	1.50	1.53
11	cA	802	CLA	C4C-C3C	2.27	1.48	1.45
11	bA	828	CLA	C1C-NC	-2.27	1.34	1.37
11	cB	802	CLA	C1B-C2B	2.27	1.48	1.43
12	bA	832	F6C	C1C-C2C	2.27	1.48	1.43
10	aA	801	CL0	C3D-C4D	-2.27	1.39	1.44
11	aB	803	CLA	C3B-C4B	2.27	1.48	1.42
12	aA	832	F6C	C1C-C2C	2.27	1.48	1.43
12	bL	202	F6C	C4C-C3C	2.27	1.49	1.44
12	bA	844	F6C	C1A-C2A	2.27	1.50	1.45
11	aB	817	CLA	C3D-C4D	-2.27	1.39	1.44
11	bA	816	CLA	C1B-C2B	2.26	1.48	1.43
15	cI	103	BCR	C30-C25	-2.26	1.50	1.53
11	bB	829	CLA	C3B-C4B	2.26	1.48	1.42
11	aA	802	CLA	C4C-C3C	2.26	1.48	1.45
11	cA	811	CLA	C1C-C2C	2.26	1.48	1.44
11	cB	831	CLA	C1C-C2C	2.26	1.48	1.44
11	cB	838	CLA	C3D-C4D	-2.26	1.39	1.44
12	cB	824	F6C	C4A-C3A	2.26	1.49	1.45
11	bA	833	CLA	C1B-C2B	2.26	1.48	1.43
11	bA	806	CLA	C3D-C4D	-2.26	1.39	1.44
11	bB	836	CLA	C1B-C2B	2.26	1.48	1.43
11	cB	803	CLA	C3B-C4B	2.26	1.48	1.42
11	cB	827	CLA	C1C-C2C	2.26	1.48	1.44
11	cL	206	CLA	C1C-C2C	2.26	1.48	1.44
11	aB	802	CLA	C1B-C2B	2.26	1.48	1.43
12	bA	826	F6C	C1C-NC	-2.26	1.35	1.37
11	aB	804	CLA	C3B-C2B	2.26	1.48	1.41
11	aB	836	CLA	C1C-C2C	2.26	1.48	1.44
11	cA	842	CLA	C1B-C2B	2.26	1.48	1.43
15	bI	101	BCR	C30-C25	-2.26	1.50	1.53
11	aB	828	CLA	C3B-C2B	2.26	1.48	1.41
11	aA	840	CLA	C4C-C3C	2.26	1.48	1.45
11	aA	831	CLA	C3B-C2B	2.26	1.48	1.41
11	aA	821	CLA	C1C-C2C	2.26	1.48	1.44
11	cA	816	CLA	C1C-C2C	2.26	1.48	1.44
11	aB	829	CLA	C3B-C4B	2.26	1.48	1.42
11	bA	825	CLA	C1B-C2B	2.26	1.48	1.43
12	bB	824	F6C	C4A-C3A	2.26	1.49	1.45
11	bA	805	CLA	C3B-C2B	2.26	1.48	1.41
11	bA	843	CLA	C4C-C3C	2.26	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bB	810	CLA	C4C-C3C	2.26	1.48	1.45
11	cB	805	CLA	C3B-C2B	2.26	1.48	1.41
11	aB	838	CLA	C3D-C4D	-2.26	1.39	1.44
15	cL	203	BCR	C33-C5	-2.26	1.47	1.50
11	aA	813	CLA	C1C-C2C	2.25	1.48	1.44
11	cB	809	CLA	C1B-C2B	2.25	1.48	1.43
10	aA	801	CL0	C1C-C2C	2.25	1.48	1.44
11	cB	826	CLA	C1C-C2C	2.25	1.48	1.44
11	cB	806	CLA	C1C-C2C	2.25	1.48	1.44
11	cB	838	CLA	C1C-C2C	2.25	1.48	1.44
11	bA	806	CLA	C4C-C3C	2.25	1.48	1.45
11	bB	816	CLA	C4C-C3C	2.25	1.48	1.45
11	bA	828	CLA	C3B-C2B	2.25	1.48	1.41
11	cA	805	CLA	C3B-C2B	2.25	1.48	1.41
11	bA	804	CLA	C4C-C3C	2.25	1.48	1.45
11	aB	834	CLA	C1B-C2B	2.25	1.48	1.43
11	cB	829	CLA	C3B-C4B	2.25	1.48	1.42
11	aA	807	CLA	C3D-C4D	-2.25	1.39	1.44
10	cA	801	CL0	C1C-C2C	2.25	1.48	1.44
11	cL	206	CLA	C3D-C4D	-2.25	1.39	1.44
11	cA	817	CLA	C3B-C2B	2.25	1.48	1.41
12	cA	832	F6C	C1C-C2C	2.25	1.48	1.43
11	aA	809	CLA	C3B-C2B	2.25	1.48	1.41
12	aB	824	F6C	C1D-C2D	2.25	1.48	1.44
11	aB	810	CLA	C4C-C3C	2.25	1.48	1.45
11	aB	827	CLA	C1C-C2C	2.25	1.48	1.44
10	bA	801	CL0	C3D-C4D	-2.24	1.39	1.44
11	aA	843	CLA	C4C-C3C	2.24	1.48	1.45
11	cA	821	CLA	C1C-C2C	2.24	1.48	1.44
11	bB	827	CLA	C1C-C2C	2.24	1.48	1.44
11	cA	807	CLA	C3D-C4D	-2.24	1.39	1.44
11	cB	812	CLA	C3B-C2B	2.24	1.48	1.41
11	aB	805	CLA	C3B-C2B	2.24	1.48	1.41
11	aB	817	CLA	C1B-C2B	2.24	1.48	1.43
11	bA	809	CLA	C3B-C2B	2.24	1.48	1.41
12	aL	202	F6C	C2B-C1B	2.24	1.49	1.44
11	cA	843	CLA	C4C-C3C	2.24	1.48	1.45
11	cA	810	CLA	C3D-C4D	-2.24	1.39	1.44
11	bA	817	CLA	C3B-C2B	2.24	1.48	1.41
11	aB	802	CLA	C3D-C4D	-2.24	1.39	1.44
11	aA	817	CLA	C3B-C2B	2.24	1.48	1.41
11	aL	205	CLA	C3D-C4D	-2.24	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bB	831	CLA	C3D-C4D	-2.24	1.39	1.44
11	cL	205	CLA	C1C-C2C	2.24	1.48	1.44
11	bA	840	CLA	C4C-C3C	2.24	1.48	1.45
12	bA	827	F6C	CHB-C4A	-2.24	1.34	1.38
11	cA	831	CLA	C3B-C2B	2.24	1.48	1.41
11	aA	810	CLA	C3D-C4D	-2.24	1.39	1.44
11	aB	808	CLA	C1B-C2B	2.24	1.48	1.43
11	aL	205	CLA	C4C-C3C	2.24	1.48	1.45
15	aK	102	BCR	C30-C25	-2.24	1.50	1.53
11	cA	809	CLA	C3B-C2B	2.24	1.48	1.41
11	bB	813	CLA	C3D-C4D	-2.24	1.39	1.44
11	bA	822	CLA	C4C-C3C	2.24	1.48	1.45
12	bL	202	F6C	CHB-C4A	-2.24	1.34	1.38
11	aB	825	CLA	C4C-C3C	2.24	1.48	1.45
11	aB	813	CLA	C3B-C2B	2.24	1.48	1.41
11	cB	813	CLA	C3D-C4D	-2.24	1.39	1.44
11	cA	806	CLA	C4C-C3C	2.23	1.48	1.45
11	bA	831	CLA	C3B-C2B	2.23	1.48	1.41
11	bB	806	CLA	C1C-C2C	2.23	1.48	1.44
11	bK	101	CLA	C1C-C2C	2.23	1.48	1.44
11	cB	816	CLA	C1C-C2C	2.23	1.48	1.44
11	bB	813	CLA	C3B-C2B	2.23	1.48	1.41
11	bL	205	CLA	C3D-C4D	-2.23	1.39	1.44
11	cB	840	CLA	C1B-C2B	2.23	1.48	1.43
11	bB	820	CLA	C1C-C2C	2.23	1.48	1.44
11	cA	824	CLA	C1B-C2B	2.23	1.48	1.43
11	bA	811	CLA	C1C-C2C	2.23	1.48	1.44
11	aA	816	CLA	C1C-C2C	2.23	1.48	1.44
11	cA	840	CLA	C1C-C2C	2.23	1.48	1.44
12	aB	824	F6C	C4A-C3A	2.23	1.49	1.45
11	bB	834	CLA	C1B-C2B	2.23	1.48	1.43
15	cK	102	BCR	C30-C25	-2.23	1.50	1.53
11	aB	825	CLA	C1C-C2C	2.23	1.48	1.44
11	bA	816	CLA	C1C-C2C	2.23	1.48	1.44
11	cB	818	CLA	C4C-C3C	2.23	1.48	1.45
11	aA	804	CLA	C4C-C3C	2.23	1.48	1.45
11	bB	838	CLA	C1C-C2C	2.23	1.48	1.44
11	aA	835	CLA	C3D-C4D	-2.23	1.39	1.44
11	bB	832	CLA	C1C-C2C	2.23	1.48	1.44
11	cB	820	CLA	C1C-C2C	2.23	1.48	1.44
11	cA	820	CLA	C1B-C2B	2.23	1.48	1.43
11	aA	824	CLA	C1B-C2B	2.22	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aA	829	CLA	C1C-C2C	2.22	1.48	1.44
11	aL	204	CLA	C1C-C2C	2.22	1.48	1.44
12	cB	824	F6C	C1D-C2D	2.22	1.48	1.44
11	aB	816	CLA	C1C-C2C	2.22	1.48	1.44
11	bB	812	CLA	C3B-C2B	2.22	1.48	1.41
11	aB	813	CLA	C3D-C4D	-2.22	1.39	1.44
11	bB	817	CLA	C3D-C4D	-2.22	1.39	1.44
11	cA	804	CLA	C4C-C3C	2.22	1.48	1.45
11	cB	810	CLA	C4C-C3C	2.22	1.48	1.45
11	aB	809	CLA	C1B-C2B	2.22	1.48	1.43
12	bA	844	F6C	C4C-C3C	2.22	1.49	1.44
11	aB	812	CLA	C3B-C2B	2.22	1.48	1.41
11	cA	829	CLA	C1C-C2C	2.22	1.48	1.44
11	cB	817	CLA	C1B-C2B	2.22	1.48	1.43
11	aA	843	CLA	C1C-C2C	2.22	1.48	1.44
11	aB	806	CLA	C1C-C2C	2.22	1.48	1.44
11	bB	818	CLA	C4C-C3C	2.22	1.48	1.45
12	bL	202	F6C	C2B-C1B	2.22	1.49	1.44
11	aB	830	CLA	C1B-C2B	2.22	1.48	1.43
11	cL	205	CLA	C4C-C3C	2.22	1.48	1.45
11	cA	840	CLA	C4C-C3C	2.22	1.48	1.45
12	aB	824	F6C	C1C-NC	-2.22	1.35	1.37
11	cB	830	CLA	C1C-C2C	2.22	1.48	1.44
11	cL	204	CLA	C1C-C2C	2.22	1.48	1.44
11	aB	831	CLA	C3D-C4D	-2.22	1.39	1.44
11	bA	807	CLA	C3D-C4D	-2.22	1.39	1.44
12	aA	832	F6C	C4C-C3C	2.22	1.49	1.44
11	bA	804	CLA	C3B-C2B	2.22	1.48	1.41
11	bA	820	CLA	C1B-C2B	2.22	1.48	1.43
11	cB	831	CLA	C3D-C4D	-2.22	1.39	1.44
11	aL	205	CLA	C1C-C2C	2.22	1.48	1.44
11	cB	832	CLA	C1C-C2C	2.22	1.48	1.44
12	aA	827	F6C	CHB-C4A	-2.22	1.34	1.38
12	aA	844	F6C	C4C-C3C	2.22	1.49	1.44
11	cB	813	CLA	C3B-C2B	2.22	1.48	1.41
11	cA	833	CLA	C4C-C3C	2.22	1.48	1.45
11	cB	835	CLA	C1C-C2C	2.22	1.48	1.44
11	bA	824	CLA	C1B-C2B	2.22	1.48	1.43
11	cB	830	CLA	C1B-C2B	2.22	1.48	1.43
11	aA	809	CLA	C4C-C3C	2.21	1.48	1.45
12	bB	824	F6C	C1C-NC	-2.21	1.35	1.37
12	bA	832	F6C	C4C-C3C	2.21	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cA	832	F6C	C1C-NC	-2.21	1.35	1.37
12	cA	844	F6C	C4C-C3C	2.21	1.49	1.44
11	cA	836	CLA	C1B-C2B	2.21	1.48	1.43
11	aB	837	CLA	C4C-C3C	2.21	1.48	1.45
11	bB	835	CLA	C1C-C2C	2.21	1.48	1.44
12	bA	844	F6C	C1D-C2D	2.21	1.48	1.44
11	aA	805	CLA	C3B-C2B	2.21	1.48	1.41
11	bB	821	CLA	C3B-C2B	2.21	1.48	1.41
11	cA	810	CLA	C3B-C2B	2.21	1.48	1.41
11	bL	205	CLA	C4C-C3C	2.21	1.48	1.45
12	cL	202	F6C	C4C-C3C	2.21	1.49	1.44
11	aA	840	CLA	C1C-C2C	2.21	1.48	1.44
11	aA	837	CLA	C4C-C3C	2.21	1.48	1.45
11	bB	840	CLA	C1B-C2B	2.21	1.48	1.43
11	bB	822	CLA	C3D-C4D	-2.21	1.39	1.44
11	bA	810	CLA	C3B-C2B	2.21	1.48	1.41
11	cA	842	CLA	C4C-C3C	2.21	1.48	1.45
11	bB	809	CLA	C1B-C2B	2.21	1.48	1.43
11	aB	838	CLA	C1C-C2C	2.21	1.48	1.44
11	bB	816	CLA	C1C-C2C	2.21	1.48	1.44
12	bA	830	F6C	CHB-C4A	-2.21	1.34	1.38
11	bA	823	CLA	C1A-CHA	2.21	1.52	1.43
11	aB	827	CLA	C3D-C4D	-2.21	1.39	1.44
11	bB	817	CLA	C1B-C2B	2.21	1.48	1.43
11	cB	834	CLA	C1B-C2B	2.21	1.48	1.43
11	bA	840	CLA	C1C-C2C	2.21	1.48	1.44
11	cL	205	CLA	C3D-C4D	-2.21	1.39	1.44
11	bB	830	CLA	C1B-C2B	2.21	1.48	1.43
12	aB	824	F6C	C1C-C2C	2.21	1.48	1.43
11	bA	823	CLA	C1C-C2C	2.21	1.48	1.44
11	bL	204	CLA	C1C-C2C	2.21	1.48	1.44
11	cA	823	CLA	C1A-CHA	2.21	1.52	1.43
11	bB	816	CLA	C3D-C4D	-2.21	1.39	1.44
11	bA	809	CLA	C4C-C3C	2.20	1.48	1.45
11	bB	827	CLA	C3D-C4D	-2.20	1.39	1.44
11	aA	836	CLA	C1C-C2C	2.20	1.48	1.44
11	bB	837	CLA	C4C-C3C	2.20	1.48	1.45
11	cB	819	CLA	C4C-C3C	2.20	1.48	1.45
11	bB	831	CLA	C1C-C2C	2.20	1.48	1.44
11	cB	827	CLA	C3D-C4D	-2.20	1.39	1.44
11	cA	808	CLA	C3B-C2B	2.20	1.48	1.41
12	cA	832	F6C	C4C-C3C	2.20	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bA	833	CLA	C4C-C3C	2.20	1.48	1.45
11	cA	822	CLA	C4C-C3C	2.20	1.48	1.45
11	aB	823	CLA	C3D-C4D	-2.20	1.39	1.44
11	aB	840	CLA	C1B-C2B	2.20	1.48	1.43
11	aL	206	CLA	C1C-C2C	2.20	1.48	1.44
11	cA	816	CLA	C3D-C4D	-2.20	1.39	1.44
11	cB	802	CLA	C3D-C4D	-2.20	1.39	1.44
11	aA	829	CLA	C3D-C4D	-2.20	1.39	1.44
12	bB	824	F6C	C1C-C2C	2.20	1.48	1.43
11	aA	816	CLA	C3B-C2B	2.20	1.48	1.41
11	cL	206	CLA	C4C-C3C	2.20	1.48	1.45
11	aA	836	CLA	C1B-C2B	2.20	1.48	1.43
11	aB	820	CLA	C3B-C2B	2.20	1.48	1.41
11	bA	808	CLA	C3B-C2B	2.20	1.48	1.41
11	bA	843	CLA	C1C-C2C	2.20	1.48	1.44
11	aA	820	CLA	C1B-C2B	2.20	1.48	1.43
11	bB	823	CLA	C3B-C2B	2.20	1.48	1.41
11	aB	818	CLA	C4C-C3C	2.20	1.48	1.45
11	cA	837	CLA	C4C-C3C	2.20	1.48	1.45
11	aB	832	CLA	C1C-C2C	2.20	1.48	1.44
11	bA	837	CLA	C3D-C4D	-2.20	1.39	1.44
11	bB	820	CLA	C3B-C2B	2.19	1.48	1.41
11	cB	821	CLA	C3B-C2B	2.19	1.48	1.41
11	bB	830	CLA	C1C-C2C	2.19	1.48	1.44
11	aA	822	CLA	C4C-C3C	2.19	1.48	1.45
11	aA	817	CLA	C1B-C2B	2.19	1.48	1.43
11	bA	833	CLA	C1C-C2C	2.19	1.48	1.44
12	cL	202	F6C	CHB-C4A	-2.19	1.34	1.38
12	aA	844	F6C	C1D-C2D	2.19	1.48	1.44
11	cA	807	CLA	C1C-C2C	2.19	1.48	1.44
11	aA	833	CLA	C4C-C3C	2.19	1.48	1.45
11	aL	206	CLA	C4C-C3C	2.19	1.48	1.45
11	bA	837	CLA	C4C-C3C	2.19	1.48	1.45
11	bL	206	CLA	C1C-C2C	2.19	1.48	1.44
11	aA	823	CLA	C1A-CHA	2.19	1.52	1.43
11	bA	829	CLA	C1C-C2C	2.19	1.48	1.44
11	aA	810	CLA	C3B-C2B	2.19	1.48	1.41
11	aB	823	CLA	C3B-C2B	2.19	1.48	1.41
11	cA	804	CLA	C3B-C2B	2.19	1.48	1.41
11	aB	821	CLA	C3B-C2B	2.19	1.48	1.41
11	bA	836	CLA	C1C-C2C	2.19	1.48	1.44
11	cB	816	CLA	C3D-C4D	-2.19	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aA	842	CLA	C4C-C3C	2.19	1.48	1.45
12	cA	830	F6C	CHB-C4A	-2.19	1.34	1.38
11	bA	835	CLA	C1C-C2C	2.19	1.48	1.44
11	cK	101	CLA	C3B-C2B	2.19	1.48	1.41
11	cA	835	CLA	C1C-C2C	2.19	1.48	1.44
11	bB	823	CLA	C3D-C4D	-2.19	1.39	1.44
11	cA	837	CLA	C3D-C4D	-2.19	1.39	1.44
11	aB	831	CLA	C1C-C2C	2.19	1.48	1.44
11	aB	835	CLA	C1C-C2C	2.19	1.48	1.44
11	aA	819	CLA	C3B-C2B	2.19	1.48	1.41
11	bB	816	CLA	C1B-C2B	2.19	1.48	1.43
11	aA	804	CLA	C3B-C2B	2.18	1.48	1.41
11	bA	813	CLA	C3B-C2B	2.18	1.48	1.41
11	cB	802	CLA	C4C-C3C	2.18	1.48	1.45
11	aA	808	CLA	C3D-C4D	-2.18	1.39	1.44
11	aA	820	CLA	C3D-C4D	-2.18	1.39	1.44
11	aB	816	CLA	C3D-C4D	-2.18	1.39	1.44
12	aA	830	F6C	C1C-NC	-2.18	1.35	1.37
11	aB	820	CLA	C1C-C2C	2.18	1.48	1.44
11	bK	101	CLA	C3B-C2B	2.18	1.48	1.41
12	bA	832	F6C	C1C-NC	-2.18	1.35	1.37
11	cB	827	CLA	C3B-C2B	2.18	1.48	1.41
12	aL	202	F6C	CHB-C4A	-2.18	1.34	1.38
11	aB	830	CLA	C1C-C2C	2.18	1.48	1.44
11	aA	804	CLA	C3D-C4D	-2.18	1.39	1.44
11	aA	814	CLA	C1C-C2C	2.18	1.48	1.44
11	aA	834	CLA	C1C-C2C	2.18	1.48	1.44
11	cA	836	CLA	C4C-C3C	2.18	1.48	1.45
11	cA	834	CLA	C1C-C2C	2.18	1.48	1.44
11	cA	817	CLA	C1B-C2B	2.18	1.48	1.43
12	aA	832	F6C	C3D-C4D	-2.18	1.38	1.43
11	aB	819	CLA	C4C-C3C	2.18	1.48	1.45
11	aA	825	CLA	C3D-C4D	-2.18	1.39	1.44
11	aB	826	CLA	C3D-C4D	-2.18	1.39	1.44
11	bA	825	CLA	C3D-C4D	-2.18	1.39	1.44
11	bA	834	CLA	C1C-C2C	2.18	1.48	1.44
11	bB	819	CLA	C4C-C3C	2.18	1.48	1.45
11	aB	822	CLA	C3D-C4D	-2.18	1.39	1.44
11	cA	822	CLA	C3D-C4D	-2.18	1.39	1.44
11	bA	807	CLA	C1C-C2C	2.18	1.48	1.44
11	cA	843	CLA	C1C-C2C	2.18	1.48	1.44
11	cB	823	CLA	C3D-C4D	-2.18	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bB	825	CLA	C1C-C2C	2.18	1.48	1.44
11	bA	836	CLA	C4C-C3C	2.18	1.48	1.45
11	bL	206	CLA	C4C-C3C	2.18	1.48	1.45
12	bA	832	F6C	C3D-C4D	-2.18	1.38	1.43
11	aB	807	CLA	C1C-C2C	2.18	1.48	1.44
11	aA	805	CLA	C4C-C3C	2.18	1.48	1.45
11	bK	101	CLA	C3D-C4D	-2.18	1.39	1.44
11	cB	822	CLA	C3D-C4D	-2.18	1.39	1.44
11	bA	805	CLA	C4C-C3C	2.18	1.48	1.45
11	aA	835	CLA	C1C-C2C	2.18	1.48	1.44
11	aB	834	CLA	C1C-C2C	2.18	1.48	1.44
11	aB	827	CLA	C3B-C2B	2.18	1.48	1.41
11	cA	805	CLA	C4C-C3C	2.18	1.48	1.45
11	aA	802	CLA	C3B-C4B	2.18	1.47	1.42
11	cB	825	CLA	C1C-C2C	2.18	1.48	1.44
12	cA	832	F6C	C2B-C1B	2.18	1.49	1.44
11	bB	826	CLA	C3B-C2B	2.18	1.48	1.41
12	cA	844	F6C	C1D-C2D	2.18	1.48	1.44
11	cA	802	CLA	C3B-C4B	2.17	1.47	1.42
12	aA	830	F6C	CHB-C4A	-2.17	1.34	1.38
11	aA	807	CLA	C1C-C2C	2.17	1.48	1.44
11	bA	816	CLA	C3D-C4D	-2.17	1.39	1.44
12	aL	202	F6C	C4C-C3C	2.17	1.48	1.44
11	bA	804	CLA	C3D-C4D	-2.17	1.39	1.44
11	cA	825	CLA	C3D-C4D	-2.17	1.39	1.44
11	aA	807	CLA	C3B-C2B	2.17	1.48	1.41
11	cB	813	CLA	C4C-C3C	2.17	1.48	1.45
11	aA	813	CLA	C3B-C2B	2.17	1.48	1.41
11	cK	103	CLA	C3D-C4D	-2.17	1.39	1.44
11	cA	813	CLA	C3B-C2B	2.17	1.48	1.41
11	cL	204	CLA	C3D-C4D	-2.17	1.39	1.44
12	aA	832	F6C	C2B-C1B	2.17	1.49	1.44
11	cB	820	CLA	C3B-C2B	2.17	1.48	1.41
11	aA	817	CLA	C3D-C4D	-2.17	1.39	1.44
12	bA	832	F6C	C2B-C1B	2.17	1.49	1.44
11	cA	823	CLA	C1C-C2C	2.17	1.48	1.44
11	cA	819	CLA	C3B-C2B	2.17	1.48	1.41
11	bB	826	CLA	C3D-C4D	-2.17	1.39	1.44
11	cA	816	CLA	C3B-C2B	2.17	1.48	1.41
15	aA	847	BCR	C30-C25	-2.17	1.50	1.53
15	cB	848	BCR	C30-C25	-2.17	1.50	1.53
11	bA	836	CLA	C1B-C2B	2.17	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aA	833	CLA	C1C-C2C	2.17	1.48	1.44
11	bB	813	CLA	C4C-C3C	2.17	1.48	1.45
11	cA	809	CLA	C4C-C3C	2.17	1.48	1.45
11	cB	837	CLA	C4C-C3C	2.17	1.48	1.45
11	cB	823	CLA	C3B-C2B	2.17	1.48	1.41
11	aK	101	CLA	C3B-C2B	2.17	1.48	1.41
11	bK	103	CLA	C3D-C4D	-2.17	1.39	1.44
11	bA	807	CLA	C3B-C2B	2.17	1.48	1.41
11	cB	819	CLA	C3D-C4D	-2.17	1.39	1.44
11	aA	823	CLA	C1C-C2C	2.17	1.48	1.44
12	cB	824	F6C	C1C-C2C	2.17	1.48	1.43
11	cA	820	CLA	C3D-C4D	-2.17	1.39	1.44
11	cK	101	CLA	C3D-C4D	-2.17	1.39	1.44
11	bB	827	CLA	C3B-C2B	2.17	1.48	1.41
11	cA	833	CLA	C1C-C2C	2.17	1.48	1.44
11	bA	814	CLA	C3B-C2B	2.17	1.48	1.41
11	bA	816	CLA	C3B-C2B	2.17	1.48	1.41
11	cA	804	CLA	C3D-C4D	-2.17	1.39	1.44
11	cA	836	CLA	C3B-C4B	2.17	1.47	1.42
11	aB	813	CLA	C1C-C2C	2.17	1.48	1.44
11	cA	836	CLA	C1C-C2C	2.17	1.48	1.44
11	aA	821	CLA	C3D-C4D	-2.17	1.39	1.44
11	bB	834	CLA	C1C-C2C	2.17	1.48	1.44
11	cB	812	CLA	C1C-C2C	2.17	1.48	1.44
11	bB	802	CLA	C3D-C4D	-2.17	1.39	1.44
11	bA	822	CLA	C3D-C4D	-2.17	1.39	1.44
11	cA	829	CLA	C3D-C4D	-2.17	1.39	1.44
11	aB	810	CLA	C1C-C2C	2.16	1.48	1.44
11	cB	815	CLA	C3D-C4D	-2.16	1.39	1.44
11	bA	842	CLA	C4C-C3C	2.16	1.48	1.45
11	cB	819	CLA	C3B-C2B	2.16	1.48	1.41
11	bA	814	CLA	C1C-C2C	2.16	1.48	1.44
10	aA	801	CL0	C4C-C3C	2.16	1.48	1.45
11	bB	819	CLA	C3B-C2B	2.16	1.48	1.41
11	aA	816	CLA	C3D-C4D	-2.16	1.39	1.44
11	aA	808	CLA	C3B-C2B	2.16	1.48	1.41
11	cA	812	CLA	C3B-C2B	2.16	1.48	1.41
11	aB	821	CLA	C3D-C4D	-2.16	1.39	1.44
12	cA	832	F6C	C1D-C2D	2.16	1.48	1.44
11	bA	817	CLA	C1B-C2B	2.16	1.48	1.43
11	cA	821	CLA	C3D-C4D	-2.16	1.39	1.44
15	bK	102	BCR	C30-C25	-2.16	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bB	807	CLA	C1C-C2C	2.16	1.48	1.44
11	bA	821	CLA	C3D-C4D	-2.16	1.39	1.44
11	cB	823	CLA	C4C-C3C	2.16	1.48	1.45
11	aB	819	CLA	C3B-C2B	2.16	1.48	1.41
12	cA	832	F6C	C3D-C4D	-2.16	1.38	1.43
11	aA	836	CLA	C4C-C3C	2.16	1.48	1.45
11	bB	815	CLA	C3D-C4D	-2.16	1.39	1.44
11	cB	833	CLA	C3D-C4D	-2.16	1.39	1.44
12	bA	832	F6C	C1D-C2D	2.16	1.48	1.44
11	aB	816	CLA	C1B-C2B	2.16	1.48	1.43
11	cA	807	CLA	C3B-C2B	2.16	1.48	1.41
11	aA	815	CLA	C1A-CHA	2.16	1.52	1.43
18	bB	847	LMG	O7-C8	-2.16	1.41	1.46
11	bA	823	CLA	C3B-C2B	2.16	1.48	1.41
11	aB	838	CLA	C3B-C2B	2.16	1.48	1.41
11	cB	833	CLA	C3B-C2B	2.16	1.48	1.41
11	aA	809	CLA	C3D-C4D	-2.16	1.39	1.44
12	bA	830	F6C	C1C-NC	-2.16	1.35	1.37
11	cA	843	CLA	C3B-C2B	2.16	1.48	1.41
10	cA	801	CL0	C4C-C3C	2.16	1.48	1.45
11	aL	204	CLA	C4C-C3C	2.16	1.48	1.45
11	aA	821	CLA	C3B-C2B	2.15	1.48	1.41
11	aB	813	CLA	C4C-C3C	2.15	1.48	1.45
11	aA	814	CLA	C3B-C2B	2.15	1.48	1.41
11	cB	826	CLA	C3B-C2B	2.15	1.48	1.41
11	cB	838	CLA	C3B-C2B	2.15	1.48	1.41
11	cL	204	CLA	C4C-C3C	2.15	1.48	1.45
11	cA	808	CLA	C3D-C4D	-2.15	1.39	1.44
11	aB	839	CLA	C3B-C2B	2.15	1.48	1.41
11	bB	822	CLA	C3B-C2B	2.15	1.48	1.41
11	aB	822	CLA	C3B-C2B	2.15	1.48	1.41
11	aA	836	CLA	C3B-C4B	2.15	1.47	1.42
11	bA	802	CLA	C3B-C4B	2.15	1.47	1.42
11	cB	826	CLA	C3D-C4D	-2.15	1.39	1.44
12	aA	832	F6C	C1C-NC	-2.15	1.35	1.37
11	bA	813	CLA	C1B-C2B	2.15	1.48	1.43
11	aB	826	CLA	C3B-C2B	2.15	1.48	1.41
11	bL	204	CLA	C4C-C3C	2.15	1.48	1.45
11	bA	819	CLA	C3B-C2B	2.15	1.48	1.41
11	bB	821	CLA	C3D-C4D	-2.15	1.39	1.44
11	cA	817	CLA	C1C-C2C	2.15	1.48	1.44
11	cB	834	CLA	C1A-CHA	2.15	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bB	833	CLA	C3D-C4D	-2.15	1.39	1.44
15	bB	842	BCR	C30-C25	-2.15	1.50	1.53
11	bA	838	CLA	C4C-C3C	2.15	1.48	1.45
11	bA	821	CLA	C3B-C2B	2.15	1.48	1.41
11	bB	811	CLA	C3B-C2B	2.15	1.48	1.41
11	cK	103	CLA	C1C-C2C	2.15	1.48	1.44
11	bA	836	CLA	C3B-C4B	2.15	1.47	1.42
11	aA	823	CLA	C3B-C2B	2.15	1.48	1.41
11	bB	838	CLA	C3B-C2B	2.15	1.48	1.41
11	bA	829	CLA	C3D-C4D	-2.15	1.39	1.44
11	aB	819	CLA	C1A-CHA	2.15	1.52	1.43
11	aK	103	CLA	C3D-C4D	-2.15	1.39	1.44
11	bB	818	CLA	C3D-C4D	-2.15	1.39	1.44
11	cA	815	CLA	C1A-CHA	2.15	1.52	1.43
11	aA	837	CLA	C3D-C4D	-2.15	1.39	1.44
11	bB	809	CLA	C1C-NC	-2.15	1.34	1.37
11	bB	817	CLA	C3B-C2B	2.15	1.48	1.41
11	cB	822	CLA	C3B-C2B	2.15	1.48	1.41
11	aB	806	CLA	C3B-C2B	2.14	1.48	1.41
11	aA	822	CLA	C3D-C4D	-2.14	1.39	1.44
11	aB	808	CLA	C3D-C4D	-2.14	1.39	1.44
11	aB	815	CLA	C3D-C4D	-2.14	1.39	1.44
11	bB	818	CLA	C1C-C2C	2.14	1.48	1.44
11	cB	821	CLA	C3D-C4D	-2.14	1.39	1.44
11	bA	812	CLA	C3B-C2B	2.14	1.48	1.41
11	aB	818	CLA	C3D-C4D	-2.14	1.39	1.44
11	bA	841	CLA	C3B-C2B	2.14	1.48	1.41
11	bB	815	CLA	C3B-C2B	2.14	1.48	1.41
11	cB	815	CLA	C3B-C2B	2.14	1.48	1.41
11	aB	819	CLA	C3D-C4D	-2.14	1.39	1.44
11	cB	818	CLA	C3D-C4D	-2.14	1.39	1.44
11	cA	814	CLA	C3B-C2B	2.14	1.48	1.41
11	cB	806	CLA	C3B-C2B	2.14	1.48	1.41
11	cA	817	CLA	C3D-C4D	-2.14	1.39	1.44
11	aA	839	CLA	C1C-C2C	2.14	1.48	1.44
12	bA	827	F6C	C1D-C2D	2.14	1.48	1.44
11	cB	839	CLA	C3B-C2B	2.14	1.48	1.41
11	cA	841	CLA	C3B-C2B	2.14	1.48	1.41
12	cA	830	F6C	C1C-NC	-2.14	1.35	1.37
11	aA	813	CLA	C3D-C4D	-2.14	1.39	1.44
11	cB	811	CLA	C3B-C2B	2.14	1.48	1.41
12	cA	827	F6C	C1D-C2D	2.14	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aA	817	CLA	C1C-C2C	2.14	1.48	1.44
11	bK	103	CLA	C1C-C2C	2.14	1.48	1.44
11	aB	818	CLA	C1C-C2C	2.14	1.48	1.44
11	aA	843	CLA	C3B-C2B	2.14	1.48	1.41
15	cB	842	BCR	C30-C25	-2.14	1.50	1.53
11	aB	811	CLA	C3B-C2B	2.14	1.48	1.41
11	aK	101	CLA	C3D-C4D	-2.14	1.39	1.44
11	bA	808	CLA	C3D-C4D	-2.14	1.39	1.44
11	aB	826	CLA	C4C-C3C	2.14	1.48	1.45
11	bK	103	CLA	C3B-C2B	2.14	1.48	1.41
11	aA	813	CLA	C1B-C2B	2.14	1.48	1.43
11	cB	807	CLA	C1C-C2C	2.14	1.48	1.44
18	cB	847	LMG	O7-C8	-2.14	1.41	1.46
11	cA	823	CLA	C3B-C2B	2.14	1.48	1.41
11	bL	204	CLA	C3D-C4D	-2.14	1.39	1.44
11	cA	809	CLA	C3D-C4D	-2.14	1.39	1.44
11	aB	833	CLA	C3B-C2B	2.14	1.48	1.41
10	bA	801	CL0	C4C-C3C	2.14	1.48	1.45
11	bA	820	CLA	C3D-C4D	-2.14	1.39	1.44
11	cB	816	CLA	C1B-C2B	2.14	1.48	1.43
11	cB	814	CLA	C3B-C2B	2.14	1.48	1.41
11	bA	817	CLA	C3D-C4D	-2.13	1.39	1.44
11	aB	815	CLA	C3B-C2B	2.13	1.48	1.41
11	bB	806	CLA	C3B-C2B	2.13	1.48	1.41
12	aA	832	F6C	C1D-C2D	2.13	1.48	1.44
11	bB	801	CLA	C3D-C4D	-2.13	1.39	1.44
11	bB	813	CLA	C1C-C2C	2.13	1.48	1.44
11	bB	833	CLA	C3B-C2B	2.13	1.48	1.41
11	cB	834	CLA	C1C-C2C	2.13	1.48	1.44
11	aB	833	CLA	C3D-C4D	-2.13	1.39	1.44
11	bB	810	CLA	C1C-C2C	2.13	1.48	1.44
11	cB	809	CLA	C1C-NC	-2.13	1.34	1.37
11	aB	812	CLA	C1C-C2C	2.13	1.48	1.44
11	aB	830	CLA	C3B-C2B	2.13	1.48	1.41
15	aB	848	BCR	C30-C25	-2.13	1.50	1.53
11	bA	813	CLA	C3D-C4D	-2.13	1.39	1.44
11	bB	819	CLA	C3D-C4D	-2.13	1.39	1.44
11	cB	810	CLA	C1C-C2C	2.13	1.48	1.44
11	bA	839	CLA	C1C-C2C	2.13	1.48	1.44
11	cB	813	CLA	C1C-C2C	2.13	1.48	1.44
11	bB	819	CLA	C1A-CHA	2.13	1.51	1.43
11	cB	808	CLA	C3D-C4D	-2.13	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	cK	103	CLA	C3B-C2B	2.13	1.48	1.41
12	aA	827	F6C	C4C-C3C	2.13	1.48	1.44
11	aA	812	CLA	C3B-C2B	2.13	1.48	1.41
11	bB	839	CLA	C3B-C2B	2.13	1.48	1.41
11	cB	801	CLA	C3D-C4D	-2.13	1.39	1.44
11	aB	801	CLA	C1C-C2C	2.13	1.48	1.44
11	aB	823	CLA	C4C-C3C	2.13	1.48	1.45
11	bA	815	CLA	C1A-CHA	2.13	1.51	1.43
11	bA	843	CLA	C3B-C2B	2.13	1.48	1.41
11	cB	803	CLA	C3B-C2B	2.13	1.48	1.41
11	cA	813	CLA	C1B-C2B	2.13	1.48	1.43
11	aB	834	CLA	C1A-CHA	2.13	1.51	1.43
11	bB	808	CLA	C3D-C4D	-2.13	1.39	1.44
11	bA	818	CLA	C3D-C4D	-2.12	1.39	1.44
11	bB	834	CLA	C1A-CHA	2.12	1.51	1.43
11	cB	819	CLA	C1A-CHA	2.12	1.51	1.43
11	aB	809	CLA	C1C-NC	-2.12	1.34	1.37
18	aB	847	LMG	O7-C8	-2.12	1.41	1.46
11	aA	818	CLA	C1A-CHA	2.12	1.51	1.43
12	cB	824	F6C	C2B-C1B	2.12	1.49	1.44
12	bB	824	F6C	C1A-C2A	2.12	1.50	1.45
11	bB	803	CLA	C3B-C2B	2.12	1.48	1.41
11	bB	814	CLA	C3B-C2B	2.12	1.48	1.41
11	aB	803	CLA	C3B-C2B	2.12	1.48	1.41
11	cB	809	CLA	C4C-C3C	2.12	1.48	1.45
11	aK	103	CLA	C1C-C2C	2.12	1.48	1.44
11	cB	830	CLA	C3B-C2B	2.12	1.48	1.41
11	bB	826	CLA	C4C-C3C	2.12	1.48	1.45
11	bB	811	CLA	C3D-C4D	-2.12	1.39	1.44
11	cA	813	CLA	C3D-C4D	-2.12	1.39	1.44
11	aL	204	CLA	C3D-C4D	-2.12	1.39	1.44
11	aB	817	CLA	C3B-C2B	2.12	1.48	1.41
11	aB	814	CLA	C3B-C2B	2.12	1.48	1.41
11	cB	837	CLA	C3B-C2B	2.12	1.48	1.41
11	aA	811	CLA	C3D-C4D	-2.12	1.39	1.44
11	cB	818	CLA	C1C-C2C	2.12	1.48	1.44
15	aB	842	BCR	C30-C25	-2.12	1.50	1.53
11	aB	827	CLA	C4C-C3C	2.12	1.48	1.45
11	cA	821	CLA	C3B-C2B	2.12	1.48	1.41
11	cA	839	CLA	C1C-C2C	2.12	1.48	1.44
11	aB	802	CLA	C4C-C3C	2.12	1.48	1.45
11	aA	841	CLA	C3B-C2B	2.12	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bB	824	F6C	C2B-C1B	2.12	1.49	1.44
11	bA	835	CLA	C4C-C3C	2.12	1.48	1.45
11	cA	834	CLA	C4C-C3C	2.12	1.48	1.45
11	bA	809	CLA	C3D-C4D	-2.12	1.39	1.44
11	aB	829	CLA	C1A-CHA	2.12	1.51	1.43
15	cA	847	BCR	C30-C25	-2.11	1.50	1.53
12	aA	827	F6C	C1D-C2D	2.11	1.48	1.44
11	cA	835	CLA	C4C-C3C	2.11	1.48	1.45
15	bB	846	BCR	C1-C6	-2.11	1.50	1.53
11	bB	823	CLA	C4C-C3C	2.11	1.48	1.45
11	cA	811	CLA	C3D-C4D	-2.11	1.39	1.44
11	aK	103	CLA	C3B-C2B	2.11	1.48	1.41
11	aA	838	CLA	C4C-C3C	2.11	1.48	1.45
11	cA	838	CLA	C4C-C3C	2.11	1.48	1.45
11	bA	834	CLA	C4C-C3C	2.11	1.48	1.45
11	cB	817	CLA	C3B-C2B	2.11	1.48	1.41
11	aA	842	CLA	C3B-C2B	2.11	1.48	1.41
11	bB	812	CLA	C1C-C2C	2.11	1.48	1.44
11	bB	808	CLA	C3B-C2B	2.11	1.48	1.41
12	cB	824	F6C	C1C-NC	-2.11	1.35	1.37
11	cB	826	CLA	C4C-C3C	2.11	1.48	1.45
15	aB	846	BCR	C1-C6	-2.11	1.50	1.53
11	aB	832	CLA	C3B-C2B	2.11	1.48	1.41
11	bB	840	CLA	C1C-C2C	2.11	1.48	1.44
11	bB	802	CLA	C4C-C3C	2.11	1.48	1.45
11	cB	827	CLA	C4C-C3C	2.11	1.48	1.45
12	cB	824	F6C	CMB-C2B	2.11	1.49	1.45
11	bB	834	CLA	C3D-C4D	-2.11	1.39	1.44
12	aB	824	F6C	C2B-C1B	2.11	1.49	1.44
11	bB	801	CLA	C1C-C2C	2.11	1.48	1.44
11	cB	829	CLA	C1A-CHA	2.10	1.51	1.43
11	aB	820	CLA	C3D-C4D	-2.10	1.39	1.44
11	bB	829	CLA	C1A-CHA	2.10	1.51	1.43
12	cA	827	F6C	C4C-C3C	2.10	1.48	1.44
11	bA	817	CLA	C1C-C2C	2.10	1.48	1.44
12	bA	827	F6C	C4C-C3C	2.10	1.48	1.44
11	aA	824	CLA	C4C-C3C	2.10	1.48	1.45
11	bB	830	CLA	C3B-C2B	2.10	1.48	1.41
11	cA	818	CLA	C1A-CHA	2.10	1.51	1.43
11	aB	808	CLA	C3B-C2B	2.10	1.48	1.41
11	bA	836	CLA	C3D-C4D	-2.10	1.39	1.44
11	cB	820	CLA	C1A-CHA	2.10	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bB	848	BCR	C30-C25	-2.10	1.50	1.53
11	aB	801	CLA	C3D-C4D	-2.10	1.39	1.44
11	aB	811	CLA	C3D-C4D	-2.10	1.39	1.44
11	cA	814	CLA	C1C-C2C	2.10	1.48	1.44
16	bA	852	LHG	P-O6	2.10	1.67	1.59
16	aA	852	LHG	P-O6	2.10	1.67	1.59
11	bA	811	CLA	C3D-C4D	-2.10	1.39	1.44
11	cA	818	CLA	C3D-C4D	-2.10	1.39	1.44
11	cB	831	CLA	C3B-C2B	2.10	1.48	1.41
11	aA	834	CLA	C4C-C3C	2.10	1.48	1.45
11	aB	840	CLA	C1C-C2C	2.10	1.48	1.44
11	bB	835	CLA	C3D-C4D	-2.10	1.39	1.44
11	bB	805	CLA	C1C-C2C	2.10	1.48	1.44
12	aB	824	F6C	CMB-C2B	2.10	1.49	1.45
11	cA	821	CLA	C1A-CHA	2.10	1.51	1.43
11	bA	831	CLA	C1C-NC	-2.10	1.34	1.37
15	bA	847	BCR	C30-C25	-2.10	1.50	1.53
11	aA	809	CLA	C1A-CHA	2.10	1.51	1.43
11	bA	815	CLA	C3D-C4D	-2.09	1.39	1.44
11	cB	840	CLA	C1C-C2C	2.09	1.48	1.44
11	bA	842	CLA	C3B-C2B	2.09	1.48	1.41
11	aB	832	CLA	C3D-C4D	-2.09	1.39	1.44
11	bB	820	CLA	C1A-CHA	2.09	1.51	1.43
11	aA	818	CLA	C3D-C4D	-2.09	1.39	1.44
11	cB	832	CLA	C3B-C2B	2.09	1.48	1.41
11	bA	818	CLA	C1A-CHA	2.09	1.51	1.43
11	bA	811	CLA	C3B-C2B	2.09	1.48	1.41
11	cA	842	CLA	C3B-C2B	2.09	1.48	1.41
11	aB	835	CLA	C3D-C4D	-2.09	1.39	1.44
11	bB	832	CLA	C3D-C4D	-2.09	1.39	1.44
11	aB	837	CLA	C3B-C2B	2.09	1.48	1.41
11	cB	839	CLA	C1B-C2B	2.09	1.48	1.43
11	bB	827	CLA	C4C-C3C	2.09	1.48	1.45
11	aB	820	CLA	C1A-CHA	2.09	1.51	1.43
11	aB	831	CLA	C3B-C2B	2.09	1.48	1.41
11	bB	832	CLA	C3B-C2B	2.09	1.48	1.41
11	bB	829	CLA	C3D-C4D	-2.09	1.39	1.44
11	cB	801	CLA	C1C-C2C	2.09	1.48	1.44
11	cA	812	CLA	C3D-C4D	-2.09	1.39	1.44
11	cB	830	CLA	C3D-C4D	-2.09	1.39	1.44
11	aB	839	CLA	C1B-C2B	2.09	1.48	1.43
12	cB	824	F6C	C1A-C2A	2.09	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aB	830	CLA	C3D-C4D	-2.09	1.39	1.44
16	cA	852	LHG	P-O6	2.09	1.67	1.59
11	aB	805	CLA	C1C-C2C	2.09	1.48	1.44
15	cB	846	BCR	C1-C6	-2.09	1.50	1.53
11	aA	835	CLA	C4C-C3C	2.09	1.48	1.45
11	cA	824	CLA	C3B-C2B	2.08	1.48	1.41
11	aA	841	CLA	C1A-CHA	2.08	1.51	1.43
11	bA	820	CLA	C1A-CHA	2.08	1.51	1.43
11	bB	837	CLA	C3B-C2B	2.08	1.48	1.41
11	cB	804	CLA	C1A-CHA	2.08	1.51	1.43
11	cA	836	CLA	C3D-C4D	-2.08	1.39	1.44
15	cL	208	BCR	C1-C6	-2.08	1.50	1.53
11	aB	803	CLA	C1A-CHA	2.08	1.51	1.43
11	cB	816	CLA	C3B-C2B	2.08	1.48	1.41
12	cA	830	F6C	C4C-C3C	2.08	1.48	1.44
11	cB	804	CLA	C4C-C3C	2.08	1.48	1.45
11	aB	804	CLA	C3D-C4D	-2.08	1.39	1.44
11	cA	811	CLA	C3B-C2B	2.08	1.48	1.41
11	cB	823	CLA	C1A-CHA	2.08	1.51	1.43
11	cB	830	CLA	C1A-CHA	2.08	1.51	1.43
12	bB	824	F6C	CMB-C2B	2.08	1.49	1.45
11	cA	815	CLA	C3D-C4D	-2.08	1.39	1.44
11	cB	835	CLA	C3D-C4D	-2.08	1.39	1.44
11	aA	821	CLA	C1A-CHA	2.08	1.51	1.43
11	aB	823	CLA	C1A-CHA	2.08	1.51	1.43
12	cA	844	F6C	C3D-C4D	-2.08	1.38	1.43
11	bB	804	CLA	C4C-C3C	2.08	1.48	1.45
11	bB	816	CLA	C3B-C2B	2.08	1.48	1.41
11	aA	811	CLA	C3B-C2B	2.08	1.48	1.41
12	aA	827	F6C	C3D-C4D	-2.08	1.38	1.43
12	cL	202	F6C	C3D-C4D	-2.08	1.38	1.43
11	cA	829	CLA	C1A-CHA	2.08	1.51	1.43
12	cL	202	F6C	C3B-C4B	2.08	1.49	1.44
11	bB	804	CLA	C1A-CHA	2.08	1.51	1.43
11	aB	816	CLA	C3B-C2B	2.08	1.48	1.41
11	bB	830	CLA	C1A-CHA	2.08	1.51	1.43
11	aA	815	CLA	C3D-C4D	-2.08	1.39	1.44
11	cB	829	CLA	C3D-C4D	-2.08	1.39	1.44
12	bL	202	F6C	C3B-C4B	2.08	1.49	1.44
11	bB	809	CLA	C4C-C3C	2.08	1.48	1.45
11	bB	831	CLA	C3B-C2B	2.08	1.48	1.41
12	aL	202	F6C	C3D-C4D	-2.08	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bA	805	CLA	C1A-CHA	2.08	1.51	1.43
11	bA	824	CLA	C3B-C2B	2.07	1.48	1.41
11	cB	808	CLA	C1A-CHA	2.07	1.51	1.43
11	cB	804	CLA	C3D-C4D	-2.07	1.39	1.44
11	bA	824	CLA	C4C-C3C	2.07	1.48	1.45
11	bA	821	CLA	C1A-CHA	2.07	1.51	1.43
11	cA	841	CLA	C1A-CHA	2.07	1.51	1.43
11	bA	819	CLA	C1B-C2B	2.07	1.48	1.43
11	aB	809	CLA	C4C-C3C	2.07	1.48	1.45
11	cA	820	CLA	C1A-CHA	2.07	1.51	1.43
11	aB	830	CLA	C1A-CHA	2.07	1.51	1.43
11	aB	829	CLA	C3D-C4D	-2.07	1.39	1.44
12	cL	202	F6C	C4D-CHA	2.07	1.47	1.42
11	bA	829	CLA	C1A-CHA	2.07	1.51	1.43
11	aA	831	CLA	C3D-C4D	-2.07	1.39	1.44
11	bL	205	CLA	C3B-C2B	2.07	1.48	1.41
11	cA	809	CLA	C1A-CHA	2.07	1.51	1.43
11	cB	808	CLA	C3B-C2B	2.07	1.48	1.41
11	bB	821	CLA	C1A-CHA	2.07	1.51	1.43
11	aA	820	CLA	C1A-CHA	2.07	1.51	1.43
11	aL	205	CLA	C3B-C2B	2.07	1.48	1.41
11	aB	804	CLA	C1A-CHA	2.07	1.51	1.43
11	cB	803	CLA	C1A-CHA	2.07	1.51	1.43
11	cB	834	CLA	C3D-C4D	-2.07	1.39	1.44
12	aB	824	F6C	C1A-C2A	2.07	1.50	1.45
11	aA	829	CLA	C1A-CHA	2.07	1.51	1.43
11	cA	824	CLA	C4C-C3C	2.07	1.48	1.45
12	aL	202	F6C	C3B-C4B	2.07	1.49	1.44
12	bL	202	F6C	C3D-C4D	-2.07	1.38	1.43
11	bA	841	CLA	C1A-CHA	2.07	1.51	1.43
11	aB	807	CLA	C3B-C2B	2.07	1.48	1.41
11	bA	809	CLA	C1A-CHA	2.06	1.51	1.43
11	cB	832	CLA	C3D-C4D	-2.06	1.39	1.44
11	bB	830	CLA	C3D-C4D	-2.06	1.39	1.44
11	aA	817	CLA	C1A-CHA	2.06	1.51	1.43
11	aA	812	CLA	C3D-C4D	-2.06	1.39	1.44
12	bL	202	F6C	C4D-CHA	2.06	1.47	1.42
11	cA	802	CLA	C3B-C2B	2.06	1.48	1.41
11	aA	824	CLA	C3B-C2B	2.06	1.48	1.41
11	aB	808	CLA	C1A-CHA	2.06	1.51	1.43
11	bA	817	CLA	C1A-CHA	2.06	1.51	1.43
11	bB	839	CLA	C1B-C2B	2.06	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bB	823	CLA	C1A-CHA	2.06	1.51	1.43
11	cB	821	CLA	C1A-CHA	2.06	1.51	1.43
11	bA	812	CLA	C3D-C4D	-2.06	1.39	1.44
11	bL	204	CLA	C1A-CHA	2.06	1.51	1.43
11	bB	817	CLA	C4C-C3C	2.06	1.48	1.45
11	aA	805	CLA	C1A-CHA	2.06	1.51	1.43
11	bB	807	CLA	C3B-C2B	2.06	1.48	1.41
11	cL	205	CLA	C3B-C2B	2.06	1.48	1.41
12	bA	844	F6C	C3D-C4D	-2.06	1.38	1.43
11	cA	805	CLA	C1A-CHA	2.06	1.51	1.43
11	aA	805	CLA	C3D-C4D	-2.06	1.39	1.44
11	bB	803	CLA	C1A-CHA	2.06	1.51	1.43
11	cA	806	CLA	C3B-C2B	2.06	1.48	1.41
11	aA	837	CLA	C1A-CHA	2.06	1.51	1.43
11	cB	811	CLA	C3D-C4D	-2.06	1.39	1.44
11	aA	806	CLA	C3B-C2B	2.06	1.48	1.41
11	cB	815	CLA	C1A-CHA	2.06	1.51	1.43
11	bB	815	CLA	C1A-CHA	2.06	1.51	1.43
11	cB	826	CLA	C1A-CHA	2.06	1.51	1.43
11	aA	802	CLA	C1C-C2C	2.06	1.48	1.44
11	bB	835	CLA	C3B-C2B	2.06	1.48	1.41
11	bA	823	CLA	C3D-C4D	-2.06	1.39	1.44
12	aL	202	F6C	C4D-CHA	2.05	1.47	1.42
11	cB	810	CLA	C3B-C2B	2.05	1.48	1.41
11	cB	817	CLA	C4C-C3C	2.05	1.48	1.45
11	bA	842	CLA	C3D-C4D	-2.05	1.39	1.44
11	cA	842	CLA	C3D-C4D	-2.05	1.39	1.44
11	cB	835	CLA	C1A-CHA	2.05	1.51	1.43
12	bA	830	F6C	C4C-C3C	2.05	1.48	1.44
11	aB	810	CLA	C3B-C2B	2.05	1.48	1.41
12	cA	827	F6C	C3D-C4D	-2.05	1.38	1.43
12	bA	827	F6C	C3D-C4D	-2.05	1.38	1.43
11	cA	819	CLA	C1B-C2B	2.05	1.48	1.43
11	aB	821	CLA	C1A-CHA	2.05	1.51	1.43
11	bB	808	CLA	C1A-CHA	2.05	1.51	1.43
11	aA	819	CLA	C1B-C2B	2.05	1.48	1.43
11	aB	834	CLA	C3D-C4D	-2.05	1.39	1.44
11	cB	820	CLA	C3D-C4D	-2.05	1.39	1.44
11	bA	805	CLA	C3D-C4D	-2.05	1.39	1.44
12	aA	830	F6C	C4C-C3C	2.05	1.48	1.44
11	bA	802	CLA	C1C-C2C	2.05	1.48	1.44
11	cB	815	CLA	C4C-C3C	2.05	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bA	825	CLA	C3B-C2B	2.05	1.48	1.41
11	bB	810	CLA	C3B-C2B	2.05	1.48	1.41
11	cB	840	CLA	C3B-C2B	2.05	1.48	1.41
11	cB	818	CLA	C1B-C2B	2.05	1.48	1.43
11	bB	835	CLA	C1A-CHA	2.05	1.51	1.43
11	aB	835	CLA	C1A-CHA	2.05	1.51	1.43
11	aA	836	CLA	C3D-C4D	-2.05	1.39	1.44
11	bB	814	CLA	C3D-C4D	-2.05	1.39	1.44
11	bA	803	CLA	C1B-C2B	2.04	1.48	1.43
11	aB	832	CLA	C1A-CHA	2.04	1.51	1.43
11	bB	804	CLA	C3D-C4D	-2.04	1.39	1.44
11	bA	806	CLA	C3B-C2B	2.04	1.48	1.41
11	aB	815	CLA	C1A-CHA	2.04	1.51	1.43
11	aB	835	CLA	C3B-C2B	2.04	1.48	1.41
15	aL	208	BCR	C1-C6	-2.04	1.51	1.53
11	aB	817	CLA	C4C-C3C	2.04	1.48	1.45
11	bB	814	CLA	C1C-NC	-2.04	1.34	1.37
11	aA	803	CLA	C1C-C2C	2.04	1.48	1.44
11	bB	820	CLA	C3D-C4D	-2.04	1.39	1.44
11	bA	837	CLA	C1A-CHA	2.04	1.51	1.43
11	bB	826	CLA	C1A-CHA	2.04	1.51	1.43
11	cB	807	CLA	C3B-C2B	2.04	1.48	1.41
11	aA	825	CLA	C3B-C2B	2.04	1.48	1.41
11	bL	206	CLA	C3B-C2B	2.04	1.48	1.41
11	cA	803	CLA	C1B-C2B	2.04	1.48	1.43
11	cL	204	CLA	C1A-CHA	2.04	1.51	1.43
11	aL	204	CLA	C1A-CHA	2.04	1.51	1.43
11	cA	817	CLA	C1A-CHA	2.04	1.51	1.43
11	aB	826	CLA	C1A-CHA	2.04	1.51	1.43
11	bA	841	CLA	C3D-C4D	-2.04	1.39	1.44
15	bL	208	BCR	C1-C6	-2.04	1.51	1.53
11	bA	803	CLA	C1C-C2C	2.04	1.48	1.44
11	aB	804	CLA	C4C-C3C	2.04	1.48	1.45
11	aA	831	CLA	C1C-NC	-2.04	1.34	1.37
11	aB	801	CLA	C1C-NC	-2.04	1.34	1.37
11	bA	831	CLA	C3D-C4D	-2.04	1.39	1.44
11	cA	802	CLA	C1C-C2C	2.04	1.48	1.44
11	aA	803	CLA	C1B-C2B	2.04	1.48	1.43
11	cB	812	CLA	C1C-NC	-2.03	1.34	1.37
11	bB	840	CLA	C3B-C2B	2.03	1.48	1.41
11	cA	806	CLA	CHB-C4A	-2.03	1.32	1.37
12	aA	844	F6C	C3D-C4D	-2.03	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aA	842	CLA	C1A-CHA	2.03	1.51	1.43
11	aA	842	CLA	C3D-C4D	-2.03	1.39	1.44
11	aB	814	CLA	C3D-C4D	-2.03	1.39	1.44
11	cB	814	CLA	C1C-NC	-2.03	1.34	1.37
11	bA	806	CLA	CHB-C4A	-2.03	1.32	1.37
11	cB	832	CLA	C1A-CHA	2.03	1.51	1.43
11	cA	823	CLA	C3D-C4D	-2.03	1.39	1.44
12	cB	824	F6C	C3D-C4D	-2.03	1.38	1.43
11	cA	805	CLA	C3D-C4D	-2.03	1.39	1.44
11	cB	835	CLA	C3B-C2B	2.03	1.48	1.41
11	bA	842	CLA	C1A-CHA	2.03	1.51	1.43
11	aA	806	CLA	CHB-C4A	-2.03	1.32	1.37
11	cA	808	CLA	C1A-CHA	2.03	1.51	1.43
11	bB	801	CLA	C3B-C2B	2.03	1.48	1.41
11	aL	206	CLA	C3B-C2B	2.03	1.48	1.41
11	bB	818	CLA	C1B-C2B	2.03	1.48	1.43
11	aA	802	CLA	C3B-C2B	2.03	1.48	1.41
11	cB	814	CLA	C3D-C4D	-2.03	1.39	1.44
11	aA	840	CLA	C3B-C2B	2.03	1.48	1.41
11	bK	103	CLA	C1A-CHA	2.03	1.51	1.43
11	bB	808	CLA	C1C-C2C	2.03	1.48	1.44
11	aA	823	CLA	C3D-C4D	-2.03	1.39	1.44
11	aB	812	CLA	C1C-NC	-2.03	1.34	1.37
11	bA	840	CLA	C3B-C2B	2.03	1.48	1.41
11	aB	840	CLA	C3B-C2B	2.03	1.48	1.41
11	cA	834	CLA	C3B-C2B	2.03	1.48	1.41
11	cA	842	CLA	C1A-CHA	2.03	1.51	1.43
11	cA	803	CLA	C1C-C2C	2.02	1.48	1.44
11	aB	801	CLA	C3B-C2B	2.02	1.48	1.41
11	bB	832	CLA	C1A-CHA	2.02	1.51	1.43
11	cA	837	CLA	C1A-CHA	2.02	1.51	1.43
11	cA	825	CLA	C1A-CHA	2.02	1.51	1.43
11	bB	815	CLA	C4C-C3C	2.02	1.48	1.45
11	cB	805	CLA	C1C-C2C	2.02	1.48	1.44
11	bA	808	CLA	C1A-CHA	2.02	1.51	1.43
11	cA	807	CLA	C1A-CHA	2.02	1.51	1.43
11	cL	206	CLA	C3B-C2B	2.02	1.48	1.41
11	bA	825	CLA	C1A-CHA	2.02	1.51	1.43
11	bA	802	CLA	C3B-C2B	2.02	1.48	1.41
11	cB	836	CLA	C3B-C2B	2.02	1.48	1.41
11	aB	814	CLA	C1A-CHA	2.02	1.51	1.43
12	bB	824	F6C	C3D-C4D	-2.02	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aA	810	CLA	C1A-CHA	2.02	1.51	1.43
11	aB	818	CLA	C3B-C2B	2.02	1.48	1.41
11	aA	816	CLA	C1A-CHA	2.02	1.51	1.43
11	bB	809	CLA	C3B-C2B	2.02	1.48	1.41
11	cB	801	CLA	C3B-C2B	2.02	1.48	1.41
12	aB	824	F6C	C3D-C4D	-2.02	1.38	1.43
11	bA	814	CLA	C1C-NC	-2.02	1.34	1.37
11	cA	831	CLA	C1C-NC	-2.02	1.34	1.37
11	cB	809	CLA	C3B-C2B	2.01	1.48	1.41
11	cA	803	CLA	C1A-CHA	2.01	1.51	1.43
12	aA	830	F6C	C3D-C4D	-2.01	1.38	1.43
11	aA	825	CLA	C1A-CHA	2.01	1.51	1.43
11	aB	813	CLA	C1A-CHA	2.01	1.51	1.43
11	cB	801	CLA	C1C-NC	-2.01	1.34	1.37
11	bA	810	CLA	C1A-CHA	2.01	1.51	1.43
11	bA	812	CLA	C1A-CHA	2.01	1.51	1.43
12	cA	830	F6C	C3D-C4D	-2.01	1.38	1.43
11	aB	808	CLA	C1C-C2C	2.01	1.48	1.44
11	aA	841	CLA	C3D-C4D	-2.01	1.39	1.44
11	aB	811	CLA	C1A-CHA	2.01	1.51	1.43
11	cB	808	CLA	C1C-C2C	2.01	1.48	1.44
11	bB	813	CLA	C1A-CHA	2.01	1.51	1.43
11	cA	840	CLA	C3B-C2B	2.01	1.48	1.41
11	bA	834	CLA	C3B-C2B	2.01	1.48	1.41
11	cA	812	CLA	C1A-CHA	2.01	1.51	1.43
11	aB	815	CLA	C4C-C3C	2.01	1.48	1.45
11	aA	812	CLA	C1A-CHA	2.01	1.51	1.43
11	aA	819	CLA	C1A-CHA	2.01	1.51	1.43
11	aA	808	CLA	C1A-CHA	2.01	1.51	1.43
11	aA	812	CLA	C1C-C2C	2.01	1.48	1.44
11	aA	807	CLA	C1A-CHA	2.01	1.51	1.43
11	aA	834	CLA	C3B-C2B	2.01	1.48	1.41
11	bB	814	CLA	C1A-CHA	2.00	1.51	1.43
11	cB	813	CLA	C1A-CHA	2.00	1.51	1.43
11	cA	816	CLA	C1A-CHA	2.00	1.51	1.43
11	cA	825	CLA	C3B-C2B	2.00	1.48	1.41
11	bA	807	CLA	C1A-CHA	2.00	1.51	1.43
11	bB	836	CLA	C3B-C2B	2.00	1.48	1.41
11	cA	841	CLA	C3D-C4D	-2.00	1.39	1.44
11	aK	103	CLA	C1A-CHA	2.00	1.51	1.43
11	cA	819	CLA	C1A-CHA	2.00	1.51	1.43
11	cK	103	CLA	C1A-CHA	2.00	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	aL	205	CLA	C1A-CHA	2.00	1.51	1.43

All (8126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aA	829	CLA	C4-C3-C5	-21.94	78.37	115.27
11	cA	829	CLA	C4-C3-C5	-21.93	78.38	115.27
11	bA	829	CLA	C4-C3-C5	-21.91	78.42	115.27
11	bA	829	CLA	C5-C3-C2	19.02	159.62	121.12
11	aA	829	CLA	C5-C3-C2	19.00	159.57	121.12
11	cA	829	CLA	C5-C3-C2	19.00	159.57	121.12
11	cA	829	CLA	C4-C3-C2	-16.51	81.32	123.68
11	bA	829	CLA	C4-C3-C2	-16.50	81.34	123.68
11	aA	829	CLA	C4-C3-C2	-16.50	81.34	123.68
12	aA	827	F6C	C1D-ND-C4D	-15.22	99.86	106.71
12	bA	827	F6C	C1D-ND-C4D	-15.17	99.89	106.71
12	cA	844	F6C	C1D-ND-C4D	-15.16	99.89	106.71
12	cA	827	F6C	C1D-ND-C4D	-15.10	99.92	106.71
12	bA	844	F6C	C1D-ND-C4D	-15.07	99.93	106.71
12	aA	844	F6C	C1D-ND-C4D	-14.98	99.97	106.71
12	aA	832	F6C	C1D-ND-C4D	-14.62	100.13	106.71
12	bA	826	F6C	C1D-ND-C4D	-14.59	100.15	106.71
12	aA	826	F6C	C1D-ND-C4D	-14.58	100.15	106.71
12	bA	832	F6C	C1D-ND-C4D	-14.56	100.16	106.71
12	cA	826	F6C	C1D-ND-C4D	-14.52	100.18	106.71
12	aA	830	F6C	C1D-ND-C4D	-14.48	100.19	106.71
12	cA	832	F6C	C1D-ND-C4D	-14.44	100.22	106.71
12	cA	830	F6C	C1D-ND-C4D	-14.41	100.23	106.71
12	bA	830	F6C	C1D-ND-C4D	-14.38	100.24	106.71
12	cL	202	F6C	C1D-ND-C4D	-14.30	100.28	106.71
12	aL	202	F6C	C1D-ND-C4D	-14.30	100.28	106.71
12	bL	202	F6C	C1D-ND-C4D	-14.23	100.31	106.71
12	cB	824	F6C	C1D-ND-C4D	-14.11	100.36	106.71
12	aB	824	F6C	C1D-ND-C4D	-14.05	100.39	106.71
12	bB	824	F6C	C1D-ND-C4D	-13.98	100.42	106.71
12	aB	824	F6C	CAA-C2A-C3A	-12.80	104.04	127.88
12	cB	824	F6C	CAA-C2A-C3A	-12.80	104.05	127.88
12	bB	824	F6C	CAA-C2A-C3A	-12.77	104.09	127.88
12	cA	827	F6C	CAA-C2A-C3A	-12.19	105.17	127.88
12	bA	827	F6C	CAA-C2A-C3A	-12.18	105.20	127.88
12	aA	827	F6C	CAA-C2A-C3A	-12.18	105.20	127.88
12	cA	832	F6C	CAA-C2A-C3A	-10.75	107.85	127.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	832	F6C	CAA-C2A-C3A	-10.75	107.85	127.88
12	aA	832	F6C	CAA-C2A-C3A	-10.73	107.90	127.88
12	aA	830	F6C	CAA-C2A-C3A	-10.29	108.71	127.88
12	bA	830	F6C	CAA-C2A-C3A	-10.26	108.78	127.88
12	cA	830	F6C	CAA-C2A-C3A	-10.24	108.81	127.88
12	cA	844	F6C	CAA-C2A-C3A	-10.18	108.92	127.88
12	bA	844	F6C	CAA-C2A-C3A	-10.17	108.94	127.88
12	cL	202	F6C	C3A-C4A-NA	10.16	117.59	110.10
12	aA	844	F6C	CAA-C2A-C3A	-10.16	108.96	127.88
12	bL	202	F6C	C3A-C4A-NA	10.11	117.55	110.10
12	aL	202	F6C	C3A-C4A-NA	10.10	117.55	110.10
12	aA	844	F6C	CMA-C3A-C4A	-10.04	107.02	124.71
12	cA	844	F6C	CMA-C3A-C4A	-10.04	107.03	124.71
12	bA	844	F6C	CMA-C3A-C4A	-10.02	107.06	124.71
11	bB	822	CLA	C1D-ND-C4D	-9.64	99.48	106.33
11	aA	803	CLA	C2D-C1D-ND	9.61	117.19	110.10
11	bA	803	CLA	C2D-C1D-ND	9.61	117.18	110.10
12	cA	832	F6C	CMA-C3A-C4A	-9.60	107.79	124.71
11	aB	822	CLA	C1D-ND-C4D	-9.60	99.52	106.33
11	cA	818	CLA	C1D-ND-C4D	-9.59	99.52	106.33
12	aA	832	F6C	CMA-C3A-C4A	-9.57	107.84	124.71
12	bB	824	F6C	CMA-C3A-C4A	-9.57	107.84	124.71
12	bA	832	F6C	CMA-C3A-C4A	-9.56	107.87	124.71
11	cA	803	CLA	C2D-C1D-ND	9.56	117.15	110.10
11	cB	822	CLA	C1D-ND-C4D	-9.55	99.55	106.33
12	aB	824	F6C	CMA-C3A-C4A	-9.55	107.88	124.71
12	cB	824	F6C	CMA-C3A-C4A	-9.55	107.88	124.71
11	bA	818	CLA	C1D-ND-C4D	-9.52	99.57	106.33
11	aA	818	CLA	C1D-ND-C4D	-9.51	99.58	106.33
11	cA	823	CLA	C2D-C1D-ND	9.47	117.08	110.10
11	aB	820	CLA	C1D-ND-C4D	-9.45	99.62	106.33
11	aA	823	CLA	C2D-C1D-ND	9.43	117.05	110.10
11	bA	823	CLA	C2D-C1D-ND	9.43	117.05	110.10
11	cB	820	CLA	C1D-ND-C4D	-9.39	99.67	106.33
11	cA	808	CLA	C1D-ND-C4D	-9.35	99.70	106.33
11	aA	808	CLA	C1D-ND-C4D	-9.35	99.70	106.33
11	bB	820	CLA	C1D-ND-C4D	-9.34	99.70	106.33
11	aA	803	CLA	C1D-ND-C4D	-9.33	99.71	106.33
11	cA	803	CLA	C1D-ND-C4D	-9.31	99.72	106.33
11	bA	808	CLA	C1D-ND-C4D	-9.31	99.72	106.33
11	bA	803	CLA	C1D-ND-C4D	-9.29	99.74	106.33
11	bA	828	CLA	C1D-ND-C4D	-9.27	99.75	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aA	828	CLA	C1D-ND-C4D	-9.27	99.75	106.33
11	cA	823	CLA	C1D-ND-C4D	-9.26	99.75	106.33
11	bB	838	CLA	C1D-ND-C4D	-9.26	99.76	106.33
11	cB	838	CLA	C1D-ND-C4D	-9.26	99.76	106.33
11	aA	840	CLA	C1D-ND-C4D	-9.26	99.76	106.33
12	aB	824	F6C	C3A-C4A-NA	9.26	116.93	110.10
11	cL	206	CLA	C1D-ND-C4D	-9.26	99.76	106.33
11	bL	206	CLA	C1D-ND-C4D	-9.25	99.76	106.33
11	cA	828	CLA	C1D-ND-C4D	-9.23	99.78	106.33
11	bA	823	CLA	C1D-ND-C4D	-9.23	99.78	106.33
11	aL	206	CLA	C1D-ND-C4D	-9.23	99.78	106.33
11	bA	840	CLA	C1D-ND-C4D	-9.23	99.78	106.33
11	bA	841	CLA	C1D-ND-C4D	-9.23	99.78	106.33
11	cA	840	CLA	C1D-ND-C4D	-9.23	99.78	106.33
11	aA	841	CLA	C1D-ND-C4D	-9.22	99.78	106.33
11	aB	838	CLA	C1D-ND-C4D	-9.22	99.79	106.33
11	aB	804	CLA	C1D-ND-C4D	-9.21	99.79	106.33
11	cB	818	CLA	C1D-ND-C4D	-9.21	99.79	106.33
11	aB	818	CLA	C1D-ND-C4D	-9.20	99.80	106.33
11	aA	823	CLA	C1D-ND-C4D	-9.20	99.80	106.33
12	cB	824	F6C	C3A-C4A-NA	9.20	116.88	110.10
11	bB	801	CLA	C1D-ND-C4D	-9.20	99.80	106.33
11	cA	818	CLA	C2D-C1D-ND	9.19	116.88	110.10
12	bA	844	F6C	C3A-C4A-NA	9.19	116.88	110.10
12	aA	830	F6C	C3A-C4A-NA	9.18	116.87	110.10
11	bB	818	CLA	C1D-ND-C4D	-9.18	99.82	106.33
12	cA	826	F6C	C3A-C4A-NA	9.17	116.86	110.10
11	cA	841	CLA	C1D-ND-C4D	-9.17	99.82	106.33
12	bB	824	F6C	C3A-C4A-NA	9.17	116.86	110.10
12	aA	844	F6C	C3A-C4A-NA	9.16	116.86	110.10
11	aB	801	CLA	C1D-ND-C4D	-9.16	99.83	106.33
12	cA	844	F6C	C3A-C4A-NA	9.16	116.86	110.10
11	aA	818	CLA	C2D-C1D-ND	9.15	116.85	110.10
11	bA	818	CLA	C2D-C1D-ND	9.13	116.83	110.10
11	aA	806	CLA	C2B-C1B-NB	9.13	116.35	110.23
12	bA	826	F6C	C3A-C4A-NA	9.12	116.83	110.10
11	cK	103	CLA	C1D-ND-C4D	-9.12	99.85	106.33
11	cB	801	CLA	C1D-ND-C4D	-9.12	99.85	106.33
12	cA	830	F6C	C3A-C4A-NA	9.12	116.83	110.10
11	cB	804	CLA	C1D-ND-C4D	-9.12	99.86	106.33
11	bK	103	CLA	C1D-ND-C4D	-9.11	99.86	106.33
12	aA	826	F6C	C3A-C4A-NA	9.11	116.82	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bB	804	CLA	C1D-ND-C4D	-9.10	99.87	106.33
11	aA	837	CLA	C1D-ND-C4D	-9.10	99.87	106.33
11	cA	837	CLA	C1D-ND-C4D	-9.09	99.88	106.33
11	cA	806	CLA	C2B-C1B-NB	9.09	116.33	110.23
11	bA	806	CLA	C2B-C1B-NB	9.09	116.33	110.23
11	bB	802	CLA	C2B-C1B-NB	9.08	116.32	110.23
11	aA	806	CLA	C1D-ND-C4D	-9.08	99.89	106.33
11	aB	833	CLA	C1D-ND-C4D	-9.08	99.89	106.33
11	bB	833	CLA	C1D-ND-C4D	-9.07	99.89	106.33
12	bA	830	F6C	C3A-C4A-NA	9.07	116.79	110.10
11	aL	205	CLA	C1D-ND-C4D	-9.07	99.89	106.33
11	cB	833	CLA	C1D-ND-C4D	-9.07	99.89	106.33
12	bA	830	F6C	CMA-C3A-C4A	-9.07	108.74	124.71
11	cA	806	CLA	C1D-ND-C4D	-9.06	99.90	106.33
11	aK	103	CLA	C1D-ND-C4D	-9.05	99.91	106.33
11	bA	806	CLA	C1D-ND-C4D	-9.05	99.91	106.33
11	cL	205	CLA	C1D-ND-C4D	-9.05	99.91	106.33
11	aB	803	CLA	C2D-C1D-ND	9.05	116.77	110.10
11	bL	205	CLA	C1D-ND-C4D	-9.04	99.91	106.33
12	aA	830	F6C	CMA-C3A-C4A	-9.04	108.78	124.71
11	cB	802	CLA	C2B-C1B-NB	9.04	116.29	110.23
11	cB	825	CLA	C1D-ND-C4D	-9.04	99.91	106.33
12	cA	830	F6C	CMA-C3A-C4A	-9.03	108.80	124.71
11	bA	837	CLA	C1D-ND-C4D	-9.03	99.92	106.33
12	aA	827	F6C	C3A-C4A-NA	9.01	116.75	110.10
12	bA	827	F6C	C3A-C4A-NA	9.00	116.74	110.10
11	bB	825	CLA	C1D-ND-C4D	-8.99	99.95	106.33
11	cA	842	CLA	C1D-ND-C4D	-8.98	99.96	106.33
11	bB	803	CLA	C2D-C1D-ND	8.98	116.72	110.10
11	cB	803	CLA	C2D-C1D-ND	8.98	116.72	110.10
11	aB	825	CLA	C1D-ND-C4D	-8.97	99.96	106.33
11	aB	802	CLA	C2B-C1B-NB	8.96	116.24	110.23
11	bA	807	CLA	C1D-ND-C4D	-8.96	99.97	106.33
11	cA	807	CLA	C1D-ND-C4D	-8.96	99.97	106.33
11	cA	819	CLA	C1D-ND-C4D	-8.96	99.97	106.33
11	cA	813	CLA	C1D-ND-C4D	-8.94	99.98	106.33
11	bA	842	CLA	C1D-ND-C4D	-8.94	99.99	106.33
10	cA	801	CL0	C1D-ND-C4D	-8.93	99.99	106.33
11	aA	842	CLA	C1D-ND-C4D	-8.93	99.99	106.33
11	bL	204	CLA	C1D-ND-C4D	-8.93	99.99	106.33
11	aA	814	CLA	C1D-ND-C4D	-8.92	99.99	106.33
12	cA	832	F6C	C3A-C4A-NA	8.92	116.68	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bA	828	CLA	C2D-C1D-ND	8.92	116.68	110.10
11	bA	816	CLA	C1D-ND-C4D	-8.91	100.00	106.33
11	cL	204	CLA	C1D-ND-C4D	-8.91	100.00	106.33
11	bA	819	CLA	C1D-ND-C4D	-8.91	100.00	106.33
11	aA	807	CLA	C1D-ND-C4D	-8.91	100.01	106.33
11	bB	817	CLA	C1D-ND-C4D	-8.91	100.01	106.33
12	aA	832	F6C	C3A-C4A-NA	8.91	116.67	110.10
11	aA	819	CLA	C1D-ND-C4D	-8.90	100.01	106.33
11	bB	826	CLA	C1D-ND-C4D	-8.90	100.01	106.33
11	cB	826	CLA	C1D-ND-C4D	-8.90	100.01	106.33
11	cA	816	CLA	C1D-ND-C4D	-8.90	100.02	106.33
12	bA	832	F6C	C3A-C4A-NA	8.89	116.66	110.10
11	aA	816	CLA	C1D-ND-C4D	-8.89	100.02	106.33
12	cA	827	F6C	C3A-C4A-NA	8.89	116.65	110.10
11	cB	817	CLA	C1D-ND-C4D	-8.89	100.02	106.33
11	aA	813	CLA	C1D-ND-C4D	-8.88	100.03	106.33
11	bA	813	CLA	C1D-ND-C4D	-8.88	100.03	106.33
11	aB	807	CLA	C1D-ND-C4D	-8.88	100.03	106.33
11	cA	814	CLA	C1D-ND-C4D	-8.88	100.03	106.33
11	cA	828	CLA	C2D-C1D-ND	8.87	116.64	110.10
11	aB	817	CLA	C1D-ND-C4D	-8.87	100.03	106.33
11	bB	807	CLA	C1D-ND-C4D	-8.87	100.04	106.33
10	aA	801	CL0	C1D-ND-C4D	-8.86	100.04	106.33
10	bA	801	CL0	C1D-ND-C4D	-8.86	100.04	106.33
11	aB	826	CLA	C1D-ND-C4D	-8.85	100.05	106.33
11	bA	804	CLA	C1D-ND-C4D	-8.85	100.05	106.33
11	bA	835	CLA	C1D-ND-C4D	-8.85	100.05	106.33
11	bB	803	CLA	C1D-ND-C4D	-8.85	100.05	106.33
11	bA	814	CLA	C1D-ND-C4D	-8.85	100.05	106.33
11	aB	803	CLA	C1D-ND-C4D	-8.85	100.05	106.33
11	bB	832	CLA	C1D-ND-C4D	-8.85	100.05	106.33
11	cK	101	CLA	C1D-ND-C4D	-8.85	100.05	106.33
11	bA	839	CLA	C1D-ND-C4D	-8.84	100.06	106.33
11	aA	839	CLA	C1D-ND-C4D	-8.84	100.06	106.33
11	aL	204	CLA	C1D-ND-C4D	-8.84	100.06	106.33
11	aB	822	CLA	C2D-C1D-ND	8.84	116.61	110.10
11	cB	807	CLA	C1D-ND-C4D	-8.83	100.06	106.33
11	cA	839	CLA	C1D-ND-C4D	-8.83	100.06	106.33
11	bB	837	CLA	C1D-ND-C4D	-8.83	100.06	106.33
11	aB	832	CLA	C1D-ND-C4D	-8.82	100.07	106.33
11	bB	822	CLA	C2D-C1D-ND	8.82	116.61	110.10
11	aB	816	CLA	C1D-ND-C4D	-8.82	100.07	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aA	810	CLA	C1D-ND-C4D	-8.82	100.07	106.33
11	cB	803	CLA	C1D-ND-C4D	-8.82	100.07	106.33
11	bK	101	CLA	C1D-ND-C4D	-8.82	100.07	106.33
11	aA	828	CLA	C2D-C1D-ND	8.82	116.60	110.10
11	bA	810	CLA	C1D-ND-C4D	-8.81	100.07	106.33
11	aK	101	CLA	C1D-ND-C4D	-8.81	100.08	106.33
11	bB	806	CLA	C1D-ND-C4D	-8.81	100.08	106.33
11	cB	832	CLA	C1D-ND-C4D	-8.81	100.08	106.33
11	cA	835	CLA	C1D-ND-C4D	-8.81	100.08	106.33
11	aA	804	CLA	C1D-ND-C4D	-8.81	100.08	106.33
11	aB	806	CLA	C1D-ND-C4D	-8.80	100.08	106.33
11	aB	836	CLA	C1D-ND-C4D	-8.80	100.09	106.33
11	cB	822	CLA	C2D-C1D-ND	8.79	116.58	110.10
11	bB	809	CLA	C1D-ND-C4D	-8.79	100.09	106.33
11	aB	815	CLA	C1D-ND-C4D	-8.79	100.09	106.33
11	aA	835	CLA	C1D-ND-C4D	-8.79	100.09	106.33
11	aB	821	CLA	C1D-ND-C4D	-8.79	100.09	106.33
11	cB	816	CLA	C1D-ND-C4D	-8.78	100.10	106.33
11	cA	804	CLA	C1D-ND-C4D	-8.77	100.10	106.33
11	cB	806	CLA	C1D-ND-C4D	-8.77	100.11	106.33
11	cB	815	CLA	C1D-ND-C4D	-8.77	100.11	106.33
11	bB	815	CLA	C1D-ND-C4D	-8.77	100.11	106.33
11	cA	810	CLA	C1D-ND-C4D	-8.76	100.11	106.33
11	aB	809	CLA	C1D-ND-C4D	-8.75	100.12	106.33
11	cB	809	CLA	C1D-ND-C4D	-8.75	100.12	106.33
11	aB	837	CLA	C1D-ND-C4D	-8.74	100.12	106.33
11	cB	835	CLA	C1D-ND-C4D	-8.74	100.13	106.33
11	cA	811	CLA	C1D-ND-C4D	-8.74	100.13	106.33
11	cA	833	CLA	C1D-ND-C4D	-8.74	100.13	106.33
11	aA	824	CLA	C1D-ND-C4D	-8.73	100.13	106.33
11	aA	811	CLA	C1D-ND-C4D	-8.73	100.13	106.33
11	bA	811	CLA	C1D-ND-C4D	-8.73	100.14	106.33
11	bB	836	CLA	C1D-ND-C4D	-8.72	100.14	106.33
11	aB	805	CLA	C1D-ND-C4D	-8.72	100.14	106.33
11	aA	833	CLA	C1D-ND-C4D	-8.72	100.14	106.33
11	bA	833	CLA	C1D-ND-C4D	-8.72	100.14	106.33
11	bB	816	CLA	C1D-ND-C4D	-8.72	100.14	106.33
12	cA	827	F6C	CAA-C2A-C1A	-8.72	104.11	128.11
11	cB	837	CLA	C1D-ND-C4D	-8.71	100.14	106.33
12	bA	827	F6C	CAA-C2A-C1A	-8.71	104.14	128.11
11	cB	821	CLA	C1D-ND-C4D	-8.70	100.15	106.33
11	bB	826	CLA	C2D-C1D-ND	8.70	116.52	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	827	F6C	CAA-C2A-C1A	-8.70	104.14	128.11
11	cB	826	CLA	C2D-C1D-ND	8.70	116.52	110.10
11	bA	834	CLA	C1D-ND-C4D	-8.70	100.16	106.33
11	cA	834	CLA	C1D-ND-C4D	-8.70	100.16	106.33
11	aA	809	CLA	C1D-ND-C4D	-8.70	100.16	106.33
11	bB	805	CLA	C1D-ND-C4D	-8.69	100.16	106.33
11	bA	805	CLA	C1D-ND-C4D	-8.69	100.16	106.33
11	aA	834	CLA	C1D-ND-C4D	-8.69	100.16	106.33
11	aB	835	CLA	C1D-ND-C4D	-8.69	100.17	106.33
11	bB	835	CLA	C1D-ND-C4D	-8.69	100.17	106.33
11	cB	836	CLA	C1D-ND-C4D	-8.68	100.17	106.33
11	cA	805	CLA	C1D-ND-C4D	-8.68	100.17	106.33
11	cB	840	CLA	C1D-ND-C4D	-8.68	100.17	106.33
11	bA	841	CLA	C2D-C1D-ND	8.68	116.50	110.10
11	bA	824	CLA	C1D-ND-C4D	-8.68	100.17	106.33
11	aB	814	CLA	C1D-ND-C4D	-8.68	100.17	106.33
11	cA	824	CLA	C1D-ND-C4D	-8.68	100.17	106.33
11	bA	821	CLA	C1D-ND-C4D	-8.67	100.18	106.33
11	bB	821	CLA	C1D-ND-C4D	-8.67	100.18	106.33
11	aA	805	CLA	C1D-ND-C4D	-8.67	100.18	106.33
11	aA	841	CLA	C2D-C1D-ND	8.67	116.49	110.10
11	bB	811	CLA	C1D-ND-C4D	-8.66	100.18	106.33
11	cA	821	CLA	C1D-ND-C4D	-8.66	100.18	106.33
11	cA	809	CLA	C1D-ND-C4D	-8.66	100.18	106.33
11	cB	805	CLA	C1D-ND-C4D	-8.65	100.19	106.33
11	bB	839	CLA	C1D-ND-C4D	-8.65	100.19	106.33
11	aB	820	CLA	C2D-C1D-ND	8.65	116.48	110.10
11	aA	836	CLA	C1D-ND-C4D	-8.65	100.19	106.33
11	bB	810	CLA	C1D-ND-C4D	-8.65	100.19	106.33
11	aA	821	CLA	C1D-ND-C4D	-8.65	100.19	106.33
11	bB	840	CLA	C1D-ND-C4D	-8.64	100.19	106.33
11	cB	811	CLA	C1D-ND-C4D	-8.64	100.20	106.33
11	cB	839	CLA	C1D-ND-C4D	-8.64	100.20	106.33
11	cA	829	CLA	C1D-ND-C4D	-8.64	100.20	106.33
11	aA	803	CLA	C2B-C1B-NB	8.64	116.02	110.23
11	bA	829	CLA	C1D-ND-C4D	-8.64	100.20	106.33
11	bA	809	CLA	C1D-ND-C4D	-8.64	100.20	106.33
11	cA	841	CLA	C2D-C1D-ND	8.64	116.47	110.10
11	aB	826	CLA	C2D-C1D-ND	8.63	116.47	110.10
11	aB	839	CLA	C1D-ND-C4D	-8.63	100.20	106.33
11	aB	811	CLA	C1D-ND-C4D	-8.63	100.21	106.33
11	cB	814	CLA	C1D-ND-C4D	-8.63	100.21	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cA	803	CLA	C2B-C1B-NB	8.62	116.01	110.23
11	bB	814	CLA	C1D-ND-C4D	-8.62	100.21	106.33
11	aA	822	CLA	C1D-ND-C4D	-8.61	100.22	106.33
11	aB	840	CLA	C1D-ND-C4D	-8.60	100.22	106.33
11	cB	820	CLA	C2D-C1D-ND	8.60	116.44	110.10
11	aB	810	CLA	C1D-ND-C4D	-8.60	100.22	106.33
11	bB	820	CLA	C2D-C1D-ND	8.60	116.44	110.10
11	bA	803	CLA	C2B-C1B-NB	8.59	115.99	110.23
11	cA	836	CLA	C1D-ND-C4D	-8.59	100.23	106.33
11	aA	829	CLA	C1D-ND-C4D	-8.59	100.23	106.33
11	bA	836	CLA	C1D-ND-C4D	-8.58	100.24	106.33
11	aB	813	CLA	C1D-ND-C4D	-8.58	100.24	106.33
11	bB	813	CLA	C1D-ND-C4D	-8.58	100.24	106.33
11	cB	825	CLA	C2D-C1D-ND	8.58	116.43	110.10
11	cA	822	CLA	C1D-ND-C4D	-8.58	100.24	106.33
11	cB	810	CLA	C1D-ND-C4D	-8.57	100.25	106.33
11	bA	822	CLA	C1D-ND-C4D	-8.57	100.25	106.33
11	cB	813	CLA	C1D-ND-C4D	-8.57	100.25	106.33
11	cB	819	CLA	C1D-ND-C4D	-8.56	100.25	106.33
11	bA	812	CLA	C1D-ND-C4D	-8.55	100.26	106.33
11	bA	838	CLA	C1D-ND-C4D	-8.54	100.27	106.33
11	aA	838	CLA	C1D-ND-C4D	-8.53	100.28	106.33
11	bB	819	CLA	C1D-ND-C4D	-8.53	100.28	106.33
11	aB	819	CLA	C1D-ND-C4D	-8.52	100.28	106.33
11	cB	831	CLA	C1D-ND-C4D	-8.52	100.28	106.33
11	bB	825	CLA	C2D-C1D-ND	8.51	116.37	110.10
11	aA	812	CLA	C1D-ND-C4D	-8.51	100.29	106.33
11	aB	825	CLA	C2D-C1D-ND	8.51	116.37	110.10
11	cA	838	CLA	C1D-ND-C4D	-8.51	100.29	106.33
11	cA	843	CLA	C1D-ND-C4D	-8.51	100.29	106.33
11	aA	843	CLA	C1D-ND-C4D	-8.49	100.30	106.33
11	bB	831	CLA	C1D-ND-C4D	-8.49	100.30	106.33
11	bA	843	CLA	C1D-ND-C4D	-8.46	100.32	106.33
12	bA	826	F6C	C3C-C4C-NC	8.46	116.09	110.21
11	aB	831	CLA	C1D-ND-C4D	-8.45	100.33	106.33
11	cA	812	CLA	C1D-ND-C4D	-8.45	100.33	106.33
11	aB	808	CLA	C1D-ND-C4D	-8.42	100.35	106.33
11	cA	805	CLA	C2B-C1B-NB	8.42	115.88	110.23
12	aA	826	F6C	C3C-C4C-NC	8.42	116.07	110.21
11	cB	808	CLA	C1D-ND-C4D	-8.42	100.35	106.33
11	bA	805	CLA	C2B-C1B-NB	8.41	115.87	110.23
11	aB	802	CLA	C1D-ND-C4D	-8.40	100.37	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bA	831	CLA	C1D-ND-C4D	-8.40	100.37	106.33
12	cA	826	F6C	C3C-C4C-NC	8.39	116.05	110.21
11	bB	832	CLA	C2B-C1B-NB	8.38	115.85	110.23
11	bB	808	CLA	C1D-ND-C4D	-8.38	100.38	106.33
11	bL	204	CLA	C2D-C1D-ND	8.37	116.28	110.10
11	aB	804	CLA	C2D-C1D-ND	8.37	116.27	110.10
11	aB	830	CLA	C1D-ND-C4D	-8.37	100.39	106.33
11	cK	103	CLA	C2D-C1D-ND	8.37	116.27	110.10
11	cB	838	CLA	C2D-C1D-ND	8.35	116.26	110.10
11	cB	802	CLA	C1D-ND-C4D	-8.35	100.41	106.33
11	bB	823	CLA	C1D-ND-C4D	-8.34	100.41	106.33
11	bK	103	CLA	C2D-C1D-ND	8.34	116.25	110.10
11	bB	830	CLA	C1D-ND-C4D	-8.33	100.42	106.33
11	aB	838	CLA	C2D-C1D-ND	8.33	116.24	110.10
11	bA	808	CLA	C2D-C1D-ND	8.33	116.24	110.10
11	bB	838	CLA	C2D-C1D-ND	8.33	116.24	110.10
11	aA	805	CLA	C2B-C1B-NB	8.32	115.81	110.23
11	cB	818	CLA	C2D-C1D-ND	8.32	116.24	110.10
11	aB	818	CLA	C2D-C1D-ND	8.32	116.23	110.10
11	cB	830	CLA	C1D-ND-C4D	-8.32	100.42	106.33
11	cL	204	CLA	C2D-C1D-ND	8.32	116.23	110.10
11	bB	801	CLA	C2D-C1D-ND	8.32	116.23	110.10
11	bA	819	CLA	C2D-C1D-ND	8.31	116.23	110.10
11	cB	801	CLA	C2D-C1D-ND	8.31	116.23	110.10
11	bB	818	CLA	C2D-C1D-ND	8.31	116.23	110.10
11	aA	831	CLA	C1D-ND-C4D	-8.31	100.43	106.33
11	aA	808	CLA	C2D-C1D-ND	8.31	116.23	110.10
11	aA	819	CLA	C2D-C1D-ND	8.30	116.22	110.10
11	aB	823	CLA	C1D-ND-C4D	-8.30	100.44	106.33
11	cB	832	CLA	C2B-C1B-NB	8.30	115.80	110.23
11	aB	801	CLA	C2D-C1D-ND	8.30	116.22	110.10
11	bB	802	CLA	C1D-ND-C4D	-8.29	100.44	106.33
11	cA	808	CLA	C2D-C1D-ND	8.29	116.21	110.10
11	cL	205	CLA	C2D-C1D-ND	8.29	116.21	110.10
11	bB	804	CLA	C2D-C1D-ND	8.29	116.21	110.10
11	cA	819	CLA	C2D-C1D-ND	8.28	116.21	110.10
11	aL	204	CLA	C2D-C1D-ND	8.28	116.21	110.10
11	aB	832	CLA	C2B-C1B-NB	8.28	115.78	110.23
11	bB	834	CLA	C1D-ND-C4D	-8.27	100.46	106.33
11	bL	205	CLA	C2D-C1D-ND	8.27	116.20	110.10
11	aK	103	CLA	C2D-C1D-ND	8.27	116.20	110.10
11	aA	842	CLA	C2D-C1D-ND	8.27	116.20	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cA	831	CLA	C1D-ND-C4D	-8.26	100.46	106.33
11	cB	823	CLA	C1D-ND-C4D	-8.26	100.46	106.33
11	cL	206	CLA	C2D-C1D-ND	8.26	116.19	110.10
11	cB	804	CLA	C2D-C1D-ND	8.25	116.19	110.10
11	bB	815	CLA	C2D-C1D-ND	8.25	116.18	110.10
11	bA	842	CLA	C2D-C1D-ND	8.25	116.18	110.10
11	cA	842	CLA	C2D-C1D-ND	8.25	116.18	110.10
11	cA	840	CLA	C2D-C1D-ND	8.24	116.18	110.10
11	bA	825	CLA	C1D-ND-C4D	-8.24	100.48	106.33
11	aL	205	CLA	C2D-C1D-ND	8.24	116.18	110.10
11	aB	834	CLA	C1D-ND-C4D	-8.24	100.48	106.33
11	aB	806	CLA	C2D-C1D-ND	8.24	116.17	110.10
11	aA	825	CLA	C1D-ND-C4D	-8.24	100.48	106.33
11	cA	825	CLA	C1D-ND-C4D	-8.23	100.49	106.33
11	bB	827	CLA	C1D-ND-C4D	-8.23	100.49	106.33
11	bA	820	CLA	C1D-ND-C4D	-8.23	100.49	106.33
11	aB	815	CLA	C2D-C1D-ND	8.22	116.16	110.10
11	cB	815	CLA	C2D-C1D-ND	8.22	116.16	110.10
11	cB	834	CLA	C1D-ND-C4D	-8.22	100.50	106.33
11	aL	206	CLA	C2D-C1D-ND	8.21	116.16	110.10
11	bL	206	CLA	C2D-C1D-ND	8.21	116.16	110.10
11	aB	805	CLA	C2B-C1B-NB	8.20	115.73	110.23
11	bA	817	CLA	C1D-ND-C4D	-8.20	100.51	106.33
11	bB	806	CLA	C2D-C1D-ND	8.20	116.15	110.10
11	bA	840	CLA	C2D-C1D-ND	8.20	116.15	110.10
11	aA	817	CLA	C1D-ND-C4D	-8.20	100.51	106.33
11	aA	840	CLA	C2D-C1D-ND	8.19	116.14	110.10
11	cB	827	CLA	C1D-ND-C4D	-8.19	100.52	106.33
11	bB	823	CLA	C2B-C1B-NB	8.19	115.72	110.23
11	bA	807	CLA	C2D-C1D-ND	8.19	116.14	110.10
11	aA	829	CLA	C2B-C1B-NB	8.18	115.72	110.23
11	aA	820	CLA	C1D-ND-C4D	-8.17	100.53	106.33
11	aA	836	CLA	C2D-C1D-ND	8.17	116.13	110.10
11	aB	807	CLA	C2D-C1D-ND	8.17	116.12	110.10
11	aA	802	CLA	C1D-ND-C4D	-8.17	100.53	106.33
11	aB	827	CLA	C1D-ND-C4D	-8.17	100.53	106.33
11	bB	805	CLA	C2B-C1B-NB	8.17	115.71	110.23
10	cA	801	CL0	C2D-C1D-ND	8.16	116.12	110.10
11	aB	816	CLA	C2B-C1B-NB	8.16	115.70	110.23
11	cB	816	CLA	C2B-C1B-NB	8.16	115.70	110.23
11	cA	820	CLA	C1D-ND-C4D	-8.16	100.54	106.33
11	cA	807	CLA	C2D-C1D-ND	8.16	116.12	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cA	802	CLA	C1D-ND-C4D	-8.15	100.55	106.33
11	aB	836	CLA	C2D-C1D-ND	8.15	116.11	110.10
11	cB	823	CLA	C2B-C1B-NB	8.14	115.69	110.23
11	bA	831	CLA	C2D-C1D-ND	8.14	116.10	110.10
11	bB	807	CLA	C2D-C1D-ND	8.14	116.10	110.10
11	cB	806	CLA	C2D-C1D-ND	8.14	116.10	110.10
11	cB	805	CLA	C2B-C1B-NB	8.14	115.69	110.23
11	cA	836	CLA	C2D-C1D-ND	8.13	116.10	110.10
11	cA	829	CLA	C2B-C1B-NB	8.13	115.68	110.23
11	aA	807	CLA	C2D-C1D-ND	8.12	116.09	110.10
11	cA	812	CLA	C2B-C1B-NB	8.11	115.67	110.23
11	cA	817	CLA	C1D-ND-C4D	-8.11	100.57	106.33
10	aA	801	CL0	C2D-C1D-ND	8.11	116.08	110.10
11	cB	836	CLA	C2D-C1D-ND	8.11	116.08	110.10
11	aA	835	CLA	C2D-C1D-ND	8.10	116.08	110.10
11	cA	813	CLA	C2D-C1D-ND	8.10	116.08	110.10
11	cA	837	CLA	C2D-C1D-ND	8.10	116.07	110.10
11	bA	829	CLA	C2B-C1B-NB	8.10	115.66	110.23
11	bA	812	CLA	C2B-C1B-NB	8.09	115.66	110.23
10	bA	801	CL0	C2D-C1D-ND	8.09	116.07	110.10
11	bA	802	CLA	C1D-ND-C4D	-8.09	100.59	106.33
11	cB	807	CLA	C2D-C1D-ND	8.09	116.07	110.10
11	aA	831	CLA	C2D-C1D-ND	8.09	116.07	110.10
11	bA	836	CLA	C2D-C1D-ND	8.09	116.06	110.10
11	aB	823	CLA	C2B-C1B-NB	8.09	115.65	110.23
12	bL	202	F6C	C2C-C1C-NC	8.09	115.65	110.23
12	cL	202	F6C	C2C-C1C-NC	8.08	115.65	110.23
11	aA	805	CLA	C2D-C1D-ND	8.08	116.06	110.10
11	cA	805	CLA	C2D-C1D-ND	8.08	116.06	110.10
11	bA	815	CLA	C1D-ND-C4D	-8.07	100.60	106.33
11	bA	835	CLA	C2D-C1D-ND	8.07	116.05	110.10
11	cA	831	CLA	C2D-C1D-ND	8.07	116.05	110.10
11	aA	813	CLA	C2D-C1D-ND	8.07	116.05	110.10
11	aB	817	CLA	C2D-C1D-ND	8.07	116.05	110.10
11	cB	817	CLA	C2D-C1D-ND	8.07	116.05	110.10
11	bA	813	CLA	C2D-C1D-ND	8.06	116.05	110.10
11	bA	805	CLA	C2D-C1D-ND	8.06	116.04	110.10
11	aA	837	CLA	C2D-C1D-ND	8.06	116.04	110.10
11	bB	836	CLA	C2D-C1D-ND	8.06	116.04	110.10
11	bB	817	CLA	C2D-C1D-ND	8.05	116.04	110.10
12	aA	827	F6C	CMA-C3A-C4A	-8.05	110.53	124.71
11	aA	815	CLA	C1D-ND-C4D	-8.05	100.62	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cA	835	CLA	C2D-C1D-ND	8.05	116.03	110.10
11	cA	815	CLA	C1D-ND-C4D	-8.05	100.62	106.33
11	bB	816	CLA	C2B-C1B-NB	8.05	115.63	110.23
11	aA	812	CLA	C2B-C1B-NB	8.04	115.62	110.23
12	bA	827	F6C	CMA-C3A-C4A	-8.04	110.54	124.71
11	bA	837	CLA	C2D-C1D-ND	8.04	116.03	110.10
12	cA	827	F6C	CMA-C3A-C4A	-8.04	110.55	124.71
12	aL	202	F6C	C2C-C1C-NC	8.01	115.60	110.23
11	aA	809	CLA	C2D-C1D-ND	7.99	115.99	110.10
11	aB	833	CLA	C2D-C1D-ND	7.99	115.99	110.10
11	aB	812	CLA	C1D-ND-C4D	-7.97	100.67	106.33
11	bB	809	CLA	C2D-C1D-ND	7.97	115.98	110.10
11	cB	809	CLA	C2D-C1D-ND	7.96	115.97	110.10
11	cA	809	CLA	C2D-C1D-ND	7.96	115.97	110.10
11	cB	833	CLA	C2D-C1D-ND	7.95	115.97	110.10
11	aB	809	CLA	C2D-C1D-ND	7.95	115.96	110.10
11	aB	814	CLA	C2B-C1B-NB	7.94	115.56	110.23
11	bB	833	CLA	C2D-C1D-ND	7.94	115.96	110.10
11	cB	814	CLA	C2B-C1B-NB	7.94	115.55	110.23
11	bA	809	CLA	C2D-C1D-ND	7.92	115.94	110.10
11	bB	829	CLA	C1D-ND-C4D	-7.92	100.71	106.33
11	aA	819	CLA	C2B-C1B-NB	7.92	115.54	110.23
11	cB	829	CLA	C1D-ND-C4D	-7.92	100.71	106.33
11	cA	816	CLA	C2D-C1D-ND	7.92	115.94	110.10
11	bA	821	CLA	C2D-C1D-ND	7.91	115.94	110.10
11	aB	814	CLA	C2D-C1D-ND	7.91	115.93	110.10
11	bB	814	CLA	C2B-C1B-NB	7.91	115.53	110.23
11	bB	812	CLA	C1D-ND-C4D	-7.90	100.72	106.33
11	aA	839	CLA	C2D-C1D-ND	7.90	115.92	110.10
11	bA	809	CLA	C2B-C1B-NB	7.89	115.52	110.23
11	bA	839	CLA	C2D-C1D-ND	7.89	115.92	110.10
11	cA	821	CLA	C2D-C1D-ND	7.89	115.92	110.10
11	bB	821	CLA	C2D-C1D-ND	7.89	115.92	110.10
11	aA	821	CLA	C2D-C1D-ND	7.88	115.91	110.10
11	aB	816	CLA	C2D-C1D-ND	7.88	115.91	110.10
11	aA	840	CLA	C2B-C1B-NB	7.88	115.51	110.23
11	aA	816	CLA	C2D-C1D-ND	7.88	115.91	110.10
12	bA	826	F6C	C2C-C1C-NC	7.87	115.51	110.23
11	bA	816	CLA	C2D-C1D-ND	7.87	115.91	110.10
11	bA	819	CLA	C2B-C1B-NB	7.86	115.50	110.23
11	aB	821	CLA	C2D-C1D-ND	7.86	115.90	110.10
11	cB	833	CLA	C2B-C1B-NB	7.86	115.50	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bB	814	CLA	C2D-C1D-ND	7.86	115.90	110.10
12	aA	826	F6C	C2C-C1C-NC	7.86	115.50	110.23
11	cB	812	CLA	C1D-ND-C4D	-7.85	100.76	106.33
11	bB	816	CLA	C2D-C1D-ND	7.85	115.89	110.10
11	cA	816	CLA	C2B-C1B-NB	7.85	115.49	110.23
11	cB	816	CLA	C2D-C1D-ND	7.84	115.88	110.10
11	aB	829	CLA	C1D-ND-C4D	-7.84	100.77	106.33
11	cB	814	CLA	C2D-C1D-ND	7.84	115.88	110.10
11	cA	819	CLA	C2B-C1B-NB	7.84	115.49	110.23
11	aA	816	CLA	C2B-C1B-NB	7.83	115.48	110.23
11	cA	839	CLA	C2D-C1D-ND	7.83	115.88	110.10
11	bB	833	CLA	C2B-C1B-NB	7.83	115.48	110.23
11	bA	806	CLA	C2D-C1D-ND	7.83	115.87	110.10
11	bB	832	CLA	C2D-C1D-ND	7.83	115.87	110.10
11	aB	833	CLA	C2B-C1B-NB	7.83	115.48	110.23
11	bA	833	CLA	C2D-C1D-ND	7.82	115.87	110.10
11	cA	840	CLA	C2B-C1B-NB	7.82	115.48	110.23
11	aA	809	CLA	C2B-C1B-NB	7.82	115.47	110.23
11	bA	840	CLA	C2B-C1B-NB	7.82	115.47	110.23
11	cA	829	CLA	C2D-C1D-ND	7.82	115.87	110.10
11	cB	821	CLA	C2D-C1D-ND	7.82	115.86	110.10
11	cA	809	CLA	C2B-C1B-NB	7.82	115.47	110.23
11	bB	837	CLA	C2D-C1D-ND	7.82	115.86	110.10
12	cB	824	F6C	CAA-C2A-C1A	-7.81	106.60	128.11
11	aA	806	CLA	C2D-C1D-ND	7.81	115.86	110.10
11	cA	818	CLA	C2B-C1B-NB	7.81	115.47	110.23
11	cA	833	CLA	C2D-C1D-ND	7.81	115.86	110.10
11	cB	840	CLA	C2D-C1D-ND	7.81	115.86	110.10
12	aB	824	F6C	CAA-C2A-C1A	-7.81	106.61	128.11
11	bA	804	CLA	C2D-C1D-ND	7.80	115.86	110.10
12	bL	202	F6C	CMA-C3A-C4A	-7.80	110.96	124.71
12	bB	824	F6C	CAA-C2A-C1A	-7.80	106.62	128.11
12	aL	202	F6C	CMA-C3A-C4A	-7.80	110.96	124.71
11	aA	833	CLA	C2D-C1D-ND	7.80	115.85	110.10
11	cB	837	CLA	C2D-C1D-ND	7.79	115.85	110.10
11	cA	842	CLA	C2B-C1B-NB	7.79	115.46	110.23
12	cL	202	F6C	CMA-C3A-C4A	-7.79	110.99	124.71
11	aB	831	CLA	C2B-C1B-NB	7.79	115.45	110.23
11	bA	829	CLA	C2D-C1D-ND	7.78	115.84	110.10
11	bB	840	CLA	C2D-C1D-ND	7.78	115.84	110.10
11	aB	802	CLA	C2D-C1D-ND	7.78	115.84	110.10
11	aB	832	CLA	C2D-C1D-ND	7.78	115.84	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bA	816	CLA	C2B-C1B-NB	7.78	115.45	110.23
12	cA	826	F6C	C2C-C1C-NC	7.78	115.45	110.23
11	aB	805	CLA	C2D-C1D-ND	7.78	115.83	110.10
11	cB	811	CLA	C2D-C1D-ND	7.77	115.83	110.10
11	bA	842	CLA	C2B-C1B-NB	7.77	115.44	110.23
11	aA	842	CLA	C2B-C1B-NB	7.77	115.44	110.23
11	cA	843	CLA	C2D-C1D-ND	7.77	115.83	110.10
11	cK	101	CLA	C2D-C1D-ND	7.77	115.83	110.10
11	aB	830	CLA	C2D-C1D-ND	7.76	115.83	110.10
11	bB	822	CLA	C2B-C1B-NB	7.76	115.44	110.23
11	aB	822	CLA	C2B-C1B-NB	7.76	115.44	110.23
11	bB	811	CLA	C2D-C1D-ND	7.76	115.82	110.10
11	bB	830	CLA	C2D-C1D-ND	7.76	115.82	110.10
11	cA	804	CLA	C2D-C1D-ND	7.76	115.82	110.10
11	aA	810	CLA	C2D-C1D-ND	7.76	115.82	110.10
11	cB	832	CLA	C2D-C1D-ND	7.76	115.82	110.10
11	bB	805	CLA	C2D-C1D-ND	7.76	115.82	110.10
11	aB	840	CLA	C2D-C1D-ND	7.75	115.82	110.10
11	aA	818	CLA	C2B-C1B-NB	7.75	115.43	110.23
11	cB	804	CLA	C2B-C1B-NB	7.75	115.43	110.23
11	cB	802	CLA	C2D-C1D-ND	7.75	115.81	110.10
11	cB	831	CLA	C2B-C1B-NB	7.75	115.43	110.23
11	aK	101	CLA	C2D-C1D-ND	7.75	115.81	110.10
11	cB	805	CLA	C2D-C1D-ND	7.75	115.81	110.10
12	aA	826	F6C	CAA-C2A-C3A	-7.75	113.45	127.88
11	aA	843	CLA	C2D-C1D-ND	7.75	115.81	110.10
11	bA	810	CLA	C2D-C1D-ND	7.75	115.81	110.10
11	cA	837	CLA	C2B-C1B-NB	7.74	115.42	110.23
11	bK	101	CLA	C2D-C1D-ND	7.74	115.81	110.10
11	cA	811	CLA	C2D-C1D-ND	7.74	115.81	110.10
11	aB	819	CLA	C2D-C1D-ND	7.74	115.81	110.10
11	cB	822	CLA	C2B-C1B-NB	7.74	115.42	110.23
11	cB	819	CLA	C2D-C1D-ND	7.74	115.81	110.10
12	cA	826	F6C	CAA-C2A-C3A	-7.74	113.47	127.88
11	bA	818	CLA	C2B-C1B-NB	7.73	115.42	110.23
11	cA	806	CLA	C2D-C1D-ND	7.73	115.80	110.10
12	bA	826	F6C	CAA-C2A-C3A	-7.73	113.48	127.88
11	aA	829	CLA	C2D-C1D-ND	7.73	115.80	110.10
11	aA	822	CLA	C2D-C1D-ND	7.72	115.79	110.10
11	bA	843	CLA	C2D-C1D-ND	7.72	115.79	110.10
11	aB	837	CLA	C2D-C1D-ND	7.72	115.79	110.10
11	aA	804	CLA	C2D-C1D-ND	7.72	115.79	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bA	811	CLA	C2D-C1D-ND	7.72	115.79	110.10
12	bB	824	F6C	C2C-C1C-NC	7.72	115.41	110.23
11	bB	831	CLA	C2B-C1B-NB	7.71	115.40	110.23
12	bA	830	F6C	C2C-C1C-NC	7.71	115.40	110.23
11	bB	819	CLA	C2D-C1D-ND	7.70	115.78	110.10
11	cA	810	CLA	C2D-C1D-ND	7.70	115.78	110.10
11	aA	811	CLA	C2D-C1D-ND	7.70	115.78	110.10
11	aK	101	CLA	C2B-C1B-NB	7.70	115.39	110.23
11	aB	811	CLA	C2D-C1D-ND	7.70	115.78	110.10
11	cA	822	CLA	C2D-C1D-ND	7.70	115.78	110.10
11	bB	802	CLA	C2D-C1D-ND	7.69	115.77	110.10
11	cB	830	CLA	C2D-C1D-ND	7.69	115.77	110.10
11	bA	822	CLA	C2D-C1D-ND	7.69	115.77	110.10
11	cA	808	CLA	C2B-C1B-NB	7.68	115.38	110.23
11	cB	830	CLA	C2B-C1B-NB	7.68	115.38	110.23
11	bA	808	CLA	C2B-C1B-NB	7.68	115.38	110.23
11	bB	804	CLA	C2B-C1B-NB	7.68	115.38	110.23
12	cB	824	F6C	C2C-C1C-NC	7.68	115.38	110.23
11	bK	101	CLA	C2B-C1B-NB	7.68	115.38	110.23
12	aB	824	F6C	C2C-C1C-NC	7.68	115.38	110.23
11	cB	835	CLA	C2D-C1D-ND	7.68	115.76	110.10
11	aA	833	CLA	C2B-C1B-NB	7.68	115.38	110.23
12	cA	830	F6C	C2C-C1C-NC	7.68	115.38	110.23
11	bA	838	CLA	C2D-C1D-ND	7.68	115.76	110.10
11	cA	802	CLA	C2B-C1B-NB	7.67	115.38	110.23
11	bB	815	CLA	C2B-C1B-NB	7.67	115.37	110.23
11	aB	804	CLA	C2B-C1B-NB	7.67	115.37	110.23
11	aB	835	CLA	C2D-C1D-ND	7.66	115.75	110.10
11	bB	835	CLA	C2D-C1D-ND	7.66	115.75	110.10
11	aA	808	CLA	C2B-C1B-NB	7.66	115.36	110.23
11	aA	837	CLA	C2B-C1B-NB	7.66	115.36	110.23
11	bA	837	CLA	C2B-C1B-NB	7.65	115.36	110.23
11	cA	814	CLA	C2B-C1B-NB	7.65	115.36	110.23
11	cB	815	CLA	C2B-C1B-NB	7.65	115.36	110.23
12	aA	830	F6C	C2C-C1C-NC	7.65	115.36	110.23
11	cK	101	CLA	C2B-C1B-NB	7.65	115.36	110.23
11	bB	828	CLA	C1D-ND-C4D	-7.64	100.91	106.33
11	cA	838	CLA	C2D-C1D-ND	7.64	115.73	110.10
11	aB	830	CLA	C2B-C1B-NB	7.64	115.35	110.23
11	cB	808	CLA	C2D-C1D-ND	7.63	115.73	110.10
11	bB	830	CLA	C2B-C1B-NB	7.63	115.34	110.23
11	cB	828	CLA	C1D-ND-C4D	-7.63	100.92	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bA	802	CLA	C2B-C1B-NB	7.62	115.34	110.23
11	bB	838	CLA	C2B-C1B-NB	7.62	115.34	110.23
11	aB	828	CLA	C1D-ND-C4D	-7.62	100.92	106.33
11	aA	838	CLA	C2D-C1D-ND	7.62	115.72	110.10
11	bA	833	CLA	C2B-C1B-NB	7.62	115.34	110.23
11	cA	841	CLA	C2B-C1B-NB	7.62	115.34	110.23
11	aB	808	CLA	C2D-C1D-ND	7.62	115.72	110.10
11	aA	802	CLA	C2B-C1B-NB	7.61	115.33	110.23
12	bA	832	F6C	C2C-C1C-NC	7.61	115.33	110.23
11	bB	810	CLA	C2D-C1D-ND	7.60	115.71	110.10
11	cB	838	CLA	C2B-C1B-NB	7.60	115.33	110.23
11	cA	833	CLA	C2B-C1B-NB	7.60	115.33	110.23
11	bA	814	CLA	C2B-C1B-NB	7.60	115.33	110.23
12	cA	832	F6C	C2C-C1C-NC	7.60	115.32	110.23
11	bA	841	CLA	C2B-C1B-NB	7.59	115.32	110.23
11	cA	815	CLA	C2B-C1B-NB	7.58	115.32	110.23
11	bA	815	CLA	C2B-C1B-NB	7.58	115.31	110.23
11	aB	823	CLA	C2D-C1D-ND	7.58	115.69	110.10
11	aB	815	CLA	C2B-C1B-NB	7.58	115.31	110.23
11	bB	823	CLA	C2D-C1D-ND	7.58	115.69	110.10
11	aA	814	CLA	C2B-C1B-NB	7.57	115.31	110.23
11	bB	811	CLA	C2B-C1B-NB	7.57	115.31	110.23
11	aA	834	CLA	C2D-C1D-ND	7.57	115.68	110.10
11	bK	103	CLA	C2B-C1B-NB	7.57	115.30	110.23
11	bA	834	CLA	C2D-C1D-ND	7.57	115.68	110.10
11	aA	815	CLA	C2B-C1B-NB	7.56	115.30	110.23
11	bB	808	CLA	C2D-C1D-ND	7.56	115.67	110.10
11	cB	810	CLA	C2D-C1D-ND	7.56	115.67	110.10
11	cA	834	CLA	C2D-C1D-ND	7.56	115.67	110.10
11	cB	811	CLA	C2B-C1B-NB	7.55	115.29	110.23
11	bA	812	CLA	C2D-C1D-ND	7.55	115.67	110.10
11	bB	827	CLA	C2D-C1D-ND	7.55	115.67	110.10
11	bB	831	CLA	C2D-C1D-ND	7.54	115.66	110.10
11	aB	831	CLA	C2D-C1D-ND	7.54	115.66	110.10
11	cK	103	CLA	C2B-C1B-NB	7.53	115.28	110.23
11	cB	831	CLA	C2D-C1D-ND	7.53	115.65	110.10
11	bB	803	CLA	C2B-C1B-NB	7.53	115.28	110.23
11	aB	810	CLA	C2D-C1D-ND	7.52	115.65	110.10
12	aA	830	F6C	C3C-C4C-NC	7.52	115.44	110.21
11	aA	841	CLA	C2B-C1B-NB	7.52	115.27	110.23
11	aB	811	CLA	C2B-C1B-NB	7.52	115.27	110.23
11	aB	838	CLA	C2B-C1B-NB	7.52	115.27	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aA	828	CLA	C2B-C1B-NB	7.51	115.27	110.23
11	cA	828	CLA	C2B-C1B-NB	7.51	115.27	110.23
11	aB	813	CLA	C2D-C1D-ND	7.51	115.64	110.10
11	cB	827	CLA	C2D-C1D-ND	7.50	115.63	110.10
11	bA	828	CLA	C2B-C1B-NB	7.50	115.26	110.23
11	aA	812	CLA	C2D-C1D-ND	7.50	115.63	110.10
11	aB	808	CLA	C2B-C1B-NB	7.50	115.26	110.23
12	cA	830	F6C	C3C-C4C-NC	7.50	115.42	110.21
12	aA	832	F6C	C2C-C1C-NC	7.50	115.26	110.23
11	cB	813	CLA	C2D-C1D-ND	7.49	115.63	110.10
12	bA	830	F6C	C3C-C4C-NC	7.49	115.42	110.21
11	cA	812	CLA	C2D-C1D-ND	7.49	115.62	110.10
11	cB	823	CLA	C2D-C1D-ND	7.49	115.62	110.10
11	bA	817	CLA	C2D-C1D-ND	7.49	115.62	110.10
11	bA	820	CLA	C2D-C1D-ND	7.48	115.61	110.10
11	cB	803	CLA	C2B-C1B-NB	7.48	115.24	110.23
11	bB	813	CLA	C2D-C1D-ND	7.47	115.61	110.10
11	bA	804	CLA	C2B-C1B-NB	7.47	115.24	110.23
11	aA	815	CLA	C2D-C1D-ND	7.46	115.60	110.10
11	aA	817	CLA	C2D-C1D-ND	7.46	115.60	110.10
11	aB	803	CLA	C2B-C1B-NB	7.46	115.23	110.23
11	aK	103	CLA	C2B-C1B-NB	7.45	115.23	110.23
11	cA	815	CLA	C2D-C1D-ND	7.45	115.60	110.10
11	aA	820	CLA	C2D-C1D-ND	7.45	115.59	110.10
11	bA	815	CLA	C2D-C1D-ND	7.45	115.59	110.10
11	aB	827	CLA	C2D-C1D-ND	7.45	115.59	110.10
11	aA	804	CLA	C2B-C1B-NB	7.44	115.22	110.23
11	aA	835	CLA	C2B-C1B-NB	7.44	115.22	110.23
11	bB	834	CLA	C2D-C1D-ND	7.44	115.59	110.10
11	cB	831	CLA	CAA-C2A-C3A	-7.43	92.42	112.78
11	cA	817	CLA	C2D-C1D-ND	7.43	115.58	110.10
11	cA	820	CLA	C2D-C1D-ND	7.43	115.58	110.10
11	bA	824	CLA	C2B-C1B-NB	7.43	115.22	110.23
11	bB	831	CLA	CAA-C2A-C3A	-7.43	92.43	112.78
11	cA	835	CLA	C2B-C1B-NB	7.43	115.21	110.23
11	bA	838	CLA	C2B-C1B-NB	7.42	115.20	110.23
11	aA	814	CLA	C2D-C1D-ND	7.41	115.56	110.10
11	aA	824	CLA	C2D-C1D-ND	7.41	115.56	110.10
11	cA	824	CLA	C2D-C1D-ND	7.41	115.56	110.10
11	bB	808	CLA	C2B-C1B-NB	7.41	115.20	110.23
11	bA	814	CLA	C2D-C1D-ND	7.40	115.56	110.10
11	aB	831	CLA	CAA-C2A-C3A	-7.40	92.51	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aA	838	CLA	C2B-C1B-NB	7.40	115.19	110.23
11	cA	804	CLA	C2B-C1B-NB	7.40	115.19	110.23
11	cA	824	CLA	C2B-C1B-NB	7.40	115.19	110.23
11	cA	802	CLA	C2D-C1D-ND	7.40	115.56	110.10
11	cB	834	CLA	C2D-C1D-ND	7.40	115.56	110.10
11	bA	835	CLA	C2B-C1B-NB	7.40	115.19	110.23
11	aB	834	CLA	C2D-C1D-ND	7.40	115.55	110.10
11	aA	824	CLA	C2B-C1B-NB	7.39	115.19	110.23
11	aA	823	CLA	C2B-C1B-NB	7.39	115.19	110.23
11	cA	838	CLA	C2B-C1B-NB	7.39	115.19	110.23
11	cB	808	CLA	C2B-C1B-NB	7.38	115.18	110.23
11	aA	802	CLA	C2D-C1D-ND	7.37	115.54	110.10
11	cA	814	CLA	C2D-C1D-ND	7.36	115.53	110.10
11	aB	812	CLA	C2B-C1B-NB	7.36	115.16	110.23
11	bA	823	CLA	C2B-C1B-NB	7.35	115.16	110.23
11	bA	825	CLA	C2D-C1D-ND	7.35	115.52	110.10
11	aB	820	CLA	C2B-C1B-NB	7.35	115.16	110.23
11	cB	837	CLA	C2B-C1B-NB	7.35	115.16	110.23
12	cA	844	F6C	CMA-C3A-C2A	-7.34	106.18	126.12
12	bA	844	F6C	CMA-C3A-C2A	-7.34	106.19	126.12
11	bA	824	CLA	C2D-C1D-ND	7.34	115.51	110.10
11	cB	836	CLA	C2B-C1B-NB	7.34	115.15	110.23
12	aA	844	F6C	CMA-C3A-C2A	-7.34	106.20	126.12
11	bA	802	CLA	C2D-C1D-ND	7.34	115.51	110.10
11	bL	205	CLA	C2B-C1B-NB	7.33	115.14	110.23
11	bB	836	CLA	C2B-C1B-NB	7.33	115.14	110.23
11	cA	823	CLA	C2B-C1B-NB	7.32	115.14	110.23
11	aA	813	CLA	C2B-C1B-NB	7.31	115.14	110.23
11	aB	827	CLA	C2B-C1B-NB	7.31	115.13	110.23
11	aB	837	CLA	C2B-C1B-NB	7.31	115.13	110.23
11	bA	813	CLA	C2B-C1B-NB	7.31	115.13	110.23
11	bB	827	CLA	C2B-C1B-NB	7.30	115.13	110.23
11	aB	836	CLA	C2B-C1B-NB	7.30	115.12	110.23
11	cB	827	CLA	C2B-C1B-NB	7.30	115.12	110.23
11	aB	825	CLA	C2B-C1B-NB	7.30	115.12	110.23
11	aL	205	CLA	C2B-C1B-NB	7.29	115.12	110.23
11	bB	837	CLA	C2B-C1B-NB	7.29	115.12	110.23
11	cB	812	CLA	C2B-C1B-NB	7.29	115.12	110.23
11	aA	825	CLA	C2D-C1D-ND	7.29	115.48	110.10
11	bB	820	CLA	C2B-C1B-NB	7.29	115.12	110.23
11	cA	813	CLA	C2B-C1B-NB	7.28	115.11	110.23
11	bA	825	CLA	C2B-C1B-NB	7.28	115.11	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cL	205	CLA	C2B-C1B-NB	7.28	115.11	110.23
11	cB	825	CLA	C2B-C1B-NB	7.28	115.11	110.23
11	bB	825	CLA	C2B-C1B-NB	7.27	115.11	110.23
11	bB	826	CLA	C2B-C1B-NB	7.27	115.11	110.23
11	bB	812	CLA	C2B-C1B-NB	7.27	115.10	110.23
11	cA	825	CLA	C2D-C1D-ND	7.27	115.46	110.10
11	cB	820	CLA	C2B-C1B-NB	7.25	115.09	110.23
12	cL	202	F6C	C3C-C4C-NC	7.23	115.24	110.21
12	bL	202	F6C	C3C-C4C-NC	7.23	115.24	110.21
12	aL	202	F6C	C3C-C4C-NC	7.22	115.23	110.21
11	bB	817	CLA	C2B-C1B-NB	7.22	115.07	110.23
11	aB	819	CLA	C2B-C1B-NB	7.21	115.07	110.23
11	cB	826	CLA	C2B-C1B-NB	7.21	115.06	110.23
11	aB	826	CLA	C2B-C1B-NB	7.20	115.06	110.23
11	cB	817	CLA	C2B-C1B-NB	7.20	115.06	110.23
11	aA	825	CLA	C2B-C1B-NB	7.19	115.05	110.23
11	bA	807	CLA	C2B-C1B-NB	7.19	115.05	110.23
11	cA	807	CLA	C2B-C1B-NB	7.18	115.05	110.23
11	aA	817	CLA	C2B-C1B-NB	7.18	115.05	110.23
11	cA	825	CLA	C2B-C1B-NB	7.18	115.05	110.23
11	bB	821	CLA	C2B-C1B-NB	7.18	115.04	110.23
11	bA	817	CLA	C2B-C1B-NB	7.17	115.04	110.23
11	cB	821	CLA	C2B-C1B-NB	7.17	115.04	110.23
11	cL	204	CLA	C2B-C1B-NB	7.17	115.04	110.23
11	cB	819	CLA	C2B-C1B-NB	7.16	115.03	110.23
11	aA	807	CLA	C2B-C1B-NB	7.15	115.03	110.23
11	aA	843	CLA	C2B-C1B-NB	7.15	115.03	110.23
12	cA	832	F6C	CMD-C2D-C1D	7.14	135.92	125.04
11	bA	840	CLA	CAA-C2A-C3A	-7.14	93.22	112.78
12	bA	832	F6C	CMD-C2D-C1D	7.14	135.92	125.04
11	bB	819	CLA	C2B-C1B-NB	7.14	115.02	110.23
12	cL	202	F6C	CMD-C2D-C1D	7.14	135.91	125.04
11	aB	821	CLA	C2B-C1B-NB	7.14	115.02	110.23
11	bL	204	CLA	C2B-C1B-NB	7.13	115.01	110.23
11	cA	840	CLA	CAA-C2A-C3A	-7.13	93.26	112.78
12	aA	832	F6C	CMD-C2D-C1D	7.13	135.89	125.04
12	aL	202	F6C	CMD-C2D-C1D	7.12	135.89	125.04
11	cB	829	CLA	C2D-C1D-ND	7.12	115.35	110.10
11	aA	840	CLA	CAA-C2A-C3A	-7.12	93.28	112.78
12	aA	830	F6C	CMA-C3A-C2A	-7.12	106.79	126.12
12	bL	202	F6C	CMD-C2D-C1D	7.12	135.88	125.04
12	cA	830	F6C	CMA-C3A-C2A	-7.11	106.81	126.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aL	204	CLA	C2B-C1B-NB	7.11	115.00	110.23
11	bB	829	CLA	C2D-C1D-ND	7.11	115.34	110.10
11	cA	843	CLA	C2B-C1B-NB	7.11	115.00	110.23
12	bA	830	F6C	CMA-C3A-C2A	-7.11	106.82	126.12
11	aB	817	CLA	C2B-C1B-NB	7.10	114.99	110.23
11	cA	811	CLA	C2B-C1B-NB	7.09	114.98	110.23
11	bB	813	CLA	C2B-C1B-NB	7.08	114.98	110.23
11	cB	806	CLA	C2B-C1B-NB	7.07	114.97	110.23
11	bA	843	CLA	C2B-C1B-NB	7.07	114.97	110.23
11	cA	817	CLA	C2B-C1B-NB	7.07	114.97	110.23
11	aB	806	CLA	C2B-C1B-NB	7.06	114.97	110.23
11	bB	835	CLA	C2B-C1B-NB	7.06	114.96	110.23
11	cB	813	CLA	C2B-C1B-NB	7.05	114.96	110.23
11	aB	829	CLA	C2D-C1D-ND	7.04	115.29	110.10
12	aA	827	F6C	C2C-C1C-NC	7.03	114.94	110.23
12	cA	827	F6C	C2C-C1C-NC	7.03	114.94	110.23
12	bA	827	F6C	C2C-C1C-NC	7.02	114.94	110.23
11	bA	811	CLA	C2B-C1B-NB	7.02	114.94	110.23
11	aB	813	CLA	C2B-C1B-NB	7.01	114.93	110.23
11	aB	835	CLA	C2B-C1B-NB	7.01	114.93	110.23
12	aA	844	F6C	C2C-C1C-NC	7.01	114.93	110.23
11	bA	820	CLA	C2B-C1B-NB	7.00	114.93	110.23
11	aA	811	CLA	C2B-C1B-NB	7.00	114.92	110.23
10	aA	801	CL0	C2B-C1B-NB	7.00	114.92	110.23
12	cA	844	F6C	CMD-C2D-C1D	6.99	135.69	125.04
11	aA	820	CLA	C2B-C1B-NB	6.99	114.92	110.23
10	cA	801	CL0	C2B-C1B-NB	6.99	114.92	110.23
11	aA	831	CLA	C2B-C1B-NB	6.98	114.91	110.23
11	aB	812	CLA	C2D-C1D-ND	6.98	115.25	110.10
11	bB	839	CLA	C2D-C1D-ND	6.98	115.25	110.10
11	bA	831	CLA	C2B-C1B-NB	6.97	114.91	110.23
12	aA	844	F6C	CMD-C2D-C1D	6.97	135.66	125.04
12	cA	844	F6C	C2C-C1C-NC	6.97	114.91	110.23
11	cA	820	CLA	C2B-C1B-NB	6.97	114.91	110.23
11	cA	834	CLA	C2B-C1B-NB	6.96	114.90	110.23
11	cB	839	CLA	C2D-C1D-ND	6.96	115.23	110.10
11	aA	834	CLA	C2B-C1B-NB	6.96	114.89	110.23
12	bA	844	F6C	CMD-C2D-C1D	6.96	135.63	125.04
11	aB	818	CLA	C2B-C1B-NB	6.95	114.89	110.23
11	bB	806	CLA	C2B-C1B-NB	6.95	114.89	110.23
11	cA	831	CLA	C2B-C1B-NB	6.95	114.89	110.23
11	aB	839	CLA	C2D-C1D-ND	6.95	115.22	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cB	824	F6C	CMA-C3A-C2A	-6.94	107.28	126.12
11	cB	835	CLA	C2B-C1B-NB	6.94	114.88	110.23
11	aB	839	CLA	C2B-C1B-NB	6.93	114.88	110.23
10	bA	801	CL0	C2B-C1B-NB	6.93	114.88	110.23
12	bA	844	F6C	C2C-C1C-NC	6.93	114.88	110.23
12	aB	824	F6C	CMA-C3A-C2A	-6.93	107.31	126.12
11	bB	839	CLA	C2B-C1B-NB	6.93	114.88	110.23
11	cB	839	CLA	C2B-C1B-NB	6.93	114.88	110.23
12	bB	824	F6C	CMA-C3A-C2A	-6.92	107.33	126.12
11	aB	828	CLA	CMD-C2D-C1D	6.92	136.91	124.71
11	cB	828	CLA	CMD-C2D-C1D	6.91	136.89	124.71
11	bB	828	CLA	CMD-C2D-C1D	6.90	136.87	124.71
11	aB	829	CLA	C2C-C1C-NC	6.88	116.41	109.97
11	cB	829	CLA	C2C-C1C-NC	6.87	116.40	109.97
11	cB	812	CLA	C2D-C1D-ND	6.86	115.16	110.10
11	bB	812	CLA	C2D-C1D-ND	6.85	115.15	110.10
11	bA	834	CLA	C2B-C1B-NB	6.84	114.82	110.23
11	cB	818	CLA	C2B-C1B-NB	6.83	114.81	110.23
11	bB	818	CLA	C2B-C1B-NB	6.83	114.81	110.23
12	bA	827	F6C	C3C-C4C-NC	6.83	114.96	110.21
12	cA	827	F6C	C3C-C4C-NC	6.82	114.95	110.21
11	bB	829	CLA	C2C-C1C-NC	6.82	116.36	109.97
12	aB	824	F6C	CMD-C2D-C1D	6.81	135.41	125.04
12	bB	824	F6C	CMD-C2D-C1D	6.81	135.41	125.04
12	cB	824	F6C	CMD-C2D-C1D	6.81	135.41	125.04
12	aA	827	F6C	CMD-C2D-C1D	6.77	135.35	125.04
12	bA	826	F6C	CMD-C2D-C1D	6.77	135.34	125.04
12	bA	827	F6C	CMD-C2D-C1D	6.77	135.34	125.04
12	aA	826	F6C	CMD-C2D-C1D	6.76	135.34	125.04
12	cA	826	F6C	CMD-C2D-C1D	6.76	135.34	125.04
12	cA	827	F6C	CMD-C2D-C1D	6.76	135.33	125.04
11	aB	833	CLA	CMD-C2D-C1D	6.75	136.61	124.71
12	aA	827	F6C	C3C-C4C-NC	6.74	114.90	110.21
11	cB	833	CLA	CMD-C2D-C1D	6.74	136.59	124.71
11	bB	833	CLA	CMD-C2D-C1D	6.73	136.57	124.71
11	bB	831	CLA	CMD-C2D-C1D	6.72	136.56	124.71
11	aB	831	CLA	CMD-C2D-C1D	6.71	136.54	124.71
11	aA	821	CLA	C2B-C1B-NB	6.71	114.73	110.23
11	cB	831	CLA	CMD-C2D-C1D	6.70	136.52	124.71
11	bA	821	CLA	C2B-C1B-NB	6.69	114.72	110.23
11	cA	821	CLA	C2B-C1B-NB	6.69	114.71	110.23
11	aA	828	CLA	CHD-C4C-C3C	-6.67	115.04	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cA	828	CLA	CHD-C4C-C3C	-6.66	115.05	124.84
11	bA	828	CLA	CHD-C4C-C3C	-6.64	115.08	124.84
12	cA	832	F6C	CMA-C3A-C2A	-6.64	108.09	126.12
12	aA	832	F6C	CMA-C3A-C2A	-6.63	108.12	126.12
11	aA	824	CLA	CMD-C2D-C1D	6.63	136.39	124.71
11	aB	810	CLA	C2B-C1B-NB	6.63	114.67	110.23
11	bB	806	CLA	CMD-C2D-C1D	6.62	136.38	124.71
11	aL	206	CLA	C2B-C1B-NB	6.62	114.67	110.23
12	bA	832	F6C	CMA-C3A-C2A	-6.62	108.15	126.12
11	cA	824	CLA	CMD-C2D-C1D	6.62	136.38	124.71
11	cB	834	CLA	C2B-C1B-NB	6.60	114.66	110.23
11	bA	824	CLA	CMD-C2D-C1D	6.60	136.35	124.71
11	cA	807	CLA	CMD-C2D-C1D	6.60	136.35	124.71
11	aB	806	CLA	CMD-C2D-C1D	6.59	136.33	124.71
11	cB	806	CLA	CMD-C2D-C1D	6.59	136.33	124.71
11	bA	807	CLA	CMD-C2D-C1D	6.59	136.32	124.71
11	aB	834	CLA	C2B-C1B-NB	6.57	114.64	110.23
11	cB	810	CLA	C2B-C1B-NB	6.57	114.64	110.23
11	aA	807	CLA	CMD-C2D-C1D	6.56	136.28	124.71
11	aA	838	CLA	CMD-C2D-C1D	6.56	136.28	124.71
11	cA	838	CLA	CMD-C2D-C1D	6.56	136.27	124.71
11	cB	822	CLA	CMD-C2D-C1D	6.56	136.27	124.71
11	aB	822	CLA	CMD-C2D-C1D	6.55	136.26	124.71
11	bA	838	CLA	CMD-C2D-C1D	6.55	136.26	124.71
11	cL	206	CLA	C2B-C1B-NB	6.54	114.62	110.23
11	cA	818	CLA	O2D-CGD-CBD	6.54	122.89	111.27
11	bB	810	CLA	C2B-C1B-NB	6.54	114.61	110.23
11	bL	206	CLA	C2B-C1B-NB	6.54	114.61	110.23
11	bB	822	CLA	CMD-C2D-C1D	6.54	136.23	124.71
11	cB	828	CLA	C2B-C1B-NB	6.54	114.61	110.23
11	bA	818	CLA	O2D-CGD-CBD	6.53	122.88	111.27
12	bA	832	F6C	C3C-C4C-NC	6.53	114.75	110.21
11	bB	834	CLA	C2B-C1B-NB	6.53	114.61	110.23
11	bA	828	CLA	CMD-C2D-C1D	6.53	136.22	124.71
11	aB	807	CLA	C2B-C1B-NB	6.52	114.60	110.23
11	aB	801	CLA	C2B-C1B-NB	6.52	114.60	110.23
11	cB	807	CLA	C2B-C1B-NB	6.52	114.60	110.23
11	aA	818	CLA	O2D-CGD-CBD	6.51	122.84	111.27
12	cA	832	F6C	C3C-C4C-NC	6.50	114.73	110.21
11	cA	828	CLA	CMD-C2D-C1D	6.50	136.16	124.71
11	aA	810	CLA	C2B-C1B-NB	6.49	114.59	110.23
11	bB	807	CLA	C2B-C1B-NB	6.49	114.58	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aA	818	CLA	CHD-C4C-C3C	-6.49	115.30	124.84
11	bB	822	CLA	CHD-C4C-C3C	-6.49	115.31	124.84
11	bB	828	CLA	C2B-C1B-NB	6.48	114.58	110.23
11	aB	834	CLA	CMD-C2D-C1D	6.48	136.14	124.71
11	cB	810	CLA	CMD-C2D-C1D	6.48	136.14	124.71
11	bA	808	CLA	CMD-C2D-C1D	6.48	136.13	124.71
11	bA	814	CLA	CMD-C2D-C1D	6.48	136.13	124.71
11	cB	825	CLA	CMD-C2D-C1D	6.48	136.13	124.71
11	cB	834	CLA	CMD-C2D-C1D	6.48	136.13	124.71
11	aA	808	CLA	CMD-C2D-C1D	6.47	136.12	124.71
11	bB	810	CLA	CMD-C2D-C1D	6.47	136.12	124.71
11	bB	834	CLA	CMD-C2D-C1D	6.47	136.12	124.71
11	aB	822	CLA	CHD-C4C-C3C	-6.47	115.33	124.84
11	aA	814	CLA	CMD-C2D-C1D	6.46	136.11	124.71
11	cB	822	CLA	CHD-C4C-C3C	-6.46	115.34	124.84
11	bA	818	CLA	CHD-C4C-C3C	-6.46	115.34	124.84
11	aA	828	CLA	CMD-C2D-C1D	6.46	136.10	124.71
11	aB	825	CLA	CMD-C2D-C1D	6.46	136.10	124.71
11	cA	839	CLA	C2B-C1B-NB	6.46	114.56	110.23
11	bB	825	CLA	CMD-C2D-C1D	6.46	136.09	124.71
11	aB	817	CLA	CMD-C2D-C1D	6.46	136.09	124.71
11	cA	814	CLA	CMD-C2D-C1D	6.46	136.09	124.71
11	aB	810	CLA	CMD-C2D-C1D	6.45	136.09	124.71
11	cA	808	CLA	CMD-C2D-C1D	6.45	136.09	124.71
11	bA	810	CLA	C2B-C1B-NB	6.45	114.56	110.23
12	aA	832	F6C	C3C-C4C-NC	6.45	114.69	110.21
11	aA	809	CLA	CMD-C2D-C1D	6.44	136.07	124.71
11	bA	829	CLA	CMD-C2D-C1D	6.44	136.07	124.71
11	cA	804	CLA	CMD-C2D-C1D	6.44	136.07	124.71
11	aA	819	CLA	CMD-C2D-C1D	6.44	136.06	124.71
11	cA	810	CLA	C2B-C1B-NB	6.44	114.55	110.23
11	bA	804	CLA	CMD-C2D-C1D	6.44	136.06	124.71
11	cA	829	CLA	CMD-C2D-C1D	6.44	136.06	124.71
11	aA	829	CLA	CMD-C2D-C1D	6.44	136.06	124.71
11	bA	819	CLA	CMD-C2D-C1D	6.44	136.06	124.71
11	aB	801	CLA	CHD-C4C-C3C	-6.44	115.38	124.84
11	bA	839	CLA	C2B-C1B-NB	6.44	114.55	110.23
11	cB	801	CLA	C2B-C1B-NB	6.44	114.55	110.23
11	aB	816	CLA	CMD-C2D-C1D	6.43	136.05	124.71
11	cB	817	CLA	CMD-C2D-C1D	6.43	136.05	124.71
11	cB	816	CLA	CMD-C2D-C1D	6.43	136.05	124.71
11	cB	801	CLA	CHD-C4C-C3C	-6.43	115.39	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cA	809	CLA	CMD-C2D-C1D	6.43	136.04	124.71
11	cA	818	CLA	CHD-C4C-C3C	-6.43	115.39	124.84
11	bB	816	CLA	CMD-C2D-C1D	6.43	136.04	124.71
11	bB	801	CLA	CHD-C4C-C3C	-6.42	115.40	124.84
11	aB	835	CLA	CMD-C2D-C1D	6.42	136.03	124.71
11	bB	832	CLA	CMD-C2D-C1D	6.42	136.03	124.71
11	cB	835	CLA	CMD-C2D-C1D	6.42	136.03	124.71
11	bA	809	CLA	CMD-C2D-C1D	6.42	136.03	124.71
11	bB	835	CLA	CMD-C2D-C1D	6.42	136.03	124.71
11	cB	829	CLA	CMD-C2D-C1D	6.42	136.03	124.71
12	cL	202	F6C	C2D-C1D-ND	6.42	115.98	109.97
11	bB	817	CLA	CMD-C2D-C1D	6.42	136.03	124.71
11	cA	819	CLA	CMD-C2D-C1D	6.42	136.03	124.71
11	bB	829	CLA	CMD-C2D-C1D	6.42	136.02	124.71
11	aA	804	CLA	CMD-C2D-C1D	6.42	136.02	124.71
11	bB	815	CLA	CMD-C2D-C1D	6.41	136.02	124.71
11	bB	801	CLA	C2B-C1B-NB	6.41	114.53	110.23
11	bA	820	CLA	CMD-C2D-C1D	6.41	136.01	124.71
11	bK	103	CLA	CMD-C2D-C1D	6.41	136.01	124.71
11	aB	828	CLA	C2B-C1B-NB	6.41	114.53	110.23
11	bB	840	CLA	CMD-C2D-C1D	6.40	136.00	124.71
11	cB	840	CLA	CMD-C2D-C1D	6.40	136.00	124.71
11	bA	819	CLA	CHD-C4C-C3C	-6.40	115.43	124.84
11	cA	819	CLA	CHD-C4C-C3C	-6.40	115.43	124.84
11	aB	829	CLA	CMD-C2D-C1D	6.40	136.00	124.71
11	cA	837	CLA	CMD-C2D-C1D	6.40	135.99	124.71
11	aA	834	CLA	CMD-C2D-C1D	6.40	135.99	124.71
11	aB	840	CLA	CMD-C2D-C1D	6.40	135.99	124.71
11	cA	812	CLA	CMD-C2D-C1D	6.40	135.99	124.71
11	cB	832	CLA	CMD-C2D-C1D	6.40	135.99	124.71
11	aK	103	CLA	CMD-C2D-C1D	6.40	135.99	124.71
11	bA	812	CLA	CMD-C2D-C1D	6.40	135.99	124.71
11	aA	839	CLA	C2B-C1B-NB	6.39	114.52	110.23
11	aB	832	CLA	CMD-C2D-C1D	6.39	135.98	124.71
11	bA	834	CLA	CMD-C2D-C1D	6.39	135.98	124.71
11	cA	811	CLA	CMD-C2D-C1D	6.39	135.98	124.71
11	bA	837	CLA	CMD-C2D-C1D	6.39	135.98	124.71
11	bA	811	CLA	CMD-C2D-C1D	6.39	135.98	124.71
11	aA	820	CLA	CMD-C2D-C1D	6.39	135.98	124.71
11	cK	103	CLA	CMD-C2D-C1D	6.39	135.97	124.71
12	bL	202	F6C	C2D-C1D-ND	6.39	115.96	109.97
11	cA	820	CLA	CMD-C2D-C1D	6.39	135.97	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aB	815	CLA	CMD-C2D-C1D	6.39	135.97	124.71
12	aL	202	F6C	C2D-C1D-ND	6.39	115.95	109.97
11	aA	842	CLA	CMD-C2D-C1D	6.38	135.96	124.71
11	aB	812	CLA	CMD-C2D-C1D	6.38	135.96	124.71
11	cB	839	CLA	CMD-C2D-C1D	6.38	135.96	124.71
11	cB	815	CLA	CMD-C2D-C1D	6.38	135.96	124.71
11	aA	819	CLA	CHD-C4C-C3C	-6.38	115.46	124.84
11	bB	839	CLA	CMD-C2D-C1D	6.38	135.95	124.71
11	aB	804	CLA	CMD-C2D-C1D	6.38	135.95	124.71
11	cK	101	CLA	CMD-C2D-C1D	6.38	135.95	124.71
11	aA	812	CLA	CMD-C2D-C1D	6.37	135.95	124.71
11	aB	839	CLA	CMD-C2D-C1D	6.37	135.94	124.71
11	cA	834	CLA	CMD-C2D-C1D	6.37	135.94	124.71
11	bB	804	CLA	CMD-C2D-C1D	6.37	135.94	124.71
12	bA	826	F6C	C2D-C1D-ND	6.37	115.94	109.97
11	aK	101	CLA	CMD-C2D-C1D	6.36	135.93	124.71
11	cA	840	CLA	CMD-C2D-C1D	6.36	135.93	124.71
11	aA	811	CLA	CMD-C2D-C1D	6.36	135.92	124.71
11	bA	806	CLA	CMD-C2D-C1D	6.36	135.92	124.71
11	cA	842	CLA	CMD-C2D-C1D	6.36	135.92	124.71
11	cB	804	CLA	CMD-C2D-C1D	6.36	135.91	124.71
11	aA	837	CLA	CMD-C2D-C1D	6.35	135.91	124.71
11	bA	842	CLA	CMD-C2D-C1D	6.35	135.91	124.71
11	bK	101	CLA	CMD-C2D-C1D	6.35	135.91	124.71
11	cB	804	CLA	CHD-C4C-C3C	-6.34	115.51	124.84
12	cA	826	F6C	C2D-C1D-ND	6.34	115.91	109.97
11	aA	840	CLA	CMD-C2D-C1D	6.34	135.89	124.71
11	cB	812	CLA	CMD-C2D-C1D	6.34	135.89	124.71
11	aB	820	CLA	CMD-C2D-C1D	6.34	135.88	124.71
11	aA	806	CLA	CMD-C2D-C1D	6.33	135.88	124.71
11	bA	840	CLA	CMD-C2D-C1D	6.33	135.88	124.71
11	cA	806	CLA	CMD-C2D-C1D	6.33	135.87	124.71
11	bB	820	CLA	CMD-C2D-C1D	6.33	135.87	124.71
11	cB	820	CLA	CMD-C2D-C1D	6.33	135.87	124.71
11	bB	828	CLA	C2C-C1C-NC	6.33	115.90	109.97
12	aA	826	F6C	C2D-C1D-ND	6.33	115.90	109.97
11	bB	804	CLA	CHD-C4C-C3C	-6.33	115.54	124.84
11	bB	812	CLA	CMD-C2D-C1D	6.32	135.85	124.71
11	cA	802	CLA	C2C-C1C-NC	6.32	115.89	109.97
12	cA	832	F6C	CAA-C2A-C1A	-6.31	110.72	128.11
11	aB	804	CLA	CHD-C4C-C3C	-6.31	115.56	124.84
11	bB	839	CLA	CHD-C4C-C3C	-6.31	115.57	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	844	F6C	C3C-C4C-NC	6.30	114.59	110.21
12	aA	832	F6C	CAA-C2A-C1A	-6.30	110.76	128.11
11	aA	833	CLA	CMD-C2D-C1D	6.30	135.81	124.71
11	cA	833	CLA	CMD-C2D-C1D	6.30	135.81	124.71
12	bA	832	F6C	CAA-C2A-C1A	-6.29	110.78	128.11
11	cB	828	CLA	C2C-C1C-NC	6.29	115.87	109.97
11	bA	833	CLA	CMD-C2D-C1D	6.29	135.80	124.71
11	aB	830	CLA	CMD-C2D-C1D	6.29	135.80	124.71
11	bB	830	CLA	CMD-C2D-C1D	6.28	135.79	124.71
12	bA	827	F6C	C2D-C1D-ND	6.28	115.86	109.97
11	aB	839	CLA	CHD-C4C-C3C	-6.28	115.61	124.84
12	aA	827	F6C	C2D-C1D-ND	6.28	115.86	109.97
12	cA	827	F6C	C2D-C1D-ND	6.28	115.86	109.97
11	cA	823	CLA	CHD-C4C-C3C	-6.28	115.62	124.84
11	cB	815	CLA	CHD-C4C-C3C	-6.27	115.62	124.84
11	aA	802	CLA	C2C-C1C-NC	6.27	115.85	109.97
11	cB	839	CLA	CHD-C4C-C3C	-6.27	115.62	124.84
11	bB	815	CLA	CHD-C4C-C3C	-6.27	115.62	124.84
11	aA	817	CLA	CMD-C2D-C1D	6.26	135.75	124.71
11	aA	823	CLA	CHD-C4C-C3C	-6.26	115.63	124.84
11	bA	823	CLA	CHD-C4C-C3C	-6.26	115.64	124.84
11	bB	821	CLA	CMD-C2D-C1D	6.26	135.75	124.71
11	cB	830	CLA	CMD-C2D-C1D	6.26	135.75	124.71
11	aB	815	CLA	CHD-C4C-C3C	-6.26	115.64	124.84
12	cA	844	F6C	C3C-C4C-NC	6.26	114.56	110.21
11	bA	825	CLA	CMD-C2D-C1D	6.26	135.74	124.71
11	cA	817	CLA	CMD-C2D-C1D	6.25	135.74	124.71
11	bA	817	CLA	CMD-C2D-C1D	6.25	135.73	124.71
11	cB	829	CLA	C2B-C1B-NB	6.25	114.42	110.23
11	cB	837	CLA	CMD-C2D-C1D	6.25	135.73	124.71
12	bB	824	F6C	C3C-C4C-NC	6.25	114.55	110.21
12	aB	824	F6C	C3C-C4C-NC	6.24	114.55	110.21
11	aB	828	CLA	C2C-C1C-NC	6.24	115.82	109.97
11	aB	829	CLA	C2B-C1B-NB	6.24	114.41	110.23
11	aB	821	CLA	CMD-C2D-C1D	6.23	135.70	124.71
11	aA	825	CLA	CMD-C2D-C1D	6.23	135.70	124.71
11	cA	825	CLA	CMD-C2D-C1D	6.23	135.69	124.71
11	bB	837	CLA	CMD-C2D-C1D	6.23	135.69	124.71
11	aA	839	CLA	CMD-C2D-C1D	6.22	135.68	124.71
11	cB	802	CLA	O2D-CGD-CBD	6.22	122.33	111.27
11	bB	829	CLA	C2B-C1B-NB	6.22	114.40	110.23
11	bA	839	CLA	CMD-C2D-C1D	6.22	135.67	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aB	837	CLA	CMD-C2D-C1D	6.22	135.67	124.71
11	bB	826	CLA	CHD-C4C-C3C	-6.21	115.71	124.84
11	cA	839	CLA	CMD-C2D-C1D	6.21	135.66	124.71
11	bB	806	CLA	CHD-C4C-C3C	-6.21	115.71	124.84
11	cB	821	CLA	CMD-C2D-C1D	6.21	135.65	124.71
12	aA	844	F6C	C3C-C4C-NC	6.20	114.52	110.21
12	cB	824	F6C	C3C-C4C-NC	6.20	114.52	110.21
11	aB	802	CLA	O2D-CGD-CBD	6.20	122.29	111.27
11	bB	802	CLA	O2D-CGD-CBD	6.20	122.29	111.27
11	bA	802	CLA	C2C-C1C-NC	6.20	115.78	109.97
11	cB	806	CLA	CHD-C4C-C3C	-6.20	115.73	124.84
11	cB	826	CLA	CHD-C4C-C3C	-6.19	115.74	124.84
11	aB	806	CLA	CHD-C4C-C3C	-6.19	115.75	124.84
11	aB	826	CLA	CHD-C4C-C3C	-6.19	115.75	124.84
11	bB	807	CLA	C2C-C1C-NC	6.18	115.76	109.97
11	bA	815	CLA	CMD-C2D-C1D	6.18	135.61	124.71
12	bA	827	F6C	CMA-C3A-C2A	-6.18	109.35	126.12
11	aA	835	CLA	CMD-C2D-C1D	6.17	135.59	124.71
11	cB	807	CLA	C2C-C1C-NC	6.17	115.75	109.97
11	cA	815	CLA	CMD-C2D-C1D	6.17	135.59	124.71
11	aA	815	CLA	CMD-C2D-C1D	6.17	135.58	124.71
11	aB	807	CLA	C2C-C1C-NC	6.17	115.75	109.97
12	aA	827	F6C	CMA-C3A-C2A	-6.17	109.37	126.12
12	cA	827	F6C	CMA-C3A-C2A	-6.17	109.38	126.12
11	cA	835	CLA	CMD-C2D-C1D	6.15	135.56	124.71
11	cB	805	CLA	CMD-C2D-C1D	6.15	135.54	124.71
11	bB	805	CLA	CMD-C2D-C1D	6.15	135.54	124.71
11	bA	835	CLA	CMD-C2D-C1D	6.14	135.54	124.71
12	cA	826	F6C	O2D-CGD-CBD	6.14	122.18	111.27
12	bA	826	F6C	O2D-CGD-CBD	6.14	122.17	111.27
11	cA	805	CLA	CMD-C2D-C1D	6.13	135.52	124.71
11	bB	834	CLA	C2C-C1C-NC	6.13	115.72	109.97
12	aA	826	F6C	O2D-CGD-CBD	6.13	122.16	111.27
11	cB	838	CLA	CMD-C2D-C1D	6.13	135.52	124.71
11	aB	805	CLA	CMD-C2D-C1D	6.13	135.51	124.71
12	cA	844	F6C	CAA-C2A-C1A	-6.13	111.24	128.11
11	aA	805	CLA	CMD-C2D-C1D	6.13	135.51	124.71
11	bB	838	CLA	CMD-C2D-C1D	6.12	135.50	124.71
11	bA	805	CLA	CMD-C2D-C1D	6.12	135.50	124.71
11	cB	811	CLA	CMD-C2D-C1D	6.12	135.50	124.71
11	aB	838	CLA	CMD-C2D-C1D	6.12	135.50	124.71
11	bB	811	CLA	CMD-C2D-C1D	6.12	135.50	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cB	834	CLA	C2C-C1C-NC	6.12	115.70	109.97
11	bB	823	CLA	CHD-C4C-C3C	-6.11	115.86	124.84
11	aB	834	CLA	C2C-C1C-NC	6.11	115.69	109.97
12	bA	844	F6C	CAA-C2A-C1A	-6.10	111.30	128.11
11	cA	816	CLA	CMD-C2D-C1D	6.10	135.47	124.71
11	cB	823	CLA	CHD-C4C-C3C	-6.10	115.87	124.84
12	cA	844	F6C	C2D-C1D-ND	6.10	115.69	109.97
11	bB	809	CLA	C2B-C1B-NB	6.10	114.32	110.23
11	cB	836	CLA	CMD-C2D-C1D	6.10	135.46	124.71
11	aA	813	CLA	CMD-C2D-C1D	6.10	135.46	124.71
12	aA	844	F6C	CAA-C2A-C1A	-6.10	111.32	128.11
11	aB	823	CLA	CHD-C4C-C3C	-6.10	115.88	124.84
11	cA	843	CLA	CMD-C2D-C1D	6.10	135.46	124.71
11	aB	836	CLA	CMD-C2D-C1D	6.09	135.45	124.71
11	bA	831	CLA	C2C-C1C-NC	6.09	115.68	109.97
11	aA	816	CLA	CMD-C2D-C1D	6.09	135.45	124.71
11	bA	813	CLA	CMD-C2D-C1D	6.09	135.45	124.71
11	aA	802	CLA	CHD-C1D-ND	-6.09	118.86	124.45
11	cA	813	CLA	CMD-C2D-C1D	6.09	135.44	124.71
11	cB	813	CLA	CMD-C2D-C1D	6.08	135.44	124.71
11	cB	801	CLA	CMD-C2D-C1D	6.08	135.44	124.71
11	cA	822	CLA	C2B-C1B-NB	6.08	114.31	110.23
11	aB	811	CLA	CMD-C2D-C1D	6.08	135.43	124.71
11	aA	843	CLA	CMD-C2D-C1D	6.08	135.43	124.71
11	bA	816	CLA	CMD-C2D-C1D	6.08	135.43	124.71
11	bA	837	CLA	CHD-C4C-C3C	-6.08	115.90	124.84
11	cA	837	CLA	CHD-C4C-C3C	-6.08	115.91	124.84
11	aB	808	CLA	CHD-C4C-C3C	-6.07	115.91	124.84
11	aB	809	CLA	C2B-C1B-NB	6.07	114.30	110.23
11	bB	801	CLA	CMD-C2D-C1D	6.07	135.41	124.71
11	bB	840	CLA	C2C-C1C-NC	6.07	115.66	109.97
11	bB	808	CLA	CHD-C4C-C3C	-6.07	115.92	124.84
11	aA	836	CLA	C2C-C1C-NC	6.07	115.66	109.97
11	cB	808	CLA	CHD-C4C-C3C	-6.07	115.92	124.84
11	cB	840	CLA	C2B-C1B-NB	6.07	114.30	110.23
11	aA	831	CLA	C2C-C1C-NC	6.07	115.66	109.97
11	cA	831	CLA	C2C-C1C-NC	6.07	115.66	109.97
11	bB	836	CLA	CMD-C2D-C1D	6.06	135.40	124.71
11	bA	822	CLA	C2B-C1B-NB	6.06	114.29	110.23
11	aB	801	CLA	CMD-C2D-C1D	6.06	135.39	124.71
12	aA	844	F6C	C2D-C1D-ND	6.06	115.65	109.97
11	bA	843	CLA	CMD-C2D-C1D	6.05	135.38	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aB	840	CLA	C2B-C1B-NB	6.05	114.29	110.23
11	bB	840	CLA	C2B-C1B-NB	6.05	114.29	110.23
11	aB	813	CLA	CMD-C2D-C1D	6.05	135.37	124.71
12	aA	830	F6C	C2D-C1D-ND	6.04	115.64	109.97
11	bB	814	CLA	CMD-C2D-C1D	6.04	135.36	124.71
11	aB	840	CLA	C2C-C1C-NC	6.04	115.63	109.97
11	cA	802	CLA	CHD-C1D-ND	-6.04	118.90	124.45
12	bA	844	F6C	C2D-C1D-ND	6.04	115.63	109.97
11	cA	836	CLA	C2C-C1C-NC	6.04	115.63	109.97
11	bA	802	CLA	CHD-C1D-ND	-6.04	118.91	124.45
11	cA	823	CLA	O2D-CGD-CBD	6.04	121.99	111.27
11	aB	814	CLA	CMD-C2D-C1D	6.03	135.35	124.71
11	bA	836	CLA	C2C-C1C-NC	6.03	115.62	109.97
11	bB	813	CLA	CMD-C2D-C1D	6.03	135.34	124.71
12	cA	830	F6C	CAA-C2A-C1A	-6.03	111.50	128.11
11	cA	836	CLA	CHD-C4C-C3C	-6.03	115.98	124.84
11	bB	833	CLA	CHD-C1D-ND	-6.03	118.92	124.45
11	aA	837	CLA	CHD-C4C-C3C	-6.03	115.98	124.84
11	aB	833	CLA	CHD-C1D-ND	-6.02	118.92	124.45
12	cA	830	F6C	C2D-C1D-ND	6.02	115.61	109.97
12	aA	830	F6C	CAA-C2A-C1A	-6.02	111.53	128.11
11	bA	817	CLA	C2C-C1C-NC	6.02	115.61	109.97
11	cB	840	CLA	C2C-C1C-NC	6.02	115.61	109.97
11	cB	814	CLA	CMD-C2D-C1D	6.02	135.32	124.71
11	bA	836	CLA	CHD-C4C-C3C	-6.02	115.99	124.84
11	bA	823	CLA	O2D-CGD-CBD	6.02	121.96	111.27
11	aA	805	CLA	CHD-C4C-C3C	-6.01	116.00	124.84
12	bA	830	F6C	CAA-C2A-C1A	-6.01	111.55	128.11
11	cB	833	CLA	CHD-C1D-ND	-6.01	118.93	124.45
11	aA	822	CLA	C2B-C1B-NB	6.01	114.26	110.23
12	bA	830	F6C	C2D-C1D-ND	6.01	115.60	109.97
11	aA	823	CLA	O2D-CGD-CBD	6.00	121.93	111.27
11	aA	836	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
11	cB	802	CLA	CHD-C4C-C3C	-5.99	116.03	124.84
11	aA	817	CLA	C2C-C1C-NC	5.98	115.58	109.97
11	bA	805	CLA	CHD-C4C-C3C	-5.98	116.05	124.84
11	cA	805	CLA	CHD-C4C-C3C	-5.98	116.05	124.84
11	bB	817	CLA	CHD-C1D-ND	-5.98	118.96	124.45
11	bB	802	CLA	CHD-C4C-C3C	-5.98	116.05	124.84
11	cA	807	CLA	CHD-C4C-C3C	-5.98	116.05	124.84
11	cA	817	CLA	C2C-C1C-NC	5.97	115.57	109.97
11	bB	825	CLA	CHD-C4C-C3C	-5.97	116.06	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cB	840	CLA	CHD-C4C-C3C	-5.97	116.06	124.84
11	bB	840	CLA	CHD-C4C-C3C	-5.97	116.07	124.84
12	cL	202	F6C	C4A-C3A-C2A	-5.96	98.23	106.94
11	aB	802	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
11	aB	840	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
11	aB	825	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
11	bA	822	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
11	cB	825	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
12	aL	202	F6C	C4A-C3A-C2A	-5.96	98.24	106.94
11	cB	809	CLA	C2B-C1B-NB	5.96	114.22	110.23
11	aA	822	CLA	CHD-C4C-C3C	-5.96	116.09	124.84
11	aA	820	CLA	C2C-C1C-NC	5.95	115.55	109.97
11	aL	204	CLA	O2D-CGD-CBD	5.95	121.84	111.27
11	bA	807	CLA	CHD-C4C-C3C	-5.94	116.11	124.84
11	aA	835	CLA	CHD-C4C-C3C	-5.94	116.11	124.84
11	bA	835	CLA	CHD-C4C-C3C	-5.94	116.11	124.84
11	cA	835	CLA	CHD-C4C-C3C	-5.94	116.11	124.84
12	bA	832	F6C	C2D-C1D-ND	5.93	115.53	109.97
12	aA	832	F6C	C2D-C1D-ND	5.93	115.53	109.97
11	aB	817	CLA	CHD-C1D-ND	-5.93	119.00	124.45
11	cB	817	CLA	CHD-C1D-ND	-5.93	119.00	124.45
11	aA	807	CLA	CHD-C4C-C3C	-5.93	116.12	124.84
11	cA	822	CLA	CHD-C4C-C3C	-5.93	116.13	124.84
11	bL	204	CLA	O2D-CGD-CBD	5.93	121.80	111.27
12	bL	202	F6C	C4A-C3A-C2A	-5.92	98.29	106.94
11	bA	820	CLA	C2C-C1C-NC	5.92	115.52	109.97
11	cA	820	CLA	C2C-C1C-NC	5.92	115.52	109.97
11	aB	828	CLA	C2D-C1D-ND	5.92	114.47	110.10
11	bA	822	CLA	CMD-C2D-C1D	5.92	135.15	124.71
11	cL	204	CLA	O2D-CGD-CBD	5.92	121.79	111.27
11	cB	818	CLA	CHD-C4C-C3C	-5.92	116.14	124.84
12	bL	202	F6C	O2D-CGD-CBD	5.91	121.77	111.27
11	aB	818	CLA	CHD-C4C-C3C	-5.91	116.15	124.84
11	bA	808	CLA	CHD-C1D-ND	-5.91	119.02	124.45
11	bB	818	CLA	CHD-C4C-C3C	-5.91	116.15	124.84
11	bB	828	CLA	C2D-C1D-ND	5.91	114.46	110.10
11	cA	822	CLA	CMD-C2D-C1D	5.91	135.12	124.71
11	cB	827	CLA	CHD-C4C-C3C	-5.91	116.16	124.84
11	bB	819	CLA	CHD-C4C-C3C	-5.90	116.16	124.84
12	aL	202	F6C	O2D-CGD-CBD	5.90	121.76	111.27
11	cB	837	CLA	CHD-C4C-C3C	-5.90	116.17	124.84
11	aB	807	CLA	CMD-C2D-C1D	5.90	135.11	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bA	836	CLA	C2B-C1B-NB	5.90	114.19	110.23
11	aA	822	CLA	CMD-C2D-C1D	5.90	135.11	124.71
11	cL	204	CLA	CMD-C2D-C1D	5.90	135.11	124.71
11	cB	828	CLA	C2D-C1D-ND	5.90	114.45	110.10
11	aL	206	CLA	CHD-C4C-C3C	-5.90	116.17	124.84
11	cL	206	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
11	cA	808	CLA	CHD-C1D-ND	-5.89	119.04	124.45
11	bB	807	CLA	CMD-C2D-C1D	5.89	135.09	124.71
11	cB	819	CLA	CHD-C4C-C3C	-5.89	116.19	124.84
11	aA	808	CLA	CHD-C1D-ND	-5.89	119.04	124.45
11	cA	821	CLA	C2C-C1C-NC	5.89	115.49	109.97
12	cL	202	F6C	O2D-CGD-CBD	5.89	121.73	111.27
11	bA	810	CLA	CHD-C4C-C3C	-5.89	116.19	124.84
11	bB	827	CLA	CHD-C4C-C3C	-5.89	116.19	124.84
11	aL	204	CLA	CMD-C2D-C1D	5.89	135.09	124.71
12	cA	832	F6C	C2D-C1D-ND	5.88	115.48	109.97
11	bL	204	CLA	CMD-C2D-C1D	5.88	135.08	124.71
11	cB	807	CLA	CMD-C2D-C1D	5.88	135.08	124.71
11	bB	821	CLA	C2C-C1C-NC	5.88	115.48	109.97
11	aA	836	CLA	C2B-C1B-NB	5.88	114.17	110.23
11	bA	821	CLA	C2C-C1C-NC	5.88	115.48	109.97
11	bA	834	CLA	CHD-C4C-C3C	-5.88	116.20	124.84
11	cA	804	CLA	CHD-C4C-C3C	-5.88	116.20	124.84
11	aA	810	CLA	CHD-C4C-C3C	-5.88	116.20	124.84
11	cA	815	CLA	C2C-C1C-NC	5.88	115.48	109.97
11	bA	831	CLA	O2D-CGD-CBD	5.88	121.71	111.27
11	aA	821	CLA	C2C-C1C-NC	5.87	115.47	109.97
11	cA	810	CLA	CHD-C4C-C3C	-5.87	116.21	124.84
11	aA	838	CLA	CHD-C4C-C3C	-5.87	116.21	124.84
11	bB	837	CLA	CHD-C4C-C3C	-5.87	116.21	124.84
11	bL	206	CLA	CHD-C4C-C3C	-5.87	116.21	124.84
11	aA	834	CLA	CHD-C4C-C3C	-5.87	116.21	124.84
11	aB	837	CLA	CHD-C4C-C3C	-5.87	116.22	124.84
11	aB	821	CLA	C2C-C1C-NC	5.87	115.47	109.97
11	bA	838	CLA	CHD-C4C-C3C	-5.87	116.22	124.84
11	cB	816	CLA	CHD-C1D-ND	-5.86	119.06	124.45
11	aB	827	CLA	CHD-C4C-C3C	-5.86	116.22	124.84
11	aA	815	CLA	C2C-C1C-NC	5.86	115.47	109.97
11	bA	804	CLA	CHD-C4C-C3C	-5.86	116.22	124.84
11	cA	834	CLA	CHD-C4C-C3C	-5.86	116.22	124.84
11	cA	838	CLA	CHD-C4C-C3C	-5.86	116.23	124.84
11	cA	831	CLA	O2D-CGD-CBD	5.85	121.67	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aB	803	CLA	CHD-C1D-ND	-5.85	119.08	124.45
11	aB	813	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
11	aB	819	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
11	cA	842	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
11	aA	831	CLA	O2D-CGD-CBD	5.85	121.66	111.27
11	bB	803	CLA	CHD-C1D-ND	-5.85	119.08	124.45
11	bB	835	CLA	C2C-C1C-NC	5.85	115.45	109.97
11	cA	810	CLA	CMD-C2D-C1D	5.85	135.02	124.71
11	cB	820	CLA	CHD-C4C-C3C	-5.85	116.25	124.84
11	bA	810	CLA	CMD-C2D-C1D	5.85	135.02	124.71
11	cA	843	CLA	CHD-C4C-C3C	-5.84	116.25	124.84
11	cB	813	CLA	CHD-C4C-C3C	-5.84	116.26	124.84
11	aA	810	CLA	CMD-C2D-C1D	5.84	135.00	124.71
11	bB	816	CLA	CHD-C1D-ND	-5.84	119.09	124.45
11	cB	821	CLA	C2C-C1C-NC	5.84	115.44	109.97
11	cA	836	CLA	C2B-C1B-NB	5.84	114.14	110.23
11	aA	804	CLA	CHD-C4C-C3C	-5.84	116.26	124.84
11	cB	835	CLA	C2C-C1C-NC	5.83	115.44	109.97
11	bA	815	CLA	C2C-C1C-NC	5.83	115.44	109.97
11	aA	842	CLA	CHD-C4C-C3C	-5.83	116.27	124.84
11	aB	822	CLA	CHD-C1D-ND	-5.83	119.09	124.45
11	cB	823	CLA	C2C-C1C-NC	5.83	115.43	109.97
11	aB	835	CLA	C2C-C1C-NC	5.83	115.43	109.97
11	bB	823	CLA	O2D-CGD-CBD	5.82	121.62	111.27
11	cB	803	CLA	CHD-C1D-ND	-5.82	119.10	124.45
11	aB	820	CLA	CHD-C4C-C3C	-5.82	116.29	124.84
11	cB	823	CLA	O2D-CGD-CBD	5.81	121.60	111.27
11	bA	843	CLA	CHD-C4C-C3C	-5.81	116.29	124.84
11	bB	820	CLA	CHD-C4C-C3C	-5.81	116.30	124.84
11	aA	806	CLA	CHD-C1D-ND	-5.81	119.11	124.45
11	bB	822	CLA	CHD-C1D-ND	-5.81	119.11	124.45
11	bL	204	CLA	CHD-C4C-C3C	-5.81	116.30	124.84
11	aA	843	CLA	CHD-C4C-C3C	-5.81	116.30	124.84
11	aB	823	CLA	O2D-CGD-CBD	5.81	121.59	111.27
11	bA	842	CLA	CHD-C4C-C3C	-5.81	116.30	124.84
11	cL	204	CLA	CHD-C4C-C3C	-5.80	116.31	124.84
11	aA	810	CLA	C2C-C1C-NC	5.80	115.41	109.97
11	aB	816	CLA	CHD-C1D-ND	-5.80	119.12	124.45
11	aL	204	CLA	CHD-C4C-C3C	-5.80	116.32	124.84
11	bB	813	CLA	CHD-C4C-C3C	-5.79	116.32	124.84
11	cB	822	CLA	CHD-C1D-ND	-5.79	119.14	124.45
11	bA	806	CLA	CHD-C1D-ND	-5.79	119.14	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aA	802	CLA	CMD-C2D-C1D	5.78	134.91	124.71
11	bA	803	CLA	CHD-C4C-C3C	-5.78	116.34	124.84
10	aA	801	CL0	CHD-C4C-C3C	-5.78	116.35	124.84
11	aB	820	CLA	CHD-C1D-ND	-5.78	119.15	124.45
10	cA	801	CL0	CHD-C4C-C3C	-5.78	116.35	124.84
11	cA	802	CLA	CMD-C2D-C1D	5.78	134.89	124.71
11	cA	810	CLA	C2C-C1C-NC	5.77	115.38	109.97
11	aB	823	CLA	C2C-C1C-NC	5.77	115.38	109.97
11	aA	840	CLA	CHD-C1D-ND	-5.77	119.15	124.45
11	bA	840	CLA	CHD-C1D-ND	-5.77	119.15	124.45
11	bB	823	CLA	C2C-C1C-NC	5.76	115.37	109.97
11	bA	802	CLA	CMD-C2D-C1D	5.76	134.87	124.71
11	aA	813	CLA	CHD-C4C-C3C	-5.76	116.37	124.84
11	cA	840	CLA	CHD-C1D-ND	-5.76	119.16	124.45
11	cA	803	CLA	CHD-C4C-C3C	-5.75	116.38	124.84
11	cB	826	CLA	CMD-C2D-C1D	5.75	134.85	124.71
11	bA	813	CLA	CHD-C4C-C3C	-5.75	116.39	124.84
11	cB	820	CLA	CHD-C1D-ND	-5.75	119.17	124.45
11	bA	810	CLA	C2C-C1C-NC	5.74	115.35	109.97
11	bB	811	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
11	aA	803	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
12	aB	824	F6C	C2D-C1D-ND	5.74	115.35	109.97
11	cA	816	CLA	CHD-C4C-C3C	-5.74	116.41	124.84
12	cB	824	F6C	C2D-C1D-ND	5.74	115.35	109.97
10	bA	801	CL0	CHD-C4C-C3C	-5.74	116.41	124.84
11	bB	826	CLA	CMD-C2D-C1D	5.74	134.82	124.71
11	cB	821	CLA	CHD-C4C-C3C	-5.74	116.41	124.84
11	cA	806	CLA	CHD-C1D-ND	-5.74	119.18	124.45
11	bB	836	CLA	CHD-C4C-C3C	-5.74	116.41	124.84
11	aA	840	CLA	CHD-C4C-C3C	-5.73	116.42	124.84
11	cL	205	CLA	CHD-C4C-C3C	-5.73	116.42	124.84
11	bB	821	CLA	CHD-C4C-C3C	-5.73	116.42	124.84
11	aB	811	CLA	CHD-C4C-C3C	-5.73	116.42	124.84
11	cA	840	CLA	CHD-C4C-C3C	-5.73	116.42	124.84
11	cB	817	CLA	C2C-C1C-NC	5.73	115.34	109.97
11	aA	816	CLA	CHD-C4C-C3C	-5.72	116.43	124.84
11	cA	813	CLA	CHD-C4C-C3C	-5.72	116.43	124.84
11	aB	821	CLA	CHD-C4C-C3C	-5.72	116.43	124.84
11	bB	831	CLA	CHD-C4C-C3C	-5.72	116.43	124.84
11	bB	817	CLA	CHD-C4C-C3C	-5.72	116.44	124.84
11	cA	817	CLA	CHD-C4C-C3C	-5.72	116.44	124.84
11	cB	835	CLA	CHD-C4C-C3C	-5.71	116.44	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bA	816	CLA	CHD-C4C-C3C	-5.71	116.44	124.84
11	aB	817	CLA	CHD-C4C-C3C	-5.71	116.44	124.84
11	bA	840	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
11	aB	817	CLA	C2C-C1C-NC	5.71	115.32	109.97
11	bB	835	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
11	bB	820	CLA	CHD-C1D-ND	-5.71	119.21	124.45
11	aB	835	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
11	aB	826	CLA	CMD-C2D-C1D	5.71	134.77	124.71
11	cB	818	CLA	CMD-C2D-C1D	5.70	134.76	124.71
11	bA	817	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
12	bB	824	F6C	C2D-C1D-ND	5.70	115.31	109.97
11	cB	831	CLA	CHD-C4C-C3C	-5.70	116.47	124.84
11	aB	831	CLA	CHD-C4C-C3C	-5.70	116.47	124.84
11	aA	808	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
11	aB	810	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
11	aL	205	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
11	cB	811	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
11	aL	204	CLA	C2C-C1C-NC	5.69	115.31	109.97
11	bB	817	CLA	C2C-C1C-NC	5.69	115.31	109.97
11	aA	817	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
11	cB	838	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
11	cB	817	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
11	cB	810	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
11	cA	829	CLA	CHD-C1D-ND	-5.69	119.22	124.45
11	bA	839	CLA	C2C-C1C-NC	5.69	115.30	109.97
11	bB	814	CLA	C2C-C1C-NC	5.69	115.30	109.97
11	bB	810	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
11	bL	204	CLA	C2C-C1C-NC	5.69	115.30	109.97
11	aB	836	CLA	CHD-C4C-C3C	-5.69	116.48	124.84
11	bB	818	CLA	CMD-C2D-C1D	5.68	134.73	124.71
11	cB	836	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
11	aB	810	CLA	C2C-C1C-NC	5.68	115.30	109.97
11	bL	205	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
11	aA	811	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
11	bB	810	CLA	CHD-C1D-ND	-5.68	119.24	124.45
11	aB	838	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
11	aB	818	CLA	CMD-C2D-C1D	5.68	134.72	124.71
11	cA	811	CLA	CHD-C4C-C3C	-5.67	116.50	124.84
11	aB	838	CLA	C2C-C1C-NC	5.67	115.29	109.97
11	aB	814	CLA	C2C-C1C-NC	5.67	115.28	109.97
11	bA	808	CLA	CHD-C4C-C3C	-5.67	116.50	124.84
11	bB	838	CLA	C2C-C1C-NC	5.67	115.28	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bA	824	CLA	CHD-C4C-C3C	-5.67	116.51	124.84
11	bK	103	CLA	CHD-C4C-C3C	-5.67	116.51	124.84
11	cL	204	CLA	C2C-C1C-NC	5.66	115.28	109.97
10	cA	801	CL0	C2C-C1C-NC	5.66	115.28	109.97
11	cA	809	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
11	bA	820	CLA	CHD-C1D-ND	-5.66	119.25	124.45
11	bA	829	CLA	CHD-C1D-ND	-5.66	119.25	124.45
11	aA	839	CLA	C2C-C1C-NC	5.66	115.28	109.97
11	cB	838	CLA	C2C-C1C-NC	5.66	115.28	109.97
11	aB	827	CLA	C2C-C1C-NC	5.66	115.28	109.97
11	cB	810	CLA	C2C-C1C-NC	5.66	115.28	109.97
11	aK	103	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
11	aA	814	CLA	CHD-C1D-ND	-5.66	119.25	124.45
11	cA	808	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
11	aB	805	CLA	CHD-C1D-ND	-5.66	119.25	124.45
11	bB	830	CLA	CHD-C4C-C3C	-5.66	116.53	124.84
11	bA	829	CLA	C2C-C1C-NC	5.66	115.27	109.97
11	aK	101	CLA	CHD-C1D-ND	-5.66	119.26	124.45
10	aA	801	CL0	C2C-C1C-NC	5.65	115.27	109.97
11	cB	831	CLA	CHD-C1D-ND	-5.65	119.26	124.45
10	bA	801	CL0	C2C-C1C-NC	5.65	115.27	109.97
11	bB	827	CLA	C2C-C1C-NC	5.65	115.27	109.97
11	cA	833	CLA	CHD-C1D-ND	-5.65	119.26	124.45
11	aB	802	CLA	CMD-C2D-C1D	5.65	134.67	124.71
11	cB	814	CLA	C2C-C1C-NC	5.65	115.26	109.97
11	bB	838	CLA	CHD-C4C-C3C	-5.65	116.54	124.84
11	aA	824	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
11	bA	811	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
12	bA	832	F6C	C1A-C2A-C3A	-5.64	101.03	106.97
11	cA	842	CLA	CHD-C1D-ND	-5.64	119.27	124.45
11	cB	813	CLA	C2C-C1C-NC	5.64	115.26	109.97
11	bA	809	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
11	cA	811	CLA	CHD-C1D-ND	-5.64	119.27	124.45
11	aA	829	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
11	cB	827	CLA	C2C-C1C-NC	5.64	115.25	109.97
11	cK	103	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
11	bB	831	CLA	CHD-C1D-ND	-5.64	119.27	124.45
11	aA	833	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
11	bA	841	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
11	cA	824	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
11	cB	802	CLA	CMD-C2D-C1D	5.64	134.65	124.71
11	cA	820	CLA	CHD-C1D-ND	-5.63	119.28	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bA	829	CLA	CHD-C4C-C3C	-5.63	116.56	124.84
11	cA	829	CLA	CHD-C4C-C3C	-5.63	116.56	124.84
11	cA	833	CLA	CHD-C4C-C3C	-5.63	116.56	124.84
11	bB	802	CLA	CMD-C2D-C1D	5.63	134.64	124.71
11	bA	833	CLA	CHD-C4C-C3C	-5.63	116.56	124.84
11	aA	809	CLA	CHD-C4C-C3C	-5.63	116.56	124.84
11	aA	837	CLA	CHD-C1D-ND	-5.63	119.28	124.45
11	aA	834	CLA	C2C-C1C-NC	5.63	115.25	109.97
11	cA	839	CLA	C2C-C1C-NC	5.63	115.25	109.97
11	aK	101	CLA	CHD-C4C-C3C	-5.63	116.56	124.84
11	cA	821	CLA	CHD-C4C-C3C	-5.63	116.56	124.84
11	cK	101	CLA	CHD-C4C-C3C	-5.63	116.56	124.84
11	bA	834	CLA	C2C-C1C-NC	5.63	115.25	109.97
11	aB	830	CLA	CHD-C4C-C3C	-5.63	116.56	124.84
11	bA	833	CLA	CHD-C1D-ND	-5.63	119.28	124.45
11	aB	831	CLA	CHD-C1D-ND	-5.63	119.28	124.45
11	aA	842	CLA	CHD-C1D-ND	-5.63	119.28	124.45
11	cB	830	CLA	CHD-C4C-C3C	-5.62	116.57	124.84
12	aA	832	F6C	C1A-C2A-C3A	-5.62	101.05	106.97
11	cA	828	CLA	O2D-CGD-CBD	5.62	121.25	111.27
11	bA	811	CLA	CHD-C1D-ND	-5.62	119.29	124.45
11	bA	842	CLA	CHD-C1D-ND	-5.62	119.29	124.45
11	aA	841	CLA	CHD-C4C-C3C	-5.62	116.58	124.84
11	aA	820	CLA	CHD-C1D-ND	-5.62	119.29	124.45
11	bA	814	CLA	CHD-C1D-ND	-5.62	119.29	124.45
11	bA	828	CLA	O2D-CGD-CBD	5.62	121.25	111.27
12	bB	824	F6C	O2D-CGD-CBD	5.62	121.25	111.27
11	aA	829	CLA	CHD-C1D-ND	-5.61	119.29	124.45
11	bA	835	CLA	CHD-C1D-ND	-5.61	119.29	124.45
11	cA	837	CLA	CHD-C1D-ND	-5.61	119.29	124.45
11	cA	829	CLA	C2C-C1C-NC	5.61	115.23	109.97
11	aA	835	CLA	CHD-C1D-ND	-5.61	119.30	124.45
11	cA	814	CLA	CHD-C1D-ND	-5.61	119.30	124.45
12	cB	824	F6C	O2D-CGD-CBD	5.61	121.24	111.27
12	cA	832	F6C	C1A-C2A-C3A	-5.61	101.06	106.97
11	aA	821	CLA	CHD-C4C-C3C	-5.61	116.60	124.84
11	bK	101	CLA	CHD-C4C-C3C	-5.61	116.60	124.84
11	cA	841	CLA	CHD-C4C-C3C	-5.61	116.60	124.84
11	cA	834	CLA	C2C-C1C-NC	5.61	115.22	109.97
11	bB	805	CLA	CHD-C1D-ND	-5.61	119.30	124.45
11	bB	810	CLA	C2C-C1C-NC	5.61	115.22	109.97
11	bK	101	CLA	CHD-C1D-ND	-5.60	119.30	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cK	101	CLA	CHD-C1D-ND	-5.60	119.31	124.45
11	bA	821	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
12	aB	824	F6C	O2D-CGD-CBD	5.60	121.22	111.27
11	cA	835	CLA	CHD-C1D-ND	-5.60	119.31	124.45
11	cB	809	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
11	aA	828	CLA	O2D-CGD-CBD	5.60	121.22	111.27
11	bB	831	CLA	C2C-C1C-NC	5.60	115.22	109.97
11	cA	821	CLA	CMD-C2D-C1D	5.60	134.58	124.71
11	aA	821	CLA	CMD-C2D-C1D	5.60	134.57	124.71
11	bB	809	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
11	aB	810	CLA	CHD-C1D-ND	-5.60	119.31	124.45
11	cA	840	CLA	C2C-C1C-NC	5.59	115.21	109.97
11	cB	810	CLA	CHD-C1D-ND	-5.59	119.31	124.45
11	bA	840	CLA	C2C-C1C-NC	5.59	115.21	109.97
11	cA	825	CLA	C2C-C1C-NC	5.59	115.21	109.97
11	bA	821	CLA	CMD-C2D-C1D	5.59	134.56	124.71
12	aA	826	F6C	CMA-C3A-C4A	-5.59	114.86	124.71
11	bA	807	CLA	CHD-C1D-ND	-5.59	119.32	124.45
11	aA	811	CLA	CHD-C1D-ND	-5.59	119.32	124.45
11	cB	831	CLA	C2C-C1C-NC	5.59	115.20	109.97
11	aB	831	CLA	C2C-C1C-NC	5.58	115.20	109.97
11	bA	804	CLA	CHD-C1D-ND	-5.58	119.32	124.45
11	bA	825	CLA	C2C-C1C-NC	5.58	115.20	109.97
11	aA	833	CLA	CHD-C1D-ND	-5.58	119.33	124.45
11	cA	804	CLA	CHD-C1D-ND	-5.58	119.33	124.45
11	cB	805	CLA	CHD-C1D-ND	-5.58	119.33	124.45
12	cA	826	F6C	CMA-C3A-C4A	-5.58	114.88	124.71
12	bA	826	F6C	CMA-C3A-C4A	-5.58	114.89	124.71
11	aB	813	CLA	C2C-C1C-NC	5.58	115.19	109.97
11	aA	804	CLA	CHD-C1D-ND	-5.57	119.33	124.45
11	bA	812	CLA	CHD-C1D-ND	-5.57	119.33	124.45
11	bB	813	CLA	C2C-C1C-NC	5.57	115.19	109.97
11	bB	812	CLA	C2C-C1C-NC	5.57	115.19	109.97
11	aB	814	CLA	O2D-CGD-CBD	5.57	121.17	111.27
11	bA	837	CLA	CHD-C1D-ND	-5.57	119.34	124.45
11	aA	825	CLA	C2C-C1C-NC	5.57	115.19	109.97
11	aA	838	CLA	C2C-C1C-NC	5.57	115.19	109.97
11	cB	820	CLA	C2C-C1C-NC	5.57	115.19	109.97
11	aB	809	CLA	CHD-C4C-C3C	-5.57	116.66	124.84
11	cB	833	CLA	CHD-C4C-C3C	-5.56	116.66	124.84
11	cB	838	CLA	CHD-C1D-ND	-5.56	119.34	124.45
11	aA	829	CLA	C2C-C1C-NC	5.56	115.18	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aB	812	CLA	C2C-C1C-NC	5.56	115.18	109.97
11	bB	830	CLA	C2C-C1C-NC	5.56	115.18	109.97
11	bB	838	CLA	CHD-C1D-ND	-5.55	119.35	124.45
11	cA	839	CLA	CHD-C1D-ND	-5.55	119.35	124.45
11	aB	830	CLA	C2C-C1C-NC	5.55	115.17	109.97
11	aB	833	CLA	CHD-C4C-C3C	-5.55	116.69	124.84
11	bA	839	CLA	CHD-C1D-ND	-5.54	119.36	124.45
11	cB	812	CLA	C2C-C1C-NC	5.54	115.16	109.97
11	aB	838	CLA	CHD-C1D-ND	-5.54	119.37	124.45
11	cK	103	CLA	C2C-C1C-NC	5.54	115.16	109.97
11	aA	840	CLA	C2C-C1C-NC	5.53	115.16	109.97
11	aA	807	CLA	C2C-C1C-NC	5.53	115.16	109.97
11	aA	839	CLA	CHD-C1D-ND	-5.53	119.37	124.45
11	bB	837	CLA	CHD-C1D-ND	-5.53	119.37	124.45
11	cA	838	CLA	C2C-C1C-NC	5.53	115.15	109.97
11	aA	809	CLA	CHD-C1D-ND	-5.53	119.37	124.45
11	aA	839	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
11	bB	833	CLA	CHD-C4C-C3C	-5.53	116.72	124.84
11	bB	835	CLA	CHD-C1D-ND	-5.53	119.38	124.45
11	aB	832	CLA	CHD-C1D-ND	-5.52	119.38	124.45
11	aB	802	CLA	CHD-C1D-ND	-5.52	119.38	124.45
11	bA	838	CLA	C2C-C1C-NC	5.52	115.14	109.97
11	cA	809	CLA	CHD-C1D-ND	-5.52	119.38	124.45
11	aA	814	CLA	O2D-CGD-CBD	5.52	121.08	111.27
11	bA	814	CLA	CHD-C4C-C3C	-5.52	116.73	124.84
11	bB	814	CLA	O2D-CGD-CBD	5.52	121.07	111.27
11	aA	807	CLA	CHD-C1D-ND	-5.52	119.38	124.45
11	cB	814	CLA	O2D-CGD-CBD	5.52	121.07	111.27
11	cB	829	CLA	CHD-C1D-ND	-5.52	119.39	124.45
11	aK	103	CLA	C2C-C1C-NC	5.52	115.14	109.97
11	bA	814	CLA	O2D-CGD-CBD	5.51	121.06	111.27
11	cA	807	CLA	CHD-C1D-ND	-5.51	119.39	124.45
11	cB	811	CLA	C2C-C1C-NC	5.51	115.14	109.97
11	aA	812	CLA	CHD-C1D-ND	-5.51	119.39	124.45
11	bA	821	CLA	O2D-CGD-CBD	5.51	121.06	111.27
11	aB	811	CLA	C2C-C1C-NC	5.51	115.13	109.97
11	cB	830	CLA	C2C-C1C-NC	5.51	115.13	109.97
11	bB	805	CLA	CHD-C4C-C3C	-5.51	116.75	124.84
11	bA	809	CLA	CHD-C1D-ND	-5.51	119.39	124.45
11	cA	807	CLA	C2C-C1C-NC	5.51	115.13	109.97
11	bB	829	CLA	CHD-C1D-ND	-5.50	119.39	124.45
11	bK	103	CLA	C2C-C1C-NC	5.50	115.13	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bA	839	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
11	aB	835	CLA	CHD-C1D-ND	-5.50	119.40	124.45
11	cB	835	CLA	CHD-C1D-ND	-5.50	119.40	124.45
11	bA	807	CLA	C2C-C1C-NC	5.50	115.13	109.97
11	cB	805	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
11	aB	816	CLA	CHD-C4C-C3C	-5.50	116.76	124.84
11	aB	809	CLA	CHD-C1D-ND	-5.50	119.40	124.45
11	bB	820	CLA	C2C-C1C-NC	5.50	115.12	109.97
11	cA	839	CLA	CHD-C4C-C3C	-5.50	116.76	124.84
11	cB	802	CLA	CHD-C1D-ND	-5.50	119.40	124.45
11	cB	832	CLA	CHD-C1D-ND	-5.50	119.40	124.45
11	aB	829	CLA	CHD-C1D-ND	-5.50	119.40	124.45
11	aB	837	CLA	CHD-C1D-ND	-5.50	119.40	124.45
11	cA	822	CLA	C2C-C1C-NC	5.49	115.12	109.97
11	aA	813	CLA	C2C-C1C-NC	5.49	115.12	109.97
11	aB	823	CLA	CMD-C2D-C1D	5.49	134.39	124.71
11	aB	820	CLA	C2C-C1C-NC	5.49	115.11	109.97
11	aA	822	CLA	C2C-C1C-NC	5.49	115.11	109.97
11	cA	802	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
11	cA	814	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
11	cA	814	CLA	O2D-CGD-CBD	5.49	121.02	111.27
11	aB	806	CLA	CHD-C1D-ND	-5.49	119.41	124.45
11	bB	809	CLA	CHD-C1D-ND	-5.49	119.41	124.45
11	cA	821	CLA	O2D-CGD-CBD	5.49	121.02	111.27
11	aB	805	CLA	CHD-C4C-C3C	-5.48	116.78	124.84
11	bB	816	CLA	CHD-C4C-C3C	-5.48	116.78	124.84
11	bA	822	CLA	C2C-C1C-NC	5.48	115.11	109.97
11	bB	832	CLA	CHD-C1D-ND	-5.48	119.42	124.45
11	aB	807	CLA	CHD-C4C-C3C	-5.48	116.79	124.84
11	cA	812	CLA	CHD-C1D-ND	-5.48	119.42	124.45
11	cB	837	CLA	CHD-C1D-ND	-5.48	119.42	124.45
11	aA	823	CLA	C2C-C1C-NC	5.47	115.10	109.97
11	cB	816	CLA	CHD-C4C-C3C	-5.47	116.79	124.84
11	cL	206	CLA	CMD-C2D-C1D	5.47	134.36	124.71
11	aA	821	CLA	O2D-CGD-CBD	5.47	120.99	111.27
11	bB	823	CLA	CMD-C2D-C1D	5.47	134.36	124.71
11	aA	802	CLA	CHD-C4C-C3C	-5.47	116.80	124.84
11	bA	813	CLA	C2C-C1C-NC	5.47	115.10	109.97
11	bA	802	CLA	CHD-C4C-C3C	-5.47	116.80	124.84
11	aB	807	CLA	O2D-CGD-CBD	5.47	120.98	111.27
11	bA	823	CLA	C2C-C1C-NC	5.47	115.09	109.97
11	bB	819	CLA	C2C-C1C-NC	5.47	115.09	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cB	809	CLA	C2C-C1C-NC	5.47	115.09	109.97
11	cB	840	CLA	CHD-C1D-ND	-5.46	119.43	124.45
11	aA	814	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
11	bB	807	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
11	aB	819	CLA	C2C-C1C-NC	5.46	115.09	109.97
11	bA	815	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
11	bL	206	CLA	CMD-C2D-C1D	5.46	134.34	124.71
11	cB	807	CLA	O2D-CGD-CBD	5.46	120.97	111.27
11	bB	840	CLA	CHD-C1D-ND	-5.46	119.44	124.45
11	cA	805	CLA	CHD-C1D-ND	-5.46	119.44	124.45
11	aB	804	CLA	CHD-C1D-ND	-5.46	119.44	124.45
11	cB	809	CLA	CHD-C1D-ND	-5.46	119.44	124.45
11	aA	841	CLA	CMD-C2D-C1D	5.46	134.33	124.71
11	bB	807	CLA	O2D-CGD-CBD	5.46	120.96	111.27
11	cA	813	CLA	C2C-C1C-NC	5.45	115.08	109.97
11	aL	206	CLA	CMD-C2D-C1D	5.45	134.32	124.71
11	bA	841	CLA	CMD-C2D-C1D	5.45	134.32	124.71
11	cB	807	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
11	aB	825	CLA	C2C-C1C-NC	5.45	115.08	109.97
11	cA	841	CLA	CMD-C2D-C1D	5.45	134.32	124.71
11	cB	823	CLA	CMD-C2D-C1D	5.45	134.32	124.71
11	cA	811	CLA	C2C-C1C-NC	5.45	115.08	109.97
11	aB	819	CLA	CMD-C2D-C1D	5.45	134.32	124.71
11	aA	824	CLA	C2C-C1C-NC	5.45	115.07	109.97
11	bB	811	CLA	C2C-C1C-NC	5.45	115.07	109.97
11	bB	825	CLA	C2C-C1C-NC	5.45	115.07	109.97
11	aA	815	CLA	CHD-C4C-C3C	-5.44	116.84	124.84
11	bA	805	CLA	CHD-C1D-ND	-5.44	119.45	124.45
11	aB	840	CLA	CHD-C1D-ND	-5.44	119.45	124.45
11	cB	805	CLA	C2C-C1C-NC	5.44	115.06	109.97
11	bB	805	CLA	C2C-C1C-NC	5.44	115.06	109.97
11	bB	802	CLA	CHD-C1D-ND	-5.43	119.46	124.45
11	bA	817	CLA	CHD-C1D-ND	-5.43	119.47	124.45
11	cA	823	CLA	C2C-C1C-NC	5.42	115.05	109.97
11	aB	805	CLA	C2C-C1C-NC	5.42	115.05	109.97
11	cB	819	CLA	CMD-C2D-C1D	5.42	134.26	124.71
11	bA	833	CLA	C2C-C1C-NC	5.42	115.05	109.97
11	bB	809	CLA	C2C-C1C-NC	5.42	115.05	109.97
11	cA	815	CLA	CHD-C4C-C3C	-5.41	116.88	124.84
11	bB	806	CLA	CHD-C1D-ND	-5.41	119.48	124.45
11	bA	809	CLA	C2C-C1C-NC	5.41	115.04	109.97
11	cB	825	CLA	C2C-C1C-NC	5.41	115.04	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aA	817	CLA	CHD-C1D-ND	-5.41	119.48	124.45
11	cA	824	CLA	CHD-C1D-ND	-5.41	119.48	124.45
11	bA	811	CLA	C2C-C1C-NC	5.41	115.04	109.97
11	bA	824	CLA	CHD-C1D-ND	-5.41	119.49	124.45
11	cA	819	CLA	CHD-C1D-ND	-5.41	119.49	124.45
11	aA	809	CLA	C2C-C1C-NC	5.41	115.04	109.97
11	cB	819	CLA	C2C-C1C-NC	5.41	115.04	109.97
11	cA	817	CLA	CHD-C1D-ND	-5.40	119.49	124.45
11	aA	833	CLA	C2C-C1C-NC	5.40	115.03	109.97
11	bB	819	CLA	CMD-C2D-C1D	5.40	134.24	124.71
11	aA	805	CLA	CHD-C1D-ND	-5.40	119.49	124.45
11	bA	824	CLA	C2C-C1C-NC	5.40	115.03	109.97
11	cA	841	CLA	C2C-C1C-NC	5.40	115.03	109.97
11	aB	809	CLA	C2C-C1C-NC	5.39	115.03	109.97
11	bK	101	CLA	C2C-C1C-NC	5.39	115.03	109.97
11	cA	808	CLA	C2C-C1C-NC	5.39	115.03	109.97
11	cA	824	CLA	C2C-C1C-NC	5.39	115.03	109.97
11	aB	808	CLA	C2C-C1C-NC	5.39	115.02	109.97
11	bA	812	CLA	C2C-C1C-NC	5.39	115.02	109.97
11	cB	834	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
11	bB	804	CLA	CHD-C1D-ND	-5.39	119.50	124.45
11	bB	834	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
11	aA	824	CLA	CHD-C1D-ND	-5.39	119.50	124.45
11	bA	843	CLA	C2C-C1C-NC	5.39	115.02	109.97
11	cB	806	CLA	CHD-C1D-ND	-5.39	119.50	124.45
11	aK	101	CLA	C2C-C1C-NC	5.39	115.02	109.97
11	bA	841	CLA	C2C-C1C-NC	5.39	115.02	109.97
11	aB	834	CLA	CHD-C4C-C3C	-5.38	116.92	124.84
11	aA	808	CLA	C2C-C1C-NC	5.38	115.02	109.97
11	aA	843	CLA	C2C-C1C-NC	5.38	115.02	109.97
11	cB	804	CLA	CHD-C1D-ND	-5.38	119.51	124.45
11	bA	802	CLA	O2D-CGD-CBD	5.38	120.83	111.27
11	aA	811	CLA	C2C-C1C-NC	5.38	115.01	109.97
11	cA	809	CLA	C2C-C1C-NC	5.38	115.01	109.97
11	aA	802	CLA	O2D-CGD-CBD	5.38	120.82	111.27
11	bA	841	CLA	CHD-C1D-ND	-5.38	119.51	124.45
11	bB	808	CLA	O2D-CGD-CBD	5.37	120.81	111.27
11	cA	802	CLA	O2D-CGD-CBD	5.37	120.81	111.27
11	cA	833	CLA	C2C-C1C-NC	5.37	115.00	109.97
12	cA	844	F6C	C1A-C2A-C3A	-5.37	101.32	106.97
11	aL	206	CLA	C2C-C1C-NC	5.36	115.00	109.97
11	cA	843	CLA	C2C-C1C-NC	5.36	115.00	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aA	837	CLA	C2C-C1C-NC	5.36	115.00	109.97
11	cK	101	CLA	C2C-C1C-NC	5.36	115.00	109.97
11	cA	841	CLA	CHD-C1D-ND	-5.36	119.53	124.45
11	cK	103	CLA	CHD-C1D-ND	-5.36	119.53	124.45
11	bA	837	CLA	C2C-C1C-NC	5.36	114.99	109.97
11	aB	802	CLA	C4A-NA-C1A	-5.36	104.30	106.71
11	aA	819	CLA	CHD-C1D-ND	-5.36	119.53	124.45
11	aA	841	CLA	CHD-C1D-ND	-5.36	119.53	124.45
12	cA	826	F6C	C1A-C2A-C3A	-5.35	101.33	106.97
11	bA	808	CLA	C2C-C1C-NC	5.35	114.99	109.97
11	bL	205	CLA	CMD-C2D-C1D	5.35	134.14	124.71
11	aB	830	CLA	CHD-C1D-ND	-5.35	119.54	124.45
12	aA	844	F6C	C1A-C2A-C3A	-5.35	101.34	106.97
11	cA	825	CLA	CHD-C4C-C3C	-5.35	116.98	124.84
11	bB	826	CLA	C2C-C1C-NC	5.34	114.98	109.97
11	bL	206	CLA	C2C-C1C-NC	5.34	114.98	109.97
11	cB	808	CLA	O2D-CGD-CBD	5.34	120.76	111.27
11	cA	812	CLA	C2C-C1C-NC	5.34	114.98	109.97
11	bB	814	CLA	CHD-C1D-ND	-5.34	119.55	124.45
11	bB	832	CLA	CHD-C4C-C3C	-5.34	116.99	124.84
11	aB	826	CLA	C2C-C1C-NC	5.34	114.97	109.97
11	aB	832	CLA	CHD-C4C-C3C	-5.34	116.99	124.84
11	bA	825	CLA	CHD-C4C-C3C	-5.34	116.99	124.84
11	aB	808	CLA	O2D-CGD-CBD	5.34	120.75	111.27
11	bB	830	CLA	CHD-C1D-ND	-5.34	119.55	124.45
11	bA	819	CLA	CHD-C1D-ND	-5.34	119.55	124.45
11	aA	812	CLA	CHD-C4C-C3C	-5.34	117.00	124.84
11	aA	840	CLA	O2D-CGD-CBD	5.33	120.75	111.27
11	cA	809	CLA	O2D-CGD-CBD	5.33	120.74	111.27
11	bA	840	CLA	O2D-CGD-CBD	5.33	120.74	111.27
11	bB	802	CLA	C4A-NA-C1A	-5.33	104.31	106.71
12	cA	830	F6C	C1A-C2A-C3A	-5.33	101.36	106.97
11	bL	205	CLA	C2C-C1C-NC	5.33	114.97	109.97
11	cB	814	CLA	CHD-C1D-ND	-5.33	119.56	124.45
11	cB	832	CLA	CHD-C4C-C3C	-5.33	117.01	124.84
11	cB	830	CLA	CHD-C1D-ND	-5.33	119.56	124.45
11	bB	808	CLA	C2C-C1C-NC	5.33	114.96	109.97
12	aA	830	F6C	C1A-C2A-C3A	-5.33	101.36	106.97
11	cB	808	CLA	C2C-C1C-NC	5.33	114.96	109.97
11	aA	825	CLA	CHD-C4C-C3C	-5.32	117.01	124.84
11	aA	809	CLA	O2D-CGD-CBD	5.32	120.73	111.27
12	bA	830	F6C	C1A-C2A-C3A	-5.32	101.36	106.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aA	812	CLA	C2C-C1C-NC	5.32	114.96	109.97
11	cA	837	CLA	C2C-C1C-NC	5.32	114.96	109.97
11	bA	812	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
11	bB	834	CLA	CHD-C1D-ND	-5.32	119.56	124.45
11	bA	809	CLA	O2D-CGD-CBD	5.32	120.72	111.27
11	aB	814	CLA	CHD-C1D-ND	-5.32	119.57	124.45
12	aA	826	F6C	C1A-C2A-C3A	-5.32	101.37	106.97
11	bA	805	CLA	O2D-CGD-CBD	5.32	120.72	111.27
11	bA	835	CLA	C2C-C1C-NC	5.31	114.95	109.97
11	aL	205	CLA	CMD-C2D-C1D	5.31	134.08	124.71
12	bA	844	F6C	C1A-C2A-C3A	-5.31	101.38	106.97
11	cA	840	CLA	O2D-CGD-CBD	5.31	120.71	111.27
11	aB	814	CLA	CHD-C4C-C3C	-5.31	117.03	124.84
11	cL	205	CLA	CMD-C2D-C1D	5.31	134.07	124.71
11	aL	205	CLA	C2C-C1C-NC	5.31	114.95	109.97
11	cL	205	CLA	C2C-C1C-NC	5.31	114.95	109.97
11	cA	812	CLA	CHD-C4C-C3C	-5.31	117.04	124.84
11	bB	809	CLA	CMD-C2D-C1D	5.31	134.07	124.71
11	bB	814	CLA	CHD-C4C-C3C	-5.31	117.04	124.84
11	aB	809	CLA	CMD-C2D-C1D	5.30	134.06	124.71
11	cB	826	CLA	C2C-C1C-NC	5.30	114.94	109.97
11	cB	834	CLA	CHD-C1D-ND	-5.30	119.58	124.45
11	cA	805	CLA	O2D-CGD-CBD	5.30	120.69	111.27
11	cB	814	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
11	cB	809	CLA	CMD-C2D-C1D	5.30	134.05	124.71
11	cL	206	CLA	C2C-C1C-NC	5.30	114.93	109.97
12	bA	826	F6C	C1A-C2A-C3A	-5.29	101.39	106.97
11	aA	805	CLA	O2D-CGD-CBD	5.29	120.67	111.27
11	cA	835	CLA	C2C-C1C-NC	5.29	114.93	109.97
11	aA	841	CLA	C2C-C1C-NC	5.29	114.93	109.97
11	bK	103	CLA	CHD-C1D-ND	-5.29	119.59	124.45
11	aB	834	CLA	CHD-C1D-ND	-5.28	119.60	124.45
11	bB	812	CLA	O2D-CGD-CBD	5.28	120.66	111.27
11	bA	838	CLA	CHD-C1D-ND	-5.28	119.60	124.45
11	aA	835	CLA	C2C-C1C-NC	5.28	114.92	109.97
11	aA	834	CLA	CHD-C1D-ND	-5.28	119.60	124.45
11	cA	842	CLA	C2C-C1C-NC	5.27	114.91	109.97
11	bA	834	CLA	CHD-C1D-ND	-5.27	119.61	124.45
11	aK	103	CLA	CHD-C1D-ND	-5.27	119.61	124.45
11	cA	834	CLA	CHD-C1D-ND	-5.26	119.62	124.45
11	bA	802	CLA	C4A-NA-C1A	-5.26	104.34	106.71
11	cB	804	CLA	O2D-CGD-CBD	5.26	120.62	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	827	F6C	C4A-C3A-C2A	-5.26	99.26	106.94
11	aB	807	CLA	CHD-C1D-ND	-5.26	119.62	124.45
11	cA	828	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
11	aA	842	CLA	C2C-C1C-NC	5.26	114.90	109.97
11	aB	812	CLA	O2D-CGD-CBD	5.25	120.61	111.27
12	bA	827	F6C	C4A-C3A-C2A	-5.25	99.27	106.94
11	aB	804	CLA	O2D-CGD-CBD	5.25	120.59	111.27
11	bA	828	CLA	C3D-C2D-C1D	-5.25	98.67	105.83
11	aA	820	CLA	CHD-C4C-C3C	-5.25	117.13	124.84
11	cA	838	CLA	CHD-C1D-ND	-5.24	119.64	124.45
11	cA	831	CLA	CHD-C4C-C3C	-5.24	117.13	124.84
11	cA	820	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
11	cB	812	CLA	O2D-CGD-CBD	5.24	120.58	111.27
11	aB	836	CLA	C2C-C1C-NC	5.24	114.88	109.97
11	aB	806	CLA	C2C-C1C-NC	5.24	114.88	109.97
12	bA	832	F6C	O2D-CGD-CBD	5.23	120.57	111.27
11	aA	831	CLA	CHD-C4C-C3C	-5.23	117.15	124.84
11	cA	804	CLA	C2C-C1C-NC	5.23	114.87	109.97
11	aA	838	CLA	CHD-C1D-ND	-5.23	119.65	124.45
11	bA	831	CLA	CHD-C4C-C3C	-5.23	117.15	124.84
11	bB	812	CLA	CHD-C4C-C3C	-5.23	117.16	124.84
11	bA	820	CLA	CHD-C4C-C3C	-5.23	117.16	124.84
11	bB	804	CLA	O2D-CGD-CBD	5.23	120.56	111.27
11	aB	832	CLA	C2C-C1C-NC	5.22	114.87	109.97
12	aA	832	F6C	O2D-CGD-CBD	5.22	120.55	111.27
11	bB	807	CLA	CHD-C1D-ND	-5.22	119.66	124.45
11	aA	804	CLA	C2C-C1C-NC	5.22	114.86	109.97
11	bB	836	CLA	C2C-C1C-NC	5.22	114.86	109.97
11	bA	842	CLA	C2C-C1C-NC	5.22	114.86	109.97
11	bB	802	CLA	C2C-C1C-NC	5.22	114.86	109.97
12	cA	832	F6C	O2D-CGD-CBD	5.21	120.53	111.27
11	bB	802	CLA	C3B-C2B-C1B	-5.21	100.87	107.16
11	aB	802	CLA	C2C-C1C-NC	5.21	114.86	109.97
11	cB	802	CLA	C2C-C1C-NC	5.21	114.85	109.97
12	cA	827	F6C	C4A-C3A-C2A	-5.21	99.33	106.94
11	cB	832	CLA	C2C-C1C-NC	5.21	114.85	109.97
11	aA	828	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
11	cB	802	CLA	C4A-NA-C1A	-5.20	104.37	106.71
11	aA	815	CLA	CHD-C1D-ND	-5.20	119.67	124.45
11	cB	836	CLA	C2C-C1C-NC	5.20	114.84	109.97
11	aB	812	CLA	CHD-C4C-C3C	-5.20	117.20	124.84
11	aB	803	CLA	C2C-C1C-NC	5.20	114.84	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cA	807	CLA	O2D-CGD-CBD	5.20	120.50	111.27
11	bA	804	CLA	C2C-C1C-NC	5.20	114.84	109.97
11	aB	818	CLA	CHD-C1D-ND	-5.19	119.68	124.45
11	cB	825	CLA	CHD-C1D-ND	-5.19	119.68	124.45
11	bB	806	CLA	C2C-C1C-NC	5.19	114.83	109.97
11	aB	825	CLA	O2D-CGD-CBD	5.19	120.49	111.27
11	cA	838	CLA	O2D-CGD-CBD	5.19	120.49	111.27
11	cA	815	CLA	CHD-C1D-ND	-5.19	119.68	124.45
11	aB	812	CLA	CHD-C1D-ND	-5.19	119.69	124.45
11	cB	807	CLA	CHD-C1D-ND	-5.19	119.69	124.45
11	cB	818	CLA	CHD-C1D-ND	-5.19	119.69	124.45
11	aB	815	CLA	CHD-C1D-ND	-5.18	119.69	124.45
11	bB	815	CLA	CHD-C1D-ND	-5.18	119.69	124.45
11	cB	802	CLA	C3B-C2B-C1B	-5.18	100.91	107.16
11	bA	823	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
11	bA	838	CLA	O2D-CGD-CBD	5.18	120.47	111.27
11	bB	825	CLA	O2D-CGD-CBD	5.18	120.47	111.27
11	bB	812	CLA	CHD-C1D-ND	-5.17	119.70	124.45
11	bA	807	CLA	O2D-CGD-CBD	5.17	120.46	111.27
11	bB	803	CLA	C2C-C1C-NC	5.17	114.82	109.97
11	cB	812	CLA	CHD-C4C-C3C	-5.17	117.24	124.84
11	bL	204	CLA	CHD-C1D-ND	-5.17	119.70	124.45
11	cB	806	CLA	C2C-C1C-NC	5.17	114.82	109.97
11	aA	838	CLA	O2D-CGD-CBD	5.17	120.46	111.27
11	bA	815	CLA	CHD-C1D-ND	-5.17	119.70	124.45
11	cB	815	CLA	CHD-C1D-ND	-5.17	119.70	124.45
11	cB	825	CLA	O2D-CGD-CBD	5.17	120.45	111.27
11	bB	818	CLA	CHD-C1D-ND	-5.17	119.71	124.45
11	aB	802	CLA	C3B-C2B-C1B	-5.16	100.93	107.16
11	aA	835	CLA	O2D-CGD-CBD	5.16	120.44	111.27
11	aA	823	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
11	bA	802	CLA	CAA-C2A-C3A	-5.16	98.65	112.78
11	aA	802	CLA	CAA-C2A-C3A	-5.16	98.65	112.78
11	cA	813	CLA	CHD-C1D-ND	-5.16	119.71	124.45
11	cA	835	CLA	O2D-CGD-CBD	5.16	120.43	111.27
12	aL	202	F6C	CAA-C2A-C3A	-5.16	118.27	127.88
11	aA	825	CLA	CHD-C1D-ND	-5.16	119.72	124.45
11	cA	823	CLA	C3D-C2D-C1D	-5.16	98.80	105.83
11	cA	825	CLA	CHD-C1D-ND	-5.16	119.72	124.45
11	bA	835	CLA	O2D-CGD-CBD	5.16	120.43	111.27
11	aA	816	CLA	C2C-C1C-NC	5.15	114.80	109.97
11	cB	811	CLA	CHD-C1D-ND	-5.15	119.72	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bL	202	F6C	CAA-C2A-C3A	-5.15	118.28	127.88
11	cA	802	CLA	CAA-C2A-C3A	-5.15	98.67	112.78
11	aA	807	CLA	O2D-CGD-CBD	5.15	120.42	111.27
10	cA	801	CL0	CMD-C2D-C1D	5.15	133.79	124.71
11	cB	812	CLA	CHD-C1D-ND	-5.15	119.72	124.45
11	bB	825	CLA	CHD-C1D-ND	-5.15	119.72	124.45
11	bA	809	CLA	C3B-C2B-C1B	-5.15	100.95	107.16
11	aA	818	CLA	CMD-C2D-C1D	5.15	133.78	124.71
11	bB	832	CLA	C2C-C1C-NC	5.14	114.79	109.97
12	cL	202	F6C	CAA-C2A-C3A	-5.14	118.30	127.88
11	aB	811	CLA	CHD-C1D-ND	-5.14	119.73	124.45
11	bA	825	CLA	CHD-C1D-ND	-5.14	119.73	124.45
12	bB	824	F6C	C1A-C2A-C3A	-5.14	101.56	106.97
11	cB	803	CLA	C2C-C1C-NC	5.14	114.79	109.97
11	bA	818	CLA	CMD-C2D-C1D	5.14	133.77	124.71
11	cA	818	CLA	CMD-C2D-C1D	5.14	133.77	124.71
10	aA	801	CL0	CMD-C2D-C1D	5.13	133.75	124.71
11	bB	811	CLA	CHD-C1D-ND	-5.13	119.74	124.45
11	bA	816	CLA	C2C-C1C-NC	5.12	114.77	109.97
11	aL	205	CLA	O2D-CGD-CBD	5.12	120.37	111.27
12	cB	824	F6C	C1A-C2A-C3A	-5.12	101.57	106.97
11	bL	205	CLA	O2D-CGD-CBD	5.12	120.37	111.27
11	bA	813	CLA	CHD-C1D-ND	-5.12	119.75	124.45
11	cA	816	CLA	C2C-C1C-NC	5.12	114.77	109.97
11	cA	802	CLA	C4A-NA-C1A	-5.12	104.41	106.71
11	cA	809	CLA	C3B-C2B-C1B	-5.12	100.98	107.16
11	cB	829	CLA	O2D-CGD-CBD	5.11	120.36	111.27
11	cL	205	CLA	O2D-CGD-CBD	5.11	120.35	111.27
11	aA	809	CLA	C3B-C2B-C1B	-5.11	100.99	107.16
11	bA	816	CLA	CHD-C1D-ND	-5.11	119.76	124.45
11	aL	204	CLA	CHD-C1D-ND	-5.11	119.76	124.45
11	aB	829	CLA	O2D-CGD-CBD	5.10	120.34	111.27
12	aB	824	F6C	C1A-C2A-C3A	-5.10	101.60	106.97
11	aB	821	CLA	CHD-C1D-ND	-5.10	119.77	124.45
12	bA	826	F6C	C4A-C3A-C2A	-5.10	99.49	106.94
10	bA	801	CL0	CMD-C2D-C1D	5.10	133.70	124.71
11	aB	825	CLA	CHD-C1D-ND	-5.10	119.77	124.45
12	aA	826	F6C	C4A-C3A-C2A	-5.10	99.49	106.94
11	bB	829	CLA	O2D-CGD-CBD	5.10	120.32	111.27
11	bA	815	CLA	O2D-CGD-CBD	5.09	120.32	111.27
11	aA	813	CLA	CHD-C1D-ND	-5.09	119.77	124.45
11	cL	204	CLA	CHD-C1D-ND	-5.09	119.78	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cA	815	CLA	O2D-CGD-CBD	5.08	120.30	111.27
12	cA	826	F6C	C4A-C3A-C2A	-5.08	99.52	106.94
11	cA	816	CLA	CHD-C1D-ND	-5.08	119.78	124.45
11	aA	816	CLA	CHD-C1D-ND	-5.08	119.79	124.45
11	cL	205	CLA	CHD-C1D-ND	-5.07	119.79	124.45
11	aA	815	CLA	O2D-CGD-CBD	5.07	120.28	111.27
11	aA	823	CLA	CMD-C2D-C1D	5.07	133.65	124.71
11	aL	205	CLA	CHD-C1D-ND	-5.07	119.79	124.45
11	cA	823	CLA	CMD-C2D-C1D	5.07	133.65	124.71
11	cA	823	CLA	CHD-C1D-ND	-5.07	119.80	124.45
11	cB	825	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
11	aA	829	CLA	C3B-C2B-C1B	-5.07	101.05	107.16
11	cB	801	CLA	C2C-C1C-NC	5.07	114.72	109.97
11	bA	825	CLA	O2D-CGD-CBD	5.06	120.26	111.27
11	bA	823	CLA	CMD-C2D-C1D	5.06	133.63	124.71
11	cB	821	CLA	CHD-C1D-ND	-5.06	119.81	124.45
11	bB	825	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
11	aA	825	CLA	O2D-CGD-CBD	5.05	120.25	111.27
11	cA	825	CLA	O2D-CGD-CBD	5.05	120.24	111.27
11	cB	822	CLA	O2D-CGD-CBD	5.05	120.24	111.27
11	aB	822	CLA	O2D-CGD-CBD	5.05	120.24	111.27
11	bL	205	CLA	CHD-C1D-ND	-5.05	119.82	124.45
11	bB	821	CLA	CHD-C1D-ND	-5.05	119.82	124.45
11	aA	822	CLA	CHD-C1D-ND	-5.04	119.82	124.45
11	cA	829	CLA	C3B-C2B-C1B	-5.04	101.07	107.16
11	aB	837	CLA	C2C-C1C-NC	5.04	114.69	109.97
11	aA	802	CLA	C4A-NA-C1A	-5.04	104.44	106.71
11	aB	825	CLA	C3D-C2D-C1D	-5.04	98.96	105.83
11	bA	829	CLA	C3B-C2B-C1B	-5.03	101.08	107.16
11	bB	822	CLA	O2D-CGD-CBD	5.03	120.21	111.27
11	bL	206	CLA	CHD-C1D-ND	-5.03	119.83	124.45
11	cB	822	CLA	C3D-C2D-C1D	-5.03	98.96	105.83
11	cA	822	CLA	CHD-C1D-ND	-5.03	119.83	124.45
11	aA	806	CLA	C2C-C1C-NC	5.03	114.68	109.97
11	cA	806	CLA	C2C-C1C-NC	5.02	114.68	109.97
12	aA	827	F6C	O2D-CGD-CBD	5.02	120.19	111.27
11	bB	822	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
12	bA	827	F6C	O2D-CGD-CBD	5.01	120.18	111.27
11	bA	822	CLA	CHD-C1D-ND	-5.01	119.85	124.45
11	aA	823	CLA	CHD-C1D-ND	-5.01	119.85	124.45
11	bA	828	CLA	CHD-C1D-ND	-5.01	119.85	124.45
11	bB	801	CLA	C2C-C1C-NC	5.01	114.67	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bB	803	CLA	C3B-C2B-C1B	-5.01	101.11	107.16
11	bA	823	CLA	CHD-C1D-ND	-5.01	119.85	124.45
11	aB	822	CLA	C3D-C2D-C1D	-5.01	99.00	105.83
11	cL	206	CLA	CHD-C1D-ND	-5.01	119.85	124.45
11	aB	838	CLA	O2D-CGD-CBD	5.00	120.16	111.27
11	bB	833	CLA	C2C-C1C-NC	5.00	114.66	109.97
11	aA	828	CLA	CHD-C1D-ND	-5.00	119.86	124.45
11	aL	206	CLA	CHD-C1D-ND	-5.00	119.86	124.45
11	cB	803	CLA	C3B-C2B-C1B	-5.00	101.12	107.16
11	cB	833	CLA	C2C-C1C-NC	5.00	114.66	109.97
11	bB	836	CLA	C4A-NA-C1A	-5.00	104.46	106.71
11	cA	828	CLA	CHD-C1D-ND	-5.00	119.86	124.45
11	cA	814	CLA	C2C-C1C-NC	5.00	114.65	109.97
11	cB	804	CLA	C2C-C1C-NC	5.00	114.65	109.97
11	aB	804	CLA	C3B-C2B-C1B	-5.00	101.13	107.16
11	cB	804	CLA	C3B-C2B-C1B	-4.99	101.13	107.16
11	cB	823	CLA	C3B-C2B-C1B	-4.99	101.13	107.16
11	bB	804	CLA	C3B-C2B-C1B	-4.99	101.14	107.16
11	cB	805	CLA	O2D-CGD-CBD	4.99	120.14	111.27
11	bB	823	CLA	C3B-C2B-C1B	-4.99	101.14	107.16
11	cB	838	CLA	O2D-CGD-CBD	4.99	120.13	111.27
11	aB	833	CLA	C2C-C1C-NC	4.98	114.64	109.97
11	aB	805	CLA	O2D-CGD-CBD	4.98	120.12	111.27
11	cA	843	CLA	CHD-C1D-ND	-4.98	119.88	124.45
12	cA	827	F6C	O2D-CGD-CBD	4.98	120.12	111.27
11	bA	805	CLA	C3B-C2B-C1B	-4.98	101.15	107.16
11	bA	806	CLA	C3B-C2B-C1B	-4.98	101.15	107.16
11	cA	806	CLA	C3B-C2B-C1B	-4.98	101.15	107.16
11	bB	805	CLA	O2D-CGD-CBD	4.98	120.11	111.27
11	bB	838	CLA	O2D-CGD-CBD	4.98	120.11	111.27
11	aB	801	CLA	C2C-C1C-NC	4.98	114.64	109.97
12	bA	844	F6C	C3D-C4D-ND	4.98	117.44	110.17
11	bA	814	CLA	C2C-C1C-NC	4.98	114.63	109.97
11	cA	805	CLA	C3B-C2B-C1B	-4.97	101.16	107.16
11	aA	806	CLA	C3B-C2B-C1B	-4.97	101.16	107.16
11	cB	817	CLA	O2D-CGD-CBD	4.97	120.10	111.27
11	aB	836	CLA	C4A-NA-C1A	-4.97	104.47	106.71
11	bB	817	CLA	O2D-CGD-CBD	4.97	120.09	111.27
12	aB	824	F6C	C4A-C3A-C2A	-4.97	99.69	106.94
11	bB	813	CLA	CHD-C1D-ND	-4.97	119.89	124.45
12	cA	844	F6C	C3D-C4D-ND	4.97	117.43	110.17
11	cB	837	CLA	C2C-C1C-NC	4.97	114.62	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aB	803	CLA	C3B-C2B-C1B	-4.97	101.17	107.16
11	aA	843	CLA	CHD-C1D-ND	-4.97	119.89	124.45
11	aB	817	CLA	O2D-CGD-CBD	4.97	120.09	111.27
11	cA	839	CLA	O2D-CGD-CBD	4.96	120.09	111.27
11	cB	826	CLA	O2D-CGD-CBD	4.96	120.07	111.27
11	aA	805	CLA	C3B-C2B-C1B	-4.95	101.18	107.16
11	aB	829	CLA	C1C-C2C-C3C	-4.95	101.75	106.96
11	bB	806	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
12	aA	844	F6C	C3D-C4D-ND	4.95	117.41	110.17
11	bA	806	CLA	C2C-C1C-NC	4.95	114.61	109.97
11	bB	804	CLA	C2C-C1C-NC	4.95	114.61	109.97
11	cB	839	CLA	C2C-C1C-NC	4.95	114.61	109.97
11	aA	803	CLA	CHD-C1D-ND	-4.95	119.91	124.45
11	aA	839	CLA	O2D-CGD-CBD	4.95	120.06	111.27
11	cB	829	CLA	C1C-C2C-C3C	-4.95	101.75	106.96
11	aB	806	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
11	bA	843	CLA	CHD-C1D-ND	-4.95	119.91	124.45
11	bB	837	CLA	C2C-C1C-NC	4.95	114.61	109.97
12	cB	824	F6C	C4A-C3A-C2A	-4.94	99.72	106.94
11	bB	829	CLA	C1C-C2C-C3C	-4.94	101.76	106.96
11	cB	806	CLA	C3D-C2D-C1D	-4.94	99.08	105.83
11	bB	826	CLA	O2D-CGD-CBD	4.94	120.05	111.27
11	bA	839	CLA	O2D-CGD-CBD	4.94	120.05	111.27
11	bB	801	CLA	CHD-C1D-ND	-4.94	119.91	124.45
11	aB	823	CLA	C3B-C2B-C1B	-4.94	101.20	107.16
10	cA	801	CL0	C3B-C2B-C1B	-4.94	101.20	107.16
11	aB	832	CLA	C3B-C2B-C1B	-4.94	101.20	107.16
10	aA	801	CL0	C3B-C2B-C1B	-4.93	101.21	107.16
11	bB	832	CLA	C3B-C2B-C1B	-4.93	101.21	107.16
11	cB	832	CLA	C3B-C2B-C1B	-4.93	101.21	107.16
11	aB	813	CLA	CHD-C1D-ND	-4.93	119.92	124.45
11	aB	801	CLA	CHD-C1D-ND	-4.93	119.93	124.45
11	cB	830	CLA	O2D-CGD-CBD	4.92	120.02	111.27
11	aB	815	CLA	C2C-C1C-NC	4.92	114.58	109.97
10	bA	801	CL0	C3B-C2B-C1B	-4.92	101.22	107.16
12	bB	824	F6C	C4A-C3A-C2A	-4.92	99.75	106.94
11	aA	814	CLA	C2C-C1C-NC	4.92	114.58	109.97
11	bA	812	CLA	C3B-C2B-C1B	-4.92	101.22	107.16
12	aA	827	F6C	C3D-C4D-ND	4.92	117.37	110.17
11	aA	803	CLA	C3B-C2B-C1B	-4.92	101.22	107.16
11	cB	836	CLA	C4A-NA-C1A	-4.92	104.49	106.71
11	aB	804	CLA	C2C-C1C-NC	4.92	114.58	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bB	830	CLA	O2D-CGD-CBD	4.92	120.01	111.27
11	cB	801	CLA	CHD-C1D-ND	-4.92	119.93	124.45
11	aB	826	CLA	O2D-CGD-CBD	4.92	120.00	111.27
11	aA	831	CLA	CMD-C2D-C1D	4.92	133.38	124.71
11	cA	803	CLA	C3B-C2B-C1B	-4.92	101.23	107.16
12	cA	827	F6C	C3D-C4D-ND	4.91	117.36	110.17
12	bA	827	F6C	C3D-C4D-ND	4.91	117.35	110.17
11	aB	830	CLA	O2D-CGD-CBD	4.91	120.00	111.27
11	bA	803	CLA	CHD-C1D-ND	-4.91	119.94	124.45
11	bA	819	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
11	bB	816	CLA	C2C-C1C-NC	4.91	114.57	109.97
11	aA	819	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
11	cA	831	CLA	CMD-C2D-C1D	4.90	133.36	124.71
11	cB	815	CLA	C2C-C1C-NC	4.90	114.57	109.97
11	cA	812	CLA	C3B-C2B-C1B	-4.90	101.24	107.16
11	cB	831	CLA	C4A-NA-C1A	-4.90	104.50	106.71
11	bA	840	CLA	C4A-NA-C1A	-4.90	104.50	106.71
11	bA	831	CLA	CMD-C2D-C1D	4.90	133.35	124.71
11	aB	816	CLA	C2C-C1C-NC	4.90	114.56	109.97
11	bB	839	CLA	C2C-C1C-NC	4.89	114.56	109.97
11	cA	819	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
11	bB	815	CLA	C2C-C1C-NC	4.89	114.55	109.97
11	aB	839	CLA	C2C-C1C-NC	4.88	114.55	109.97
11	cB	802	CLA	CAA-C2A-C3A	-4.88	99.41	112.78
12	cA	826	F6C	CAA-C2A-C1A	-4.88	114.66	128.11
11	bA	803	CLA	C3B-C2B-C1B	-4.88	101.27	107.16
11	cA	803	CLA	CHD-C1D-ND	-4.88	119.97	124.45
12	aA	826	F6C	CAA-C2A-C1A	-4.88	114.67	128.11
11	cB	812	CLA	C3B-C2B-C1B	-4.88	101.27	107.16
11	aB	812	CLA	C3B-C2B-C1B	-4.88	101.27	107.16
11	aA	835	CLA	C3B-C2B-C1B	-4.88	101.28	107.16
11	cA	837	CLA	C3B-C2B-C1B	-4.87	101.28	107.16
12	bA	826	F6C	CAA-C2A-C1A	-4.87	114.69	128.11
11	aB	802	CLA	CAA-C2A-C3A	-4.87	99.43	112.78
11	bB	802	CLA	CAA-C2A-C3A	-4.87	99.44	112.78
11	aA	812	CLA	C3B-C2B-C1B	-4.87	101.28	107.16
11	cB	813	CLA	CHD-C1D-ND	-4.87	119.98	124.45
11	cB	822	CLA	C3B-C2B-C1B	-4.87	101.29	107.16
11	cB	805	CLA	C3B-C2B-C1B	-4.86	101.29	107.16
11	cB	816	CLA	C2C-C1C-NC	4.86	114.53	109.97
11	bA	831	CLA	CHD-C1D-ND	-4.86	119.99	124.45
11	aB	822	CLA	C3B-C2B-C1B	-4.85	101.30	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aA	840	CLA	C4A-NA-C1A	-4.85	104.52	106.71
11	bB	831	CLA	C4A-NA-C1A	-4.85	104.52	106.71
11	cA	835	CLA	C3B-C2B-C1B	-4.85	101.31	107.16
12	aA	830	F6C	C4A-C3A-C2A	-4.85	99.86	106.94
11	aA	808	CLA	C3B-C2B-C1B	-4.84	101.31	107.16
11	cA	828	CLA	C3B-C2B-C1B	-4.84	101.32	107.16
11	cA	808	CLA	C3B-C2B-C1B	-4.84	101.32	107.16
11	bK	103	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
11	cK	103	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
12	cA	830	F6C	C4A-C3A-C2A	-4.84	99.88	106.94
11	aB	803	CLA	CMD-C2D-C1D	4.84	133.24	124.71
11	bA	816	CLA	O2D-CGD-CBD	4.84	119.86	111.27
11	bB	822	CLA	C3B-C2B-C1B	-4.84	101.32	107.16
11	cB	836	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
11	cB	803	CLA	CMD-C2D-C1D	4.83	133.23	124.71
11	aB	805	CLA	C4A-NA-C1A	-4.83	104.53	106.71
11	bA	835	CLA	C3B-C2B-C1B	-4.83	101.33	107.16
12	bA	844	F6C	C4A-C3A-C2A	-4.83	99.88	106.94
11	bA	828	CLA	C3B-C2B-C1B	-4.83	101.33	107.16
11	bB	812	CLA	C3B-C2B-C1B	-4.83	101.33	107.16
11	bB	828	CLA	CHD-C4C-C3C	-4.83	117.74	124.84
11	aA	816	CLA	O2D-CGD-CBD	4.83	119.85	111.27
11	aB	805	CLA	C3B-C2B-C1B	-4.83	101.33	107.16
11	bB	836	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
12	cA	844	F6C	C4A-C3A-C2A	-4.83	99.89	106.94
11	aA	837	CLA	C3B-C2B-C1B	-4.83	101.33	107.16
11	bB	803	CLA	CMD-C2D-C1D	4.83	133.22	124.71
11	aA	828	CLA	C3B-C2B-C1B	-4.83	101.33	107.16
11	aB	836	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
11	bB	819	CLA	O2D-CGD-CBD	4.83	119.84	111.27
11	bA	837	CLA	C3B-C2B-C1B	-4.83	101.33	107.16
11	cB	819	CLA	O2D-CGD-CBD	4.83	119.84	111.27
11	bB	815	CLA	C3D-C2D-C1D	-4.83	99.25	105.83
11	bA	808	CLA	C3B-C2B-C1B	-4.83	101.34	107.16
12	aA	844	F6C	C4A-C3A-C2A	-4.82	99.89	106.94
11	aA	806	CLA	CHD-C4C-C3C	-4.82	117.75	124.84
11	aB	820	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
12	bA	830	F6C	C4A-C3A-C2A	-4.82	99.90	106.94
11	cB	828	CLA	CHD-C4C-C3C	-4.82	117.75	124.84
11	bB	805	CLA	C3B-C2B-C1B	-4.82	101.34	107.16
11	bB	815	CLA	C3B-C2B-C1B	-4.82	101.34	107.16
11	aB	819	CLA	O2D-CGD-CBD	4.82	119.83	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cA	836	CLA	CMD-C2D-C1D	4.82	133.21	124.71
11	aB	825	CLA	C3B-C2B-C1B	-4.82	101.34	107.16
11	aB	816	CLA	C3B-C2B-C1B	-4.82	101.35	107.16
11	cA	816	CLA	O2D-CGD-CBD	4.82	119.83	111.27
11	bA	806	CLA	CHD-C4C-C3C	-4.82	117.76	124.84
10	cA	801	CL0	CAA-C2A-C3A	-4.81	99.60	112.78
11	cB	808	CLA	CMD-C2D-C1D	4.81	133.19	124.71
11	cA	806	CLA	CHD-C4C-C3C	-4.81	117.77	124.84
11	cB	815	CLA	C3D-C2D-C1D	-4.81	99.26	105.83
11	aB	808	CLA	CMD-C2D-C1D	4.81	133.19	124.71
11	aA	836	CLA	CMD-C2D-C1D	4.81	133.19	124.71
11	bB	820	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
11	aB	828	CLA	CHD-C4C-C3C	-4.81	117.77	124.84
11	aB	827	CLA	C3B-C2B-C1B	-4.81	101.36	107.16
10	aA	801	CL0	CAA-C2A-C3A	-4.81	99.61	112.78
11	bA	836	CLA	CMD-C2D-C1D	4.81	133.19	124.71
11	aK	103	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
12	aA	830	F6C	C3D-C4D-ND	4.81	117.20	110.17
11	aB	819	CLA	C3B-C2B-C1B	-4.80	101.36	107.16
11	cB	825	CLA	C3B-C2B-C1B	-4.80	101.36	107.16
11	cB	820	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
12	bA	830	F6C	C3D-C4D-ND	4.80	117.19	110.17
11	bB	827	CLA	C3B-C2B-C1B	-4.80	101.37	107.16
11	cB	815	CLA	C3B-C2B-C1B	-4.80	101.37	107.16
11	aB	836	CLA	CHD-C1D-ND	-4.80	120.04	124.45
11	cB	831	CLA	O2D-CGD-CBD	4.80	119.79	111.27
10	bA	801	CL0	CAA-C2A-C3A	-4.80	99.64	112.78
11	cB	827	CLA	C3B-C2B-C1B	-4.79	101.37	107.16
11	bB	825	CLA	C3B-C2B-C1B	-4.79	101.38	107.16
11	cA	840	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
11	aB	815	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
11	aB	815	CLA	C3B-C2B-C1B	-4.79	101.38	107.16
11	bA	838	CLA	C3B-C2B-C1B	-4.79	101.38	107.16
11	bA	804	CLA	C3B-C2B-C1B	-4.79	101.38	107.16
11	bB	819	CLA	C3B-C2B-C1B	-4.79	101.38	107.16
11	bB	808	CLA	CMD-C2D-C1D	4.79	133.15	124.71
11	cA	840	CLA	C4A-NA-C1A	-4.79	104.55	106.71
11	cA	841	CLA	C3B-C2B-C1B	-4.79	101.39	107.16
11	aB	801	CLA	C3B-C2B-C1B	-4.78	101.39	107.16
12	cA	830	F6C	C3D-C4D-ND	4.78	117.16	110.17
11	aA	831	CLA	CHD-C1D-ND	-4.78	120.06	124.45
11	bB	801	CLA	C3B-C2B-C1B	-4.78	101.39	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cA	808	CLA	O2D-CGD-CBD	4.78	119.76	111.27
11	bA	808	CLA	O2D-CGD-CBD	4.78	119.76	111.27
11	cB	831	CLA	C3B-C2B-C1B	-4.78	101.39	107.16
11	bA	807	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
11	bB	818	CLA	C2C-C1C-NC	4.78	114.45	109.97
11	cA	838	CLA	C3B-C2B-C1B	-4.78	101.39	107.16
11	cB	818	CLA	C2C-C1C-NC	4.78	114.45	109.97
11	aA	807	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
11	aA	808	CLA	O2D-CGD-CBD	4.78	119.75	111.27
12	bB	824	F6C	C3D-C4D-ND	4.78	117.15	110.17
10	cA	801	CL0	CMA-C3A-C4A	-4.78	98.94	111.77
11	bB	831	CLA	O2D-CGD-CBD	4.78	119.75	111.27
11	aB	831	CLA	C3B-C2B-C1B	-4.78	101.40	107.16
11	bB	826	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
11	aB	831	CLA	O2D-CGD-CBD	4.77	119.75	111.27
11	cB	816	CLA	C3B-C2B-C1B	-4.77	101.40	107.16
11	cA	807	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
11	bB	826	CLA	CHD-C1D-ND	-4.77	120.07	124.45
11	aA	820	CLA	C4A-NA-C1A	-4.77	104.56	106.71
11	aB	826	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
11	cB	801	CLA	C3B-C2B-C1B	-4.77	101.41	107.16
10	aA	801	CL0	CMA-C3A-C4A	-4.77	98.96	111.77
11	bB	816	CLA	C3B-C2B-C1B	-4.77	101.41	107.16
11	cB	826	CLA	C3D-C2D-C1D	-4.77	99.33	105.83
11	bA	840	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
12	cB	824	F6C	C3D-C4D-ND	4.76	117.13	110.17
11	aA	840	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
10	bA	801	CL0	CMA-C3A-C4A	-4.76	98.98	111.77
11	aA	838	CLA	C3B-C2B-C1B	-4.76	101.42	107.16
10	bA	801	CL0	CHD-C1D-ND	-4.76	120.08	124.45
12	aB	824	F6C	C3D-C4D-ND	4.76	117.13	110.17
11	aB	818	CLA	C2C-C1C-NC	4.76	114.43	109.97
11	cA	831	CLA	CHD-C1D-ND	-4.76	120.08	124.45
10	cA	801	CL0	CHD-C1D-ND	-4.76	120.08	124.45
11	cB	826	CLA	CHD-C1D-ND	-4.76	120.08	124.45
11	bA	820	CLA	C4A-NA-C1A	-4.76	104.57	106.71
12	bA	827	F6C	C1A-C2A-C3A	-4.75	101.96	106.97
11	cB	836	CLA	CHD-C1D-ND	-4.75	120.09	124.45
11	aA	841	CLA	C3B-C2B-C1B	-4.75	101.42	107.16
11	cB	806	CLA	C3B-C2B-C1B	-4.75	101.42	107.16
11	cA	818	CLA	C3B-C2B-C1B	-4.75	101.43	107.16
11	aA	818	CLA	C3D-C2D-C1D	-4.75	99.35	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aB	806	CLA	C3B-C2B-C1B	-4.75	101.43	107.16
11	aB	826	CLA	CHD-C1D-ND	-4.75	120.09	124.45
11	aA	818	CLA	C3B-C2B-C1B	-4.75	101.43	107.16
11	aA	823	CLA	C3B-C2B-C1B	-4.75	101.43	107.16
11	bA	814	CLA	C3B-C2B-C1B	-4.75	101.43	107.16
11	cA	804	CLA	C3B-C2B-C1B	-4.75	101.43	107.16
11	bB	837	CLA	C3B-C2B-C1B	-4.75	101.43	107.16
11	cB	819	CLA	C3B-C2B-C1B	-4.75	101.43	107.16
11	cB	836	CLA	C3B-C2B-C1B	-4.75	101.43	107.16
11	cA	835	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
11	aK	101	CLA	C3B-C2B-C1B	-4.74	101.43	107.16
11	bB	836	CLA	CHD-C1D-ND	-4.74	120.09	124.45
11	bK	103	CLA	C3B-C2B-C1B	-4.74	101.44	107.16
12	cA	830	F6C	CMD-C2D-C1D	4.74	132.26	125.04
11	bA	818	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
11	aA	804	CLA	C3B-C2B-C1B	-4.74	101.44	107.16
11	cB	817	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
11	bB	838	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
11	cA	833	CLA	C3B-C2B-C1B	-4.74	101.44	107.16
11	aA	835	CLA	C3D-C2D-C1D	-4.74	99.37	105.83
12	aA	827	F6C	C1A-C2A-C3A	-4.74	101.98	106.97
12	cA	827	F6C	C1A-C2A-C3A	-4.74	101.98	106.97
11	bA	841	CLA	C3B-C2B-C1B	-4.74	101.44	107.16
11	aB	813	CLA	O2D-CGD-CBD	4.74	119.68	111.27
11	bB	813	CLA	O2D-CGD-CBD	4.74	119.68	111.27
11	aB	820	CLA	C3B-C2B-C1B	-4.73	101.45	107.16
11	aB	838	CLA	C3D-C2D-C1D	-4.73	99.37	105.83
11	bB	820	CLA	C3B-C2B-C1B	-4.73	101.45	107.16
11	aB	817	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
10	aA	801	CL0	CHD-C1D-ND	-4.73	120.11	124.45
11	aB	831	CLA	C4A-NA-C1A	-4.73	104.58	106.71
12	aA	830	F6C	CMD-C2D-C1D	4.73	132.24	125.04
11	cB	838	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
11	cB	813	CLA	O2D-CGD-CBD	4.73	119.67	111.27
11	cB	837	CLA	C3B-C2B-C1B	-4.73	101.46	107.16
11	cB	820	CLA	C3B-C2B-C1B	-4.73	101.46	107.16
11	cK	103	CLA	C3B-C2B-C1B	-4.73	101.46	107.16
11	cA	818	CLA	C3D-C2D-C1D	-4.72	99.38	105.83
11	bA	818	CLA	C3B-C2B-C1B	-4.72	101.46	107.16
11	aB	837	CLA	C3B-C2B-C1B	-4.72	101.46	107.16
11	aK	103	CLA	C3B-C2B-C1B	-4.72	101.46	107.16
11	cA	814	CLA	C3B-C2B-C1B	-4.72	101.46	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bA	819	CLA	C3B-C2B-C1B	-4.72	101.46	107.16
11	bK	101	CLA	C3B-C2B-C1B	-4.72	101.46	107.16
11	bB	805	CLA	C4A-NA-C1A	-4.72	104.58	106.71
11	cK	101	CLA	C3B-C2B-C1B	-4.72	101.46	107.16
11	aA	833	CLA	C3B-C2B-C1B	-4.72	101.46	107.16
11	bA	805	CLA	C2C-C1C-NC	4.72	114.39	109.97
11	cB	833	CLA	C3B-C2B-C1B	-4.72	101.47	107.16
12	aL	202	F6C	CHB-C4A-C3A	-4.72	115.58	125.48
11	aA	814	CLA	C3B-C2B-C1B	-4.72	101.47	107.16
11	bB	831	CLA	C3B-C2B-C1B	-4.72	101.47	107.16
12	bA	830	F6C	CMD-C2D-C1D	4.72	132.22	125.04
11	bA	842	CLA	C3D-C2D-C1D	-4.72	99.40	105.83
11	cB	811	CLA	C3B-C2B-C1B	-4.72	101.47	107.16
11	bA	835	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
11	bB	811	CLA	C3B-C2B-C1B	-4.71	101.47	107.16
11	bB	836	CLA	C3B-C2B-C1B	-4.71	101.47	107.16
11	bA	808	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
11	aA	819	CLA	C3B-C2B-C1B	-4.71	101.47	107.16
11	bA	823	CLA	C3B-C2B-C1B	-4.71	101.48	107.16
11	cA	823	CLA	C3B-C2B-C1B	-4.71	101.48	107.16
11	aA	842	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
11	bA	841	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
11	cA	808	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
11	aB	833	CLA	C3B-C2B-C1B	-4.71	101.48	107.16
12	aA	832	F6C	C3D-C4D-ND	4.71	117.05	110.17
11	bB	826	CLA	C3C-C4C-NC	4.70	115.85	110.57
11	aA	808	CLA	C3D-C2D-C1D	-4.70	99.41	105.83
12	cL	202	F6C	CHB-C4A-C3A	-4.70	115.61	125.48
11	aB	811	CLA	C3B-C2B-C1B	-4.70	101.48	107.16
11	bB	806	CLA	C3B-C2B-C1B	-4.70	101.48	107.16
11	bB	817	CLA	C3D-C2D-C1D	-4.70	99.41	105.83
11	aB	836	CLA	C3B-C2B-C1B	-4.70	101.49	107.16
11	bB	833	CLA	C3B-C2B-C1B	-4.70	101.49	107.16
12	bA	832	F6C	C3D-C4D-ND	4.70	117.04	110.17
11	cA	842	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
11	aB	803	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
12	cA	832	F6C	C3D-C4D-ND	4.70	117.04	110.17
12	cA	826	F6C	CHD-C4C-C3C	-4.69	115.10	125.36
11	cA	843	CLA	O2D-CGD-CBD	4.69	119.61	111.27
11	aA	841	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
11	bL	204	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
11	aA	803	CLA	C3D-C2D-C1D	-4.69	99.43	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bB	828	CLA	CHD-C1D-ND	-4.69	120.15	124.45
11	cA	819	CLA	C3B-C2B-C1B	-4.69	101.50	107.16
11	cL	204	CLA	C3D-C2D-C1D	-4.69	99.44	105.83
11	bA	833	CLA	C3B-C2B-C1B	-4.69	101.50	107.16
11	cA	833	CLA	C3D-C2D-C1D	-4.69	99.44	105.83
11	cA	841	CLA	C3D-C2D-C1D	-4.69	99.44	105.83
11	aA	833	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
11	cB	826	CLA	C3C-C4C-NC	4.68	115.82	110.57
11	bB	832	CLA	O2D-CGD-CBD	4.68	119.58	111.27
12	aA	826	F6C	CHD-C4C-C3C	-4.68	115.13	125.36
11	bB	831	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
11	aB	828	CLA	CHD-C1D-ND	-4.68	120.16	124.45
11	aB	807	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
11	cB	805	CLA	C4A-NA-C1A	-4.68	104.60	106.71
11	aL	204	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
11	bA	803	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
11	aB	832	CLA	O2D-CGD-CBD	4.67	119.57	111.27
11	cA	837	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
11	cA	805	CLA	C2C-C1C-NC	4.67	114.35	109.97
12	bL	202	F6C	CHB-C4A-C3A	-4.67	115.68	125.48
12	cA	832	F6C	C4A-C3A-C2A	-4.67	100.12	106.94
11	bB	807	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
12	bA	826	F6C	CHD-C4C-C3C	-4.67	115.16	125.36
11	cB	807	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
11	cB	803	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
11	aA	839	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
11	aB	804	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
11	aB	826	CLA	C3C-C4C-NC	4.66	115.80	110.57
11	cB	828	CLA	CHD-C1D-ND	-4.66	120.17	124.45
11	cA	803	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
11	bA	837	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
11	bA	807	CLA	C3B-C2B-C1B	-4.66	101.53	107.16
11	bA	843	CLA	O2D-CGD-CBD	4.66	119.55	111.27
11	cB	832	CLA	O2D-CGD-CBD	4.66	119.55	111.27
11	aA	843	CLA	O2D-CGD-CBD	4.66	119.55	111.27
11	aA	807	CLA	C3B-C2B-C1B	-4.66	101.54	107.16
11	bA	811	CLA	C4A-NA-C1A	-4.66	104.61	106.71
11	bB	805	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
11	cB	814	CLA	C3B-C2B-C1B	-4.66	101.54	107.16
11	aB	831	CLA	C3D-C2D-C1D	-4.66	99.48	105.83
11	bA	833	CLA	C3D-C2D-C1D	-4.66	99.48	105.83
11	aA	805	CLA	C3D-C2D-C1D	-4.66	99.48	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cB	822	CLA	C3C-C4C-NC	4.66	115.79	110.57
12	aA	832	F6C	C4A-C3A-C2A	-4.65	100.14	106.94
11	aA	842	CLA	C4A-NA-C1A	-4.65	104.61	106.71
11	cA	820	CLA	C4A-NA-C1A	-4.65	104.61	106.71
11	bB	803	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
11	aB	822	CLA	C3C-C4C-NC	4.65	115.79	110.57
12	bA	832	F6C	C4A-C3A-C2A	-4.65	100.15	106.94
11	bB	822	CLA	C3C-C4C-NC	4.65	115.79	110.57
11	cB	833	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
11	aA	809	CLA	C3D-C2D-C1D	-4.64	99.49	105.83
11	bB	814	CLA	C3B-C2B-C1B	-4.64	101.56	107.16
11	bA	805	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
11	aB	809	CLA	CAA-C2A-C3A	-4.64	100.07	112.78
11	bA	839	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
11	bB	820	CLA	O2D-CGD-CBD	4.64	119.52	111.27
11	cL	204	CLA	C3B-C2B-C1B	-4.64	101.56	107.16
11	cB	805	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
11	bB	804	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
11	cA	842	CLA	C3B-C2B-C1B	-4.64	101.56	107.16
11	aB	805	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
11	bB	833	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
11	bB	809	CLA	CAA-C2A-C3A	-4.64	100.08	112.78
11	aA	805	CLA	C2C-C1C-NC	4.64	114.31	109.97
11	cB	804	CLA	C3D-C2D-C1D	-4.64	99.51	105.83
11	aB	833	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
11	aB	814	CLA	C3B-C2B-C1B	-4.63	101.57	107.16
11	cB	831	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
11	cA	809	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
11	aA	842	CLA	C3B-C2B-C1B	-4.63	101.57	107.16
11	cA	807	CLA	C3B-C2B-C1B	-4.63	101.57	107.16
11	cA	805	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
11	cA	818	CLA	CHD-C1D-ND	-4.63	120.20	124.45
11	cB	836	CLA	O2D-CGD-CBD	4.63	119.49	111.27
11	cA	839	CLA	C3D-C2D-C1D	-4.63	99.52	105.83
11	cA	834	CLA	C3B-C2B-C1B	-4.63	101.58	107.16
11	aA	806	CLA	O2D-CGD-CBD	4.63	119.49	111.27
11	bA	842	CLA	C3B-C2B-C1B	-4.62	101.58	107.16
11	cA	811	CLA	C4A-NA-C1A	-4.62	104.63	106.71
11	bA	809	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
11	cB	821	CLA	O2D-CGD-CBD	4.62	119.48	111.27
11	cB	809	CLA	CAA-C2A-C3A	-4.62	100.12	112.78
11	aB	830	CLA	C3D-C2D-C1D	-4.62	99.52	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aB	820	CLA	O2D-CGD-CBD	4.62	119.48	111.27
11	bL	204	CLA	C3B-C2B-C1B	-4.62	101.58	107.16
11	bB	802	CLA	C3C-C4C-NC	4.62	115.75	110.57
11	aA	837	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
11	bB	821	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
11	cA	842	CLA	C4A-NA-C1A	-4.62	104.63	106.71
11	bA	843	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
11	aK	103	CLA	O2D-CGD-CBD	4.62	119.47	111.27
11	cB	840	CLA	C3D-C2D-C1D	-4.61	99.53	105.83
12	bL	202	F6C	C3D-C2D-C1D	-4.61	99.15	105.83
11	cL	205	CLA	C3B-C2B-C1B	-4.61	101.59	107.16
11	bB	821	CLA	O2D-CGD-CBD	4.61	119.46	111.27
11	bL	205	CLA	C3B-C2B-C1B	-4.61	101.60	107.16
11	bB	836	CLA	O2D-CGD-CBD	4.61	119.46	111.27
11	bB	813	CLA	C3B-C2B-C1B	-4.61	101.60	107.16
11	cB	820	CLA	O2D-CGD-CBD	4.61	119.45	111.27
11	bB	840	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
12	cL	202	F6C	C3D-C2D-C1D	-4.61	99.16	105.83
11	cB	813	CLA	C3B-C2B-C1B	-4.60	101.60	107.16
11	aL	204	CLA	C3B-C2B-C1B	-4.60	101.61	107.16
11	cB	802	CLA	C3C-C4C-NC	4.60	115.73	110.57
11	aB	840	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
11	bB	830	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
11	aB	836	CLA	O2D-CGD-CBD	4.60	119.44	111.27
11	aB	821	CLA	O2D-CGD-CBD	4.60	119.44	111.27
11	aA	834	CLA	C3B-C2B-C1B	-4.59	101.62	107.16
12	aL	202	F6C	C3D-C2D-C1D	-4.59	99.18	105.83
11	cA	831	CLA	C3B-C4B-NB	4.59	114.77	110.52
11	aB	821	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
11	cA	843	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
11	cA	806	CLA	O2D-CGD-CBD	4.59	119.42	111.27
11	aA	843	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
11	cK	103	CLA	O2D-CGD-CBD	4.59	119.42	111.27
11	aB	802	CLA	C3C-C4C-NC	4.59	115.72	110.57
11	bK	103	CLA	O2D-CGD-CBD	4.59	119.42	111.27
11	aA	831	CLA	C3B-C4B-NB	4.59	114.77	110.52
11	bA	834	CLA	C3B-C2B-C1B	-4.58	101.63	107.16
11	cB	821	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
11	aL	205	CLA	C3B-C2B-C1B	-4.58	101.63	107.16
11	bA	818	CLA	C2C-C1C-NC	4.58	114.26	109.97
11	aB	813	CLA	C3B-C2B-C1B	-4.58	101.63	107.16
11	cB	830	CLA	C3D-C2D-C1D	-4.58	99.58	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cB	830	CLA	C3B-C2B-C1B	-4.58	101.64	107.16
11	bA	818	CLA	CHD-C1D-ND	-4.58	120.25	124.45
11	aA	818	CLA	CHD-C1D-ND	-4.58	120.25	124.45
11	bA	815	CLA	C3B-C2B-C1B	-4.58	101.64	107.16
11	bL	206	CLA	O2D-CGD-CBD	4.58	119.40	111.27
10	aA	801	CL0	CMA-C3A-C2A	-4.58	95.37	113.83
11	cL	206	CLA	O2D-CGD-CBD	4.58	119.40	111.27
11	cB	827	CLA	C3C-C4C-NC	4.57	115.70	110.57
11	aA	829	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
11	bA	829	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
11	bA	804	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
11	bA	806	CLA	O2D-CGD-CBD	4.57	119.39	111.27
11	cA	829	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
11	aL	206	CLA	O2D-CGD-CBD	4.57	119.39	111.27
11	bB	837	CLA	O2D-CGD-CBD	4.57	119.39	111.27
17	aA	853	LMT	C6B-C5B-C4B	-4.57	102.30	113.00
17	cA	853	LMT	C6B-C5B-C4B	-4.57	102.31	113.00
11	aB	816	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
11	bB	816	CLA	C3D-C2D-C1D	-4.56	99.60	105.83
10	cA	801	CL0	CMA-C3A-C2A	-4.56	95.42	113.83
11	cA	836	CLA	C3C-C4C-NC	4.56	115.69	110.57
11	bB	801	CLA	CMB-C2B-C1B	4.56	132.32	125.37
11	bK	101	CLA	C3D-C2D-C1D	-4.56	99.60	105.83
11	aA	810	CLA	CHD-C1D-ND	-4.56	120.26	124.45
11	aA	836	CLA	C3C-C4C-NC	4.56	115.69	110.57
11	aB	803	CLA	CAC-C3C-C4C	4.56	130.73	124.81
11	bA	842	CLA	C4A-NA-C1A	-4.56	104.66	106.71
10	bA	801	CL0	CMA-C3A-C2A	-4.56	95.43	113.83
11	bA	838	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
11	aB	830	CLA	C3B-C2B-C1B	-4.56	101.66	107.16
11	cB	837	CLA	O2D-CGD-CBD	4.56	119.36	111.27
11	cA	820	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
11	aB	801	CLA	CMB-C2B-C1B	4.55	132.31	125.37
11	cA	833	CLA	O2D-CGD-CBD	4.55	119.36	111.27
11	cB	803	CLA	CAC-C3C-C4C	4.55	130.72	124.81
11	aA	838	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
11	cB	816	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
11	cK	101	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
17	bA	853	LMT	C6B-C5B-C4B	-4.55	102.35	113.00
11	aB	814	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
11	bA	838	CLA	C4A-NA-C1A	-4.55	104.66	106.71
11	bA	836	CLA	C3C-C4C-NC	4.55	115.67	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bB	814	CLA	C3D-C2D-C1D	-4.55	99.63	105.83
11	aA	820	CLA	C3D-C2D-C1D	-4.55	99.63	105.83
11	aB	837	CLA	O2D-CGD-CBD	4.55	119.35	111.27
11	bB	810	CLA	C3D-C2D-C1D	-4.55	99.63	105.83
11	aA	804	CLA	C3D-C2D-C1D	-4.55	99.63	105.83
11	aA	810	CLA	C3B-C2B-C1B	-4.54	101.67	107.16
11	cA	810	CLA	C3B-C2B-C1B	-4.54	101.67	107.16
11	bB	823	CLA	C3C-C4C-NC	4.54	115.67	110.57
11	bB	827	CLA	C3C-C4C-NC	4.54	115.67	110.57
11	bA	831	CLA	C3B-C4B-NB	4.54	114.73	110.52
11	aA	819	CLA	C2C-C1C-NC	4.54	114.23	109.97
11	cB	818	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
11	bA	833	CLA	O2D-CGD-CBD	4.54	119.34	111.27
11	cB	814	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
11	cA	838	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
11	cA	804	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
11	cB	810	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
11	aA	813	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
11	cA	815	CLA	C3B-C2B-C1B	-4.54	101.68	107.16
11	cL	205	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
11	aB	818	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
11	cB	837	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
11	cA	828	CLA	C3C-C4C-NC	4.54	115.66	110.57
11	cA	802	CLA	C3B-C2B-C1B	-4.54	101.69	107.16
12	aA	826	F6C	CHB-C4A-C3A	-4.54	115.97	125.48
11	bB	818	CLA	C3D-C2D-C1D	-4.53	99.64	105.83
11	cA	813	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
11	bB	832	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
11	bB	837	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
11	aB	810	CLA	C4A-NA-C1A	-4.53	104.67	106.71
11	aB	840	CLA	C1C-C2C-C3C	-4.53	102.19	106.96
11	bL	205	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
11	bB	803	CLA	CAC-C3C-C4C	4.53	130.68	124.81
11	aA	819	CLA	C4A-NA-C1A	-4.53	104.67	106.71
11	aB	812	CLA	C4A-NA-C1A	-4.53	104.67	106.71
11	aB	827	CLA	C3C-C4C-NC	4.53	115.65	110.57
12	cA	826	F6C	CHB-C4A-C3A	-4.52	115.99	125.48
11	bB	835	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
11	bB	840	CLA	C1C-C2C-C3C	-4.52	102.20	106.96
11	aK	101	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
11	bA	802	CLA	C3B-C2B-C1B	-4.52	101.70	107.16
11	bA	820	CLA	C3D-C2D-C1D	-4.52	99.66	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bB	830	CLA	C3B-C2B-C1B	-4.52	101.71	107.16
11	aB	809	CLA	C3D-C2D-C1D	-4.52	99.67	105.83
11	aA	815	CLA	C3B-C2B-C1B	-4.52	101.71	107.16
11	aA	816	CLA	C3B-C2B-C1B	-4.52	101.71	107.16
11	aA	818	CLA	C3C-C4C-NC	4.51	115.63	110.57
11	aB	810	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
11	aA	833	CLA	O2D-CGD-CBD	4.51	119.29	111.27
11	cA	816	CLA	C3B-C2B-C1B	-4.51	101.71	107.16
11	cB	801	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
11	bB	801	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
11	bB	821	CLA	C3B-C2B-C1B	-4.51	101.72	107.16
11	cB	840	CLA	C1C-C2C-C3C	-4.51	102.21	106.96
11	aA	817	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
11	bA	810	CLA	CHD-C1D-ND	-4.51	120.31	124.45
11	cA	817	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
11	bA	813	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
11	bA	817	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
11	bB	809	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
11	bB	817	CLA	C3B-C2B-C1B	-4.51	101.72	107.16
11	cB	838	CLA	C3B-C2B-C1B	-4.51	101.72	107.16
11	cB	812	CLA	C4A-NA-C1A	-4.50	104.68	106.71
11	cB	801	CLA	CMB-C2B-C1B	4.50	132.23	125.37
11	aB	839	CLA	C3C-C4C-NC	4.50	115.62	110.57
11	cB	829	CLA	CAC-C3C-C4C	4.50	130.65	124.81
12	bA	826	F6C	CHB-C4A-C3A	-4.50	116.04	125.48
11	aA	828	CLA	C3C-C4C-NC	4.50	115.62	110.57
11	aA	828	CLA	C2C-C1C-NC	4.50	114.19	109.97
11	cB	835	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
11	bA	810	CLA	C3B-C2B-C1B	-4.50	101.73	107.16
11	aA	811	CLA	C4A-NA-C1A	-4.50	104.68	106.71
11	aL	205	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
11	cA	828	CLA	C2C-C1C-NC	4.50	114.19	109.97
11	cB	837	CLA	C4A-NA-C1A	-4.50	104.68	106.71
11	cA	816	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
11	aB	808	CLA	C3B-C2B-C1B	-4.50	101.73	107.16
11	bB	834	CLA	C3D-C2D-C1D	-4.50	99.70	105.83
11	aB	835	CLA	C3D-C2D-C1D	-4.50	99.70	105.83
11	cA	818	CLA	C2C-C1C-NC	4.49	114.18	109.97
11	cB	823	CLA	C3C-C4C-NC	4.49	115.61	110.57
11	aA	815	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
11	aB	817	CLA	C3B-C2B-C1B	-4.49	101.74	107.16
11	cB	817	CLA	C3B-C2B-C1B	-4.49	101.74	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aB	801	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
11	aB	837	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
11	bB	801	CLA	C3C-C4C-NC	4.49	115.61	110.57
11	aA	803	CLA	C2C-C1C-NC	4.49	114.18	109.97
11	bA	828	CLA	C2C-C1C-NC	4.49	114.18	109.97
11	cB	809	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
11	cA	811	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
11	aA	802	CLA	C3B-C2B-C1B	-4.49	101.75	107.16
11	aB	832	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
11	bB	838	CLA	C3B-C2B-C1B	-4.49	101.75	107.16
11	aA	818	CLA	C2C-C1C-NC	4.49	114.17	109.97
11	cB	832	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
11	cB	801	CLA	C3C-C4C-NC	4.49	115.60	110.57
11	aB	823	CLA	C3C-C4C-NC	4.48	115.60	110.57
11	cA	815	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
11	cA	824	CLA	O2D-CGD-CBD	4.48	119.23	111.27
11	bA	815	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
11	bA	816	CLA	C3B-C2B-C1B	-4.48	101.76	107.16
11	aB	828	CLA	C3B-C4B-NB	4.48	114.67	110.52
11	bA	828	CLA	C3C-C4C-NC	4.48	115.59	110.57
11	aB	834	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
11	cB	808	CLA	C3B-C2B-C1B	-4.48	101.76	107.16
11	cB	821	CLA	C3B-C2B-C1B	-4.47	101.76	107.16
11	bA	802	CLA	C3B-C4B-NB	4.47	114.67	110.52
11	bA	818	CLA	C3C-C4C-NC	4.47	115.59	110.57
11	cA	812	CLA	C3D-C2D-C1D	-4.47	99.72	105.83
11	aB	821	CLA	C3B-C2B-C1B	-4.47	101.76	107.16
11	cA	802	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
11	bB	837	CLA	C4A-NA-C1A	-4.47	104.69	106.71
11	cA	803	CLA	C2C-C1C-NC	4.47	114.16	109.97
11	bB	829	CLA	CAC-C3C-C4C	4.47	130.61	124.81
11	cA	810	CLA	CHD-C1D-ND	-4.47	120.34	124.45
11	bB	839	CLA	C3C-C4C-NC	4.47	115.59	110.57
11	cA	819	CLA	C2C-C1C-NC	4.47	114.16	109.97
11	aB	802	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
11	bB	808	CLA	C3B-C2B-C1B	-4.47	101.77	107.16
11	bA	819	CLA	C2C-C1C-NC	4.47	114.16	109.97
11	aB	839	CLA	O2D-CGD-CBD	4.47	119.21	111.27
11	cB	828	CLA	C3B-C4B-NB	4.46	114.66	110.52
11	bA	811	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
11	aB	829	CLA	CAC-C3C-C4C	4.46	130.60	124.81
11	cA	806	CLA	CAC-C3C-C4C	4.46	130.60	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cA	818	CLA	C3C-C4C-NC	4.46	115.57	110.57
11	aB	838	CLA	C3B-C2B-C1B	-4.46	101.78	107.16
11	bL	206	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
11	cB	834	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
11	cB	839	CLA	O2D-CGD-CBD	4.46	119.19	111.27
11	bB	811	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
11	aA	811	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
11	cB	840	CLA	O2D-CGD-CBD	4.46	119.19	111.27
11	aB	801	CLA	C3C-C4C-NC	4.45	115.57	110.57
11	bA	812	CLA	C3D-C2D-C1D	-4.45	99.75	105.83
11	cL	206	CLA	C3D-C2D-C1D	-4.45	99.75	105.83
11	bA	824	CLA	O2D-CGD-CBD	4.45	119.18	111.27
11	cA	802	CLA	C3B-C4B-NB	4.45	114.65	110.52
11	bB	839	CLA	O2D-CGD-CBD	4.45	119.18	111.27
11	aA	824	CLA	O2D-CGD-CBD	4.45	119.18	111.27
11	bB	840	CLA	O2D-CGD-CBD	4.45	119.18	111.27
11	cB	802	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
11	bB	804	CLA	C3C-C4C-NC	4.45	115.56	110.57
11	bB	828	CLA	C3B-C4B-NB	4.45	114.64	110.52
11	aA	816	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
12	aB	824	F6C	OMB-CMB-C2B	-4.45	115.62	125.69
11	cB	811	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
11	aA	802	CLA	C3B-C4B-NB	4.45	114.64	110.52
11	aA	838	CLA	C4A-NA-C1A	-4.45	104.71	106.71
11	bA	839	CLA	C4A-NA-C1A	-4.45	104.71	106.71
11	aB	840	CLA	O2D-CGD-CBD	4.45	119.17	111.27
11	bB	826	CLA	C3B-C2B-C1B	-4.45	101.79	107.16
11	aA	831	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
12	cB	824	F6C	CHB-C4A-C3A	-4.45	116.16	125.48
11	cB	839	CLA	C3C-C4C-NC	4.44	115.55	110.57
12	bA	826	F6C	C3D-C4D-ND	4.44	116.67	110.17
11	aA	802	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
11	bB	808	CLA	C3C-C4C-NC	4.44	115.55	110.57
11	aA	812	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
11	aL	206	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
12	aA	826	F6C	C3D-C4D-ND	4.44	116.66	110.17
11	bA	803	CLA	C2C-C1C-NC	4.44	114.13	109.97
11	bB	836	CLA	C3C-C4C-NC	4.44	115.55	110.57
12	cB	824	F6C	OMB-CMB-C2B	-4.44	115.65	125.69
11	aB	811	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
11	bA	816	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
11	bA	806	CLA	CAC-C3C-C4C	4.44	130.57	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bA	831	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
11	bB	802	CLA	C3D-C2D-C1D	-4.44	99.78	105.83
12	bB	824	F6C	OMB-CMB-C2B	-4.44	115.66	125.69
11	bA	806	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
11	cB	804	CLA	C3C-C4C-NC	4.43	115.54	110.57
12	aB	824	F6C	CHB-C4A-C3A	-4.43	116.18	125.48
11	bA	834	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
11	aA	836	CLA	CHD-C1D-ND	-4.43	120.38	124.45
11	aB	808	CLA	C3C-C4C-NC	4.43	115.54	110.57
11	aB	826	CLA	C3B-C2B-C1B	-4.43	101.81	107.16
11	cB	826	CLA	C3B-C2B-C1B	-4.43	101.81	107.16
11	cB	808	CLA	C3C-C4C-NC	4.43	115.54	110.57
11	aA	806	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
11	aA	806	CLA	CAC-C3C-C4C	4.43	130.55	124.81
11	cA	819	CLA	C4A-NA-C1A	-4.43	104.72	106.71
12	cA	826	F6C	C3D-C4D-ND	4.43	116.64	110.17
12	bB	824	F6C	CHB-C4A-C3A	-4.43	116.20	125.48
11	bB	829	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
11	aA	834	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
11	bB	812	CLA	CAC-C3C-C4C	4.42	130.54	124.81
11	cB	810	CLA	C4A-NA-C1A	-4.42	104.72	106.71
11	aB	804	CLA	C3C-C4C-NC	4.42	115.53	110.57
11	bA	802	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
11	cB	827	CLA	C4A-NA-C1A	-4.42	104.72	106.71
11	cA	831	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
11	bA	824	CLA	C3B-C2B-C1B	-4.42	101.83	107.16
11	aA	839	CLA	C4A-NA-C1A	-4.42	104.72	106.71
11	aB	812	CLA	CAC-C3C-C4C	4.41	130.53	124.81
12	bA	844	F6C	CHB-C4A-C3A	-4.41	116.23	125.48
11	bB	839	CLA	CHD-C1D-ND	-4.41	120.40	124.45
11	cB	829	CLA	CHD-C4C-C3C	-4.41	118.36	124.84
12	cA	844	F6C	CHB-C4A-C3A	-4.41	116.23	125.48
11	cB	829	CLA	C3D-C2D-C1D	-4.41	99.82	105.83
11	bB	829	CLA	CHD-C4C-C3C	-4.41	118.36	124.84
11	bB	810	CLA	C4A-NA-C1A	-4.41	104.72	106.71
11	cA	824	CLA	C3D-C2D-C1D	-4.41	99.82	105.83
11	bB	835	CLA	C3B-C2B-C1B	-4.40	101.84	107.16
11	aA	824	CLA	C3D-C2D-C1D	-4.40	99.82	105.83
11	aB	835	CLA	C3B-C2B-C1B	-4.40	101.85	107.16
11	aB	839	CLA	C3B-C2B-C1B	-4.40	101.85	107.16
11	cA	834	CLA	C3D-C2D-C1D	-4.40	99.82	105.83
11	bA	810	CLA	C3C-C4C-NC	4.40	115.51	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cB	836	CLA	C3C-C4C-NC	4.40	115.51	110.57
11	cB	835	CLA	C3B-C2B-C1B	-4.40	101.85	107.16
11	bA	825	CLA	C3B-C2B-C1B	-4.40	101.85	107.16
11	aB	829	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
11	aB	836	CLA	C3C-C4C-NC	4.40	115.50	110.57
11	cA	824	CLA	C3B-C2B-C1B	-4.40	101.85	107.16
11	cA	806	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
11	aA	810	CLA	C3C-C4C-NC	4.40	115.50	110.57
11	bB	812	CLA	C4A-NA-C1A	-4.40	104.73	106.71
11	cA	838	CLA	C4A-NA-C1A	-4.40	104.73	106.71
11	cB	839	CLA	CHD-C1D-ND	-4.39	120.42	124.45
11	aA	828	CLA	C1D-CHD-C4C	-4.39	116.58	126.06
11	aB	829	CLA	CHD-C4C-C3C	-4.39	118.39	124.84
11	cA	836	CLA	CHD-C1D-ND	-4.39	120.42	124.45
11	bB	822	CLA	C1D-CHD-C4C	-4.39	116.59	126.06
11	cA	810	CLA	C3C-C4C-NC	4.39	115.49	110.57
11	aB	828	CLA	O2D-CGD-CBD	4.38	119.06	111.27
11	aA	824	CLA	C3B-C2B-C1B	-4.38	101.87	107.16
11	cA	825	CLA	C3B-C2B-C1B	-4.38	101.87	107.16
11	cB	839	CLA	C3B-C2B-C1B	-4.38	101.87	107.16
11	cB	803	CLA	CHD-C4C-C3C	-4.38	118.40	124.84
11	bB	828	CLA	O2D-CGD-CBD	4.38	119.06	111.27
12	aA	844	F6C	CHB-C4A-C3A	-4.38	116.29	125.48
11	bA	828	CLA	C1D-CHD-C4C	-4.38	116.60	126.06
11	aL	206	CLA	C3B-C2B-C1B	-4.38	101.87	107.16
11	aA	843	CLA	C4A-NA-C1A	-4.38	104.74	106.71
11	bA	819	CLA	C4A-NA-C1A	-4.38	104.74	106.71
11	bA	843	CLA	C4A-NA-C1A	-4.38	104.74	106.71
11	bA	824	CLA	C3D-C2D-C1D	-4.38	99.86	105.83
11	cB	812	CLA	CAC-C3C-C4C	4.38	130.49	124.81
11	cA	828	CLA	C1D-CHD-C4C	-4.38	116.62	126.06
11	cA	843	CLA	C4A-NA-C1A	-4.37	104.74	106.71
11	cB	822	CLA	C1D-CHD-C4C	-4.37	116.62	126.06
11	aA	825	CLA	C3B-C2B-C1B	-4.37	101.88	107.16
11	aA	829	CLA	O2D-CGD-CBD	4.37	119.04	111.27
11	cA	840	CLA	C3B-C2B-C1B	-4.37	101.88	107.16
11	cB	828	CLA	O2D-CGD-CBD	4.37	119.04	111.27
11	aB	803	CLA	CHD-C4C-C3C	-4.37	118.42	124.84
11	bA	840	CLA	C3B-C2B-C1B	-4.37	101.89	107.16
11	aB	822	CLA	C1D-CHD-C4C	-4.37	116.63	126.06
11	bB	803	CLA	CHD-C4C-C3C	-4.37	118.42	124.84
11	aB	823	CLA	CHD-C1D-ND	-4.37	120.44	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bB	806	CLA	C4A-NA-C1A	-4.37	104.74	106.71
11	cA	819	CLA	C3C-C4C-NC	4.37	115.47	110.57
11	bB	819	CLA	CHD-C1D-ND	-4.37	120.44	124.45
11	cB	835	CLA	O2D-CGD-CBD	4.36	119.02	111.27
11	cB	819	CLA	CHD-C1D-ND	-4.36	120.44	124.45
12	aL	202	F6C	C4C-CHD-C1D	-4.36	115.99	126.34
11	aB	812	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
11	bB	835	CLA	O2D-CGD-CBD	4.36	119.02	111.27
12	cL	202	F6C	C4C-CHD-C1D	-4.36	116.00	126.34
11	cB	807	CLA	C3B-C2B-C1B	-4.36	101.90	107.16
11	aB	839	CLA	CHD-C1D-ND	-4.36	120.45	124.45
11	aB	807	CLA	C3B-C2B-C1B	-4.36	101.90	107.16
11	aA	840	CLA	C3B-C2B-C1B	-4.36	101.90	107.16
11	bB	839	CLA	C3B-C2B-C1B	-4.36	101.90	107.16
11	cA	829	CLA	O2D-CGD-CBD	4.36	119.01	111.27
11	bB	807	CLA	C3B-C2B-C1B	-4.35	101.91	107.16
11	bA	825	CLA	C3D-C2D-C1D	-4.35	99.89	105.83
11	bB	825	CLA	C3C-C4C-NC	4.35	115.45	110.57
12	cA	832	F6C	CHB-C4A-C3A	-4.35	116.36	125.48
11	aB	810	CLA	O2D-CGD-CBD	4.35	119.00	111.27
11	bA	820	CLA	O2D-CGD-CBD	4.35	119.00	111.27
11	bA	829	CLA	O2D-CGD-CBD	4.35	119.00	111.27
11	bA	819	CLA	C3C-C4C-NC	4.35	115.45	110.57
11	cA	820	CLA	O2D-CGD-CBD	4.35	119.00	111.27
12	bL	202	F6C	C4C-CHD-C1D	-4.35	116.03	126.34
11	bB	827	CLA	C4A-NA-C1A	-4.35	104.75	106.71
11	bB	823	CLA	CHD-C1D-ND	-4.35	120.46	124.45
11	bA	836	CLA	CHD-C1D-ND	-4.35	120.46	124.45
11	bA	822	CLA	C3D-C2D-C1D	-4.34	99.90	105.83
11	cA	839	CLA	C4A-NA-C1A	-4.34	104.75	106.71
12	bA	826	F6C	C3D-C2D-C1D	-4.34	99.54	105.83
11	aB	825	CLA	C3C-C4C-NC	4.34	115.44	110.57
11	cA	822	CLA	C3D-C2D-C1D	-4.34	99.91	105.83
12	cA	826	F6C	C3D-C2D-C1D	-4.34	99.55	105.83
12	bA	832	F6C	CHB-C4A-C3A	-4.34	116.38	125.48
11	aB	835	CLA	O2D-CGD-CBD	4.34	118.98	111.27
11	aA	819	CLA	C3C-C4C-NC	4.34	115.44	110.57
12	cA	826	F6C	CHD-C4C-NC	4.34	128.85	124.26
11	aB	819	CLA	CHD-C1D-ND	-4.34	120.47	124.45
11	cB	810	CLA	O2D-CGD-CBD	4.34	118.97	111.27
11	aA	822	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
11	aA	820	CLA	O2D-CGD-CBD	4.33	118.96	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	827	F6C	C3D-C2D-C1D	-4.33	99.56	105.83
11	cB	812	CLA	C3D-C2D-C1D	-4.33	99.93	105.83
11	aB	801	CLA	C1D-CHD-C4C	-4.32	116.73	126.06
11	cL	206	CLA	C3B-C2B-C1B	-4.32	101.94	107.16
11	bL	206	CLA	C3B-C2B-C1B	-4.32	101.94	107.16
11	aB	837	CLA	C4A-NA-C1A	-4.32	104.76	106.71
12	aA	832	F6C	CHB-C4A-C3A	-4.32	116.42	125.48
11	bB	810	CLA	O2D-CGD-CBD	4.32	118.94	111.27
11	bA	821	CLA	C3C-C4C-NC	4.32	115.41	110.57
11	cB	801	CLA	C1D-CHD-C4C	-4.32	116.74	126.06
11	cB	806	CLA	C4A-NA-C1A	-4.32	104.77	106.71
11	bB	801	CLA	C1D-CHD-C4C	-4.31	116.75	126.06
11	aA	814	CLA	C3D-C4D-ND	4.31	117.22	110.24
11	bB	812	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
12	aA	827	F6C	C3D-C2D-C1D	-4.31	99.59	105.83
12	aA	826	F6C	C3D-C2D-C1D	-4.31	99.59	105.83
11	aA	825	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
12	bA	827	F6C	C3D-C2D-C1D	-4.31	99.59	105.83
11	bA	810	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
11	cB	820	CLA	C1C-C2C-C3C	-4.31	102.43	106.96
11	aB	808	CLA	C1D-CHD-C4C	-4.31	116.77	126.06
11	cB	808	CLA	C1D-CHD-C4C	-4.31	116.77	126.06
10	aA	801	CL0	C3D-C2D-C1D	-4.30	99.96	105.83
11	bA	836	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
10	cA	801	CL0	C3D-C2D-C1D	-4.30	99.97	105.83
11	aB	827	CLA	C4A-NA-C1A	-4.30	104.77	106.71
12	aA	830	F6C	O2D-CGD-CBD	4.30	118.90	111.27
11	bB	808	CLA	C1D-CHD-C4C	-4.30	116.79	126.06
11	cA	836	CLA	C3D-C2D-C1D	-4.30	99.97	105.83
11	cA	825	CLA	C3D-C2D-C1D	-4.29	99.97	105.83
11	cB	829	CLA	CMB-C2B-C1B	4.29	131.91	125.37
11	cA	821	CLA	C3C-C4C-NC	4.29	115.38	110.57
11	cA	811	CLA	C3B-C2B-C1B	-4.29	101.98	107.16
11	bB	815	CLA	C3C-C4C-NC	4.29	115.38	110.57
11	cA	814	CLA	C3D-C4D-ND	4.29	117.18	110.24
12	aA	826	F6C	CHD-C4C-NC	4.29	128.80	124.26
11	aA	836	CLA	C3D-C2D-C1D	-4.29	99.98	105.83
11	cB	813	CLA	C3D-C2D-C1D	-4.29	99.98	105.83
11	bA	821	CLA	CHD-C1D-ND	-4.29	120.52	124.45
11	cB	823	CLA	CHD-C1D-ND	-4.29	120.52	124.45
11	aA	843	CLA	C3B-C2B-C1B	-4.28	101.99	107.16
11	bB	820	CLA	C1C-C2C-C3C	-4.28	102.45	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aB	815	CLA	C3C-C4C-NC	4.28	115.37	110.57
10	aA	801	CL0	C3C-C4C-NC	4.28	115.37	110.57
11	bA	814	CLA	C3D-C4D-ND	4.28	117.16	110.24
11	bA	810	CLA	O2D-CGD-CBD	4.28	118.86	111.27
12	cA	830	F6C	O2D-CGD-CBD	4.27	118.86	111.27
11	cA	821	CLA	C3D-C2D-C1D	-4.27	100.00	105.83
11	cA	814	CLA	C3D-C2D-C1D	-4.27	100.00	105.83
11	aB	818	CLA	C3C-C4C-NC	4.27	115.36	110.57
11	bB	839	CLA	C4A-NA-C1A	-4.27	104.78	106.71
11	bA	821	CLA	C3D-C2D-C1D	-4.27	100.00	105.83
10	bA	801	CL0	C3D-C2D-C1D	-4.27	100.00	105.83
11	cB	825	CLA	C3C-C4C-NC	4.27	115.36	110.57
11	aA	817	CLA	C3B-C2B-C1B	-4.27	102.01	107.16
11	aB	829	CLA	CMB-C2B-C1B	4.27	131.87	125.37
12	aA	827	F6C	CHD-C4C-NC	4.27	128.77	124.26
11	aL	206	CLA	C3D-C4D-ND	4.26	117.14	110.24
11	bA	814	CLA	C3D-C2D-C1D	-4.26	100.01	105.83
11	bB	829	CLA	CMB-C2B-C1B	4.26	131.86	125.37
11	aA	821	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
11	aB	813	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
11	cA	843	CLA	C3B-C2B-C1B	-4.26	102.02	107.16
11	cA	810	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
10	cA	801	CL0	C3C-C4C-NC	4.26	115.35	110.57
11	bL	206	CLA	C3D-C4D-ND	4.26	117.12	110.24
11	aA	810	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
11	aA	810	CLA	O2D-CGD-CBD	4.26	118.83	111.27
12	bA	830	F6C	O2D-CGD-CBD	4.25	118.83	111.27
12	aA	827	F6C	CHB-C4A-C3A	-4.25	116.56	125.48
11	aB	820	CLA	C1C-C2C-C3C	-4.25	102.49	106.96
11	aA	821	CLA	C3C-C4C-NC	4.25	115.34	110.57
11	bB	813	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
11	cA	810	CLA	O2D-CGD-CBD	4.25	118.82	111.27
11	cB	815	CLA	C3C-C4C-NC	4.25	115.34	110.57
11	cL	206	CLA	C3D-C4D-ND	4.25	117.11	110.24
11	bA	843	CLA	C3B-C2B-C1B	-4.25	102.03	107.16
11	bB	819	CLA	C3C-C4C-NC	4.25	115.33	110.57
11	aA	814	CLA	C3D-C2D-C1D	-4.24	100.04	105.83
11	cB	839	CLA	C4A-NA-C1A	-4.24	104.80	106.71
11	bA	811	CLA	C3B-C2B-C1B	-4.24	102.04	107.16
12	bA	827	F6C	CHB-C4A-C3A	-4.24	116.58	125.48
12	bA	826	F6C	CHD-C4C-NC	4.24	128.75	124.26
12	bA	832	F6C	C3D-C2D-C1D	-4.24	99.69	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cA	821	CLA	CHD-C1D-ND	-4.24	120.56	124.45
12	cA	830	F6C	CHD-C4C-C3C	-4.24	116.10	125.36
11	cA	817	CLA	C3B-C2B-C1B	-4.24	102.05	107.16
12	aA	830	F6C	CHD-C4C-C3C	-4.24	116.11	125.36
12	cA	827	F6C	CHD-C4C-NC	4.24	128.74	124.26
11	aA	821	CLA	C3B-C2B-C1B	-4.24	102.05	107.16
11	bA	817	CLA	C3B-C2B-C1B	-4.24	102.05	107.16
10	bA	801	CL0	C3C-C4C-NC	4.23	115.32	110.57
11	aA	811	CLA	C3B-C2B-C1B	-4.23	102.05	107.16
11	bA	819	CLA	O2D-CGD-CBD	4.23	118.79	111.27
11	aB	839	CLA	C4A-NA-C1A	-4.23	104.80	106.71
12	aA	832	F6C	C3D-C2D-C1D	-4.23	99.71	105.83
11	cA	808	CLA	C3D-C4D-ND	4.23	117.07	110.24
11	aA	808	CLA	C3D-C4D-ND	4.22	117.07	110.24
12	bA	830	F6C	CHD-C4C-C3C	-4.22	116.13	125.36
11	cB	819	CLA	C3C-C4C-NC	4.22	115.31	110.57
11	bB	801	CLA	CMA-C3A-C2A	-4.22	96.79	113.83
11	cB	801	CLA	CMA-C3A-C2A	-4.22	96.80	113.83
11	aB	801	CLA	CMA-C3A-C2A	-4.22	96.80	113.83
11	aB	811	CLA	C3C-C4C-NC	4.22	115.31	110.57
11	bB	807	CLA	C3C-C4C-NC	4.22	115.30	110.57
11	aA	819	CLA	O2D-CGD-CBD	4.22	118.77	111.27
11	aA	821	CLA	CHD-C1D-ND	-4.22	120.58	124.45
11	cB	818	CLA	C3C-C4C-NC	4.22	115.30	110.57
11	bA	821	CLA	C3B-C2B-C1B	-4.22	102.07	107.16
11	aA	807	CLA	C1C-C2C-C3C	-4.22	102.52	106.96
12	bA	827	F6C	CHD-C4C-NC	4.22	128.72	124.26
11	aB	806	CLA	C4A-NA-C1A	-4.22	104.81	106.71
11	bA	812	CLA	C4A-NA-C1A	-4.22	104.81	106.71
11	bB	828	CLA	C4A-NA-C1A	-4.21	104.81	106.71
11	bB	818	CLA	C3C-C4C-NC	4.21	115.29	110.57
12	cA	827	F6C	CHB-C4A-C3A	-4.21	116.65	125.48
11	cA	821	CLA	C3B-C2B-C1B	-4.21	102.08	107.16
12	cA	832	F6C	C3D-C2D-C1D	-4.21	99.74	105.83
11	aA	802	CLA	C3C-C4C-NC	4.21	115.29	110.57
11	cA	822	CLA	C3C-C4C-NC	4.21	115.29	110.57
11	aL	206	CLA	C3C-C4C-NC	4.20	115.28	110.57
11	cL	206	CLA	C3C-C4C-NC	4.20	115.28	110.57
11	aA	822	CLA	C3C-C4C-NC	4.20	115.28	110.57
11	aB	819	CLA	C3C-C4C-NC	4.20	115.28	110.57
11	bL	206	CLA	C3C-C4C-NC	4.20	115.28	110.57
11	aB	807	CLA	C3C-C4C-NC	4.20	115.28	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aA	843	CLA	C3C-C4C-NC	4.19	115.27	110.57
11	cA	806	CLA	C3D-C4D-ND	4.19	117.02	110.24
11	cA	802	CLA	C3C-C4C-NC	4.19	115.27	110.57
11	cA	819	CLA	O2D-CGD-CBD	4.19	118.71	111.27
11	cB	807	CLA	C3C-C4C-NC	4.19	115.27	110.57
11	cB	809	CLA	O2D-CGD-CBD	4.19	118.71	111.27
11	bB	809	CLA	O2D-CGD-CBD	4.19	118.71	111.27
11	cA	843	CLA	C3C-C4C-NC	4.19	115.27	110.57
11	bA	808	CLA	C3D-C4D-ND	4.19	117.01	110.24
11	cB	834	CLA	O2D-CGD-CBD	4.19	118.70	111.27
11	cB	818	CLA	C3D-C4D-ND	4.18	117.01	110.24
11	bA	807	CLA	C1C-C2C-C3C	-4.18	102.56	106.96
11	cA	812	CLA	C4A-NA-C1A	-4.18	104.83	106.71
11	cB	829	CLA	C3B-C4B-NB	4.18	114.39	110.52
11	bA	843	CLA	C3C-C4C-NC	4.18	115.26	110.57
11	aA	840	CLA	C3D-C4D-ND	4.18	117.00	110.24
11	bB	818	CLA	C3D-C4D-ND	4.18	117.00	110.24
11	aB	818	CLA	C3D-C4D-ND	4.18	116.99	110.24
11	bA	814	CLA	C4A-NA-C1A	-4.18	104.83	106.71
11	cB	819	CLA	C3D-C2D-C1D	-4.17	100.14	105.83
11	aB	809	CLA	O2D-CGD-CBD	4.17	118.68	111.27
11	bA	837	CLA	C3C-C4C-NC	4.17	115.25	110.57
11	bB	809	CLA	C3D-C4D-ND	4.17	116.98	110.24
11	bA	802	CLA	C3C-C4C-NC	4.17	115.25	110.57
11	aA	823	CLA	C1C-C2C-C3C	-4.17	102.57	106.96
11	cB	838	CLA	C3D-C4D-ND	4.17	116.98	110.24
11	cA	803	CLA	C3C-C4C-NC	4.17	115.25	110.57
11	cB	811	CLA	C3C-C4C-NC	4.17	115.25	110.57
11	cA	802	CLA	C1C-C2C-C3C	-4.17	102.58	106.96
11	cA	807	CLA	C1C-C2C-C3C	-4.17	102.58	106.96
11	bB	838	CLA	C3D-C4D-ND	4.17	116.98	110.24
11	bB	811	CLA	C3C-C4C-NC	4.17	115.24	110.57
11	aB	819	CLA	C3D-C2D-C1D	-4.17	100.15	105.83
11	bB	821	CLA	C3C-C4C-NC	4.16	115.24	110.57
11	aB	809	CLA	C3D-C4D-ND	4.16	116.97	110.24
16	aA	852	LHG	O4-P-O5	4.16	132.82	112.24
16	cA	852	LHG	O4-P-O5	4.16	132.82	112.24
12	cA	830	F6C	CHB-C4A-C3A	-4.16	116.75	125.48
11	aL	205	CLA	C3D-C4D-ND	4.16	116.97	110.24
16	bA	852	LHG	O4-P-O5	4.16	132.81	112.24
11	bB	834	CLA	O2D-CGD-CBD	4.16	118.66	111.27
11	cA	813	CLA	O2D-CGD-CBD	4.16	118.66	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	844	F6C	C3D-C2D-C1D	-4.16	99.81	105.83
11	bA	822	CLA	C3C-C4C-NC	4.16	115.23	110.57
11	aB	807	CLA	C4A-NA-C1A	-4.16	104.84	106.71
11	cA	823	CLA	C1C-C2C-C3C	-4.16	102.59	106.96
11	bA	823	CLA	C1C-C2C-C3C	-4.16	102.59	106.96
11	aB	829	CLA	C3B-C4B-NB	4.15	114.37	110.52
11	cB	821	CLA	C3C-C4C-NC	4.15	115.23	110.57
11	bA	840	CLA	C3D-C4D-ND	4.15	116.96	110.24
11	aB	823	CLA	C3D-C2D-C1D	-4.15	100.16	105.83
11	aA	812	CLA	C4A-NA-C1A	-4.15	104.84	106.71
12	aA	830	F6C	CHB-C4A-C3A	-4.15	116.77	125.48
11	aA	817	CLA	C1C-C2C-C3C	-4.15	102.59	106.96
11	cA	840	CLA	C3D-C4D-ND	4.15	116.95	110.24
11	bA	806	CLA	C3D-C4D-ND	4.15	116.95	110.24
11	aB	828	CLA	C4A-NA-C1A	-4.15	104.84	106.71
11	aB	834	CLA	O2D-CGD-CBD	4.15	118.64	111.27
12	cA	827	F6C	CHD-C4C-C3C	-4.15	116.30	125.36
11	aB	838	CLA	C3D-C4D-ND	4.14	116.94	110.24
11	aB	821	CLA	C3C-C4C-NC	4.14	115.22	110.57
12	bA	830	F6C	CHB-C4A-C3A	-4.14	116.79	125.48
11	bB	823	CLA	C3D-C2D-C1D	-4.14	100.18	105.83
11	aA	806	CLA	C3D-C4D-ND	4.14	116.94	110.24
11	bA	813	CLA	O2D-CGD-CBD	4.14	118.63	111.27
11	bL	205	CLA	C3D-C4D-ND	4.14	116.94	110.24
11	bA	803	CLA	C3C-C4C-NC	4.14	115.22	110.57
11	cB	833	CLA	O2D-CGD-CBD	4.14	118.62	111.27
11	bB	819	CLA	C3D-C2D-C1D	-4.14	100.18	105.83
11	aA	802	CLA	C1C-C2C-C3C	-4.14	102.61	106.96
12	bA	827	F6C	CHD-C4C-C3C	-4.14	116.32	125.36
12	cL	202	F6C	C3D-C4D-ND	4.14	116.22	110.17
12	bA	844	F6C	C3D-C2D-C1D	-4.14	99.84	105.83
12	aA	827	F6C	CHD-C4C-C3C	-4.14	116.32	125.36
11	aA	813	CLA	O2D-CGD-CBD	4.14	118.62	111.27
11	cB	809	CLA	C3D-C4D-ND	4.13	116.93	110.24
12	aA	844	F6C	C3D-C2D-C1D	-4.13	99.84	105.83
11	aA	803	CLA	C3C-C4C-NC	4.13	115.21	110.57
11	aA	813	CLA	C3C-C4C-NC	4.13	115.21	110.57
11	bA	805	CLA	C3C-C4C-NC	4.13	115.21	110.57
11	cA	837	CLA	C3C-C4C-NC	4.13	115.21	110.57
11	aA	837	CLA	C3D-C4D-ND	4.13	116.92	110.24
11	cL	205	CLA	C3D-C4D-ND	4.13	116.92	110.24
11	aA	805	CLA	C3C-C4C-NC	4.13	115.20	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bB	829	CLA	C3B-C4B-NB	4.13	114.34	110.52
11	aB	833	CLA	O2D-CGD-CBD	4.12	118.60	111.27
12	aL	202	F6C	C3D-C4D-ND	4.12	116.20	110.17
11	cA	805	CLA	C3C-C4C-NC	4.12	115.20	110.57
11	cB	823	CLA	C3D-C2D-C1D	-4.12	100.20	105.83
11	bB	833	CLA	O2D-CGD-CBD	4.12	118.59	111.27
12	cA	844	F6C	O2D-CGD-CBD	4.12	118.59	111.27
11	aA	837	CLA	C3C-C4C-NC	4.12	115.19	110.57
11	aL	204	CLA	C3C-C4C-NC	4.12	115.19	110.57
12	bL	202	F6C	C3D-C4D-ND	4.12	116.19	110.17
11	cB	828	CLA	C4A-NA-C1A	-4.11	104.86	106.71
11	cL	204	CLA	C3C-C4C-NC	4.11	115.18	110.57
11	cA	815	CLA	C3B-C4B-NB	4.11	114.33	110.52
11	cA	817	CLA	C1C-C2C-C3C	-4.11	102.64	106.96
11	bB	822	CLA	C3D-C4D-ND	4.11	116.89	110.24
12	bA	844	F6C	O2D-CGD-CBD	4.11	118.57	111.27
11	cA	837	CLA	C3D-C4D-ND	4.11	116.88	110.24
11	bA	817	CLA	C1C-C2C-C3C	-4.11	102.64	106.96
11	aB	817	CLA	C1C-C2C-C3C	-4.11	102.64	106.96
11	aB	813	CLA	C3C-C4C-NC	4.11	115.17	110.57
11	cA	831	CLA	C3C-C4C-NC	4.10	115.17	110.57
11	bA	815	CLA	C3B-C4B-NB	4.10	114.32	110.52
11	aA	829	CLA	C3C-C4C-NC	4.10	115.17	110.57
11	cB	817	CLA	C1C-C2C-C3C	-4.10	102.64	106.96
11	cA	820	CLA	C3B-C2B-C1B	-4.10	102.21	107.16
11	bB	809	CLA	C3C-C4C-NC	4.10	115.17	110.57
11	bA	837	CLA	C3D-C4D-ND	4.10	116.87	110.24
11	cA	839	CLA	C3D-C4D-ND	4.10	116.87	110.24
11	cA	838	CLA	C3C-C4C-NC	4.10	115.17	110.57
11	cB	833	CLA	C3D-C4D-ND	4.10	116.87	110.24
11	aB	822	CLA	C3D-C4D-ND	4.10	116.87	110.24
11	bA	803	CLA	CMD-C2D-C1D	4.09	131.93	124.71
11	bA	802	CLA	C1C-C2C-C3C	-4.09	102.65	106.96
11	bB	828	CLA	C1C-C2C-C3C	-4.09	102.65	106.96
11	cB	822	CLA	C3D-C4D-ND	4.09	116.86	110.24
11	aA	815	CLA	C3B-C4B-NB	4.09	114.31	110.52
11	bK	103	CLA	C3C-C4C-NC	4.09	115.16	110.57
11	bB	817	CLA	C1C-C2C-C3C	-4.09	102.65	106.96
11	aB	809	CLA	C3C-C4C-NC	4.09	115.16	110.57
11	bL	204	CLA	C3C-C4C-NC	4.09	115.16	110.57
12	aA	844	F6C	O2D-CGD-CBD	4.09	118.54	111.27
11	aB	837	CLA	C3D-C4D-ND	4.09	116.86	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bA	839	CLA	C3D-C4D-ND	4.09	116.85	110.24
11	cB	809	CLA	C3C-C4C-NC	4.09	115.16	110.57
11	bK	101	CLA	C3D-C4D-ND	4.09	116.85	110.24
11	cK	101	CLA	C3D-C4D-ND	4.09	116.85	110.24
11	cB	810	CLA	C3B-C2B-C1B	-4.09	102.23	107.16
11	cB	813	CLA	C3C-C4C-NC	4.09	115.16	110.57
11	aA	820	CLA	C3B-C2B-C1B	-4.09	102.23	107.16
11	cA	829	CLA	C3C-C4C-NC	4.09	115.16	110.57
11	cB	828	CLA	C1C-C2C-C3C	-4.08	102.66	106.96
11	bA	820	CLA	C3B-C2B-C1B	-4.08	102.23	107.16
11	aA	839	CLA	C3D-C4D-ND	4.08	116.84	110.24
11	bA	804	CLA	O2D-CGD-CBD	4.08	118.53	111.27
11	cA	814	CLA	C4A-NA-C1A	-4.08	104.87	106.71
11	cB	807	CLA	C4A-NA-C1A	-4.08	104.87	106.71
11	aA	803	CLA	CMD-C2D-C1D	4.08	131.91	124.71
11	bB	837	CLA	C3D-C4D-ND	4.08	116.84	110.24
11	bA	813	CLA	C3C-C4C-NC	4.08	115.15	110.57
11	bB	833	CLA	C3D-C4D-ND	4.08	116.84	110.24
11	cB	837	CLA	C3C-C4C-NC	4.08	115.14	110.57
11	aA	816	CLA	C3C-C4C-NC	4.08	115.14	110.57
11	cA	816	CLA	C3C-C4C-NC	4.08	115.14	110.57
11	aA	823	CLA	C3C-C4C-NC	4.08	115.14	110.57
11	aA	831	CLA	C3C-C4C-NC	4.08	115.14	110.57
11	aK	101	CLA	C3D-C4D-ND	4.07	116.83	110.24
11	bA	820	CLA	C1C-C2C-C3C	-4.07	102.67	106.96
11	aB	838	CLA	C3C-C4C-NC	4.07	115.14	110.57
11	aB	807	CLA	C1C-C2C-C3C	-4.07	102.68	106.96
11	bA	829	CLA	C3C-C4C-NC	4.07	115.14	110.57
11	cA	804	CLA	O2D-CGD-CBD	4.07	118.50	111.27
11	aA	841	CLA	C3D-C4D-ND	4.07	116.82	110.24
11	bB	813	CLA	C3C-C4C-NC	4.07	115.14	110.57
11	bA	841	CLA	C3D-C4D-ND	4.07	116.82	110.24
11	aB	805	CLA	C3D-C4D-ND	4.06	116.81	110.24
11	cA	813	CLA	C3C-C4C-NC	4.06	115.13	110.57
11	aB	833	CLA	C3D-C4D-ND	4.06	116.81	110.24
11	aA	804	CLA	O2D-CGD-CBD	4.06	118.48	111.27
11	bA	834	CLA	C3C-C4C-NC	4.06	115.12	110.57
11	aA	802	CLA	C3D-C4D-ND	4.06	116.81	110.24
11	bB	839	CLA	C3D-C4D-ND	4.06	116.81	110.24
11	bA	823	CLA	C3C-C4C-NC	4.06	115.12	110.57
11	bA	839	CLA	C3B-C2B-C1B	-4.06	102.26	107.16
11	cB	837	CLA	C3D-C4D-ND	4.06	116.80	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bB	823	CLA	C4A-NA-C1A	-4.06	104.88	106.71
11	cA	803	CLA	CMD-C2D-C1D	4.06	131.86	124.71
11	bA	804	CLA	C3D-C4D-ND	4.06	116.80	110.24
11	bA	831	CLA	C3C-C4C-NC	4.06	115.12	110.57
11	cA	839	CLA	C3B-C2B-C1B	-4.06	102.27	107.16
11	aA	838	CLA	C3C-C4C-NC	4.06	115.12	110.57
11	aA	814	CLA	C4A-NA-C1A	-4.05	104.88	106.71
11	cB	817	CLA	C3D-C4D-ND	4.05	116.80	110.24
11	cA	823	CLA	C3C-C4C-NC	4.05	115.12	110.57
11	aB	820	CLA	C3D-C4D-ND	4.05	116.80	110.24
11	cA	841	CLA	C3D-C4D-ND	4.05	116.80	110.24
11	aB	810	CLA	C3B-C2B-C1B	-4.05	102.27	107.16
11	aA	804	CLA	C3D-C4D-ND	4.05	116.79	110.24
11	aB	816	CLA	C3D-C4D-ND	4.05	116.79	110.24
11	bB	805	CLA	C3D-C4D-ND	4.05	116.79	110.24
11	aB	823	CLA	C4A-NA-C1A	-4.05	104.88	106.71
11	bB	807	CLA	C4A-NA-C1A	-4.05	104.88	106.71
11	bB	817	CLA	C3D-C4D-ND	4.05	116.79	110.24
12	cA	830	F6C	C1-C2-C3	-4.05	119.04	126.04
11	aB	839	CLA	C3D-C4D-ND	4.05	116.79	110.24
11	aA	820	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
11	aK	103	CLA	C3C-C4C-NC	4.05	115.11	110.57
11	cB	829	CLA	C3B-C2B-C1B	-4.05	102.28	107.16
12	aA	832	F6C	CHD-C4C-NC	4.05	128.54	124.26
11	cA	802	CLA	C3D-C4D-ND	4.04	116.78	110.24
11	bA	838	CLA	C3C-C4C-NC	4.04	115.11	110.57
11	cL	205	CLA	C3C-C4C-NC	4.04	115.11	110.57
11	aA	811	CLA	C3D-C4D-ND	4.04	116.78	110.24
11	bB	822	CLA	C2C-C1C-NC	4.04	113.76	109.97
11	aA	824	CLA	C3D-C4D-ND	4.04	116.78	110.24
11	cB	839	CLA	C3D-C4D-ND	4.04	116.78	110.24
11	aA	839	CLA	C3B-C2B-C1B	-4.04	102.28	107.16
11	aB	839	CLA	C1D-CHD-C4C	-4.04	117.34	126.06
11	bB	816	CLA	C4A-NA-C1A	-4.04	104.89	106.71
11	bB	826	CLA	C4A-NA-C1A	-4.04	104.89	106.71
11	aB	828	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
11	aB	822	CLA	C2C-C1C-NC	4.04	113.76	109.97
11	cA	820	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
11	bB	816	CLA	O2D-CGD-CBD	4.04	118.45	111.27
11	bB	839	CLA	C1D-CHD-C4C	-4.04	117.34	126.06
11	cB	823	CLA	C4A-NA-C1A	-4.04	104.89	106.71
11	bB	812	CLA	C3C-C4C-NC	4.04	115.10	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bB	810	CLA	C3B-C2B-C1B	-4.04	102.29	107.16
11	bB	827	CLA	C1D-CHD-C4C	-4.04	117.35	126.06
12	bB	824	F6C	C3D-C2D-C1D	-4.04	99.98	105.83
11	bA	802	CLA	C3D-C4D-ND	4.04	116.77	110.24
11	cA	811	CLA	C3D-C4D-ND	4.04	116.77	110.24
11	cB	827	CLA	C1D-CHD-C4C	-4.04	117.35	126.06
11	aB	816	CLA	O2D-CGD-CBD	4.04	118.44	111.27
11	cB	820	CLA	C3D-C4D-ND	4.04	116.77	110.24
11	bA	816	CLA	C3C-C4C-NC	4.04	115.10	110.57
11	bA	837	CLA	O2D-CGD-CBD	4.04	118.44	111.27
11	cB	805	CLA	C3D-C4D-ND	4.03	116.77	110.24
11	aB	826	CLA	C4A-NA-C1A	-4.03	104.89	106.71
11	cB	816	CLA	C4A-NA-C1A	-4.03	104.89	106.71
11	aB	829	CLA	C3B-C2B-C1B	-4.03	102.29	107.16
11	bB	811	CLA	O2D-CGD-CBD	4.03	118.44	111.27
11	bB	820	CLA	C3D-C4D-ND	4.03	116.76	110.24
11	cB	839	CLA	C1D-CHD-C4C	-4.03	117.36	126.06
11	bB	807	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
11	bB	829	CLA	C3B-C2B-C1B	-4.03	102.29	107.16
11	aB	817	CLA	C3D-C4D-ND	4.03	116.76	110.24
11	cB	808	CLA	CHD-C1D-ND	-4.03	120.75	124.45
11	cB	816	CLA	O2D-CGD-CBD	4.03	118.43	111.27
11	cK	103	CLA	C3C-C4C-NC	4.03	115.09	110.57
12	aB	824	F6C	C3D-C2D-C1D	-4.03	99.99	105.83
12	cA	832	F6C	CHD-C4C-NC	4.03	128.52	124.26
12	aA	830	F6C	C1-C2-C3	-4.03	119.07	126.04
11	cA	837	CLA	O2D-CGD-CBD	4.03	118.43	111.27
11	aB	808	CLA	CHD-C1D-ND	-4.03	120.75	124.45
11	bB	808	CLA	CHD-C1D-ND	-4.03	120.75	124.45
11	bA	824	CLA	C3D-C4D-ND	4.03	116.76	110.24
11	cB	822	CLA	C2C-C1C-NC	4.03	113.75	109.97
11	aA	833	CLA	C3D-C4D-ND	4.03	116.75	110.24
11	bA	811	CLA	C3D-C4D-ND	4.03	116.75	110.24
11	aB	837	CLA	C3C-C4C-NC	4.03	115.09	110.57
11	bA	841	CLA	C3C-C4C-NC	4.03	115.09	110.57
11	bB	830	CLA	C3C-C4C-NC	4.03	115.09	110.57
11	cA	834	CLA	C3C-C4C-NC	4.03	115.09	110.57
11	cB	830	CLA	C3C-C4C-NC	4.02	115.08	110.57
11	aA	834	CLA	C3C-C4C-NC	4.02	115.08	110.57
12	cB	824	F6C	C3D-C2D-C1D	-4.02	100.00	105.83
11	cA	804	CLA	C3D-C4D-ND	4.02	116.75	110.24
11	bA	835	CLA	C3D-C4D-ND	4.02	116.74	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cB	816	CLA	C3D-C4D-ND	4.02	116.74	110.24
11	aB	812	CLA	C3C-C4C-NC	4.02	115.08	110.57
11	cB	838	CLA	C3C-C4C-NC	4.02	115.08	110.57
12	bA	830	F6C	C1-C2-C3	-4.02	119.09	126.04
11	aB	811	CLA	O2D-CGD-CBD	4.02	118.41	111.27
11	cB	835	CLA	C3D-C4D-ND	4.02	116.74	110.24
11	bA	829	CLA	C3B-C4B-NB	4.02	114.24	110.52
11	cB	838	CLA	C4A-NA-C1A	-4.02	104.90	106.71
11	bL	205	CLA	C3C-C4C-NC	4.02	115.08	110.57
11	aA	837	CLA	O2D-CGD-CBD	4.02	118.40	111.27
11	cB	806	CLA	C3C-C4C-NC	4.02	115.07	110.57
11	cB	813	CLA	C1D-CHD-C4C	-4.01	117.40	126.06
11	aB	834	CLA	C3C-C4C-NC	4.01	115.07	110.57
11	aA	829	CLA	C3B-C4B-NB	4.01	114.24	110.52
12	aA	844	F6C	CHD-C4C-NC	4.01	128.51	124.26
11	aB	827	CLA	C1D-CHD-C4C	-4.01	117.40	126.06
11	cB	807	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
11	cA	833	CLA	C3D-C4D-ND	4.01	116.72	110.24
12	bA	827	F6C	CHA-C1A-C2A	-4.01	118.97	129.84
11	cA	824	CLA	C3D-C4D-ND	4.01	116.72	110.24
11	aA	841	CLA	C3C-C4C-NC	4.01	115.07	110.57
11	bB	834	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
12	cA	844	F6C	CHD-C4C-NC	4.01	128.50	124.26
11	aB	830	CLA	C3C-C4C-NC	4.01	115.06	110.57
11	aB	813	CLA	C1D-CHD-C4C	-4.01	117.41	126.06
12	aA	827	F6C	CHA-C1A-C2A	-4.01	118.97	129.84
11	cB	812	CLA	C3C-C4C-NC	4.01	115.06	110.57
11	aB	834	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
11	bA	816	CLA	C3D-C4D-ND	4.00	116.72	110.24
11	bB	816	CLA	C3D-C4D-ND	4.00	116.72	110.24
11	cB	811	CLA	O2D-CGD-CBD	4.00	118.38	111.27
11	cB	826	CLA	C4A-NA-C1A	-4.00	104.91	106.71
11	cA	835	CLA	C3D-C4D-ND	4.00	116.71	110.24
11	bA	841	CLA	O2D-CGD-CBD	4.00	118.38	111.27
11	cA	841	CLA	C3C-C4C-NC	4.00	115.06	110.57
11	aA	841	CLA	O2D-CGD-CBD	4.00	118.38	111.27
11	cB	835	CLA	C4A-NA-C1A	-4.00	104.91	106.71
11	bB	807	CLA	C3D-C4D-ND	4.00	116.71	110.24
10	aA	801	CL0	C3D-C4D-ND	4.00	116.71	110.24
10	cA	801	CL0	C3D-C4D-ND	4.00	116.71	110.24
11	cB	834	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
11	bA	822	CLA	C4A-NA-C1A	-4.00	104.91	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	832	F6C	CHD-C4C-NC	4.00	128.49	124.26
12	bA	844	F6C	CHD-C4C-NC	4.00	128.49	124.26
11	cA	829	CLA	C3B-C4B-NB	4.00	114.22	110.52
11	bA	833	CLA	C3D-C4D-ND	4.00	116.70	110.24
12	cA	827	F6C	CHA-C1A-C2A	-4.00	119.01	129.84
11	bB	837	CLA	C3C-C4C-NC	3.99	115.05	110.57
11	aA	838	CLA	C1C-C2C-C3C	-3.99	102.76	106.96
11	cA	841	CLA	O2D-CGD-CBD	3.99	118.36	111.27
11	cA	816	CLA	C3D-C4D-ND	3.99	116.69	110.24
11	aB	806	CLA	C3C-C4C-NC	3.99	115.05	110.57
12	cA	830	F6C	CHD-C4C-NC	3.99	128.48	124.26
11	bA	834	CLA	C3D-C4D-ND	3.98	116.68	110.24
11	cA	834	CLA	C3D-C4D-ND	3.98	116.68	110.24
11	bB	838	CLA	C3C-C4C-NC	3.98	115.04	110.57
11	aB	804	CLA	C3D-C4D-ND	3.98	116.68	110.24
11	aB	810	CLA	C3D-C4D-ND	3.98	116.68	110.24
11	aB	835	CLA	C3D-C4D-ND	3.98	116.68	110.24
11	bA	818	CLA	C3D-C4D-ND	3.98	116.68	110.24
11	aA	808	CLA	C3C-C4C-NC	3.98	115.04	110.57
11	bB	835	CLA	C3D-C4D-ND	3.98	116.68	110.24
11	cB	832	CLA	C3D-C4D-ND	3.98	116.68	110.24
11	bB	818	CLA	O2D-CGD-CBD	3.98	118.34	111.27
11	aA	835	CLA	C3D-C4D-ND	3.98	116.67	110.24
11	bB	806	CLA	C3C-C4C-NC	3.98	115.03	110.57
11	aB	807	CLA	C3D-C4D-ND	3.98	116.67	110.24
11	bA	813	CLA	C3B-C2B-C1B	-3.98	102.36	107.16
11	aL	205	CLA	C3C-C4C-NC	3.98	115.03	110.57
10	bA	801	CL0	C3D-C4D-ND	3.97	116.67	110.24
11	aA	816	CLA	C3D-C4D-ND	3.97	116.67	110.24
11	bK	101	CLA	C4A-NA-C1A	-3.97	104.92	106.71
11	cB	804	CLA	C3D-C4D-ND	3.97	116.67	110.24
11	aA	834	CLA	C3D-C4D-ND	3.97	116.67	110.24
11	aA	835	CLA	C3C-C4C-NC	3.97	115.03	110.57
11	bB	832	CLA	C3D-C4D-ND	3.97	116.66	110.24
11	cA	831	CLA	C1D-CHD-C4C	-3.97	117.49	126.06
11	cA	806	CLA	CHB-C4A-NA	3.97	130.00	124.51
11	aB	829	CLA	CHC-C1C-C2C	-3.97	115.70	126.73
11	cB	807	CLA	C3D-C4D-ND	3.97	116.66	110.24
11	cB	804	CLA	C1D-CHD-C4C	-3.97	117.50	126.06
11	bB	813	CLA	C1D-CHD-C4C	-3.97	117.50	126.06
11	aA	822	CLA	C4A-NA-C1A	-3.97	104.92	106.71
11	aA	822	CLA	C3D-C4D-ND	3.97	116.65	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bB	804	CLA	C3D-C4D-ND	3.97	116.65	110.24
11	cB	813	CLA	C3D-C4D-ND	3.97	116.65	110.24
11	cA	822	CLA	C3D-C4D-ND	3.97	116.65	110.24
12	aA	830	F6C	CHD-C4C-NC	3.96	128.45	124.26
11	bA	806	CLA	CHB-C4A-NA	3.96	129.99	124.51
11	bA	819	CLA	C1D-CHD-C4C	-3.96	117.51	126.06
11	cB	834	CLA	C3C-C4C-NC	3.96	115.02	110.57
11	cA	813	CLA	C3D-C4D-ND	3.96	116.65	110.24
11	cA	818	CLA	C3D-C4D-ND	3.96	116.65	110.24
11	cB	810	CLA	C3D-C4D-ND	3.96	116.65	110.24
11	bB	804	CLA	C1D-CHD-C4C	-3.96	117.51	126.06
12	bL	202	F6C	C1A-C2A-C3A	-3.96	102.80	106.97
11	aB	818	CLA	O2D-CGD-CBD	3.96	118.31	111.27
11	cA	803	CLA	C3D-C4D-ND	3.96	116.64	110.24
11	aA	831	CLA	C1D-CHD-C4C	-3.96	117.51	126.06
11	bB	810	CLA	C3D-C4D-ND	3.96	116.64	110.24
11	bA	822	CLA	C3D-C4D-ND	3.96	116.64	110.24
12	bA	830	F6C	CHD-C4C-NC	3.96	128.45	124.26
11	cB	829	CLA	CHC-C1C-C2C	-3.96	115.74	126.73
11	bB	805	CLA	C3B-C4B-NB	3.96	114.19	110.52
11	cB	835	CLA	C1C-C2C-C3C	-3.96	102.80	106.96
11	aB	838	CLA	C4A-NA-C1A	-3.95	104.93	106.71
11	aB	832	CLA	C3D-C4D-ND	3.95	116.64	110.24
11	aA	804	CLA	C3C-C4C-NC	3.95	115.00	110.57
11	cB	818	CLA	O2D-CGD-CBD	3.95	118.29	111.27
11	aL	204	CLA	C1C-C2C-C3C	-3.95	102.80	106.96
11	cA	835	CLA	C3C-C4C-NC	3.95	115.00	110.57
12	cL	202	F6C	C1A-C2A-C3A	-3.95	102.81	106.97
11	aA	803	CLA	C3D-C4D-ND	3.95	116.63	110.24
11	aA	818	CLA	C3D-C4D-ND	3.95	116.63	110.24
11	bA	810	CLA	C3D-C4D-ND	3.95	116.63	110.24
11	bB	829	CLA	CHC-C1C-C2C	-3.95	115.76	126.73
11	aB	804	CLA	C1D-CHD-C4C	-3.95	117.54	126.06
11	bB	835	CLA	C1C-C2C-C3C	-3.95	102.81	106.96
11	bA	831	CLA	C1D-CHD-C4C	-3.95	117.54	126.06
11	bA	803	CLA	C3D-C4D-ND	3.95	116.62	110.24
11	cA	842	CLA	C3D-C4D-ND	3.95	116.62	110.24
11	bL	204	CLA	C1C-C2C-C3C	-3.95	102.81	106.96
11	bA	817	CLA	C3C-C4C-NC	3.95	115.00	110.57
11	aB	816	CLA	C4A-NA-C1A	-3.95	104.93	106.71
11	bA	808	CLA	C3C-C4C-NC	3.95	115.00	110.57
11	aA	819	CLA	C1D-CHD-C4C	-3.94	117.55	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aB	813	CLA	C3D-C4D-ND	3.94	116.62	110.24
11	aA	806	CLA	CHB-C4A-NA	3.94	129.97	124.51
11	aA	836	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
11	cA	804	CLA	C3C-C4C-NC	3.94	114.99	110.57
11	aA	813	CLA	C3B-C2B-C1B	-3.94	102.40	107.16
11	cA	838	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
11	bA	835	CLA	C3C-C4C-NC	3.94	114.99	110.57
12	cA	832	F6C	CHD-C4C-C3C	-3.94	116.75	125.36
11	cA	817	CLA	C3C-C4C-NC	3.94	114.99	110.57
11	bA	838	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
11	cA	810	CLA	C3D-C4D-ND	3.94	116.61	110.24
11	aA	813	CLA	C3D-C4D-ND	3.94	116.61	110.24
11	aA	810	CLA	C3D-C4D-ND	3.94	116.61	110.24
12	aL	202	F6C	C1A-C2A-C3A	-3.94	102.82	106.97
11	aB	827	CLA	C3D-C4D-ND	3.94	116.61	110.24
11	aA	842	CLA	C3C-C4C-NC	3.94	114.99	110.57
11	bB	835	CLA	C3C-C4C-NC	3.94	114.99	110.57
11	bB	813	CLA	C3D-C4D-ND	3.94	116.61	110.24
11	bB	827	CLA	C3D-C4D-ND	3.94	116.61	110.24
11	cA	808	CLA	C3C-C4C-NC	3.94	114.98	110.57
11	cA	819	CLA	C1D-CHD-C4C	-3.94	117.57	126.06
12	bA	832	F6C	CHD-C4C-C3C	-3.94	116.76	125.36
11	cB	835	CLA	C3C-C4C-NC	3.93	114.98	110.57
11	aB	814	CLA	C3D-C4D-ND	3.93	116.60	110.24
11	cA	813	CLA	C3B-C2B-C1B	-3.93	102.41	107.16
11	bB	803	CLA	CAA-C2A-C3A	-3.93	102.01	112.78
12	aA	832	F6C	CHD-C4C-C3C	-3.93	116.77	125.36
11	aB	803	CLA	CAA-C2A-C3A	-3.93	102.01	112.78
11	aK	101	CLA	C4A-NA-C1A	-3.93	104.94	106.71
11	aB	835	CLA	C1C-C2C-C3C	-3.93	102.82	106.96
11	cB	809	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
11	cL	204	CLA	C1C-C2C-C3C	-3.93	102.82	106.96
11	cB	815	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
11	bB	821	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
12	cA	826	F6C	CAC-C3C-C2C	3.93	133.16	126.86
11	bK	103	CLA	C3D-C4D-ND	3.93	116.59	110.24
11	aB	805	CLA	C3B-C4B-NB	3.93	114.16	110.52
11	cB	806	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
11	bB	834	CLA	C3C-C4C-NC	3.93	114.98	110.57
11	bA	836	CLA	C3D-C4D-ND	3.93	116.59	110.24
11	cL	204	CLA	C3D-C4D-ND	3.93	116.59	110.24
11	cK	101	CLA	C4A-NA-C1A	-3.93	104.94	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bB	809	CLA	C3B-C2B-C1B	-3.93	102.42	107.16
11	aB	810	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
11	cB	803	CLA	CAA-C2A-C3A	-3.93	102.02	112.78
11	bA	812	CLA	C3D-C4D-ND	3.93	116.59	110.24
11	bL	204	CLA	C3D-C4D-ND	3.93	116.59	110.24
11	bB	806	CLA	C1D-CHD-C4C	-3.93	117.59	126.06
11	cA	803	CLA	O2D-CGD-CBD	3.93	118.25	111.27
11	aB	835	CLA	C3C-C4C-NC	3.93	114.97	110.57
11	aA	817	CLA	C3C-C4C-NC	3.93	114.97	110.57
11	cA	840	CLA	C3C-C4C-NC	3.93	114.97	110.57
11	aK	103	CLA	C3D-C4D-ND	3.92	116.58	110.24
11	aA	824	CLA	C1D-CHD-C4C	-3.92	117.59	126.06
11	bA	804	CLA	C3C-C4C-NC	3.92	114.97	110.57
11	aA	834	CLA	C1C-C2C-C3C	-3.92	102.83	106.96
11	aB	813	CLA	C3B-C4B-NB	3.92	114.15	110.52
11	cA	842	CLA	C3C-C4C-NC	3.92	114.97	110.57
11	bA	818	CLA	C1D-CHD-C4C	-3.92	117.60	126.06
11	aB	811	CLA	C3D-C4D-ND	3.92	116.58	110.24
11	aB	814	CLA	C1D-CHD-C4C	-3.92	117.60	126.06
11	aB	815	CLA	C1D-CHD-C4C	-3.92	117.61	126.06
11	bB	815	CLA	C1D-CHD-C4C	-3.92	117.61	126.06
11	bA	833	CLA	C1C-C2C-C3C	-3.92	102.84	106.96
12	bA	826	F6C	CAC-C3C-C2C	3.92	133.14	126.86
11	aB	806	CLA	C1D-CHD-C4C	-3.92	117.61	126.06
11	bB	811	CLA	C3D-C4D-ND	3.92	116.57	110.24
11	cB	840	CLA	C3D-C4D-ND	3.92	116.57	110.24
11	bA	803	CLA	O2D-CGD-CBD	3.92	118.23	111.27
11	cA	843	CLA	C1D-CHD-C4C	-3.92	117.61	126.06
11	aB	801	CLA	O2D-CGD-CBD	3.92	118.23	111.27
11	aA	818	CLA	C1D-CHD-C4C	-3.92	117.61	126.06
11	bB	809	CLA	C1D-CHD-C4C	-3.92	117.61	126.06
11	cB	811	CLA	C3D-C4D-ND	3.91	116.57	110.24
11	bA	843	CLA	C1D-CHD-C4C	-3.91	117.61	126.06
11	cA	810	CLA	C1D-CHD-C4C	-3.91	117.61	126.06
11	aA	803	CLA	O2D-CGD-CBD	3.91	118.22	111.27
11	cA	812	CLA	C3D-C4D-ND	3.91	116.57	110.24
11	bA	822	CLA	C3B-C2B-C1B	-3.91	102.44	107.16
11	bA	810	CLA	C1D-CHD-C4C	-3.91	117.62	126.06
11	bA	831	CLA	C1C-C2C-C3C	-3.91	102.84	106.96
11	cB	827	CLA	C3D-C4D-ND	3.91	116.57	110.24
11	bB	801	CLA	O2D-CGD-CBD	3.91	118.22	111.27
11	aA	812	CLA	C3D-C4D-ND	3.91	116.57	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bA	813	CLA	C3D-C4D-ND	3.91	116.56	110.24
11	cA	809	CLA	C3C-C4C-NC	3.91	114.96	110.57
11	cA	836	CLA	C1C-C2C-C3C	-3.91	102.84	106.96
11	cA	802	CLA	C1D-CHD-C4C	-3.91	117.62	126.06
11	aA	822	CLA	C3B-C2B-C1B	-3.91	102.44	107.16
11	cA	822	CLA	C3B-C2B-C1B	-3.91	102.44	107.16
11	bB	801	CLA	CAA-C2A-C3A	-3.91	102.07	112.78
11	cB	805	CLA	C3B-C4B-NB	3.91	114.14	110.52
11	aA	842	CLA	C3D-C4D-ND	3.91	116.56	110.24
11	bA	836	CLA	C1D-CHD-C4C	-3.91	117.62	126.06
11	cB	810	CLA	C1C-C2C-C3C	-3.91	102.85	106.96
11	bB	840	CLA	C3D-C4D-ND	3.91	116.56	110.24
11	aA	843	CLA	C1D-CHD-C4C	-3.91	117.63	126.06
12	aA	826	F6C	CAC-C3C-C2C	3.91	133.12	126.86
10	bA	801	CL0	C1C-C2C-C3C	-3.90	102.85	106.96
11	cB	821	CLA	C1C-C2C-C3C	-3.90	102.85	106.96
11	bA	824	CLA	C1D-CHD-C4C	-3.90	117.63	126.06
11	bB	840	CLA	C3C-C4C-NC	3.90	114.95	110.57
11	cA	824	CLA	C1D-CHD-C4C	-3.90	117.64	126.06
11	cA	836	CLA	C1D-CHD-C4C	-3.90	117.64	126.06
11	bB	838	CLA	C4A-NA-C1A	-3.90	104.95	106.71
11	cB	830	CLA	C4A-NA-C1A	-3.90	104.95	106.71
11	cB	814	CLA	C3D-C4D-ND	3.90	116.55	110.24
11	aA	831	CLA	C1C-C2C-C3C	-3.90	102.85	106.96
11	bA	815	CLA	C1D-CHD-C4C	-3.90	117.64	126.06
11	aB	801	CLA	CAA-C2A-C3A	-3.90	102.09	112.78
11	bB	831	CLA	C3C-C4C-NC	3.90	114.95	110.57
11	aA	805	CLA	C4A-NA-C1A	-3.90	104.95	106.71
11	cA	836	CLA	C3D-C4D-ND	3.90	116.55	110.24
11	aA	833	CLA	C1C-C2C-C3C	-3.90	102.86	106.96
11	cB	801	CLA	CAA-C2A-C3A	-3.90	102.10	112.78
11	aB	840	CLA	C3D-C4D-ND	3.90	116.55	110.24
11	aB	809	CLA	C3B-C2B-C1B	-3.90	102.45	107.16
11	aA	817	CLA	O2D-CGD-CBD	3.90	118.20	111.27
11	cA	818	CLA	C1D-CHD-C4C	-3.90	117.65	126.06
11	cB	827	CLA	O2D-CGD-CBD	3.90	118.20	111.27
11	bA	842	CLA	C3C-C4C-NC	3.90	114.94	110.57
11	aL	204	CLA	C3D-C4D-ND	3.90	116.54	110.24
11	bA	836	CLA	C1C-C2C-C3C	-3.90	102.86	106.96
11	aB	808	CLA	C3D-C2D-C1D	-3.90	100.51	105.83
11	bB	814	CLA	C3D-C4D-ND	3.90	116.54	110.24
11	bB	809	CLA	C4A-NA-C1A	-3.89	104.95	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cA	833	CLA	C4A-NA-C1A	-3.89	104.95	106.71
11	aA	836	CLA	C3D-C4D-ND	3.89	116.54	110.24
11	bA	842	CLA	C3D-C4D-ND	3.89	116.54	110.24
11	cB	808	CLA	C3D-C2D-C1D	-3.89	100.52	105.83
11	cB	814	CLA	C1D-CHD-C4C	-3.89	117.66	126.06
11	aB	808	CLA	C3D-C4D-ND	3.89	116.54	110.24
11	cB	840	CLA	C3C-C4C-NC	3.89	114.94	110.57
11	aB	809	CLA	C1D-CHD-C4C	-3.89	117.66	126.06
11	aB	821	CLA	C1C-C2C-C3C	-3.89	102.86	106.96
11	aA	810	CLA	C1D-CHD-C4C	-3.89	117.66	126.06
11	aA	836	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
11	bA	802	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
10	cA	801	CL0	C1C-C2C-C3C	-3.89	102.87	106.96
11	aA	840	CLA	C3C-C4C-NC	3.89	114.93	110.57
11	bB	814	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
11	cB	801	CLA	O2D-CGD-CBD	3.89	118.17	111.27
11	cB	810	CLA	C3C-C4C-NC	3.89	114.93	110.57
11	aA	833	CLA	C4A-NA-C1A	-3.89	104.96	106.71
11	cK	103	CLA	C3D-C4D-ND	3.89	116.52	110.24
11	bB	827	CLA	O2D-CGD-CBD	3.88	118.17	111.27
12	aL	202	F6C	CHD-C4C-C3C	-3.88	116.87	125.36
10	aA	801	CL0	C1C-C2C-C3C	-3.88	102.87	106.96
11	bA	834	CLA	C1C-C2C-C3C	-3.88	102.87	106.96
15	bA	847	BCR	C2-C1-C6	3.88	116.46	110.48
11	bB	803	CLA	C3C-C4C-NC	3.88	114.92	110.57
11	cA	807	CLA	C3D-C4D-ND	3.88	116.52	110.24
11	aB	827	CLA	O2D-CGD-CBD	3.88	118.17	111.27
12	bL	202	F6C	CHD-C4C-C3C	-3.88	116.88	125.36
11	bB	835	CLA	C4A-NA-C1A	-3.88	104.96	106.71
11	cB	831	CLA	C3D-C4D-ND	3.88	116.52	110.24
11	bB	810	CLA	C3C-C4C-NC	3.88	114.92	110.57
11	bB	808	CLA	C3D-C4D-ND	3.88	116.52	110.24
11	cB	819	CLA	C1D-CHD-C4C	-3.88	117.69	126.06
11	cB	809	CLA	C3B-C2B-C1B	-3.88	102.48	107.16
11	cB	803	CLA	C3C-C4C-NC	3.88	114.92	110.57
11	aB	801	CLA	C3D-C4D-ND	3.88	116.51	110.24
11	bB	822	CLA	C4C-C3C-C2C	-3.88	101.25	106.90
11	cB	823	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
12	cL	202	F6C	CHD-C4C-C3C	-3.88	116.89	125.36
11	cB	808	CLA	C3D-C4D-ND	3.88	116.51	110.24
11	aB	803	CLA	C3D-C4D-ND	3.87	116.51	110.24
11	aB	803	CLA	C3C-C4C-NC	3.87	114.92	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aB	840	CLA	C3C-C4C-NC	3.87	114.92	110.57
11	bB	819	CLA	C1D-CHD-C4C	-3.87	117.70	126.06
11	bA	809	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
11	aB	818	CLA	C3B-C2B-C1B	-3.87	102.49	107.16
11	aB	819	CLA	C1D-CHD-C4C	-3.87	117.70	126.06
11	cB	822	CLA	C4C-C3C-C2C	-3.87	101.26	106.90
11	aB	810	CLA	C3C-C4C-NC	3.87	114.91	110.57
11	aB	823	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
11	bA	823	CLA	C1D-CHD-C4C	-3.87	117.71	126.06
11	cA	815	CLA	C1D-CHD-C4C	-3.87	117.71	126.06
11	bA	840	CLA	C3C-C4C-NC	3.87	114.91	110.57
11	aA	802	CLA	C1D-CHD-C4C	-3.87	117.71	126.06
11	aA	812	CLA	O2D-CGD-CBD	3.87	118.14	111.27
15	cA	847	BCR	C2-C1-C6	3.87	116.44	110.48
11	bB	818	CLA	C1D-CHD-C4C	-3.87	117.72	126.06
11	bB	808	CLA	C3D-C2D-C1D	-3.87	100.56	105.83
11	aB	822	CLA	C4C-C3C-C2C	-3.87	101.26	106.90
11	cA	831	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
11	aA	815	CLA	C1D-CHD-C4C	-3.87	117.72	126.06
11	cA	815	CLA	C1C-C2C-C3C	-3.86	102.89	106.96
11	cA	809	CLA	C3D-C4D-ND	3.86	116.49	110.24
12	bA	844	F6C	CHD-C4C-C3C	-3.86	116.92	125.36
11	cA	811	CLA	C3C-C4C-NC	3.86	114.90	110.57
11	aA	817	CLA	C4A-NA-C1A	-3.86	104.97	106.71
11	bA	805	CLA	C4A-NA-C1A	-3.86	104.97	106.71
11	cA	834	CLA	C1C-C2C-C3C	-3.86	102.89	106.96
11	bB	815	CLA	C4A-NA-C1A	-3.86	104.97	106.71
15	aA	847	BCR	C2-C1-C6	3.86	116.42	110.48
11	cB	823	CLA	C1D-CHD-C4C	-3.86	117.73	126.06
11	aA	823	CLA	C1D-CHD-C4C	-3.86	117.73	126.06
11	bA	812	CLA	O2D-CGD-CBD	3.86	118.13	111.27
11	aB	821	CLA	C3D-C4D-ND	3.86	116.48	110.24
11	cB	803	CLA	C3D-C4D-ND	3.86	116.48	110.24
11	cA	822	CLA	C4A-NA-C1A	-3.86	104.97	106.71
11	bA	817	CLA	O2D-CGD-CBD	3.86	118.12	111.27
11	bB	836	CLA	C1D-CHD-C4C	-3.86	117.73	126.06
11	cA	833	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
11	bA	834	CLA	O2D-CGD-CBD	3.86	118.12	111.27
11	bB	831	CLA	C3D-C4D-ND	3.86	116.48	110.24
11	aA	809	CLA	C3C-C4C-NC	3.86	114.90	110.57
11	cB	818	CLA	C1D-CHD-C4C	-3.86	117.74	126.06
11	bA	807	CLA	C3D-C4D-ND	3.86	116.47	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bB	803	CLA	C3D-C4D-ND	3.86	116.47	110.24
12	cA	844	F6C	CHD-C4C-C3C	-3.85	116.94	125.36
11	bB	801	CLA	C3D-C4D-ND	3.85	116.47	110.24
11	aA	809	CLA	C3D-C4D-ND	3.85	116.47	110.24
11	bB	813	CLA	C3B-C4B-NB	3.85	114.09	110.52
11	bA	829	CLA	C3D-C4D-ND	3.85	116.47	110.24
11	aA	807	CLA	C3D-C4D-ND	3.85	116.47	110.24
11	aA	809	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
11	bB	823	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
11	cB	813	CLA	C3B-C4B-NB	3.85	114.09	110.52
12	bL	202	F6C	O2A-CGA-CBA	3.85	123.99	111.91
11	bB	810	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
11	cA	823	CLA	C1D-CHD-C4C	-3.85	117.75	126.06
11	aB	812	CLA	C3D-C4D-ND	3.85	116.47	110.24
11	cB	826	CLA	C1D-CHD-C4C	-3.85	117.75	126.06
11	bA	840	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
11	cA	840	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
11	cB	831	CLA	C3C-C4C-NC	3.85	114.89	110.57
11	bB	823	CLA	C1D-CHD-C4C	-3.85	117.76	126.06
11	aA	829	CLA	C3D-C4D-ND	3.85	116.46	110.24
11	aB	818	CLA	C1D-CHD-C4C	-3.85	117.76	126.06
11	cA	817	CLA	O2D-CGD-CBD	3.85	118.10	111.27
11	aA	836	CLA	C3B-C2B-C1B	-3.85	102.52	107.16
11	cA	834	CLA	O2D-CGD-CBD	3.85	118.10	111.27
11	bA	824	CLA	C4A-NA-C1A	-3.85	104.98	106.71
11	aA	811	CLA	C3C-C4C-NC	3.85	114.88	110.57
11	cB	801	CLA	C3D-C4D-ND	3.85	116.46	110.24
11	aA	838	CLA	C3D-C4D-ND	3.85	116.46	110.24
11	aA	834	CLA	O2D-CGD-CBD	3.84	118.10	111.27
11	bB	826	CLA	C1D-CHD-C4C	-3.84	117.76	126.06
11	cA	834	CLA	C1D-CHD-C4C	-3.84	117.76	126.06
11	aB	823	CLA	C1D-CHD-C4C	-3.84	117.77	126.06
11	aB	831	CLA	C3C-C4C-NC	3.84	114.88	110.57
11	cB	815	CLA	C4A-NA-C1A	-3.84	104.98	106.71
11	bA	809	CLA	C3C-C4C-NC	3.84	114.88	110.57
11	bB	812	CLA	C3D-C4D-ND	3.84	116.45	110.24
11	cB	821	CLA	C3D-C4D-ND	3.84	116.45	110.24
12	cL	202	F6C	O2A-CGA-CBA	3.84	123.96	111.91
11	aB	815	CLA	C4A-NA-C1A	-3.84	104.98	106.71
11	aB	835	CLA	C4A-NA-C1A	-3.84	104.98	106.71
12	aA	844	F6C	CHD-C4C-C3C	-3.84	116.97	125.36
11	cB	818	CLA	C3B-C2B-C1B	-3.84	102.53	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bA	811	CLA	C3C-C4C-NC	3.84	114.88	110.57
11	cB	836	CLA	C1D-CHD-C4C	-3.84	117.78	126.06
11	aB	836	CLA	C1D-CHD-C4C	-3.84	117.78	126.06
11	aA	815	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
11	bB	839	CLA	C3D-C2D-C1D	-3.84	100.59	105.83
11	aB	802	CLA	C3D-C4D-ND	3.84	116.45	110.24
11	bA	809	CLA	C3D-C4D-ND	3.84	116.45	110.24
11	bA	834	CLA	C1D-CHD-C4C	-3.84	117.78	126.06
11	bB	818	CLA	C3B-C2B-C1B	-3.84	102.53	107.16
11	aA	834	CLA	C1D-CHD-C4C	-3.84	117.78	126.06
11	cB	801	CLA	CMA-C3A-C4A	-3.84	101.47	111.77
11	aB	826	CLA	C1D-CHD-C4C	-3.83	117.79	126.06
11	cA	819	CLA	C3D-C4D-ND	3.83	116.44	110.24
11	cB	831	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
11	bA	836	CLA	C3B-C2B-C1B	-3.83	102.53	107.16
11	cA	812	CLA	O2D-CGD-CBD	3.83	118.08	111.27
12	bB	824	F6C	CHD-C4C-NC	3.83	128.31	124.26
11	bB	802	CLA	C1D-CHD-C4C	-3.83	117.79	126.06
11	aA	819	CLA	C3D-C4D-ND	3.83	116.44	110.24
12	aL	202	F6C	O2A-CGA-CBA	3.83	123.93	111.91
11	cA	822	CLA	O2D-CGD-CBD	3.83	118.07	111.27
11	bB	819	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
11	aA	839	CLA	C3C-C4C-NC	3.83	114.87	110.57
11	aA	822	CLA	O2D-CGD-CBD	3.83	118.07	111.27
11	aA	825	CLA	C3D-C4D-ND	3.83	116.43	110.24
11	bA	839	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
11	bA	805	CLA	C3D-C4D-ND	3.83	116.43	110.24
11	cB	812	CLA	C3D-C4D-ND	3.83	116.43	110.24
12	cB	824	F6C	CHD-C4C-NC	3.83	128.31	124.26
11	cB	802	CLA	C1D-CHD-C4C	-3.83	117.80	126.06
10	aA	801	CL0	O2D-CGD-CBD	3.83	118.07	111.27
11	aK	101	CLA	C3C-C4C-NC	3.83	114.86	110.57
11	cA	809	CLA	C1C-C2C-C3C	-3.83	102.94	106.96
11	bA	819	CLA	C3D-C4D-ND	3.82	116.42	110.24
11	aB	839	CLA	C3D-C2D-C1D	-3.82	100.61	105.83
11	cA	834	CLA	C4A-NA-C1A	-3.82	104.99	106.71
11	cA	836	CLA	C4A-NA-C1A	-3.82	104.99	106.71
11	cB	809	CLA	C4A-NA-C1A	-3.82	104.99	106.71
11	cA	838	CLA	C3D-C4D-ND	3.82	116.42	110.24
11	aA	817	CLA	C3D-C4D-ND	3.82	116.42	110.24
11	bA	825	CLA	C1D-CHD-C4C	-3.82	117.81	126.06
11	cA	836	CLA	C3B-C2B-C1B	-3.82	102.55	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bK	101	CLA	C3C-C4C-NC	3.82	114.86	110.57
11	bB	801	CLA	CMA-C3A-C4A	-3.82	101.50	111.77
12	aB	824	F6C	CHD-C4C-NC	3.82	128.30	124.26
11	bB	836	CLA	CAC-C3C-C4C	3.82	129.77	124.81
11	cA	829	CLA	C3D-C4D-ND	3.82	116.42	110.24
10	bA	801	CL0	O2D-CGD-CBD	3.82	118.06	111.27
11	cA	825	CLA	C3D-C4D-ND	3.82	116.42	110.24
11	aA	805	CLA	C3D-C4D-ND	3.82	116.42	110.24
11	bA	825	CLA	C3D-C4D-ND	3.82	116.42	110.24
11	cB	802	CLA	C3D-C4D-ND	3.82	116.42	110.24
11	aB	828	CLA	C3D-C4D-ND	3.82	116.42	110.24
11	aB	801	CLA	CMA-C3A-C4A	-3.82	101.51	111.77
11	aA	840	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
11	bB	831	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
11	bB	815	CLA	O2D-CGD-CBD	3.82	118.05	111.27
11	aB	802	CLA	C1D-CHD-C4C	-3.82	117.83	126.06
11	bB	838	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
11	bB	821	CLA	C3D-C4D-ND	3.82	116.41	110.24
11	aA	821	CLA	C1D-CHD-C4C	-3.81	117.83	126.06
11	bB	828	CLA	C1D-CHD-C4C	-3.81	117.83	126.06
11	bB	802	CLA	C3D-C4D-ND	3.81	116.41	110.24
11	aA	839	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
11	cK	101	CLA	C3C-C4C-NC	3.81	114.85	110.57
11	cA	817	CLA	C3B-C4B-NB	3.81	114.05	110.52
11	bA	839	CLA	C3C-C4C-NC	3.81	114.85	110.57
11	cA	839	CLA	C3C-C4C-NC	3.81	114.85	110.57
11	aB	831	CLA	C3D-C4D-ND	3.81	116.40	110.24
11	bA	817	CLA	C3D-C4D-ND	3.81	116.40	110.24
11	cA	821	CLA	C1D-CHD-C4C	-3.81	117.84	126.06
11	cA	825	CLA	C1D-CHD-C4C	-3.81	117.84	126.06
11	bA	817	CLA	C4A-NA-C1A	-3.81	104.99	106.71
11	cA	837	CLA	C1D-CHD-C4C	-3.81	117.84	126.06
11	aB	819	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
11	aK	103	CLA	C1D-CHD-C4C	-3.81	117.84	126.06
10	cA	801	CL0	O2D-CGD-CBD	3.81	118.04	111.27
11	aA	843	CLA	C3D-C4D-ND	3.81	116.40	110.24
11	bA	820	CLA	C3D-C4D-ND	3.81	116.40	110.24
11	cB	819	CLA	C3D-C4D-ND	3.81	116.40	110.24
11	aA	812	CLA	C1D-CHD-C4C	-3.81	117.84	126.06
11	bK	103	CLA	C1D-CHD-C4C	-3.81	117.84	126.06
11	bA	837	CLA	C1D-CHD-C4C	-3.81	117.84	126.06
11	cB	828	CLA	C1D-CHD-C4C	-3.81	117.84	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cB	839	CLA	C3D-C2D-C1D	-3.81	100.64	105.83
11	bA	815	CLA	C1C-C2C-C3C	-3.81	102.96	106.96
11	cA	821	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
11	aA	825	CLA	C1D-CHD-C4C	-3.80	117.86	126.06
11	bA	831	CLA	C3D-C4D-ND	3.80	116.39	110.24
11	aA	821	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
11	aA	815	CLA	C3C-C4C-NC	3.80	114.83	110.57
11	aB	825	CLA	C1D-CHD-C4C	-3.80	117.86	126.06
11	bA	838	CLA	C3D-C4D-ND	3.80	116.39	110.24
11	bB	819	CLA	C3D-C4D-ND	3.80	116.39	110.24
11	bA	813	CLA	C1D-CHD-C4C	-3.80	117.86	126.06
12	aA	844	F6C	CHA-C1A-C2A	-3.80	119.54	129.84
11	cA	821	CLA	C3D-C4D-ND	3.80	116.38	110.24
11	bB	828	CLA	C3D-C4D-ND	3.80	116.38	110.24
11	aB	806	CLA	C1C-C2C-C3C	-3.80	102.97	106.96
11	bA	821	CLA	C1C-C2C-C3C	-3.80	102.97	106.96
11	cB	838	CLA	C1C-C2C-C3C	-3.80	102.97	106.96
11	aB	819	CLA	C3D-C4D-ND	3.80	116.38	110.24
11	aA	842	CLA	C1C-C2C-C3C	-3.80	102.97	106.96
11	bA	822	CLA	O2D-CGD-CBD	3.80	118.01	111.27
11	aA	820	CLA	C3D-C4D-ND	3.80	116.38	110.24
11	cA	805	CLA	C4A-NA-C1A	-3.79	105.00	106.71
11	bB	806	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
11	aB	828	CLA	C1D-CHD-C4C	-3.79	117.87	126.06
11	bB	825	CLA	C1D-CHD-C4C	-3.79	117.87	126.06
11	cA	805	CLA	C3D-C4D-ND	3.79	116.38	110.24
11	aB	838	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
11	aA	813	CLA	C1D-CHD-C4C	-3.79	117.87	126.06
12	cL	202	F6C	CMA-C3A-C2A	-3.79	115.82	126.12
11	aA	821	CLA	C3D-C4D-ND	3.79	116.37	110.24
11	cK	103	CLA	C1D-CHD-C4C	-3.79	117.88	126.06
12	aL	202	F6C	CMA-C3A-C2A	-3.79	115.82	126.12
11	cA	812	CLA	C1D-CHD-C4C	-3.79	117.88	126.06
11	aB	813	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
11	bA	843	CLA	C3D-C4D-ND	3.79	116.37	110.24
11	bB	806	CLA	C3D-C4D-ND	3.79	116.37	110.24
11	cA	811	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
11	bA	814	CLA	C3C-C4C-NC	3.79	114.82	110.57
11	bB	811	CLA	C1D-CHD-C4C	-3.79	117.88	126.06
11	cB	806	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
11	bA	836	CLA	C4A-NA-C1A	-3.79	105.00	106.71
11	cB	828	CLA	C3D-C4D-ND	3.79	116.36	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	844	F6C	CHA-C1A-C2A	-3.79	119.57	129.84
11	cA	839	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
11	cA	843	CLA	C3D-C4D-ND	3.79	116.36	110.24
11	cB	806	CLA	C3D-C4D-ND	3.79	116.36	110.24
11	cB	825	CLA	C1D-CHD-C4C	-3.79	117.89	126.06
11	aA	811	CLA	C1C-C2C-C3C	-3.79	102.98	106.96
11	bA	821	CLA	C1D-CHD-C4C	-3.78	117.89	126.06
11	cL	206	CLA	C1D-CHD-C4C	-3.78	117.89	126.06
11	aA	831	CLA	C3D-C4D-ND	3.78	116.36	110.24
11	cB	840	CLA	C3B-C2B-C1B	-3.78	102.59	107.16
11	bA	815	CLA	C3C-C4C-NC	3.78	114.81	110.57
11	cA	822	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
11	cB	819	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
12	bL	202	F6C	CMA-C3A-C2A	-3.78	115.84	126.12
11	aB	836	CLA	CAC-C3C-C4C	3.78	129.72	124.81
11	bA	812	CLA	C1D-CHD-C4C	-3.78	117.90	126.06
11	aB	831	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
11	cB	836	CLA	CAC-C3C-C4C	3.78	129.72	124.81
11	cA	831	CLA	C3D-C4D-ND	3.78	116.36	110.24
11	bA	813	CLA	C4A-NA-C1A	-3.78	105.01	106.71
11	bA	842	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
11	cB	815	CLA	O2D-CGD-CBD	3.78	117.99	111.27
11	cA	820	CLA	C3D-C4D-ND	3.78	116.35	110.24
11	cB	833	CLA	CMA-C3A-C4A	-3.78	101.61	111.77
11	cB	813	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
11	aA	818	CLA	O2D-CGD-O1D	-3.78	116.45	123.84
15	bL	207	BCR	C3-C4-C5	-3.78	107.33	114.08
11	bA	818	CLA	O2D-CGD-O1D	-3.78	116.45	123.84
11	cB	805	CLA	C3C-C4C-NC	3.78	114.81	110.57
11	bB	833	CLA	CMA-C3A-C4A	-3.78	101.62	111.77
11	cA	818	CLA	O2D-CGD-O1D	-3.78	116.45	123.84
11	aA	837	CLA	C1D-CHD-C4C	-3.78	117.91	126.06
11	aL	206	CLA	C1D-CHD-C4C	-3.78	117.91	126.06
11	bB	830	CLA	C4A-NA-C1A	-3.78	105.01	106.71
15	aL	207	BCR	C3-C4-C5	-3.78	107.33	114.08
11	cA	813	CLA	C1D-CHD-C4C	-3.78	117.91	126.06
11	aA	822	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
11	aA	824	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
11	cA	817	CLA	C3D-C4D-ND	3.77	116.34	110.24
11	aB	833	CLA	CMA-C3A-C4A	-3.77	101.63	111.77
11	cA	814	CLA	C3C-C4C-NC	3.77	114.80	110.57
11	bA	821	CLA	C3D-C4D-ND	3.77	116.34	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aB	815	CLA	O2D-CGD-CBD	3.77	117.97	111.27
11	aA	839	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
11	bA	822	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
11	bA	824	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
11	bA	817	CLA	C3B-C4B-NB	3.77	114.01	110.52
12	bA	844	F6C	CHA-C1A-C2A	-3.77	119.61	129.84
11	aB	815	CLA	C3D-C4D-ND	3.77	116.33	110.24
11	bA	834	CLA	C4A-NA-C1A	-3.77	105.01	106.71
12	bB	824	F6C	CHD-C4C-C3C	-3.77	117.13	125.36
11	cA	824	CLA	C1C-C2C-C3C	-3.77	103.00	106.96
11	aA	838	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
11	cA	810	CLA	C1C-C2C-C3C	-3.77	103.00	106.96
11	aA	816	CLA	C4A-NA-C1A	-3.77	105.01	106.71
11	cA	815	CLA	C3C-C4C-NC	3.76	114.79	110.57
11	bA	804	CLA	C4A-NA-C1A	-3.76	105.01	106.71
11	aB	811	CLA	C1D-CHD-C4C	-3.76	117.94	126.06
11	bA	838	CLA	C1D-CHD-C4C	-3.76	117.94	126.06
11	aB	836	CLA	C3D-C4D-ND	3.76	116.32	110.24
11	bA	811	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
11	cA	842	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
11	aB	834	CLA	C3B-C2B-C1B	-3.76	102.62	107.16
11	bB	840	CLA	C3B-C2B-C1B	-3.76	102.62	107.16
11	bL	206	CLA	C1D-CHD-C4C	-3.76	117.94	126.06
15	cL	207	BCR	C3-C4-C5	-3.76	107.36	114.08
12	aB	824	F6C	CHD-C4C-C3C	-3.76	117.14	125.36
11	bB	805	CLA	C3C-C4C-NC	3.76	114.79	110.57
11	cB	811	CLA	C1D-CHD-C4C	-3.76	117.95	126.06
11	aB	806	CLA	C3D-C4D-ND	3.76	116.32	110.24
11	aA	814	CLA	C3C-C4C-NC	3.76	114.79	110.57
11	cB	840	CLA	C1D-CHD-C4C	-3.76	117.95	126.06
11	bA	822	CLA	C1D-CHD-C4C	-3.76	117.95	126.06
11	cA	807	CLA	C1D-CHD-C4C	-3.76	117.95	126.06
11	aB	834	CLA	C3D-C4D-ND	3.76	116.31	110.24
11	bA	839	CLA	C1D-CHD-C4C	-3.76	117.95	126.06
11	bB	840	CLA	C1D-CHD-C4C	-3.76	117.96	126.06
11	aB	803	CLA	C4C-C3C-C2C	-3.75	101.42	106.90
10	aA	801	CL0	C3B-C4B-NB	3.75	114.00	110.52
11	cB	803	CLA	C4C-C3C-C2C	-3.75	101.43	106.90
12	cB	824	F6C	CHD-C4C-C3C	-3.75	117.16	125.36
11	cB	815	CLA	C3D-C4D-ND	3.75	116.31	110.24
11	cA	838	CLA	C1D-CHD-C4C	-3.75	117.97	126.06
11	aB	840	CLA	C1D-CHD-C4C	-3.75	117.97	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aB	817	CLA	C4-C3-C5	3.75	121.58	115.27
11	aB	814	CLA	C3C-C4C-NC	3.75	114.78	110.57
11	aA	817	CLA	C3B-C4B-NB	3.75	113.99	110.52
11	bB	826	CLA	C3D-C4D-ND	3.75	116.30	110.24
11	aA	810	CLA	C1C-C2C-C3C	-3.75	103.01	106.96
11	aA	835	CLA	C1D-CHD-C4C	-3.75	117.97	126.06
11	bA	835	CLA	C1D-CHD-C4C	-3.75	117.97	126.06
11	bB	815	CLA	C3D-C4D-ND	3.75	116.30	110.24
11	aA	822	CLA	C1D-CHD-C4C	-3.75	117.97	126.06
11	bB	834	CLA	C3B-C2B-C1B	-3.75	102.64	107.16
11	cA	816	CLA	C1D-CHD-C4C	-3.75	117.97	126.06
11	aA	807	CLA	C3C-C4C-NC	3.75	114.77	110.57
12	aA	832	F6C	CHA-C1A-C2A	-3.75	119.68	129.84
11	bB	836	CLA	C3D-C4D-ND	3.75	116.30	110.24
11	cA	829	CLA	C1C-C2C-C3C	-3.75	103.02	106.96
11	aA	834	CLA	C4A-NA-C1A	-3.75	105.02	106.71
12	cA	830	F6C	C4C-CHD-C1D	-3.75	117.45	126.34
11	aB	831	CLA	C1D-CHD-C4C	-3.75	117.98	126.06
12	cA	832	F6C	CHA-C1A-C2A	-3.75	119.68	129.84
11	cA	835	CLA	C1D-CHD-C4C	-3.74	117.98	126.06
11	cA	839	CLA	C1D-CHD-C4C	-3.74	117.98	126.06
11	bA	823	CLA	C3D-C4D-ND	3.74	116.30	110.24
11	aA	820	CLA	C1D-CHD-C4C	-3.74	117.98	126.06
11	cB	817	CLA	C4-C3-C5	3.74	121.57	115.27
11	cA	828	CLA	C4C-C3C-C2C	-3.74	101.44	106.90
11	aA	816	CLA	C1D-CHD-C4C	-3.74	117.98	126.06
11	aA	823	CLA	C3D-C4D-ND	3.74	116.29	110.24
11	cA	807	CLA	C3C-C4C-NC	3.74	114.77	110.57
11	aA	808	CLA	C1C-C2C-C3C	-3.74	103.02	106.96
11	bB	834	CLA	C3D-C4D-ND	3.74	116.29	110.24
11	cB	834	CLA	C3D-C4D-ND	3.74	116.29	110.24
11	cA	817	CLA	C4A-NA-C1A	-3.74	105.02	106.71
11	bB	831	CLA	C1D-CHD-C4C	-3.74	117.99	126.06
12	aA	830	F6C	C4C-CHD-C1D	-3.74	117.47	126.34
11	cB	834	CLA	C3B-C2B-C1B	-3.74	102.65	107.16
12	bA	832	F6C	CHA-C1A-C2A	-3.74	119.70	129.84
11	bB	803	CLA	C4C-C3C-C2C	-3.74	101.45	106.90
11	bB	817	CLA	C4-C3-C5	3.74	121.56	115.27
11	cB	825	CLA	C3D-C4D-ND	3.74	116.29	110.24
11	cA	822	CLA	C1D-CHD-C4C	-3.74	117.99	126.06
11	cA	823	CLA	C3D-C4D-ND	3.74	116.28	110.24
11	cB	821	CLA	C1D-CHD-C4C	-3.74	118.00	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cB	831	CLA	C1D-CHD-C4C	-3.74	118.00	126.06
11	aA	813	CLA	C4A-NA-C1A	-3.74	105.03	106.71
11	aA	836	CLA	C4A-NA-C1A	-3.74	105.03	106.71
11	cA	813	CLA	C4A-NA-C1A	-3.74	105.03	106.71
11	cB	826	CLA	C3D-C4D-ND	3.74	116.28	110.24
11	bB	823	CLA	C3D-C4D-ND	3.73	116.28	110.24
11	aA	807	CLA	C1D-CHD-C4C	-3.73	118.00	126.06
11	bA	816	CLA	C1D-CHD-C4C	-3.73	118.00	126.06
11	bB	813	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
11	cA	812	CLA	C3C-C4C-NC	3.73	114.76	110.57
11	bB	821	CLA	C1D-CHD-C4C	-3.73	118.00	126.06
12	bB	824	F6C	CHA-C1A-C2A	-3.73	119.72	129.84
11	bA	829	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
10	cA	801	CL0	C3B-C4B-NB	3.73	113.98	110.52
11	aB	840	CLA	C3B-C2B-C1B	-3.73	102.66	107.16
11	cL	204	CLA	C1D-CHD-C4C	-3.73	118.01	126.06
11	cB	830	CLA	C3D-C4D-ND	3.73	116.27	110.24
11	cB	836	CLA	C3D-C4D-ND	3.73	116.27	110.24
11	aA	812	CLA	C3C-C4C-NC	3.73	114.75	110.57
11	bA	833	CLA	C3C-C4C-NC	3.73	114.75	110.57
12	aB	824	F6C	CHA-C1A-C2A	-3.73	119.72	129.84
11	bA	825	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
11	cB	810	CLA	C1D-CHD-C4C	-3.73	118.01	126.06
12	cB	824	F6C	CHA-C1A-C2A	-3.73	119.73	129.84
12	bA	830	F6C	C4C-CHD-C1D	-3.73	117.50	126.34
11	aB	810	CLA	C1D-CHD-C4C	-3.73	118.02	126.06
11	bB	822	CLA	CAC-C3C-C4C	3.73	129.65	124.81
11	aB	830	CLA	C3D-C4D-ND	3.73	116.27	110.24
11	bA	812	CLA	C3C-C4C-NC	3.73	114.75	110.57
11	cB	814	CLA	C3C-C4C-NC	3.73	114.75	110.57
11	bA	841	CLA	C1C-C2C-C3C	-3.73	103.04	106.96
11	cA	825	CLA	C1C-C2C-C3C	-3.73	103.04	106.96
11	cA	820	CLA	C1D-CHD-C4C	-3.73	118.02	126.06
11	cA	824	CLA	C4A-NA-C1A	-3.73	105.03	106.71
11	bA	807	CLA	C3C-C4C-NC	3.73	114.75	110.57
11	aB	832	CLA	C3C-C4C-NC	3.72	114.75	110.57
11	cA	804	CLA	C1C-C2C-C3C	-3.72	103.04	106.96
11	bA	833	CLA	C4A-NA-C1A	-3.72	105.03	106.71
11	aB	826	CLA	C3D-C4D-ND	3.72	116.26	110.24
11	aB	822	CLA	CAC-C3C-C4C	3.72	129.64	124.81
11	bA	807	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
11	bB	814	CLA	C3C-C4C-NC	3.72	114.75	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cA	841	CLA	C1C-C2C-C3C	-3.72	103.04	106.96
12	aA	830	F6C	CHA-C1A-C2A	-3.72	119.75	129.84
11	aB	821	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
11	cB	823	CLA	C3D-C4D-ND	3.72	116.26	110.24
11	aA	840	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
12	bA	830	F6C	CHA-C1A-C2A	-3.72	119.75	129.84
11	bA	804	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
11	bA	820	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
11	aA	825	CLA	C3C-C4C-NC	3.72	114.74	110.57
11	aA	833	CLA	C3C-C4C-NC	3.72	114.74	110.57
11	cB	805	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
11	aB	809	CLA	C4A-NA-C1A	-3.72	105.03	106.71
11	cA	804	CLA	C4A-NA-C1A	-3.72	105.03	106.71
11	aL	204	CLA	C3B-C4B-NB	3.72	113.97	110.52
11	cB	822	CLA	CAC-C3C-C4C	3.72	129.63	124.81
11	bL	204	CLA	C1D-CHD-C4C	-3.72	118.04	126.06
11	aA	829	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
11	aA	828	CLA	C3D-C4D-ND	3.72	116.25	110.24
11	bA	840	CLA	C1D-CHD-C4C	-3.72	118.04	126.06
11	cA	837	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
11	aB	825	CLA	C3D-C4D-ND	3.72	116.25	110.24
11	cA	817	CLA	C1D-CHD-C4C	-3.72	118.04	126.06
11	bA	808	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
11	cA	833	CLA	C3C-C4C-NC	3.72	114.74	110.57
11	aB	805	CLA	C1D-CHD-C4C	-3.72	118.04	126.06
11	bA	824	CLA	C4-C3-C5	3.71	120.23	115.98
11	bA	810	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
11	aL	204	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
11	bB	805	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
11	bA	828	CLA	C4C-C3C-C2C	-3.71	101.48	106.90
11	aB	823	CLA	C3D-C4D-ND	3.71	116.25	110.24
11	aA	828	CLA	C4C-C3C-C2C	-3.71	101.49	106.90
11	bB	832	CLA	C3C-C4C-NC	3.71	114.73	110.57
11	cA	840	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
11	aA	824	CLA	C4-C3-C5	3.71	120.23	115.98
11	aA	817	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
11	cA	842	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
11	bA	828	CLA	C3D-C4D-ND	3.71	116.24	110.24
11	bA	817	CLA	C1D-CHD-C4C	-3.71	118.06	126.06
11	aB	827	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
11	cA	808	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
12	cA	830	F6C	CHA-C1A-C2A	-3.71	119.78	129.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bA	804	CLA	C1D-CHD-C4C	-3.71	118.06	126.06
11	bB	810	CLA	C1D-CHD-C4C	-3.71	118.06	126.06
11	cK	101	CLA	C1D-CHD-C4C	-3.71	118.06	126.06
11	cB	829	CLA	C1D-CHD-C4C	-3.71	118.06	126.06
11	cA	804	CLA	C1D-CHD-C4C	-3.71	118.06	126.06
11	bB	829	CLA	C1D-CHD-C4C	-3.71	118.06	126.06
11	aB	805	CLA	C3C-C4C-NC	3.70	114.73	110.57
11	bB	830	CLA	C3D-C4D-ND	3.70	116.23	110.24
11	cL	205	CLA	C1D-CHD-C4C	-3.70	118.07	126.06
11	aA	824	CLA	C4A-NA-C1A	-3.70	105.04	106.71
11	bA	842	CLA	C1D-CHD-C4C	-3.70	118.07	126.06
11	bB	825	CLA	C3D-C4D-ND	3.70	116.22	110.24
11	bA	831	CLA	C3B-C2B-C1B	-3.70	102.69	107.16
11	aA	842	CLA	C1D-CHD-C4C	-3.70	118.08	126.06
11	cA	828	CLA	C3D-C4D-ND	3.70	116.22	110.24
11	cB	829	CLA	C3D-C4D-ND	3.70	116.22	110.24
11	cA	835	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
11	cB	827	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
12	cA	830	F6C	C3D-C2D-C1D	-3.70	100.47	105.83
11	bB	829	CLA	C3D-C4D-ND	3.70	116.22	110.24
11	aL	205	CLA	C1D-CHD-C4C	-3.70	118.08	126.06
11	bK	101	CLA	C1D-CHD-C4C	-3.70	118.08	126.06
11	aB	829	CLA	C1D-CHD-C4C	-3.70	118.09	126.06
11	aK	101	CLA	C1C-C2C-C3C	-3.69	103.07	106.96
11	aB	811	CLA	C4A-NA-C1A	-3.69	105.05	106.71
11	aA	804	CLA	C1C-C2C-C3C	-3.69	103.07	106.96
11	cB	816	CLA	C3C-C4C-NC	3.69	114.71	110.57
11	bL	205	CLA	C1D-CHD-C4C	-3.69	118.09	126.06
11	aA	837	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
11	bB	827	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
11	cA	824	CLA	C4-C3-C5	3.69	120.20	115.98
11	bA	816	CLA	C4A-NA-C1A	-3.69	105.05	106.71
11	bB	817	CLA	C1D-CHD-C4C	-3.69	118.10	126.06
11	cA	825	CLA	C3C-C4C-NC	3.69	114.71	110.57
11	bB	830	CLA	C1D-CHD-C4C	-3.69	118.10	126.06
11	aB	817	CLA	C1D-CHD-C4C	-3.69	118.11	126.06
11	aA	809	CLA	C4A-NA-C1A	-3.69	105.05	106.71
12	aA	830	F6C	C3D-C2D-C1D	-3.68	100.50	105.83
11	cB	832	CLA	C3C-C4C-NC	3.68	114.70	110.57
12	bA	832	F6C	OMB-CMB-C2B	-3.68	117.36	125.69
11	bL	204	CLA	C3B-C4B-NB	3.68	113.93	110.52
11	cB	817	CLA	C3C-C4C-NC	3.68	114.70	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aK	101	CLA	C1D-CHD-C4C	-3.68	118.12	126.06
11	cB	817	CLA	C1D-CHD-C4C	-3.68	118.12	126.06
11	aA	841	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
11	aB	829	CLA	C3D-C4D-ND	3.68	116.19	110.24
11	aB	835	CLA	C1D-CHD-C4C	-3.68	118.12	126.06
11	bK	101	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
11	aA	804	CLA	C1D-CHD-C4C	-3.68	118.12	126.06
11	cB	835	CLA	C1D-CHD-C4C	-3.68	118.12	126.06
11	bA	825	CLA	C3C-C4C-NC	3.68	114.70	110.57
11	bA	835	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
11	aA	835	CLA	C1C-C2C-C3C	-3.67	103.09	106.96
11	aB	830	CLA	C1D-CHD-C4C	-3.67	118.13	126.06
11	cA	831	CLA	C3B-C2B-C1B	-3.67	102.73	107.16
11	bA	837	CLA	C1C-C2C-C3C	-3.67	103.09	106.96
11	bA	814	CLA	C1D-CHD-C4C	-3.67	118.14	126.06
11	bB	814	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
11	aA	831	CLA	C3B-C2B-C1B	-3.67	102.73	107.16
11	bB	805	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
11	cB	830	CLA	C1D-CHD-C4C	-3.67	118.14	126.06
10	cA	801	CL0	C1D-CHD-C4C	-3.67	118.14	126.06
11	bB	817	CLA	C3C-C4C-NC	3.67	114.68	110.57
11	bB	835	CLA	C1D-CHD-C4C	-3.67	118.15	126.06
11	aB	817	CLA	C3C-C4C-NC	3.67	114.68	110.57
11	cK	101	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
11	aA	829	CLA	C1D-CHD-C4C	-3.67	118.15	126.06
12	cA	832	F6C	OMB-CMB-C2B	-3.66	117.40	125.69
11	cA	813	CLA	C1C-C2C-C3C	-3.66	103.10	106.96
12	aA	832	F6C	OMB-CMB-C2B	-3.66	117.40	125.69
11	aB	812	CLA	C1D-CHD-C4C	-3.66	118.16	126.06
11	bB	812	CLA	C1D-CHD-C4C	-3.66	118.16	126.06
11	cB	837	CLA	C1D-CHD-C4C	-3.66	118.16	126.06
11	cA	814	CLA	C1D-CHD-C4C	-3.66	118.16	126.06
11	aA	811	CLA	C1D-CHD-C4C	-3.66	118.16	126.06
11	aA	833	CLA	C1D-CHD-C4C	-3.66	118.16	126.06
11	aB	805	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
11	bB	816	CLA	C3C-C4C-NC	3.66	114.68	110.57
11	cA	829	CLA	C1D-CHD-C4C	-3.66	118.16	126.06
10	bA	801	CL0	C3B-C4B-NB	3.66	113.91	110.52
11	cB	838	CLA	C1D-CHD-C4C	-3.66	118.16	126.06
11	aA	804	CLA	C4A-NA-C1A	-3.66	105.06	106.71
10	aA	801	CL0	C1D-CHD-C4C	-3.66	118.17	126.06
11	bA	829	CLA	C1D-CHD-C4C	-3.66	118.17	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bB	837	CLA	C1D-CHD-C4C	-3.66	118.17	126.06
12	bA	830	F6C	C3D-C2D-C1D	-3.66	100.54	105.83
11	aB	838	CLA	C1D-CHD-C4C	-3.66	118.17	126.06
11	cA	816	CLA	C4A-NA-C1A	-3.65	105.06	106.71
11	bB	830	CLA	C1C-C2C-C3C	-3.65	103.11	106.96
11	bA	815	CLA	C3D-C4D-ND	3.65	116.15	110.24
11	aA	825	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
11	bA	833	CLA	C1D-CHD-C4C	-3.65	118.18	126.06
11	bA	809	CLA	C1D-CHD-C4C	-3.65	118.18	126.06
11	cB	812	CLA	C1D-CHD-C4C	-3.65	118.18	126.06
11	cB	830	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
11	aA	809	CLA	C1D-CHD-C4C	-3.65	118.18	126.06
11	bB	818	CLA	C4A-NA-C1A	-3.65	105.06	106.71
11	bA	813	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
11	cL	204	CLA	C3B-C4B-NB	3.65	113.90	110.52
11	aB	816	CLA	C3C-C4C-NC	3.65	114.66	110.57
11	aB	803	CLA	C3B-C4B-NB	3.65	113.90	110.52
10	bA	801	CL0	C1D-CHD-C4C	-3.65	118.19	126.06
11	cB	820	CLA	C3C-C4C-NC	3.65	114.66	110.57
11	cA	809	CLA	C1D-CHD-C4C	-3.64	118.20	126.06
11	cB	833	CLA	C1C-C2C-C3C	-3.64	103.12	106.96
11	aB	837	CLA	C1D-CHD-C4C	-3.64	118.20	126.06
11	bB	838	CLA	C1D-CHD-C4C	-3.64	118.20	126.06
11	cA	829	CLA	C1-C2-C3	-3.64	119.74	126.04
11	bB	827	CLA	C4-C3-C5	3.64	121.40	115.27
11	cB	803	CLA	C3B-C4B-NB	3.64	113.89	110.52
11	aB	820	CLA	C3C-C4C-NC	3.64	114.65	110.57
11	cB	828	CLA	C3C-C4C-NC	3.64	114.65	110.57
11	aB	827	CLA	C3D-C2D-C1D	-3.64	100.86	105.83
11	bB	827	CLA	C3D-C2D-C1D	-3.64	100.86	105.83
11	bB	820	CLA	C1D-CHD-C4C	-3.64	118.20	126.06
11	aA	815	CLA	C3D-C4D-ND	3.64	116.13	110.24
11	aA	813	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
11	aB	830	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
11	bA	835	CLA	C4A-NA-C1A	-3.64	105.07	106.71
11	cB	827	CLA	C4-C3-C5	3.64	121.39	115.27
11	cB	820	CLA	C1D-CHD-C4C	-3.64	118.21	126.06
11	aB	830	CLA	C4A-NA-C1A	-3.64	105.07	106.71
11	cB	827	CLA	C3D-C2D-C1D	-3.64	100.87	105.83
11	cB	805	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
11	aA	814	CLA	C1D-CHD-C4C	-3.64	118.22	126.06
11	bA	811	CLA	C1D-CHD-C4C	-3.64	118.22	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bA	842	CLA	O2D-CGD-CBD	3.63	117.73	111.27
11	cA	833	CLA	C1D-CHD-C4C	-3.63	118.22	126.06
11	cB	807	CLA	C1D-CHD-C4C	-3.63	118.22	126.06
11	cA	825	CLA	CAC-C3C-C4C	3.63	129.53	124.81
11	aB	833	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
11	bL	205	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
11	cB	814	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
11	aB	814	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
11	aA	829	CLA	C1-C2-C3	-3.63	119.76	126.04
11	cA	835	CLA	C4A-NA-C1A	-3.63	105.07	106.71
11	aA	805	CLA	C1D-CHD-C4C	-3.63	118.22	126.06
11	cA	811	CLA	C1D-CHD-C4C	-3.63	118.22	126.06
11	aB	807	CLA	C1D-CHD-C4C	-3.63	118.22	126.06
11	bB	832	CLA	C1D-CHD-C4C	-3.63	118.23	126.06
11	cA	842	CLA	O2D-CGD-CBD	3.63	117.71	111.27
15	aB	848	BCR	C3-C4-C5	-3.63	107.60	114.08
11	aB	832	CLA	C1D-CHD-C4C	-3.62	118.24	126.06
11	cL	205	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
11	cA	815	CLA	C3D-C4D-ND	3.62	116.10	110.24
11	aB	827	CLA	C4-C3-C5	3.62	121.37	115.27
11	cB	833	CLA	C3C-C4C-NC	3.62	114.63	110.57
11	bB	828	CLA	C3C-C4C-NC	3.62	114.63	110.57
11	aA	825	CLA	CAC-C3C-C4C	3.62	129.51	124.81
11	aA	842	CLA	O2D-CGD-CBD	3.62	117.70	111.27
11	bB	807	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
11	aB	820	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
11	bB	833	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
11	aB	828	CLA	C3D-C2D-C1D	-3.62	100.89	105.83
11	bB	803	CLA	C3B-C4B-NB	3.62	113.87	110.52
12	cA	826	F6C	C4C-CHD-C1D	-3.62	117.76	126.34
11	cB	832	CLA	C1D-CHD-C4C	-3.62	118.26	126.06
11	bA	825	CLA	CAC-C3C-C4C	3.62	129.50	124.81
11	aB	833	CLA	C3C-C4C-NC	3.61	114.62	110.57
11	aB	828	CLA	C3C-C4C-NC	3.61	114.62	110.57
11	cA	809	CLA	C4A-NA-C1A	-3.61	105.08	106.71
11	cL	206	CLA	C4A-NA-C1A	-3.61	105.08	106.71
15	cB	848	BCR	C3-C4-C5	-3.61	107.63	114.08
11	aL	205	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
11	cB	811	CLA	C4A-NA-C1A	-3.61	105.08	106.71
11	bA	824	CLA	C3C-C4C-NC	3.61	114.62	110.57
11	bA	820	CLA	C3B-C4B-NB	3.61	113.86	110.52
11	bB	811	CLA	C4A-NA-C1A	-3.61	105.08	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bA	829	CLA	C1-C2-C3	-3.61	119.80	126.04
11	aA	820	CLA	C3B-C4B-NB	3.61	113.86	110.52
11	bA	805	CLA	C1D-CHD-C4C	-3.61	118.28	126.06
11	bB	834	CLA	C1D-CHD-C4C	-3.61	118.28	126.06
11	aB	811	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
15	bB	848	BCR	C3-C4-C5	-3.60	107.64	114.08
11	cB	811	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
12	aA	826	F6C	C4C-CHD-C1D	-3.60	117.80	126.34
11	cB	828	CLA	C3D-C2D-C1D	-3.60	100.92	105.83
12	aA	827	F6C	C1-C2-C3	-3.60	119.82	126.04
11	cB	834	CLA	C1D-CHD-C4C	-3.60	118.30	126.06
11	bB	802	CLA	C3B-C4B-NB	3.59	113.85	110.52
11	bB	833	CLA	C3C-C4C-NC	3.59	114.60	110.57
11	cA	805	CLA	C1D-CHD-C4C	-3.59	118.31	126.06
12	bA	826	F6C	C4C-CHD-C1D	-3.59	117.82	126.34
11	bB	820	CLA	C3C-C4C-NC	3.59	114.60	110.57
11	bB	828	CLA	C3D-C2D-C1D	-3.59	100.93	105.83
11	cA	824	CLA	C3C-C4C-NC	3.59	114.60	110.57
12	bA	827	F6C	C1-C2-C3	-3.59	119.84	126.04
11	aB	834	CLA	C1D-CHD-C4C	-3.59	118.32	126.06
11	aB	818	CLA	C4A-NA-C1A	-3.59	105.09	106.71
11	aB	803	CLA	CHC-C1C-C2C	-3.59	116.77	126.73
11	bB	834	CLA	C3B-C4B-NB	3.58	113.84	110.52
11	aA	835	CLA	C4A-NA-C1A	-3.58	105.09	106.71
12	cA	827	F6C	C1-C2-C3	-3.58	119.85	126.04
11	bB	828	CLA	C3B-C2B-C1B	-3.58	102.84	107.16
11	bL	206	CLA	C4A-NA-C1A	-3.58	105.10	106.71
11	cB	828	CLA	C3B-C2B-C1B	-3.58	102.84	107.16
11	cB	833	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
11	aB	832	CLA	C1C-C2C-C3C	-3.58	103.20	106.96
11	aL	206	CLA	C1C-C2C-C3C	-3.58	103.20	106.96
11	bA	809	CLA	C4A-NA-C1A	-3.58	105.10	106.71
11	aB	802	CLA	O2D-CGD-O1D	-3.58	116.85	123.84
11	aB	810	CLA	C3B-C4B-NB	3.58	113.83	110.52
11	aB	833	CLA	C1D-CHD-C4C	-3.57	118.35	126.06
11	bL	205	CLA	C4A-NA-C1A	-3.57	105.10	106.71
11	bB	823	CLA	C3B-C4B-NB	3.57	113.83	110.52
11	bB	802	CLA	O2D-CGD-O1D	-3.57	116.85	123.84
11	cB	802	CLA	O2D-CGD-O1D	-3.57	116.85	123.84
11	cB	818	CLA	C4A-NA-C1A	-3.57	105.10	106.71
11	aA	824	CLA	C3C-C4C-NC	3.57	114.58	110.57
11	bB	821	CLA	C4A-NA-C1A	-3.57	105.10	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bB	811	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
11	aA	841	CLA	C1D-CHD-C4C	-3.57	118.36	126.06
11	cB	803	CLA	CHC-C1C-C2C	-3.57	116.82	126.73
11	cB	802	CLA	C3B-C4B-NB	3.57	113.83	110.52
11	bB	836	CLA	C4C-C3C-C2C	-3.57	101.70	106.90
11	bA	841	CLA	C1D-CHD-C4C	-3.57	118.36	126.06
11	cA	838	CLA	C3B-C4B-NB	3.57	113.82	110.52
12	cA	827	F6C	C4C-CHD-C1D	-3.57	117.88	126.34
11	bB	803	CLA	CHC-C1C-C2C	-3.56	116.83	126.73
11	bA	828	CLA	C3B-C4B-NB	3.56	113.82	110.52
11	bB	810	CLA	C3B-C4B-NB	3.56	113.82	110.52
11	cA	820	CLA	C3B-C4B-NB	3.56	113.82	110.52
11	bB	808	CLA	CAA-C2A-C3A	-3.56	103.02	112.78
11	aB	802	CLA	C3B-C4B-NB	3.56	113.82	110.52
11	bB	833	CLA	C1D-CHD-C4C	-3.56	118.38	126.06
11	cL	206	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
11	bB	834	CLA	C4A-NA-C1A	-3.56	105.11	106.71
11	bL	206	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
11	aA	828	CLA	C3B-C4B-NB	3.55	113.81	110.52
11	aB	808	CLA	CAA-C2A-C3A	-3.55	103.05	112.78
11	cB	808	CLA	CAA-C2A-C3A	-3.55	103.06	112.78
11	aA	806	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
11	cB	834	CLA	C3B-C4B-NB	3.55	113.81	110.52
11	cA	841	CLA	C1D-CHD-C4C	-3.55	118.40	126.06
12	bA	827	F6C	C4C-CHD-C1D	-3.55	117.92	126.34
11	bB	827	CLA	CMD-C2D-C1D	3.55	130.97	124.71
12	aA	827	F6C	C4C-CHD-C1D	-3.55	117.93	126.34
11	bB	828	CLA	CHC-C1C-C2C	-3.55	116.88	126.73
11	aA	837	CLA	C4A-NA-C1A	-3.55	105.11	106.71
11	aB	836	CLA	C4C-C3C-C2C	-3.54	101.73	106.90
11	cB	809	CLA	C3B-C4B-NB	3.54	113.80	110.52
11	cB	810	CLA	C3B-C4B-NB	3.54	113.80	110.52
11	cB	801	CLA	C3B-C4B-NB	3.54	113.80	110.52
11	aB	828	CLA	CHC-C1C-C2C	-3.54	116.89	126.73
11	cK	103	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
12	bB	824	F6C	C1C-C2C-C3C	-3.54	102.69	106.83
11	cB	828	CLA	CHC-C1C-C2C	-3.54	116.91	126.73
11	aB	825	CLA	C1C-C2C-C3C	-3.54	103.24	106.96
11	aB	828	CLA	C3B-C2B-C1B	-3.54	102.89	107.16
15	aB	848	BCR	C15-C16-C17	-3.53	116.23	123.47
15	cB	848	BCR	C15-C16-C17	-3.53	116.24	123.47
11	cB	823	CLA	C3B-C4B-NB	3.53	113.79	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cB	828	CLA	CAC-C3C-C4C	3.53	129.39	124.81
11	bB	809	CLA	C3B-C4B-NB	3.53	113.79	110.52
15	aI	101	BCR	C2-C1-C6	3.53	115.91	110.48
11	aB	834	CLA	C3B-C4B-NB	3.53	113.79	110.52
11	cB	836	CLA	C4C-C3C-C2C	-3.53	101.76	106.90
11	aA	838	CLA	C3B-C4B-NB	3.53	113.79	110.52
11	bA	838	CLA	C3B-C4B-NB	3.53	113.79	110.52
11	cA	828	CLA	C3B-C4B-NB	3.52	113.78	110.52
11	cB	832	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
11	aA	806	CLA	C1D-CHD-C4C	-3.52	118.46	126.06
11	cA	806	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
11	bA	806	CLA	C1C-C2C-C3C	-3.52	103.26	106.96
11	cA	806	CLA	C1D-CHD-C4C	-3.52	118.47	126.06
11	bK	103	CLA	C1C-C2C-C3C	-3.52	103.26	106.96
11	aL	205	CLA	C4A-NA-C1A	-3.52	105.12	106.71
11	cB	808	CLA	C3B-C4B-NB	3.52	113.78	110.52
11	bA	837	CLA	C4A-NA-C1A	-3.51	105.13	106.71
11	bB	808	CLA	C3B-C4B-NB	3.51	113.77	110.52
11	bA	814	CLA	C1-C2-C3	-3.51	119.97	126.04
11	cA	820	CLA	C3C-C4C-NC	3.51	114.51	110.57
11	bA	806	CLA	C1D-CHD-C4C	-3.51	118.48	126.06
11	aB	809	CLA	C3B-C4B-NB	3.51	113.77	110.52
11	bA	811	CLA	CAA-C2A-C3A	-3.51	103.17	112.78
15	bB	848	BCR	C15-C16-C17	-3.51	116.28	123.47
11	aB	833	CLA	C4A-NA-C1A	-3.51	105.13	106.71
12	aB	824	F6C	C1C-C2C-C3C	-3.51	102.73	106.83
11	aA	808	CLA	C1D-CHD-C4C	-3.51	118.49	126.06
11	aB	828	CLA	CAC-C3C-C4C	3.51	129.36	124.81
11	aB	817	CLA	C4A-NA-C1A	-3.51	105.13	106.71
11	aL	204	CLA	C4A-NA-C1A	-3.51	105.13	106.71
11	aB	816	CLA	C1C-C2C-C3C	-3.51	103.27	106.96
11	bB	832	CLA	C1C-C2C-C3C	-3.51	103.27	106.96
15	cI	103	BCR	C2-C1-C6	3.51	115.88	110.48
12	cA	844	F6C	C4C-CHD-C1D	-3.50	118.03	126.34
12	bA	844	F6C	C4C-CHD-C1D	-3.50	118.03	126.34
11	aK	103	CLA	C1C-C2C-C3C	-3.50	103.27	106.96
11	bB	816	CLA	C1C-C2C-C3C	-3.50	103.27	106.96
15	bI	101	BCR	C2-C1-C6	3.50	115.87	110.48
11	aA	803	CLA	CHB-C4A-NA	3.50	129.36	124.51
11	cA	811	CLA	CAA-C2A-C3A	-3.50	103.19	112.78
11	cA	808	CLA	C1D-CHD-C4C	-3.50	118.50	126.06
13	cB	841	PQN	C11-C12-C13	-3.50	120.96	126.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aB	816	CLA	C1D-CHD-C4C	-3.50	118.51	126.06
11	aA	811	CLA	CAA-C2A-C3A	-3.50	103.20	112.78
11	aB	801	CLA	C3B-C4B-NB	3.50	113.76	110.52
11	cA	837	CLA	C4A-NA-C1A	-3.50	105.13	106.71
11	aB	827	CLA	CMD-C2D-C1D	3.50	130.88	124.71
11	bB	825	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
11	bB	814	CLA	C3B-C4B-NB	3.50	113.76	110.52
11	bB	814	CLA	C4A-NA-C1A	-3.50	105.13	106.71
11	aB	837	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
11	cB	816	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
11	cB	827	CLA	CMD-C2D-C1D	3.50	130.87	124.71
11	cB	809	CLA	C1C-C2C-C3C	-3.49	103.28	106.96
11	cA	803	CLA	C1D-CHD-C4C	-3.49	118.52	126.06
11	cB	825	CLA	C1C-C2C-C3C	-3.49	103.28	106.96
11	bB	801	CLA	C3B-C4B-NB	3.49	113.75	110.52
11	aB	814	CLA	C4A-NA-C1A	-3.49	105.14	106.71
11	bA	808	CLA	C4A-NA-C1A	-3.49	105.14	106.71
11	bA	818	CLA	CMC-C2C-C1C	3.49	130.36	125.04
11	cA	837	CLA	CAA-C2A-C3A	-3.49	103.22	112.78
11	cL	205	CLA	C4A-NA-C1A	-3.49	105.14	106.71
12	cB	824	F6C	C1C-C2C-C3C	-3.49	102.75	106.83
11	bA	808	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
12	bA	826	F6C	C1C-C2C-C3C	-3.49	102.75	106.83
11	aA	814	CLA	C1-C2-C3	-3.49	120.01	126.04
11	bA	803	CLA	C1D-CHD-C4C	-3.49	118.54	126.06
11	bB	833	CLA	C4A-NA-C1A	-3.49	105.14	106.71
11	aB	823	CLA	C3B-C4B-NB	3.48	113.75	110.52
12	aA	826	F6C	C1C-C2C-C3C	-3.48	102.75	106.83
11	cB	804	CLA	C1C-C2C-C3C	-3.48	103.29	106.96
12	aA	844	F6C	C4C-CHD-C1D	-3.48	118.08	126.34
11	cB	814	CLA	C3B-C4B-NB	3.48	113.75	110.52
11	aB	809	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
11	cB	837	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
11	aL	206	CLA	C4A-NA-C1A	-3.48	105.14	106.71
11	cA	834	CLA	CMB-C2B-C1B	3.48	130.67	125.37
11	cA	814	CLA	C1-C2-C3	-3.48	120.03	126.04
11	bB	828	CLA	CAC-C3C-C4C	3.48	129.32	124.81
11	aA	834	CLA	CMB-C2B-C1B	3.48	130.66	125.37
11	cB	812	CLA	C3B-C4B-NB	3.48	113.74	110.52
11	bA	820	CLA	C3C-C4C-NC	3.47	114.47	110.57
11	bB	837	CLA	C1C-C2C-C3C	-3.47	103.30	106.96
11	cA	803	CLA	CHB-C4A-NA	3.47	129.31	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aA	820	CLA	CBA-CAA-C2A	3.47	124.11	113.86
11	aB	834	CLA	C4A-NA-C1A	-3.47	105.14	106.71
11	cA	825	CLA	C4A-NA-C1A	-3.47	105.14	106.71
11	aA	820	CLA	CAC-C3C-C4C	3.47	129.31	124.81
11	bB	816	CLA	C1D-CHD-C4C	-3.47	118.57	126.06
12	bL	202	F6C	C1C-C2C-C3C	-3.47	102.77	106.83
11	aB	804	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
12	cA	832	F6C	C4C-CHD-C1D	-3.47	118.11	126.34
11	aA	837	CLA	CAA-C2A-C3A	-3.47	103.27	112.78
11	bB	809	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
11	bB	825	CLA	C4A-NA-C1A	-3.47	105.15	106.71
11	bA	837	CLA	CAA-C2A-C3A	-3.47	103.28	112.78
11	aB	821	CLA	C4A-NA-C1A	-3.47	105.15	106.71
13	aB	841	PQN	C11-C12-C13	-3.47	121.02	126.79
13	bB	841	PQN	C11-C12-C13	-3.46	121.02	126.79
11	bB	817	CLA	C3B-C4B-NB	3.46	113.73	110.52
11	aA	820	CLA	C3C-C4C-NC	3.46	114.46	110.57
11	aA	803	CLA	C1D-CHD-C4C	-3.46	118.59	126.06
11	bA	803	CLA	CHB-C4A-NA	3.46	129.30	124.51
11	cA	818	CLA	CMC-C2C-C1C	3.46	130.31	125.04
12	bA	832	F6C	C4C-CHD-C1D	-3.46	118.13	126.34
11	bA	820	CLA	CBA-CAA-C2A	3.46	124.08	113.86
12	aL	202	F6C	C1C-C2C-C3C	-3.46	102.78	106.83
11	cA	820	CLA	CBA-CAA-C2A	3.46	124.07	113.86
11	bA	820	CLA	CAC-C3C-C4C	3.46	129.29	124.81
11	aB	815	CLA	CMC-C2C-C1C	3.46	130.30	125.04
12	cL	202	F6C	C1C-C2C-C3C	-3.46	102.79	106.83
11	bB	826	CLA	C3B-C4B-NB	3.46	113.72	110.52
11	bB	817	CLA	C4A-NA-C1A	-3.45	105.15	106.71
12	aA	832	F6C	C4C-CHD-C1D	-3.45	118.15	126.34
11	cA	837	CLA	C3B-C4B-NB	3.45	113.72	110.52
11	cB	834	CLA	C4A-NA-C1A	-3.45	105.16	106.71
11	cB	840	CLA	C4A-NA-C1A	-3.45	105.16	106.71
11	aB	808	CLA	O2A-CGA-CBA	3.45	122.73	111.91
11	aB	808	CLA	C3B-C4B-NB	3.45	113.71	110.52
11	cB	815	CLA	CMC-C2C-C1C	3.45	130.29	125.04
11	bA	834	CLA	CMB-C2B-C1B	3.45	130.62	125.37
12	cA	826	F6C	C1C-C2C-C3C	-3.45	102.80	106.83
11	bB	808	CLA	O2A-CGA-CBA	3.45	122.72	111.91
11	cB	816	CLA	C1D-CHD-C4C	-3.45	118.62	126.06
11	cB	821	CLA	C4A-NA-C1A	-3.45	105.16	106.71
11	aB	814	CLA	C3B-C4B-NB	3.45	113.71	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bB	812	CLA	C3B-C4B-NB	3.44	113.71	110.52
11	cB	803	CLA	C1D-CHD-C4C	-3.44	118.63	126.06
11	bA	825	CLA	C4A-NA-C1A	-3.44	105.16	106.71
11	cB	814	CLA	C4A-NA-C1A	-3.44	105.16	106.71
11	bA	836	CLA	C3B-C4B-NB	3.44	113.71	110.52
12	bA	832	F6C	C1C-C2C-C3C	-3.44	102.81	106.83
11	aB	808	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
11	cB	808	CLA	O2A-CGA-CBA	3.44	122.70	111.91
11	cA	820	CLA	CAC-C3C-C4C	3.44	129.27	124.81
12	aL	202	F6C	C1-C2-C3	-3.44	120.10	126.04
11	aA	818	CLA	CMC-C2C-C1C	3.44	130.27	125.04
11	aB	835	CLA	C3B-C4B-NB	3.44	113.70	110.52
11	cB	826	CLA	C3B-C4B-NB	3.44	113.70	110.52
11	bA	829	CLA	C4A-NA-C1A	-3.43	105.16	106.71
11	aB	817	CLA	C3B-C4B-NB	3.43	113.70	110.52
12	bL	202	F6C	C1-C2-C3	-3.43	120.11	126.04
11	aB	818	CLA	C4C-C3C-C2C	-3.43	101.90	106.90
11	aB	803	CLA	C1D-CHD-C4C	-3.43	118.66	126.06
11	bB	815	CLA	CMC-C2C-C1C	3.43	130.26	125.04
11	cA	815	CLA	CHC-C1C-C2C	-3.43	117.21	126.73
11	bB	804	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
11	bA	808	CLA	C3B-C4B-NB	3.43	113.69	110.52
11	bA	837	CLA	C3B-C4B-NB	3.43	113.69	110.52
12	cL	202	F6C	C1-C2-C3	-3.43	120.11	126.04
11	aB	815	CLA	CAC-C3C-C4C	3.43	129.26	124.81
11	bB	803	CLA	C1D-CHD-C4C	-3.43	118.67	126.06
12	aL	202	F6C	CHD-C4C-NC	3.43	127.88	124.26
12	bB	824	F6C	CHC-C1C-C2C	-3.43	117.56	127.24
11	bB	835	CLA	C3B-C4B-NB	3.42	113.69	110.52
11	cA	803	CLA	C3B-C4B-NB	3.42	113.69	110.52
11	cB	815	CLA	CAC-C3C-C4C	3.42	129.25	124.81
12	bL	202	F6C	CHD-C4C-NC	3.42	127.88	124.26
11	cB	818	CLA	C4C-C3C-C2C	-3.42	101.91	106.90
11	cA	843	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
11	cB	835	CLA	C3B-C4B-NB	3.42	113.69	110.52
12	aB	824	F6C	CHC-C1C-C2C	-3.42	117.58	127.24
12	aA	844	F6C	CHD-C1D-ND	-3.42	119.02	124.20
12	aA	826	F6C	CHA-C1A-C2A	-3.42	120.57	129.84
11	bB	815	CLA	CAC-C3C-C4C	3.42	129.24	124.81
11	bB	818	CLA	C4C-C3C-C2C	-3.42	101.92	106.90
12	cA	832	F6C	C1C-C2C-C3C	-3.42	102.83	106.83
12	bA	826	F6C	CHA-C1A-C2A	-3.42	120.58	129.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	844	F6C	CHD-C1D-ND	-3.41	119.02	124.20
11	aA	837	CLA	C3B-C4B-NB	3.41	113.68	110.52
12	cA	826	F6C	CHA-C1A-C2A	-3.41	120.58	129.84
11	aB	840	CLA	C3B-C4B-NB	3.41	113.68	110.52
11	cA	836	CLA	C3B-C4B-NB	3.41	113.68	110.52
11	aB	832	CLA	C4A-NA-C1A	-3.41	105.17	106.71
11	aA	836	CLA	C3B-C4B-NB	3.41	113.68	110.52
15	bL	207	BCR	C2-C1-C6	3.41	115.73	110.48
11	aA	815	CLA	CHC-C1C-C2C	-3.41	117.27	126.73
11	bB	834	CLA	CHC-C1C-C2C	-3.41	117.27	126.73
12	cL	202	F6C	CHD-C4C-NC	3.41	127.86	124.26
11	bB	803	CLA	CHB-C4A-NA	3.41	129.22	124.51
11	cA	820	CLA	CHC-C1C-C2C	-3.40	117.27	126.73
11	cB	834	CLA	CHC-C1C-C2C	-3.40	117.27	126.73
11	bA	811	CLA	O2D-CGD-CBD	3.40	117.32	111.27
11	aB	834	CLA	CHC-C1C-C2C	-3.40	117.27	126.73
11	bA	815	CLA	CHC-C1C-C2C	-3.40	117.27	126.73
11	bA	820	CLA	CHC-C1C-C2C	-3.40	117.28	126.73
11	bA	843	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
12	aA	832	F6C	C1C-C2C-C3C	-3.40	102.85	106.83
11	bB	832	CLA	C4A-NA-C1A	-3.40	105.18	106.71
11	aB	812	CLA	C3B-C4B-NB	3.40	113.67	110.52
11	aB	826	CLA	C3B-C4B-NB	3.40	113.67	110.52
11	cA	808	CLA	C3B-C4B-NB	3.40	113.67	110.52
11	cA	833	CLA	C3B-C4B-NB	3.40	113.67	110.52
11	aA	843	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
11	cB	833	CLA	C4A-NA-C1A	-3.40	105.18	106.71
11	aA	820	CLA	CHC-C1C-C2C	-3.40	117.29	126.73
15	aB	848	BCR	C2-C1-C6	3.40	115.71	110.48
11	aA	829	CLA	C4A-NA-C1A	-3.40	105.18	106.71
11	aB	831	CLA	O2D-CGD-O1D	-3.40	117.19	123.84
11	cA	811	CLA	O2D-CGD-CBD	3.40	117.30	111.27
11	bB	808	CLA	C1C-C2C-C3C	-3.40	103.39	106.96
11	aB	803	CLA	CHB-C4A-NA	3.40	129.21	124.51
11	cB	831	CLA	O2D-CGD-O1D	-3.40	117.20	123.84
11	bA	803	CLA	C3B-C4B-NB	3.39	113.66	110.52
11	aA	811	CLA	O2D-CGD-CBD	3.39	117.30	111.27
15	cB	848	BCR	C2-C1-C6	3.39	115.70	110.48
11	aA	833	CLA	C3B-C4B-NB	3.39	113.66	110.52
11	cB	817	CLA	C3B-C4B-NB	3.39	113.66	110.52
15	aL	207	BCR	C2-C1-C6	3.39	115.70	110.48
12	cB	824	F6C	CHD-C1D-ND	-3.39	119.06	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bL	206	CLA	C1-C2-C3	-3.39	120.18	126.04
12	cB	824	F6C	CHC-C1C-C2C	-3.39	117.67	127.24
11	cA	807	CLA	C4A-NA-C1A	-3.39	105.18	106.71
12	bA	844	F6C	CHD-C1D-ND	-3.39	119.06	124.20
15	cL	207	BCR	C2-C1-C6	3.39	115.69	110.48
11	aB	809	CLA	CMA-C3A-C2A	-3.39	100.17	113.83
12	bA	844	F6C	C1-C2-C3	-3.38	120.19	126.04
11	bB	809	CLA	CMA-C3A-C2A	-3.38	100.17	113.83
11	bB	826	CLA	C4C-C3C-C2C	-3.38	101.97	106.90
11	aA	806	CLA	C3B-C4B-NB	3.38	113.65	110.52
11	cL	204	CLA	C4A-NA-C1A	-3.38	105.19	106.71
11	bB	826	CLA	CAC-C3C-C4C	3.38	129.20	124.81
11	aB	808	CLA	O2A-CGA-O1A	-3.38	115.06	123.59
11	cB	809	CLA	CMA-C3A-C2A	-3.38	100.19	113.83
11	aA	841	CLA	C4A-NA-C1A	-3.38	105.19	106.71
11	bA	842	CLA	CAA-C2A-C3A	-3.38	103.52	112.78
11	cA	806	CLA	C3B-C4B-NB	3.38	113.65	110.52
11	cL	206	CLA	C3B-C4B-NB	3.38	113.65	110.52
11	cB	804	CLA	C1-C2-C3	-3.38	121.28	126.75
11	cA	831	CLA	C4A-NA-C1A	-3.38	105.19	106.71
11	bA	831	CLA	CHC-C1C-C2C	-3.38	117.35	126.73
11	bA	806	CLA	C3B-C4B-NB	3.38	113.65	110.52
11	cB	808	CLA	O2A-CGA-O1A	-3.38	115.07	123.59
11	cB	839	CLA	C1C-C2C-C3C	-3.38	103.41	106.96
11	cB	826	CLA	C4C-C3C-C2C	-3.37	101.98	106.90
11	aB	826	CLA	CAC-C3C-C4C	3.37	129.19	124.81
11	aA	808	CLA	C3B-C4B-NB	3.37	113.64	110.52
11	bA	814	CLA	CAC-C3C-C4C	3.37	129.19	124.81
11	bB	831	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
11	bB	808	CLA	C4A-NA-C1A	-3.37	105.19	106.71
11	bL	204	CLA	C4A-NA-C1A	-3.37	105.19	106.71
11	aL	206	CLA	C1-C2-C3	-3.37	120.21	126.04
15	bB	848	BCR	C2-C1-C6	3.37	115.67	110.48
11	cA	808	CLA	C4A-NA-C1A	-3.37	105.19	106.71
11	aB	826	CLA	C4C-C3C-C2C	-3.37	101.99	106.90
11	bA	833	CLA	C3B-C4B-NB	3.37	113.64	110.52
11	aA	825	CLA	C4A-NA-C1A	-3.37	105.19	106.71
12	bB	824	F6C	C4C-CHD-C1D	-3.37	118.35	126.34
12	aB	824	F6C	CHD-C1D-ND	-3.37	119.10	124.20
11	bB	804	CLA	C1-C2-C3	-3.37	121.31	126.75
11	aA	814	CLA	CAC-C3C-C4C	3.37	129.18	124.81
11	aA	816	CLA	C1C-C2C-C3C	-3.37	103.42	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bA	807	CLA	C4A-NA-C1A	-3.37	105.19	106.71
11	aA	842	CLA	CAA-C2A-C3A	-3.36	103.56	112.78
11	cA	842	CLA	CAA-C2A-C3A	-3.36	103.57	112.78
11	aA	803	CLA	C3B-C4B-NB	3.36	113.63	110.52
12	aA	827	F6C	CHD-C1D-ND	-3.36	119.10	124.20
11	cB	840	CLA	C3B-C4B-NB	3.36	113.63	110.52
11	bB	840	CLA	C4A-NA-C1A	-3.36	105.19	106.71
12	aA	832	F6C	CHD-C1D-ND	-3.36	119.10	124.20
11	cA	831	CLA	CHC-C1C-C2C	-3.36	117.39	126.73
11	bB	808	CLA	O2A-CGA-O1A	-3.36	115.11	123.59
11	cB	808	CLA	C1C-C2C-C3C	-3.36	103.42	106.96
11	aA	831	CLA	CHC-C1C-C2C	-3.36	117.40	126.73
11	cA	817	CLA	CHC-C1C-C2C	-3.36	117.40	126.73
12	cA	844	F6C	C1-C2-C3	-3.36	120.24	126.04
11	cA	841	CLA	C4A-NA-C1A	-3.36	105.20	106.71
11	cA	812	CLA	C3B-C4B-NB	3.36	113.63	110.52
11	bA	816	CLA	C1C-C2C-C3C	-3.36	103.43	106.96
11	cB	832	CLA	C4A-NA-C1A	-3.35	105.20	106.71
11	bB	803	CLA	O2D-CGD-CBD	3.35	117.23	111.27
11	cA	816	CLA	C1C-C2C-C3C	-3.35	103.43	106.96
11	cB	803	CLA	CHB-C4A-NA	3.35	129.15	124.51
12	bA	830	F6C	C1C-C2C-C3C	-3.35	102.91	106.83
17	aA	853	LMT	O3'-C3'-C2'	-3.35	102.60	110.35
17	cA	853	LMT	O3'-C3'-C2'	-3.35	102.60	110.35
11	cB	817	CLA	C4A-NA-C1A	-3.35	105.20	106.71
11	cB	835	CLA	CAA-C2A-C3A	-3.35	103.61	112.78
12	aB	824	F6C	C4C-CHD-C1D	-3.35	118.39	126.34
11	bL	206	CLA	C3B-C4B-NB	3.35	113.62	110.52
12	aA	844	F6C	C1-C2-C3	-3.35	120.25	126.04
11	bA	817	CLA	CHC-C1C-C2C	-3.35	117.43	126.73
11	bA	812	CLA	C1C-C2C-C3C	-3.35	103.44	106.96
11	aB	803	CLA	O2D-CGD-CBD	3.35	117.22	111.27
11	aB	840	CLA	C4A-NA-C1A	-3.35	105.20	106.71
11	cB	803	CLA	O2D-CGD-CBD	3.35	117.21	111.27
10	cA	801	CL0	C4A-NA-C1A	-3.35	105.20	106.71
11	aB	808	CLA	C4A-NA-C1A	-3.35	105.20	106.71
11	aB	832	CLA	C3B-C4B-NB	3.34	113.62	110.52
11	cA	814	CLA	CAC-C3C-C4C	3.34	129.15	124.81
11	bA	814	CLA	C3B-C4B-NB	3.34	113.62	110.52
12	cB	824	F6C	C4C-CHD-C1D	-3.34	118.41	126.34
17	bA	853	LMT	O3'-C3'-C2'	-3.34	102.62	110.35
11	bB	835	CLA	CAA-C2A-C3A	-3.34	103.63	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	827	F6C	CHD-C1D-ND	-3.34	119.14	124.20
11	bB	802	CLA	C1C-C2C-C3C	-3.34	103.45	106.96
11	cK	103	CLA	C4A-NA-C1A	-3.34	105.20	106.71
11	aA	817	CLA	CHC-C1C-C2C	-3.34	117.46	126.73
12	cA	830	F6C	C1C-C2C-C3C	-3.34	102.93	106.83
11	cB	832	CLA	C3B-C4B-NB	3.34	113.61	110.52
11	cB	826	CLA	CAC-C3C-C4C	3.34	129.14	124.81
11	cL	206	CLA	C1-C2-C3	-3.34	120.27	126.04
11	aB	835	CLA	CAA-C2A-C3A	-3.34	103.64	112.78
12	bB	824	F6C	CHD-C1D-ND	-3.34	119.14	124.20
11	aA	824	CLA	C3B-C4B-NB	3.34	113.61	110.52
12	aA	830	F6C	C1C-C2C-C3C	-3.34	102.93	106.83
11	cA	812	CLA	C1C-C2C-C3C	-3.33	103.45	106.96
11	bA	805	CLA	C1C-C2C-C3C	-3.33	103.45	106.96
11	aB	804	CLA	C1-C2-C3	-3.33	121.36	126.75
11	cA	829	CLA	C4A-NA-C1A	-3.33	105.21	106.71
11	bA	834	CLA	C3B-C4B-NB	3.33	113.60	110.52
11	cA	821	CLA	CAC-C3C-C4C	3.33	129.13	124.81
11	aA	812	CLA	C1C-C2C-C3C	-3.33	103.46	106.96
17	cA	853	LMT	C1'-C2'-C3'	3.33	116.92	110.00
11	bB	825	CLA	C3B-C4B-NB	3.33	113.60	110.52
12	cA	827	F6C	CHD-C1D-ND	-3.33	119.16	124.20
17	bA	853	LMT	C1'-C2'-C3'	3.33	116.92	110.00
11	bA	803	CLA	C4C-C3C-C2C	-3.32	102.05	106.90
12	bA	832	F6C	CHD-C1D-ND	-3.32	119.16	124.20
11	cB	825	CLA	C4A-NA-C1A	-3.32	105.21	106.71
11	bA	814	CLA	C1C-C2C-C3C	-3.32	103.46	106.96
11	aA	811	CLA	C3B-C4B-NB	3.32	113.60	110.52
11	bB	826	CLA	C1C-C2C-C3C	-3.32	103.47	106.96
11	bB	832	CLA	C3B-C4B-NB	3.32	113.59	110.52
11	cA	834	CLA	C3B-C4B-NB	3.32	113.59	110.52
11	bA	812	CLA	C3B-C4B-NB	3.32	113.59	110.52
11	aB	802	CLA	C1C-C2C-C3C	-3.32	103.47	106.96
11	aA	814	CLA	C3B-C4B-NB	3.32	113.59	110.52
11	aA	807	CLA	C4A-NA-C1A	-3.32	105.22	106.71
11	bA	821	CLA	CAC-C3C-C4C	3.32	129.11	124.81
11	bA	811	CLA	C3B-C4B-NB	3.31	113.59	110.52
11	bB	840	CLA	C3B-C4B-NB	3.31	113.59	110.52
11	cA	814	CLA	C3B-C4B-NB	3.31	113.59	110.52
10	aA	801	CL0	C4A-NA-C1A	-3.31	105.22	106.71
11	aA	808	CLA	C4A-NA-C1A	-3.31	105.22	106.71
11	cB	808	CLA	C4A-NA-C1A	-3.31	105.22	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bB	814	CLA	CHC-C1C-C2C	-3.31	117.53	126.73
17	aA	853	LMT	C1'-C2'-C3'	3.31	116.89	110.00
11	aB	839	CLA	C1C-C2C-C3C	-3.31	103.47	106.96
12	bA	832	F6C	CHC-C1C-C2C	-3.31	117.89	127.24
11	aA	821	CLA	CAC-C3C-C4C	3.31	129.10	124.81
12	cA	832	F6C	CHC-C1C-C2C	-3.31	117.90	127.24
11	cA	823	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
11	aA	814	CLA	C1C-C2C-C3C	-3.31	103.48	106.96
11	cA	818	CLA	C3B-C4B-NB	3.30	113.58	110.52
11	aA	818	CLA	C3B-C4B-NB	3.30	113.58	110.52
11	aA	834	CLA	C3B-C4B-NB	3.30	113.58	110.52
11	aB	814	CLA	CHC-C1C-C2C	-3.30	117.56	126.73
11	aL	206	CLA	C3B-C4B-NB	3.30	113.58	110.52
11	aB	815	CLA	C1C-C2C-C3C	-3.30	103.49	106.96
11	bB	807	CLA	C3B-C4B-NB	3.30	113.58	110.52
11	cA	814	CLA	C1C-C2C-C3C	-3.30	103.49	106.96
11	cB	814	CLA	CHC-C1C-C2C	-3.30	117.57	126.73
12	cA	832	F6C	CHD-C1D-ND	-3.30	119.20	124.20
11	aB	826	CLA	C1C-C2C-C3C	-3.30	103.49	106.96
11	aA	809	CLA	C3B-C4B-NB	3.30	113.57	110.52
11	bA	823	CLA	C3B-C4B-NB	3.30	113.57	110.52
11	bB	825	CLA	C4C-C3C-C2C	-3.29	102.10	106.90
11	cA	811	CLA	C3B-C4B-NB	3.29	113.57	110.52
11	bK	103	CLA	C4A-NA-C1A	-3.29	105.23	106.71
11	cB	802	CLA	C4C-C3C-C2C	-3.29	102.10	106.90
11	aA	805	CLA	C1C-C2C-C3C	-3.29	103.50	106.96
11	aA	831	CLA	C4A-NA-C1A	-3.29	105.23	106.71
11	cA	805	CLA	C1C-C2C-C3C	-3.29	103.50	106.96
11	bA	823	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
11	aB	825	CLA	C4A-NA-C1A	-3.29	105.23	106.71
11	aB	807	CLA	C3B-C4B-NB	3.29	113.56	110.52
11	cB	815	CLA	C1C-C2C-C3C	-3.29	103.50	106.96
11	bA	824	CLA	C3B-C4B-NB	3.29	113.56	110.52
11	bA	841	CLA	C4A-NA-C1A	-3.29	105.23	106.71
11	bB	815	CLA	C1C-C2C-C3C	-3.28	103.50	106.96
11	bB	839	CLA	C1C-C2C-C3C	-3.28	103.50	106.96
11	bA	818	CLA	C3B-C4B-NB	3.28	113.56	110.52
11	cA	803	CLA	C4C-C3C-C2C	-3.28	102.11	106.90
12	aA	832	F6C	CHC-C1C-C2C	-3.28	117.98	127.24
11	bB	807	CLA	CAC-C3C-C4C	3.28	129.06	124.81
11	bA	831	CLA	C4A-NA-C1A	-3.28	105.23	106.71
11	cB	802	CLA	C1C-C2C-C3C	-3.28	103.51	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cB	825	CLA	C4C-C3C-C2C	-3.27	102.13	106.90
11	aB	807	CLA	CAC-C3C-C4C	3.27	129.06	124.81
11	cB	827	CLA	CHD-C1D-ND	-3.27	121.45	124.45
11	aK	103	CLA	C4A-NA-C1A	-3.27	105.24	106.71
11	cB	826	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
11	cA	824	CLA	C3B-C4B-NB	3.27	113.55	110.52
11	cB	807	CLA	C3B-C4B-NB	3.27	113.55	110.52
11	aA	825	CLA	C3B-C4B-NB	3.27	113.55	110.52
11	cB	817	CLA	CHC-C1C-C2C	-3.27	117.66	126.73
11	aA	812	CLA	C3B-C4B-NB	3.27	113.55	110.52
11	bA	807	CLA	C3B-C4B-NB	3.27	113.54	110.52
11	aB	812	CLA	C4C-C3C-C2C	-3.26	102.14	106.90
11	aA	823	CLA	C3B-C4B-NB	3.26	113.54	110.52
11	bB	812	CLA	C4C-C3C-C2C	-3.26	102.14	106.90
11	aB	825	CLA	C4C-C3C-C2C	-3.26	102.14	106.90
11	aB	817	CLA	CHC-C1C-C2C	-3.26	117.68	126.73
11	bB	805	CLA	CAC-C3C-C4C	3.26	129.04	124.81
11	bA	843	CLA	C4-C3-C5	3.26	119.71	115.98
11	aA	828	CLA	CHD-C4C-NC	3.26	129.34	124.20
11	bB	827	CLA	CHD-C1D-ND	-3.26	121.46	124.45
11	aA	803	CLA	C4C-C3C-C2C	-3.26	102.15	106.90
11	bB	839	CLA	C4C-C3C-C2C	-3.26	102.15	106.90
11	cB	825	CLA	C3B-C4B-NB	3.26	113.54	110.52
12	aA	844	F6C	C1C-C2C-C3C	-3.26	103.02	106.83
11	aB	825	CLA	C3B-C4B-NB	3.26	113.53	110.52
11	cA	807	CLA	C3B-C4B-NB	3.26	113.53	110.52
11	cA	823	CLA	C3B-C4B-NB	3.26	113.53	110.52
11	bA	824	CLA	CHC-C1C-C2C	-3.25	117.69	126.73
11	bB	817	CLA	CHC-C1C-C2C	-3.25	117.69	126.73
11	aA	812	CLA	CHC-C1C-C2C	-3.25	117.69	126.73
11	cA	834	CLA	CAA-C2A-C3A	-3.25	103.87	112.78
11	cB	840	CLA	CHC-C1C-C2C	-3.25	117.69	126.73
11	aB	827	CLA	CHD-C1D-ND	-3.25	121.47	124.45
11	bB	840	CLA	CHC-C1C-C2C	-3.25	117.70	126.73
11	bA	828	CLA	CHD-C4C-NC	3.25	129.33	124.20
11	aB	840	CLA	CHC-C1C-C2C	-3.25	117.70	126.73
11	aA	823	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
11	cA	812	CLA	CAC-C3C-C4C	3.25	129.03	124.81
11	cB	808	CLA	C4C-C3C-C2C	-3.25	102.16	106.90
11	aA	812	CLA	CAC-C3C-C4C	3.25	129.02	124.81
11	cA	812	CLA	CHC-C1C-C2C	-3.25	117.71	126.73
11	cA	824	CLA	CHC-C1C-C2C	-3.25	117.71	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bA	812	CLA	CHC-C1C-C2C	-3.25	117.71	126.73
12	cA	844	F6C	C1C-C2C-C3C	-3.25	103.03	106.83
11	aB	802	CLA	C4C-C3C-C2C	-3.24	102.17	106.90
11	bA	809	CLA	C3B-C4B-NB	3.24	113.53	110.52
11	cA	825	CLA	CHC-C1C-C2C	-3.24	117.72	126.73
11	bB	802	CLA	C4C-C3C-C2C	-3.24	102.17	106.90
11	cB	805	CLA	CAC-C3C-C4C	3.24	129.02	124.81
11	aA	824	CLA	CHC-C1C-C2C	-3.24	117.73	126.73
11	cB	807	CLA	CAC-C3C-C4C	3.24	129.01	124.81
11	aA	806	CLA	CHC-C1C-C2C	-3.24	117.73	126.73
11	aB	825	CLA	CAA-C2A-C3A	-3.24	103.91	112.78
11	bA	825	CLA	CHC-C1C-C2C	-3.24	117.74	126.73
11	aA	825	CLA	CHC-C1C-C2C	-3.24	117.74	126.73
12	bA	844	F6C	C1C-C2C-C3C	-3.24	103.05	106.83
11	aA	834	CLA	CAA-C2A-C3A	-3.23	103.92	112.78
11	bA	825	CLA	C3B-C4B-NB	3.23	113.52	110.52
11	bB	808	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
11	bA	806	CLA	CHC-C1C-C2C	-3.23	117.76	126.73
11	cA	806	CLA	CHC-C1C-C2C	-3.23	117.76	126.73
11	bA	834	CLA	CAA-C2A-C3A	-3.23	103.93	112.78
11	cB	801	CLA	C1C-C2C-C3C	-3.23	103.56	106.96
11	aB	808	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
11	cA	819	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
11	cA	828	CLA	CHD-C4C-NC	3.23	129.29	124.20
11	cA	809	CLA	C3B-C4B-NB	3.23	113.51	110.52
11	bA	812	CLA	CAC-C3C-C4C	3.23	129.00	124.81
11	bB	825	CLA	CAA-C2A-C3A	-3.23	103.94	112.78
13	cA	845	PQN	C14-C13-C15	3.23	120.70	115.27
11	aA	807	CLA	C3B-C4B-NB	3.23	113.51	110.52
11	aB	839	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
13	aA	845	PQN	C14-C13-C15	3.22	120.69	115.27
11	bA	819	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
11	cB	801	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
11	bB	802	CLA	CAC-C3C-C4C	3.22	128.99	124.81
15	cB	845	BCR	C15-C16-C17	-3.22	116.87	123.47
11	cB	812	CLA	C1C-C2C-C3C	-3.22	103.57	106.96
11	aA	819	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
11	cB	812	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
15	aB	846	BCR	C2-C1-C6	3.22	115.44	110.48
15	cB	846	BCR	C2-C1-C6	3.22	115.44	110.48
11	bB	801	CLA	C1C-C2C-C3C	-3.22	103.57	106.96
15	aB	845	BCR	C15-C16-C17	-3.22	116.88	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cL	206	CLA	CAA-C2A-C3A	-3.22	103.97	112.78
11	aA	843	CLA	C4-C3-C5	3.22	119.66	115.98
15	bB	845	BCR	C15-C16-C17	-3.22	116.89	123.47
11	aA	818	CLA	C4C-C3C-C2C	-3.21	102.21	106.90
11	aB	802	CLA	CAC-C3C-C4C	3.21	128.98	124.81
11	bB	801	CLA	C4C-C3C-C2C	-3.21	102.21	106.90
11	cB	825	CLA	CAA-C2A-C3A	-3.21	103.98	112.78
12	aA	827	F6C	C1C-C2C-C3C	-3.21	103.07	106.83
11	aB	801	CLA	C1C-C2C-C3C	-3.21	103.58	106.96
11	aB	812	CLA	C1C-C2C-C3C	-3.21	103.58	106.96
11	cA	823	CLA	CHD-C4C-NC	3.21	129.26	124.20
11	cA	840	CLA	CBA-CAA-C2A	3.21	123.34	113.86
11	bB	812	CLA	C1C-C2C-C3C	-3.21	103.58	106.96
12	cA	827	F6C	C1C-C2C-C3C	-3.21	103.08	106.83
11	cA	843	CLA	C4-C3-C5	3.21	119.65	115.98
11	cB	802	CLA	CAC-C3C-C4C	3.21	128.97	124.81
11	aB	801	CLA	C4C-C3C-C2C	-3.21	102.22	106.90
13	bA	845	PQN	C14-C13-C15	3.21	120.67	115.27
15	bB	846	BCR	C2-C1-C6	3.21	115.42	110.48
11	aL	206	CLA	CAA-C2A-C3A	-3.21	104.00	112.78
11	aA	840	CLA	CBA-CAA-C2A	3.20	123.32	113.86
11	aA	818	CLA	CAC-C3C-C4C	3.20	128.97	124.81
11	bB	806	CLA	CHD-C4C-NC	3.20	129.25	124.20
11	cA	803	CLA	CAA-C2A-C3A	-3.20	104.01	112.78
11	aA	803	CLA	CAA-C2A-C3A	-3.20	104.01	112.78
11	bB	811	CLA	C4C-C3C-C2C	-3.20	102.23	106.90
11	bL	206	CLA	CAA-C2A-C3A	-3.20	104.01	112.78
11	cB	839	CLA	C4C-C3C-C2C	-3.20	102.23	106.90
11	aA	819	CLA	CMC-C2C-C1C	3.20	129.91	125.04
11	aB	835	CLA	CHC-C1C-C2C	-3.20	117.84	126.73
11	aL	206	CLA	CMB-C2B-C1B	3.20	130.24	125.37
11	bA	840	CLA	CBA-CAA-C2A	3.20	123.30	113.86
11	aB	809	CLA	CHC-C1C-C2C	-3.20	117.85	126.73
11	bA	823	CLA	CHD-C4C-NC	3.20	129.24	124.20
11	bB	835	CLA	CHC-C1C-C2C	-3.19	117.86	126.73
11	aB	811	CLA	C4C-C3C-C2C	-3.19	102.24	106.90
11	bB	809	CLA	CHC-C1C-C2C	-3.19	117.86	126.73
10	bA	801	CL0	C4A-NA-C1A	-3.19	105.27	106.71
11	aA	821	CLA	CHC-C1C-C2C	-3.19	117.86	126.73
11	cB	835	CLA	CHC-C1C-C2C	-3.19	117.86	126.73
11	cA	825	CLA	C3B-C4B-NB	3.19	113.48	110.52
11	bA	818	CLA	C4C-C3C-C2C	-3.19	102.25	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bB	835	CLA	CMB-C2B-C1B	3.19	130.23	125.37
11	aA	836	CLA	CHC-C1C-C2C	-3.19	117.87	126.73
11	cA	819	CLA	CMC-C2C-C1C	3.19	129.89	125.04
12	bA	827	F6C	C1C-C2C-C3C	-3.19	103.10	106.83
11	cB	827	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
11	cB	818	CLA	CAC-C3C-C4C	3.19	128.95	124.81
11	bA	821	CLA	CHC-C1C-C2C	-3.19	117.88	126.73
11	cB	809	CLA	CHC-C1C-C2C	-3.19	117.88	126.73
11	bA	819	CLA	CMC-C2C-C1C	3.19	129.89	125.04
11	aA	823	CLA	CHD-C4C-NC	3.19	129.22	124.20
11	cB	814	CLA	CAC-C3C-C4C	3.19	128.94	124.81
11	cA	818	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
11	cA	821	CLA	CHC-C1C-C2C	-3.19	117.88	126.73
11	aB	806	CLA	O2D-CGD-CBD	3.18	116.93	111.27
11	aB	835	CLA	CMB-C2B-C1B	3.18	130.22	125.37
11	cA	816	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
11	bA	810	CLA	CAC-C3C-C4C	3.18	128.94	124.81
11	cA	836	CLA	CHC-C1C-C2C	-3.18	117.90	126.73
15	cA	851	BCR	C15-C16-C17	-3.18	116.96	123.47
11	bA	835	CLA	CMB-C2B-C1B	3.18	130.21	125.37
15	bA	851	BCR	C15-C16-C17	-3.18	116.96	123.47
11	aB	810	CLA	CHC-C1C-C2C	-3.18	117.90	126.73
11	aB	818	CLA	CAC-C3C-C4C	3.18	128.93	124.81
11	cB	806	CLA	O2D-CGD-CBD	3.18	116.91	111.27
11	bB	814	CLA	CAC-C3C-C4C	3.18	128.93	124.81
11	cB	810	CLA	CHC-C1C-C2C	-3.18	117.91	126.73
11	bB	832	CLA	CAC-C3C-C4C	3.18	128.93	124.81
11	bA	803	CLA	CAA-C2A-C3A	-3.18	104.08	112.78
11	bB	809	CLA	C4C-C3C-C2C	-3.18	102.27	106.90
12	bA	832	F6C	C1-C2-C3	-3.17	121.61	126.75
11	aB	806	CLA	CHD-C4C-NC	3.17	129.21	124.20
11	bB	827	CLA	C4C-C3C-C2C	-3.17	102.27	106.90
11	cA	835	CLA	CMB-C2B-C1B	3.17	130.20	125.37
11	cL	206	CLA	CMB-C2B-C1B	3.17	130.20	125.37
11	aB	814	CLA	CAC-C3C-C4C	3.17	128.93	124.81
11	bA	839	CLA	C3B-C4B-NB	3.17	113.46	110.52
11	aA	835	CLA	CMB-C2B-C1B	3.17	130.20	125.37
11	cA	810	CLA	CAC-C3C-C4C	3.17	128.93	124.81
11	bA	836	CLA	CHC-C1C-C2C	-3.17	117.92	126.73
11	cB	817	CLA	CAA-C2A-C3A	-3.17	104.09	112.78
11	aB	805	CLA	CAC-C3C-C4C	3.17	128.92	124.81
11	cB	809	CLA	C4C-C3C-C2C	-3.17	102.28	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aB	827	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
11	aA	810	CLA	CAC-C3C-C4C	3.17	128.92	124.81
11	bB	810	CLA	CHC-C1C-C2C	-3.17	117.93	126.73
11	cB	811	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
11	cB	806	CLA	CHD-C4C-NC	3.17	129.19	124.20
15	aA	851	BCR	C15-C16-C17	-3.16	116.99	123.47
11	bA	816	CLA	C4C-C3C-C2C	-3.16	102.29	106.90
11	cA	843	CLA	C4C-C3C-C2C	-3.16	102.29	106.90
11	bB	806	CLA	O2D-CGD-CBD	3.16	116.89	111.27
11	cA	818	CLA	CAC-C3C-C4C	3.16	128.91	124.81
12	cA	832	F6C	C1-C2-C3	-3.16	121.64	126.75
11	aB	809	CLA	C4C-C3C-C2C	-3.16	102.29	106.90
11	bB	817	CLA	CAA-C2A-C3A	-3.16	104.13	112.78
11	aA	816	CLA	C4C-C3C-C2C	-3.16	102.29	106.90
11	aA	829	CLA	CAC-C3C-C4C	3.16	128.91	124.81
11	cA	807	CLA	CHD-C4C-NC	3.16	129.18	124.20
11	cB	822	CLA	C3B-C4B-NB	3.16	113.44	110.52
11	aA	843	CLA	C4C-C3C-C2C	-3.16	102.30	106.90
11	aB	820	CLA	C3B-C4B-NB	3.16	113.44	110.52
11	aB	817	CLA	CAA-C2A-C3A	-3.15	104.14	112.78
11	bL	206	CLA	CMB-C2B-C1B	3.15	130.17	125.37
11	bA	829	CLA	CAC-C3C-C4C	3.15	128.90	124.81
11	cA	819	CLA	CAC-C3C-C4C	3.15	128.90	124.81
11	bB	830	CLA	CHC-C1C-C2C	-3.15	117.98	126.73
11	bA	843	CLA	C4C-C3C-C2C	-3.15	102.30	106.90
11	bB	804	CLA	C4A-NA-C1A	-3.15	105.29	106.71
11	cA	815	CLA	C4A-NA-C1A	-3.15	105.29	106.71
11	bB	804	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
12	bL	202	F6C	CHD-C1D-ND	-3.15	119.43	124.20
11	bB	818	CLA	CAC-C3C-C4C	3.15	128.89	124.81
11	cB	833	CLA	CHB-C4A-NA	3.15	128.86	124.51
11	aA	802	CLA	CHC-C1C-C2C	-3.15	117.99	126.73
11	bA	802	CLA	CHC-C1C-C2C	-3.15	117.99	126.73
12	aA	832	F6C	C1-C2-C3	-3.14	121.66	126.75
11	aB	832	CLA	CAC-C3C-C4C	3.14	128.89	124.81
11	cA	802	CLA	CHC-C1C-C2C	-3.14	118.00	126.73
11	bB	821	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
11	bA	806	CLA	C4A-NA-C1A	-3.14	105.29	106.71
12	aL	202	F6C	CHD-C1D-ND	-3.14	119.44	124.20
11	cB	835	CLA	CMB-C2B-C1B	3.14	130.15	125.37
12	cL	202	F6C	CHD-C1D-ND	-3.14	119.44	124.20
11	aK	103	CLA	C4C-C3C-C2C	-3.14	102.32	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bB	821	CLA	CHC-C1C-C2C	-3.14	118.01	126.73
11	aL	206	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
11	bK	103	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
12	aA	826	F6C	CHC-C1C-C2C	-3.14	118.37	127.24
11	cB	831	CLA	C3B-C4B-NB	3.14	113.43	110.52
11	cB	820	CLA	C3B-C4B-NB	3.14	113.43	110.52
11	cA	829	CLA	CAC-C3C-C4C	3.14	128.88	124.81
11	bA	807	CLA	CHD-C4C-NC	3.14	129.14	124.20
11	cB	826	CLA	C1-C2-C3	-3.13	120.62	126.04
11	aB	821	CLA	CHC-C1C-C2C	-3.13	118.02	126.73
11	cA	806	CLA	C4A-NA-C1A	-3.13	105.30	106.71
12	bA	826	F6C	CHC-C1C-C2C	-3.13	118.39	127.24
11	cK	103	CLA	CHC-C1C-C2C	-3.13	118.03	126.73
11	bA	805	CLA	CMC-C2C-C1C	3.13	129.81	125.04
11	bB	833	CLA	CHB-C4A-NA	3.13	128.84	124.51
11	cA	839	CLA	CHC-C1C-C2C	-3.13	118.03	126.73
11	cB	804	CLA	C4C-C3C-C2C	-3.13	102.33	106.90
11	aB	804	CLA	C4A-NA-C1A	-3.13	105.30	106.71
11	aA	839	CLA	CHC-C1C-C2C	-3.13	118.04	126.73
11	aB	830	CLA	CHC-C1C-C2C	-3.13	118.04	126.73
11	bB	805	CLA	CHC-C1C-C2C	-3.13	118.04	126.73
11	cB	804	CLA	C3B-C4B-NB	3.13	113.42	110.52
11	cA	843	CLA	CAC-C3C-C4C	3.13	128.87	124.81
11	cB	821	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
11	bA	818	CLA	CAC-C3C-C4C	3.13	128.87	124.81
11	bB	820	CLA	C3B-C4B-NB	3.13	113.42	110.52
11	bK	103	CLA	C3B-C4B-NB	3.13	113.42	110.52
11	cB	821	CLA	CHC-C1C-C2C	-3.13	118.05	126.73
11	aB	826	CLA	C1-C2-C3	-3.13	120.64	126.04
11	cB	830	CLA	CHC-C1C-C2C	-3.13	118.05	126.73
11	aA	824	CLA	CBC-CAC-C3C	-3.12	103.82	112.43
11	cB	820	CLA	CHC-C1C-C2C	-3.12	118.05	126.73
11	bA	819	CLA	C1-C2-C3	-3.12	120.64	126.04
11	aB	821	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
11	aA	815	CLA	C4A-NA-C1A	-3.12	105.30	106.71
11	bB	826	CLA	C1-C2-C3	-3.12	120.64	126.04
11	bA	819	CLA	CHD-C4C-NC	3.12	129.12	124.20
11	aB	833	CLA	CHB-C4A-NA	3.12	128.83	124.51
11	cB	805	CLA	CHB-C4A-NA	3.12	128.83	124.51
11	cK	103	CLA	C4-C3-C5	3.12	119.55	115.98
11	bA	839	CLA	CHC-C1C-C2C	-3.12	118.07	126.73
11	bK	103	CLA	CHC-C1C-C2C	-3.12	118.07	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bA	824	CLA	CBC-CAC-C3C	-3.12	103.84	112.43
11	bK	103	CLA	C4-C3-C5	3.12	119.55	115.98
11	cK	103	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
11	cL	206	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
11	aA	819	CLA	CAC-C3C-C4C	3.12	128.85	124.81
11	aA	839	CLA	CAC-C3C-C4C	3.12	128.85	124.81
11	aB	805	CLA	CHC-C1C-C2C	-3.12	118.07	126.73
15	cB	842	BCR	C15-C16-C17	-3.11	117.09	123.47
11	bL	206	CLA	C4C-C3C-C2C	-3.11	102.36	106.90
11	bB	821	CLA	C3B-C4B-NB	3.11	113.40	110.52
12	cA	826	F6C	CHC-C1C-C2C	-3.11	118.44	127.24
11	bA	812	CLA	C4C-C3C-C2C	-3.11	102.36	106.90
11	aA	843	CLA	CAC-C3C-C4C	3.11	128.85	124.81
11	cB	832	CLA	CAC-C3C-C4C	3.11	128.85	124.81
11	aB	808	CLA	CHC-C1C-C2C	-3.11	118.08	126.73
11	aK	103	CLA	CHC-C1C-C2C	-3.11	118.08	126.73
11	bA	819	CLA	CAC-C3C-C4C	3.11	128.85	124.81
11	aB	822	CLA	C3B-C4B-NB	3.11	113.40	110.52
11	bB	831	CLA	C3B-C4B-NB	3.11	113.40	110.52
11	aA	812	CLA	C4C-C3C-C2C	-3.11	102.36	106.90
11	aA	807	CLA	CHD-C4C-NC	3.11	129.10	124.20
11	aB	831	CLA	C3B-C4B-NB	3.11	113.40	110.52
11	aA	806	CLA	C4A-NA-C1A	-3.11	105.31	106.71
11	bB	820	CLA	CHD-C4C-NC	3.11	129.10	124.20
11	cA	819	CLA	CHD-C4C-NC	3.11	129.10	124.20
11	cB	831	CLA	CHC-C1C-C2C	-3.11	118.09	126.73
11	aA	819	CLA	CHD-C4C-NC	3.11	129.10	124.20
11	cB	813	CLA	CHC-C1C-C2C	-3.11	118.10	126.73
11	bB	822	CLA	C3B-C4B-NB	3.11	113.40	110.52
11	bA	836	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
11	cB	822	CLA	CAA-C2A-C3A	-3.11	104.27	112.78
11	aB	813	CLA	CHC-C1C-C2C	-3.11	118.10	126.73
11	cA	812	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
11	bB	820	CLA	CHC-C1C-C2C	-3.11	118.10	126.73
11	cB	805	CLA	CHC-C1C-C2C	-3.11	118.10	126.73
11	cA	824	CLA	CBC-CAC-C3C	-3.11	103.87	112.43
11	aA	805	CLA	CMC-C2C-C1C	3.11	129.77	125.04
11	cA	805	CLA	CMC-C2C-C1C	3.10	129.77	125.04
11	cB	820	CLA	CHD-C4C-NC	3.10	129.09	124.20
12	bL	202	F6C	CHC-C1C-C2C	-3.10	118.47	127.24
12	aA	844	F6C	CHC-C1C-C2C	-3.10	118.47	127.24
11	aB	804	CLA	C4C-C3C-C2C	-3.10	102.38	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cB	817	CLA	O2A-CGA-CBA	3.10	121.64	111.91
11	aA	808	CLA	CAC-C3C-C4C	3.10	128.84	124.81
11	cA	836	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
11	bB	822	CLA	CAA-C2A-C3A	-3.10	104.28	112.78
11	cB	821	CLA	C3B-C4B-NB	3.10	113.39	110.52
11	cA	839	CLA	CAC-C3C-C4C	3.10	128.83	124.81
12	bA	844	F6C	CHC-C1C-C2C	-3.10	118.48	127.24
11	aB	807	CLA	CHC-C1C-C2C	-3.10	118.12	126.73
18	aB	847	LMG	O6-C1-O1	-3.10	102.64	109.97
11	aA	810	CLA	C4A-NA-C1A	-3.10	105.31	106.71
11	cA	831	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
11	aB	821	CLA	C3B-C4B-NB	3.10	113.39	110.52
11	aA	813	CLA	CAC-C3C-C4C	3.10	128.83	124.81
15	bB	842	BCR	C15-C16-C17	-3.10	117.13	123.47
11	aB	830	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
12	cA	844	F6C	CHC-C1C-C2C	-3.10	118.49	127.24
11	aB	820	CLA	CHC-C1C-C2C	-3.10	118.13	126.73
12	cA	826	F6C	C4C-C3C-C2C	-3.10	102.02	106.89
11	bB	817	CLA	O2A-CGA-CBA	3.10	121.62	111.91
11	aB	822	CLA	CAA-C2A-C3A	-3.10	104.30	112.78
11	cA	833	CLA	CAA-C2A-C3A	-3.09	104.30	112.78
11	aK	103	CLA	C4-C3-C5	3.09	119.52	115.98
11	aB	817	CLA	O2A-CGA-CBA	3.09	121.61	111.91
11	cA	808	CLA	CAC-C3C-C4C	3.09	128.82	124.81
11	cB	810	CLA	CAA-C2A-C3A	-3.09	104.31	112.78
11	bB	807	CLA	CHC-C1C-C2C	-3.09	118.14	126.73
12	bA	826	F6C	C4C-C3C-C2C	-3.09	102.03	106.89
11	bA	839	CLA	CAC-C3C-C4C	3.09	128.82	124.81
11	aA	819	CLA	C1-C2-C3	-3.09	120.70	126.04
11	aB	838	CLA	C3B-C4B-NB	3.09	113.38	110.52
11	bB	830	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
11	bB	831	CLA	CHC-C1C-C2C	-3.09	118.15	126.73
11	cB	830	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
11	cA	819	CLA	C1-C2-C3	-3.09	120.70	126.04
11	cA	840	CLA	CAC-C3C-C4C	3.09	128.82	124.81
11	bA	815	CLA	C4A-NA-C1A	-3.09	105.32	106.71
12	cL	202	F6C	CHC-C1C-C2C	-3.09	118.52	127.24
15	aB	842	BCR	C15-C16-C17	-3.09	117.15	123.47
11	bB	838	CLA	C3B-C4B-NB	3.09	113.38	110.52
11	bA	843	CLA	CAC-C3C-C4C	3.09	128.81	124.81
11	cB	807	CLA	CHC-C1C-C2C	-3.09	118.16	126.73
11	aK	103	CLA	C3B-C4B-NB	3.09	113.38	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cK	103	CLA	C3B-C4B-NB	3.09	113.38	110.52
11	bB	808	CLA	CHC-C1C-C2C	-3.09	118.16	126.73
11	bA	818	CLA	CHD-C4C-NC	3.09	129.06	124.20
11	aB	831	CLA	CHC-C1C-C2C	-3.08	118.16	126.73
18	bB	847	LMG	O6-C1-O1	-3.08	102.67	109.97
18	cB	847	LMG	O6-C1-O1	-3.08	102.67	109.97
12	aL	202	F6C	CHC-C1C-C2C	-3.08	118.53	127.24
11	bB	804	CLA	C3B-C4B-NB	3.08	113.38	110.52
11	cA	839	CLA	C3B-C4B-NB	3.08	113.38	110.52
11	aA	818	CLA	CHD-C4C-NC	3.08	129.06	124.20
11	aA	807	CLA	CHC-C1C-C2C	-3.08	118.17	126.73
11	bB	813	CLA	CHC-C1C-C2C	-3.08	118.17	126.73
11	aA	833	CLA	CAA-C2A-C3A	-3.08	104.34	112.78
11	cA	807	CLA	CHC-C1C-C2C	-3.08	118.17	126.73
11	bA	814	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
12	cL	202	F6C	O2D-CGD-O1D	-3.08	117.82	123.84
11	cB	808	CLA	CHC-C1C-C2C	-3.08	118.18	126.73
11	bA	808	CLA	CAC-C3C-C4C	3.08	128.81	124.81
11	bK	103	CLA	CAC-C3C-C4C	3.08	128.81	124.81
11	aB	820	CLA	CHD-C4C-NC	3.08	129.06	124.20
11	aA	831	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
11	bB	810	CLA	CAA-C2A-C3A	-3.08	104.35	112.78
11	aB	801	CLA	CHD-C4C-NC	3.08	129.05	124.20
11	cB	808	CLA	C4-C3-C5	3.08	120.45	115.27
12	aA	826	F6C	C4C-C3C-C2C	-3.08	102.05	106.89
11	aA	836	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
11	bA	831	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
11	cA	814	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
11	bA	833	CLA	CAA-C2A-C3A	-3.07	104.36	112.78
11	cB	838	CLA	CAA-C2A-C3A	-3.07	104.36	112.78
11	aB	808	CLA	C4-C3-C5	3.07	120.44	115.27
11	aA	811	CLA	CHC-C1C-C2C	-3.07	118.19	126.73
11	bB	808	CLA	C4-C3-C5	3.07	120.44	115.27
11	cB	815	CLA	CHD-C4C-NC	3.07	129.04	124.20
11	aB	810	CLA	CAA-C2A-C3A	-3.07	104.37	112.78
12	bL	202	F6C	O2D-CGD-O1D	-3.07	117.83	123.84
11	bA	808	CLA	C1-C2-C3	-3.07	120.73	126.04
11	aB	804	CLA	C3B-C4B-NB	3.07	113.36	110.52
12	bA	827	F6C	C4-C3-C5	3.07	120.43	115.27
12	aL	202	F6C	O2D-CGD-O1D	-3.07	117.84	123.84
12	cA	827	F6C	C4-C3-C5	3.07	120.43	115.27
11	aB	805	CLA	CHB-C4A-NA	3.07	128.75	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bB	830	CLA	C3B-C4B-NB	3.07	113.36	110.52
11	cA	843	CLA	C3B-C4B-NB	3.07	113.36	110.52
11	cB	838	CLA	C3B-C4B-NB	3.07	113.36	110.52
11	cA	808	CLA	C1-C2-C3	-3.07	120.74	126.04
11	bA	818	CLA	C1C-C2C-C3C	-3.06	103.73	106.96
12	aA	826	F6C	CHD-C1D-ND	-3.06	119.55	124.20
11	bB	805	CLA	CHB-C4A-NA	3.06	128.75	124.51
11	bA	807	CLA	CHC-C1C-C2C	-3.06	118.22	126.73
11	cB	804	CLA	CMC-C2C-C1C	3.06	129.71	125.04
11	cA	818	CLA	CHD-C4C-NC	3.06	129.03	124.20
11	aA	813	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
11	cA	811	CLA	CHC-C1C-C2C	-3.06	118.23	126.73
15	bA	848	BCR	C24-C23-C22	-3.06	121.61	126.23
12	bA	826	F6C	CHD-C1D-ND	-3.06	119.56	124.20
12	cA	830	F6C	CHC-C1C-C2C	-3.06	118.60	127.24
11	aK	101	CLA	CHC-C1C-C2C	-3.06	118.24	126.73
11	bA	811	CLA	CHC-C1C-C2C	-3.06	118.24	126.73
11	cK	101	CLA	CAA-C2A-C3A	-3.06	106.62	114.26
11	aA	808	CLA	C1-C2-C3	-3.06	120.76	126.04
11	aA	814	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
11	aA	813	CLA	CHC-C1C-C2C	-3.06	118.24	126.73
11	aB	832	CLA	CHC-C1C-C2C	-3.06	118.24	126.73
11	aB	838	CLA	CAA-C2A-C3A	-3.06	104.41	112.78
11	bA	813	CLA	CAC-C3C-C4C	3.06	128.77	124.81
12	aA	830	F6C	CHC-C1C-C2C	-3.05	118.61	127.24
11	cA	821	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
11	aB	816	CLA	CAA-C2A-C3A	-3.05	104.42	112.78
11	aA	840	CLA	CAC-C3C-C4C	3.05	128.77	124.81
11	bB	838	CLA	CAA-C2A-C3A	-3.05	104.42	112.78
11	cB	804	CLA	C4A-NA-C1A	-3.05	105.33	106.71
11	cK	101	CLA	CHC-C1C-C2C	-3.05	118.25	126.73
11	cB	804	CLA	CAA-C2A-C3A	-3.05	104.42	112.78
11	cA	816	CLA	CHC-C1C-C2C	-3.05	118.26	126.73
11	bA	810	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
12	bA	830	F6C	CHC-C1C-C2C	-3.05	118.62	127.24
11	cB	801	CLA	CHD-C4C-NC	3.05	129.01	124.20
11	cA	843	CLA	CHC-C1C-C2C	-3.05	118.26	126.73
11	bB	816	CLA	CAA-C2A-C3A	-3.05	104.42	112.78
11	aB	817	CLA	CBA-CAA-C2A	3.05	122.87	113.86
11	bK	101	CLA	CAA-C2A-C3A	-3.05	106.64	114.26
11	aA	839	CLA	C3B-C4B-NB	3.05	113.34	110.52
11	cB	817	CLA	CBA-CAA-C2A	3.05	122.86	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	826	F6C	CHD-C1D-ND	-3.05	119.58	124.20
11	aA	834	CLA	CHC-C1C-C2C	-3.05	118.27	126.73
11	aA	810	CLA	C4C-C3C-C2C	-3.05	102.46	106.90
11	bA	821	CLA	C4C-C3C-C2C	-3.05	102.46	106.90
11	aB	804	CLA	CAA-C2A-C3A	-3.05	104.44	112.78
11	aK	101	CLA	CAA-C2A-C3A	-3.05	106.65	114.26
11	bA	816	CLA	CHC-C1C-C2C	-3.05	118.27	126.73
11	bA	843	CLA	CHC-C1C-C2C	-3.05	118.27	126.73
12	aA	827	F6C	CHC-C1C-C2C	-3.05	118.64	127.24
11	bB	804	CLA	CAA-C2A-C3A	-3.04	104.44	112.78
11	bA	833	CLA	CHC-C1C-C2C	-3.04	118.27	126.73
11	aB	840	CLA	CHD-C4C-NC	3.04	129.00	124.20
11	aA	823	CLA	CHC-C1C-C2C	-3.04	118.28	126.73
11	cA	813	CLA	CAC-C3C-C4C	3.04	128.76	124.81
11	aA	816	CLA	CHC-C1C-C2C	-3.04	118.28	126.73
11	bA	843	CLA	C3B-C4B-NB	3.04	113.34	110.52
11	bK	101	CLA	CHC-C1C-C2C	-3.04	118.28	126.73
11	aA	810	CLA	CHC-C1C-C2C	-3.04	118.28	126.73
15	aA	848	BCR	C24-C23-C22	-3.04	121.64	126.23
11	aB	812	CLA	CHC-C1C-C2C	-3.04	118.28	126.73
11	bB	838	CLA	CHC-C1C-C2C	-3.04	118.28	126.73
11	cA	835	CLA	CAA-C2A-C3A	-3.04	104.45	112.78
11	cB	840	CLA	CHD-C4C-NC	3.04	129.00	124.20
11	bB	819	CLA	CHC-C1C-C2C	-3.04	118.28	126.73
11	cA	813	CLA	CHC-C1C-C2C	-3.04	118.28	126.73
11	aK	103	CLA	CAC-C3C-C4C	3.04	128.76	124.81
11	bB	815	CLA	CHD-C4C-NC	3.04	129.00	124.20
11	cB	832	CLA	CHC-C1C-C2C	-3.04	118.28	126.73
12	cA	827	F6C	CHC-C1C-C2C	-3.04	118.65	127.24
11	bB	801	CLA	CHD-C4C-NC	3.04	128.99	124.20
11	aA	835	CLA	CAA-C2A-C3A	-3.04	104.45	112.78
11	aA	843	CLA	CHC-C1C-C2C	-3.04	118.29	126.73
11	cA	810	CLA	C4A-NA-C1A	-3.04	105.34	106.71
11	bA	834	CLA	CHC-C1C-C2C	-3.04	118.29	126.73
11	bB	817	CLA	CBA-CAA-C2A	3.04	122.83	113.86
11	bA	813	CLA	CHC-C1C-C2C	-3.04	118.29	126.73
11	bA	835	CLA	CAA-C2A-C3A	-3.04	104.46	112.78
11	cB	811	CLA	CHC-C1C-C2C	-3.04	118.30	126.73
11	aA	821	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
11	aB	815	CLA	CHD-C4C-NC	3.04	128.99	124.20
11	bA	823	CLA	CHC-C1C-C2C	-3.03	118.30	126.73
11	cA	834	CLA	CHC-C1C-C2C	-3.03	118.30	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bB	811	CLA	CHC-C1C-C2C	-3.03	118.30	126.73
11	cB	812	CLA	CHC-C1C-C2C	-3.03	118.30	126.73
10	aA	801	CL0	C4C-C3C-C2C	-3.03	102.48	106.90
12	bA	827	F6C	CHC-C1C-C2C	-3.03	118.67	127.24
11	aB	811	CLA	CHC-C1C-C2C	-3.03	118.30	126.73
11	cB	819	CLA	CHC-C1C-C2C	-3.03	118.30	126.73
11	cL	204	CLA	CHC-C1C-C2C	-3.03	118.30	126.73
10	cA	801	CL0	C4C-C3C-C2C	-3.03	102.48	106.90
11	cA	806	CLA	C4-C3-C5	3.03	120.37	115.27
11	bA	807	CLA	C1-C2-C3	-3.03	120.80	126.04
11	cB	816	CLA	CAA-C2A-C3A	-3.03	104.48	112.78
11	bB	840	CLA	CHD-C4C-NC	3.03	128.98	124.20
11	cB	815	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
11	cA	818	CLA	C1C-C2C-C3C	-3.03	103.77	106.96
11	cK	103	CLA	CAC-C3C-C4C	3.03	128.74	124.81
15	aA	849	BCR	C15-C16-C17	-3.03	117.27	123.47
11	aA	818	CLA	C1C-C2C-C3C	-3.03	103.77	106.96
11	cA	823	CLA	CHC-C1C-C2C	-3.03	118.32	126.73
11	aA	833	CLA	CHC-C1C-C2C	-3.03	118.32	126.73
11	bA	810	CLA	C4A-NA-C1A	-3.03	105.34	106.71
11	aB	814	CLA	C4C-C3C-C2C	-3.03	102.49	106.90
11	cA	829	CLA	CHC-C1C-C2C	-3.03	118.33	126.73
11	bB	815	CLA	C4C-C3C-C2C	-3.03	102.49	106.90
11	bB	812	CLA	CHC-C1C-C2C	-3.03	118.33	126.73
12	aA	827	F6C	C4-C3-C5	3.03	120.36	115.27
11	aB	836	CLA	C1C-C2C-C3C	-3.03	103.78	106.96
11	cA	810	CLA	CHC-C1C-C2C	-3.02	118.33	126.73
11	aA	843	CLA	C3B-C4B-NB	3.02	113.32	110.52
11	cA	833	CLA	CHC-C1C-C2C	-3.02	118.33	126.73
11	bL	204	CLA	CHC-C1C-C2C	-3.02	118.33	126.73
11	cA	831	CLA	CAC-C3C-C4C	3.02	128.73	124.81
11	bB	828	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
11	aB	819	CLA	CHC-C1C-C2C	-3.02	118.33	126.73
11	bB	832	CLA	CHC-C1C-C2C	-3.02	118.33	126.73
11	aB	815	CLA	C4C-C3C-C2C	-3.02	102.49	106.90
11	aL	204	CLA	CHC-C1C-C2C	-3.02	118.34	126.73
11	cA	802	CLA	CAC-C3C-C4C	3.02	128.73	124.81
11	aA	807	CLA	C1-C2-C3	-3.02	120.82	126.04
11	aA	803	CLA	C1C-C2C-C3C	-3.02	103.78	106.96
11	aB	838	CLA	CHC-C1C-C2C	-3.02	118.34	126.73
11	cB	814	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
11	cB	828	CLA	O2D-CGD-O1D	-3.02	117.94	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cB	836	CLA	C1C-C2C-C3C	-3.02	103.78	106.96
11	bB	814	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
11	aB	801	CLA	CAC-C3C-C4C	3.02	128.72	124.81
11	cA	810	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
11	aA	825	CLA	O2A-CGA-CBA	3.02	121.37	111.91
11	cB	838	CLA	CHC-C1C-C2C	-3.02	118.35	126.73
11	bB	804	CLA	CMC-C2C-C1C	3.02	129.63	125.04
11	cL	205	CLA	CAC-C3C-C4C	3.02	128.72	124.81
15	cA	849	BCR	C15-C16-C17	-3.01	117.30	123.47
11	cA	841	CLA	CHC-C1C-C2C	-3.01	118.36	126.73
11	aB	821	CLA	C4C-C3C-C2C	-3.01	102.50	106.90
11	bB	801	CLA	CAC-C3C-C4C	3.01	128.72	124.81
11	cB	836	CLA	CMB-C2B-C1B	3.01	129.96	125.37
11	aA	831	CLA	CAC-C3C-C4C	3.01	128.72	124.81
11	bB	836	CLA	C1C-C2C-C3C	-3.01	103.79	106.96
11	bA	829	CLA	CHC-C1C-C2C	-3.01	118.36	126.73
11	bB	833	CLA	CMA-C3A-C2A	-3.01	101.68	113.83
11	aA	841	CLA	C3B-C4B-NB	3.01	113.31	110.52
11	aB	830	CLA	C3B-C4B-NB	3.01	113.31	110.52
11	aB	804	CLA	CMC-C2C-C1C	3.01	129.62	125.04
11	bA	840	CLA	CAC-C3C-C4C	3.01	128.72	124.81
11	aB	825	CLA	CHC-C1C-C2C	-3.01	118.37	126.73
11	bA	810	CLA	CHC-C1C-C2C	-3.01	118.37	126.73
11	aB	833	CLA	CMA-C3A-C2A	-3.01	101.69	113.83
11	bA	806	CLA	C4-C3-C5	3.01	120.33	115.27
11	bA	813	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
11	aB	828	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
11	cA	836	CLA	CAC-C3C-C4C	3.01	128.71	124.81
11	bA	841	CLA	C3B-C4B-NB	3.01	113.31	110.52
11	bA	825	CLA	O2A-CGA-CBA	3.01	121.34	111.91
11	cB	804	CLA	CHD-C4C-NC	3.01	128.94	124.20
11	bB	830	CLA	C4C-C3C-C2C	-3.01	102.52	106.90
11	bB	821	CLA	C4C-C3C-C2C	-3.00	102.52	106.90
11	bB	836	CLA	CMB-C2B-C1B	3.00	129.94	125.37
11	aA	829	CLA	CHC-C1C-C2C	-3.00	118.39	126.73
11	bB	832	CLA	CMB-C2B-C1B	3.00	129.94	125.37
11	cA	807	CLA	C1-C2-C3	-3.00	120.85	126.04
11	cB	833	CLA	CMA-C3A-C2A	-3.00	101.72	113.83
11	aA	802	CLA	CAC-C3C-C4C	3.00	128.71	124.81
11	bL	205	CLA	CHC-C1C-C2C	-3.00	118.39	126.73
11	aB	827	CLA	C3B-C4B-NB	3.00	113.30	110.52
11	cB	801	CLA	CAC-C3C-C4C	3.00	128.71	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aB	836	CLA	CMB-C2B-C1B	3.00	129.94	125.37
11	cA	825	CLA	O2A-CGA-CBA	3.00	121.33	111.91
11	bA	841	CLA	CHC-C1C-C2C	-3.00	118.39	126.73
11	bA	822	CLA	CHC-C1C-C2C	-3.00	118.39	126.73
11	bA	809	CLA	CHC-C1C-C2C	-3.00	118.40	126.73
11	aB	832	CLA	CMB-C2B-C1B	3.00	129.94	125.37
10	bA	801	CL0	C4C-C3C-C2C	-3.00	102.53	106.90
11	bA	831	CLA	CAC-C3C-C4C	3.00	128.70	124.81
11	bB	825	CLA	CHC-C1C-C2C	-3.00	118.40	126.73
11	bA	837	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
11	aB	810	CLA	CMA-C3A-C2A	-3.00	101.73	113.83
11	cL	205	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
11	cL	205	CLA	CHC-C1C-C2C	-3.00	118.40	126.73
11	cA	805	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
11	cB	825	CLA	CHC-C1C-C2C	-3.00	118.41	126.73
15	bA	849	BCR	C15-C16-C17	-3.00	117.34	123.47
11	cB	827	CLA	CHC-C1C-C2C	-3.00	118.41	126.73
11	cA	821	CLA	C3B-C4B-NB	3.00	113.29	110.52
12	cA	826	F6C	C1-C2-C3	-3.00	120.86	126.04
11	cB	809	CLA	CAC-C3C-C4C	3.00	128.70	124.81
15	cA	848	BCR	C24-C23-C22	-2.99	121.71	126.23
11	bB	827	CLA	C3B-C4B-NB	2.99	113.29	110.52
11	cB	836	CLA	C4-C3-C5	2.99	119.41	115.98
11	aB	816	CLA	CHC-C1C-C2C	-2.99	118.41	126.73
11	cA	813	CLA	C4C-C3C-C2C	-2.99	102.53	106.90
11	cA	803	CLA	C1C-C2C-C3C	-2.99	103.81	106.96
11	bB	809	CLA	CAC-C3C-C4C	2.99	128.69	124.81
11	bA	822	CLA	C3B-C4B-NB	2.99	113.29	110.52
11	cB	810	CLA	CMA-C3A-C2A	-2.99	101.75	113.83
11	aL	205	CLA	CHC-C1C-C2C	-2.99	118.42	126.73
11	bB	827	CLA	CHC-C1C-C2C	-2.99	118.42	126.73
11	aA	805	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
11	cB	821	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
12	bA	826	F6C	C1-C2-C3	-2.99	120.87	126.04
11	aA	841	CLA	CHC-C1C-C2C	-2.99	118.42	126.73
11	aB	827	CLA	CHC-C1C-C2C	-2.99	118.42	126.73
11	bB	818	CLA	CHC-C1C-C2C	-2.99	118.42	126.73
11	cB	816	CLA	CHC-C1C-C2C	-2.99	118.42	126.73
11	aA	821	CLA	C3B-C4B-NB	2.99	113.29	110.52
11	aA	836	CLA	CAC-C3C-C4C	2.99	128.69	124.81
11	cB	830	CLA	C3B-C4B-NB	2.99	113.29	110.52
11	aB	818	CLA	CAA-C2A-C3A	-2.99	104.59	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aA	806	CLA	C4-C3-C5	2.99	120.30	115.27
11	bA	836	CLA	CAC-C3C-C4C	2.99	128.69	124.81
11	aB	838	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
11	cA	822	CLA	CHC-C1C-C2C	-2.99	118.43	126.73
11	cA	835	CLA	CHC-C1C-C2C	-2.99	118.43	126.73
11	bA	804	CLA	C3B-C4B-NB	2.99	113.29	110.52
11	aB	830	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
12	aA	826	F6C	C1-C2-C3	-2.99	120.88	126.04
11	aB	804	CLA	CHD-C4C-NC	2.99	128.91	124.20
11	bB	816	CLA	CHC-C1C-C2C	-2.99	118.44	126.73
11	bA	829	CLA	C4C-C3C-C2C	-2.99	102.55	106.90
11	cB	837	CLA	C4C-C3C-C2C	-2.99	102.55	106.90
11	bA	802	CLA	CAC-C3C-C4C	2.98	128.68	124.81
11	cB	816	CLA	C1-C2-C3	-2.98	120.88	126.04
11	aA	809	CLA	CHC-C1C-C2C	-2.98	118.44	126.73
11	cB	838	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
11	aA	805	CLA	CAC-C3C-C4C	2.98	128.68	124.81
11	aB	809	CLA	CAC-C3C-C4C	2.98	128.68	124.81
11	cK	101	CLA	C3B-C4B-NB	2.98	113.28	110.52
11	bB	810	CLA	CMA-C3A-C2A	-2.98	101.80	113.83
11	bB	822	CLA	CHD-C4C-NC	2.98	128.90	124.20
11	bB	818	CLA	CAA-C2A-C3A	-2.98	104.61	112.78
11	cB	832	CLA	CMB-C2B-C1B	2.98	129.91	125.37
10	bA	801	CL0	CHB-C4A-NA	2.98	128.63	124.51
11	aA	822	CLA	CHC-C1C-C2C	-2.98	118.45	126.73
11	aB	818	CLA	CHC-C1C-C2C	-2.98	118.45	126.73
11	aB	811	CLA	C3B-C4B-NB	2.98	113.28	110.52
11	bA	821	CLA	C3B-C4B-NB	2.98	113.28	110.52
11	cB	818	CLA	CAA-C2A-C3A	-2.98	104.62	112.78
11	bA	805	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
11	bA	835	CLA	CHC-C1C-C2C	-2.98	118.46	126.73
11	cA	809	CLA	CHC-C1C-C2C	-2.98	118.46	126.73
11	cA	822	CLA	C3B-C4B-NB	2.98	113.28	110.52
11	bB	804	CLA	CHD-C4C-NC	2.98	128.89	124.20
11	cA	809	CLA	CAC-C3C-C4C	2.98	128.67	124.81
11	aA	808	CLA	CAA-C2A-C3A	-2.98	104.63	112.78
11	aL	205	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
11	bA	835	CLA	CHD-C4C-NC	2.98	128.89	124.20
11	cA	808	CLA	CAA-C2A-C3A	-2.98	104.63	112.78
11	cA	829	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
11	bB	816	CLA	C1-C2-C3	-2.97	120.90	126.04
11	cB	830	CLA	C4C-C3C-C2C	-2.97	102.56	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aB	821	CLA	C4-C3-C5	2.97	120.27	115.27
11	bA	841	CLA	CAC-C3C-C4C	2.97	128.67	124.81
11	aA	835	CLA	CHC-C1C-C2C	-2.97	118.47	126.73
11	cB	818	CLA	CHC-C1C-C2C	-2.97	118.47	126.73
12	aA	826	F6C	CHB-C4A-NA	2.97	127.19	124.45
11	aA	829	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
11	aB	802	CLA	CMC-C2C-C1C	2.97	129.56	125.04
11	aK	101	CLA	CAC-C3C-C4C	2.97	128.66	124.81
11	cA	805	CLA	CAC-C3C-C4C	2.97	128.66	124.81
11	cA	837	CLA	CHD-C4C-NC	2.97	128.88	124.20
11	cB	813	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
11	bB	817	CLA	CHD-C4C-NC	2.97	128.88	124.20
11	cA	835	CLA	CHD-C4C-NC	2.97	128.88	124.20
11	bB	838	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
11	aL	205	CLA	CAC-C3C-C4C	2.97	128.66	124.81
11	bA	840	CLA	CHC-C1C-C2C	-2.97	118.49	126.73
11	aB	838	CLA	CAC-C3C-C4C	2.97	128.66	124.81
12	bB	824	F6C	C1-C2-C3	-2.96	120.92	126.04
11	aA	837	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
11	aB	833	CLA	CHC-C1C-C2C	-2.96	118.50	126.73
11	bL	205	CLA	C3B-C4B-NB	2.96	113.27	110.52
11	aB	813	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
11	cK	101	CLA	CAC-C3C-C4C	2.96	128.66	124.81
11	cA	819	CLA	C1C-C2C-C3C	-2.96	103.84	106.96
11	aB	822	CLA	CHD-C4C-NC	2.96	128.87	124.20
11	aA	824	CLA	CHD-C4C-NC	2.96	128.87	124.20
11	aA	819	CLA	C1C-C2C-C3C	-2.96	103.84	106.96
11	bL	205	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
11	cA	837	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
11	cB	833	CLA	CHC-C1C-C2C	-2.96	118.50	126.73
11	aB	817	CLA	CHD-C4C-NC	2.96	128.87	124.20
11	bB	813	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
12	cB	824	F6C	C1-C2-C3	-2.96	120.92	126.04
11	bA	819	CLA	C1C-C2C-C3C	-2.96	103.84	106.96
11	cA	806	CLA	C3C-C4C-NC	2.96	113.89	110.57
11	bB	814	CLA	CAA-C2A-C3A	-2.96	104.67	112.78
11	aB	837	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
11	bA	841	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
11	aB	822	CLA	C4A-NA-C1A	-2.96	105.38	106.71
12	cA	826	F6C	O2D-CGD-O1D	-2.96	118.05	123.84
11	cB	802	CLA	CMC-C2C-C1C	2.96	129.55	125.04
11	aB	816	CLA	C1-C2-C3	-2.96	120.92	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bA	805	CLA	CAC-C3C-C4C	2.96	128.65	124.81
11	bB	802	CLA	CMC-C2C-C1C	2.96	129.55	125.04
11	bA	808	CLA	CAA-C2A-C3A	-2.96	104.67	112.78
11	bB	836	CLA	C4-C3-C5	2.96	119.36	115.98
11	aA	835	CLA	CHD-C4C-NC	2.96	128.86	124.20
11	cB	822	CLA	CHD-C4C-NC	2.96	128.86	124.20
11	bA	804	CLA	CHC-C1C-C2C	-2.96	118.52	126.73
11	bA	824	CLA	CHD-C4C-NC	2.96	128.86	124.20
11	cB	814	CLA	CAA-C2A-C3A	-2.96	104.69	112.78
11	cA	840	CLA	CHC-C1C-C2C	-2.96	118.52	126.73
11	aB	814	CLA	CAA-C2A-C3A	-2.96	104.69	112.78
11	bK	101	CLA	CAC-C3C-C4C	2.95	128.64	124.81
10	bA	801	CL0	CHC-C1C-C2C	-2.95	118.52	126.73
11	cB	811	CLA	C3B-C4B-NB	2.95	113.26	110.52
15	cM	101	BCR	C15-C16-C17	-2.95	117.42	123.47
10	cA	801	CL0	CHC-C1C-C2C	-2.95	118.53	126.73
11	cA	841	CLA	C3B-C4B-NB	2.95	113.25	110.52
11	cB	827	CLA	C3B-C4B-NB	2.95	113.25	110.52
11	bA	806	CLA	C3C-C4C-NC	2.95	113.88	110.57
15	aM	101	BCR	C15-C16-C17	-2.95	117.43	123.47
11	aA	841	CLA	CAC-C3C-C4C	2.95	128.64	124.81
11	bL	205	CLA	CAC-C3C-C4C	2.95	128.64	124.81
11	aA	804	CLA	CHC-C1C-C2C	-2.95	118.53	126.73
11	bB	837	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
11	cA	804	CLA	CHC-C1C-C2C	-2.95	118.53	126.73
11	bA	831	CLA	C1-C2-C3	-2.95	120.94	126.04
11	bB	833	CLA	CHC-C1C-C2C	-2.95	118.54	126.73
10	aA	801	CL0	CHB-C4A-NA	2.95	128.59	124.51
11	bB	821	CLA	C4-C3-C5	2.95	120.23	115.27
11	bA	803	CLA	C1C-C2C-C3C	-2.95	103.86	106.96
11	cB	823	CLA	CMC-C2C-C1C	2.95	129.53	125.04
11	bB	811	CLA	C3B-C4B-NB	2.95	113.25	110.52
11	bA	837	CLA	CHD-C4C-NC	2.95	128.85	124.20
10	aA	801	CL0	CHC-C1C-C2C	-2.95	118.55	126.73
11	bA	840	CLA	C3B-C4B-NB	2.95	113.25	110.52
11	aA	831	CLA	C1-C2-C3	-2.95	120.95	126.04
12	aB	824	F6C	C1-C2-C3	-2.95	120.95	126.04
11	aA	840	CLA	CHC-C1C-C2C	-2.95	118.55	126.73
11	bB	839	CLA	CHD-C4C-NC	2.95	128.84	124.20
11	aA	841	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
11	cA	841	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
11	bB	822	CLA	C4A-NA-C1A	-2.94	105.38	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bA	808	CLA	CHC-C1C-C2C	-2.94	118.55	126.73
11	aA	822	CLA	C3B-C4B-NB	2.94	113.25	110.52
11	cA	824	CLA	CHD-C4C-NC	2.94	128.84	124.20
11	bA	822	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
11	cA	831	CLA	C1-C2-C3	-2.94	120.95	126.04
11	aB	836	CLA	C4-C3-C5	2.94	119.35	115.98
11	aL	205	CLA	C3B-C4B-NB	2.94	113.25	110.52
11	cB	821	CLA	C4-C3-C5	2.94	120.22	115.27
11	cB	838	CLA	CAC-C3C-C4C	2.94	128.63	124.81
12	aA	826	F6C	O2D-CGD-O1D	-2.94	118.09	123.84
12	bA	826	F6C	O2D-CGD-O1D	-2.94	118.09	123.84
11	bB	838	CLA	O2A-CGA-CBA	2.94	121.14	111.91
11	aA	804	CLA	C3B-C4B-NB	2.94	113.24	110.52
11	cB	838	CLA	O2A-CGA-CBA	2.94	121.14	111.91
11	aB	834	CLA	CAC-C3C-C4C	2.94	128.62	124.81
11	aA	822	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
11	bB	807	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
11	cA	841	CLA	CAC-C3C-C4C	2.94	128.62	124.81
11	aA	806	CLA	C3C-C4C-NC	2.94	113.87	110.57
11	aA	808	CLA	CHC-C1C-C2C	-2.94	118.57	126.73
11	cA	804	CLA	C3B-C4B-NB	2.94	113.24	110.52
10	cA	801	CL0	CHB-C4A-NA	2.94	128.57	124.51
11	aB	838	CLA	O2A-CGA-CBA	2.94	121.12	111.91
11	cA	837	CLA	CHC-C1C-C2C	-2.93	118.58	126.73
11	cB	817	CLA	CHD-C4C-NC	2.93	128.83	124.20
11	cA	816	CLA	CAC-C3C-C4C	2.93	128.62	124.81
11	cA	808	CLA	CHC-C1C-C2C	-2.93	118.58	126.73
11	aA	837	CLA	CHD-C4C-NC	2.93	128.82	124.20
11	cB	839	CLA	CHD-C4C-NC	2.93	128.82	124.20
11	cB	823	CLA	CHC-C1C-C2C	-2.93	118.58	126.73
11	cA	822	CLA	C4C-C3C-C2C	-2.93	102.62	106.90
11	cB	807	CLA	C4C-C3C-C2C	-2.93	102.62	106.90
11	bB	823	CLA	CHC-C1C-C2C	-2.93	118.59	126.73
11	cA	840	CLA	C3B-C4B-NB	2.93	113.23	110.52
11	bL	206	CLA	C4-C3-C5	2.93	120.20	115.27
11	aA	815	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
11	aA	828	CLA	CHC-C1C-C2C	-2.93	118.60	126.73
11	aA	837	CLA	CHC-C1C-C2C	-2.93	118.60	126.73
11	bA	815	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
11	aK	101	CLA	C3B-C4B-NB	2.93	113.23	110.52
11	aA	808	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
11	bK	101	CLA	C3B-C4B-NB	2.93	113.23	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bA	837	CLA	CHC-C1C-C2C	-2.93	118.60	126.73
11	bA	809	CLA	CAC-C3C-C4C	2.93	128.61	124.81
11	aB	818	CLA	C3B-C4B-NB	2.93	113.23	110.52
11	cB	807	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
11	bB	807	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
11	cL	205	CLA	C3B-C4B-NB	2.92	113.23	110.52
12	aA	827	F6C	O2D-CGD-O1D	-2.92	118.12	123.84
11	bA	808	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
11	aA	810	CLA	C3B-C4B-NB	2.92	113.23	110.52
11	cB	834	CLA	CAC-C3C-C4C	2.92	128.60	124.81
11	bB	832	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
11	cA	808	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
11	bA	804	CLA	CHD-C4C-NC	2.92	128.81	124.20
11	bB	823	CLA	CMC-C2C-C1C	2.92	129.49	125.04
15	bM	101	BCR	C15-C16-C17	-2.92	117.49	123.47
11	aA	809	CLA	CAC-C3C-C4C	2.92	128.60	124.81
11	aB	823	CLA	CHC-C1C-C2C	-2.92	118.62	126.73
11	aB	831	CLA	CBA-CAA-C2A	2.92	122.48	113.86
11	bB	823	CLA	CAC-C3C-C4C	2.92	128.60	124.81
11	aB	823	CLA	CMC-C2C-C1C	2.92	129.49	125.04
11	cA	841	CLA	O2A-CGA-CBA	2.92	121.07	111.91
11	cB	832	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
11	bA	829	CLA	CAA-C2A-C3A	-2.92	104.78	112.78
12	bA	827	F6C	O2D-CGD-O1D	-2.92	118.13	123.84
11	cA	804	CLA	CHD-C4C-NC	2.92	128.80	124.20
12	bB	824	F6C	C4-C3-C5	2.92	120.18	115.27
11	bB	818	CLA	C1C-C2C-C3C	-2.92	103.89	106.96
11	aA	816	CLA	CAC-C3C-C4C	2.92	128.59	124.81
11	cB	805	CLA	C4C-C3C-C2C	-2.92	102.65	106.90
11	aA	838	CLA	CHC-C1C-C2C	-2.92	118.63	126.73
11	bA	828	CLA	CHC-C1C-C2C	-2.92	118.63	126.73
11	bB	819	CLA	C4C-C3C-C2C	-2.92	102.65	106.90
11	cA	828	CLA	CHC-C1C-C2C	-2.92	118.63	126.73
11	aA	805	CLA	CHD-C4C-NC	2.92	128.80	124.20
11	aA	829	CLA	CAA-C2A-C3A	-2.91	104.80	112.78
11	bA	842	CLA	CHC-C1C-C2C	-2.91	118.64	126.73
11	bB	823	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
11	cA	829	CLA	CAA-C2A-C3A	-2.91	104.80	112.78
12	cL	202	F6C	CHA-C1A-C2A	-2.91	121.94	129.84
15	aL	208	BCR	C2-C1-C6	2.91	114.96	110.48
11	cA	842	CLA	CHD-C4C-NC	2.91	128.79	124.20
11	bA	822	CLA	CMB-C2B-C1B	2.91	129.80	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aB	832	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
11	bB	831	CLA	CBA-CAA-C2A	2.91	122.46	113.86
11	bA	803	CLA	CAC-C3C-C4C	2.91	128.59	124.81
11	aB	807	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
11	aA	840	CLA	C3B-C4B-NB	2.91	113.22	110.52
11	cB	818	CLA	C1C-C2C-C3C	-2.91	103.90	106.96
11	cB	831	CLA	CBA-CAA-C2A	2.91	122.45	113.86
11	bA	814	CLA	CHC-C1C-C2C	-2.91	118.65	126.73
11	bA	838	CLA	CHC-C1C-C2C	-2.91	118.65	126.73
11	cA	839	CLA	CMB-C2B-C1B	2.91	129.80	125.37
12	bL	202	F6C	CHA-C1A-C2A	-2.91	121.95	129.84
11	bB	808	CLA	CAC-C3C-C4C	2.91	128.58	124.81
12	aL	202	F6C	CHA-C1A-C2A	-2.91	121.95	129.84
11	aL	206	CLA	C4-C3-C5	2.91	120.16	115.27
12	aB	824	F6C	C4-C3-C5	2.91	120.16	115.27
11	cB	806	CLA	CHC-C1C-C2C	-2.91	118.66	126.73
11	cA	814	CLA	CHC-C1C-C2C	-2.91	118.66	126.73
11	aA	814	CLA	CHC-C1C-C2C	-2.90	118.66	126.73
11	aB	808	CLA	CAC-C3C-C4C	2.90	128.58	124.81
11	bA	841	CLA	O2A-CGA-CBA	2.90	121.02	111.91
11	aA	842	CLA	CHC-C1C-C2C	-2.90	118.66	126.73
11	aL	206	CLA	CHC-C1C-C2C	-2.90	118.66	126.73
15	cL	208	BCR	C2-C1-C6	2.90	114.95	110.48
11	aA	821	CLA	CMB-C2B-C1B	2.90	129.79	125.37
11	bB	834	CLA	CAC-C3C-C4C	2.90	128.58	124.81
11	bB	838	CLA	CAC-C3C-C4C	2.90	128.58	124.81
11	cA	815	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
11	cL	206	CLA	C4-C3-C5	2.90	120.15	115.27
11	bA	810	CLA	C3B-C4B-NB	2.90	113.21	110.52
11	cB	823	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
11	bB	830	CLA	CAC-C3C-C4C	2.90	128.57	124.81
11	bB	818	CLA	C3B-C4B-NB	2.90	113.21	110.52
11	aA	814	CLA	CAA-C2A-C3A	-2.90	104.83	112.78
11	cB	819	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
11	cA	842	CLA	CHC-C1C-C2C	-2.90	118.67	126.73
11	cB	830	CLA	CAC-C3C-C4C	2.90	128.57	124.81
11	cA	822	CLA	CMB-C2B-C1B	2.90	129.79	125.37
11	aB	839	CLA	CHD-C4C-NC	2.90	128.77	124.20
11	cA	838	CLA	CHC-C1C-C2C	-2.90	118.67	126.73
11	cB	827	CLA	CAC-C3C-C4C	2.90	128.57	124.81
11	bB	805	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
11	bA	818	CLA	C4A-NA-C1A	-2.90	105.40	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bA	814	CLA	CAA-C2A-C3A	-2.90	104.84	112.78
11	bB	806	CLA	CHC-C1C-C2C	-2.90	118.68	126.73
11	aA	841	CLA	O2A-CGA-CBA	2.90	121.00	111.91
11	bA	816	CLA	CAC-C3C-C4C	2.90	128.57	124.81
11	aA	818	CLA	C4A-NA-C1A	-2.90	105.40	106.71
12	cA	826	F6C	CHB-C4A-NA	2.90	127.11	124.45
12	cB	824	F6C	C4-C3-C5	2.90	120.14	115.27
11	cB	823	CLA	CAC-C3C-C4C	2.89	128.57	124.81
11	aB	818	CLA	C1C-C2C-C3C	-2.89	103.91	106.96
15	bL	208	BCR	C2-C1-C6	2.89	114.94	110.48
11	cL	206	CLA	CHC-C1C-C2C	-2.89	118.69	126.73
11	bA	840	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
11	bA	839	CLA	CMB-C2B-C1B	2.89	129.77	125.37
11	bA	834	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
11	cA	810	CLA	C3B-C4B-NB	2.89	113.20	110.52
11	aB	807	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
11	aB	823	CLA	CAC-C3C-C4C	2.89	128.56	124.81
11	aB	834	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
10	bA	801	CL0	C1-C2-C3	-2.89	121.05	126.04
11	aB	806	CLA	CHC-C1C-C2C	-2.89	118.71	126.73
11	bL	206	CLA	CHC-C1C-C2C	-2.89	118.71	126.73
11	aL	205	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
11	aA	839	CLA	CMB-C2B-C1B	2.89	129.77	125.37
11	cA	805	CLA	CHD-C4C-NC	2.89	128.75	124.20
12	bA	826	F6C	CHB-C4A-NA	2.89	127.11	124.45
11	bA	842	CLA	CHD-C4C-NC	2.89	128.75	124.20
11	aB	823	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
11	cB	816	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
11	bL	205	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
12	cA	827	F6C	O2D-CGD-O1D	-2.88	118.20	123.84
11	cL	204	CLA	C4C-C3C-C2C	-2.88	102.69	106.90
11	bB	827	CLA	CAC-C3C-C4C	2.88	128.55	124.81
11	bA	821	CLA	CMB-C2B-C1B	2.88	129.76	125.37
11	aA	842	CLA	CHD-C4C-NC	2.88	128.75	124.20
11	bA	805	CLA	CHD-C4C-NC	2.88	128.75	124.20
11	bB	826	CLA	CHC-C1C-C2C	-2.88	118.72	126.73
11	cB	834	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
11	cA	839	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
12	bL	202	F6C	O2A-CGA-O1A	-2.88	116.32	123.59
10	aA	801	CL0	C1-C2-C3	-2.88	121.06	126.04
11	bB	837	CLA	CHD-C4C-NC	2.88	128.74	124.20
11	aA	822	CLA	CMB-C2B-C1B	2.88	129.75	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bB	804	CLA	CBA-CAA-C2A	2.88	122.36	113.86
11	cA	814	CLA	CAA-C2A-C3A	-2.88	104.90	112.78
11	aL	204	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
11	bA	835	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
11	cA	803	CLA	CAC-C3C-C4C	2.88	128.54	124.81
11	cL	205	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
11	aA	835	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
11	aB	826	CLA	CHC-C1C-C2C	-2.87	118.75	126.73
11	aA	839	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
11	cA	834	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
11	cA	835	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
15	aA	849	BCR	C11-C10-C9	-2.87	123.21	127.31
11	aB	804	CLA	CBA-CAA-C2A	2.87	122.35	113.86
11	cB	801	CLA	CMC-C2C-C1C	2.87	129.42	125.04
11	aB	831	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
11	bK	103	CLA	O2A-CGA-CBA	2.87	120.92	111.91
11	aA	804	CLA	CHD-C4C-NC	2.87	128.73	124.20
11	aA	840	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
11	cB	804	CLA	CBA-CAA-C2A	2.87	122.34	113.86
11	bB	810	CLA	CAC-C3C-C4C	2.87	128.54	124.81
11	cB	826	CLA	CHC-C1C-C2C	-2.87	118.75	126.73
10	cA	801	CL0	C1-C2-C3	-2.87	121.08	126.04
11	bB	837	CLA	CHC-C1C-C2C	-2.87	118.75	126.73
11	aK	101	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
11	aB	837	CLA	CHC-C1C-C2C	-2.87	118.76	126.73
12	aL	202	F6C	O2A-CGA-O1A	-2.87	116.35	123.59
11	bB	831	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
11	cK	101	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
11	aB	819	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
11	bL	204	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
11	cK	103	CLA	O2A-CGA-CBA	2.87	120.91	111.91
12	cL	202	F6C	O2A-CGA-O1A	-2.87	116.35	123.59
11	cB	808	CLA	CAC-C3C-C4C	2.87	128.53	124.81
11	cB	801	CLA	CHC-C1C-C2C	-2.87	118.77	126.73
11	aB	830	CLA	CAC-C3C-C4C	2.87	128.53	124.81
11	aA	802	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
11	cB	837	CLA	CHC-C1C-C2C	-2.87	118.77	126.73
11	aB	816	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
11	cA	821	CLA	CMB-C2B-C1B	2.86	129.73	125.37
11	bB	834	CLA	C4C-C3C-C2C	-2.86	102.72	106.90
15	bA	849	BCR	C11-C10-C9	-2.86	123.22	127.31
11	aB	806	CLA	CAA-C2A-C3A	-2.86	104.94	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cA	840	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
11	cB	822	CLA	C4A-NA-C1A	-2.86	105.42	106.71
11	aA	834	CLA	C4C-C3C-C2C	-2.86	102.72	106.90
11	cA	840	CLA	C4C-C3C-C2C	-2.86	102.72	106.90
11	bA	802	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
11	bK	101	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
11	bA	835	CLA	C3B-C4B-NB	2.86	113.17	110.52
11	aB	801	CLA	CHC-C1C-C2C	-2.86	118.78	126.73
11	aA	803	CLA	CAC-C3C-C4C	2.86	128.52	124.81
11	aB	836	CLA	CHC-C1C-C2C	-2.86	118.78	126.73
11	bB	801	CLA	CHC-C1C-C2C	-2.86	118.79	126.73
11	cA	835	CLA	C3B-C4B-NB	2.86	113.17	110.52
11	cA	817	CLA	CAA-C2A-C3A	-2.86	104.95	112.78
11	aA	825	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
11	bA	839	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
11	aK	103	CLA	O2A-CGA-CBA	2.86	120.88	111.91
11	aA	833	CLA	CHD-C4C-NC	2.86	128.71	124.20
11	cB	833	CLA	CHD-C4C-NC	2.86	128.71	124.20
11	aA	834	CLA	CHD-C4C-NC	2.86	128.70	124.20
11	cA	833	CLA	CHD-C4C-NC	2.86	128.70	124.20
11	cB	836	CLA	CHC-C1C-C2C	-2.86	118.80	126.73
11	aB	805	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
11	bB	836	CLA	CHC-C1C-C2C	-2.85	118.80	126.73
11	bA	822	CLA	C4-C3-C5	2.85	120.07	115.27
11	bB	816	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
10	bA	801	CL0	CMB-C2B-C1B	2.85	129.71	125.37
10	cA	801	CL0	CMB-C2B-C1B	2.85	129.71	125.37
11	bB	806	CLA	CAA-C2A-C3A	-2.85	104.97	112.78
11	aB	837	CLA	CHD-C4C-NC	2.85	128.70	124.20
11	cB	801	CLA	C1-C2-C3	-2.85	121.11	126.04
11	cA	811	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
11	aA	840	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
15	cA	849	BCR	C11-C10-C9	-2.85	123.24	127.31
11	bB	801	CLA	C1-C2-C3	-2.85	121.12	126.04
11	cB	806	CLA	CAA-C2A-C3A	-2.85	104.98	112.78
11	cA	834	CLA	CHD-C4C-NC	2.85	128.69	124.20
11	cB	837	CLA	CHD-C4C-NC	2.85	128.69	124.20
11	aB	833	CLA	CHD-C4C-NC	2.85	128.69	124.20
11	cA	835	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
10	aA	801	CL0	CMB-C2B-C1B	2.85	129.70	125.37
11	bB	816	CLA	CAC-C3C-C4C	2.85	128.50	124.81
11	bA	817	CLA	CAA-C2A-C3A	-2.85	104.99	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bB	835	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
11	cA	818	CLA	C4A-NA-C1A	-2.84	105.43	106.71
11	bA	833	CLA	CHD-C4C-NC	2.84	128.69	124.20
11	aB	801	CLA	C1-C2-C3	-2.84	121.12	126.04
11	aB	801	CLA	CMC-C2C-C1C	2.84	129.37	125.04
12	aL	202	F6C	CAC-C3C-C4C	2.84	128.86	124.92
11	aB	827	CLA	CAC-C3C-C4C	2.84	128.50	124.81
11	cA	842	CLA	C4C-C3C-C2C	-2.84	102.75	106.90
11	cB	835	CLA	C4C-C3C-C2C	-2.84	102.75	106.90
11	bA	822	CLA	CHD-C4C-NC	2.84	128.68	124.20
11	bB	833	CLA	CHD-C4C-NC	2.84	128.68	124.20
11	bB	819	CLA	CAC-C3C-C4C	2.84	128.50	124.81
11	aA	803	CLA	CHC-C1C-C2C	-2.84	118.84	126.73
11	aA	835	CLA	C3B-C4B-NB	2.84	113.15	110.52
11	cB	818	CLA	C3B-C4B-NB	2.84	113.15	110.52
11	bA	835	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
11	aA	817	CLA	CAA-C2A-C3A	-2.84	105.00	112.78
11	aB	810	CLA	CAC-C3C-C4C	2.84	128.50	124.81
11	cB	810	CLA	CAC-C3C-C4C	2.84	128.50	124.81
11	cB	833	CLA	C3B-C4B-NB	2.84	113.15	110.52
11	bB	801	CLA	CMC-C2C-C1C	2.84	129.36	125.04
11	bB	807	CLA	CMB-C2B-C1B	2.84	129.69	125.37
11	aA	806	CLA	CMC-C2C-C1C	2.84	129.36	125.04
11	cA	802	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
11	cB	831	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
11	cA	803	CLA	CHC-C1C-C2C	-2.84	118.84	126.73
11	aB	808	CLA	CBA-CAA-C2A	2.84	122.24	113.86
11	bA	834	CLA	CHD-C4C-NC	2.84	128.68	124.20
11	cA	806	CLA	CMC-C2C-C1C	2.84	129.36	125.04
11	aB	835	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
11	bB	831	CLA	CAC-C3C-C4C	2.84	128.49	124.81
11	cB	816	CLA	CAC-C3C-C4C	2.84	128.49	124.81
11	bA	838	CLA	CHD-C4C-NC	2.84	128.67	124.20
11	cB	826	CLA	CAA-C2A-C3A	-2.84	105.01	112.78
11	bB	823	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
11	cB	807	CLA	CMB-C2B-C1B	2.83	129.69	125.37
11	bA	803	CLA	CHC-C1C-C2C	-2.83	118.86	126.73
11	aA	838	CLA	CHD-C4C-NC	2.83	128.67	124.20
11	cB	837	CLA	CAC-C3C-C4C	2.83	128.49	124.81
11	aA	811	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
11	bA	811	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
11	bA	840	CLA	C4C-C3C-C2C	-2.83	102.77	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aB	807	CLA	CMB-C2B-C1B	2.83	129.68	125.37
11	cB	808	CLA	CBA-CAA-C2A	2.83	122.22	113.86
11	cA	822	CLA	C4-C3-C5	2.83	120.03	115.27
11	aA	804	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
11	cB	819	CLA	CAC-C3C-C4C	2.83	128.48	124.81
11	bB	808	CLA	CBA-CAA-C2A	2.83	122.21	113.86
15	aB	848	BCR	C27-C26-C25	2.83	126.84	122.73
12	bL	202	F6C	CAC-C3C-C4C	2.83	128.84	124.92
11	cA	804	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
12	cL	202	F6C	CAC-C3C-C4C	2.82	128.84	124.92
11	aB	826	CLA	CAA-C2A-C3A	-2.82	105.05	112.78
11	bA	806	CLA	CMC-C2C-C1C	2.82	129.34	125.04
11	aA	840	CLA	CHD-C4C-NC	2.82	128.65	124.20
10	cA	801	CL0	O2A-CGA-CBA	2.82	120.77	111.91
11	aB	831	CLA	CHD-C4C-NC	2.82	128.65	124.20
11	aA	838	CLA	CAC-C3C-C4C	2.82	128.47	124.81
11	bA	824	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
11	bB	826	CLA	CAA-C2A-C3A	-2.82	105.05	112.78
11	cA	825	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
11	aA	842	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
11	aA	822	CLA	C4-C3-C5	2.82	120.01	115.27
11	bA	840	CLA	CHD-C4C-NC	2.82	128.65	124.20
11	cB	831	CLA	CHD-C4C-NC	2.82	128.65	124.20
10	bA	801	CL0	O2A-CGA-CBA	2.82	120.75	111.91
12	bL	202	F6C	C4C-C3C-C2C	-2.82	102.46	106.89
11	aA	835	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
10	aA	801	CL0	O2A-CGA-CBA	2.82	120.75	111.91
11	aB	823	CLA	O2D-CGD-O1D	-2.81	118.33	123.84
11	aB	828	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
11	bA	825	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
11	bB	833	CLA	C3B-C4B-NB	2.81	113.13	110.52
11	bA	804	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
11	aB	825	CLA	O2A-CGA-CBA	2.81	120.74	111.91
11	bB	833	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
11	aA	822	CLA	CHD-C4C-NC	2.81	128.63	124.20
11	cB	823	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
12	bA	844	F6C	CAC-C3C-C4C	2.81	128.82	124.92
12	cA	844	F6C	CAC-C3C-C4C	2.81	128.82	124.92
11	aB	833	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
15	cB	848	BCR	C27-C26-C25	2.81	126.81	122.73
11	aA	811	CLA	CHD-C4C-NC	2.81	128.63	124.20
11	bB	810	CLA	C4C-C3C-C2C	-2.81	102.81	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cB	833	CLA	C4C-C3C-C2C	-2.81	102.81	106.90
12	aA	844	F6C	CAC-C3C-C4C	2.81	128.81	124.92
11	bA	842	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
11	bB	828	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
11	aL	204	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
11	cA	838	CLA	CAC-C3C-C4C	2.80	128.45	124.81
11	bA	838	CLA	CMC-C2C-C1C	2.80	129.31	125.04
11	aB	816	CLA	CAC-C3C-C4C	2.80	128.45	124.81
11	bB	831	CLA	CHD-C4C-NC	2.80	128.62	124.20
11	cB	835	CLA	CAC-C3C-C4C	2.80	128.44	124.81
11	aB	810	CLA	CHD-C4C-NC	2.80	128.62	124.20
12	cL	202	F6C	C4C-C3C-C2C	-2.80	102.49	106.89
15	cA	850	BCR	C15-C16-C17	-2.80	117.74	123.47
11	aA	838	CLA	CMC-C2C-C1C	2.80	129.30	125.04
11	cA	809	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
11	bB	825	CLA	O2A-CGA-CBA	2.80	120.69	111.91
11	bA	805	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
11	aA	840	CLA	CMB-C2B-C1B	2.80	129.63	125.37
11	cA	805	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
11	bB	802	CLA	C4-C3-C5	2.80	119.97	115.27
11	aA	805	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
11	cB	802	CLA	C4-C3-C5	2.79	119.97	115.27
12	aL	202	F6C	C4C-C3C-C2C	-2.79	102.50	106.89
11	cA	840	CLA	CHD-C4C-NC	2.79	128.60	124.20
11	aB	837	CLA	CAC-C3C-C4C	2.79	128.43	124.81
11	cB	831	CLA	CAC-C3C-C4C	2.79	128.43	124.81
11	bB	806	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
11	cB	806	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
11	aB	833	CLA	C3B-C4B-NB	2.79	113.11	110.52
11	bB	810	CLA	CHD-C4C-NC	2.79	128.60	124.20
11	cB	828	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
11	cL	204	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
11	cB	825	CLA	O2A-CGA-CBA	2.79	120.66	111.91
15	cL	203	BCR	C7-C8-C9	-2.79	122.02	126.23
11	aB	833	CLA	CAC-C3C-C4C	2.79	128.43	124.81
11	bL	204	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
11	cA	838	CLA	CHD-C4C-NC	2.79	128.60	124.20
11	aB	831	CLA	CAC-C3C-C4C	2.79	128.43	124.81
11	cA	811	CLA	CHD-C4C-NC	2.79	128.60	124.20
11	cB	810	CLA	CHD-C4C-NC	2.79	128.60	124.20
11	aB	802	CLA	C4-C3-C5	2.79	119.96	115.27
11	cB	815	CLA	C3B-C4B-NB	2.79	113.10	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cA	824	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
11	cA	838	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
11	aL	206	CLA	CAC-C3C-C4C	2.79	128.43	124.81
11	bB	835	CLA	CAC-C3C-C4C	2.79	128.43	124.81
15	bA	850	BCR	C15-C16-C17	-2.79	117.77	123.47
11	cA	840	CLA	CMB-C2B-C1B	2.79	129.61	125.37
11	cB	836	CLA	O2A-CGA-CBA	2.79	120.65	111.91
12	bA	832	F6C	O2A-CGA-CBA	2.78	120.65	111.91
15	aA	849	BCR	C15-C14-C13	-2.78	123.34	127.31
12	cA	830	F6C	C4C-C3C-C2C	-2.78	102.52	106.89
11	bA	821	CLA	C4A-NA-C1A	-2.78	105.45	106.71
11	cA	803	CLA	CMB-C2B-C3B	2.78	133.33	126.59
12	aA	832	F6C	O2A-CGA-CBA	2.78	120.64	111.91
11	cB	813	CLA	CHD-C4C-NC	2.78	128.59	124.20
11	cK	101	CLA	CHD-C4C-NC	2.78	128.59	124.20
15	bA	849	BCR	C15-C14-C13	-2.78	123.34	127.31
11	bA	838	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
11	cA	808	CLA	C4-C3-C5	2.78	119.16	115.98
11	cB	810	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
11	cA	822	CLA	CHD-C4C-NC	2.78	128.58	124.20
11	aA	803	CLA	CMB-C2B-C3B	2.78	133.32	126.59
12	aA	830	F6C	C4C-C3C-C2C	-2.78	102.52	106.89
11	bB	836	CLA	O2A-CGA-CBA	2.78	120.63	111.91
11	bA	840	CLA	CMB-C2B-C1B	2.78	129.60	125.37
11	bB	806	CLA	C3B-C4B-NB	2.78	113.09	110.52
11	aB	813	CLA	CHD-C4C-NC	2.78	128.58	124.20
11	cB	833	CLA	CAC-C3C-C4C	2.78	128.41	124.81
11	aA	802	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
11	aA	821	CLA	C4A-NA-C1A	-2.78	105.46	106.71
11	aB	801	CLA	C4A-NA-C1A	-2.78	105.46	106.71
11	aA	841	CLA	C1-C2-C3	-2.78	122.26	126.75
11	bA	823	CLA	CMB-C2B-C1B	2.78	129.60	125.37
11	aB	810	CLA	C4C-C3C-C2C	-2.78	102.85	106.90
11	cB	815	CLA	CHC-C1C-C2C	-2.78	119.02	126.73
12	cA	832	F6C	O2A-CGA-CBA	2.78	120.62	111.91
11	aB	816	CLA	CHD-C4C-NC	2.78	128.58	124.20
11	aA	824	CLA	C4C-C3C-C2C	-2.78	102.85	106.90
15	aA	850	BCR	C15-C16-C17	-2.78	117.79	123.47
11	aK	101	CLA	CHD-C4C-NC	2.77	128.58	124.20
11	bA	811	CLA	CHD-C4C-NC	2.77	128.58	124.20
11	cA	817	CLA	CHD-C4C-NC	2.77	128.57	124.20
11	aA	838	CLA	C4C-C3C-C2C	-2.77	102.85	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cB	835	CLA	CHD-C4C-NC	2.77	128.57	124.20
15	cA	849	BCR	C15-C14-C13	-2.77	123.35	127.31
11	cB	802	CLA	CHB-C1B-C2B	-2.77	119.40	127.24
11	cB	818	CLA	C4-C3-C5	2.77	119.94	115.27
11	aB	806	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
11	cA	835	CLA	C1-C2-C3	-2.77	121.25	126.04
11	aB	835	CLA	CHD-C4C-NC	2.77	128.57	124.20
11	aB	835	CLA	CAC-C3C-C4C	2.77	128.41	124.81
11	bA	838	CLA	CAC-C3C-C4C	2.77	128.41	124.81
11	bA	809	CLA	CHD-C4C-NC	2.77	128.57	124.20
11	cA	838	CLA	CMC-C2C-C1C	2.77	129.26	125.04
11	aB	815	CLA	CHC-C1C-C2C	-2.77	119.03	126.73
11	bA	803	CLA	CMB-C2B-C3B	2.77	133.30	126.59
15	bB	848	BCR	C27-C26-C25	2.77	126.75	122.73
11	cA	821	CLA	C4A-NA-C1A	-2.77	105.46	106.71
11	cB	820	CLA	C4A-NA-C1A	-2.77	105.46	106.71
15	aL	203	BCR	C7-C8-C9	-2.77	122.05	126.23
11	bK	103	CLA	CMB-C2B-C1B	2.77	129.59	125.37
11	aB	819	CLA	CAC-C3C-C4C	2.77	128.40	124.81
11	bB	815	CLA	C3B-C4B-NB	2.77	113.08	110.52
11	bB	835	CLA	CHD-C4C-NC	2.77	128.56	124.20
11	bB	837	CLA	CAC-C3C-C4C	2.77	128.40	124.81
11	bA	840	CLA	O2A-CGA-CBA	2.77	120.59	111.91
11	cA	814	CLA	CAA-CBA-CGA	-2.77	105.17	113.25
11	cA	802	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
11	cA	818	CLA	C4-C3-C5	2.77	119.92	115.27
11	bB	833	CLA	CAC-C3C-C4C	2.77	128.40	124.81
11	bB	802	CLA	CHB-C1B-C2B	-2.77	119.43	127.24
11	bA	835	CLA	C1-C2-C3	-2.76	121.26	126.04
11	cB	818	CLA	CHD-C4C-NC	2.76	128.56	124.20
11	cA	817	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
11	aB	836	CLA	O2A-CGA-CBA	2.76	120.58	111.91
11	bA	836	CLA	CMB-C2B-C1B	2.76	129.58	125.37
11	bA	817	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
12	bA	830	F6C	C4C-C3C-C2C	-2.76	102.55	106.89
11	bA	802	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
11	bB	817	CLA	C1-O2A-CGA	2.76	123.69	116.44
11	aA	809	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
11	cL	206	CLA	CAC-C3C-C4C	2.76	128.40	124.81
11	bA	814	CLA	CAA-CBA-CGA	-2.76	105.18	113.25
11	cA	803	CLA	C4A-NA-C1A	-2.76	105.46	106.71
11	aA	817	CLA	CHD-C4C-NC	2.76	128.56	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bB	818	CLA	CHD-C4C-NC	2.76	128.56	124.20
11	aA	811	CLA	CAC-C3C-C4C	2.76	128.39	124.81
11	bA	822	CLA	CAC-C3C-C4C	2.76	128.39	124.81
11	bA	841	CLA	C1-C2-C3	-2.76	122.28	126.75
11	cB	825	CLA	CHD-C4C-NC	2.76	128.55	124.20
11	bB	815	CLA	CHC-C1C-C2C	-2.76	119.06	126.73
11	aB	802	CLA	CHB-C1B-C2B	-2.76	119.44	127.24
11	bA	818	CLA	C4-C3-C5	2.76	119.91	115.27
11	bA	809	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
11	bA	839	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
11	aL	206	CLA	CHD-C4C-NC	2.76	128.55	124.20
11	aA	840	CLA	O2A-CGA-CBA	2.76	120.56	111.91
11	cB	839	CLA	CMC-C2C-C1C	2.76	129.24	125.04
11	cB	803	CLA	CHC-C1C-NC	2.76	128.39	124.20
11	cA	836	CLA	CMB-C2B-C1B	2.76	129.57	125.37
11	aA	814	CLA	CAA-CBA-CGA	-2.76	105.20	113.25
11	bK	101	CLA	CHD-C4C-NC	2.76	128.55	124.20
11	bB	816	CLA	CHB-C4A-NA	2.76	128.32	124.51
11	aB	815	CLA	C3B-C4B-NB	2.76	113.07	110.52
11	aA	818	CLA	C4-C3-C5	2.75	119.91	115.27
11	bB	818	CLA	C4-C3-C5	2.75	119.91	115.27
11	aB	808	CLA	CHD-C4C-NC	2.75	128.54	124.20
11	aA	816	CLA	C3B-C4B-NB	2.75	113.07	110.52
11	aA	809	CLA	CHD-C4C-NC	2.75	128.54	124.20
11	cL	206	CLA	CHD-C4C-NC	2.75	128.54	124.20
15	bL	203	BCR	C7-C8-C9	-2.75	122.07	126.23
15	cK	102	BCR	C20-C21-C22	-2.75	123.38	127.31
11	bB	816	CLA	CHD-C4C-NC	2.75	128.54	124.20
11	aB	823	CLA	C1-O2A-CGA	2.75	123.67	116.44
11	aB	803	CLA	CHC-C1C-NC	2.75	128.38	124.20
11	bA	817	CLA	CHD-C4C-NC	2.75	128.54	124.20
11	bB	813	CLA	CHD-C4C-NC	2.75	128.54	124.20
11	cB	808	CLA	CHD-C4C-NC	2.75	128.54	124.20
11	aA	822	CLA	CAC-C3C-C4C	2.75	128.38	124.81
11	bL	206	CLA	CAC-C3C-C4C	2.75	128.38	124.81
11	cA	833	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
11	cK	103	CLA	CMB-C2B-C1B	2.75	129.56	125.37
11	aA	835	CLA	C1-C2-C3	-2.75	121.29	126.04
11	cA	840	CLA	O2A-CGA-CBA	2.75	120.53	111.91
11	cA	841	CLA	C1-C2-C3	-2.75	122.31	126.75
11	bL	204	CLA	CHD-C4C-NC	2.75	128.53	124.20
11	aB	818	CLA	C4-C3-C5	2.75	119.89	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cA	816	CLA	C3B-C4B-NB	2.75	113.06	110.52
11	aA	835	CLA	CAC-C3C-C4C	2.75	128.37	124.81
11	bB	808	CLA	CHD-C4C-NC	2.75	128.53	124.20
11	aB	816	CLA	C3B-C4B-NB	2.74	113.06	110.52
11	cA	809	CLA	CHD-C4C-NC	2.74	128.53	124.20
11	bB	832	CLA	CHB-C1B-NB	-2.74	121.35	124.26
11	aB	823	CLA	CHD-C4C-NC	2.74	128.52	124.20
15	bK	102	BCR	C20-C21-C22	-2.74	123.40	127.31
11	aA	828	CLA	C4-C3-C5	2.74	119.88	115.27
15	bI	101	BCR	C3-C4-C5	-2.74	109.18	114.08
11	aA	823	CLA	CMB-C2B-C1B	2.74	129.54	125.37
12	aB	824	F6C	CAC-C3C-C4C	2.74	128.72	124.92
11	aB	817	CLA	C1-O2A-CGA	2.74	123.63	116.44
11	cB	817	CLA	C1-O2A-CGA	2.74	123.63	116.44
11	aB	806	CLA	C3B-C4B-NB	2.74	113.06	110.52
11	cB	823	CLA	CHD-C4C-NC	2.74	128.52	124.20
11	cA	802	CLA	C1-C2-C3	-2.74	121.31	126.04
11	cB	823	CLA	C1-O2A-CGA	2.74	123.63	116.44
11	bA	808	CLA	C4-C3-C5	2.74	119.11	115.98
15	cL	207	BCR	C15-C16-C17	-2.74	117.87	123.47
11	bA	807	CLA	CMB-C2B-C1B	2.74	129.54	125.37
12	aA	826	F6C	O2A-CGA-CBA	2.74	120.50	111.91
11	aB	816	CLA	CHB-C4A-NA	2.74	128.29	124.51
11	aA	807	CLA	CAA-C2A-C3A	-2.74	105.29	112.78
11	aK	103	CLA	CMB-C2B-C1B	2.73	129.53	125.37
11	cA	811	CLA	CAC-C3C-C4C	2.73	128.36	124.81
11	cB	819	CLA	C4A-NA-C1A	-2.73	105.48	106.71
11	bL	206	CLA	CHD-C4C-NC	2.73	128.51	124.20
11	bB	826	CLA	O2A-CGA-CBA	2.73	120.49	111.91
11	aA	836	CLA	CMB-C2B-C1B	2.73	129.53	125.37
12	bA	832	F6C	CHB-C4A-NA	2.73	126.97	124.45
15	cI	103	BCR	C3-C4-C5	-2.73	109.20	114.08
11	bB	819	CLA	C4A-NA-C1A	-2.73	105.48	106.71
11	cA	822	CLA	CAC-C3C-C4C	2.73	128.35	124.81
11	cA	835	CLA	CAC-C3C-C4C	2.73	128.35	124.81
11	cB	819	CLA	CHD-C4C-NC	2.73	128.51	124.20
15	aL	207	BCR	C15-C16-C17	-2.73	117.88	123.47
12	cA	832	F6C	CHB-C4A-NA	2.73	126.96	124.45
11	aB	826	CLA	O2A-CGA-CBA	2.73	120.47	111.91
11	aA	808	CLA	C4-C3-C5	2.73	119.10	115.98
12	bB	824	F6C	CAC-C3C-C4C	2.73	128.70	124.92
11	aB	829	CLA	CMC-C2C-C1C	2.73	129.19	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aA	833	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
11	bB	819	CLA	CHD-C4C-NC	2.73	128.50	124.20
15	aK	102	BCR	C20-C21-C22	-2.73	123.42	127.31
11	bA	802	CLA	CHA-C1A-NA	-2.73	120.15	126.40
11	bB	823	CLA	C1-O2A-CGA	2.73	123.60	116.44
11	bB	803	CLA	CHC-C1C-NC	2.73	128.34	124.20
12	cB	824	F6C	CHB-C4A-NA	2.73	126.96	124.45
15	aL	207	BCR	C27-C26-C25	2.73	126.69	122.73
11	bB	840	CLA	CBC-CAC-C3C	-2.73	104.91	112.43
12	bA	844	F6C	C4-C3-C5	2.73	119.86	115.27
10	aA	801	CL0	CHB-C1B-NB	-2.73	121.37	124.26
11	aB	829	CLA	CHB-C1B-NB	-2.73	121.37	124.26
11	cL	204	CLA	CHD-C4C-NC	2.73	128.50	124.20
11	bA	808	CLA	CHD-C4C-NC	2.73	128.50	124.20
11	bA	833	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
15	bL	207	BCR	C15-C16-C17	-2.73	117.89	123.47
11	cA	807	CLA	CAA-C2A-C3A	-2.73	105.31	112.78
12	bA	826	F6C	O2A-CGA-CBA	2.73	120.46	111.91
11	aL	205	CLA	CHD-C4C-NC	2.72	128.50	124.20
11	bA	822	CLA	CMC-C2C-C1C	2.72	129.19	125.04
12	aA	844	F6C	C4-C3-C5	2.72	119.85	115.27
12	cA	826	F6C	O2A-CGA-CBA	2.72	120.46	111.91
11	cB	806	CLA	C3B-C4B-NB	2.72	113.04	110.52
11	bB	839	CLA	CMC-C2C-C1C	2.72	129.19	125.04
11	bA	835	CLA	CAC-C3C-C4C	2.72	128.34	124.81
11	aA	808	CLA	CHD-C4C-NC	2.72	128.49	124.20
11	bA	816	CLA	C3B-C4B-NB	2.72	113.04	110.52
11	aB	805	CLA	CHD-C4C-NC	2.72	128.49	124.20
11	aB	812	CLA	CMC-C2C-C1C	2.72	129.18	125.04
11	cA	822	CLA	CMC-C2C-C1C	2.72	129.18	125.04
11	cA	808	CLA	CHD-C4C-NC	2.72	128.49	124.20
11	cB	816	CLA	CHD-C4C-NC	2.72	128.49	124.20
11	cA	839	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
11	cA	823	CLA	CMB-C2B-C1B	2.72	129.51	125.37
15	aI	101	BCR	C3-C4-C5	-2.72	109.22	114.08
11	bA	837	CLA	CAC-C3C-C4C	2.72	128.34	124.81
11	cB	813	CLA	CAC-C3C-C4C	2.72	128.34	124.81
11	aB	840	CLA	CBC-CAC-C3C	-2.72	104.93	112.43
11	aA	807	CLA	CMB-C2B-C1B	2.72	129.51	125.37
11	cA	807	CLA	CMB-C2B-C1B	2.72	129.51	125.37
11	cB	829	CLA	CHB-C1B-NB	-2.72	121.38	124.26
11	cB	826	CLA	O2A-CGA-CBA	2.72	120.44	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aB	813	CLA	CAC-C3C-C4C	2.72	128.34	124.81
11	cB	840	CLA	CBC-CAC-C3C	-2.72	104.94	112.43
11	cB	819	CLA	C3B-C4B-NB	2.72	113.04	110.52
11	aA	839	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
12	bA	827	F6C	C4C-C3C-C2C	-2.72	102.62	106.89
11	aB	819	CLA	C4A-NA-C1A	-2.72	105.48	106.71
11	aB	818	CLA	CHD-C4C-NC	2.72	128.49	124.20
11	cB	816	CLA	C3B-C4B-NB	2.72	113.04	110.52
11	bB	825	CLA	CHD-C4C-NC	2.72	128.49	124.20
11	bB	813	CLA	CHB-C4A-NA	2.72	128.27	124.51
11	aB	839	CLA	CMC-C2C-C1C	2.72	129.18	125.04
11	aL	204	CLA	CHD-C4C-NC	2.72	128.48	124.20
15	bI	101	BCR	C11-C10-C9	-2.72	123.43	127.31
15	bL	207	BCR	C27-C26-C25	2.72	126.67	122.73
11	aB	832	CLA	CHB-C1B-NB	-2.72	121.38	124.26
11	cA	820	CLA	C1-C2-C3	-2.72	121.35	126.04
12	cA	844	F6C	C4-C3-C5	2.71	119.84	115.27
11	bA	807	CLA	CAA-C2A-C3A	-2.71	105.34	112.78
11	aB	819	CLA	CHD-C4C-NC	2.71	128.48	124.20
11	cB	832	CLA	CHB-C1B-NB	-2.71	121.38	124.26
11	aA	802	CLA	C11-C12-C13	-2.71	107.15	115.92
11	aA	817	CLA	C4C-C3C-C2C	-2.71	102.94	106.90
12	aA	844	F6C	OMB-CMB-C2B	-2.71	119.55	125.69
12	bA	830	F6C	OMB-CMB-C2B	-2.71	119.55	125.69
11	cA	843	CLA	CHD-C4C-NC	2.71	128.48	124.20
11	cB	829	CLA	CMC-C2C-C1C	2.71	129.17	125.04
11	cA	834	CLA	C4-C3-C5	2.71	119.83	115.27
11	aA	822	CLA	CMC-C2C-C1C	2.71	129.17	125.04
11	aB	822	CLA	CMB-C2B-C1B	2.71	129.50	125.37
11	bB	822	CLA	CMB-C2B-C1B	2.71	129.50	125.37
11	bA	802	CLA	C11-C12-C13	-2.71	107.16	115.92
11	bA	805	CLA	CHC-C1C-C2C	-2.71	119.20	126.73
11	aB	825	CLA	CHD-C4C-NC	2.71	128.47	124.20
11	bB	823	CLA	CHD-C4C-NC	2.71	128.47	124.20
12	bB	824	F6C	CHB-C4A-NA	2.71	126.94	124.45
11	cL	205	CLA	CHD-C4C-NC	2.71	128.47	124.20
11	bA	811	CLA	CAC-C3C-C4C	2.71	128.32	124.81
11	cA	809	CLA	CHB-C4A-NA	2.71	128.26	124.51
11	cA	805	CLA	CHC-C1C-C2C	-2.71	119.21	126.73
11	cA	828	CLA	C4-C3-C5	2.71	119.82	115.27
11	bB	802	CLA	CHC-C1C-C2C	-2.71	119.22	126.73
12	aA	830	F6C	OMB-CMB-C2B	-2.70	119.57	125.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	827	F6C	C4C-C3C-C2C	-2.70	102.64	106.89
11	cA	828	CLA	CAC-C3C-C4C	2.70	128.32	124.81
11	bB	805	CLA	CHD-C4C-NC	2.70	128.46	124.20
11	cB	825	CLA	C4-C3-C5	2.70	119.82	115.27
11	aB	812	CLA	C1-C2-C3	-2.70	121.37	126.04
11	bA	802	CLA	C1-C2-C3	-2.70	121.37	126.04
12	cB	824	F6C	CAC-C3C-C4C	2.70	128.67	124.92
11	bB	825	CLA	C4-C3-C5	2.70	119.82	115.27
11	cA	837	CLA	CAC-C3C-C4C	2.70	128.32	124.81
11	aA	806	CLA	CMB-C2B-C1B	2.70	129.49	125.37
11	cB	813	CLA	CHB-C4A-NA	2.70	128.25	124.51
11	cA	805	CLA	C3B-C4B-NB	2.70	113.02	110.52
11	bA	813	CLA	CHD-C4C-NC	2.70	128.46	124.20
11	cA	806	CLA	CMB-C2B-C1B	2.70	129.48	125.37
11	bB	805	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
11	cA	802	CLA	C11-C12-C13	-2.70	107.19	115.92
11	aA	815	CLA	CAC-C3C-C4C	2.70	128.31	124.81
11	cB	820	CLA	CMC-C2C-C1C	2.70	129.15	125.04
11	bA	828	CLA	C4-C3-C5	2.70	119.81	115.27
11	bA	803	CLA	C4A-NA-C1A	-2.70	105.49	106.71
12	cA	830	F6C	OMB-CMB-C2B	-2.70	119.58	125.69
11	bA	816	CLA	CHD-C4C-NC	2.70	128.46	124.20
11	cB	822	CLA	CMB-C2B-C1B	2.70	129.48	125.37
11	bB	819	CLA	C3B-C4B-NB	2.70	113.02	110.52
11	aA	802	CLA	C1-C2-C3	-2.70	121.38	126.04
11	bA	831	CLA	C4-C3-C5	2.70	119.81	115.27
13	bB	841	PQN	C14-C13-C15	2.70	119.81	115.27
12	aA	827	F6C	C4C-C3C-C2C	-2.70	102.65	106.89
11	bB	812	CLA	C1-C2-C3	-2.70	121.38	126.04
11	aA	828	CLA	CAC-C3C-C4C	2.70	128.31	124.81
15	cB	845	BCR	C27-C26-C25	2.70	126.65	122.73
15	cI	103	BCR	C11-C10-C9	-2.70	123.46	127.31
11	cB	805	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
11	aB	813	CLA	CHB-C4A-NA	2.70	128.24	124.51
11	bA	804	CLA	CMB-C2B-C1B	2.70	129.48	125.37
11	cB	839	CLA	CHC-C1C-C2C	-2.70	119.24	126.73
11	bA	828	CLA	CAC-C3C-C4C	2.70	128.31	124.81
11	aB	826	CLA	CHD-C4C-NC	2.70	128.45	124.20
11	bA	814	CLA	CHD-C4C-NC	2.70	128.45	124.20
11	cA	816	CLA	CHD-C4C-NC	2.69	128.45	124.20
11	bA	805	CLA	C3B-C4B-NB	2.69	113.02	110.52
15	aI	101	BCR	C11-C10-C9	-2.69	123.47	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	844	F6C	OMB-CMB-C2B	-2.69	119.60	125.69
11	cB	838	CLA	CHD-C4C-NC	2.69	128.45	124.20
11	aB	825	CLA	C4-C3-C5	2.69	119.80	115.27
11	bA	809	CLA	CHB-C4A-NA	2.69	128.24	124.51
11	bB	812	CLA	CMC-C2C-C1C	2.69	129.14	125.04
11	cB	802	CLA	CHC-C1C-C2C	-2.69	119.25	126.73
11	bB	812	CLA	O2A-CGA-CBA	2.69	120.36	111.91
15	bB	845	BCR	C27-C26-C25	2.69	126.64	122.73
11	bB	839	CLA	CAC-C3C-C4C	2.69	128.30	124.81
11	aA	805	CLA	CHC-C1C-C2C	-2.69	119.25	126.73
11	bA	843	CLA	CHD-C4C-NC	2.69	128.44	124.20
11	cA	813	CLA	CHD-C4C-NC	2.69	128.44	124.20
11	cA	802	CLA	CHA-C1A-NA	-2.69	120.23	126.40
12	cA	832	F6C	CAC-C3C-C4C	2.69	128.65	124.92
11	bB	826	CLA	CHD-C4C-NC	2.69	128.44	124.20
11	cB	816	CLA	CHB-C4A-NA	2.69	128.23	124.51
11	bA	834	CLA	C4-C3-C5	2.69	119.79	115.27
11	bB	829	CLA	CHB-C1B-NB	-2.69	121.41	124.26
11	bA	810	CLA	CMB-C2B-C1B	2.69	129.46	125.37
11	bA	803	CLA	CHD-C4C-NC	2.69	128.44	124.20
12	cA	844	F6C	OMB-CMB-C2B	-2.69	119.61	125.69
11	bB	829	CLA	CMC-C2C-C1C	2.69	129.13	125.04
11	cB	812	CLA	C1-C2-C3	-2.69	121.39	126.04
11	aA	802	CLA	CHA-C1A-NA	-2.69	120.24	126.40
11	aA	834	CLA	C4-C3-C5	2.69	119.79	115.27
11	bA	828	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
11	aA	820	CLA	C1-C2-C3	-2.69	121.40	126.04
11	cB	806	CLA	C1-C2-C3	-2.69	121.40	126.04
11	bL	205	CLA	CHD-C4C-NC	2.69	128.44	124.20
11	cA	828	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
11	aB	806	CLA	C1-C2-C3	-2.69	121.40	126.04
15	cL	207	BCR	C27-C26-C25	2.68	126.63	122.73
11	cB	805	CLA	CHD-C4C-NC	2.68	128.43	124.20
11	aB	812	CLA	O2A-CGA-CBA	2.68	120.33	111.91
11	cB	826	CLA	CHD-C4C-NC	2.68	128.43	124.20
12	aA	826	F6C	C4-C3-C5	2.68	119.79	115.27
11	bA	815	CLA	CAC-C3C-C4C	2.68	128.29	124.81
11	aB	805	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
11	aB	802	CLA	CHC-C1C-C2C	-2.68	119.28	126.73
11	aB	806	CLA	CMC-C2C-C1C	2.68	129.12	125.04
11	aB	831	CLA	CMB-C2B-C1B	2.68	129.46	125.37
10	bA	801	CL0	CHB-C1B-NB	-2.68	121.42	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cB	812	CLA	O2A-CGA-CBA	2.68	120.33	111.91
11	bB	813	CLA	CAC-C3C-C4C	2.68	128.29	124.81
11	cB	812	CLA	CMC-C2C-C1C	2.68	129.12	125.04
11	aA	809	CLA	CHB-C4A-NA	2.68	128.22	124.51
11	aA	816	CLA	CHD-C4C-NC	2.68	128.43	124.20
15	aB	845	BCR	C27-C26-C25	2.68	126.62	122.73
11	aA	828	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
11	cA	815	CLA	CAC-C3C-C4C	2.68	128.29	124.81
11	cA	831	CLA	C4-C3-C5	2.68	119.78	115.27
11	bB	839	CLA	CHC-C1C-C2C	-2.68	119.29	126.73
11	bA	806	CLA	CMB-C2B-C1B	2.68	129.45	125.37
11	cB	806	CLA	CMC-C2C-C1C	2.68	129.12	125.04
11	cA	814	CLA	CHD-C4C-NC	2.68	128.42	124.20
11	bB	806	CLA	C1-C2-C3	-2.68	121.41	126.04
13	aB	841	PQN	C14-C13-C15	2.68	119.77	115.27
11	aA	837	CLA	CAC-C3C-C4C	2.68	128.28	124.81
11	aA	810	CLA	CMB-C2B-C1B	2.68	129.44	125.37
11	aA	839	CLA	CHD-C4C-NC	2.68	128.42	124.20
11	aA	843	CLA	CHD-C4C-NC	2.68	128.42	124.20
11	bB	820	CLA	CMC-C2C-C1C	2.68	129.11	125.04
12	aA	832	F6C	CHB-C4A-NA	2.68	126.91	124.45
12	bA	832	F6C	CAC-C3C-C4C	2.68	128.63	124.92
12	cA	827	F6C	CAC-C3C-C4C	2.68	128.63	124.92
11	aA	831	CLA	C4-C3-C5	2.68	119.77	115.27
11	bA	820	CLA	C1-C2-C3	-2.68	121.42	126.04
11	aA	813	CLA	CHD-C4C-NC	2.68	128.42	124.20
11	bB	838	CLA	CHD-C4C-NC	2.68	128.42	124.20
11	cA	804	CLA	CAC-C3C-C4C	2.68	128.28	124.81
12	bA	830	F6C	C4-C3-C5	2.68	119.77	115.27
11	cA	804	CLA	CMB-C2B-C1B	2.67	129.44	125.37
11	aB	839	CLA	CHC-C1C-C2C	-2.67	119.30	126.73
11	aA	842	CLA	C3B-C4B-NB	2.67	113.00	110.52
10	cA	801	CL0	CHB-C1B-NB	-2.67	121.43	124.26
11	aB	839	CLA	CAC-C3C-C4C	2.67	128.28	124.81
11	bB	816	CLA	C3B-C4B-NB	2.67	112.99	110.52
11	aA	820	CLA	CHD-C4C-NC	2.67	128.41	124.20
11	bB	806	CLA	CMC-C2C-C1C	2.67	129.11	125.04
13	cB	841	PQN	C14-C13-C15	2.67	119.77	115.27
11	cA	802	CLA	O2A-CGA-CBA	2.67	120.29	111.91
11	bB	801	CLA	C4A-NA-C1A	-2.67	105.50	106.71
11	cB	806	CLA	C4-C3-C5	2.67	119.76	115.27
12	bA	826	F6C	C4-C3-C5	2.67	119.76	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cA	805	CLA	CHB-C4A-NA	2.67	128.21	124.51
11	cB	819	CLA	CMB-C2B-C1B	2.67	129.44	125.37
11	cB	831	CLA	CMB-C2B-C1B	2.67	129.44	125.37
11	bB	828	CLA	C1-C2-C3	-2.67	121.43	126.04
12	cA	830	F6C	C4-C3-C5	2.67	119.76	115.27
11	cA	810	CLA	CMB-C2B-C1B	2.67	129.43	125.37
12	cA	844	F6C	CHB-C4A-NA	2.67	126.91	124.45
11	aA	802	CLA	O2A-CGA-CBA	2.67	120.28	111.91
11	cB	801	CLA	C4A-NA-C1A	-2.67	105.51	106.71
12	aA	827	F6C	O2A-CGA-CBA	2.67	120.28	111.91
12	cA	826	F6C	C4-C3-C5	2.67	119.76	115.27
11	cB	804	CLA	CHC-C1C-C2C	-2.67	119.33	126.73
11	bA	836	CLA	O2D-CGD-CBD	2.67	116.00	111.27
11	bA	839	CLA	CHD-C4C-NC	2.67	128.40	124.20
11	cB	839	CLA	CAC-C3C-C4C	2.67	128.27	124.81
11	cA	824	CLA	O2A-CGA-CBA	2.67	120.27	111.91
11	aA	814	CLA	CHD-C4C-NC	2.66	128.40	124.20
12	bA	827	F6C	CAC-C3C-C4C	2.66	128.61	124.92
11	aB	828	CLA	C1-C2-C3	-2.66	121.44	126.04
11	bB	804	CLA	CHC-C1C-C2C	-2.66	119.33	126.73
15	aB	844	BCR	C27-C26-C25	2.66	126.59	122.73
12	aA	832	F6C	CAC-C3C-C4C	2.66	128.61	124.92
15	cB	844	BCR	C27-C26-C25	2.66	126.59	122.73
12	aA	830	F6C	C4-C3-C5	2.66	119.75	115.27
11	cA	839	CLA	CHD-C4C-NC	2.66	128.39	124.20
12	aA	830	F6C	C4A-NA-C1A	-2.66	104.45	106.33
12	bA	827	F6C	O2A-CGA-CBA	2.66	120.25	111.91
11	aA	805	CLA	C3B-C4B-NB	2.66	112.98	110.52
11	aB	819	CLA	C3B-C4B-NB	2.66	112.98	110.52
11	aB	804	CLA	CHC-C1C-C2C	-2.66	119.35	126.73
11	aA	803	CLA	CHD-C4C-NC	2.66	128.39	124.20
11	bA	807	CLA	O2A-CGA-CBA	2.66	120.25	111.91
11	aA	813	CLA	C3B-C4B-NB	2.66	112.98	110.52
12	aA	830	F6C	CAC-C3C-C4C	2.66	128.60	124.92
15	cK	102	BCR	C15-C14-C13	-2.66	123.52	127.31
11	bB	830	CLA	CHD-C4C-NC	2.66	128.39	124.20
11	bA	824	CLA	O2A-CGA-CBA	2.65	120.24	111.91
11	aA	823	CLA	C4C-C3C-C2C	-2.65	103.03	106.90
11	bB	806	CLA	C4-C3-C5	2.65	119.73	115.27
11	cA	802	CLA	C4-C3-C5	2.65	119.73	115.27
11	aA	806	CLA	CHD-C4C-NC	2.65	128.38	124.20
11	aA	824	CLA	O2A-CGA-CBA	2.65	120.23	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cB	828	CLA	C1-C2-C3	-2.65	121.45	126.04
11	aA	804	CLA	CAC-C3C-C4C	2.65	128.25	124.81
12	aB	824	F6C	CHB-C4A-NA	2.65	126.89	124.45
15	aK	102	BCR	C15-C14-C13	-2.65	123.53	127.31
12	cA	827	F6C	O2A-CGA-CBA	2.65	120.23	111.91
11	aA	807	CLA	O2A-CGA-CBA	2.65	120.23	111.91
12	cA	830	F6C	CAC-C3C-C4C	2.65	128.59	124.92
11	aB	820	CLA	CMC-C2C-C1C	2.65	129.07	125.04
11	bA	831	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
11	cA	831	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
11	cA	823	CLA	C4C-C3C-C2C	-2.65	103.04	106.90
12	aA	827	F6C	CAC-C3C-C4C	2.65	128.59	124.92
11	aB	801	CLA	CHB-C1B-NB	-2.65	121.45	124.26
11	bA	820	CLA	CHD-C4C-NC	2.65	128.38	124.20
11	bA	823	CLA	C4C-C3C-C2C	-2.65	103.04	106.90
11	bA	802	CLA	O2A-CGA-CBA	2.65	120.21	111.91
12	bA	844	F6C	CHB-C4A-NA	2.65	126.89	124.45
11	aB	830	CLA	CHD-C4C-NC	2.64	128.37	124.20
11	bA	815	CLA	CHD-C4C-NC	2.64	128.37	124.20
11	aK	103	CLA	CHD-C4C-NC	2.64	128.37	124.20
11	cA	803	CLA	CHD-C4C-NC	2.64	128.37	124.20
11	aB	819	CLA	CMB-C2B-C1B	2.64	129.40	125.37
11	cA	841	CLA	CMB-C2B-C1B	2.64	129.40	125.37
12	bA	830	F6C	CAC-C3C-C4C	2.64	128.59	124.92
11	cA	807	CLA	O2A-CGA-CBA	2.64	120.20	111.91
11	aB	822	CLA	CHC-C1C-C2C	-2.64	119.39	126.73
11	aB	838	CLA	CHD-C4C-NC	2.64	128.37	124.20
11	cA	836	CLA	O2D-CGD-CBD	2.64	115.96	111.27
11	bB	831	CLA	CMB-C2B-C1B	2.64	129.39	125.37
18	cB	847	LMG	O1-C1-C2	-2.64	104.18	108.30
11	bB	811	CLA	CAA-C2A-C3A	-2.64	105.55	112.78
11	aB	806	CLA	C4-C3-C5	2.64	119.71	115.27
11	bB	822	CLA	CHC-C1C-C2C	-2.64	119.40	126.73
11	cB	821	CLA	CHD-C4C-NC	2.64	128.36	124.20
11	bB	819	CLA	CMB-C2B-C1B	2.64	129.39	125.37
11	aB	820	CLA	C4A-NA-C1A	-2.64	105.52	106.71
11	cB	803	CLA	CMB-C2B-C1B	2.64	129.39	125.37
11	cA	802	CLA	CHB-C1B-C2B	-2.64	119.79	127.24
11	bA	805	CLA	CHB-C4A-NA	2.64	128.16	124.51
15	bB	844	BCR	C27-C26-C25	2.64	126.56	122.73
11	bA	841	CLA	CHD-C4C-NC	2.64	128.36	124.20
11	bB	811	CLA	CHD-C4C-NC	2.64	128.36	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bA	802	CLA	C4-C3-C5	2.64	119.71	115.27
11	cA	812	CLA	CMB-C2B-C1B	2.64	129.38	125.37
11	cA	813	CLA	C3B-C4B-NB	2.64	112.96	110.52
11	cA	842	CLA	C3B-C4B-NB	2.64	112.96	110.52
15	cB	845	BCR	C15-C14-C13	-2.64	123.55	127.31
11	bA	806	CLA	CHD-C4C-NC	2.64	128.36	124.20
11	cK	103	CLA	CHD-C4C-NC	2.64	128.36	124.20
12	aB	824	F6C	C4A-NA-C1A	-2.64	104.46	106.33
11	bA	809	CLA	CMC-C2C-C1C	2.64	129.05	125.04
11	aA	804	CLA	CMB-C2B-C1B	2.63	129.38	125.37
11	cA	820	CLA	CHD-C4C-NC	2.63	128.35	124.20
11	aB	803	CLA	CHB-C1B-NB	-2.63	121.47	124.26
11	cB	822	CLA	CHC-C1C-C2C	-2.63	119.42	126.73
11	aB	821	CLA	CHD-C4C-NC	2.63	128.35	124.20
11	aB	811	CLA	CAA-C2A-C3A	-2.63	105.57	112.78
15	bK	102	BCR	C15-C14-C13	-2.63	123.56	127.31
11	aA	841	CLA	CHD-C4C-NC	2.63	128.35	124.20
11	cA	835	CLA	CMC-C2C-C1C	2.63	129.04	125.04
11	bA	842	CLA	C3B-C4B-NB	2.63	112.95	110.52
12	aB	824	F6C	CHC-C1C-NC	2.63	127.04	124.26
11	cB	830	CLA	CHD-C4C-NC	2.63	128.34	124.20
11	bA	840	CLA	CMC-C2C-C1C	2.63	129.04	125.04
11	cB	811	CLA	CAA-C2A-C3A	-2.63	105.58	112.78
11	bA	802	CLA	CHB-C1B-C2B	-2.63	119.82	127.24
11	bB	808	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
11	bL	205	CLA	CMB-C2B-C1B	2.63	129.37	125.37
11	cA	806	CLA	CHD-C4C-NC	2.63	128.34	124.20
11	aA	809	CLA	CMC-C2C-C1C	2.63	129.04	125.04
11	cL	204	CLA	CAC-C3C-C4C	2.63	128.22	124.81
11	cA	841	CLA	CHD-C4C-NC	2.63	128.34	124.20
12	aL	202	F6C	CHB-C4A-NA	2.62	126.87	124.45
12	bB	824	F6C	CHC-C1C-NC	2.62	127.03	124.26
11	bA	812	CLA	CMB-C2B-C1B	2.62	129.36	125.37
11	bL	204	CLA	CAC-C3C-C4C	2.62	128.21	124.81
15	aB	845	BCR	C15-C14-C13	-2.62	123.57	127.31
11	bA	819	CLA	O2A-CGA-CBA	2.62	120.14	111.91
11	bB	821	CLA	CHD-C4C-NC	2.62	128.34	124.20
11	bB	803	CLA	CMB-C2B-C1B	2.62	129.36	125.37
11	cA	819	CLA	O2A-CGA-CBA	2.62	120.14	111.91
11	bA	836	CLA	CHD-C4C-NC	2.62	128.34	124.20
11	cA	836	CLA	CHD-C4C-NC	2.62	128.34	124.20
11	aA	840	CLA	CAA-CBA-CGA	-2.62	105.59	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bB	828	CLA	C4-C3-C5	2.62	119.68	115.27
11	cB	837	CLA	C3B-C4B-NB	2.62	112.95	110.52
11	aA	831	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
11	bB	813	CLA	C4A-NA-C1A	-2.62	105.53	106.71
11	aA	812	CLA	CMB-C2B-C1B	2.62	129.36	125.37
11	bA	804	CLA	CAC-C3C-C4C	2.62	128.21	124.81
11	bA	840	CLA	CAA-CBA-CGA	-2.62	105.60	113.25
11	aA	819	CLA	O2A-CGA-CBA	2.62	120.13	111.91
11	bA	821	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
12	cB	824	F6C	C4A-NA-C1A	-2.62	104.47	106.33
11	aA	802	CLA	C4-C3-C5	2.62	119.67	115.27
11	cB	801	CLA	CHB-C4A-NA	2.62	128.13	124.51
11	bA	837	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
11	cB	801	CLA	CHB-C1B-NB	-2.62	121.49	124.26
11	aA	815	CLA	CHD-C4C-NC	2.62	128.33	124.20
11	aA	836	CLA	O2D-CGD-CBD	2.62	115.92	111.27
11	bK	103	CLA	CHD-C4C-NC	2.62	128.33	124.20
11	cA	815	CLA	CHD-C4C-NC	2.62	128.33	124.20
11	bB	820	CLA	C4A-NA-C1A	-2.62	105.53	106.71
11	cA	840	CLA	CAA-CBA-CGA	-2.62	105.61	113.25
11	aB	828	CLA	C4-C3-C5	2.61	119.67	115.27
11	aL	204	CLA	CAC-C3C-C4C	2.61	128.20	124.81
18	bB	847	LMG	O1-C1-C2	-2.61	104.22	108.30
11	aA	805	CLA	CHB-C4A-NA	2.61	128.13	124.51
11	cA	808	CLA	CMC-C2C-C1C	2.61	129.02	125.04
11	bA	841	CLA	CMB-C2B-C1B	2.61	129.35	125.37
11	aB	807	CLA	CAA-C2A-C3A	-2.61	105.62	112.78
11	aB	808	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
11	aA	802	CLA	CHB-C1B-C2B	-2.61	119.86	127.24
15	cB	848	BCR	C37-C22-C21	-2.61	119.26	122.92
11	cA	804	CLA	CAA-C2A-C3A	-2.61	105.62	112.78
11	cB	808	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
11	cA	809	CLA	CMC-C2C-C1C	2.61	129.01	125.04
11	bA	818	CLA	C1-O2A-CGA	2.61	123.29	116.44
11	aA	815	CLA	CHB-C4A-NA	2.61	128.12	124.51
11	cB	813	CLA	C4A-NA-C1A	-2.61	105.53	106.71
11	bB	803	CLA	CHB-C1B-NB	-2.61	121.50	124.26
11	cA	837	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
11	bB	807	CLA	CAA-C2A-C3A	-2.61	105.64	112.78
11	aB	812	CLA	C4-C3-C5	2.61	119.66	115.27
11	cB	807	CLA	CAA-C2A-C3A	-2.61	105.64	112.78
11	aB	820	CLA	CMB-C2B-C1B	2.61	129.34	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	844	F6C	CHB-C4A-NA	2.61	126.85	124.45
11	bA	825	CLA	CHD-C4C-NC	2.61	128.31	124.20
12	bA	830	F6C	C4A-NA-C1A	-2.61	104.48	106.33
11	aA	808	CLA	CMC-C2C-C1C	2.61	129.01	125.04
11	cA	825	CLA	CHD-C4C-NC	2.61	128.31	124.20
11	bB	837	CLA	C3B-C4B-NB	2.61	112.93	110.52
11	bB	838	CLA	CMB-C2B-C1B	2.60	129.34	125.37
12	bA	844	F6C	C4C-C3C-C2C	-2.60	102.80	106.89
11	bA	833	CLA	C1-C2-C3	-2.60	121.54	126.04
11	aA	804	CLA	CAA-C2A-C3A	-2.60	105.65	112.78
11	bA	810	CLA	CHD-C4C-NC	2.60	128.31	124.20
10	cA	801	CL0	CHD-C4C-NC	2.60	128.30	124.20
11	cA	819	CLA	CHC-C1C-C2C	-2.60	119.50	126.73
11	cB	812	CLA	C4-C3-C5	2.60	119.65	115.27
11	bA	815	CLA	CHB-C4A-NA	2.60	128.11	124.51
11	bA	813	CLA	C3B-C4B-NB	2.60	112.93	110.52
11	bA	829	CLA	CHD-C4C-NC	2.60	128.30	124.20
11	cA	818	CLA	C1-O2A-CGA	2.60	123.27	116.44
11	aB	803	CLA	CMB-C2B-C1B	2.60	129.33	125.37
11	bA	825	CLA	CHB-C4A-NA	2.60	128.11	124.51
11	aB	817	CLA	C4C-C3C-C2C	-2.60	103.11	106.90
11	bA	834	CLA	CAC-C3C-C4C	2.60	128.18	124.81
11	bA	819	CLA	CHC-C1C-C2C	-2.60	119.51	126.73
11	aA	825	CLA	CHB-C4A-NA	2.60	128.11	124.51
11	cA	810	CLA	CHD-C4C-NC	2.60	128.30	124.20
11	cA	840	CLA	CMC-C2C-C1C	2.60	129.00	125.04
15	bB	848	BCR	C15-C14-C13	-2.60	123.60	127.31
11	cB	817	CLA	C4C-C3C-C2C	-2.60	103.11	106.90
11	aB	837	CLA	CMC-C2C-C1C	2.60	129.00	125.04
15	bB	845	BCR	C15-C14-C13	-2.60	123.60	127.31
11	aA	810	CLA	CHD-C4C-NC	2.60	128.30	124.20
11	cB	806	CLA	CMB-C2B-C1B	2.60	129.32	125.37
11	aA	819	CLA	CHC-C1C-C2C	-2.60	119.52	126.73
11	bA	818	CLA	CHC-C1C-C2C	-2.60	119.52	126.73
11	aA	841	CLA	CMB-C2B-C1B	2.60	129.32	125.37
11	cB	819	CLA	CHB-C4A-NA	2.60	128.10	124.51
11	aA	840	CLA	CMC-C2C-C1C	2.60	128.99	125.04
11	bA	808	CLA	CMC-C2C-C1C	2.60	128.99	125.04
12	bA	832	F6C	O2D-CGD-O1D	-2.60	118.76	123.84
11	cA	820	CLA	C4C-C3C-C2C	-2.60	103.11	106.90
15	bL	207	BCR	C15-C14-C13	-2.60	123.61	127.31
15	cB	848	BCR	C15-C14-C13	-2.60	123.61	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bK	102	BCR	C38-C26-C27	-2.59	108.63	113.62
11	aB	816	CLA	O2A-CGA-CBA	2.59	120.05	111.91
15	aB	848	BCR	C37-C22-C21	-2.59	119.29	122.92
11	cA	821	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
11	aA	835	CLA	CMC-C2C-C1C	2.59	128.99	125.04
11	bB	820	CLA	CMB-C2B-C1B	2.59	129.32	125.37
11	cB	832	CLA	CHD-C4C-NC	2.59	128.29	124.20
11	bB	819	CLA	CHB-C4A-NA	2.59	128.10	124.51
11	bB	817	CLA	C4C-C3C-C2C	-2.59	103.12	106.90
11	aA	836	CLA	CHD-C4C-NC	2.59	128.29	124.20
11	aA	818	CLA	C1-O2A-CGA	2.59	123.25	116.44
12	cA	832	F6C	O2D-CGD-O1D	-2.59	118.77	123.84
11	cA	840	CLA	C4-C3-C5	2.59	119.63	115.27
18	cB	847	LMG	O1-C7-C8	-2.59	104.65	110.90
11	cB	837	CLA	CMC-C2C-C1C	2.59	128.99	125.04
11	cL	205	CLA	CMB-C2B-C1B	2.59	129.31	125.37
11	bA	804	CLA	CAA-C2A-C3A	-2.59	105.69	112.78
10	aA	801	CL0	CHD-C4C-NC	2.59	128.28	124.20
11	cA	829	CLA	CHD-C4C-NC	2.59	128.28	124.20
11	cB	811	CLA	CHD-C4C-NC	2.59	128.28	124.20
11	cB	803	CLA	CHB-C1B-NB	-2.59	121.52	124.26
12	cA	844	F6C	C4C-C3C-C2C	-2.59	102.82	106.89
11	cA	804	CLA	CMC-C2C-C1C	2.59	128.98	125.04
11	cA	810	CLA	CMC-C2C-C1C	2.59	128.98	125.04
11	aB	813	CLA	C4A-NA-C1A	-2.59	105.54	106.71
11	bB	811	CLA	CMB-C2B-C1B	2.59	129.31	125.37
11	aB	819	CLA	CHB-C4A-NA	2.59	128.09	124.51
11	cA	807	CLA	CMC-C2C-C1C	2.59	128.98	125.04
11	cB	838	CLA	CMB-C2B-C1B	2.59	129.31	125.37
11	aB	838	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
12	aA	844	F6C	C4C-C3C-C2C	-2.59	102.82	106.89
11	cB	829	CLA	CHB-C4A-NA	2.59	128.09	124.51
11	cA	833	CLA	C1-C2-C3	-2.59	121.57	126.04
11	bB	812	CLA	C4-C3-C5	2.59	119.62	115.27
11	cB	837	CLA	CMB-C2B-C1B	2.59	129.31	125.37
11	cB	839	CLA	C1-C2-C3	-2.59	121.57	126.04
11	aA	802	CLA	CBC-CAC-C3C	-2.59	105.30	112.43
11	cB	815	CLA	CMB-C2B-C1B	2.59	129.31	125.37
12	cL	202	F6C	CAA-C2A-C1A	-2.59	120.99	128.11
11	aA	829	CLA	CHD-C4C-NC	2.59	128.28	124.20
18	aB	847	LMG	O1-C1-C2	-2.59	104.27	108.30
12	bL	202	F6C	CAA-C2A-C1A	-2.58	120.99	128.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aA	803	CLA	C4A-NA-C1A	-2.58	105.54	106.71
11	cB	832	CLA	CHB-C4A-NA	2.58	128.09	124.51
11	cB	822	CLA	O2D-CGD-O1D	-2.58	118.78	123.84
15	aB	848	BCR	C15-C14-C13	-2.58	123.62	127.31
11	bA	835	CLA	CMC-C2C-C1C	2.58	128.97	125.04
10	bA	801	CL0	CHD-C4C-NC	2.58	128.28	124.20
11	cA	818	CLA	CHC-C1C-C2C	-2.58	119.55	126.73
11	bB	832	CLA	CHD-C4C-NC	2.58	128.27	124.20
11	aA	807	CLA	CMC-C2C-C1C	2.58	128.97	125.04
11	aA	821	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
11	cB	838	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
12	bB	824	F6C	C4A-NA-C1A	-2.58	104.50	106.33
11	aB	811	CLA	CHD-C4C-NC	2.58	128.27	124.20
11	aA	810	CLA	CMC-C2C-C1C	2.58	128.97	125.04
11	cB	816	CLA	O2A-CGA-CBA	2.58	120.01	111.91
11	cB	814	CLA	CMB-C2B-C1B	2.58	129.30	125.37
15	bB	848	BCR	C37-C22-C21	-2.58	119.31	122.92
11	aA	820	CLA	C4C-C3C-C2C	-2.58	103.14	106.90
11	aB	839	CLA	C1-C2-C3	-2.58	121.58	126.04
11	bB	815	CLA	CMB-C2B-C1B	2.58	129.30	125.37
11	aA	817	CLA	CAC-C3C-C4C	2.58	128.16	124.81
11	aA	834	CLA	CAC-C3C-C4C	2.58	128.16	124.81
11	cB	821	CLA	CAC-C3C-C4C	2.58	128.16	124.81
11	bA	840	CLA	C4-C3-C5	2.58	119.61	115.27
11	aB	829	CLA	CHB-C4A-NA	2.58	128.08	124.51
11	aA	804	CLA	CMC-C2C-C1C	2.58	128.97	125.04
18	aB	847	LMG	O1-C7-C8	-2.58	104.68	110.90
12	aL	202	F6C	CAA-C2A-C1A	-2.58	121.01	128.11
11	aB	806	CLA	CMB-C2B-C1B	2.58	129.29	125.37
15	aL	208	BCR	C15-C16-C17	-2.58	118.19	123.47
11	cA	817	CLA	CAC-C3C-C4C	2.58	128.15	124.81
11	cB	820	CLA	CMB-C2B-C1B	2.58	129.29	125.37
11	aL	205	CLA	CMB-C2B-C1B	2.58	129.29	125.37
12	aA	832	F6C	O2D-CGD-O1D	-2.58	118.80	123.84
11	bA	824	CLA	CAC-C3C-C4C	2.58	128.15	124.81
11	aA	840	CLA	C4-C3-C5	2.58	119.60	115.27
15	aK	102	BCR	C38-C26-C27	-2.57	108.67	113.62
11	bB	831	CLA	C4-C3-C5	2.57	119.60	115.27
11	aB	832	CLA	CHD-C4C-NC	2.57	128.26	124.20
11	bB	837	CLA	CMC-C2C-C1C	2.57	128.96	125.04
11	bB	816	CLA	O2A-CGA-CBA	2.57	119.98	111.91
11	aA	837	CLA	O2D-CGD-O1D	-2.57	118.81	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	bB	847	LMG	O1-C7-C8	-2.57	104.69	110.90
11	cA	802	CLA	CBC-CAC-C3C	-2.57	105.34	112.43
11	cB	828	CLA	C4-C3-C5	2.57	119.60	115.27
11	cA	833	CLA	CAC-C3C-C4C	2.57	128.15	124.81
11	bA	833	CLA	CAC-C3C-C4C	2.57	128.15	124.81
15	cL	207	BCR	C38-C26-C27	-2.57	108.68	113.62
11	bA	804	CLA	CMC-C2C-C1C	2.57	128.96	125.04
11	aA	818	CLA	CHC-C1C-C2C	-2.57	119.59	126.73
11	bA	817	CLA	CAC-C3C-C4C	2.57	128.15	124.81
11	bL	206	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
11	bB	806	CLA	CMB-C2B-C1B	2.57	129.28	125.37
11	bB	829	CLA	C3C-C4C-NC	2.57	113.45	110.57
11	bA	805	CLA	CAA-C2A-C3A	-2.57	105.74	112.78
11	bA	802	CLA	CBC-CAC-C3C	-2.57	105.35	112.43
11	aA	833	CLA	CAC-C3C-C4C	2.57	128.14	124.81
11	cB	801	CLA	CBC-CAC-C3C	-2.57	105.35	112.43
11	cA	805	CLA	CAA-C2A-C3A	-2.57	105.74	112.78
11	bB	829	CLA	CHB-C4A-NA	2.57	128.06	124.51
12	bA	844	F6C	C4A-NA-C1A	-2.57	104.51	106.33
11	bB	826	CLA	CMC-C2C-C1C	2.57	128.95	125.04
11	cB	831	CLA	C4-C3-C5	2.57	119.59	115.27
11	bB	801	CLA	CHB-C1B-NB	-2.57	121.54	124.26
12	cB	824	F6C	O2D-CGD-O1D	-2.57	118.82	123.84
11	cB	817	CLA	C5-C3-C2	-2.57	115.92	121.12
15	aL	207	BCR	C15-C14-C13	-2.57	123.65	127.31
12	bA	832	F6C	C4C-C3C-C2C	-2.57	102.86	106.89
11	cA	834	CLA	CAC-C3C-C4C	2.57	128.14	124.81
11	bB	801	CLA	CBC-CAC-C3C	-2.57	105.36	112.43
11	aA	812	CLA	CHD-C4C-NC	2.57	128.25	124.20
11	aB	838	CLA	CMB-C2B-C1B	2.57	129.28	125.37
13	aA	845	PQN	C2M-C2-C3	-2.57	120.22	124.40
11	cA	825	CLA	CHB-C4A-NA	2.57	128.06	124.51
11	cB	811	CLA	CMB-C2B-C1B	2.56	129.28	125.37
11	aB	801	CLA	CBC-CAC-C3C	-2.56	105.36	112.43
11	aB	803	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
11	bA	807	CLA	CMC-C2C-C1C	2.56	128.94	125.04
11	bB	819	CLA	CMC-C2C-C1C	2.56	128.94	125.04
11	aA	825	CLA	CHD-C4C-NC	2.56	128.24	124.20
12	cA	832	F6C	C4C-C3C-C2C	-2.56	102.86	106.89
11	bA	810	CLA	CMC-C2C-C1C	2.56	128.94	125.04
11	bB	832	CLA	CHB-C4A-NA	2.56	128.06	124.51
12	aA	844	F6C	C4A-NA-C1A	-2.56	104.52	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cA	815	CLA	CHB-C4A-NA	2.56	128.05	124.51
11	aA	841	CLA	CAA-C2A-C3A	-2.56	105.76	112.78
11	bB	814	CLA	CMB-C2B-C1B	2.56	129.27	125.37
12	bB	824	F6C	O2D-CGD-O1D	-2.56	118.83	123.84
11	aB	814	CLA	CMB-C2B-C1B	2.56	129.27	125.37
11	bA	820	CLA	C4C-C3C-C2C	-2.56	103.17	106.90
15	bL	207	BCR	C38-C26-C27	-2.56	108.70	113.62
11	bB	836	CLA	CAA-C2A-C3A	-2.56	105.77	112.78
11	bB	839	CLA	C1-C2-C3	-2.56	121.62	126.04
11	cB	802	CLA	CHD-C4C-NC	2.56	128.24	124.20
11	bB	822	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
11	aB	815	CLA	CMB-C2B-C1B	2.56	129.27	125.37
15	cL	207	BCR	C15-C14-C13	-2.56	123.66	127.31
11	cB	809	CLA	CHD-C4C-NC	2.56	128.23	124.20
12	cA	830	F6C	C4A-NA-C1A	-2.56	104.52	106.33
11	aB	826	CLA	CMC-C2C-C1C	2.56	128.93	125.04
15	cL	208	BCR	C15-C16-C17	-2.56	118.23	123.47
15	aL	207	BCR	C38-C26-C27	-2.56	108.70	113.62
11	aL	206	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
11	bA	837	CLA	CMC-C2C-C1C	2.56	128.93	125.04
11	bA	841	CLA	CAA-C2A-C3A	-2.56	105.78	112.78
11	bA	812	CLA	CHD-C4C-NC	2.56	128.23	124.20
11	aB	837	CLA	C3B-C4B-NB	2.56	112.89	110.52
15	bL	208	BCR	C15-C16-C17	-2.56	118.24	123.47
15	cL	203	BCR	C11-C10-C9	-2.55	123.66	127.31
11	aA	833	CLA	C1-C2-C3	-2.55	121.62	126.04
11	cA	841	CLA	CAA-C2A-C3A	-2.55	105.78	112.78
11	bB	821	CLA	CAC-C3C-C4C	2.55	128.12	124.81
11	cA	837	CLA	CMC-C2C-C1C	2.55	128.93	125.04
13	cA	845	PQN	C2M-C2-C3	-2.55	120.23	124.40
11	bB	801	CLA	CHB-C4A-NA	2.55	128.04	124.51
11	aB	836	CLA	CAA-C2A-C3A	-2.55	105.79	112.78
11	bA	838	CLA	CBC-CAC-C3C	-2.55	105.40	112.43
11	bA	814	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
11	cL	206	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
11	cB	836	CLA	CAA-C2A-C3A	-2.55	105.79	112.78
11	aB	822	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
11	aB	821	CLA	CAC-C3C-C4C	2.55	128.12	124.81
11	aB	831	CLA	C4-C3-C5	2.55	119.56	115.27
11	aB	837	CLA	CMB-C2B-C1B	2.55	129.25	125.37
11	bB	803	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
11	cB	829	CLA	C3C-C4C-NC	2.55	113.43	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	cA	801	CL0	CAC-C3C-C4C	2.55	128.12	124.81
11	aA	814	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
11	aB	827	CLA	CMA-C3A-C2A	-2.55	103.56	113.83
11	aA	807	CLA	CBC-CAC-C3C	-2.55	105.41	112.43
11	aA	805	CLA	CAA-C2A-C3A	-2.55	105.81	112.78
17	cA	853	LMT	O5B-C5B-C4B	2.55	114.32	109.69
11	cB	827	CLA	CMA-C3A-C2A	-2.55	103.56	113.83
11	bA	807	CLA	CBC-CAC-C3C	-2.55	105.41	112.43
11	cA	807	CLA	CBC-CAC-C3C	-2.55	105.41	112.43
12	cB	824	F6C	CHC-C1C-NC	2.55	126.95	124.26
12	cL	202	F6C	CHB-C4A-NA	2.55	126.79	124.45
11	bB	813	CLA	CMB-C2B-C1B	2.54	129.25	125.37
11	aB	832	CLA	CHB-C4A-NA	2.54	128.03	124.51
11	cA	828	CLA	C4A-NA-C1A	-2.54	105.56	106.71
11	cA	802	CLA	CMC-C2C-C1C	2.54	128.91	125.04
11	bB	809	CLA	CHD-C4C-NC	2.54	128.21	124.20
11	aA	839	CLA	CAA-C2A-C3A	-2.54	105.81	112.78
11	aB	811	CLA	CMB-C2B-C1B	2.54	129.24	125.37
11	bB	821	CLA	CMB-C2B-C1B	2.54	129.24	125.37
11	bB	827	CLA	CMA-C3A-C2A	-2.54	103.57	113.83
11	bB	814	CLA	CHD-C4C-NC	2.54	128.21	124.20
11	cB	829	CLA	CHD-C4C-NC	2.54	128.21	124.20
15	cK	102	BCR	C38-C26-C27	-2.54	108.73	113.62
11	bB	811	CLA	CAC-C3C-C4C	2.54	128.11	124.81
12	aA	832	F6C	C4C-C3C-C2C	-2.54	102.89	106.89
11	cA	814	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
11	cB	813	CLA	C1-C2-C3	-2.54	121.65	126.04
11	bB	837	CLA	CMB-C2B-C1B	2.54	129.24	125.37
10	aA	801	CL0	CAC-C3C-C4C	2.54	128.11	124.81
15	aL	203	BCR	C11-C10-C9	-2.54	123.69	127.31
13	bA	845	PQN	C2M-C2-C3	-2.54	120.26	124.40
11	aB	802	CLA	CHD-C4C-NC	2.54	128.21	124.20
11	aB	829	CLA	CHD-C4C-NC	2.54	128.21	124.20
11	cA	812	CLA	CHD-C4C-NC	2.54	128.21	124.20
11	aB	819	CLA	CMC-C2C-C1C	2.54	128.91	125.04
11	aB	821	CLA	CMB-C2B-C1B	2.54	129.24	125.37
11	cA	821	CLA	C1-C2-C3	-2.54	121.65	126.04
12	bA	826	F6C	OMB-CMB-C2B	-2.54	119.95	125.69
16	aA	852	LHG	O8-C23-C24	2.54	119.87	111.91
11	aB	821	CLA	O2A-CGA-CBA	2.54	119.87	111.91
11	aB	817	CLA	C5-C3-C2	-2.54	115.98	121.12
17	bA	853	LMT	O5B-C5B-C4B	2.54	114.30	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cB	814	CLA	CHB-C4A-NA	2.54	128.02	124.51
11	aB	831	CLA	C1-C2-C3	-2.54	121.66	126.04
11	aB	801	CLA	CHB-C4A-NA	2.54	128.02	124.51
11	cB	803	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
11	aA	837	CLA	CMC-C2C-C1C	2.54	128.90	125.04
11	cB	821	CLA	CMB-C2B-C1B	2.54	129.23	125.37
16	bA	852	LHG	O8-C23-C24	2.54	119.86	111.91
11	cB	814	CLA	CHD-C4C-NC	2.54	128.20	124.20
11	cA	838	CLA	CBC-CAC-C3C	-2.53	105.44	112.43
11	bB	814	CLA	CHB-C4A-NA	2.53	128.02	124.51
11	bB	813	CLA	CAA-C2A-C3A	-2.53	105.84	112.78
11	cB	826	CLA	CMC-C2C-C1C	2.53	128.90	125.04
12	aA	832	F6C	C4A-NA-C1A	-2.53	104.53	106.33
11	cA	824	CLA	CAC-C3C-C4C	2.53	128.10	124.81
11	aB	813	CLA	CMB-C2B-C1B	2.53	129.23	125.37
11	cB	813	CLA	CMB-C2B-C1B	2.53	129.23	125.37
11	aA	838	CLA	CBC-CAC-C3C	-2.53	105.45	112.43
11	aB	811	CLA	CAC-C3C-C4C	2.53	128.10	124.81
11	cA	807	CLA	C4C-C3C-C2C	-2.53	103.21	106.90
17	aA	853	LMT	O5B-C5B-C4B	2.53	114.29	109.69
11	cA	839	CLA	CAA-C2A-C3A	-2.53	105.84	112.78
11	cB	807	CLA	CMC-C2C-C1C	2.53	128.90	125.04
11	cA	817	CLA	CBC-CAC-C3C	-2.53	105.45	112.43
11	bB	802	CLA	CHD-C4C-NC	2.53	128.19	124.20
11	bB	817	CLA	C5-C3-C2	-2.53	115.99	121.12
11	bB	821	CLA	O2A-CGA-CBA	2.53	119.85	111.91
11	bA	839	CLA	CAA-C2A-C3A	-2.53	105.85	112.78
11	bB	811	CLA	CHB-C4A-NA	2.53	128.01	124.51
11	bB	838	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
11	bB	813	CLA	C1-C2-C3	-2.53	121.67	126.04
11	aA	814	CLA	CHB-C4A-NA	2.53	128.01	124.51
11	cA	802	CLA	C6-C5-C3	-2.53	106.82	113.45
12	aB	824	F6C	O2D-CGD-O1D	-2.53	118.89	123.84
11	cB	840	CLA	C4C-C3C-C2C	-2.53	103.21	106.90
11	aB	829	CLA	C3C-C4C-NC	2.53	113.41	110.57
11	cA	818	CLA	CHB-C4A-NA	2.53	128.01	124.51
11	cB	811	CLA	CHB-C4A-NA	2.53	128.01	124.51
11	aA	802	CLA	CMC-C2C-C1C	2.53	128.89	125.04
11	aB	814	CLA	CHD-C4C-NC	2.53	128.19	124.20
11	bB	840	CLA	C4C-C3C-C2C	-2.53	103.21	106.90
11	aA	802	CLA	C6-C5-C3	-2.53	106.83	113.45
11	cB	813	CLA	CAA-C2A-C3A	-2.53	105.86	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bA	821	CLA	C1-C2-C3	-2.52	121.68	126.04
11	bB	829	CLA	CHD-C4C-NC	2.52	128.18	124.20
11	aB	813	CLA	CAA-C2A-C3A	-2.52	105.86	112.78
11	aA	824	CLA	CAC-C3C-C4C	2.52	128.09	124.81
12	cA	844	F6C	C4A-NA-C1A	-2.52	104.54	106.33
11	aA	817	CLA	CBC-CAC-C3C	-2.52	105.47	112.43
11	cB	819	CLA	O2A-CGA-CBA	2.52	119.83	111.91
11	aB	813	CLA	C1-C2-C3	-2.52	121.68	126.04
11	cB	811	CLA	CAC-C3C-C4C	2.52	128.08	124.81
11	aB	809	CLA	CHD-C4C-NC	2.52	128.18	124.20
11	aB	814	CLA	CHB-C4A-NA	2.52	128.00	124.51
11	bA	817	CLA	CBC-CAC-C3C	-2.52	105.48	112.43
15	bL	203	BCR	C11-C10-C9	-2.52	123.71	127.31
11	cA	806	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
10	aA	801	CL0	O2D-CGD-O1D	-2.52	118.91	123.84
11	bB	819	CLA	O2A-CGA-CBA	2.52	119.81	111.91
16	cA	852	LHG	O8-C23-C24	2.52	119.81	111.91
11	aB	840	CLA	C4C-C3C-C2C	-2.52	103.23	106.90
11	cB	819	CLA	CMC-C2C-C1C	2.52	128.87	125.04
12	cA	826	F6C	OMB-CMB-C2B	-2.52	119.99	125.69
11	cB	821	CLA	O2A-CGA-CBA	2.52	119.81	111.91
13	cA	845	PQN	C11-C12-C13	-2.52	122.60	126.79
15	bB	846	BCR	C3-C4-C5	-2.52	109.58	114.08
13	aA	845	PQN	C11-C12-C13	-2.52	122.60	126.79
11	cA	814	CLA	CHB-C4A-NA	2.52	127.99	124.51
15	aL	208	BCR	C11-C10-C9	-2.52	123.72	127.31
11	aB	819	CLA	O2A-CGA-CBA	2.52	119.80	111.91
11	bB	831	CLA	C1-C2-C3	-2.51	121.69	126.04
11	bA	802	CLA	CMC-C2C-C1C	2.51	128.87	125.04
12	bL	202	F6C	CHB-C4A-NA	2.51	126.76	124.45
11	bA	802	CLA	C6-C5-C3	-2.51	106.87	113.45
11	aB	807	CLA	CMC-C2C-C1C	2.51	128.86	125.04
10	bA	801	CL0	CAC-C3C-C4C	2.51	128.07	124.81
11	cA	806	CLA	C4C-C3C-C2C	-2.51	103.24	106.90
11	bA	835	CLA	CHB-C4A-NA	2.51	127.98	124.51
10	bA	801	CL0	O2D-CGD-O1D	-2.51	118.93	123.84
12	aA	826	F6C	OMB-CMB-C2B	-2.51	120.02	125.69
11	bA	806	CLA	C4C-C3C-C2C	-2.51	103.24	106.90
15	aA	848	BCR	C27-C26-C25	2.51	126.37	122.73
11	cA	842	CLA	CMC-C2C-C1C	2.50	128.85	125.04
18	cB	847	LMG	C40-C39-C38	-2.50	101.71	114.42
12	aB	824	F6C	C4C-C3C-C2C	-2.50	102.95	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aA	821	CLA	C1-C2-C3	-2.50	121.71	126.04
11	aA	818	CLA	CHB-C4A-NA	2.50	127.97	124.51
11	cA	834	CLA	CHB-C4A-NA	2.50	127.97	124.51
11	aA	806	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
15	cB	846	BCR	C3-C4-C5	-2.50	109.61	114.08
10	cA	801	CL0	O2D-CGD-O1D	-2.50	118.95	123.84
16	cA	852	LHG	C11-C10-C9	-2.50	101.73	114.42
11	aA	834	CLA	CHB-C4A-NA	2.50	127.97	124.51
18	bB	847	LMG	C40-C39-C38	-2.50	101.73	114.42
15	bL	208	BCR	C11-C10-C9	-2.50	123.74	127.31
15	bB	842	BCR	C15-C14-C13	-2.50	123.74	127.31
12	bA	832	F6C	C4A-NA-C1A	-2.50	104.56	106.33
11	cA	828	CLA	CAA-C2A-C3A	-2.50	105.93	112.78
15	aM	101	BCR	C24-C23-C22	-2.50	122.46	126.23
11	bB	827	CLA	CHD-C4C-NC	2.50	128.14	124.20
15	bK	102	BCR	C27-C26-C25	2.50	126.36	122.73
15	cM	101	BCR	C24-C23-C22	-2.50	122.46	126.23
11	cB	827	CLA	CHD-C4C-NC	2.50	128.14	124.20
15	cL	208	BCR	C11-C10-C9	-2.50	123.75	127.31
18	aB	847	LMG	C40-C39-C38	-2.50	101.74	114.42
12	aA	827	F6C	C4A-NA-C1A	-2.50	104.56	106.33
11	cB	815	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
16	bA	852	LHG	C11-C10-C9	-2.50	101.75	114.42
11	aB	811	CLA	CHB-C4A-NA	2.50	127.96	124.51
11	aA	820	CLA	CAA-C2A-C3A	-2.50	105.94	112.78
11	aA	842	CLA	CMC-C2C-C1C	2.50	128.84	125.04
11	bB	807	CLA	CMC-C2C-C1C	2.50	128.84	125.04
11	aA	843	CLA	O2A-CGA-CBA	2.50	119.74	111.91
12	bB	824	F6C	C4C-C3C-C2C	-2.50	102.97	106.89
11	aB	817	CLA	CAC-C3C-C4C	2.49	128.05	124.81
11	aA	829	CLA	O2A-CGA-CBA	2.49	119.74	111.91
11	bA	806	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
16	aA	852	LHG	C11-C10-C9	-2.49	101.77	114.42
11	bA	842	CLA	CMC-C2C-C1C	2.49	128.84	125.04
11	bA	818	CLA	CHB-C4A-NA	2.49	127.96	124.51
11	cB	828	CLA	O2A-CGA-CBA	2.49	119.73	111.91
11	cB	831	CLA	C1-C2-C3	-2.49	121.73	126.04
11	aB	827	CLA	CHD-C4C-NC	2.49	128.13	124.20
11	bB	815	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
11	aA	828	CLA	CHB-C1B-NB	-2.49	121.62	124.26
11	cA	808	CLA	CHB-C4A-NA	2.49	127.96	124.51
11	cA	843	CLA	O2A-CGA-CBA	2.49	119.72	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aB	842	BCR	C15-C14-C13	-2.49	123.75	127.31
11	aB	828	CLA	O2A-CGA-CBA	2.49	119.72	111.91
11	bA	820	CLA	CAA-C2A-C3A	-2.49	105.96	112.78
11	cA	829	CLA	O2A-CGA-CBA	2.49	119.72	111.91
13	bA	845	PQN	C11-C12-C13	-2.49	122.65	126.79
12	cB	824	F6C	C4C-C3C-C2C	-2.49	102.98	106.89
11	bA	831	CLA	CAA-C2A-C3A	-2.49	105.96	112.78
11	bA	829	CLA	O2A-CGA-CBA	2.49	119.72	111.91
11	aA	808	CLA	CHB-C4A-NA	2.49	127.95	124.51
11	bA	820	CLA	C2A-C3A-C4A	-2.49	97.85	101.87
11	bA	807	CLA	C4C-C3C-C2C	-2.49	103.27	106.90
11	cB	833	CLA	CMB-C2B-C1B	2.49	129.16	125.37
11	bA	843	CLA	O2A-CGA-CBA	2.49	119.71	111.91
11	aA	806	CLA	C4C-C3C-C2C	-2.49	103.27	106.90
15	aK	102	BCR	C27-C26-C25	2.49	126.34	122.73
11	bA	802	CLA	C6-C7-C8	-2.49	107.89	115.92
12	bA	827	F6C	C4A-NA-C1A	-2.48	104.57	106.33
11	aA	835	CLA	CHB-C4A-NA	2.48	127.95	124.51
11	bA	814	CLA	CHB-C4A-NA	2.48	127.95	124.51
11	bA	823	CLA	CHB-C4A-NA	2.48	127.95	124.51
15	bM	101	BCR	C24-C23-C22	-2.48	122.48	126.23
11	aA	813	CLA	CMC-C2C-C1C	2.48	128.82	125.04
15	bM	101	BCR	C28-C27-C26	-2.48	109.64	114.08
11	cA	820	CLA	CAA-C2A-C3A	-2.48	105.98	112.78
11	bB	815	CLA	C4-C3-C5	2.48	119.45	115.27
11	aA	823	CLA	CHB-C4A-NA	2.48	127.94	124.51
11	bA	841	CLA	CHB-C4A-NA	2.48	127.94	124.51
11	cB	839	CLA	C4-C3-C5	2.48	119.44	115.27
11	cB	823	CLA	CHA-C1A-NA	-2.48	120.72	126.40
15	aL	207	BCR	C7-C8-C9	-2.48	122.49	126.23
11	aA	807	CLA	C4C-C3C-C2C	-2.48	103.28	106.90
11	aK	101	CLA	CMB-C2B-C1B	2.48	129.15	125.37
12	bL	202	F6C	OMB-CMB-C2B	-2.48	120.08	125.69
11	aB	839	CLA	C4-C3-C5	2.48	119.44	115.27
11	bK	101	CLA	CMB-C2B-C1B	2.48	129.14	125.37
11	aA	828	CLA	CAA-C2A-C3A	-2.48	105.99	112.78
11	aA	814	CLA	C4-C3-C5	2.48	119.44	115.27
15	aM	101	BCR	C28-C27-C26	-2.48	109.65	114.08
15	aB	846	BCR	C3-C4-C5	-2.48	109.65	114.08
11	cA	820	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
11	bA	828	CLA	CAA-C2A-C3A	-2.48	106.00	112.78
11	aB	823	CLA	CHA-C1A-NA	-2.48	120.73	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bA	851	BCR	C27-C26-C25	2.48	126.33	122.73
11	cA	808	CLA	CMB-C2B-C1B	2.48	129.14	125.37
11	cK	101	CLA	CMB-C2B-C1B	2.48	129.14	125.37
11	bA	814	CLA	C4-C3-C5	2.47	119.43	115.27
11	bB	823	CLA	CMB-C2B-C1B	2.47	129.14	125.37
11	bB	834	CLA	CHD-C4C-NC	2.47	128.10	124.20
11	bB	823	CLA	CHA-C1A-NA	-2.47	120.73	126.40
11	aA	823	CLA	CMC-C2C-C1C	2.47	128.81	125.04
11	bB	838	CLA	O2A-CGA-O1A	-2.47	117.35	123.59
11	bA	828	CLA	C4A-NA-C1A	-2.47	105.59	106.71
11	cB	826	CLA	CBA-CAA-C2A	2.47	121.16	113.86
12	cL	202	F6C	OMB-CMB-C2B	-2.47	120.10	125.69
11	aB	826	CLA	CBA-CAA-C2A	2.47	121.16	113.86
11	bB	817	CLA	CAC-C3C-C4C	2.47	128.01	124.81
11	bA	828	CLA	CHB-C1B-NB	-2.47	121.64	124.26
11	aA	831	CLA	CAA-C2A-C3A	-2.47	106.02	112.78
11	bA	820	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
11	cB	837	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
11	cA	828	CLA	CHB-C1B-NB	-2.47	121.64	124.26
11	cA	820	CLA	C2A-C3A-C4A	-2.47	97.88	101.87
11	aA	808	CLA	CMB-C2B-C1B	2.47	129.13	125.37
11	cA	831	CLA	CAA-C2A-C3A	-2.47	106.02	112.78
12	bA	827	F6C	OMB-CMB-C2B	-2.47	120.11	125.69
11	aA	802	CLA	C6-C7-C8	-2.47	107.94	115.92
11	bA	808	CLA	CMB-C2B-C1B	2.47	129.13	125.37
11	cA	835	CLA	CHB-C4A-NA	2.47	127.92	124.51
12	aL	202	F6C	OMB-CMB-C2B	-2.47	120.11	125.69
11	aB	838	CLA	O2A-CGA-O1A	-2.47	117.37	123.59
11	bB	828	CLA	O2A-CGA-CBA	2.47	119.65	111.91
15	cB	842	BCR	C15-C14-C13	-2.47	123.79	127.31
11	aA	828	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
11	aB	823	CLA	CMB-C2B-C1B	2.47	129.12	125.37
12	cA	832	F6C	C4A-NA-C1A	-2.46	104.58	106.33
11	aB	803	CLA	O2A-CGA-CBA	2.46	119.64	111.91
11	aA	809	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
11	cA	829	CLA	CHB-C4A-NA	2.46	127.92	124.51
11	cB	838	CLA	O2A-CGA-O1A	-2.46	117.37	123.59
11	bB	833	CLA	CMB-C2B-C1B	2.46	129.12	125.37
15	cL	207	BCR	C7-C8-C9	-2.46	122.51	126.23
11	bB	812	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
11	cA	802	CLA	C6-C7-C8	-2.46	107.96	115.92
11	bB	826	CLA	CBA-CAA-C2A	2.46	121.13	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cB	823	CLA	CMB-C2B-C1B	2.46	129.12	125.37
11	cB	817	CLA	CAC-C3C-C4C	2.46	128.00	124.81
11	bA	833	CLA	CBC-CAC-C3C	-2.46	105.65	112.43
15	cA	851	BCR	C27-C26-C25	2.46	126.30	122.73
15	cK	102	BCR	C27-C26-C25	2.46	126.30	122.73
11	cA	823	CLA	CHB-C4A-NA	2.46	127.91	124.51
11	cA	813	CLA	CMC-C2C-C1C	2.46	128.78	125.04
11	bA	809	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
11	cA	829	CLA	CMC-C2C-C1C	2.46	128.78	125.04
11	bA	834	CLA	CHB-C4A-NA	2.46	127.91	124.51
11	cB	801	CLA	C4-C3-C5	2.46	119.41	115.27
11	bA	823	CLA	CMC-C2C-C1C	2.46	128.78	125.04
15	bA	848	BCR	C27-C26-C25	2.46	126.30	122.73
11	cA	819	CLA	CBA-CAA-C2A	2.46	121.12	113.86
11	aB	804	CLA	CHB-C4A-NA	2.46	127.91	124.51
11	bB	830	CLA	CAA-C2A-C3A	-2.46	106.05	112.78
11	cB	815	CLA	C4-C3-C5	2.46	119.41	115.27
11	aA	833	CLA	CBC-CAC-C3C	-2.46	105.66	112.43
11	cA	833	CLA	CBC-CAC-C3C	-2.46	105.66	112.43
11	aA	819	CLA	CBA-CAA-C2A	2.46	121.11	113.86
11	bA	841	CLA	CMC-C2C-C1C	2.46	128.78	125.04
11	bA	829	CLA	CHB-C4A-NA	2.46	127.91	124.51
11	aB	833	CLA	CMB-C2B-C1B	2.46	129.11	125.37
11	aB	815	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
12	cA	827	F6C	OMB-CMB-C2B	-2.45	120.14	125.69
11	bB	803	CLA	O2A-CGA-CBA	2.45	119.61	111.91
15	aB	848	BCR	C7-C8-C9	-2.45	122.53	126.23
11	bA	834	CLA	O2A-CGA-CBA	2.45	119.61	111.91
15	cM	101	BCR	C28-C27-C26	-2.45	109.70	114.08
11	cA	834	CLA	O2A-CGA-CBA	2.45	119.60	111.91
11	bA	819	CLA	CBA-CAA-C2A	2.45	121.10	113.86
11	bB	839	CLA	C4-C3-C5	2.45	119.40	115.27
11	cB	834	CLA	CHD-C4C-NC	2.45	128.07	124.20
11	cB	830	CLA	CAA-C2A-C3A	-2.45	106.06	112.78
11	aB	805	CLA	C4-C3-C5	2.45	119.39	115.27
15	cA	848	BCR	C27-C26-C25	2.45	126.29	122.73
11	bB	801	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
11	aA	812	CLA	CHB-C4A-NA	2.45	127.90	124.51
11	cA	841	CLA	CMC-C2C-C1C	2.45	128.77	125.04
11	cA	841	CLA	CHB-C4A-NA	2.45	127.90	124.51
11	aA	825	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
11	aB	812	CLA	O2D-CGD-O1D	-2.45	119.05	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cA	812	CLA	CHB-C4A-NA	2.45	127.90	124.51
15	cB	848	BCR	C7-C8-C9	-2.45	122.53	126.23
13	cB	841	PQN	C2M-C2-C3	-2.45	120.41	124.40
11	aA	821	CLA	CHD-C4C-NC	2.45	128.06	124.20
11	bA	813	CLA	CMC-C2C-C1C	2.45	128.77	125.04
11	cA	814	CLA	C4-C3-C5	2.45	119.39	115.27
11	aA	834	CLA	O2A-CGA-CBA	2.45	119.59	111.91
11	aA	820	CLA	C2A-C3A-C4A	-2.45	97.92	101.87
12	aA	827	F6C	OMB-CMB-C2B	-2.45	120.16	125.69
13	aB	841	PQN	C2M-C2-C3	-2.44	120.41	124.40
11	cA	809	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
11	aA	842	CLA	CAC-C3C-C4C	2.44	127.98	124.81
11	cB	803	CLA	O2A-CGA-CBA	2.44	119.58	111.91
15	bL	207	BCR	C7-C8-C9	-2.44	122.54	126.23
11	cA	816	CLA	CAA-C2A-C3A	-2.44	106.09	112.78
11	aK	103	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
13	bB	841	PQN	C2M-C2-C3	-2.44	120.41	124.40
11	cA	821	CLA	CHD-C4C-NC	2.44	128.05	124.20
11	aA	829	CLA	CHB-C4A-NA	2.44	127.89	124.51
11	aA	803	CLA	C4-C3-C5	2.44	119.38	115.27
11	bB	801	CLA	C4-C3-C5	2.44	119.38	115.27
12	cA	844	F6C	O2A-CGA-CBA	2.44	119.57	111.91
11	cA	842	CLA	CAC-C3C-C4C	2.44	127.98	124.81
11	bA	816	CLA	CAA-C2A-C3A	-2.44	106.09	112.78
12	aA	844	F6C	O2A-CGA-CBA	2.44	119.57	111.91
11	bA	829	CLA	CMC-C2C-C1C	2.44	128.75	125.04
11	aA	841	CLA	CHB-C4A-NA	2.44	127.89	124.51
12	bA	844	F6C	O2A-CGA-CBA	2.44	119.56	111.91
11	cB	804	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
12	cA	827	F6C	CHB-C4A-NA	2.44	126.69	124.45
11	aA	834	CLA	CMC-C2C-C1C	2.44	128.75	125.04
15	cA	851	BCR	C15-C14-C13	-2.44	123.83	127.31
11	aB	815	CLA	C4-C3-C5	2.44	119.37	115.27
12	cA	827	F6C	C4A-NA-C1A	-2.44	104.60	106.33
11	bB	804	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
11	bB	837	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
11	aA	816	CLA	CAA-C2A-C3A	-2.44	106.11	112.78
15	cL	208	BCR	C27-C26-C25	2.44	126.27	122.73
11	bB	805	CLA	C4-C3-C5	2.44	119.37	115.27
15	bB	848	BCR	C7-C8-C9	-2.44	122.56	126.23
11	aB	830	CLA	CAA-C2A-C3A	-2.43	106.11	112.78
11	bB	831	CLA	CHB-C4A-NA	2.43	127.88	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bB	836	CLA	CHD-C4C-NC	2.43	128.04	124.20
11	aB	837	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
12	aA	827	F6C	CHB-C4A-NA	2.43	126.69	124.45
11	cA	839	CLA	C1-C2-C3	-2.43	121.83	126.04
11	cB	812	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
11	bB	810	CLA	CBC-CAC-C3C	-2.43	105.72	112.43
11	aA	836	CLA	CMC-C2C-C1C	2.43	128.74	125.04
11	aL	205	CLA	CMC-C2C-C1C	2.43	128.74	125.04
11	aA	820	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
11	cA	807	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
11	aB	831	CLA	CHB-C4A-NA	2.43	127.88	124.51
11	cB	810	CLA	CBC-CAC-C3C	-2.43	105.73	112.43
12	cB	824	F6C	CBC-CAC-C3C	-2.43	105.73	112.43
11	aB	801	CLA	C4-C3-C5	2.43	119.36	115.27
11	bB	804	CLA	CHB-C4A-NA	2.43	127.87	124.51
11	bA	839	CLA	C4-C3-C5	2.43	119.36	115.27
15	bK	102	BCR	C37-C22-C21	-2.43	119.52	122.92
11	aA	815	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
11	aB	801	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
11	cA	836	CLA	CMC-C2C-C1C	2.43	128.74	125.04
11	bA	825	CLA	CMC-C2C-C1C	2.43	128.74	125.04
11	cL	205	CLA	CMC-C2C-C1C	2.43	128.74	125.04
11	cA	828	CLA	O2A-CGA-CBA	2.43	119.53	111.91
11	bA	828	CLA	C1C-C2C-C3C	-2.43	104.40	106.96
15	bA	851	BCR	C15-C14-C13	-2.43	123.84	127.31
11	bA	834	CLA	CMC-C2C-C1C	2.43	128.74	125.04
11	bA	836	CLA	CMC-C2C-C1C	2.43	128.74	125.04
11	cA	823	CLA	CMC-C2C-C1C	2.43	128.74	125.04
12	aB	824	F6C	CBC-CAC-C3C	-2.43	105.74	112.43
11	bA	842	CLA	CAC-C3C-C4C	2.43	127.96	124.81
11	cB	804	CLA	CHB-C4A-NA	2.43	127.87	124.51
11	cA	803	CLA	C4-C3-C5	2.43	119.35	115.27
11	cA	828	CLA	C1C-C2C-C3C	-2.43	104.41	106.96
11	aA	841	CLA	CMC-C2C-C1C	2.43	128.73	125.04
11	aB	829	CLA	CHC-C1C-NC	2.43	127.88	124.20
11	bA	815	CLA	O2D-CGD-O1D	-2.43	119.10	123.84
11	cA	814	CLA	CMC-C2C-C1C	2.42	128.73	125.04
15	aA	847	BCR	C28-C27-C26	-2.42	109.75	114.08
11	bB	829	CLA	CHC-C1C-NC	2.42	127.88	124.20
12	bB	824	F6C	CBC-CAC-C3C	-2.42	105.75	112.43
12	bA	827	F6C	CHB-C4A-NA	2.42	126.68	124.45
11	aA	807	CLA	C4-C3-C5	2.42	119.34	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	830	F6C	CHD-C1D-ND	-2.42	120.53	124.20
11	aA	823	CLA	CHB-C1B-NB	-2.42	121.69	124.26
11	cA	821	CLA	C4-C3-C5	2.42	119.34	115.27
11	aA	829	CLA	CMC-C2C-C1C	2.42	128.72	125.04
11	bA	814	CLA	CMC-C2C-C1C	2.42	128.72	125.04
11	cA	825	CLA	CMC-C2C-C1C	2.42	128.72	125.04
11	cA	815	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
11	cB	805	CLA	C4-C3-C5	2.42	119.34	115.27
11	aB	804	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
11	bB	813	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
11	bA	825	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
11	aB	804	CLA	CAC-C3C-C4C	2.42	127.95	124.81
11	aA	821	CLA	CMC-C2C-C1C	2.42	128.72	125.04
11	cK	103	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
11	aB	810	CLA	CBC-CAC-C3C	-2.42	105.77	112.43
15	aK	102	BCR	C37-C22-C21	-2.42	119.54	122.92
11	cA	812	CLA	O2A-CGA-CBA	2.42	119.50	111.91
15	aA	851	BCR	C27-C26-C25	2.42	126.24	122.73
11	aB	836	CLA	CHD-C4C-NC	2.42	128.01	124.20
11	cB	813	CLA	CBC-CAC-C3C	-2.42	105.77	112.43
11	bB	813	CLA	CBC-CAC-C3C	-2.42	105.77	112.43
18	aB	847	LMG	C38-C37-C36	-2.42	102.16	114.42
11	bA	808	CLA	CHB-C4A-NA	2.42	127.85	124.51
11	bA	803	CLA	C4-C3-C5	2.42	119.33	115.27
11	bA	828	CLA	O2A-CGA-CBA	2.41	119.49	111.91
11	bA	812	CLA	CHB-C4A-NA	2.41	127.85	124.51
11	aA	828	CLA	O2A-CGA-CBA	2.41	119.48	111.91
11	cB	836	CLA	CHD-C4C-NC	2.41	128.01	124.20
11	cA	825	CLA	O2A-CGA-O1A	-2.41	117.50	123.59
11	cA	839	CLA	C4-C3-C5	2.41	119.33	115.27
11	cA	821	CLA	CMC-C2C-C1C	2.41	128.72	125.04
11	bL	205	CLA	CMC-C2C-C1C	2.41	128.71	125.04
12	aA	830	F6C	CHD-C1D-ND	-2.41	120.54	124.20
11	cL	204	CLA	CMC-C2C-C1C	2.41	128.71	125.04
11	aA	825	CLA	CMC-C2C-C1C	2.41	128.71	125.04
11	cB	801	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
11	cB	813	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
11	bA	834	CLA	O2A-CGA-O1A	-2.41	117.51	123.59
11	aB	834	CLA	CHD-C4C-NC	2.41	128.00	124.20
11	bA	812	CLA	O2A-CGA-CBA	2.41	119.47	111.91
11	aA	812	CLA	O2A-CGA-CBA	2.41	119.47	111.91
11	bB	804	CLA	CAC-C3C-C4C	2.41	127.94	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cB	829	CLA	CHC-C1C-NC	2.41	127.86	124.20
15	aB	843	BCR	C15-C16-C17	-2.41	118.54	123.47
18	cB	847	LMG	C38-C37-C36	-2.41	102.19	114.42
11	aB	813	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
11	aA	838	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
15	cK	102	BCR	C37-C22-C21	-2.41	119.55	122.92
11	bB	817	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
11	bA	807	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
15	aL	208	BCR	C27-C26-C25	2.41	126.22	122.73
11	bA	821	CLA	C4-C3-C5	2.41	119.32	115.27
18	bB	847	LMG	C38-C37-C36	-2.41	102.21	114.42
11	bA	807	CLA	C4-C3-C5	2.41	119.32	115.27
11	cA	824	CLA	CAA-C2A-C3A	-2.41	106.19	112.78
11	bA	807	CLA	CHB-C4A-NA	2.40	127.84	124.51
15	cA	847	BCR	C28-C27-C26	-2.40	109.78	114.08
11	cA	838	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
12	cA	830	F6C	CHD-C1D-ND	-2.40	120.56	124.20
15	bA	847	BCR	C28-C27-C26	-2.40	109.79	114.08
11	cB	817	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
11	aB	810	CLA	CMC-C2C-C1C	2.40	128.70	125.04
11	cA	834	CLA	CMC-C2C-C1C	2.40	128.70	125.04
15	cA	850	BCR	C15-C14-C13	-2.40	123.88	127.31
11	aA	821	CLA	C4-C3-C5	2.40	119.31	115.27
10	cA	801	CL0	CMC-C2C-C1C	2.40	128.69	125.04
11	aB	813	CLA	CBC-CAC-C3C	-2.40	105.81	112.43
15	bB	843	BCR	C15-C16-C17	-2.40	118.56	123.47
11	aL	204	CLA	CMC-C2C-C1C	2.40	128.69	125.04
11	cB	839	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
11	cA	813	CLA	O2A-CGA-CBA	2.40	119.43	111.91
15	bL	208	BCR	C27-C26-C25	2.40	126.21	122.73
11	cA	807	CLA	C4-C3-C5	2.40	119.30	115.27
11	aB	839	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
11	aB	814	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
11	bA	839	CLA	C1-C2-C3	-2.40	121.90	126.04
11	bB	839	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
11	bA	824	CLA	CAA-C2A-C3A	-2.40	106.22	112.78
11	bK	103	CLA	O2D-CGD-O1D	-2.40	119.16	123.84
11	cB	804	CLA	CAC-C3C-C4C	2.39	127.92	124.81
11	aA	839	CLA	C4-C3-C5	2.39	119.30	115.27
12	aL	202	F6C	C4-C3-C5	2.39	119.30	115.27
15	bA	849	BCR	C27-C26-C25	2.39	126.21	122.73
11	cB	810	CLA	CMC-C2C-C1C	2.39	128.69	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bA	821	CLA	CHD-C4C-NC	2.39	127.98	124.20
11	bA	831	CLA	CMB-C2B-C3B	2.39	132.39	126.59
11	bA	821	CLA	CMC-C2C-C1C	2.39	128.68	125.04
11	aA	813	CLA	O2A-CGA-CBA	2.39	119.42	111.91
15	cB	843	BCR	C15-C16-C17	-2.39	118.58	123.47
15	aA	851	BCR	C15-C14-C13	-2.39	123.90	127.31
11	cB	820	CLA	C4C-C3C-C2C	-2.39	103.41	106.90
10	bA	801	CL0	CMC-C2C-C1C	2.39	128.68	125.04
11	cA	834	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
15	cA	849	BCR	C27-C26-C25	2.39	126.20	122.73
15	bA	850	BCR	C15-C14-C13	-2.39	123.90	127.31
11	aB	826	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
11	aA	825	CLA	C4-C3-C5	2.39	119.29	115.27
11	aA	839	CLA	C1-C2-C3	-2.39	121.91	126.04
11	aA	807	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
11	bL	204	CLA	CMC-C2C-C1C	2.39	128.68	125.04
11	bA	833	CLA	C4-C3-C5	2.39	119.29	115.27
11	aA	807	CLA	CHB-C4A-NA	2.39	127.81	124.51
11	cB	826	CLA	O2A-CGA-O1A	-2.39	117.57	123.59
15	cL	208	BCR	C15-C14-C13	-2.39	123.90	127.31
11	bA	813	CLA	O2A-CGA-CBA	2.39	119.40	111.91
11	cB	808	CLA	CBC-CAC-C3C	-2.39	105.85	112.43
11	cB	831	CLA	CHB-C4A-NA	2.39	127.81	124.51
11	cA	838	CLA	CAA-C2A-C3A	-2.39	106.24	112.78
11	aA	813	CLA	C1-C2-C3	-2.39	121.92	126.04
11	aB	806	CLA	CBC-CAC-C3C	-2.39	105.86	112.43
15	cB	844	BCR	C40-C30-C25	2.39	114.17	110.30
15	aL	208	BCR	C15-C14-C13	-2.39	123.91	127.31
12	cL	202	F6C	C4-C3-C5	2.38	119.28	115.27
11	aA	834	CLA	O2A-CGA-O1A	-2.38	117.57	123.59
11	bA	825	CLA	C4-C3-C5	2.38	119.28	115.27
11	aA	814	CLA	CMC-C2C-C1C	2.38	128.67	125.04
11	bB	803	CLA	C4-C3-C5	2.38	119.28	115.27
12	bL	202	F6C	C4-C3-C5	2.38	119.28	115.27
11	bB	806	CLA	O2A-CGA-CBA	2.38	119.39	111.91
12	cA	832	F6C	CHC-C1C-NC	2.38	126.78	124.26
11	aB	820	CLA	C4C-C3C-C2C	-2.38	103.42	106.90
11	aA	812	CLA	C1-C2-C3	-2.38	121.92	126.04
11	bB	808	CLA	CBC-CAC-C3C	-2.38	105.86	112.43
12	bA	832	F6C	CHC-C1C-NC	2.38	126.78	124.26
11	cA	831	CLA	CMB-C2B-C3B	2.38	132.35	126.59
11	cA	812	CLA	C1-C2-C3	-2.38	121.92	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aA	824	CLA	CAA-C2A-C3A	-2.38	106.26	112.78
11	bA	838	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
11	aA	806	CLA	CHB-C1B-NB	-2.38	121.74	124.26
11	cA	802	CLA	CHD-C4C-NC	2.38	127.95	124.20
15	aA	850	BCR	C15-C14-C13	-2.38	123.91	127.31
11	bA	802	CLA	CHD-C4C-NC	2.38	127.95	124.20
11	aA	831	CLA	CMB-C2B-C3B	2.38	132.35	126.59
11	bB	826	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
11	cA	807	CLA	CHB-C4A-NA	2.38	127.80	124.51
11	aB	817	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
15	aA	849	BCR	C27-C26-C25	2.38	126.18	122.73
12	aA	844	F6C	CBC-CAC-C3C	-2.38	105.88	112.43
11	aB	808	CLA	CBC-CAC-C3C	-2.38	105.88	112.43
11	bL	205	CLA	O2A-CGA-CBA	2.38	119.37	111.91
11	cB	803	CLA	C4-C3-C5	2.38	119.27	115.27
11	bA	812	CLA	C1-C2-C3	-2.38	121.93	126.04
10	aA	801	CL0	CMC-C2C-C1C	2.38	128.66	125.04
11	aA	831	CLA	O1D-CGD-CBD	-2.38	119.62	124.48
11	bB	829	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
12	cB	824	F6C	O2A-CGA-CBA	2.37	119.36	111.91
11	bB	810	CLA	CMC-C2C-C1C	2.37	128.66	125.04
11	cA	825	CLA	C4-C3-C5	2.37	119.27	115.27
11	aB	829	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
11	aL	205	CLA	O2A-CGA-CBA	2.37	119.36	111.91
11	cB	806	CLA	O2A-CGA-CBA	2.37	119.36	111.91
11	cB	807	CLA	CBC-CAC-C3C	-2.37	105.89	112.43
15	aL	207	BCR	C11-C10-C9	-2.37	123.92	127.31
11	cA	833	CLA	C4-C3-C5	2.37	119.26	115.27
11	bA	838	CLA	CAA-C2A-C3A	-2.37	106.28	112.78
12	bB	824	F6C	O2A-CGA-CBA	2.37	119.35	111.91
11	cB	825	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
11	bK	103	CLA	CAA-CBA-CGA	-2.37	106.32	113.25
11	bA	831	CLA	O1D-CGD-CBD	-2.37	119.63	124.48
12	aA	832	F6C	CHC-C1C-NC	2.37	126.77	124.26
11	bB	806	CLA	CBC-CAC-C3C	-2.37	105.89	112.43
11	bA	834	CLA	C1-C2-C3	-2.37	121.94	126.04
11	bB	825	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
11	cA	808	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
11	cB	814	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
11	aB	814	CLA	O1D-CGD-CBD	-2.37	119.64	124.48
11	cK	103	CLA	CAA-CBA-CGA	-2.37	106.33	113.25
11	bA	839	CLA	O2A-CGA-O1A	-2.37	117.61	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aA	839	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
11	aB	806	CLA	O2A-CGA-CBA	2.37	119.34	111.91
11	aK	103	CLA	CAA-CBA-CGA	-2.37	106.33	113.25
11	aA	834	CLA	C1-C2-C3	-2.37	121.95	126.04
11	aB	830	CLA	CHB-C4A-NA	2.37	127.79	124.51
11	aB	807	CLA	CHD-C4C-NC	2.37	127.93	124.20
11	aA	838	CLA	CAA-C2A-C3A	-2.37	106.30	112.78
11	bA	838	CLA	CMB-C2B-C3B	2.37	132.32	126.59
11	cL	205	CLA	O2A-CGA-CBA	2.37	119.33	111.91
11	cA	843	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
11	bB	814	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
11	bA	813	CLA	C1-C2-C3	-2.36	121.95	126.04
11	bB	838	CLA	CHB-C4A-NA	2.36	127.78	124.51
11	bB	804	CLA	CMB-C2B-C1B	2.36	128.97	125.37
11	aB	803	CLA	C4-C3-C5	2.36	119.24	115.27
11	cB	828	CLA	CMD-C2D-C3D	-2.36	122.18	127.61
15	bL	207	BCR	C11-C10-C9	-2.36	123.94	127.31
12	bA	832	F6C	C5-C3-C4	2.36	119.82	114.60
11	aB	825	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
11	bB	806	CLA	CAC-C3C-C4C	2.36	127.87	124.81
15	aL	203	BCR	C27-C26-C25	2.36	126.16	122.73
15	bI	101	BCR	C27-C26-C25	2.36	126.16	122.73
12	aB	824	F6C	O2A-CGA-CBA	2.36	119.31	111.91
11	bB	820	CLA	C4C-C3C-C2C	-2.36	103.46	106.90
15	bL	208	BCR	C15-C14-C13	-2.36	123.94	127.31
11	bB	807	CLA	CBC-CAC-C3C	-2.36	105.93	112.43
11	cB	836	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
11	bB	802	CLA	O2A-CGA-CBA	2.36	119.31	111.91
11	cB	806	CLA	CBC-CAC-C3C	-2.36	105.93	112.43
11	bA	808	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
11	cA	813	CLA	C1-C2-C3	-2.36	121.97	126.04
11	bB	814	CLA	O1D-CGD-CBD	-2.36	119.66	124.48
15	aB	844	BCR	C30-C25-C26	-2.36	119.30	122.61
11	aB	807	CLA	CBC-CAC-C3C	-2.36	105.94	112.43
11	aA	833	CLA	C4-C3-C5	2.36	119.23	115.27
12	cA	830	F6C	O2A-CGA-CBA	2.36	119.30	111.91
11	aA	802	CLA	CHD-C4C-NC	2.36	127.92	124.20
11	aB	828	CLA	CMD-C2D-C3D	-2.36	122.20	127.61
11	cB	829	CLA	O2D-CGD-O1D	-2.35	119.23	123.84
11	bA	825	CLA	CMB-C2B-C1B	2.35	128.96	125.37
11	cB	802	CLA	O2A-CGA-CBA	2.35	119.30	111.91
12	bA	830	F6C	O2A-CGA-CBA	2.35	119.30	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bA	823	CLA	CHB-C1B-NB	-2.35	121.77	124.26
12	cA	832	F6C	C5-C3-C4	2.35	119.80	114.60
11	aA	828	CLA	C4A-NA-C1A	-2.35	105.65	106.71
12	cA	830	F6C	CMC-C2C-C1C	2.35	128.95	125.37
11	aB	802	CLA	O2A-CGA-CBA	2.35	119.29	111.91
11	cA	806	CLA	C1-C2-C3	-2.35	121.97	126.04
11	bB	828	CLA	CMD-C2D-C3D	-2.35	122.20	127.61
11	bA	833	CLA	CMC-C2C-C1C	2.35	128.62	125.04
11	aB	825	CLA	CAC-C3C-C4C	2.35	127.86	124.81
12	aA	830	F6C	O2A-CGA-CBA	2.35	119.29	111.91
11	bA	811	CLA	CMC-C2C-C1C	2.35	128.62	125.04
11	cA	831	CLA	O1D-CGD-CBD	-2.35	119.67	124.48
11	aL	205	CLA	C1-C2-C3	-2.35	121.98	126.04
11	cA	806	CLA	CHB-C1B-NB	-2.35	121.77	124.26
11	cA	823	CLA	CHB-C1B-NB	-2.35	121.77	124.26
11	cA	838	CLA	CMB-C2B-C3B	2.35	132.28	126.59
11	bA	803	CLA	C1-C2-C3	-2.35	121.98	126.04
11	cA	820	CLA	CMC-C2C-C1C	2.35	128.62	125.04
15	cL	207	BCR	C11-C10-C9	-2.35	123.96	127.31
11	cA	824	CLA	CHB-C4A-NA	2.35	127.76	124.51
11	cB	814	CLA	O1D-CGD-CBD	-2.35	119.68	124.48
11	cB	807	CLA	CHD-C4C-NC	2.35	127.90	124.20
11	cA	814	CLA	CMB-C2B-C1B	2.35	128.94	125.37
11	aA	838	CLA	CMB-C2B-C3B	2.35	132.27	126.59
11	aA	820	CLA	CMC-C2C-C1C	2.35	128.61	125.04
11	bA	843	CLA	CMC-C2C-C1C	2.35	128.61	125.04
11	cA	843	CLA	CMC-C2C-C1C	2.35	128.61	125.04
11	cB	806	CLA	CAC-C3C-C4C	2.35	127.86	124.81
11	cB	808	CLA	CHB-C4A-NA	2.35	127.76	124.51
12	bA	844	F6C	CBC-CAC-C3C	-2.35	105.96	112.43
11	cA	839	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
15	aB	844	BCR	C40-C30-C25	2.35	114.10	110.30
11	aA	806	CLA	C1-C2-C3	-2.35	121.99	126.04
11	cA	836	CLA	CAA-C2A-C3A	-2.34	106.36	112.78
12	cA	844	F6C	CBC-CAC-C3C	-2.34	105.97	112.43
15	cM	101	BCR	C15-C14-C13	-2.34	123.96	127.31
18	bB	847	LMG	O3-C3-C2	-2.34	104.93	110.35
11	cA	834	CLA	C1-C2-C3	-2.34	121.99	126.04
11	cB	804	CLA	CMB-C2B-C1B	2.34	128.94	125.37
15	aM	101	BCR	C15-C14-C13	-2.34	123.97	127.31
11	cA	821	CLA	CHB-C4A-NA	2.34	127.75	124.51
12	aA	830	F6C	CMC-C2C-C1C	2.34	128.94	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aB	838	CLA	CHB-C4A-NA	2.34	127.75	124.51
11	aA	843	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
11	aA	833	CLA	CMC-C2C-C1C	2.34	128.60	125.04
15	bB	844	BCR	C30-C25-C26	-2.34	119.32	122.61
12	bA	830	F6C	CMC-C2C-C1C	2.34	128.93	125.37
15	bB	844	BCR	C40-C30-C25	2.34	114.09	110.30
18	cB	847	LMG	O3-C3-C2	-2.34	104.94	110.35
11	bB	836	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
11	cA	833	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
11	bB	828	CLA	CMB-C2B-C3B	2.34	132.25	126.59
12	aA	832	F6C	C5-C3-C4	2.34	119.76	114.60
11	bA	843	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
11	cA	811	CLA	CMC-C2C-C1C	2.34	128.60	125.04
11	aA	821	CLA	CHB-C4A-NA	2.34	127.74	124.51
11	bB	807	CLA	CHD-C4C-NC	2.34	127.88	124.20
11	aA	808	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
11	bA	833	CLA	O2D-CGD-O1D	-2.33	119.27	123.84
11	cB	831	CLA	CBC-CAC-C3C	-2.33	106.00	112.43
11	bB	830	CLA	CHB-C4A-NA	2.33	127.74	124.51
11	cB	838	CLA	CHB-C4A-NA	2.33	127.74	124.51
11	bA	806	CLA	C1-C2-C3	-2.33	122.01	126.04
11	bA	820	CLA	CMC-C2C-C1C	2.33	128.59	125.04
11	cA	803	CLA	C1-C2-C3	-2.33	122.01	126.04
11	aB	836	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
11	cL	205	CLA	C1-C2-C3	-2.33	122.01	126.04
11	aB	809	CLA	CBC-CAC-C3C	-2.33	106.01	112.43
11	aA	811	CLA	CMC-C2C-C1C	2.33	128.59	125.04
11	aA	836	CLA	CAA-C2A-C3A	-2.33	106.40	112.78
11	bA	837	CLA	CHB-C4A-NA	2.33	127.73	124.51
11	cA	816	CLA	CHB-C4A-NA	2.33	127.73	124.51
11	cA	833	CLA	CMC-C2C-C1C	2.33	128.59	125.04
11	bL	205	CLA	C1-C2-C3	-2.33	122.02	126.04
11	bA	823	CLA	C4A-NA-C1A	-2.33	105.66	106.71
15	cI	103	BCR	C27-C26-C25	2.33	126.11	122.73
11	bA	836	CLA	CAA-C2A-C3A	-2.33	106.40	112.78
11	bA	814	CLA	CMB-C2B-C1B	2.33	128.91	125.37
16	bA	852	LHG	C18-C17-C16	-2.33	102.61	114.42
11	aA	815	CLA	CBC-CAC-C3C	-2.33	106.01	112.43
11	aB	831	CLA	CBC-CAC-C3C	-2.33	106.01	112.43
15	bA	851	BCR	C24-C23-C22	-2.33	122.72	126.23
15	aI	101	BCR	C27-C26-C25	2.33	126.11	122.73
11	aB	808	CLA	CHB-C4A-NA	2.33	127.73	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aA	814	CLA	CMB-C2B-C1B	2.33	128.91	125.37
11	aB	840	CLA	CMC-C2C-C1C	2.33	128.58	125.04
11	aB	820	CLA	CHB-C4A-NA	2.33	127.73	124.51
11	bB	809	CLA	CBC-CAC-C3C	-2.33	106.02	112.43
11	aB	828	CLA	CMB-C2B-C3B	2.33	132.22	126.59
11	aA	807	CLA	CHB-C1B-NB	-2.33	121.80	124.26
11	bB	840	CLA	CMC-C2C-C1C	2.33	128.58	125.04
15	aB	843	BCR	C33-C5-C6	-2.33	121.92	124.53
11	bA	821	CLA	CHB-C4A-NA	2.32	127.73	124.51
15	bM	101	BCR	C15-C14-C13	-2.32	123.99	127.31
12	bA	826	F6C	O1D-CGD-CBD	-2.32	119.73	124.48
11	bA	806	CLA	CHB-C1B-NB	-2.32	121.80	124.26
15	cL	203	BCR	C27-C26-C25	2.32	126.11	122.73
11	bK	101	CLA	CMC-C2C-C1C	2.32	128.58	125.04
16	cA	852	LHG	C18-C17-C16	-2.32	102.62	114.42
11	aK	101	CLA	CMC-C2C-C1C	2.32	128.58	125.04
15	cB	844	BCR	C30-C25-C26	-2.32	119.34	122.61
16	aA	852	LHG	C18-C17-C16	-2.32	102.63	114.42
11	bB	825	CLA	CAC-C3C-C4C	2.32	127.82	124.81
11	bB	809	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
11	cB	840	CLA	CMC-C2C-C1C	2.32	128.57	125.04
11	aA	833	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
11	bA	834	CLA	CBC-CAC-C3C	-2.32	106.03	112.43
11	aA	837	CLA	CHB-C4A-NA	2.32	127.72	124.51
11	aB	802	CLA	CHA-C1A-NA	-2.32	121.08	126.40
11	bA	807	CLA	CHB-C1B-NB	-2.32	121.80	124.26
11	cB	825	CLA	CAC-C3C-C4C	2.32	127.82	124.81
15	cB	844	BCR	C15-C16-C17	-2.32	118.72	123.47
18	aB	847	LMG	O3-C3-C2	-2.32	104.99	110.35
11	bA	815	CLA	CBC-CAC-C3C	-2.32	106.04	112.43
11	bK	103	CLA	CHB-C4A-NA	2.32	127.72	124.51
15	aA	851	BCR	C1-C6-C5	-2.32	119.35	122.61
12	aA	826	F6C	O1D-CGD-CBD	-2.32	119.74	124.48
11	bB	831	CLA	CBC-CAC-C3C	-2.32	106.04	112.43
11	cB	828	CLA	CMB-C2B-C3B	2.32	132.20	126.59
12	bA	832	F6C	CBC-CAC-C3C	-2.32	106.04	112.43
11	aB	804	CLA	CMB-C2B-C1B	2.32	128.90	125.37
11	bB	808	CLA	CHB-C4A-NA	2.32	127.72	124.51
11	cB	805	CLA	CMA-C3A-C2A	-2.32	104.48	113.83
11	aA	824	CLA	CHB-C4A-NA	2.32	127.72	124.51
15	aA	851	BCR	C24-C23-C22	-2.32	122.73	126.23
11	aB	806	CLA	CAC-C3C-C4C	2.32	127.82	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aB	828	CLA	CBC-CAC-C3C	-2.32	106.05	112.43
12	aA	832	F6C	CBC-CAC-C3C	-2.32	106.05	112.43
11	aA	803	CLA	C1-C2-C3	-2.32	122.04	126.04
11	aL	204	CLA	CBC-CAC-C3C	-2.32	106.05	112.43
11	aB	805	CLA	CMA-C3A-C2A	-2.32	104.49	113.83
11	cA	806	CLA	CAA-C2A-C3A	-2.32	106.44	112.78
10	aA	801	CL0	C4-C3-C5	2.32	119.17	115.27
12	cA	832	F6C	CBC-CAC-C3C	-2.31	106.05	112.43
11	cB	830	CLA	CHB-C4A-NA	2.31	127.71	124.51
15	bB	844	BCR	C15-C16-C17	-2.31	118.73	123.47
11	bB	805	CLA	CMA-C3A-C2A	-2.31	104.50	113.83
11	aA	843	CLA	CMC-C2C-C1C	2.31	128.56	125.04
11	aL	206	CLA	CMC-C2C-C1C	2.31	128.56	125.04
11	cA	807	CLA	CHB-C1B-NB	-2.31	121.81	124.26
11	aA	825	CLA	CMB-C2B-C1B	2.31	128.89	125.37
11	cB	809	CLA	CBC-CAC-C3C	-2.31	106.06	112.43
11	aB	822	CLA	CHB-C1B-NB	-2.31	121.81	124.26
11	aB	813	CLA	O2A-CGA-CBA	2.31	119.16	111.91
15	bB	843	BCR	C33-C5-C6	-2.31	121.93	124.53
11	cA	834	CLA	CBC-CAC-C3C	-2.31	106.06	112.43
11	aA	806	CLA	CAA-C2A-C3A	-2.31	106.45	112.78
11	cK	101	CLA	CMC-C2C-C1C	2.31	128.56	125.04
15	aB	844	BCR	C15-C16-C17	-2.31	118.74	123.47
11	cA	815	CLA	CBC-CAC-C3C	-2.31	106.07	112.43
11	aA	834	CLA	CBC-CAC-C3C	-2.31	106.07	112.43
12	cA	826	F6C	O1D-CGD-CBD	-2.31	119.76	124.48
11	bB	819	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
11	cB	813	CLA	O2A-CGA-CBA	2.31	119.15	111.91
11	bA	812	CLA	C4-C3-C5	2.31	119.15	115.27
11	cB	828	CLA	CBC-CAC-C3C	-2.31	106.07	112.43
11	bB	804	CLA	O2A-CGA-CBA	2.31	119.14	111.91
11	bA	838	CLA	O2A-CGA-CBA	2.31	119.14	111.91
11	aB	812	CLA	CAA-C2A-C3A	-2.30	106.47	112.78
11	cA	837	CLA	CHB-C4A-NA	2.30	127.70	124.51
11	bB	835	CLA	O2D-CGD-O1D	-2.30	119.33	123.84
11	bB	828	CLA	CBC-CAC-C3C	-2.30	106.08	112.43
11	aB	809	CLA	O2D-CGD-O1D	-2.30	119.33	123.84
11	cL	204	CLA	CBC-CAC-C3C	-2.30	106.08	112.43
11	cA	825	CLA	CMB-C2B-C1B	2.30	128.88	125.37
11	cA	812	CLA	C4-C3-C5	2.30	119.14	115.27
11	bB	802	CLA	CHA-C1A-NA	-2.30	121.12	126.40
15	aA	850	BCR	C27-C26-C25	2.30	126.07	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aK	103	CLA	CHB-C4A-NA	2.30	127.70	124.51
11	cB	839	CLA	C3B-C4B-NB	2.30	112.65	110.52
11	aA	825	CLA	CBC-CAC-C3C	-2.30	106.08	112.43
11	bB	829	CLA	C4A-NA-C1A	-2.30	105.67	106.71
15	bA	849	BCR	C29-C30-C25	2.30	114.03	110.48
15	bL	203	BCR	C27-C26-C25	2.30	126.07	122.73
11	cA	825	CLA	CBC-CAC-C3C	-2.30	106.09	112.43
11	cB	835	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
12	cL	202	F6C	CHB-C1B-NB	-2.30	120.58	124.20
11	cB	809	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
15	cB	846	BCR	C27-C26-C25	2.30	126.07	122.73
11	aB	833	CLA	CMC-C2C-C1C	2.30	128.54	125.04
11	bB	833	CLA	CMC-C2C-C1C	2.30	128.54	125.04
11	cB	815	CLA	C1-C2-C3	-2.30	122.07	126.04
11	cB	812	CLA	CAA-C2A-C3A	-2.30	106.48	112.78
10	bA	801	CL0	C4-C3-C5	2.30	119.14	115.27
11	bL	204	CLA	CBC-CAC-C3C	-2.30	106.09	112.43
11	bB	838	CLA	CMC-C2C-C1C	2.30	128.54	125.04
11	bA	824	CLA	CHB-C4A-NA	2.30	127.69	124.51
12	bL	202	F6C	CHB-C1B-NB	-2.30	120.58	124.20
11	bB	839	CLA	C3B-C4B-NB	2.30	112.65	110.52
15	cA	851	BCR	C24-C23-C22	-2.30	122.76	126.23
11	bB	839	CLA	O2A-CGA-CBA	2.30	119.12	111.91
11	aB	819	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
11	aA	812	CLA	C4-C3-C5	2.30	119.14	115.27
11	bA	825	CLA	CBC-CAC-C3C	-2.30	106.10	112.43
11	bL	206	CLA	CMC-C2C-C1C	2.30	128.54	125.04
15	cA	849	BCR	C29-C30-C25	2.30	114.02	110.48
11	bB	812	CLA	CAA-C2A-C3A	-2.30	106.49	112.78
11	aA	804	CLA	CBC-CAC-C3C	-2.29	106.11	112.43
11	bB	820	CLA	CHB-C4A-NA	2.29	127.69	124.51
11	cA	842	CLA	CMB-C2B-C1B	2.29	128.86	125.37
11	aB	835	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
11	bB	813	CLA	O2A-CGA-CBA	2.29	119.10	111.91
11	cB	802	CLA	CHA-C1A-NA	-2.29	121.15	126.40
10	cA	801	CL0	C4-C3-C5	2.29	119.13	115.27
15	cB	843	BCR	C33-C5-C6	-2.29	121.95	124.53
11	cB	819	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
11	aA	828	CLA	CHB-C4A-NA	2.29	127.68	124.51
11	cA	823	CLA	C4A-NA-C1A	-2.29	105.68	106.71
15	cA	851	BCR	C1-C6-C5	-2.29	119.39	122.61
11	cB	820	CLA	CHB-C4A-NA	2.29	127.68	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cK	103	CLA	CHB-C4A-NA	2.29	127.68	124.51
11	cB	822	CLA	CMC-C2C-C1C	2.29	128.53	125.04
11	aA	838	CLA	O2A-CGA-CBA	2.29	119.09	111.91
15	cA	847	BCR	C11-C10-C9	-2.29	124.04	127.31
11	aB	804	CLA	O2A-CGA-CBA	2.29	119.09	111.91
11	bA	816	CLA	CHB-C4A-NA	2.29	127.68	124.51
11	cA	804	CLA	CBC-CAC-C3C	-2.29	106.12	112.43
11	cB	804	CLA	O2A-CGA-CBA	2.29	119.09	111.91
15	aB	846	BCR	C16-C15-C14	-2.29	118.79	123.47
11	bA	804	CLA	CBC-CAC-C3C	-2.29	106.12	112.43
11	aB	815	CLA	C1-C2-C3	-2.29	122.09	126.04
11	bA	843	CLA	C1-C2-C3	-2.29	122.09	126.04
11	cK	101	CLA	CHB-C4A-NA	2.29	127.67	124.51
15	aA	849	BCR	C29-C30-C25	2.29	114.00	110.48
11	bA	806	CLA	CAA-C2A-C3A	-2.29	106.52	112.78
12	cA	830	F6C	CBC-CAC-C3C	-2.29	106.13	112.43
11	aL	204	CLA	O1D-CGD-CBD	-2.29	119.81	124.48
15	bA	847	BCR	C11-C10-C9	-2.29	124.05	127.31
11	cB	823	CLA	CHB-C4A-NA	2.29	127.67	124.51
11	aB	822	CLA	CMC-C2C-C1C	2.29	128.52	125.04
15	aL	207	BCR	C30-C25-C26	-2.29	119.39	122.61
11	aB	839	CLA	O2A-CGA-CBA	2.28	119.08	111.91
12	aA	830	F6C	CBC-CAC-C3C	-2.28	106.14	112.43
11	cB	833	CLA	CMC-C2C-C1C	2.28	128.52	125.04
11	cB	839	CLA	O2A-CGA-CBA	2.28	119.07	111.91
11	cB	821	CLA	CHB-C4A-NA	2.28	127.67	124.51
11	bL	204	CLA	O1D-CGD-CBD	-2.28	119.82	124.48
11	aA	803	CLA	CHB-C1B-C2B	-2.28	120.79	127.24
12	bL	202	F6C	CMC-C2C-C1C	2.28	128.84	125.37
11	cB	804	CLA	CHB-C1B-NB	-2.28	121.84	124.26
11	aB	821	CLA	CHB-C4A-NA	2.28	127.67	124.51
11	aA	843	CLA	C1-C2-C3	-2.28	122.10	126.04
11	aB	823	CLA	CHB-C4A-NA	2.28	127.66	124.51
11	bB	823	CLA	CHB-C4A-NA	2.28	127.66	124.51
11	aB	838	CLA	CMC-C2C-C1C	2.28	128.51	125.04
11	bB	822	CLA	CMC-C2C-C1C	2.28	128.51	125.04
11	cA	838	CLA	O2A-CGA-CBA	2.28	119.06	111.91
11	bB	822	CLA	CHB-C1B-NB	-2.28	121.84	124.26
15	cB	846	BCR	C16-C15-C14	-2.28	118.81	123.47
11	bA	831	CLA	O2A-CGA-CBA	2.28	119.05	111.91
11	aA	831	CLA	O2A-CGA-CBA	2.28	119.05	111.91
11	bB	826	CLA	O1D-CGD-CBD	-2.28	119.83	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aA	816	CLA	CHB-C4A-NA	2.28	127.66	124.51
15	cA	850	BCR	C27-C26-C25	2.27	126.03	122.73
11	cL	204	CLA	O1D-CGD-CBD	-2.27	119.83	124.48
11	bB	820	CLA	O2D-CGD-O1D	-2.27	119.39	123.84
11	bB	815	CLA	C1-C2-C3	-2.27	122.11	126.04
12	aL	202	F6C	CHB-C1B-NB	-2.27	120.62	124.20
11	cB	838	CLA	CMC-C2C-C1C	2.27	128.50	125.04
11	cA	831	CLA	O2A-CGA-CBA	2.27	119.04	111.91
11	bA	828	CLA	CHB-C4A-NA	2.27	127.66	124.51
16	aA	852	LHG	C20-C19-C18	-2.27	102.89	114.42
16	bA	852	LHG	C20-C19-C18	-2.27	102.89	114.42
12	bA	830	F6C	CBC-CAC-C3C	-2.27	106.17	112.43
11	aK	101	CLA	CHB-C4A-NA	2.27	127.65	124.51
11	aB	831	CLA	CMC-C2C-C1C	2.27	128.50	125.04
11	cB	822	CLA	CHB-C1B-NB	-2.27	121.85	124.26
11	aB	839	CLA	C3B-C4B-NB	2.27	112.62	110.52
15	bA	851	BCR	C1-C6-C5	-2.27	119.42	122.61
15	aK	102	BCR	C30-C25-C26	-2.27	119.42	122.61
11	cB	826	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
12	aA	830	F6C	O2D-CGD-O1D	-2.27	119.40	123.84
11	bB	815	CLA	CHB-C4A-NA	2.27	127.65	124.51
11	cL	205	CLA	CHB-C4A-NA	2.27	127.65	124.51
11	cA	820	CLA	C4-C3-C5	2.27	119.09	115.27
15	cK	102	BCR	C30-C25-C26	-2.27	119.42	122.61
16	cA	852	LHG	C20-C19-C18	-2.27	102.91	114.42
11	aL	205	CLA	CHB-C4A-NA	2.27	127.65	124.51
18	bB	847	LMG	C42-C41-C40	-2.27	102.92	114.42
11	cA	839	CLA	CMC-C2C-C1C	2.27	128.49	125.04
15	aA	847	BCR	C11-C10-C9	-2.27	124.08	127.31
17	aA	853	LMT	C3B-C4B-C5B	2.27	114.28	110.24
15	bL	207	BCR	C30-C25-C26	-2.27	119.42	122.61
11	aB	826	CLA	O1D-CGD-CBD	-2.27	119.85	124.48
11	aB	815	CLA	CHB-C4A-NA	2.26	127.64	124.51
18	cB	847	LMG	C42-C41-C40	-2.26	102.93	114.42
11	cB	831	CLA	CMC-C2C-C1C	2.26	128.49	125.04
11	aB	829	CLA	C4A-NA-C1A	-2.26	105.69	106.71
11	aB	820	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
15	bB	846	BCR	C27-C26-C25	2.26	126.02	122.73
11	bB	831	CLA	CMC-C2C-C1C	2.26	128.49	125.04
11	cB	826	CLA	CHA-C1A-NA	-2.26	121.22	126.40
11	bB	821	CLA	CHB-C4A-NA	2.26	127.64	124.51
15	aA	851	BCR	C7-C8-C9	-2.26	122.82	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bA	806	CLA	CHC-C1C-NC	2.26	127.63	124.20
12	cL	202	F6C	CMC-C2C-C1C	2.26	128.81	125.37
11	cA	803	CLA	CHB-C1B-C2B	-2.26	120.85	127.24
15	bA	850	BCR	C27-C26-C25	2.26	126.01	122.73
15	bB	846	BCR	C16-C15-C14	-2.26	118.84	123.47
12	cA	830	F6C	O2D-CGD-O1D	-2.26	119.42	123.84
11	bA	803	CLA	CHB-C1B-C2B	-2.26	120.86	127.24
11	cA	817	CLA	O2A-CGA-CBA	2.26	119.00	111.91
11	aA	821	CLA	CAA-C2A-C1A	2.26	119.38	111.97
11	aB	812	CLA	CMB-C2B-C1B	2.26	128.81	125.37
15	aB	846	BCR	C27-C26-C25	2.26	126.01	122.73
11	cA	834	CLA	CMA-C3A-C4A	-2.26	105.70	111.77
11	bK	101	CLA	CHB-C4A-NA	2.26	127.64	124.51
11	cA	809	CLA	CBA-CAA-C2A	2.26	120.53	113.86
11	cA	843	CLA	C1-C2-C3	-2.26	122.14	126.04
18	aB	847	LMG	C42-C41-C40	-2.26	102.97	114.42
17	bA	853	LMT	C3B-C4B-C5B	2.26	114.27	110.24
15	cB	845	BCR	C11-C10-C9	-2.26	124.09	127.31
11	aA	839	CLA	CMC-C2C-C1C	2.26	128.48	125.04
11	bA	839	CLA	CMC-C2C-C1C	2.26	128.48	125.04
11	bA	840	CLA	CHB-C4A-NA	2.26	127.63	124.51
11	cA	828	CLA	CHB-C4A-NA	2.26	127.63	124.51
11	cB	826	CLA	CHB-C4A-NA	2.26	127.63	124.51
11	bA	834	CLA	CMA-C3A-C4A	-2.26	105.71	111.77
11	bA	842	CLA	CMB-C2B-C1B	2.26	128.81	125.37
12	bA	830	F6C	O2D-CGD-O1D	-2.26	119.43	123.84
11	cL	206	CLA	CMC-C2C-C1C	2.26	128.47	125.04
11	aA	842	CLA	CMB-C2B-C1B	2.26	128.80	125.37
11	bL	205	CLA	CHB-C4A-NA	2.25	127.63	124.51
11	bA	817	CLA	O2A-CGA-CBA	2.25	118.98	111.91
15	bK	102	BCR	C30-C25-C26	-2.25	119.44	122.61
11	cB	805	CLA	CMC-C2C-C1C	2.25	128.47	125.04
15	aL	203	BCR	C33-C5-C6	-2.25	122.00	124.53
11	aA	834	CLA	CMA-C3A-C4A	-2.25	105.72	111.77
11	cB	815	CLA	CHB-C4A-NA	2.25	127.63	124.51
11	cB	817	CLA	C2A-C3A-C4A	-2.25	98.23	101.87
11	cA	841	CLA	CED-O2D-CGD	2.25	121.03	115.94
11	cB	835	CLA	CBC-CAC-C3C	-2.25	106.23	112.43
11	bB	825	CLA	C1-C2-C3	-2.25	122.15	126.04
11	cA	821	CLA	CAA-C2A-C1A	2.25	119.35	111.97
12	bA	844	F6C	CHC-C1C-NC	2.25	126.64	124.26
11	aA	802	CLA	O2A-CGA-O1A	-2.25	117.92	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bA	820	CLA	CMB-C2B-C1B	2.25	128.79	125.37
15	bB	845	BCR	C24-C23-C22	-2.25	122.84	126.23
11	aA	804	CLA	CHB-C4A-NA	2.25	127.62	124.51
11	aA	820	CLA	C4-C3-C5	2.25	119.05	115.27
15	cB	845	BCR	C24-C23-C22	-2.25	122.84	126.23
11	cB	804	CLA	CAA-C2A-C1A	2.25	119.34	111.97
11	cB	820	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
11	cA	840	CLA	CBC-CAC-C3C	-2.25	106.23	112.43
11	cA	820	CLA	CMB-C2B-C1B	2.25	128.79	125.37
11	aB	804	CLA	CAA-C2A-C1A	2.25	119.34	111.97
11	bB	826	CLA	CHA-C1A-NA	-2.25	121.25	126.40
11	cA	824	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
12	aB	824	F6C	O1D-CGD-CBD	-2.25	119.89	124.48
11	bA	802	CLA	C16-C15-C13	-2.25	108.66	115.92
11	bA	809	CLA	CBA-CAA-C2A	2.25	120.49	113.86
11	bA	841	CLA	CED-O2D-CGD	2.25	121.02	115.94
15	aA	847	BCR	C24-C23-C22	-2.25	122.84	126.23
11	bB	815	CLA	O2A-CGA-CBA	2.25	118.95	111.91
12	aL	202	F6C	CMC-C2C-C1C	2.24	128.79	125.37
11	cA	804	CLA	CHB-C4A-NA	2.24	127.62	124.51
11	aA	842	CLA	CED-O2D-CGD	2.24	121.01	115.94
15	aA	848	BCR	C37-C22-C21	-2.24	119.78	122.92
11	bA	818	CLA	CAA-C2A-C3A	-2.24	106.63	112.78
11	bB	812	CLA	CHD-C4C-NC	2.24	127.74	124.20
11	aA	841	CLA	C5-C3-C4	2.24	119.56	114.60
11	bB	840	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
15	bA	851	BCR	C7-C8-C9	-2.24	122.84	126.23
11	bB	825	CLA	CHB-C1B-NB	-2.24	121.88	124.26
11	cA	841	CLA	C5-C3-C4	2.24	119.56	114.60
11	cA	818	CLA	CAA-C2A-C3A	-2.24	106.64	112.78
11	aA	817	CLA	O2A-CGA-CBA	2.24	118.94	111.91
11	aB	804	CLA	CHB-C1B-NB	-2.24	121.88	124.26
11	bA	841	CLA	C5-C3-C4	2.24	119.56	114.60
11	aA	819	CLA	CHB-C4A-NA	2.24	127.61	124.51
11	aB	825	CLA	CHB-C4A-NA	2.24	127.61	124.51
11	cA	802	CLA	C16-C15-C13	-2.24	108.68	115.92
11	bB	835	CLA	CBC-CAC-C3C	-2.24	106.25	112.43
18	aB	847	LMG	O2-C2-C1	-2.24	104.60	110.05
11	aB	835	CLA	CBC-CAC-C3C	-2.24	106.25	112.43
15	bA	847	BCR	C24-C23-C22	-2.24	122.85	126.23
15	aB	845	BCR	C11-C10-C9	-2.24	124.11	127.31
11	aA	818	CLA	CAA-C2A-C3A	-2.24	106.64	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bA	809	CLA	CMB-C2B-C1B	2.24	128.78	125.37
11	bB	826	CLA	CHB-C4A-NA	2.24	127.61	124.51
11	aB	826	CLA	CHA-C1A-NA	-2.24	121.27	126.40
11	bA	840	CLA	CBC-CAC-C3C	-2.24	106.26	112.43
11	aA	828	CLA	CMB-C2B-C1B	2.24	128.78	125.37
11	aA	809	CLA	CBA-CAA-C2A	2.24	120.47	113.86
17	cA	853	LMT	C3B-C4B-C5B	2.24	114.23	110.24
11	bA	821	CLA	CAA-C2A-C1A	2.24	119.31	111.97
11	aA	820	CLA	CMB-C2B-C1B	2.24	128.78	125.37
11	aA	841	CLA	CED-O2D-CGD	2.24	121.00	115.94
10	cA	801	CL0	O2A-CGA-O1A	-2.24	117.95	123.59
11	cB	801	CLA	C11-C12-C13	-2.24	108.69	115.92
11	bA	820	CLA	C4-C3-C5	2.24	119.03	115.27
11	aA	835	CLA	O2A-CGA-CBA	2.24	118.93	111.91
11	bA	836	CLA	CHB-C4A-NA	2.24	127.61	124.51
11	aB	817	CLA	C2A-C3A-C4A	-2.24	98.26	101.87
11	bA	828	CLA	CMB-C2B-C1B	2.24	128.78	125.37
18	bB	847	LMG	O2-C2-C1	-2.24	104.61	110.05
11	bA	825	CLA	CMA-C3A-C4A	-2.24	105.77	111.77
11	aA	840	CLA	CBC-CAC-C3C	-2.24	106.27	112.43
11	cA	802	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
11	cA	828	CLA	CMB-C2B-C1B	2.24	128.77	125.37
11	aB	805	CLA	C1-C2-C3	-2.23	122.18	126.04
11	aB	810	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
11	aB	815	CLA	O2A-CGA-CBA	2.23	118.92	111.91
12	aA	827	F6C	CMC-C2C-C1C	2.23	128.77	125.37
11	bB	812	CLA	CHB-C4A-NA	2.23	127.60	124.51
11	bB	804	CLA	CHB-C1B-NB	-2.23	121.89	124.26
10	aA	801	CL0	O2A-CGA-O1A	-2.23	117.96	123.59
11	aB	826	CLA	CHB-C4A-NA	2.23	127.60	124.51
15	cA	847	BCR	C24-C23-C22	-2.23	122.86	126.23
11	aB	812	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
11	cA	842	CLA	CED-O2D-CGD	2.23	120.98	115.94
11	bA	819	CLA	CHB-C4A-NA	2.23	127.60	124.51
15	cA	848	BCR	C37-C22-C21	-2.23	119.80	122.92
11	aB	812	CLA	CHD-C4C-NC	2.23	127.72	124.20
11	bA	831	CLA	CHD-C4C-NC	2.23	127.72	124.20
18	cB	847	LMG	O2-C2-C1	-2.23	104.63	110.05
11	cA	813	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
11	bB	801	CLA	C11-C12-C13	-2.23	108.71	115.92
11	bA	843	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
11	bB	817	CLA	C2A-C3A-C4A	-2.23	98.27	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aA	802	CLA	C16-C15-C13	-2.23	108.71	115.92
11	aA	806	CLA	CHC-C1C-NC	2.23	127.59	124.20
12	bB	824	F6C	O1D-CGD-CBD	-2.23	119.92	124.48
11	aA	824	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
15	cA	851	BCR	C7-C8-C9	-2.23	122.87	126.23
11	bA	835	CLA	O2A-CGA-CBA	2.23	118.90	111.91
11	cA	843	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
11	bB	810	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
12	aL	202	F6C	CBC-CAC-C3C	-2.23	106.29	112.43
11	aB	825	CLA	C1-C2-C3	-2.23	122.19	126.04
15	bB	845	BCR	C11-C10-C9	-2.23	124.13	127.31
11	cA	803	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
11	bB	804	CLA	CAA-C2A-C1A	2.23	119.27	111.97
11	aA	836	CLA	CHB-C4A-NA	2.23	127.59	124.51
11	aB	801	CLA	C11-C12-C13	-2.23	108.72	115.92
11	bB	805	CLA	CMC-C2C-C1C	2.23	128.43	125.04
11	bL	206	CLA	CHB-C4A-NA	2.23	127.59	124.51
15	aB	845	BCR	C24-C23-C22	-2.23	122.87	126.23
11	aA	843	CLA	CAA-C2A-C3A	-2.23	106.68	112.78
11	cB	825	CLA	C1-C2-C3	-2.23	122.19	126.04
11	aA	803	CLA	CMC-C2C-C1C	2.23	128.43	125.04
11	cA	819	CLA	CHB-C4A-NA	2.23	127.59	124.51
11	aA	840	CLA	CHB-C4A-NA	2.22	127.59	124.51
11	cA	840	CLA	CHB-C4A-NA	2.22	127.59	124.51
11	aA	825	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
15	cL	207	BCR	C30-C25-C26	-2.22	119.48	122.61
11	cB	840	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
11	aB	802	CLA	C4-C3-C2	-2.22	117.97	123.68
11	aA	810	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
11	aA	834	CLA	CHB-C1B-NB	-2.22	121.90	124.26
11	aA	831	CLA	CHD-C4C-NC	2.22	127.71	124.20
11	aL	206	CLA	C11-C10-C8	-2.22	108.73	115.92
11	cB	815	CLA	O2A-CGA-CBA	2.22	118.88	111.91
10	bA	801	CL0	O2A-CGA-O1A	-2.22	117.99	123.59
11	aL	206	CLA	CHB-C4A-NA	2.22	127.58	124.51
11	bA	824	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
11	bA	842	CLA	CED-O2D-CGD	2.22	120.96	115.94
11	bB	812	CLA	CMB-C2B-C1B	2.22	128.75	125.37
12	cB	824	F6C	O1D-CGD-CBD	-2.22	119.94	124.48
11	bA	803	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
11	cA	803	CLA	CMC-C2C-C1C	2.22	128.42	125.04
11	bB	812	CLA	O2A-CGA-O1A	-2.22	117.99	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aA	825	CLA	CMA-C3A-C4A	-2.22	105.81	111.77
11	cB	812	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
11	cB	825	CLA	CHB-C4A-NA	2.22	127.58	124.51
11	cL	206	CLA	C11-C10-C8	-2.22	108.75	115.92
11	bA	833	CLA	CHB-C4A-NA	2.22	127.58	124.51
11	cB	810	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
11	cB	837	CLA	C4-C3-C5	2.22	119.00	115.27
11	aA	813	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
11	aA	819	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
11	bA	825	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
11	cA	835	CLA	O2A-CGA-CBA	2.22	118.86	111.91
11	cB	812	CLA	CMB-C2B-C1B	2.22	128.75	125.37
15	aM	101	BCR	C7-C8-C9	-2.22	122.89	126.23
11	bA	819	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
12	cA	844	F6C	CHC-C1C-NC	2.22	126.60	124.26
11	bA	810	CLA	O2D-CGD-O1D	-2.22	119.51	123.84
11	bB	802	CLA	C4-C3-C2	-2.22	117.99	123.68
11	cB	812	CLA	CHD-C4C-NC	2.22	127.69	124.20
11	cA	813	CLA	C4-C3-C5	2.22	119.00	115.27
12	cA	827	F6C	CMC-C2C-C1C	2.22	128.74	125.37
11	bA	811	CLA	CED-O2D-CGD	2.22	120.95	115.94
11	cB	837	CLA	CAA-C2A-C3A	-2.21	106.71	112.78
11	cA	806	CLA	CHC-C1C-NC	2.21	127.56	124.20
12	cL	202	F6C	CBC-CAC-C3C	-2.21	106.33	112.43
15	bA	848	BCR	C37-C22-C21	-2.21	119.82	122.92
11	aB	820	CLA	CAC-C3C-C4C	2.21	127.68	124.81
11	aB	840	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
11	cB	805	CLA	C1-C2-C3	-2.21	122.21	126.04
11	cB	825	CLA	CMB-C2B-C1B	2.21	128.74	125.37
11	cB	829	CLA	C4A-NA-C1A	-2.21	105.71	106.71
11	bA	813	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
11	aB	805	CLA	CMC-C2C-C1C	2.21	128.41	125.04
11	aA	803	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
11	cA	825	CLA	CMA-C3A-C4A	-2.21	105.83	111.77
12	aA	844	F6C	CHC-C1C-NC	2.21	126.60	124.26
11	bB	807	CLA	CMA-C3A-C2A	-2.21	104.91	113.83
11	cA	825	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
11	bB	839	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
11	cB	802	CLA	C4-C3-C2	-2.21	118.01	123.68
11	bA	802	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
11	aB	837	CLA	CHB-C4A-NA	2.21	127.57	124.51
15	bM	101	BCR	C2-C1-C6	2.21	113.88	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cA	831	CLA	CHD-C4C-NC	2.21	127.69	124.20
11	cB	834	CLA	CHB-C4A-NA	2.21	127.57	124.51
11	bB	805	CLA	C1-C2-C3	-2.21	122.22	126.04
11	bL	206	CLA	C11-C10-C8	-2.21	108.78	115.92
11	aA	839	CLA	O2A-CGA-CBA	2.21	118.84	111.91
11	bB	808	CLA	CHB-C1B-C2B	-2.21	121.00	127.24
11	aB	837	CLA	CAA-C2A-C3A	-2.21	106.73	112.78
11	aB	825	CLA	CMB-C2B-C1B	2.21	128.73	125.37
12	bA	827	F6C	CMC-C2C-C1C	2.21	128.73	125.37
11	aA	835	CLA	CBC-CAC-C3C	-2.21	106.34	112.43
11	aB	839	CLA	CAA-C2A-C3A	-2.21	106.73	112.78
12	aA	826	F6C	CMC-C2C-C3C	2.21	130.38	125.61
11	bA	803	CLA	CMC-C2C-C1C	2.21	128.40	125.04
11	aB	813	CLA	CMC-C2C-C1C	2.21	128.40	125.04
12	aA	844	F6C	CMC-C2C-C1C	2.21	128.73	125.37
11	aB	837	CLA	C4-C3-C5	2.21	118.98	115.27
11	bB	837	CLA	CAA-C2A-C3A	-2.21	106.74	112.78
15	bA	848	BCR	C33-C5-C6	-2.20	122.05	124.53
11	cB	839	CLA	CAA-C2A-C3A	-2.20	106.74	112.78
11	bA	813	CLA	C4-C3-C5	2.20	118.98	115.27
11	cB	820	CLA	CAC-C3C-C4C	2.20	127.67	124.81
11	cB	807	CLA	CMA-C3A-C2A	-2.20	104.94	113.83
11	bA	820	CLA	CHB-C1B-C2B	-2.20	121.01	127.24
11	bB	837	CLA	C4-C3-C5	2.20	118.98	115.27
11	aA	820	CLA	CBC-CAC-C3C	-2.20	106.36	112.43
12	bL	202	F6C	CBC-CAC-C3C	-2.20	106.36	112.43
11	bA	804	CLA	CHB-C4A-NA	2.20	127.56	124.51
11	cA	817	CLA	CHB-C4A-NA	2.20	127.56	124.51
11	aB	808	CLA	CHB-C1B-C2B	-2.20	121.02	127.24
11	cB	813	CLA	CMC-C2C-C1C	2.20	128.39	125.04
11	aB	807	CLA	CMA-C3A-C2A	-2.20	104.94	113.83
11	cA	833	CLA	CHB-C4A-NA	2.20	127.56	124.51
15	bK	102	BCR	C15-C16-C17	-2.20	118.96	123.47
11	cA	820	CLA	CBC-CAC-C3C	-2.20	106.36	112.43
11	cL	206	CLA	CHB-C4A-NA	2.20	127.56	124.51
11	aA	819	CLA	C3B-C4B-NB	2.20	112.56	110.52
12	cA	826	F6C	CMC-C2C-C3C	2.20	130.37	125.61
11	bB	803	CLA	CED-O2D-CGD	2.20	120.92	115.94
11	bA	839	CLA	O2A-CGA-CBA	2.20	118.81	111.91
12	bA	826	F6C	CMC-C2C-C3C	2.20	130.37	125.61
11	bB	813	CLA	CMC-C2C-C1C	2.20	128.39	125.04
11	bA	824	CLA	C1-C2-C3	-2.20	122.24	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cA	824	CLA	C1-C2-C3	-2.20	122.24	126.04
15	cM	101	BCR	C7-C8-C9	-2.20	122.91	126.23
11	bA	819	CLA	C3B-C4B-NB	2.20	112.56	110.52
11	cB	808	CLA	CHB-C1B-C2B	-2.20	121.03	127.24
11	cA	835	CLA	CBC-CAC-C3C	-2.20	106.37	112.43
11	cB	835	CLA	CMC-C2C-C1C	2.20	128.38	125.04
15	cL	203	BCR	C33-C5-C6	-2.20	122.06	124.53
11	aB	803	CLA	CED-O2D-CGD	2.20	120.91	115.94
11	cA	811	CLA	CED-O2D-CGD	2.20	120.91	115.94
11	aA	811	CLA	CED-O2D-CGD	2.20	120.91	115.94
15	aM	101	BCR	C2-C1-C6	2.20	113.86	110.48
11	aB	835	CLA	CMC-C2C-C1C	2.20	128.38	125.04
12	bA	844	F6C	CMC-C2C-C1C	2.20	128.71	125.37
15	cK	102	BCR	C15-C16-C17	-2.19	118.98	123.47
11	aA	809	CLA	CMB-C2B-C1B	2.19	128.71	125.37
11	cA	834	CLA	CMA-C3A-C2A	-2.19	104.98	113.83
15	aK	102	BCR	C15-C16-C17	-2.19	118.98	123.47
11	cA	810	CLA	CMA-C3A-C4A	2.19	117.67	111.77
11	bB	835	CLA	CMC-C2C-C1C	2.19	128.38	125.04
11	aB	825	CLA	CHB-C1B-NB	-2.19	121.94	124.26
11	aA	834	CLA	CMA-C3A-C2A	-2.19	104.98	113.83
11	cA	839	CLA	O2A-CGA-CBA	2.19	118.79	111.91
11	bB	836	CLA	C1-C2-C3	-2.19	122.25	126.04
15	bL	203	BCR	C33-C5-C6	-2.19	122.07	124.53
11	aA	813	CLA	C4-C3-C5	2.19	118.96	115.27
11	bB	825	CLA	CHB-C4A-NA	2.19	127.54	124.51
11	aB	836	CLA	C1-C2-C3	-2.19	122.25	126.04
11	cB	818	CLA	CHB-C4A-NA	2.19	127.54	124.51
11	cB	803	CLA	CED-O2D-CGD	2.19	120.89	115.94
11	cA	820	CLA	CHB-C1B-C2B	-2.19	121.06	127.24
11	bB	834	CLA	CHB-C4A-NA	2.19	127.54	124.51
11	cA	819	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
11	cA	809	CLA	CMB-C2B-C1B	2.19	128.70	125.37
11	aB	812	CLA	CHB-C4A-NA	2.19	127.54	124.51
11	bA	820	CLA	CBC-CAC-C3C	-2.19	106.40	112.43
11	aA	820	CLA	CHB-C1B-C2B	-2.19	121.06	127.24
11	bA	835	CLA	CBC-CAC-C3C	-2.19	106.40	112.43
11	aA	833	CLA	CHB-C4A-NA	2.19	127.53	124.51
11	aB	835	CLA	CHB-C4A-NA	2.19	127.53	124.51
11	bA	834	CLA	CMA-C3A-C2A	-2.19	105.01	113.83
11	bB	834	CLA	CHA-C1A-NA	-2.19	121.39	126.40
11	aA	837	CLA	O2A-CGA-CBA	2.19	121.05	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aA	818	CLA	CBC-CAC-C3C	-2.19	106.41	112.43
11	aA	810	CLA	CMA-C3A-C4A	2.18	117.64	111.77
11	cB	825	CLA	CHB-C1B-NB	-2.18	121.94	124.26
11	cA	810	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
11	cA	836	CLA	CHB-C4A-NA	2.18	127.53	124.51
11	cB	827	CLA	CMC-C2C-C1C	2.18	128.36	125.04
15	cA	848	BCR	C33-C5-C6	-2.18	122.08	124.53
11	bB	827	CLA	CMC-C2C-C1C	2.18	128.36	125.04
15	aA	848	BCR	C33-C5-C6	-2.18	122.08	124.53
11	aA	839	CLA	C6-C7-C8	-2.18	108.87	115.92
12	aA	844	F6C	CAA-CBA-CGA	-2.18	107.09	113.43
11	aA	817	CLA	CHB-C4A-NA	2.18	127.53	124.51
11	aB	801	CLA	O2A-CGA-CBA	2.18	118.75	111.91
11	cA	816	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
11	aA	810	CLA	CBC-CAC-C3C	-2.18	106.42	112.43
11	bA	837	CLA	O2A-CGA-CBA	2.18	121.03	114.03
11	cB	834	CLA	CHA-C1A-NA	-2.18	121.41	126.40
11	aB	827	CLA	CMC-C2C-C1C	2.18	128.36	125.04
11	cA	828	CLA	C1-C2-C3	-2.18	122.28	126.04
11	aB	834	CLA	CHB-C4A-NA	2.18	127.52	124.51
11	bA	839	CLA	C6-C7-C8	-2.18	108.88	115.92
11	cB	801	CLA	O2A-CGA-CBA	2.18	118.74	111.91
11	bA	810	CLA	CBC-CAC-C3C	-2.18	106.43	112.43
11	cB	840	CLA	CMB-C2B-C1B	2.18	128.68	125.37
12	cA	844	F6C	CMC-C2C-C1C	2.18	128.68	125.37
11	cA	818	CLA	CBC-CAC-C3C	-2.18	106.43	112.43
15	bL	203	BCR	C15-C14-C13	-2.18	124.20	127.31
11	aA	824	CLA	C1-C2-C3	-2.18	122.28	126.04
15	cL	203	BCR	C15-C14-C13	-2.18	124.20	127.31
11	cA	810	CLA	CBC-CAC-C3C	-2.17	106.44	112.43
11	cB	812	CLA	CHB-C4A-NA	2.17	127.52	124.51
11	aA	803	CLA	CBC-CAC-C3C	-2.17	106.44	112.43
11	bB	828	CLA	CHD-C4C-NC	2.17	127.63	124.20
11	bB	837	CLA	CHB-C4A-NA	2.17	127.52	124.51
15	cM	101	BCR	C2-C1-C6	2.17	113.83	110.48
11	cA	829	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
15	bB	842	BCR	C33-C5-C6	-2.17	122.09	124.53
11	bA	810	CLA	CMA-C3A-C4A	2.17	117.61	111.77
11	bA	834	CLA	CHB-C1B-NB	-2.17	121.96	124.26
11	cA	837	CLA	CBA-CAA-C2A	2.17	120.27	113.86
11	cA	837	CLA	O2A-CGA-CBA	2.17	121.00	114.03
11	bB	831	CLA	O2A-CGA-CBA	2.17	118.72	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aA	814	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
11	cA	803	CLA	CBC-CAC-C3C	-2.17	106.45	112.43
12	aA	826	F6C	CMA-C3A-C2A	-2.17	120.23	126.12
11	bA	817	CLA	CHB-C4A-NA	2.17	127.51	124.51
11	cB	837	CLA	CHB-C4A-NA	2.17	127.51	124.51
11	cA	822	CLA	O2A-CGA-CBA	2.17	118.71	111.91
15	aB	842	BCR	C33-C5-C6	-2.17	122.09	124.53
11	cA	839	CLA	C6-C7-C8	-2.17	108.91	115.92
11	bA	828	CLA	C1-C2-C3	-2.17	122.29	126.04
12	cA	826	F6C	CMA-C3A-C2A	-2.17	120.23	126.12
11	bA	818	CLA	CBC-CAC-C3C	-2.17	106.45	112.43
11	cB	831	CLA	O2A-CGA-CBA	2.17	118.71	111.91
11	bA	829	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
11	bA	822	CLA	O2A-CGA-CBA	2.17	118.71	111.91
11	cB	813	CLA	CHB-C1B-NB	-2.17	121.96	124.26
11	aA	822	CLA	C6-C7-C8	-2.17	108.92	115.92
11	bA	803	CLA	CBC-CAC-C3C	-2.17	106.46	112.43
15	cB	842	BCR	C27-C26-C25	2.17	125.88	122.73
12	bA	826	F6C	CMA-C3A-C2A	-2.17	120.24	126.12
11	cA	819	CLA	C3B-C4B-NB	2.17	112.52	110.52
11	cB	823	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
11	bA	837	CLA	CBA-CAA-C2A	2.17	120.25	113.86
11	aB	811	CLA	O2D-CGD-O1D	-2.17	119.61	123.84
11	bA	816	CLA	O2D-CGD-O1D	-2.17	119.61	123.84
11	aA	837	CLA	CBA-CAA-C2A	2.16	120.25	113.86
11	cB	836	CLA	C1-C2-C3	-2.16	122.30	126.04
12	bA	844	F6C	CAA-CBA-CGA	-2.16	107.14	113.43
11	bB	801	CLA	O2A-CGA-CBA	2.16	118.70	111.91
11	aB	831	CLA	O2A-CGA-CBA	2.16	118.69	111.91
15	aL	203	BCR	C15-C14-C13	-2.16	124.22	127.31
15	bM	101	BCR	C7-C8-C9	-2.16	122.97	126.23
11	aA	822	CLA	O2A-CGA-CBA	2.16	118.69	111.91
11	bB	825	CLA	CMB-C2B-C1B	2.16	128.66	125.37
15	cA	848	BCR	C16-C15-C14	-2.16	119.05	123.47
12	cA	844	F6C	CAA-CBA-CGA	-2.16	107.15	113.43
11	bA	814	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
11	cB	827	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
11	bB	826	CLA	C4-C3-C5	2.16	118.90	115.27
11	bB	820	CLA	CAC-C3C-C4C	2.16	127.61	124.81
11	aA	813	CLA	CHB-C4A-NA	2.16	127.50	124.51
11	aB	816	CLA	CED-O2D-CGD	2.16	120.82	115.94
11	aB	828	CLA	CHD-C4C-NC	2.16	127.61	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bB	840	CLA	CMB-C2B-C1B	2.16	128.66	125.37
15	cB	842	BCR	C33-C5-C6	-2.16	122.10	124.53
15	aB	842	BCR	C27-C26-C25	2.16	125.86	122.73
11	cB	834	CLA	CMB-C2B-C1B	2.16	128.66	125.37
11	aB	823	CLA	O1D-CGD-CBD	-2.16	120.07	124.48
11	aB	840	CLA	CHB-C4A-NA	2.16	127.50	124.51
11	cA	822	CLA	C6-C7-C8	-2.16	108.95	115.92
11	aA	816	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
11	aB	837	CLA	O2A-CGA-CBA	2.16	118.68	111.91
11	aB	834	CLA	CHA-C1A-NA	-2.16	121.46	126.40
15	bB	842	BCR	C27-C26-C25	2.16	125.86	122.73
11	aB	840	CLA	CMB-C2B-C1B	2.15	128.65	125.37
12	cA	844	F6C	O2D-CGD-O1D	-2.15	119.63	123.84
11	bB	835	CLA	CHB-C4A-NA	2.15	127.49	124.51
11	bK	103	CLA	CHA-C1A-NA	-2.15	121.47	126.40
11	bB	837	CLA	O2A-CGA-CBA	2.15	118.66	111.91
11	aB	813	CLA	CHB-C1B-NB	-2.15	121.98	124.26
11	bB	813	CLA	CHB-C1B-NB	-2.15	121.98	124.26
11	cA	842	CLA	CHB-C1B-C2B	-2.15	121.16	127.24
11	aA	831	CLA	CHB-C4A-NA	2.15	127.49	124.51
11	bB	823	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
11	bB	802	CLA	CMB-C2B-C3B	2.15	131.80	126.59
11	bB	817	CLA	CMC-C2C-C1C	2.15	128.31	125.04
11	bB	801	CLA	C11-C10-C8	-2.15	108.97	115.92
11	cB	837	CLA	O2A-CGA-CBA	2.15	118.66	111.91
11	cA	834	CLA	CHB-C1B-NB	-2.15	121.98	124.26
11	cB	817	CLA	CMC-C2C-C1C	2.15	128.31	125.04
11	aB	826	CLA	C4-C3-C5	2.15	118.89	115.27
11	aK	101	CLA	OBD-CAD-C3D	-2.15	125.19	128.74
11	aA	822	CLA	CAA-C2A-C3A	-2.15	106.89	112.78
11	aA	823	CLA	C4A-NA-C1A	-2.15	105.74	106.71
11	cA	814	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
11	cB	828	CLA	CHD-C4C-NC	2.15	127.59	124.20
11	cA	825	CLA	CAA-C2A-C3A	-2.15	106.90	112.78
15	bB	844	BCR	C38-C26-C27	-2.15	109.49	113.62
11	bK	101	CLA	OBD-CAD-C3D	-2.15	125.19	128.74
11	aB	817	CLA	CMC-C2C-C1C	2.15	128.31	125.04
11	aK	103	CLA	CHA-C1A-NA	-2.15	121.48	126.40
11	bB	811	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
11	cB	835	CLA	CHB-C4A-NA	2.15	127.48	124.51
11	aB	805	CLA	CHB-C1B-NB	-2.15	121.99	124.26
11	bA	825	CLA	O1D-CGD-CBD	-2.15	120.09	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	830	F6C	CHB-C4A-NA	2.14	126.42	124.45
11	aA	828	CLA	C1-C2-C3	-2.14	122.33	126.04
11	bA	825	CLA	CAA-C2A-C3A	-2.14	106.91	112.78
15	cB	844	BCR	C38-C26-C27	-2.14	109.50	113.62
11	aA	829	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
11	bB	832	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
11	cK	103	CLA	CHA-C1A-NA	-2.14	121.49	126.40
11	cB	816	CLA	CMC-C2C-C1C	2.14	128.30	125.04
11	bB	816	CLA	CED-O2D-CGD	2.14	120.78	115.94
11	cB	826	CLA	C4-C3-C5	2.14	118.88	115.27
11	bA	838	CLA	C1-C2-C3	-2.14	122.34	126.04
11	aB	834	CLA	CMB-C2B-C1B	2.14	128.63	125.37
12	bA	830	F6C	CHB-C4A-NA	2.14	126.42	124.45
12	bA	844	F6C	O2D-CGD-O1D	-2.14	119.65	123.84
11	cA	807	CLA	CAC-C3C-C4C	2.14	127.59	124.81
11	cB	801	CLA	C11-C10-C8	-2.14	109.00	115.92
15	aA	848	BCR	C16-C15-C14	-2.14	119.09	123.47
11	bA	822	CLA	CAA-C2A-C3A	-2.14	106.92	112.78
11	bB	840	CLA	CHB-C4A-NA	2.14	127.47	124.51
11	aA	842	CLA	CHB-C1B-C2B	-2.14	121.20	127.24
11	cA	825	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
11	bA	831	CLA	CHB-C4A-NA	2.14	127.47	124.51
11	bB	805	CLA	CHB-C1B-NB	-2.14	121.99	124.26
15	aI	101	BCR	C15-C14-C13	-2.14	124.26	127.31
11	bB	834	CLA	CMB-C2B-C1B	2.14	128.62	125.37
11	aB	836	CLA	C3B-C4B-NB	2.14	112.50	110.52
11	cB	802	CLA	CMB-C2B-C3B	2.14	131.76	126.59
15	aM	101	BCR	C29-C30-C25	2.14	113.77	110.48
11	bA	807	CLA	CAC-C3C-C4C	2.14	127.58	124.81
11	aB	836	CLA	CHA-C1A-NA	-2.14	121.51	126.40
11	bB	827	CLA	O2D-CGD-O1D	-2.13	119.66	123.84
11	aB	816	CLA	CMC-C2C-C1C	2.13	128.29	125.04
11	bA	822	CLA	C6-C7-C8	-2.13	109.02	115.92
15	bA	847	BCR	C29-C30-C25	2.13	113.77	110.48
11	cA	822	CLA	CAA-C2A-C3A	-2.13	106.94	112.78
11	cB	805	CLA	CAA-C2A-C3A	-2.13	106.94	112.78
11	aB	818	CLA	CHB-C4A-NA	2.13	127.46	124.51
11	cA	831	CLA	CHB-C4A-NA	2.13	127.46	124.51
11	bA	803	CLA	O2A-CGA-CBA	2.13	118.59	111.91
15	cL	203	BCR	C16-C15-C14	-2.13	119.11	123.47
11	bB	816	CLA	CMC-C2C-C1C	2.13	128.28	125.04
11	cA	803	CLA	O2A-CGA-CBA	2.13	118.59	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aB	801	CLA	C11-C10-C8	-2.13	109.04	115.92
15	aL	203	BCR	C16-C15-C14	-2.13	119.11	123.47
11	aA	825	CLA	CAA-C2A-C3A	-2.13	106.95	112.78
11	cA	813	CLA	CHC-C4B-NB	-2.13	122.00	124.26
11	cA	838	CLA	C1-C2-C3	-2.13	122.36	126.04
11	aB	802	CLA	CMB-C2B-C3B	2.13	131.74	126.59
15	bA	847	BCR	C15-C16-C17	-2.13	119.11	123.47
11	cB	816	CLA	CED-O2D-CGD	2.13	120.75	115.94
11	cB	814	CLA	CBC-CAC-C3C	-2.13	106.56	112.43
11	aB	805	CLA	CAA-C2A-C3A	-2.13	106.95	112.78
11	bB	836	CLA	CHA-C1A-NA	-2.13	121.53	126.40
11	cA	815	CLA	CHB-C1B-NB	-2.13	122.00	124.26
11	aA	838	CLA	C1-C2-C3	-2.13	122.36	126.04
11	cB	836	CLA	C3B-C4B-NB	2.13	112.49	110.52
11	bA	809	CLA	CAA-C2A-C3A	-2.13	106.95	112.78
12	cA	844	F6C	CED-O2D-CGD	2.13	120.75	115.94
11	cA	810	CLA	CAA-C2A-C1A	2.13	118.94	111.97
11	aA	825	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
15	cI	103	BCR	C15-C14-C13	-2.13	124.28	127.31
15	bA	848	BCR	C16-C15-C14	-2.13	119.12	123.47
11	aA	803	CLA	O2A-CGA-CBA	2.12	118.58	111.91
11	bA	842	CLA	CHB-C1B-C2B	-2.12	121.24	127.24
15	bB	843	BCR	C27-C26-C25	2.12	125.81	122.73
11	aB	827	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
11	cA	842	CLA	CHB-C4A-NA	2.12	127.45	124.51
11	bA	813	CLA	CHC-C4B-NB	-2.12	122.01	124.26
15	bI	101	BCR	C15-C14-C13	-2.12	124.28	127.31
11	cA	809	CLA	CAA-C2A-C3A	-2.12	106.97	112.78
11	aB	832	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
12	aA	844	F6C	O2D-CGD-O1D	-2.12	119.69	123.84
11	bA	810	CLA	CAA-C2A-C1A	2.12	118.92	111.97
15	aB	844	BCR	C38-C26-C27	-2.12	109.54	113.62
11	bB	805	CLA	CAA-C2A-C3A	-2.12	106.97	112.78
11	bB	818	CLA	CHB-C4A-NA	2.12	127.44	124.51
11	bB	836	CLA	C3B-C4B-NB	2.12	112.48	110.52
11	bA	842	CLA	CHB-C4A-NA	2.12	127.44	124.51
13	aA	845	PQN	C2M-C2-C1	2.12	119.78	116.27
11	aA	838	CLA	O2A-C1-C2	2.12	114.20	108.64
11	cA	813	CLA	CHB-C4A-NA	2.12	127.44	124.51
11	cB	832	CLA	O2D-CGD-O1D	-2.12	119.70	123.84
11	aB	832	CLA	CMC-C2C-C1C	2.12	128.26	125.04
11	bB	814	CLA	CBC-CAC-C3C	-2.12	106.59	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aB	833	CLA	O2D-CGD-O1D	-2.12	119.70	123.84
11	cB	810	CLA	CHB-C4A-NA	2.12	127.44	124.51
11	cB	840	CLA	CHB-C4A-NA	2.12	127.44	124.51
11	cB	834	CLA	O2D-CGD-O1D	-2.12	119.70	123.84
11	cB	806	CLA	CHB-C4A-NA	2.12	127.44	124.51
11	aA	810	CLA	CAA-C2A-C1A	2.12	118.91	111.97
11	cK	101	CLA	OBD-CAD-C3D	-2.12	125.24	128.74
11	bB	827	CLA	CBC-CAC-C3C	-2.12	106.60	112.43
15	aA	847	BCR	C29-C30-C25	2.12	113.74	110.48
11	cB	811	CLA	O2D-CGD-O1D	-2.11	119.70	123.84
11	cB	807	CLA	O2A-CGA-CBA	2.11	118.54	111.91
11	bA	813	CLA	CHB-C4A-NA	2.11	127.44	124.51
15	aA	847	BCR	C15-C16-C17	-2.11	119.14	123.47
11	bB	815	CLA	CBC-CAC-C3C	-2.11	106.60	112.43
11	bB	807	CLA	O2A-CGA-CBA	2.11	118.54	111.91
11	bA	838	CLA	C1-O2A-CGA	2.11	121.99	116.44
11	bA	828	CLA	OBD-CAD-C3D	-2.11	123.43	128.52
11	cB	819	CLA	CBA-CAA-C2A	2.11	120.10	113.86
11	cA	828	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
11	aA	809	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
15	cL	208	BCR	C24-C23-C22	-2.11	123.04	126.23
11	cA	809	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
11	aA	828	CLA	OBD-CAD-C3D	-2.11	123.44	128.52
11	cB	836	CLA	CHA-C1A-NA	-2.11	121.56	126.40
12	bA	844	F6C	CED-O2D-CGD	2.11	120.71	115.94
13	cB	841	PQN	C11-C3-C4	2.11	120.76	118.50
11	aB	819	CLA	CBA-CAA-C2A	2.11	120.09	113.86
11	aA	813	CLA	CHC-C4B-NB	-2.11	122.02	124.26
15	cA	847	BCR	C29-C30-C25	2.11	113.73	110.48
15	bL	203	BCR	C16-C15-C14	-2.11	119.15	123.47
15	cA	847	BCR	C15-C16-C17	-2.11	119.15	123.47
11	aB	827	CLA	CBC-CAC-C3C	-2.11	106.61	112.43
11	bA	828	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
11	aB	807	CLA	O2A-CGA-CBA	2.11	118.53	111.91
11	bA	806	CLA	C6-C7-C8	-2.11	109.10	115.92
11	cA	838	CLA	O2A-C1-C2	2.11	114.18	108.64
11	bA	805	CLA	CHB-C1B-C2B	-2.11	121.28	127.24
11	bK	101	CLA	CBC-CAC-C3C	-2.11	106.62	112.43
13	bA	845	PQN	C2M-C2-C1	2.11	119.76	116.27
11	bB	819	CLA	CBA-CAA-C2A	2.11	120.08	113.86
11	aB	834	CLA	O2D-CGD-O1D	-2.11	119.72	123.84
11	bA	843	CLA	CHB-C4A-NA	2.11	127.43	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	aB	814	CLA	CBC-CAC-C3C	-2.11	106.62	112.43
13	cA	845	PQN	C2M-C2-C1	2.11	119.76	116.27
11	aA	842	CLA	CHB-C4A-NA	2.11	127.42	124.51
11	cK	101	CLA	CBC-CAC-C3C	-2.11	106.63	112.43
15	cB	843	BCR	C27-C26-C25	2.11	125.79	122.73
11	cA	815	CLA	CHA-C1A-NA	-2.11	121.58	126.40
11	aL	204	CLA	C1-C2-C3	-2.11	122.40	126.04
15	aB	843	BCR	C27-C26-C25	2.10	125.79	122.73
11	aA	807	CLA	CAC-C3C-C4C	2.10	127.54	124.81
11	aA	815	CLA	CHA-C1A-NA	-2.10	121.58	126.40
11	bB	810	CLA	CHB-C4A-NA	2.10	127.42	124.51
11	aA	838	CLA	C1-O2A-CGA	2.10	121.96	116.44
11	aA	828	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
15	bM	101	BCR	C29-C30-C25	2.10	113.72	110.48
11	cB	813	CLA	C4-C3-C5	2.10	118.81	115.27
11	aA	806	CLA	C6-C7-C8	-2.10	109.13	115.92
12	aA	844	F6C	CED-O2D-CGD	2.10	120.69	115.94
11	bA	838	CLA	O2A-C1-C2	2.10	114.16	108.64
11	cA	843	CLA	CHB-C4A-NA	2.10	127.41	124.51
11	cB	833	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
11	cB	837	CLA	C1-C2-C3	-2.10	122.41	126.04
12	bB	824	F6C	C1-O2A-CGA	2.10	121.95	116.44
11	cA	806	CLA	C6-C7-C8	-2.10	109.14	115.92
11	cA	828	CLA	OBD-CAD-C3D	-2.10	123.47	128.52
11	aA	815	CLA	CHB-C1B-NB	-2.10	122.04	124.26
15	cL	208	BCR	C7-C8-C9	-2.10	123.07	126.23
11	cB	802	CLA	CHB-C4A-NA	2.10	127.41	124.51
11	aB	806	CLA	CHB-C4A-NA	2.10	127.41	124.51
16	cA	852	LHG	C27-C26-C25	-2.10	103.79	114.42
15	aA	851	BCR	C11-C10-C9	-2.09	124.32	127.31
11	cB	805	CLA	CHB-C1B-NB	-2.09	122.04	124.26
12	cB	824	F6C	C1-O2A-CGA	2.09	121.94	116.44
11	bB	834	CLA	O2D-CGD-O1D	-2.09	119.74	123.84
15	bA	847	BCR	C16-C15-C14	-2.09	119.19	123.47
11	aA	843	CLA	CMB-C2B-C1B	2.09	128.56	125.37
11	cB	805	CLA	CBA-CAA-C2A	2.09	120.04	113.86
11	bA	815	CLA	CHA-C1A-NA	-2.09	121.61	126.40
11	cB	809	CLA	CHB-C4A-NA	2.09	127.41	124.51
11	aA	802	CLA	C11-C10-C8	-2.09	109.16	115.92
12	bA	832	F6C	O2A-CGA-O1A	-2.09	118.31	123.59
12	cA	832	F6C	O2A-CGA-O1A	-2.09	118.31	123.59
11	cA	838	CLA	C1-O2A-CGA	2.09	121.93	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aB	824	F6C	C1-O2A-CGA	2.09	121.93	116.44
11	cB	827	CLA	CBC-CAC-C3C	-2.09	106.67	112.43
11	cA	838	CLA	CHB-C4A-NA	2.09	127.40	124.51
11	bA	820	CLA	CAA-CBA-CGA	2.09	119.36	113.25
11	cA	820	CLA	CAA-CBA-CGA	2.09	119.36	113.25
11	cA	843	CLA	CMB-C2B-C1B	2.09	128.55	125.37
11	aB	815	CLA	CBC-CAC-C3C	-2.09	106.67	112.43
11	aB	814	CLA	CHB-C1B-NB	-2.09	122.05	124.26
11	aA	843	CLA	CHB-C4A-NA	2.09	127.40	124.51
11	bL	204	CLA	C1-C2-C3	-2.09	122.43	126.04
11	bB	833	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
11	aK	101	CLA	CBC-CAC-C3C	-2.09	106.67	112.43
15	aL	208	BCR	C24-C23-C22	-2.09	123.08	126.23
16	aA	852	LHG	C27-C26-C25	-2.09	103.83	114.42
11	aB	809	CLA	CHB-C4A-NA	2.09	127.40	124.51
11	cA	802	CLA	C11-C10-C8	-2.09	109.17	115.92
11	aB	820	CLA	CHB-C1B-NB	-2.09	122.05	124.26
15	cA	847	BCR	C16-C15-C14	-2.09	119.20	123.47
11	aB	810	CLA	CMB-C2B-C1B	2.09	128.55	125.37
16	bA	852	LHG	C27-C26-C25	-2.09	103.83	114.42
11	cA	812	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
11	cA	805	CLA	CHB-C1B-C2B	-2.09	121.34	127.24
11	aA	821	CLA	O1D-CGD-CBD	-2.09	120.22	124.48
11	cA	821	CLA	O1D-CGD-CBD	-2.09	120.22	124.48
11	cB	822	CLA	CHB-C4A-NA	2.09	127.40	124.51
11	aA	809	CLA	O1D-CGD-CBD	-2.09	120.22	124.48
11	aA	804	CLA	CHB-C1B-NB	-2.08	122.05	124.26
11	bA	809	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
11	cL	204	CLA	C1-C2-C3	-2.08	122.44	126.04
11	bB	802	CLA	CHB-C4A-NA	2.08	127.39	124.51
15	aI	101	BCR	C38-C26-C27	-2.08	109.61	113.62
11	aA	819	CLA	CHB-C1B-C2B	-2.08	121.35	127.24
11	cB	815	CLA	CBC-CAC-C3C	-2.08	106.69	112.43
11	bB	837	CLA	C1-C2-C3	-2.08	122.44	126.04
11	bA	802	CLA	C11-C10-C8	-2.08	109.19	115.92
12	aA	832	F6C	O2A-CGA-O1A	-2.08	118.34	123.59
11	aB	810	CLA	CHB-C4A-NA	2.08	127.39	124.51
11	bA	821	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
11	cB	807	CLA	CHB-C4A-NA	2.08	127.39	124.51
11	aA	816	CLA	CMB-C2B-C1B	2.08	128.54	125.37
11	aA	838	CLA	CHB-C4A-NA	2.08	127.39	124.51
15	aA	847	BCR	C16-C15-C14	-2.08	119.21	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bL	208	BCR	C24-C23-C22	-2.08	123.09	126.23
11	aA	812	CLA	CAA-C2A-C3A	-2.08	107.08	112.78
11	cB	832	CLA	O2A-CGA-CBA	2.08	120.71	114.03
11	cB	810	CLA	CMB-C2B-C1B	2.08	128.53	125.37
15	aL	208	BCR	C7-C8-C9	-2.08	123.10	126.23
11	aB	805	CLA	CBA-CAA-C2A	2.08	119.99	113.86
11	bA	819	CLA	CHB-C1B-C2B	-2.08	121.37	127.24
12	aA	830	F6C	CHB-C4A-NA	2.08	126.36	124.45
11	aA	812	CLA	CHC-C1C-NC	2.08	127.35	124.20
11	aA	831	CLA	CBC-CAC-C3C	-2.08	106.71	112.43
11	bB	805	CLA	CBA-CAA-C2A	2.07	119.99	113.86
15	aB	848	BCR	C30-C25-C26	-2.07	119.69	122.61
11	aA	820	CLA	CAA-CBA-CGA	2.07	119.32	113.25
11	bA	831	CLA	CBC-CAC-C3C	-2.07	106.71	112.43
11	bB	806	CLA	CHB-C4A-NA	2.07	127.38	124.51
11	aB	804	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
11	aA	805	CLA	CHB-C1B-C2B	-2.07	121.38	127.24
11	bB	830	CLA	CMC-C2C-C1C	2.07	128.19	125.04
11	cB	807	CLA	C4-C3-C5	2.07	118.76	115.27
15	cM	101	BCR	C29-C30-C25	2.07	113.67	110.48
11	bB	832	CLA	O2A-CGA-CBA	2.07	120.68	114.03
11	aB	807	CLA	C4-C3-C5	2.07	118.75	115.27
11	bB	810	CLA	CMB-C2B-C1B	2.07	128.52	125.37
11	cB	827	CLA	CMB-C2B-C1B	2.07	128.52	125.37
11	aB	832	CLA	O2A-CGA-CBA	2.07	120.68	114.03
11	bA	815	CLA	CHB-C1B-NB	-2.07	122.06	124.26
15	bI	101	BCR	C38-C26-C27	-2.07	109.64	113.62
11	bB	839	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
11	cA	822	CLA	CHB-C4A-NA	2.07	127.37	124.51
11	bB	813	CLA	C4-C3-C5	2.07	118.75	115.27
11	cB	804	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
12	bA	832	F6C	CMC-C2C-C1C	2.07	128.52	125.37
11	bB	816	CLA	C4-C3-C5	2.07	118.75	115.27
11	bB	827	CLA	CMB-C2B-C1B	2.07	128.52	125.37
11	cB	814	CLA	CHB-C1B-NB	-2.07	122.07	124.26
11	bA	841	CLA	CBC-CAC-C3C	-2.07	106.73	112.43
11	aB	837	CLA	C1-C2-C3	-2.07	122.47	126.04
11	cB	832	CLA	CMC-C2C-C1C	2.07	128.19	125.04
15	cB	848	BCR	C30-C25-C26	-2.07	119.70	122.61
11	bB	807	CLA	CHB-C4A-NA	2.07	127.37	124.51
11	bB	820	CLA	CHB-C1B-NB	-2.07	122.07	124.26
11	aA	841	CLA	CBC-CAC-C3C	-2.07	106.74	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cI	103	BCR	C38-C26-C27	-2.07	109.65	113.62
11	cA	841	CLA	CBC-CAC-C3C	-2.07	106.74	112.43
11	aB	813	CLA	C4-C3-C5	2.06	118.74	115.27
11	bB	807	CLA	C4-C3-C5	2.06	118.74	115.27
11	bB	836	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
11	cB	834	CLA	CED-O2D-CGD	2.06	120.61	115.94
11	cA	816	CLA	CMB-C2B-C1B	2.06	128.51	125.37
12	bA	830	F6C	CAA-CBA-CGA	-2.06	107.43	113.43
11	aA	829	CLA	CHB-C1B-C2B	-2.06	121.41	127.24
11	cB	816	CLA	CMB-C2B-C1B	2.06	128.51	125.37
11	aA	807	CLA	C11-C12-C13	-2.06	109.25	115.92
11	bA	838	CLA	C4-C3-C5	2.06	118.34	115.98
11	aB	804	CLA	C5-C3-C4	2.06	119.15	114.60
11	cA	831	CLA	CBC-CAC-C3C	-2.06	106.75	112.43
11	bB	804	CLA	C5-C3-C4	2.06	119.15	114.60
11	aB	827	CLA	CMB-C2B-C1B	2.06	128.51	125.37
11	bB	822	CLA	CHB-C4A-NA	2.06	127.36	124.51
11	bA	843	CLA	CMB-C2B-C1B	2.06	128.50	125.37
11	aB	816	CLA	O2D-CGD-O1D	-2.06	119.81	123.84
12	cA	830	F6C	CAA-CBA-CGA	-2.06	107.44	113.43
11	bA	816	CLA	CMB-C2B-C1B	2.06	128.50	125.37
11	cA	807	CLA	C11-C12-C13	-2.06	109.27	115.92
11	cA	811	CLA	CMB-C2B-C1B	2.06	128.50	125.37
11	bA	838	CLA	CHB-C4A-NA	2.06	127.36	124.51
11	cB	836	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
13	bB	841	PQN	C11-C3-C4	2.06	120.70	118.50
11	cA	819	CLA	CHB-C1B-C2B	-2.06	121.43	127.24
11	aA	821	CLA	CHA-C1A-NA	-2.06	121.69	126.40
11	aB	802	CLA	CHB-C4A-NA	2.06	127.36	124.51
11	cB	836	CLA	CHB-C4A-NA	2.06	127.36	124.51
11	cL	206	CLA	O2A-CGA-CBA	2.06	118.36	111.91
11	cA	821	CLA	CHA-C1A-NA	-2.06	121.69	126.40
11	bA	812	CLA	CAA-C2A-C3A	-2.05	107.15	112.78
11	cB	830	CLA	CHB-C1B-C2B	-2.05	121.44	127.24
11	aA	824	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
11	bL	206	CLA	O2A-CGA-CBA	2.05	118.35	111.91
11	cB	820	CLA	CHB-C1B-NB	-2.05	122.08	124.26
11	bB	809	CLA	CMB-C2B-C1B	2.05	128.50	125.37
11	bA	829	CLA	CMA-C3A-C2A	-2.05	105.55	113.83
11	cA	815	CLA	CHC-C1C-NC	2.05	127.32	124.20
11	aB	825	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
11	aB	830	CLA	CMC-C2C-C1C	2.05	128.16	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cA	812	CLA	CHC-C1C-NC	2.05	127.31	124.20
11	bB	834	CLA	CED-O2D-CGD	2.05	120.58	115.94
15	cA	851	BCR	C11-C10-C9	-2.05	124.38	127.31
11	bB	832	CLA	CMC-C2C-C1C	2.05	128.16	125.04
15	bA	851	BCR	C11-C10-C9	-2.05	124.39	127.31
11	aB	807	CLA	CHB-C4A-NA	2.05	127.34	124.51
12	aA	830	F6C	CAA-CBA-CGA	-2.05	107.47	113.43
11	cA	829	CLA	CMA-C3A-C2A	-2.05	105.57	113.83
11	aB	830	CLA	CHB-C1B-C2B	-2.05	121.45	127.24
11	bA	829	CLA	CHB-C1B-C2B	-2.05	121.45	127.24
11	bA	821	CLA	CHA-C1A-NA	-2.05	121.71	126.40
11	bA	822	CLA	CHB-C4A-NA	2.05	127.34	124.51
11	cB	804	CLA	C5-C3-C4	2.05	119.12	114.60
11	aB	828	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
11	cB	816	CLA	O2D-CGD-O1D	-2.05	119.84	123.84
11	bA	811	CLA	CMB-C2B-C1B	2.05	128.49	125.37
11	bB	821	CLA	CAA-C2A-C3A	-2.05	107.17	112.78
11	aB	816	CLA	CMB-C2B-C1B	2.05	128.49	125.37
11	aL	206	CLA	O2A-CGA-CBA	2.05	118.33	111.91
11	aB	839	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
11	bA	824	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
11	cA	821	CLA	CHB-C1B-NB	-2.05	122.09	124.26
11	aB	836	CLA	CHB-C4A-NA	2.04	127.34	124.51
11	cA	829	CLA	CHB-C1B-C2B	-2.04	121.46	127.24
11	aB	836	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
12	aA	827	F6C	CHC-C1C-NC	2.04	126.42	124.26
11	bB	821	CLA	CMC-C2C-C1C	2.04	128.15	125.04
11	cB	823	CLA	CBC-CAC-C3C	-2.04	106.81	112.43
11	bA	807	CLA	C11-C12-C13	-2.04	109.32	115.92
11	bB	812	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
11	bB	823	CLA	CBC-CAC-C3C	-2.04	106.81	112.43
11	cA	824	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
11	cB	828	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
11	aB	822	CLA	CHB-C4A-NA	2.04	127.33	124.51
11	aB	834	CLA	CED-O2D-CGD	2.04	120.55	115.94
11	bB	804	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
11	cB	830	CLA	CBC-CAC-C3C	-2.04	106.81	112.43
11	cB	816	CLA	C4-C3-C5	2.04	118.70	115.27
11	aB	805	CLA	CHA-C1A-NA	-2.04	121.73	126.40
11	cB	821	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
11	bB	816	CLA	CMB-C2B-C1B	2.04	128.47	125.37
11	bB	816	CLA	O2D-CGD-O1D	-2.04	119.86	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cA	836	CLA	CBC-CAC-C3C	-2.04	106.82	112.43
11	aB	816	CLA	C4-C3-C5	2.04	118.70	115.27
11	bB	814	CLA	CHB-C1B-NB	-2.04	122.10	124.26
11	bA	815	CLA	CHC-C1C-NC	2.03	127.29	124.20
11	bB	830	CLA	CHB-C1B-C2B	-2.03	121.49	127.24
11	aA	838	CLA	C4-C3-C5	2.03	118.31	115.98
11	aL	205	CLA	CBC-CAC-C3C	-2.03	106.82	112.43
11	bA	836	CLA	CBC-CAC-C3C	-2.03	106.82	112.43
11	cB	816	CLA	CBC-CAC-C3C	-2.03	106.83	112.43
11	aB	821	CLA	CMC-C2C-C1C	2.03	128.13	125.04
15	bL	208	BCR	C7-C8-C9	-2.03	123.16	126.23
15	bB	848	BCR	C30-C25-C26	-2.03	119.75	122.61
11	aB	828	CLA	CHC-C1C-NC	2.03	127.29	124.20
11	aA	822	CLA	O2D-CGD-O1D	-2.03	119.86	123.84
15	cK	102	BCR	C7-C8-C9	-2.03	123.17	126.23
11	aA	819	CLA	CHA-C1A-NA	-2.03	121.75	126.40
12	cA	827	F6C	CHC-C1C-NC	2.03	126.41	124.26
11	aA	817	CLA	CHB-C1B-C2B	-2.03	121.50	127.24
11	cB	812	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
11	cA	817	CLA	CHB-C1B-C2B	-2.03	121.50	127.24
11	bB	833	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
11	aB	823	CLA	CBC-CAC-C3C	-2.03	106.83	112.43
12	cA	832	F6C	CMC-C2C-C1C	2.03	128.46	125.37
11	bA	838	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
11	bA	817	CLA	CHB-C1B-C2B	-2.03	121.50	127.24
11	aA	829	CLA	CMA-C3A-C2A	-2.03	105.64	113.83
11	bB	809	CLA	CHB-C4A-NA	2.03	127.32	124.51
11	bL	204	CLA	CHB-C4A-NA	2.03	127.32	124.51
11	bA	828	CLA	CBC-CAC-C3C	-2.03	106.83	112.43
11	bB	825	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
11	bB	823	CLA	CAA-C2A-C1A	2.03	118.63	111.97
11	cA	828	CLA	CBC-CAC-C3C	-2.03	106.84	112.43
11	aB	823	CLA	CAA-C2A-C1A	2.03	118.62	111.97
11	cB	830	CLA	CMC-C2C-C1C	2.03	128.13	125.04
11	aA	811	CLA	CMB-C2B-C1B	2.03	128.46	125.37
13	aB	841	PQN	C11-C3-C4	2.03	120.67	118.50
11	aB	812	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
11	cB	839	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
11	bA	810	CLA	CHA-C1A-NA	-2.03	121.75	126.40
12	cA	827	F6C	CBC-CAC-C3C	-2.03	106.84	112.43
11	aB	816	CLA	CBC-CAC-C3C	-2.03	106.84	112.43
11	aA	828	CLA	CBC-CAC-C3C	-2.03	106.84	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cB	830	CLA	CHA-C1A-NA	-2.03	121.76	126.40
11	bA	824	CLA	CHC-C1C-NC	2.03	127.28	124.20
11	aA	821	CLA	CHB-C1B-NB	-2.03	122.11	124.26
11	aB	819	CLA	CHB-C1B-NB	-2.03	122.11	124.26
11	cB	833	CLA	CAA-C2A-C3A	-2.03	107.23	112.78
15	aK	102	BCR	C7-C8-C9	-2.02	123.18	126.23
11	cA	804	CLA	CHB-C1B-NB	-2.02	122.11	124.26
15	aB	846	BCR	C10-C11-C12	-2.02	116.90	123.22
11	aA	806	CLA	CBA-CAA-C2A	2.02	119.84	113.86
11	aA	836	CLA	CBC-CAC-C3C	-2.02	106.85	112.43
12	bA	827	F6C	CBC-CAC-C3C	-2.02	106.85	112.43
11	cK	103	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
11	cB	818	CLA	C1-O2A-CGA	2.02	121.75	116.44
15	bA	849	BCR	C24-C23-C22	-2.02	123.18	126.23
11	aB	829	CLA	CBA-CAA-C2A	2.02	119.84	113.86
11	aA	814	CLA	CHB-C1B-NB	-2.02	122.11	124.26
11	cL	205	CLA	CBC-CAC-C3C	-2.02	106.85	112.43
11	aA	810	CLA	CHA-C1A-NA	-2.02	121.77	126.40
11	aB	809	CLA	CMB-C2B-C1B	2.02	128.45	125.37
11	bA	840	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
11	bB	829	CLA	CBA-CAA-C2A	2.02	119.83	113.86
11	cA	810	CLA	CHA-C1A-NA	-2.02	121.77	126.40
11	bK	103	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
11	cB	825	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
12	bL	202	F6C	O1D-CGD-CBD	-2.02	120.35	124.48
11	bA	838	CLA	CHA-C1A-NA	-2.02	121.77	126.40
11	cA	838	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
11	bB	828	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
11	aA	815	CLA	CHC-C1C-NC	2.02	127.27	124.20
11	cA	806	CLA	CBA-CAA-C2A	2.02	119.82	113.86
11	aB	819	CLA	CBC-CAC-C3C	-2.02	106.86	112.43
11	bA	812	CLA	CHC-C1C-NC	2.02	127.27	124.20
11	cB	823	CLA	CAA-C2A-C1A	2.02	118.59	111.97
11	aB	830	CLA	CBC-CAC-C3C	-2.02	106.87	112.43
11	bA	840	CLA	CHA-C1A-NA	-2.02	121.78	126.40
15	aA	851	BCR	C37-C22-C21	-2.02	120.10	122.92
11	cA	838	CLA	C4-C3-C5	2.02	118.29	115.98
11	cB	809	CLA	CMB-C2B-C1B	2.02	128.44	125.37
11	cL	204	CLA	CHB-C4A-NA	2.02	127.30	124.51
11	cA	824	CLA	CHC-C1C-NC	2.02	127.26	124.20
12	aL	202	F6C	O1D-CGD-CBD	-2.02	120.36	124.48
11	aB	812	CLA	CHA-C1A-NA	-2.02	121.78	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bB	819	CLA	CBC-CAC-C3C	-2.02	106.87	112.43
11	aB	833	CLA	CAA-C2A-C3A	-2.02	107.26	112.78
11	bB	830	CLA	CBC-CAC-C3C	-2.02	106.87	112.43
12	bA	827	F6C	CHC-C1C-NC	2.02	126.39	124.26
11	aA	840	CLA	CHB-C1B-C2B	-2.01	121.55	127.24
11	cB	829	CLA	O2A-CGA-CBA	2.01	120.50	114.03
11	aA	812	CLA	CBC-CAC-C3C	-2.01	106.88	112.43
15	cA	851	BCR	C37-C22-C21	-2.01	120.10	122.92
15	aA	850	BCR	C33-C5-C6	-2.01	122.27	124.53
11	cA	812	CLA	CBC-CAC-C3C	-2.01	106.88	112.43
11	aA	817	CLA	CHA-C1A-NA	-2.01	121.78	126.40
11	bB	818	CLA	C1-O2A-CGA	2.01	121.73	116.44
15	bM	101	BCR	C31-C1-C6	2.01	113.56	110.30
11	bB	816	CLA	CBC-CAC-C3C	-2.01	106.88	112.43
11	aB	828	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
11	cB	805	CLA	CHA-C1A-NA	-2.01	121.79	126.40
11	bL	205	CLA	CBC-CAC-C3C	-2.01	106.88	112.43
11	cA	840	CLA	CHB-C1B-C2B	-2.01	121.55	127.24
11	cA	812	CLA	CHB-C1B-NB	-2.01	122.13	124.26
11	aB	829	CLA	O2A-CGA-CBA	2.01	120.49	114.03
11	cA	822	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
15	bB	846	BCR	C10-C11-C12	-2.01	116.94	123.22
11	bA	824	CLA	CMB-C2B-C1B	2.01	128.43	125.37
11	aB	831	CLA	CHB-C1B-C2B	-2.01	121.56	127.24
11	bA	840	CLA	CHB-C1B-C2B	-2.01	121.56	127.24
11	cB	817	CLA	CBC-CAC-C3C	-2.01	106.89	112.43
11	cA	811	CLA	CHB-C4A-NA	2.01	127.29	124.51
12	bA	827	F6C	O2A-CGA-O1A	-2.01	118.52	123.59
11	bB	818	CLA	C1-C2-C3	-2.01	122.57	126.04
11	bA	821	CLA	CHB-C1B-NB	-2.01	122.13	124.26
11	cA	840	CLA	CHA-C1A-NA	-2.01	121.80	126.40
11	aA	840	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
11	aB	821	CLA	CAA-C2A-C3A	-2.01	107.28	112.78
11	cB	829	CLA	CBA-CAA-C2A	2.01	119.79	113.86
11	aL	206	CLA	CAA-C2A-C1A	-2.01	105.39	111.97
12	aA	832	F6C	CMC-C2C-C1C	2.01	128.43	125.37
11	bA	817	CLA	CHA-C1A-NA	-2.01	121.80	126.40
11	aB	827	CLA	O2A-CGA-CBA	2.01	118.21	111.91
11	bA	812	CLA	CBC-CAC-C3C	-2.01	106.90	112.43
11	bA	807	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
11	bB	829	CLA	O2A-CGA-CBA	2.01	120.48	114.03
11	aA	824	CLA	CMB-C2B-C1B	2.01	128.43	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bB	805	CLA	CHA-C1A-NA	-2.01	121.80	126.40
11	aB	818	CLA	C1-O2A-CGA	2.01	121.71	116.44
11	cB	806	CLA	CHA-C1A-NA	-2.01	121.80	126.40
11	aA	807	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
12	aA	827	F6C	O2A-CGA-O1A	-2.00	118.53	123.59
11	cB	819	CLA	CBC-CAC-C3C	-2.00	106.90	112.43
11	bA	806	CLA	CBA-CAA-C2A	2.00	119.78	113.86
11	cA	840	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
11	cB	821	CLA	CMC-C2C-C1C	2.00	128.09	125.04
15	cB	846	BCR	C10-C11-C12	-2.00	116.96	123.22
11	cB	818	CLA	C1-C2-C3	-2.00	122.58	126.04
11	cA	817	CLA	CHA-C1A-NA	-2.00	121.81	126.40
15	aL	208	BCR	C16-C15-C14	-2.00	119.37	123.47
12	aA	827	F6C	CBC-CAC-C3C	-2.00	106.91	112.43
11	cA	824	CLA	CMB-C2B-C1B	2.00	128.42	125.37
15	bA	851	BCR	C37-C22-C21	-2.00	120.12	122.92
11	cB	827	CLA	O2A-CGA-CBA	2.00	118.19	111.91
11	bB	831	CLA	CHA-C1A-NA	-2.00	121.81	126.40
11	cA	807	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
11	aK	103	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
11	bB	836	CLA	CHB-C4A-NA	2.00	127.28	124.51
11	cA	819	CLA	CHA-C1A-NA	-2.00	121.81	126.40
15	bA	850	BCR	C33-C5-C6	-2.00	122.28	124.53
11	cA	814	CLA	CHB-C1B-NB	-2.00	122.14	124.26
11	cB	828	CLA	CAA-C2A-C3A	-2.00	107.30	112.78

All (24) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	aA	826	F6C	NA
12	aA	827	F6C	C8
12	aA	827	F6C	NA
12	aA	830	F6C	NA
12	aA	832	F6C	NA
12	aA	844	F6C	NA
12	aB	824	F6C	NA
12	aL	202	F6C	NA
12	bA	826	F6C	NA
12	bA	827	F6C	C8
12	bA	827	F6C	NA
12	bA	830	F6C	NA
12	bA	832	F6C	NA

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Mol	Chain	Res	Type	Atom
12	bA	844	F6C	NA
12	bB	824	F6C	NA
12	bL	202	F6C	NA
12	cA	826	F6C	NA
12	cA	827	F6C	C8
12	cA	827	F6C	NA
12	cA	830	F6C	NA
12	cA	832	F6C	NA
12	cA	844	F6C	NA
12	cB	824	F6C	NA
12	cL	202	F6C	NA

All (3337) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	aA	804	CLA	C2B-C3B-CAB-CBB
11	aA	804	CLA	C4B-C3B-CAB-CBB
11	aA	804	CLA	CBD-CGD-O2D-CED
11	aA	805	CLA	CHA-CBD-CGD-O1D
11	aA	805	CLA	CHA-CBD-CGD-O2D
11	aA	806	CLA	C1A-C2A-CAA-CBA
11	aA	806	CLA	C3A-C2A-CAA-CBA
11	aA	806	CLA	CHA-CBD-CGD-O1D
11	aA	807	CLA	C2B-C3B-CAB-CBB
11	aA	807	CLA	C4B-C3B-CAB-CBB
11	aA	809	CLA	C3A-C2A-CAA-CBA
11	aA	812	CLA	C2B-C3B-CAB-CBB
11	aA	812	CLA	C4B-C3B-CAB-CBB
11	aA	818	CLA	CHA-CBD-CGD-O2D
11	aA	819	CLA	C3A-C2A-CAA-CBA
11	aA	820	CLA	C1A-C2A-CAA-CBA
11	aA	820	CLA	C3A-C2A-CAA-CBA
11	aA	820	CLA	C2B-C3B-CAB-CBB
11	aA	820	CLA	C4B-C3B-CAB-CBB
11	aA	821	CLA	C1A-C2A-CAA-CBA
11	aA	823	CLA	C1A-C2A-CAA-CBA
11	aA	823	CLA	C3A-C2A-CAA-CBA
11	aA	824	CLA	O1A-CGA-O2A-C1
11	aA	824	CLA	C4B-C3B-CAB-CBB
11	aA	824	CLA	C2-C3-C5-C6
11	aA	824	CLA	C4-C3-C5-C6
11	aA	825	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	aA	834	CLA	C2B-C3B-CAB-CBB
11	aA	834	CLA	C4B-C3B-CAB-CBB
11	aA	835	CLA	CHA-CBD-CGD-O1D
11	aA	835	CLA	CHA-CBD-CGD-O2D
11	aA	837	CLA	C1A-C2A-CAA-CBA
11	aA	837	CLA	CHA-CBD-CGD-O1D
11	aA	837	CLA	CHA-CBD-CGD-O2D
11	aA	840	CLA	C1A-C2A-CAA-CBA
11	aA	841	CLA	CHA-CBD-CGD-O1D
11	aA	841	CLA	CHA-CBD-CGD-O2D
11	aA	842	CLA	CHA-CBD-CGD-O1D
11	aA	842	CLA	CHA-CBD-CGD-O2D
11	aA	842	CLA	CBD-CGD-O2D-CED
11	aB	801	CLA	C2B-C3B-CAB-CBB
11	aB	801	CLA	C4B-C3B-CAB-CBB
11	aB	801	CLA	CHA-CBD-CGD-O1D
11	aB	802	CLA	C1A-C2A-CAA-CBA
11	aB	802	CLA	C3A-C2A-CAA-CBA
11	aB	804	CLA	C1A-C2A-CAA-CBA
11	aB	804	CLA	C3A-C2A-CAA-CBA
11	aB	805	CLA	C1A-C2A-CAA-CBA
11	aB	805	CLA	C3A-C2A-CAA-CBA
11	aB	806	CLA	C2B-C3B-CAB-CBB
11	aB	806	CLA	C4B-C3B-CAB-CBB
11	aB	806	CLA	C11-C10-C8-C7
11	aB	807	CLA	C2B-C3B-CAB-CBB
11	aB	807	CLA	C4B-C3B-CAB-CBB
11	aB	809	CLA	C1A-C2A-CAA-CBA
11	aB	812	CLA	C1A-C2A-CAA-CBA
11	aB	812	CLA	C3A-C2A-CAA-CBA
11	aB	815	CLA	CBD-CGD-O2D-CED
11	aB	817	CLA	C1A-C2A-CAA-CBA
11	aB	817	CLA	C2-C3-C5-C6
11	aB	817	CLA	C4-C3-C5-C6
11	aB	818	CLA	CBD-CGD-O2D-CED
11	aB	819	CLA	C3A-C2A-CAA-CBA
11	aB	819	CLA	C2B-C3B-CAB-CBB
11	aB	819	CLA	C4B-C3B-CAB-CBB
11	aB	821	CLA	C2A-CAA-CBA-CGA
11	aB	821	CLA	C2-C3-C5-C6
11	aB	821	CLA	C4-C3-C5-C6
11	aB	822	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
11	aB	822	CLA	C4B-C3B-CAB-CBB
11	aB	822	CLA	CHA-CBD-CGD-O1D
11	aB	822	CLA	CHA-CBD-CGD-O2D
11	aB	823	CLA	CHA-CBD-CGD-O1D
11	aB	823	CLA	CHA-CBD-CGD-O2D
11	aB	826	CLA	C1A-C2A-CAA-CBA
11	aB	827	CLA	C1A-C2A-CAA-CBA
11	aB	827	CLA	C3A-C2A-CAA-CBA
11	aB	829	CLA	C3A-C2A-CAA-CBA
11	aB	829	CLA	C2B-C3B-CAB-CBB
11	aB	829	CLA	C4B-C3B-CAB-CBB
11	aB	832	CLA	C1A-C2A-CAA-CBA
11	aB	832	CLA	C2B-C3B-CAB-CBB
11	aB	832	CLA	C4B-C3B-CAB-CBB
11	aB	832	CLA	CBD-CGD-O2D-CED
11	aB	836	CLA	C2-C3-C5-C6
11	aL	205	CLA	C1A-C2A-CAA-CBA
11	aL	205	CLA	C3A-C2A-CAA-CBA
11	aL	205	CLA	C2B-C3B-CAB-CBB
11	aL	205	CLA	C4B-C3B-CAB-CBB
11	aL	205	CLA	C6-C7-C8-C9
11	bA	804	CLA	C2B-C3B-CAB-CBB
11	bA	804	CLA	C4B-C3B-CAB-CBB
11	bA	804	CLA	CBD-CGD-O2D-CED
11	bA	805	CLA	CHA-CBD-CGD-O1D
11	bA	805	CLA	CHA-CBD-CGD-O2D
11	bA	806	CLA	C1A-C2A-CAA-CBA
11	bA	806	CLA	C3A-C2A-CAA-CBA
11	bA	806	CLA	CHA-CBD-CGD-O1D
11	bA	807	CLA	C2B-C3B-CAB-CBB
11	bA	807	CLA	C4B-C3B-CAB-CBB
11	bA	809	CLA	C3A-C2A-CAA-CBA
11	bA	812	CLA	C2B-C3B-CAB-CBB
11	bA	812	CLA	C4B-C3B-CAB-CBB
11	bA	818	CLA	CHA-CBD-CGD-O2D
11	bA	819	CLA	C3A-C2A-CAA-CBA
11	bA	820	CLA	C1A-C2A-CAA-CBA
11	bA	820	CLA	C3A-C2A-CAA-CBA
11	bA	820	CLA	C2B-C3B-CAB-CBB
11	bA	820	CLA	C4B-C3B-CAB-CBB
11	bA	821	CLA	C1A-C2A-CAA-CBA
11	bA	823	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
11	bA	823	CLA	C3A-C2A-CAA-CBA
11	bA	824	CLA	O1A-CGA-O2A-C1
11	bA	824	CLA	C4B-C3B-CAB-CBB
11	bA	824	CLA	C2-C3-C5-C6
11	bA	824	CLA	C4-C3-C5-C6
11	bA	825	CLA	CBD-CGD-O2D-CED
11	bA	834	CLA	C2B-C3B-CAB-CBB
11	bA	834	CLA	C4B-C3B-CAB-CBB
11	bA	835	CLA	CHA-CBD-CGD-O1D
11	bA	835	CLA	CHA-CBD-CGD-O2D
11	bA	837	CLA	C1A-C2A-CAA-CBA
11	bA	837	CLA	CHA-CBD-CGD-O1D
11	bA	837	CLA	CHA-CBD-CGD-O2D
11	bA	840	CLA	C1A-C2A-CAA-CBA
11	bA	841	CLA	CHA-CBD-CGD-O1D
11	bA	841	CLA	CHA-CBD-CGD-O2D
11	bA	842	CLA	CHA-CBD-CGD-O1D
11	bA	842	CLA	CHA-CBD-CGD-O2D
11	bA	842	CLA	CBD-CGD-O2D-CED
11	bB	801	CLA	C2B-C3B-CAB-CBB
11	bB	801	CLA	C4B-C3B-CAB-CBB
11	bB	801	CLA	CHA-CBD-CGD-O1D
11	bB	802	CLA	C1A-C2A-CAA-CBA
11	bB	802	CLA	C3A-C2A-CAA-CBA
11	bB	804	CLA	C1A-C2A-CAA-CBA
11	bB	804	CLA	C3A-C2A-CAA-CBA
11	bB	805	CLA	C1A-C2A-CAA-CBA
11	bB	805	CLA	C3A-C2A-CAA-CBA
11	bB	806	CLA	C2B-C3B-CAB-CBB
11	bB	806	CLA	C4B-C3B-CAB-CBB
11	bB	806	CLA	C11-C10-C8-C7
11	bB	807	CLA	C2B-C3B-CAB-CBB
11	bB	807	CLA	C4B-C3B-CAB-CBB
11	bB	809	CLA	C1A-C2A-CAA-CBA
11	bB	812	CLA	C1A-C2A-CAA-CBA
11	bB	812	CLA	C3A-C2A-CAA-CBA
11	bB	815	CLA	CBD-CGD-O2D-CED
11	bB	817	CLA	C1A-C2A-CAA-CBA
11	bB	817	CLA	C2-C3-C5-C6
11	bB	817	CLA	C4-C3-C5-C6
11	bB	818	CLA	CBD-CGD-O2D-CED
11	bB	819	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
11	bB	819	CLA	C2B-C3B-CAB-CBB
11	bB	819	CLA	C4B-C3B-CAB-CBB
11	bB	821	CLA	C2A-CAA-CBA-CGA
11	bB	821	CLA	C2-C3-C5-C6
11	bB	821	CLA	C4-C3-C5-C6
11	bB	822	CLA	C2B-C3B-CAB-CBB
11	bB	822	CLA	C4B-C3B-CAB-CBB
11	bB	822	CLA	CHA-CBD-CGD-O1D
11	bB	822	CLA	CHA-CBD-CGD-O2D
11	bB	823	CLA	CHA-CBD-CGD-O1D
11	bB	823	CLA	CHA-CBD-CGD-O2D
11	bB	826	CLA	C1A-C2A-CAA-CBA
11	bB	827	CLA	C1A-C2A-CAA-CBA
11	bB	827	CLA	C3A-C2A-CAA-CBA
11	bB	829	CLA	C3A-C2A-CAA-CBA
11	bB	829	CLA	C2B-C3B-CAB-CBB
11	bB	829	CLA	C4B-C3B-CAB-CBB
11	bB	832	CLA	C1A-C2A-CAA-CBA
11	bB	832	CLA	C2B-C3B-CAB-CBB
11	bB	832	CLA	C4B-C3B-CAB-CBB
11	bB	832	CLA	CBD-CGD-O2D-CED
11	bB	836	CLA	C2-C3-C5-C6
11	bL	205	CLA	C1A-C2A-CAA-CBA
11	bL	205	CLA	C3A-C2A-CAA-CBA
11	bL	205	CLA	C2B-C3B-CAB-CBB
11	bL	205	CLA	C4B-C3B-CAB-CBB
11	bL	205	CLA	C6-C7-C8-C9
11	cA	804	CLA	C2B-C3B-CAB-CBB
11	cA	804	CLA	C4B-C3B-CAB-CBB
11	cA	804	CLA	CBD-CGD-O2D-CED
11	cA	805	CLA	CHA-CBD-CGD-O1D
11	cA	805	CLA	CHA-CBD-CGD-O2D
11	cA	806	CLA	C1A-C2A-CAA-CBA
11	cA	806	CLA	C3A-C2A-CAA-CBA
11	cA	806	CLA	CHA-CBD-CGD-O1D
11	cA	807	CLA	C2B-C3B-CAB-CBB
11	cA	807	CLA	C4B-C3B-CAB-CBB
11	cA	809	CLA	C3A-C2A-CAA-CBA
11	cA	812	CLA	C2B-C3B-CAB-CBB
11	cA	812	CLA	C4B-C3B-CAB-CBB
11	cA	818	CLA	CHA-CBD-CGD-O2D
11	cA	819	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
11	cA	820	CLA	C1A-C2A-CAA-CBA
11	cA	820	CLA	C3A-C2A-CAA-CBA
11	cA	820	CLA	C2B-C3B-CAB-CBB
11	cA	820	CLA	C4B-C3B-CAB-CBB
11	cA	821	CLA	C1A-C2A-CAA-CBA
11	cA	823	CLA	C1A-C2A-CAA-CBA
11	cA	823	CLA	C3A-C2A-CAA-CBA
11	cA	824	CLA	O1A-CGA-O2A-C1
11	cA	824	CLA	C4B-C3B-CAB-CBB
11	cA	824	CLA	C2-C3-C5-C6
11	cA	824	CLA	C4-C3-C5-C6
11	cA	825	CLA	CBD-CGD-O2D-CED
11	cA	834	CLA	C2B-C3B-CAB-CBB
11	cA	834	CLA	C4B-C3B-CAB-CBB
11	cA	835	CLA	CHA-CBD-CGD-O1D
11	cA	835	CLA	CHA-CBD-CGD-O2D
11	cA	837	CLA	C1A-C2A-CAA-CBA
11	cA	837	CLA	CHA-CBD-CGD-O1D
11	cA	837	CLA	CHA-CBD-CGD-O2D
11	cA	840	CLA	C1A-C2A-CAA-CBA
11	cA	841	CLA	CHA-CBD-CGD-O1D
11	cA	841	CLA	CHA-CBD-CGD-O2D
11	cA	842	CLA	CHA-CBD-CGD-O1D
11	cA	842	CLA	CHA-CBD-CGD-O2D
11	cA	842	CLA	CBD-CGD-O2D-CED
11	cB	801	CLA	C2B-C3B-CAB-CBB
11	cB	801	CLA	C4B-C3B-CAB-CBB
11	cB	801	CLA	CHA-CBD-CGD-O1D
11	cB	802	CLA	C1A-C2A-CAA-CBA
11	cB	802	CLA	C3A-C2A-CAA-CBA
11	cB	804	CLA	C1A-C2A-CAA-CBA
11	cB	804	CLA	C3A-C2A-CAA-CBA
11	cB	805	CLA	C1A-C2A-CAA-CBA
11	cB	805	CLA	C3A-C2A-CAA-CBA
11	cB	806	CLA	C2B-C3B-CAB-CBB
11	cB	806	CLA	C4B-C3B-CAB-CBB
11	cB	806	CLA	C11-C10-C8-C7
11	cB	807	CLA	C2B-C3B-CAB-CBB
11	cB	807	CLA	C4B-C3B-CAB-CBB
11	cB	809	CLA	C1A-C2A-CAA-CBA
11	cB	812	CLA	C1A-C2A-CAA-CBA
11	cB	812	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
11	cB	815	CLA	CBD-CGD-O2D-CED
11	cB	817	CLA	C1A-C2A-CAA-CBA
11	cB	817	CLA	C2-C3-C5-C6
11	cB	817	CLA	C4-C3-C5-C6
11	cB	818	CLA	CBD-CGD-O2D-CED
11	cB	819	CLA	C3A-C2A-CAA-CBA
11	cB	819	CLA	C2B-C3B-CAB-CBB
11	cB	819	CLA	C4B-C3B-CAB-CBB
11	cB	821	CLA	C2A-CAA-CBA-CGA
11	cB	821	CLA	C2-C3-C5-C6
11	cB	821	CLA	C4-C3-C5-C6
11	cB	822	CLA	C2B-C3B-CAB-CBB
11	cB	822	CLA	C4B-C3B-CAB-CBB
11	cB	822	CLA	CHA-CBD-CGD-O1D
11	cB	822	CLA	CHA-CBD-CGD-O2D
11	cB	823	CLA	CHA-CBD-CGD-O1D
11	cB	823	CLA	CHA-CBD-CGD-O2D
11	cB	826	CLA	C1A-C2A-CAA-CBA
11	cB	827	CLA	C1A-C2A-CAA-CBA
11	cB	827	CLA	C3A-C2A-CAA-CBA
11	cB	829	CLA	C3A-C2A-CAA-CBA
11	cB	829	CLA	C2B-C3B-CAB-CBB
11	cB	829	CLA	C4B-C3B-CAB-CBB
11	cB	832	CLA	C1A-C2A-CAA-CBA
11	cB	832	CLA	C2B-C3B-CAB-CBB
11	cB	832	CLA	C4B-C3B-CAB-CBB
11	cB	832	CLA	CBD-CGD-O2D-CED
11	cB	836	CLA	C2-C3-C5-C6
11	cL	205	CLA	C1A-C2A-CAA-CBA
11	cL	205	CLA	C3A-C2A-CAA-CBA
11	cL	205	CLA	C2B-C3B-CAB-CBB
11	cL	205	CLA	C4B-C3B-CAB-CBB
11	cL	205	CLA	C6-C7-C8-C9
12	aA	826	F6C	C2C-C3C-CAC-CBC
12	aA	830	F6C	C3A-C2A-CAA-CBA
12	aA	832	F6C	C3B-C2B-CMB-OMB
12	aA	844	F6C	C2A-CAA-CBA-CGA
12	aB	824	F6C	C1A-C2A-CAA-CBA
12	aB	824	F6C	C3A-C2A-CAA-CBA
12	aB	824	F6C	CHA-CBD-CGD-O2D
12	aB	824	F6C	C1B-C2B-CMB-OMB
12	aB	824	F6C	C3B-C2B-CMB-OMB

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Mol	Chain	Res	Type	Atoms
12	aL	202	F6C	C3B-C2B-CMB-OMB
12	aL	202	F6C	C2-C3-C5-C6
12	aL	202	F6C	C4-C3-C5-C6
12	bA	826	F6C	C2C-C3C-CAC-CBC
12	bA	830	F6C	C3A-C2A-CAA-CBA
12	bA	832	F6C	C3B-C2B-CMB-OMB
12	bA	844	F6C	C2A-CAA-CBA-CGA
12	bB	824	F6C	C1A-C2A-CAA-CBA
12	bB	824	F6C	C3A-C2A-CAA-CBA
12	bB	824	F6C	CHA-CBD-CGD-O2D
12	bB	824	F6C	C1B-C2B-CMB-OMB
12	bB	824	F6C	C3B-C2B-CMB-OMB
12	bL	202	F6C	C3B-C2B-CMB-OMB
12	bL	202	F6C	C2-C3-C5-C6
12	bL	202	F6C	C4-C3-C5-C6
12	cA	826	F6C	C2C-C3C-CAC-CBC
12	cA	830	F6C	C3A-C2A-CAA-CBA
12	cA	832	F6C	C3B-C2B-CMB-OMB
12	cA	844	F6C	C2A-CAA-CBA-CGA
12	cB	824	F6C	C1A-C2A-CAA-CBA
12	cB	824	F6C	C3A-C2A-CAA-CBA
12	cB	824	F6C	CHA-CBD-CGD-O2D
12	cB	824	F6C	C1B-C2B-CMB-OMB
12	cB	824	F6C	C3B-C2B-CMB-OMB
12	cL	202	F6C	C3B-C2B-CMB-OMB
12	cL	202	F6C	C2-C3-C5-C6
12	cL	202	F6C	C4-C3-C5-C6
15	aA	847	BCR	C1-C6-C7-C8
15	aA	847	BCR	C37-C22-C23-C24
15	aA	848	BCR	C6-C7-C8-C9
15	aA	848	BCR	C7-C8-C9-C34
15	aA	848	BCR	C11-C12-C13-C35
15	aA	848	BCR	C20-C21-C22-C23
15	aA	848	BCR	C20-C21-C22-C37
15	aA	848	BCR	C37-C22-C23-C24
15	aA	849	BCR	C1-C6-C7-C8
15	aA	849	BCR	C7-C8-C9-C34
15	aA	849	BCR	C20-C21-C22-C37
15	aA	849	BCR	C21-C22-C23-C24
15	aA	849	BCR	C37-C22-C23-C24
15	aA	849	BCR	C22-C23-C24-C25
15	aA	850	BCR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
15	aA	851	BCR	C6-C7-C8-C9
15	aA	851	BCR	C18-C19-C20-C21
15	aA	851	BCR	C20-C21-C22-C23
15	aA	851	BCR	C20-C21-C22-C37
15	aA	851	BCR	C21-C22-C23-C24
15	aA	851	BCR	C22-C23-C24-C25
15	aB	842	BCR	C6-C7-C8-C9
15	aB	842	BCR	C7-C8-C9-C10
15	aB	842	BCR	C37-C22-C23-C24
15	aB	843	BCR	C7-C8-C9-C10
15	aB	843	BCR	C7-C8-C9-C34
15	aB	843	BCR	C21-C22-C23-C24
15	aB	843	BCR	C37-C22-C23-C24
15	aB	844	BCR	C1-C6-C7-C8
15	aB	844	BCR	C37-C22-C23-C24
15	aB	845	BCR	C6-C7-C8-C9
15	aB	845	BCR	C10-C11-C12-C13
15	aB	845	BCR	C11-C12-C13-C35
15	aB	845	BCR	C18-C19-C20-C21
15	aB	846	BCR	C7-C8-C9-C10
15	aB	846	BCR	C18-C19-C20-C21
15	aB	846	BCR	C20-C21-C22-C23
15	aB	846	BCR	C20-C21-C22-C37
15	aB	848	BCR	C1-C6-C7-C8
15	aB	848	BCR	C7-C8-C9-C34
15	aB	848	BCR	C16-C17-C18-C19
15	aB	848	BCR	C16-C17-C18-C36
15	aB	848	BCR	C20-C21-C22-C23
15	aB	848	BCR	C20-C21-C22-C37
15	aB	848	BCR	C37-C22-C23-C24
15	aB	848	BCR	C22-C23-C24-C25
15	aB	848	BCR	C23-C24-C25-C26
15	aB	848	BCR	C23-C24-C25-C30
15	aI	101	BCR	C1-C6-C7-C8
15	aI	101	BCR	C7-C8-C9-C10
15	aI	101	BCR	C7-C8-C9-C34
15	aI	101	BCR	C20-C21-C22-C23
15	aI	101	BCR	C21-C22-C23-C24
15	aI	101	BCR	C37-C22-C23-C24
15	aK	102	BCR	C1-C6-C7-C8
15	aK	102	BCR	C7-C8-C9-C10
15	aK	102	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
15	aK	102	BCR	C21-C22-C23-C24
15	aK	102	BCR	C37-C22-C23-C24
15	aL	203	BCR	C23-C24-C25-C30
15	aL	207	BCR	C1-C6-C7-C8
15	aL	208	BCR	C7-C8-C9-C34
15	aM	101	BCR	C1-C6-C7-C8
15	aM	101	BCR	C7-C8-C9-C34
15	aM	101	BCR	C22-C23-C24-C25
15	bA	847	BCR	C1-C6-C7-C8
15	bA	847	BCR	C37-C22-C23-C24
15	bA	848	BCR	C6-C7-C8-C9
15	bA	848	BCR	C7-C8-C9-C34
15	bA	848	BCR	C11-C12-C13-C35
15	bA	848	BCR	C20-C21-C22-C23
15	bA	848	BCR	C20-C21-C22-C37
15	bA	848	BCR	C37-C22-C23-C24
15	bA	849	BCR	C1-C6-C7-C8
15	bA	849	BCR	C7-C8-C9-C34
15	bA	849	BCR	C20-C21-C22-C37
15	bA	849	BCR	C21-C22-C23-C24
15	bA	849	BCR	C37-C22-C23-C24
15	bA	849	BCR	C22-C23-C24-C25
15	bA	850	BCR	C22-C23-C24-C25
15	bA	851	BCR	C6-C7-C8-C9
15	bA	851	BCR	C18-C19-C20-C21
15	bA	851	BCR	C20-C21-C22-C23
15	bA	851	BCR	C20-C21-C22-C37
15	bA	851	BCR	C21-C22-C23-C24
15	bA	851	BCR	C22-C23-C24-C25
15	bB	842	BCR	C6-C7-C8-C9
15	bB	842	BCR	C7-C8-C9-C10
15	bB	842	BCR	C37-C22-C23-C24
15	bB	843	BCR	C7-C8-C9-C10
15	bB	843	BCR	C7-C8-C9-C34
15	bB	843	BCR	C21-C22-C23-C24
15	bB	843	BCR	C37-C22-C23-C24
15	bB	844	BCR	C1-C6-C7-C8
15	bB	844	BCR	C37-C22-C23-C24
15	bB	845	BCR	C6-C7-C8-C9
15	bB	845	BCR	C10-C11-C12-C13
15	bB	845	BCR	C11-C12-C13-C35
15	bB	845	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
15	bB	846	BCR	C7-C8-C9-C10
15	bB	846	BCR	C18-C19-C20-C21
15	bB	846	BCR	C20-C21-C22-C23
15	bB	846	BCR	C20-C21-C22-C37
15	bB	848	BCR	C1-C6-C7-C8
15	bB	848	BCR	C7-C8-C9-C34
15	bB	848	BCR	C16-C17-C18-C19
15	bB	848	BCR	C16-C17-C18-C36
15	bB	848	BCR	C20-C21-C22-C23
15	bB	848	BCR	C20-C21-C22-C37
15	bB	848	BCR	C37-C22-C23-C24
15	bB	848	BCR	C22-C23-C24-C25
15	bB	848	BCR	C23-C24-C25-C26
15	bB	848	BCR	C23-C24-C25-C30
15	bI	101	BCR	C1-C6-C7-C8
15	bI	101	BCR	C7-C8-C9-C10
15	bI	101	BCR	C7-C8-C9-C34
15	bI	101	BCR	C20-C21-C22-C23
15	bI	101	BCR	C21-C22-C23-C24
15	bI	101	BCR	C37-C22-C23-C24
15	bK	102	BCR	C1-C6-C7-C8
15	bK	102	BCR	C7-C8-C9-C10
15	bK	102	BCR	C7-C8-C9-C34
15	bK	102	BCR	C21-C22-C23-C24
15	bK	102	BCR	C37-C22-C23-C24
15	bL	203	BCR	C23-C24-C25-C30
15	bL	207	BCR	C1-C6-C7-C8
15	bL	208	BCR	C7-C8-C9-C34
15	bM	101	BCR	C1-C6-C7-C8
15	bM	101	BCR	C7-C8-C9-C34
15	bM	101	BCR	C22-C23-C24-C25
15	cA	847	BCR	C1-C6-C7-C8
15	cA	847	BCR	C37-C22-C23-C24
15	cA	848	BCR	C6-C7-C8-C9
15	cA	848	BCR	C7-C8-C9-C34
15	cA	848	BCR	C11-C12-C13-C35
15	cA	848	BCR	C20-C21-C22-C23
15	cA	848	BCR	C20-C21-C22-C37
15	cA	848	BCR	C37-C22-C23-C24
15	cA	849	BCR	C1-C6-C7-C8
15	cA	849	BCR	C7-C8-C9-C34
15	cA	849	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
15	cA	849	BCR	C21-C22-C23-C24
15	cA	849	BCR	C37-C22-C23-C24
15	cA	849	BCR	C22-C23-C24-C25
15	cA	850	BCR	C22-C23-C24-C25
15	cA	851	BCR	C6-C7-C8-C9
15	cA	851	BCR	C18-C19-C20-C21
15	cA	851	BCR	C20-C21-C22-C23
15	cA	851	BCR	C20-C21-C22-C37
15	cA	851	BCR	C21-C22-C23-C24
15	cA	851	BCR	C22-C23-C24-C25
15	cB	842	BCR	C6-C7-C8-C9
15	cB	842	BCR	C7-C8-C9-C10
15	cB	842	BCR	C37-C22-C23-C24
15	cB	843	BCR	C7-C8-C9-C10
15	cB	843	BCR	C7-C8-C9-C34
15	cB	843	BCR	C21-C22-C23-C24
15	cB	843	BCR	C37-C22-C23-C24
15	cB	844	BCR	C1-C6-C7-C8
15	cB	844	BCR	C37-C22-C23-C24
15	cB	845	BCR	C6-C7-C8-C9
15	cB	845	BCR	C10-C11-C12-C13
15	cB	845	BCR	C11-C12-C13-C35
15	cB	845	BCR	C18-C19-C20-C21
15	cB	846	BCR	C7-C8-C9-C10
15	cB	846	BCR	C18-C19-C20-C21
15	cB	846	BCR	C20-C21-C22-C23
15	cB	846	BCR	C20-C21-C22-C37
15	cB	848	BCR	C1-C6-C7-C8
15	cB	848	BCR	C7-C8-C9-C34
15	cB	848	BCR	C16-C17-C18-C19
15	cB	848	BCR	C16-C17-C18-C36
15	cB	848	BCR	C20-C21-C22-C23
15	cB	848	BCR	C20-C21-C22-C37
15	cB	848	BCR	C37-C22-C23-C24
15	cB	848	BCR	C22-C23-C24-C25
15	cB	848	BCR	C23-C24-C25-C26
15	cB	848	BCR	C23-C24-C25-C30
15	cI	103	BCR	C1-C6-C7-C8
15	cI	103	BCR	C7-C8-C9-C10
15	cI	103	BCR	C7-C8-C9-C34
15	cI	103	BCR	C20-C21-C22-C23
15	cI	103	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
15	cI	103	BCR	C37-C22-C23-C24
15	cK	102	BCR	C1-C6-C7-C8
15	cK	102	BCR	C7-C8-C9-C10
15	cK	102	BCR	C7-C8-C9-C34
15	cK	102	BCR	C21-C22-C23-C24
15	cK	102	BCR	C37-C22-C23-C24
15	cL	203	BCR	C23-C24-C25-C30
15	cL	207	BCR	C1-C6-C7-C8
15	cL	208	BCR	C7-C8-C9-C34
15	cM	101	BCR	C1-C6-C7-C8
15	cM	101	BCR	C7-C8-C9-C34
15	cM	101	BCR	C22-C23-C24-C25
16	aA	852	LHG	C3-O3-P-O4
16	bA	852	LHG	C3-O3-P-O4
16	cA	852	LHG	C3-O3-P-O4
17	aA	853	LMT	C2'-C1'-O1'-C1
17	aA	853	LMT	O5'-C1'-O1'-C1
17	bA	853	LMT	C2'-C1'-O1'-C1
17	bA	853	LMT	O5'-C1'-O1'-C1
17	cA	853	LMT	C2'-C1'-O1'-C1
17	cA	853	LMT	O5'-C1'-O1'-C1
11	aA	806	CLA	CBD-CGD-O2D-CED
11	aA	810	CLA	CBD-CGD-O2D-CED
11	aA	812	CLA	CBD-CGD-O2D-CED
11	aA	816	CLA	CBD-CGD-O2D-CED
11	aA	817	CLA	CBD-CGD-O2D-CED
11	aA	818	CLA	CBD-CGD-O2D-CED
11	aA	822	CLA	CBD-CGD-O2D-CED
11	aA	824	CLA	CBD-CGD-O2D-CED
11	aA	836	CLA	CBD-CGD-O2D-CED
11	aB	806	CLA	CBD-CGD-O2D-CED
11	bA	806	CLA	CBD-CGD-O2D-CED
11	bA	810	CLA	CBD-CGD-O2D-CED
11	bA	812	CLA	CBD-CGD-O2D-CED
11	bA	816	CLA	CBD-CGD-O2D-CED
11	bA	817	CLA	CBD-CGD-O2D-CED
11	bA	818	CLA	CBD-CGD-O2D-CED
11	bA	822	CLA	CBD-CGD-O2D-CED
11	bA	824	CLA	CBD-CGD-O2D-CED
11	bA	836	CLA	CBD-CGD-O2D-CED
11	bB	806	CLA	CBD-CGD-O2D-CED
11	cA	806	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	cA	810	CLA	CBD-CGD-O2D-CED
11	cA	816	CLA	CBD-CGD-O2D-CED
11	cA	817	CLA	CBD-CGD-O2D-CED
11	cA	818	CLA	CBD-CGD-O2D-CED
11	cA	822	CLA	CBD-CGD-O2D-CED
11	cA	824	CLA	CBD-CGD-O2D-CED
11	cA	836	CLA	CBD-CGD-O2D-CED
11	cB	806	CLA	CBD-CGD-O2D-CED
11	aA	821	CLA	O1A-CGA-O2A-C1
11	bA	821	CLA	O1A-CGA-O2A-C1
11	cA	821	CLA	O1A-CGA-O2A-C1
11	aB	806	CLA	O1D-CGD-O2D-CED
11	bB	806	CLA	O1D-CGD-O2D-CED
11	cB	806	CLA	O1D-CGD-O2D-CED
11	aA	804	CLA	O1D-CGD-O2D-CED
11	aA	842	CLA	O1D-CGD-O2D-CED
11	aB	815	CLA	O1D-CGD-O2D-CED
11	aB	818	CLA	O1D-CGD-O2D-CED
11	aB	832	CLA	O1D-CGD-O2D-CED
11	bA	804	CLA	O1D-CGD-O2D-CED
11	bA	842	CLA	O1D-CGD-O2D-CED
11	bB	815	CLA	O1D-CGD-O2D-CED
11	bB	818	CLA	O1D-CGD-O2D-CED
11	bB	832	CLA	O1D-CGD-O2D-CED
11	cA	804	CLA	O1D-CGD-O2D-CED
11	cA	842	CLA	O1D-CGD-O2D-CED
11	cB	815	CLA	O1D-CGD-O2D-CED
11	cB	818	CLA	O1D-CGD-O2D-CED
11	cB	832	CLA	O1D-CGD-O2D-CED
11	aA	807	CLA	CBD-CGD-O2D-CED
11	aA	835	CLA	CBD-CGD-O2D-CED
11	aA	840	CLA	CBD-CGD-O2D-CED
11	aA	843	CLA	CBD-CGD-O2D-CED
11	aB	809	CLA	CBD-CGD-O2D-CED
11	aB	810	CLA	CBD-CGD-O2D-CED
11	aB	820	CLA	CBD-CGD-O2D-CED
11	aB	826	CLA	CBD-CGD-O2D-CED
11	bA	807	CLA	CBD-CGD-O2D-CED
11	bA	835	CLA	CBD-CGD-O2D-CED
11	bA	840	CLA	CBD-CGD-O2D-CED
11	bA	843	CLA	CBD-CGD-O2D-CED
11	bB	801	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	bB	809	CLA	CBD-CGD-O2D-CED
11	bB	810	CLA	CBD-CGD-O2D-CED
11	bB	820	CLA	CBD-CGD-O2D-CED
11	bB	826	CLA	CBD-CGD-O2D-CED
11	cA	807	CLA	CBD-CGD-O2D-CED
11	cA	812	CLA	CBD-CGD-O2D-CED
11	cA	835	CLA	CBD-CGD-O2D-CED
11	cA	840	CLA	CBD-CGD-O2D-CED
11	cA	843	CLA	CBD-CGD-O2D-CED
11	cB	801	CLA	CBD-CGD-O2D-CED
11	cB	809	CLA	CBD-CGD-O2D-CED
11	cB	810	CLA	CBD-CGD-O2D-CED
11	cB	820	CLA	CBD-CGD-O2D-CED
11	cB	826	CLA	CBD-CGD-O2D-CED
11	aA	822	CLA	O1A-CGA-O2A-C1
11	aA	829	CLA	O1A-CGA-O2A-C1
11	bA	822	CLA	O1A-CGA-O2A-C1
11	bA	829	CLA	O1A-CGA-O2A-C1
11	cA	822	CLA	O1A-CGA-O2A-C1
11	cA	829	CLA	O1A-CGA-O2A-C1
12	aL	202	F6C	O1A-CGA-O2A-C1
12	bL	202	F6C	O1A-CGA-O2A-C1
12	cL	202	F6C	O1A-CGA-O2A-C1
12	aA	826	F6C	C4C-C3C-CAC-CBC
12	bA	826	F6C	C4C-C3C-CAC-CBC
12	cA	826	F6C	C4C-C3C-CAC-CBC
11	aA	809	CLA	CBD-CGD-O2D-CED
11	aA	815	CLA	CBD-CGD-O2D-CED
11	aB	801	CLA	CBD-CGD-O2D-CED
11	aB	822	CLA	CBD-CGD-O2D-CED
11	bA	809	CLA	CBD-CGD-O2D-CED
11	bA	815	CLA	CBD-CGD-O2D-CED
11	bB	822	CLA	CBD-CGD-O2D-CED
11	cA	809	CLA	CBD-CGD-O2D-CED
11	cA	815	CLA	CBD-CGD-O2D-CED
11	cB	822	CLA	CBD-CGD-O2D-CED
11	aB	802	CLA	O1A-CGA-O2A-C1
11	bB	802	CLA	O1A-CGA-O2A-C1
11	cB	802	CLA	O1A-CGA-O2A-C1
11	aA	803	CLA	C3-C5-C6-C7
11	aA	807	CLA	C3-C5-C6-C7
11	aA	819	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
11	aA	828	CLA	C3-C5-C6-C7
11	aA	829	CLA	C3-C5-C6-C7
11	aA	833	CLA	C3-C5-C6-C7
11	aA	839	CLA	C3-C5-C6-C7
11	aB	802	CLA	C3-C5-C6-C7
11	aB	806	CLA	C3-C5-C6-C7
11	aB	813	CLA	C3-C5-C6-C7
11	aB	831	CLA	C3-C5-C6-C7
11	aB	839	CLA	C3-C5-C6-C7
11	bA	803	CLA	C3-C5-C6-C7
11	bA	807	CLA	C3-C5-C6-C7
11	bA	819	CLA	C3-C5-C6-C7
11	bA	828	CLA	C3-C5-C6-C7
11	bA	829	CLA	C3-C5-C6-C7
11	bA	833	CLA	C3-C5-C6-C7
11	bA	839	CLA	C3-C5-C6-C7
11	bB	802	CLA	C3-C5-C6-C7
11	bB	806	CLA	C3-C5-C6-C7
11	bB	813	CLA	C3-C5-C6-C7
11	bB	831	CLA	C3-C5-C6-C7
11	bB	839	CLA	C3-C5-C6-C7
11	cA	803	CLA	C3-C5-C6-C7
11	cA	807	CLA	C3-C5-C6-C7
11	cA	819	CLA	C3-C5-C6-C7
11	cA	828	CLA	C3-C5-C6-C7
11	cA	829	CLA	C3-C5-C6-C7
11	cA	833	CLA	C3-C5-C6-C7
11	cA	839	CLA	C3-C5-C6-C7
11	cB	802	CLA	C3-C5-C6-C7
11	cB	806	CLA	C3-C5-C6-C7
11	cB	813	CLA	C3-C5-C6-C7
11	cB	831	CLA	C3-C5-C6-C7
11	cB	839	CLA	C3-C5-C6-C7
11	aA	820	CLA	CBA-CGA-O2A-C1
11	aA	821	CLA	CBA-CGA-O2A-C1
11	aA	822	CLA	CBA-CGA-O2A-C1
11	aA	824	CLA	CBA-CGA-O2A-C1
11	bA	820	CLA	CBA-CGA-O2A-C1
11	bA	821	CLA	CBA-CGA-O2A-C1
11	bA	822	CLA	CBA-CGA-O2A-C1
11	bA	824	CLA	CBA-CGA-O2A-C1
11	cA	820	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
11	cA	821	CLA	CBA-CGA-O2A-C1
11	cA	822	CLA	CBA-CGA-O2A-C1
11	cA	824	CLA	CBA-CGA-O2A-C1
11	aA	825	CLA	O1D-CGD-O2D-CED
11	bA	825	CLA	O1D-CGD-O2D-CED
11	cA	825	CLA	O1D-CGD-O2D-CED
11	aA	833	CLA	C4-C3-C5-C6
11	bA	833	CLA	C4-C3-C5-C6
11	cA	833	CLA	C4-C3-C5-C6
11	aA	812	CLA	C2A-CAA-CBA-CGA
11	aB	811	CLA	C2A-CAA-CBA-CGA
11	aB	839	CLA	C2A-CAA-CBA-CGA
11	bA	812	CLA	C2A-CAA-CBA-CGA
11	bB	811	CLA	C2A-CAA-CBA-CGA
11	bB	839	CLA	C2A-CAA-CBA-CGA
11	cA	812	CLA	C2A-CAA-CBA-CGA
11	cB	811	CLA	C2A-CAA-CBA-CGA
11	cB	839	CLA	C2A-CAA-CBA-CGA
11	aA	824	CLA	O1D-CGD-O2D-CED
11	bA	824	CLA	O1D-CGD-O2D-CED
11	cA	824	CLA	O1D-CGD-O2D-CED
11	aA	818	CLA	C3-C5-C6-C7
11	aA	820	CLA	C3-C5-C6-C7
11	aA	831	CLA	C3-C5-C6-C7
11	aB	808	CLA	C3-C5-C6-C7
11	aB	817	CLA	C3-C5-C6-C7
11	bA	818	CLA	C3-C5-C6-C7
11	bA	820	CLA	C3-C5-C6-C7
11	bA	831	CLA	C3-C5-C6-C7
11	bB	808	CLA	C3-C5-C6-C7
11	bB	817	CLA	C3-C5-C6-C7
11	cA	818	CLA	C3-C5-C6-C7
11	cA	820	CLA	C3-C5-C6-C7
11	cA	831	CLA	C3-C5-C6-C7
11	cB	808	CLA	C3-C5-C6-C7
11	cB	817	CLA	C3-C5-C6-C7
11	aA	829	CLA	CBA-CGA-O2A-C1
11	aA	838	CLA	CBA-CGA-O2A-C1
11	aB	804	CLA	CBA-CGA-O2A-C1
11	bA	829	CLA	CBA-CGA-O2A-C1
11	bA	838	CLA	CBA-CGA-O2A-C1
11	bB	804	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
11	bB	828	CLA	CBA-CGA-O2A-C1
11	cA	829	CLA	CBA-CGA-O2A-C1
11	cA	838	CLA	CBA-CGA-O2A-C1
11	cB	804	CLA	CBA-CGA-O2A-C1
12	aL	202	F6C	CBA-CGA-O2A-C1
12	bL	202	F6C	CBA-CGA-O2A-C1
12	cL	202	F6C	CBA-CGA-O2A-C1
12	aA	826	F6C	C1A-C2A-CAA-CBA
12	aA	827	F6C	C1A-C2A-CAA-CBA
12	aL	202	F6C	C1A-C2A-CAA-CBA
12	bA	826	F6C	C1A-C2A-CAA-CBA
12	bA	827	F6C	C1A-C2A-CAA-CBA
12	bL	202	F6C	C1A-C2A-CAA-CBA
12	cA	826	F6C	C1A-C2A-CAA-CBA
12	cA	827	F6C	C1A-C2A-CAA-CBA
12	cL	202	F6C	C1A-C2A-CAA-CBA
11	aA	817	CLA	O1D-CGD-O2D-CED
11	aA	836	CLA	O1D-CGD-O2D-CED
11	bA	817	CLA	O1D-CGD-O2D-CED
11	bA	836	CLA	O1D-CGD-O2D-CED
11	cA	817	CLA	O1D-CGD-O2D-CED
11	cA	836	CLA	O1D-CGD-O2D-CED
11	aA	838	CLA	O1A-CGA-O2A-C1
11	bA	838	CLA	O1A-CGA-O2A-C1
11	cA	838	CLA	O1A-CGA-O2A-C1
12	aA	844	F6C	O1A-CGA-O2A-C1
12	bA	844	F6C	O1A-CGA-O2A-C1
12	cA	844	F6C	O1A-CGA-O2A-C1
15	aA	851	BCR	C19-C20-C21-C22
15	aB	848	BCR	C19-C20-C21-C22
15	bA	851	BCR	C19-C20-C21-C22
15	bB	848	BCR	C19-C20-C21-C22
15	cA	851	BCR	C19-C20-C21-C22
15	cB	848	BCR	C19-C20-C21-C22
11	aB	830	CLA	CBD-CGD-O2D-CED
11	aB	838	CLA	CBD-CGD-O2D-CED
11	bB	830	CLA	CBD-CGD-O2D-CED
11	bB	838	CLA	CBD-CGD-O2D-CED
11	cB	830	CLA	CBD-CGD-O2D-CED
11	cB	838	CLA	CBD-CGD-O2D-CED
12	aB	824	F6C	C3-C5-C6-C7
12	bB	824	F6C	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
12	cB	824	F6C	C3-C5-C6-C7
11	aA	840	CLA	CBA-CGA-O2A-C1
11	aB	821	CLA	CBA-CGA-O2A-C1
11	aB	828	CLA	CBA-CGA-O2A-C1
11	bA	840	CLA	CBA-CGA-O2A-C1
11	bB	821	CLA	CBA-CGA-O2A-C1
11	cA	840	CLA	CBA-CGA-O2A-C1
11	cB	821	CLA	CBA-CGA-O2A-C1
11	cB	828	CLA	CBA-CGA-O2A-C1
12	aA	844	F6C	CBA-CGA-O2A-C1
12	bA	844	F6C	CBA-CGA-O2A-C1
12	cA	844	F6C	CBA-CGA-O2A-C1
11	aA	820	CLA	O1A-CGA-O2A-C1
11	aB	804	CLA	O1A-CGA-O2A-C1
11	bA	820	CLA	O1A-CGA-O2A-C1
11	bB	804	CLA	O1A-CGA-O2A-C1
11	cA	820	CLA	O1A-CGA-O2A-C1
11	cB	804	CLA	O1A-CGA-O2A-C1
11	aA	810	CLA	O1D-CGD-O2D-CED
11	bA	810	CLA	O1D-CGD-O2D-CED
11	cA	810	CLA	O1D-CGD-O2D-CED
11	aB	814	CLA	CBD-CGD-O2D-CED
11	bB	814	CLA	CBD-CGD-O2D-CED
11	cB	814	CLA	CBD-CGD-O2D-CED
11	aA	818	CLA	O1D-CGD-O2D-CED
11	bA	818	CLA	O1D-CGD-O2D-CED
11	cA	818	CLA	O1D-CGD-O2D-CED
11	aB	802	CLA	CBA-CGA-O2A-C1
11	bB	802	CLA	CBA-CGA-O2A-C1
11	cB	802	CLA	CBA-CGA-O2A-C1
11	aB	821	CLA	O1A-CGA-O2A-C1
11	aB	828	CLA	O1A-CGA-O2A-C1
11	bB	821	CLA	O1A-CGA-O2A-C1
11	cB	821	CLA	O1A-CGA-O2A-C1
12	aA	830	F6C	C2A-CAA-CBA-CGA
12	bA	830	F6C	C2A-CAA-CBA-CGA
12	cA	830	F6C	C2A-CAA-CBA-CGA
11	aB	827	CLA	C4-C3-C5-C6
11	bB	827	CLA	C4-C3-C5-C6
11	cB	827	CLA	C4-C3-C5-C6
11	aA	833	CLA	C2-C3-C5-C6
11	aB	827	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
11	bA	833	CLA	C2-C3-C5-C6
11	bB	827	CLA	C2-C3-C5-C6
11	cA	833	CLA	C2-C3-C5-C6
11	cB	827	CLA	C2-C3-C5-C6
11	aA	806	CLA	O1D-CGD-O2D-CED
11	bA	806	CLA	O1D-CGD-O2D-CED
11	cA	806	CLA	O1D-CGD-O2D-CED
11	bB	828	CLA	O1A-CGA-O2A-C1
11	cB	828	CLA	O1A-CGA-O2A-C1
11	aA	812	CLA	O1D-CGD-O2D-CED
11	bA	812	CLA	O1D-CGD-O2D-CED
11	cA	812	CLA	O1D-CGD-O2D-CED
11	aA	816	CLA	O1D-CGD-O2D-CED
11	aA	822	CLA	O1D-CGD-O2D-CED
11	bA	816	CLA	O1D-CGD-O2D-CED
11	bA	822	CLA	O1D-CGD-O2D-CED
11	cA	816	CLA	O1D-CGD-O2D-CED
11	cA	822	CLA	O1D-CGD-O2D-CED
11	aA	840	CLA	O1A-CGA-O2A-C1
11	bA	840	CLA	O1A-CGA-O2A-C1
11	cA	840	CLA	O1A-CGA-O2A-C1
11	aB	821	CLA	C3-C5-C6-C7
11	bB	821	CLA	C3-C5-C6-C7
11	cB	821	CLA	C3-C5-C6-C7
11	aA	812	CLA	CBA-CGA-O2A-C1
11	aA	817	CLA	CBA-CGA-O2A-C1
11	aA	828	CLA	CBA-CGA-O2A-C1
11	aB	817	CLA	CBA-CGA-O2A-C1
11	aB	830	CLA	CBA-CGA-O2A-C1
11	bA	812	CLA	CBA-CGA-O2A-C1
11	bA	817	CLA	CBA-CGA-O2A-C1
11	bA	828	CLA	CBA-CGA-O2A-C1
11	bB	817	CLA	CBA-CGA-O2A-C1
11	bB	830	CLA	CBA-CGA-O2A-C1
11	cA	812	CLA	CBA-CGA-O2A-C1
11	cA	817	CLA	CBA-CGA-O2A-C1
11	cA	828	CLA	CBA-CGA-O2A-C1
11	cB	817	CLA	CBA-CGA-O2A-C1
11	cB	830	CLA	CBA-CGA-O2A-C1
11	aA	841	CLA	CBD-CGD-O2D-CED
11	aB	828	CLA	CBD-CGD-O2D-CED
11	bA	841	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	bB	828	CLA	CBD-CGD-O2D-CED
11	cA	841	CLA	CBD-CGD-O2D-CED
11	cB	828	CLA	CBD-CGD-O2D-CED
18	aB	847	LMG	C28-C29-C30-C31
18	cB	847	LMG	C28-C29-C30-C31
12	aA	832	F6C	C3A-C2A-CAA-CBA
12	bA	832	F6C	C3A-C2A-CAA-CBA
12	cA	832	F6C	C3A-C2A-CAA-CBA
11	aB	827	CLA	C5-C6-C7-C8
11	bB	827	CLA	C5-C6-C7-C8
11	cB	827	CLA	C5-C6-C7-C8
18	bB	847	LMG	C28-C29-C30-C31
11	aA	828	CLA	O1A-CGA-O2A-C1
11	aB	830	CLA	O1A-CGA-O2A-C1
11	bA	828	CLA	O1A-CGA-O2A-C1
11	bB	830	CLA	O1A-CGA-O2A-C1
11	cA	828	CLA	O1A-CGA-O2A-C1
11	cB	830	CLA	O1A-CGA-O2A-C1
11	aB	806	CLA	C4-C3-C5-C6
11	bB	806	CLA	C4-C3-C5-C6
11	cB	806	CLA	C4-C3-C5-C6
11	aA	814	CLA	C11-C12-C13-C14
11	aA	822	CLA	C11-C10-C8-C9
11	aA	825	CLA	C11-C12-C13-C14
11	aA	833	CLA	C6-C7-C8-C9
11	aA	833	CLA	C14-C13-C15-C16
11	aA	840	CLA	C14-C13-C15-C16
11	aB	812	CLA	C11-C12-C13-C14
11	aL	206	CLA	C14-C13-C15-C16
11	bA	814	CLA	C11-C12-C13-C14
11	bA	822	CLA	C11-C10-C8-C9
11	bA	825	CLA	C11-C12-C13-C14
11	bA	833	CLA	C6-C7-C8-C9
11	bA	833	CLA	C14-C13-C15-C16
11	bA	840	CLA	C14-C13-C15-C16
11	bB	812	CLA	C11-C12-C13-C14
11	bL	206	CLA	C14-C13-C15-C16
11	cA	814	CLA	C11-C12-C13-C14
11	cA	822	CLA	C11-C10-C8-C9
11	cA	825	CLA	C11-C12-C13-C14
11	cA	833	CLA	C6-C7-C8-C9
11	cA	833	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
11	cA	840	CLA	C14-C13-C15-C16
11	cB	812	CLA	C11-C12-C13-C14
12	aA	844	F6C	C11-C12-C13-C14
12	bA	844	F6C	C11-C12-C13-C14
12	cA	844	F6C	C11-C12-C13-C14
11	aA	807	CLA	O1D-CGD-O2D-CED
11	aB	809	CLA	O1D-CGD-O2D-CED
11	bA	807	CLA	O1D-CGD-O2D-CED
11	bB	809	CLA	O1D-CGD-O2D-CED
11	cA	807	CLA	O1D-CGD-O2D-CED
11	cB	809	CLA	O1D-CGD-O2D-CED
11	aB	806	CLA	C15-C16-C17-C18
11	bA	825	CLA	C10-C11-C12-C13
11	bB	806	CLA	C15-C16-C17-C18
11	cA	825	CLA	C10-C11-C12-C13
11	cB	806	CLA	C15-C16-C17-C18
11	aA	809	CLA	C2A-CAA-CBA-CGA
11	aB	829	CLA	C2A-CAA-CBA-CGA
11	bA	809	CLA	C2A-CAA-CBA-CGA
11	bB	829	CLA	C2A-CAA-CBA-CGA
11	cA	809	CLA	C2A-CAA-CBA-CGA
11	cB	829	CLA	C2A-CAA-CBA-CGA
15	aA	851	BCR	C36-C18-C19-C20
15	aA	851	BCR	C37-C22-C23-C24
15	aB	842	BCR	C7-C8-C9-C34
15	aB	844	BCR	C11-C12-C13-C35
15	bA	851	BCR	C36-C18-C19-C20
15	bA	851	BCR	C37-C22-C23-C24
15	bB	842	BCR	C7-C8-C9-C34
15	bB	844	BCR	C11-C12-C13-C35
15	cA	851	BCR	C36-C18-C19-C20
15	cA	851	BCR	C37-C22-C23-C24
15	cB	842	BCR	C7-C8-C9-C34
15	cB	844	BCR	C11-C12-C13-C35
15	aA	847	BCR	C21-C22-C23-C24
15	aB	842	BCR	C21-C22-C23-C24
15	aL	207	BCR	C21-C22-C23-C24
15	bA	847	BCR	C21-C22-C23-C24
15	bB	842	BCR	C21-C22-C23-C24
15	bL	207	BCR	C21-C22-C23-C24
15	cA	847	BCR	C21-C22-C23-C24
15	cB	842	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
15	cL	207	BCR	C21-C22-C23-C24
11	aA	814	CLA	C5-C6-C7-C8
11	aA	814	CLA	C15-C16-C17-C18
11	aA	825	CLA	C10-C11-C12-C13
11	aA	831	CLA	C13-C15-C16-C17
11	aB	812	CLA	C15-C16-C17-C18
11	bA	814	CLA	C5-C6-C7-C8
11	bA	814	CLA	C15-C16-C17-C18
11	bA	831	CLA	C13-C15-C16-C17
11	bB	812	CLA	C15-C16-C17-C18
11	cA	814	CLA	C5-C6-C7-C8
11	cA	814	CLA	C15-C16-C17-C18
11	cA	831	CLA	C13-C15-C16-C17
11	cB	812	CLA	C15-C16-C17-C18
11	aB	820	CLA	O1D-CGD-O2D-CED
11	bB	820	CLA	O1D-CGD-O2D-CED
11	cB	820	CLA	O1D-CGD-O2D-CED
11	aB	840	CLA	CBD-CGD-O2D-CED
11	bB	840	CLA	CBD-CGD-O2D-CED
11	cB	840	CLA	CBD-CGD-O2D-CED
11	aA	831	CLA	CBA-CGA-O2A-C1
11	bA	831	CLA	CBA-CGA-O2A-C1
11	cA	831	CLA	CBA-CGA-O2A-C1
11	aA	833	CLA	C5-C6-C7-C8
11	aA	834	CLA	C5-C6-C7-C8
11	aB	808	CLA	C10-C11-C12-C13
11	aL	204	CLA	C13-C15-C16-C17
11	bA	833	CLA	C5-C6-C7-C8
11	bA	834	CLA	C5-C6-C7-C8
11	bB	808	CLA	C10-C11-C12-C13
11	bL	204	CLA	C13-C15-C16-C17
11	cA	833	CLA	C5-C6-C7-C8
11	cA	834	CLA	C5-C6-C7-C8
11	cB	808	CLA	C10-C11-C12-C13
11	cL	204	CLA	C13-C15-C16-C17
12	aA	827	F6C	C5-C6-C7-C8
12	aL	202	F6C	C15-C16-C17-C18
12	bA	827	F6C	C5-C6-C7-C8
12	bL	202	F6C	C15-C16-C17-C18
12	cA	827	F6C	C5-C6-C7-C8
12	cL	202	F6C	C15-C16-C17-C18
11	aA	812	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
11	aA	840	CLA	C13-C15-C16-C17
11	aL	205	CLA	C8-C10-C11-C12
11	aL	206	CLA	C5-C6-C7-C8
11	bA	840	CLA	C13-C15-C16-C17
11	bL	205	CLA	C8-C10-C11-C12
11	bL	206	CLA	C5-C6-C7-C8
11	cA	840	CLA	C13-C15-C16-C17
11	cL	205	CLA	C8-C10-C11-C12
11	cL	206	CLA	C5-C6-C7-C8
11	aB	810	CLA	O1D-CGD-O2D-CED
11	bB	810	CLA	O1D-CGD-O2D-CED
11	cB	810	CLA	O1D-CGD-O2D-CED
11	bA	812	CLA	C8-C10-C11-C12
11	cA	812	CLA	C8-C10-C11-C12
11	aA	840	CLA	O1D-CGD-O2D-CED
11	bA	840	CLA	O1D-CGD-O2D-CED
11	aB	805	CLA	C15-C16-C17-C18
11	aL	204	CLA	C10-C11-C12-C13
11	bB	805	CLA	C15-C16-C17-C18
11	bL	204	CLA	C10-C11-C12-C13
11	cB	805	CLA	C15-C16-C17-C18
11	cL	204	CLA	C10-C11-C12-C13
11	bA	835	CLA	O1D-CGD-O2D-CED
11	bA	843	CLA	O1D-CGD-O2D-CED
11	bB	822	CLA	O1D-CGD-O2D-CED
11	cA	835	CLA	O1D-CGD-O2D-CED
11	cA	843	CLA	O1D-CGD-O2D-CED
11	aA	822	CLA	C11-C10-C8-C7
11	aL	205	CLA	C6-C7-C8-C10
11	aL	206	CLA	C11-C12-C13-C15
11	bA	822	CLA	C11-C10-C8-C7
11	bL	205	CLA	C6-C7-C8-C10
11	bL	206	CLA	C11-C12-C13-C15
11	cA	822	CLA	C11-C10-C8-C7
11	cL	205	CLA	C6-C7-C8-C10
11	cL	206	CLA	C11-C12-C13-C15
11	aA	812	CLA	O1A-CGA-O2A-C1
11	bA	812	CLA	O1A-CGA-O2A-C1
11	cA	812	CLA	O1A-CGA-O2A-C1
11	aA	802	CLA	C2A-CAA-CBA-CGA
11	bA	802	CLA	C2A-CAA-CBA-CGA
11	cA	802	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
11	aA	835	CLA	O1D-CGD-O2D-CED
11	aA	843	CLA	O1D-CGD-O2D-CED
11	aB	822	CLA	O1D-CGD-O2D-CED
11	cA	840	CLA	O1D-CGD-O2D-CED
11	cB	822	CLA	O1D-CGD-O2D-CED
11	aA	840	CLA	C10-C11-C12-C13
11	aB	806	CLA	C5-C6-C7-C8
11	aL	204	CLA	C15-C16-C17-C18
11	bA	840	CLA	C10-C11-C12-C13
11	bB	806	CLA	C5-C6-C7-C8
11	bL	204	CLA	C15-C16-C17-C18
11	cA	840	CLA	C10-C11-C12-C13
11	cB	806	CLA	C5-C6-C7-C8
11	cL	204	CLA	C15-C16-C17-C18
11	aL	206	CLA	C15-C16-C17-C18
11	bL	206	CLA	C15-C16-C17-C18
11	cL	206	CLA	C15-C16-C17-C18
11	aB	826	CLA	O1D-CGD-O2D-CED
11	bB	826	CLA	O1D-CGD-O2D-CED
11	cB	826	CLA	O1D-CGD-O2D-CED
15	aB	842	BCR	C10-C11-C12-C13
15	aB	848	BCR	C18-C19-C20-C21
15	aL	207	BCR	C10-C11-C12-C13
15	aM	101	BCR	C18-C19-C20-C21
15	bB	842	BCR	C10-C11-C12-C13
15	bB	848	BCR	C18-C19-C20-C21
15	bL	207	BCR	C10-C11-C12-C13
15	bM	101	BCR	C18-C19-C20-C21
15	cB	842	BCR	C10-C11-C12-C13
15	cB	848	BCR	C18-C19-C20-C21
15	cL	207	BCR	C10-C11-C12-C13
15	cM	101	BCR	C18-C19-C20-C21
16	aA	852	LHG	O2-C2-C3-O3
16	bA	852	LHG	O2-C2-C3-O3
16	cA	852	LHG	O2-C2-C3-O3
11	aA	803	CLA	C5-C6-C7-C8
11	aA	840	CLA	C15-C16-C17-C18
11	aB	802	CLA	C5-C6-C7-C8
11	bA	803	CLA	C5-C6-C7-C8
11	bA	840	CLA	C15-C16-C17-C18
11	bB	802	CLA	C5-C6-C7-C8
11	cA	803	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
11	cA	840	CLA	C15-C16-C17-C18
11	cB	802	CLA	C5-C6-C7-C8
11	aA	817	CLA	O1A-CGA-O2A-C1
11	aA	831	CLA	O1A-CGA-O2A-C1
11	aB	817	CLA	O1A-CGA-O2A-C1
11	bA	817	CLA	O1A-CGA-O2A-C1
11	bA	831	CLA	O1A-CGA-O2A-C1
11	bB	817	CLA	O1A-CGA-O2A-C1
11	cA	817	CLA	O1A-CGA-O2A-C1
11	cA	831	CLA	O1A-CGA-O2A-C1
11	cB	817	CLA	O1A-CGA-O2A-C1
11	aB	808	CLA	C13-C15-C16-C17
11	aA	839	CLA	C15-C16-C17-C18
11	aB	812	CLA	C10-C11-C12-C13
11	bA	839	CLA	C15-C16-C17-C18
11	bB	808	CLA	C13-C15-C16-C17
11	bB	812	CLA	C10-C11-C12-C13
11	cA	839	CLA	C15-C16-C17-C18
11	cB	808	CLA	C13-C15-C16-C17
11	cB	812	CLA	C10-C11-C12-C13
16	aA	852	LHG	C3-O3-P-O6
16	bA	852	LHG	C3-O3-P-O6
16	cA	852	LHG	C3-O3-P-O6
11	aA	834	CLA	C3-C5-C6-C7
11	bA	834	CLA	C3-C5-C6-C7
11	cA	834	CLA	C3-C5-C6-C7
12	aA	832	F6C	CBA-CGA-O2A-C1
12	bA	832	F6C	CBA-CGA-O2A-C1
12	cA	832	F6C	CBA-CGA-O2A-C1
11	aA	809	CLA	O1D-CGD-O2D-CED
11	bA	809	CLA	O1D-CGD-O2D-CED
11	bB	801	CLA	O1D-CGD-O2D-CED
11	cA	809	CLA	O1D-CGD-O2D-CED
16	aA	852	LHG	C1-C2-C3-O3
16	bA	852	LHG	C1-C2-C3-O3
16	cA	852	LHG	C1-C2-C3-O3
11	cB	801	CLA	O1D-CGD-O2D-CED
11	aA	813	CLA	C2A-CAA-CBA-CGA
11	aB	809	CLA	C2A-CAA-CBA-CGA
11	aB	826	CLA	C2A-CAA-CBA-CGA
11	bB	809	CLA	C2A-CAA-CBA-CGA
11	bB	826	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
11	cA	813	CLA	C2A-CAA-CBA-CGA
11	cB	809	CLA	C2A-CAA-CBA-CGA
11	cB	826	CLA	C2A-CAA-CBA-CGA
11	aL	205	CLA	C3-C5-C6-C7
11	bL	205	CLA	C3-C5-C6-C7
11	cL	205	CLA	C3-C5-C6-C7
11	aB	801	CLA	O1D-CGD-O2D-CED
11	aA	808	CLA	CBA-CGA-O2A-C1
11	aB	826	CLA	CBA-CGA-O2A-C1
11	bA	808	CLA	CBA-CGA-O2A-C1
11	bB	826	CLA	CBA-CGA-O2A-C1
11	cA	808	CLA	CBA-CGA-O2A-C1
11	cB	826	CLA	CBA-CGA-O2A-C1
11	aA	815	CLA	O1D-CGD-O2D-CED
11	aA	822	CLA	C8-C10-C11-C12
11	bA	822	CLA	C8-C10-C11-C12
11	cA	822	CLA	C8-C10-C11-C12
15	aA	847	BCR	C20-C21-C22-C37
15	aB	843	BCR	C20-C21-C22-C37
15	aB	846	BCR	C11-C10-C9-C34
15	aI	101	BCR	C20-C21-C22-C37
15	aL	208	BCR	C20-C21-C22-C37
15	bA	847	BCR	C20-C21-C22-C37
15	bB	843	BCR	C20-C21-C22-C37
15	bB	846	BCR	C11-C10-C9-C34
15	bI	101	BCR	C20-C21-C22-C37
15	bL	208	BCR	C20-C21-C22-C37
15	cA	847	BCR	C20-C21-C22-C37
15	cB	843	BCR	C20-C21-C22-C37
15	cB	846	BCR	C11-C10-C9-C34
15	cI	103	BCR	C20-C21-C22-C37
15	cL	208	BCR	C20-C21-C22-C37
18	aB	847	LMG	C29-C30-C31-C32
18	bB	847	LMG	C29-C30-C31-C32
18	cB	847	LMG	C29-C30-C31-C32
11	bA	815	CLA	O1D-CGD-O2D-CED
11	cA	815	CLA	O1D-CGD-O2D-CED
11	aA	822	CLA	C13-C15-C16-C17
11	bA	822	CLA	C13-C15-C16-C17
11	cA	822	CLA	C13-C15-C16-C17
16	aA	852	LHG	C34-C35-C36-C37
16	bA	852	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
16	cA	852	LHG	C34-C35-C36-C37
18	aB	847	LMG	C39-C40-C41-C42
18	bB	847	LMG	C39-C40-C41-C42
18	cB	847	LMG	C39-C40-C41-C42
15	aA	847	BCR	C16-C17-C18-C19
15	aA	849	BCR	C20-C21-C22-C23
15	aB	848	BCR	C11-C10-C9-C8
15	aK	102	BCR	C20-C21-C22-C23
15	aL	203	BCR	C20-C21-C22-C23
15	aL	208	BCR	C20-C21-C22-C23
15	bA	847	BCR	C16-C17-C18-C19
15	bA	849	BCR	C20-C21-C22-C23
15	bB	848	BCR	C11-C10-C9-C8
15	bK	102	BCR	C20-C21-C22-C23
15	bL	203	BCR	C20-C21-C22-C23
15	bL	208	BCR	C20-C21-C22-C23
15	cA	847	BCR	C16-C17-C18-C19
15	cA	849	BCR	C20-C21-C22-C23
15	cB	848	BCR	C11-C10-C9-C8
15	cK	102	BCR	C20-C21-C22-C23
15	cL	203	BCR	C20-C21-C22-C23
15	cL	208	BCR	C20-C21-C22-C23
11	aB	809	CLA	CBA-CGA-O2A-C1
11	bB	809	CLA	CBA-CGA-O2A-C1
11	cB	809	CLA	CBA-CGA-O2A-C1
16	aA	852	LHG	C32-C33-C34-C35
16	bA	852	LHG	C32-C33-C34-C35
16	cA	852	LHG	C32-C33-C34-C35
11	aB	837	CLA	C6-C7-C8-C10
11	bB	837	CLA	C6-C7-C8-C10
11	cB	837	CLA	C6-C7-C8-C10
11	aA	806	CLA	C4-C3-C5-C6
11	aB	815	CLA	C4-C3-C5-C6
11	bA	806	CLA	C4-C3-C5-C6
11	bB	815	CLA	C4-C3-C5-C6
11	cA	806	CLA	C4-C3-C5-C6
11	cB	815	CLA	C4-C3-C5-C6
11	aB	823	CLA	C5-C6-C7-C8
11	bB	823	CLA	C5-C6-C7-C8
11	cB	823	CLA	C5-C6-C7-C8
17	aA	853	LMT	C2-C3-C4-C5
17	bA	853	LMT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
17	cA	853	LMT	C2-C3-C4-C5
11	aA	803	CLA	C6-C7-C8-C9
11	aA	831	CLA	C11-C10-C8-C9
11	aB	805	CLA	C6-C7-C8-C9
11	aB	825	CLA	C14-C13-C15-C16
11	bA	803	CLA	C6-C7-C8-C9
11	bA	831	CLA	C11-C10-C8-C9
11	bB	805	CLA	C6-C7-C8-C9
11	bB	825	CLA	C14-C13-C15-C16
11	cA	831	CLA	C11-C10-C8-C9
11	cB	805	CLA	C6-C7-C8-C9
11	cB	825	CLA	C14-C13-C15-C16
11	cL	206	CLA	C14-C13-C15-C16
11	aB	827	CLA	C2A-CAA-CBA-CGA
11	bA	813	CLA	C2A-CAA-CBA-CGA
11	bB	827	CLA	C2A-CAA-CBA-CGA
11	cB	827	CLA	C2A-CAA-CBA-CGA
12	aA	832	F6C	O1A-CGA-O2A-C1
12	bA	832	F6C	O1A-CGA-O2A-C1
12	cA	832	F6C	O1A-CGA-O2A-C1
15	aL	207	BCR	C37-C22-C23-C24
15	bL	207	BCR	C37-C22-C23-C24
15	cB	845	BCR	C7-C8-C9-C34
15	cL	207	BCR	C37-C22-C23-C24
15	aL	207	BCR	C7-C8-C9-C10
15	bL	207	BCR	C7-C8-C9-C10
15	cL	207	BCR	C7-C8-C9-C10
11	aA	831	CLA	C8-C10-C11-C12
11	aL	206	CLA	C8-C10-C11-C12
11	bA	831	CLA	C8-C10-C11-C12
11	bL	206	CLA	C8-C10-C11-C12
11	cA	831	CLA	C8-C10-C11-C12
11	cL	206	CLA	C8-C10-C11-C12
16	aA	852	LHG	C28-C29-C30-C31
16	bA	852	LHG	C28-C29-C30-C31
16	cA	852	LHG	C28-C29-C30-C31
11	aA	810	CLA	C4B-C3B-CAB-CBB
11	aA	811	CLA	C4B-C3B-CAB-CBB
11	aA	814	CLA	C4B-C3B-CAB-CBB
11	aA	822	CLA	C4B-C3B-CAB-CBB
11	aA	823	CLA	C4B-C3B-CAB-CBB
11	aA	825	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
11	aA	835	CLA	C4B-C3B-CAB-CBB
11	aA	836	CLA	C4B-C3B-CAB-CBB
11	aA	841	CLA	C4B-C3B-CAB-CBB
11	aB	815	CLA	C4B-C3B-CAB-CBB
11	aB	816	CLA	C4B-C3B-CAB-CBB
11	aB	820	CLA	C4B-C3B-CAB-CBB
11	aB	830	CLA	C4B-C3B-CAB-CBB
11	aB	835	CLA	C4B-C3B-CAB-CBB
11	aB	837	CLA	C4B-C3B-CAB-CBB
11	bA	810	CLA	C4B-C3B-CAB-CBB
11	bA	811	CLA	C4B-C3B-CAB-CBB
11	bA	814	CLA	C4B-C3B-CAB-CBB
11	bA	822	CLA	C4B-C3B-CAB-CBB
11	bA	823	CLA	C4B-C3B-CAB-CBB
11	bA	825	CLA	C4B-C3B-CAB-CBB
11	bA	835	CLA	C4B-C3B-CAB-CBB
11	bA	836	CLA	C4B-C3B-CAB-CBB
11	bA	841	CLA	C4B-C3B-CAB-CBB
11	bB	815	CLA	C4B-C3B-CAB-CBB
11	bB	816	CLA	C4B-C3B-CAB-CBB
11	bB	820	CLA	C4B-C3B-CAB-CBB
11	bB	830	CLA	C4B-C3B-CAB-CBB
11	bB	834	CLA	C4B-C3B-CAB-CBB
11	bB	835	CLA	C4B-C3B-CAB-CBB
11	bB	837	CLA	C4B-C3B-CAB-CBB
11	cA	810	CLA	C4B-C3B-CAB-CBB
11	cA	811	CLA	C4B-C3B-CAB-CBB
11	cA	814	CLA	C4B-C3B-CAB-CBB
11	cA	822	CLA	C4B-C3B-CAB-CBB
11	cA	823	CLA	C4B-C3B-CAB-CBB
11	cA	825	CLA	C4B-C3B-CAB-CBB
11	cA	835	CLA	C4B-C3B-CAB-CBB
11	cA	836	CLA	C4B-C3B-CAB-CBB
11	cA	841	CLA	C4B-C3B-CAB-CBB
11	cB	815	CLA	C4B-C3B-CAB-CBB
11	cB	816	CLA	C4B-C3B-CAB-CBB
11	cB	820	CLA	C4B-C3B-CAB-CBB
11	cB	830	CLA	C4B-C3B-CAB-CBB
11	cB	834	CLA	C4B-C3B-CAB-CBB
11	cB	835	CLA	C4B-C3B-CAB-CBB
11	cB	837	CLA	C4B-C3B-CAB-CBB
11	aB	806	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
11	cB	806	CLA	C10-C11-C12-C13
18	cB	847	LMG	C41-C42-C43-C44
18	aB	847	LMG	C41-C42-C43-C44
18	bB	847	LMG	C41-C42-C43-C44
11	aB	806	CLA	C10-C11-C12-C13
11	bB	806	CLA	C10-C11-C12-C13
11	bB	806	CLA	C13-C15-C16-C17
11	cB	806	CLA	C13-C15-C16-C17
11	aB	826	CLA	O1A-CGA-O2A-C1
11	bA	808	CLA	O1A-CGA-O2A-C1
11	bB	826	CLA	O1A-CGA-O2A-C1
11	cA	808	CLA	O1A-CGA-O2A-C1
11	cB	826	CLA	O1A-CGA-O2A-C1
18	aB	847	LMG	C35-C36-C37-C38
11	bB	838	CLA	O1D-CGD-O2D-CED
11	aA	802	CLA	C3A-C2A-CAA-CBA
11	aA	804	CLA	C3A-C2A-CAA-CBA
11	aA	814	CLA	C3A-C2A-CAA-CBA
11	aA	821	CLA	C3A-C2A-CAA-CBA
11	aA	837	CLA	C3A-C2A-CAA-CBA
11	aA	838	CLA	C3A-C2A-CAA-CBA
11	aB	825	CLA	C3A-C2A-CAA-CBA
11	aB	826	CLA	C3A-C2A-CAA-CBA
11	aB	836	CLA	C3A-C2A-CAA-CBA
11	bA	802	CLA	C3A-C2A-CAA-CBA
11	bA	804	CLA	C3A-C2A-CAA-CBA
11	bA	814	CLA	C3A-C2A-CAA-CBA
11	bA	821	CLA	C3A-C2A-CAA-CBA
11	bA	837	CLA	C3A-C2A-CAA-CBA
11	bA	838	CLA	C3A-C2A-CAA-CBA
11	bB	825	CLA	C3A-C2A-CAA-CBA
11	bB	826	CLA	C3A-C2A-CAA-CBA
11	bB	836	CLA	C3A-C2A-CAA-CBA
11	cA	802	CLA	C3A-C2A-CAA-CBA
11	cA	804	CLA	C3A-C2A-CAA-CBA
11	cA	814	CLA	C3A-C2A-CAA-CBA
11	cA	821	CLA	C3A-C2A-CAA-CBA
11	cA	837	CLA	C3A-C2A-CAA-CBA
11	cA	838	CLA	C3A-C2A-CAA-CBA
11	cB	825	CLA	C3A-C2A-CAA-CBA
11	cB	826	CLA	C3A-C2A-CAA-CBA
11	cB	836	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
16	aA	852	LHG	C27-C28-C29-C30
16	bA	852	LHG	C27-C28-C29-C30
16	cA	852	LHG	C27-C28-C29-C30
18	bB	847	LMG	C35-C36-C37-C38
18	cB	847	LMG	C35-C36-C37-C38
11	aA	808	CLA	O1A-CGA-O2A-C1
11	aB	838	CLA	O1D-CGD-O2D-CED
11	cB	838	CLA	O1D-CGD-O2D-CED
15	aB	842	BCR	C14-C15-C16-C17
15	aB	848	BCR	C14-C15-C16-C17
15	bB	842	BCR	C14-C15-C16-C17
15	bB	848	BCR	C14-C15-C16-C17
15	cB	842	BCR	C14-C15-C16-C17
15	cB	848	BCR	C14-C15-C16-C17
11	aA	807	CLA	CBA-CGA-O2A-C1
11	aB	831	CLA	CBA-CGA-O2A-C1
11	bA	807	CLA	CBA-CGA-O2A-C1
11	bB	831	CLA	CBA-CGA-O2A-C1
11	cA	807	CLA	CBA-CGA-O2A-C1
11	cB	831	CLA	CBA-CGA-O2A-C1
11	aA	835	CLA	C2-C3-C5-C6
11	bA	835	CLA	C2-C3-C5-C6
11	cA	835	CLA	C2-C3-C5-C6
11	aB	809	CLA	O1A-CGA-O2A-C1
11	bB	809	CLA	O1A-CGA-O2A-C1
11	cB	809	CLA	O1A-CGA-O2A-C1
11	aA	810	CLA	C2B-C3B-CAB-CBB
11	aA	811	CLA	C2B-C3B-CAB-CBB
11	aA	814	CLA	C2B-C3B-CAB-CBB
11	aA	822	CLA	C2B-C3B-CAB-CBB
11	aA	823	CLA	C2B-C3B-CAB-CBB
11	aA	824	CLA	C2B-C3B-CAB-CBB
11	aA	825	CLA	C2B-C3B-CAB-CBB
11	aA	835	CLA	C2B-C3B-CAB-CBB
11	aA	836	CLA	C2B-C3B-CAB-CBB
11	aA	841	CLA	C2B-C3B-CAB-CBB
11	aB	811	CLA	C2B-C3B-CAB-CBB
11	aB	815	CLA	C2B-C3B-CAB-CBB
11	aB	816	CLA	C2B-C3B-CAB-CBB
11	aB	820	CLA	C2B-C3B-CAB-CBB
11	aB	830	CLA	C2B-C3B-CAB-CBB
11	aB	831	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
11	aB	834	CLA	C2B-C3B-CAB-CBB
11	aB	835	CLA	C2B-C3B-CAB-CBB
11	aB	837	CLA	C2B-C3B-CAB-CBB
11	aB	839	CLA	C2B-C3B-CAB-CBB
11	aB	840	CLA	C2B-C3B-CAB-CBB
11	aK	101	CLA	C2B-C3B-CAB-CBB
11	aK	103	CLA	C2B-C3B-CAB-CBB
11	bA	810	CLA	C2B-C3B-CAB-CBB
11	bA	811	CLA	C2B-C3B-CAB-CBB
11	bA	814	CLA	C2B-C3B-CAB-CBB
11	bA	822	CLA	C2B-C3B-CAB-CBB
11	bA	823	CLA	C2B-C3B-CAB-CBB
11	bA	824	CLA	C2B-C3B-CAB-CBB
11	bA	825	CLA	C2B-C3B-CAB-CBB
11	bA	835	CLA	C2B-C3B-CAB-CBB
11	bA	836	CLA	C2B-C3B-CAB-CBB
11	bA	841	CLA	C2B-C3B-CAB-CBB
11	bB	811	CLA	C2B-C3B-CAB-CBB
11	bB	815	CLA	C2B-C3B-CAB-CBB
11	bB	816	CLA	C2B-C3B-CAB-CBB
11	bB	820	CLA	C2B-C3B-CAB-CBB
11	bB	830	CLA	C2B-C3B-CAB-CBB
11	bB	831	CLA	C2B-C3B-CAB-CBB
11	bB	834	CLA	C2B-C3B-CAB-CBB
11	bB	835	CLA	C2B-C3B-CAB-CBB
11	bB	837	CLA	C2B-C3B-CAB-CBB
11	bB	839	CLA	C2B-C3B-CAB-CBB
11	bB	840	CLA	C2B-C3B-CAB-CBB
11	bK	103	CLA	C2B-C3B-CAB-CBB
11	cA	810	CLA	C2B-C3B-CAB-CBB
11	cA	811	CLA	C2B-C3B-CAB-CBB
11	cA	814	CLA	C2B-C3B-CAB-CBB
11	cA	822	CLA	C2B-C3B-CAB-CBB
11	cA	823	CLA	C2B-C3B-CAB-CBB
11	cA	824	CLA	C2B-C3B-CAB-CBB
11	cA	825	CLA	C2B-C3B-CAB-CBB
11	cA	835	CLA	C2B-C3B-CAB-CBB
11	cA	836	CLA	C2B-C3B-CAB-CBB
11	cA	841	CLA	C2B-C3B-CAB-CBB
11	cB	811	CLA	C2B-C3B-CAB-CBB
11	cB	815	CLA	C2B-C3B-CAB-CBB
11	cB	816	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
11	cB	820	CLA	C2B-C3B-CAB-CBB
11	cB	830	CLA	C2B-C3B-CAB-CBB
11	cB	831	CLA	C2B-C3B-CAB-CBB
11	cB	834	CLA	C2B-C3B-CAB-CBB
11	cB	835	CLA	C2B-C3B-CAB-CBB
11	cB	837	CLA	C2B-C3B-CAB-CBB
11	cB	839	CLA	C2B-C3B-CAB-CBB
11	cB	840	CLA	C2B-C3B-CAB-CBB
11	cK	103	CLA	C2B-C3B-CAB-CBB
10	aA	801	CL0	C15-C16-C17-C18
10	bA	801	CL0	C15-C16-C17-C18
10	cA	801	CL0	C15-C16-C17-C18
12	aL	202	F6C	C13-C15-C16-C17
12	bL	202	F6C	C13-C15-C16-C17
12	cL	202	F6C	C13-C15-C16-C17
17	aA	853	LMT	C1-C2-C3-C4
17	bA	853	LMT	C1-C2-C3-C4
17	cA	853	LMT	C1-C2-C3-C4
11	aA	821	CLA	C2-C1-O2A-CGA
11	aA	829	CLA	C2-C1-O2A-CGA
11	aB	802	CLA	C2-C1-O2A-CGA
11	bA	821	CLA	C2-C1-O2A-CGA
11	bA	829	CLA	C2-C1-O2A-CGA
11	bB	802	CLA	C2-C1-O2A-CGA
11	cA	821	CLA	C2-C1-O2A-CGA
11	cA	829	CLA	C2-C1-O2A-CGA
11	cB	802	CLA	C2-C1-O2A-CGA
12	aA	826	F6C	C2-C1-O2A-CGA
12	bA	826	F6C	C2-C1-O2A-CGA
12	cA	826	F6C	C2-C1-O2A-CGA
11	bB	803	CLA	C10-C11-C12-C13
11	cB	803	CLA	C10-C11-C12-C13
10	aA	801	CL0	C3-C5-C6-C7
10	bA	801	CL0	C3-C5-C6-C7
10	cA	801	CL0	C3-C5-C6-C7
11	aB	818	CLA	C3-C5-C6-C7
11	aL	206	CLA	C3-C5-C6-C7
11	bB	818	CLA	C3-C5-C6-C7
11	bL	206	CLA	C3-C5-C6-C7
11	cB	818	CLA	C3-C5-C6-C7
11	cL	206	CLA	C3-C5-C6-C7
12	aA	844	F6C	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
12	bA	844	F6C	C3-C5-C6-C7
12	cA	844	F6C	C3-C5-C6-C7
15	aA	847	BCR	C5-C6-C7-C8
15	aA	847	BCR	C23-C24-C25-C26
15	aA	847	BCR	C23-C24-C25-C30
15	aA	848	BCR	C1-C6-C7-C8
15	aA	848	BCR	C5-C6-C7-C8
15	aA	848	BCR	C23-C24-C25-C26
15	aA	848	BCR	C23-C24-C25-C30
15	aA	849	BCR	C5-C6-C7-C8
15	aA	850	BCR	C1-C6-C7-C8
15	aA	850	BCR	C5-C6-C7-C8
15	aB	842	BCR	C1-C6-C7-C8
15	aB	842	BCR	C5-C6-C7-C8
15	aB	843	BCR	C1-C6-C7-C8
15	aB	843	BCR	C5-C6-C7-C8
15	aB	844	BCR	C5-C6-C7-C8
15	aB	845	BCR	C1-C6-C7-C8
15	aB	845	BCR	C5-C6-C7-C8
15	aB	845	BCR	C23-C24-C25-C26
15	aB	845	BCR	C23-C24-C25-C30
15	aB	848	BCR	C5-C6-C7-C8
15	aI	101	BCR	C5-C6-C7-C8
15	aK	102	BCR	C5-C6-C7-C8
15	aL	203	BCR	C1-C6-C7-C8
15	aL	203	BCR	C5-C6-C7-C8
15	aL	203	BCR	C23-C24-C25-C26
15	aL	207	BCR	C5-C6-C7-C8
15	aL	208	BCR	C23-C24-C25-C26
15	aL	208	BCR	C23-C24-C25-C30
15	aM	101	BCR	C5-C6-C7-C8
15	bA	847	BCR	C5-C6-C7-C8
15	bA	847	BCR	C23-C24-C25-C26
15	bA	847	BCR	C23-C24-C25-C30
15	bA	848	BCR	C1-C6-C7-C8
15	bA	848	BCR	C5-C6-C7-C8
15	bA	848	BCR	C23-C24-C25-C26
15	bA	848	BCR	C23-C24-C25-C30
15	bA	849	BCR	C5-C6-C7-C8
15	bA	850	BCR	C1-C6-C7-C8
15	bA	850	BCR	C5-C6-C7-C8
15	bB	842	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
15	bB	842	BCR	C5-C6-C7-C8
15	bB	843	BCR	C1-C6-C7-C8
15	bB	843	BCR	C5-C6-C7-C8
15	bB	844	BCR	C5-C6-C7-C8
15	bB	845	BCR	C1-C6-C7-C8
15	bB	845	BCR	C5-C6-C7-C8
15	bB	845	BCR	C23-C24-C25-C26
15	bB	845	BCR	C23-C24-C25-C30
15	bB	848	BCR	C5-C6-C7-C8
15	bI	101	BCR	C5-C6-C7-C8
15	bK	102	BCR	C5-C6-C7-C8
15	bL	203	BCR	C1-C6-C7-C8
15	bL	203	BCR	C5-C6-C7-C8
15	bL	203	BCR	C23-C24-C25-C26
15	bL	207	BCR	C5-C6-C7-C8
15	bL	208	BCR	C23-C24-C25-C26
15	bL	208	BCR	C23-C24-C25-C30
15	bM	101	BCR	C5-C6-C7-C8
15	cA	847	BCR	C5-C6-C7-C8
15	cA	847	BCR	C23-C24-C25-C26
15	cA	847	BCR	C23-C24-C25-C30
15	cA	848	BCR	C1-C6-C7-C8
15	cA	848	BCR	C5-C6-C7-C8
15	cA	848	BCR	C23-C24-C25-C26
15	cA	848	BCR	C23-C24-C25-C30
15	cA	849	BCR	C5-C6-C7-C8
15	cA	849	BCR	C23-C24-C25-C26
15	cA	850	BCR	C1-C6-C7-C8
15	cA	850	BCR	C5-C6-C7-C8
15	cB	842	BCR	C1-C6-C7-C8
15	cB	842	BCR	C5-C6-C7-C8
15	cB	843	BCR	C1-C6-C7-C8
15	cB	843	BCR	C5-C6-C7-C8
15	cB	844	BCR	C5-C6-C7-C8
15	cB	845	BCR	C1-C6-C7-C8
15	cB	845	BCR	C5-C6-C7-C8
15	cB	845	BCR	C23-C24-C25-C26
15	cB	845	BCR	C23-C24-C25-C30
15	cB	848	BCR	C5-C6-C7-C8
15	cI	103	BCR	C5-C6-C7-C8
15	cK	102	BCR	C5-C6-C7-C8
15	cL	203	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
15	cL	203	BCR	C5-C6-C7-C8
15	cL	203	BCR	C23-C24-C25-C26
15	cL	207	BCR	C5-C6-C7-C8
15	cL	208	BCR	C23-C24-C25-C26
15	cL	208	BCR	C23-C24-C25-C30
15	cM	101	BCR	C5-C6-C7-C8
11	aB	836	CLA	CBA-CGA-O2A-C1
11	bB	836	CLA	CBA-CGA-O2A-C1
11	cB	836	CLA	CBA-CGA-O2A-C1
11	aB	803	CLA	C10-C11-C12-C13
11	bB	804	CLA	CBD-CGD-O2D-CED
11	cB	804	CLA	CBD-CGD-O2D-CED
18	aB	847	LMG	C36-C37-C38-C39
18	bB	847	LMG	C36-C37-C38-C39
18	cB	847	LMG	C36-C37-C38-C39
11	aA	822	CLA	C4-C3-C5-C6
11	aA	835	CLA	C4-C3-C5-C6
11	aB	823	CLA	C4-C3-C5-C6
11	bA	822	CLA	C4-C3-C5-C6
11	bA	835	CLA	C4-C3-C5-C6
11	bB	823	CLA	C4-C3-C5-C6
11	cA	822	CLA	C4-C3-C5-C6
11	cA	835	CLA	C4-C3-C5-C6
11	cB	823	CLA	C4-C3-C5-C6
11	aA	806	CLA	C2-C3-C5-C6
11	aA	814	CLA	C11-C12-C13-C15
11	aA	814	CLA	C12-C13-C15-C16
11	aA	831	CLA	C11-C10-C8-C7
11	aA	833	CLA	C6-C7-C8-C10
11	aB	806	CLA	C2-C3-C5-C6
11	aB	815	CLA	C2-C3-C5-C6
11	aB	816	CLA	C11-C10-C8-C7
11	aB	825	CLA	C12-C13-C15-C16
11	aL	205	CLA	C11-C12-C13-C15
11	bA	806	CLA	C2-C3-C5-C6
11	bA	814	CLA	C11-C12-C13-C15
11	bA	814	CLA	C12-C13-C15-C16
11	bA	831	CLA	C11-C10-C8-C7
11	bA	833	CLA	C6-C7-C8-C10
11	bB	806	CLA	C2-C3-C5-C6
11	bB	815	CLA	C2-C3-C5-C6
11	bB	816	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
11	bB	825	CLA	C12-C13-C15-C16
11	bL	205	CLA	C11-C12-C13-C15
11	cA	806	CLA	C2-C3-C5-C6
11	cA	814	CLA	C11-C12-C13-C15
11	cA	814	CLA	C12-C13-C15-C16
11	cA	831	CLA	C11-C10-C8-C7
11	cA	833	CLA	C6-C7-C8-C10
11	cB	806	CLA	C2-C3-C5-C6
11	cB	815	CLA	C2-C3-C5-C6
11	cB	816	CLA	C11-C10-C8-C7
11	cB	825	CLA	C12-C13-C15-C16
11	cL	205	CLA	C11-C12-C13-C15
11	aA	807	CLA	O1A-CGA-O2A-C1
11	aB	831	CLA	O1A-CGA-O2A-C1
11	bA	807	CLA	O1A-CGA-O2A-C1
11	bB	831	CLA	O1A-CGA-O2A-C1
11	cA	807	CLA	O1A-CGA-O2A-C1
11	cB	831	CLA	O1A-CGA-O2A-C1
12	aA	844	F6C	C1A-C2A-CAA-CBA
12	bA	844	F6C	C1A-C2A-CAA-CBA
12	cA	844	F6C	C1A-C2A-CAA-CBA
11	aA	834	CLA	CBD-CGD-O2D-CED
11	aB	804	CLA	CBD-CGD-O2D-CED
11	aB	837	CLA	C6-C7-C8-C9
11	bB	837	CLA	C6-C7-C8-C9
11	cB	837	CLA	C6-C7-C8-C9
11	aA	819	CLA	CBA-CGA-O2A-C1
11	aA	833	CLA	CBA-CGA-O2A-C1
11	aB	812	CLA	CBA-CGA-O2A-C1
11	bA	819	CLA	CBA-CGA-O2A-C1
11	bA	833	CLA	CBA-CGA-O2A-C1
11	bB	812	CLA	CBA-CGA-O2A-C1
11	cA	819	CLA	CBA-CGA-O2A-C1
11	cA	833	CLA	CBA-CGA-O2A-C1
11	cB	812	CLA	CBA-CGA-O2A-C1
11	aA	824	CLA	C2A-CAA-CBA-CGA
11	aB	815	CLA	C2A-CAA-CBA-CGA
11	aL	206	CLA	C2A-CAA-CBA-CGA
11	bA	824	CLA	C2A-CAA-CBA-CGA
11	bB	815	CLA	C2A-CAA-CBA-CGA
11	bL	206	CLA	C2A-CAA-CBA-CGA
11	cA	824	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
11	cB	815	CLA	C2A-CAA-CBA-CGA
11	cL	206	CLA	C2A-CAA-CBA-CGA
11	bA	834	CLA	CBD-CGD-O2D-CED
11	cA	834	CLA	CBD-CGD-O2D-CED
11	aA	818	CLA	C5-C6-C7-C8
11	bA	818	CLA	C5-C6-C7-C8
11	cA	818	CLA	C5-C6-C7-C8
18	aB	847	LMG	C38-C39-C40-C41
18	bB	847	LMG	C38-C39-C40-C41
18	cB	847	LMG	C38-C39-C40-C41
15	aA	849	BCR	C6-C7-C8-C9
15	aB	846	BCR	C22-C23-C24-C25
15	bA	849	BCR	C6-C7-C8-C9
15	bB	846	BCR	C22-C23-C24-C25
15	cA	849	BCR	C6-C7-C8-C9
15	cB	846	BCR	C22-C23-C24-C25
11	aL	206	CLA	C13-C15-C16-C17
11	bL	206	CLA	C13-C15-C16-C17
11	cL	206	CLA	C13-C15-C16-C17
16	aA	852	LHG	C8-C7-O7-C5
16	bA	852	LHG	C8-C7-O7-C5
16	cA	852	LHG	C8-C7-O7-C5
11	aA	835	CLA	C13-C15-C16-C17
11	cA	835	CLA	C13-C15-C16-C17
11	aA	805	CLA	CBD-CGD-O2D-CED
11	bA	805	CLA	CBD-CGD-O2D-CED
11	cA	805	CLA	CBD-CGD-O2D-CED
11	bA	835	CLA	C13-C15-C16-C17
11	aB	839	CLA	C13-C15-C16-C17
11	cB	839	CLA	C13-C15-C16-C17
11	aA	818	CLA	C4-C3-C5-C6
11	bA	818	CLA	C4-C3-C5-C6
11	cA	818	CLA	C4-C3-C5-C6
11	aB	806	CLA	C11-C10-C8-C9
11	aL	205	CLA	C11-C12-C13-C14
11	aL	206	CLA	C11-C12-C13-C14
11	bB	806	CLA	C11-C10-C8-C9
11	bL	205	CLA	C11-C12-C13-C14
11	bL	206	CLA	C11-C12-C13-C14
11	cA	803	CLA	C6-C7-C8-C9
11	cB	806	CLA	C11-C10-C8-C9
11	cL	205	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
11	cL	206	CLA	C11-C12-C13-C14
11	bB	839	CLA	C13-C15-C16-C17
11	bB	830	CLA	O1D-CGD-O2D-CED
11	aA	838	CLA	C2A-CAA-CBA-CGA
11	aB	819	CLA	C2A-CAA-CBA-CGA
11	bA	838	CLA	C2A-CAA-CBA-CGA
11	bB	819	CLA	C2A-CAA-CBA-CGA
11	cA	838	CLA	C2A-CAA-CBA-CGA
11	cB	819	CLA	C2A-CAA-CBA-CGA
15	aB	845	BCR	C7-C8-C9-C34
15	aB	846	BCR	C7-C8-C9-C34
15	bB	845	BCR	C7-C8-C9-C34
15	bB	846	BCR	C7-C8-C9-C34
15	cB	846	BCR	C7-C8-C9-C34
11	aB	830	CLA	O1D-CGD-O2D-CED
11	cB	830	CLA	O1D-CGD-O2D-CED
11	aB	836	CLA	O1A-CGA-O2A-C1
11	bB	836	CLA	O1A-CGA-O2A-C1
11	cB	836	CLA	O1A-CGA-O2A-C1
11	aA	804	CLA	C1A-C2A-CAA-CBA
11	aA	808	CLA	C1A-C2A-CAA-CBA
11	aA	809	CLA	C1A-C2A-CAA-CBA
11	aA	814	CLA	C1A-C2A-CAA-CBA
11	aA	817	CLA	C1A-C2A-CAA-CBA
11	aA	819	CLA	C1A-C2A-CAA-CBA
11	aA	833	CLA	C1A-C2A-CAA-CBA
11	aA	838	CLA	C1A-C2A-CAA-CBA
11	aB	810	CLA	C1A-C2A-CAA-CBA
11	aB	814	CLA	C1A-C2A-CAA-CBA
11	aB	818	CLA	C1A-C2A-CAA-CBA
11	aB	819	CLA	C1A-C2A-CAA-CBA
11	aB	825	CLA	C1A-C2A-CAA-CBA
11	aB	829	CLA	C1A-C2A-CAA-CBA
11	aB	836	CLA	C1A-C2A-CAA-CBA
11	aB	838	CLA	C1A-C2A-CAA-CBA
11	bA	804	CLA	C1A-C2A-CAA-CBA
11	bA	808	CLA	C1A-C2A-CAA-CBA
11	bA	809	CLA	C1A-C2A-CAA-CBA
11	bA	814	CLA	C1A-C2A-CAA-CBA
11	bA	817	CLA	C1A-C2A-CAA-CBA
11	bA	819	CLA	C1A-C2A-CAA-CBA
11	bA	833	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
11	bA	838	CLA	C1A-C2A-CAA-CBA
11	bB	810	CLA	C1A-C2A-CAA-CBA
11	bB	814	CLA	C1A-C2A-CAA-CBA
11	bB	818	CLA	C1A-C2A-CAA-CBA
11	bB	819	CLA	C1A-C2A-CAA-CBA
11	bB	825	CLA	C1A-C2A-CAA-CBA
11	bB	829	CLA	C1A-C2A-CAA-CBA
11	bB	836	CLA	C1A-C2A-CAA-CBA
11	bB	838	CLA	C1A-C2A-CAA-CBA
11	cA	804	CLA	C1A-C2A-CAA-CBA
11	cA	808	CLA	C1A-C2A-CAA-CBA
11	cA	809	CLA	C1A-C2A-CAA-CBA
11	cA	814	CLA	C1A-C2A-CAA-CBA
11	cA	817	CLA	C1A-C2A-CAA-CBA
11	cA	819	CLA	C1A-C2A-CAA-CBA
11	cA	833	CLA	C1A-C2A-CAA-CBA
11	cA	838	CLA	C1A-C2A-CAA-CBA
11	cB	810	CLA	C1A-C2A-CAA-CBA
11	cB	814	CLA	C1A-C2A-CAA-CBA
11	cB	818	CLA	C1A-C2A-CAA-CBA
11	cB	819	CLA	C1A-C2A-CAA-CBA
11	cB	825	CLA	C1A-C2A-CAA-CBA
11	cB	829	CLA	C1A-C2A-CAA-CBA
11	cB	836	CLA	C1A-C2A-CAA-CBA
11	cB	838	CLA	C1A-C2A-CAA-CBA
11	aA	822	CLA	C16-C17-C18-C19
11	bA	822	CLA	C16-C17-C18-C19
11	cA	822	CLA	C16-C17-C18-C19
11	aA	840	CLA	C3-C5-C6-C7
11	bA	840	CLA	C3-C5-C6-C7
11	cA	840	CLA	C3-C5-C6-C7
11	aB	805	CLA	CBA-CGA-O2A-C1
11	bB	805	CLA	CBA-CGA-O2A-C1
11	cB	805	CLA	CBA-CGA-O2A-C1
17	aA	853	LMT	C3-C4-C5-C6
17	bA	853	LMT	C3-C4-C5-C6
17	cA	853	LMT	C3-C4-C5-C6
11	aB	808	CLA	C15-C16-C17-C18
11	bB	808	CLA	C15-C16-C17-C18
11	cB	808	CLA	C15-C16-C17-C18
13	aA	845	PQN	C23-C25-C26-C27
13	bA	845	PQN	C23-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
13	cA	845	PQN	C23-C25-C26-C27
11	aA	819	CLA	O1A-CGA-O2A-C1
11	aA	833	CLA	O1A-CGA-O2A-C1
11	bA	819	CLA	O1A-CGA-O2A-C1
11	bA	833	CLA	O1A-CGA-O2A-C1
11	cA	819	CLA	O1A-CGA-O2A-C1
11	cA	833	CLA	O1A-CGA-O2A-C1
11	cB	812	CLA	O1A-CGA-O2A-C1
16	aA	852	LHG	C29-C30-C31-C32
16	cA	852	LHG	C29-C30-C31-C32
16	bA	852	LHG	C29-C30-C31-C32
11	aA	818	CLA	C6-C7-C8-C9
11	bA	818	CLA	C6-C7-C8-C9
11	cA	818	CLA	C6-C7-C8-C9
11	aB	812	CLA	O1A-CGA-O2A-C1
11	bB	812	CLA	O1A-CGA-O2A-C1
11	aB	815	CLA	CAA-CBA-CGA-O2A
11	bB	815	CLA	CAA-CBA-CGA-O2A
11	cB	815	CLA	CAA-CBA-CGA-O2A
11	bK	103	CLA	CBA-CGA-O2A-C1
11	aA	814	CLA	C10-C11-C12-C13
11	bA	814	CLA	C10-C11-C12-C13
11	cA	814	CLA	C10-C11-C12-C13
15	aB	844	BCR	C20-C21-C22-C37
15	bB	844	BCR	C20-C21-C22-C37
15	cB	844	BCR	C20-C21-C22-C37
17	aA	853	LMT	O5B-C5B-C6B-O6B
17	bA	853	LMT	O5B-C5B-C6B-O6B
17	cA	853	LMT	O5B-C5B-C6B-O6B
11	aA	807	CLA	C4-C3-C5-C6
11	bA	807	CLA	C4-C3-C5-C6
11	cA	807	CLA	C4-C3-C5-C6
11	aB	816	CLA	CBA-CGA-O2A-C1
11	aK	103	CLA	CBA-CGA-O2A-C1
11	bB	816	CLA	CBA-CGA-O2A-C1
11	cB	816	CLA	CBA-CGA-O2A-C1
11	cK	103	CLA	CBA-CGA-O2A-C1
11	aA	829	CLA	CBD-CGD-O2D-CED
11	aB	813	CLA	CBD-CGD-O2D-CED
11	bA	829	CLA	CBD-CGD-O2D-CED
11	bB	813	CLA	CBD-CGD-O2D-CED
11	cA	829	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	cB	813	CLA	CBD-CGD-O2D-CED
11	aA	840	CLA	C5-C6-C7-C8
11	aB	805	CLA	C13-C15-C16-C17
11	aB	816	CLA	C8-C10-C11-C12
11	aB	825	CLA	C8-C10-C11-C12
11	bA	840	CLA	C5-C6-C7-C8
11	bB	805	CLA	C13-C15-C16-C17
11	bB	816	CLA	C8-C10-C11-C12
11	bB	825	CLA	C8-C10-C11-C12
11	cA	840	CLA	C5-C6-C7-C8
11	cB	805	CLA	C13-C15-C16-C17
11	cB	816	CLA	C8-C10-C11-C12
11	cB	825	CLA	C8-C10-C11-C12
11	aB	814	CLA	O1D-CGD-O2D-CED
11	cB	814	CLA	O1D-CGD-O2D-CED
11	aB	817	CLA	C2-C1-O2A-CGA
11	bB	817	CLA	C2-C1-O2A-CGA
11	cB	817	CLA	C2-C1-O2A-CGA
12	aL	202	F6C	C2-C1-O2A-CGA
12	bL	202	F6C	C2-C1-O2A-CGA
12	cL	202	F6C	C2-C1-O2A-CGA
16	bA	852	LHG	C35-C36-C37-C38
16	cA	852	LHG	C35-C36-C37-C38
11	aB	840	CLA	O1D-CGD-O2D-CED
11	cB	828	CLA	O1D-CGD-O2D-CED
11	cB	840	CLA	O1D-CGD-O2D-CED
16	aA	852	LHG	C35-C36-C37-C38
11	aB	828	CLA	O1D-CGD-O2D-CED
11	bB	814	CLA	O1D-CGD-O2D-CED
11	bB	828	CLA	O1D-CGD-O2D-CED
11	bB	840	CLA	O1D-CGD-O2D-CED
11	aA	833	CLA	C10-C11-C12-C13
11	bA	833	CLA	C10-C11-C12-C13
11	cA	833	CLA	C10-C11-C12-C13
11	bA	841	CLA	O1D-CGD-O2D-CED
11	aK	103	CLA	O1A-CGA-O2A-C1
11	bK	103	CLA	O1A-CGA-O2A-C1
11	cK	103	CLA	O1A-CGA-O2A-C1
11	aB	806	CLA	C8-C10-C11-C12
11	bB	806	CLA	C8-C10-C11-C12
11	aA	841	CLA	O1D-CGD-O2D-CED
15	aB	846	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
15	aL	207	BCR	C20-C21-C22-C23
15	bB	846	BCR	C11-C10-C9-C8
15	bL	207	BCR	C20-C21-C22-C23
15	cB	846	BCR	C11-C10-C9-C8
15	cL	207	BCR	C20-C21-C22-C23
16	aA	852	LHG	O7-C5-C6-O8
16	bA	852	LHG	O7-C5-C6-O8
16	cA	852	LHG	O7-C5-C6-O8
11	aA	807	CLA	C5-C6-C7-C8
11	bA	807	CLA	C5-C6-C7-C8
11	cA	807	CLA	C5-C6-C7-C8
11	cB	806	CLA	C8-C10-C11-C12
11	aA	803	CLA	C4-C3-C5-C6
11	bA	803	CLA	C4-C3-C5-C6
11	cA	803	CLA	C4-C3-C5-C6
11	aA	803	CLA	C2-C3-C5-C6
11	aA	807	CLA	C2-C3-C5-C6
11	aA	825	CLA	C11-C12-C13-C15
11	aA	828	CLA	C6-C7-C8-C10
11	aA	840	CLA	C12-C13-C15-C16
11	aB	812	CLA	C11-C12-C13-C15
11	aB	825	CLA	C11-C12-C13-C15
11	bA	803	CLA	C2-C3-C5-C6
11	bA	807	CLA	C2-C3-C5-C6
11	bA	825	CLA	C11-C12-C13-C15
11	bA	828	CLA	C6-C7-C8-C10
11	bA	840	CLA	C12-C13-C15-C16
11	bB	812	CLA	C11-C12-C13-C15
11	bB	825	CLA	C11-C12-C13-C15
11	cA	803	CLA	C2-C3-C5-C6
11	cA	807	CLA	C2-C3-C5-C6
11	cA	825	CLA	C11-C12-C13-C15
11	cA	828	CLA	C6-C7-C8-C10
11	cA	840	CLA	C12-C13-C15-C16
11	cB	812	CLA	C11-C12-C13-C15
11	cB	825	CLA	C11-C12-C13-C15
12	aL	202	F6C	C3-C5-C6-C7
11	aA	814	CLA	C14-C13-C15-C16
11	aB	812	CLA	C14-C13-C15-C16
11	bA	814	CLA	C14-C13-C15-C16
11	bB	812	CLA	C14-C13-C15-C16
11	cA	814	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
11	cB	812	CLA	C14-C13-C15-C16
13	aB	841	PQN	C16-C17-C18-C19
13	bB	841	PQN	C16-C17-C18-C19
13	cB	841	PQN	C16-C17-C18-C19
11	cA	841	CLA	O1D-CGD-O2D-CED
15	aA	851	BCR	C7-C8-C9-C34
15	bA	851	BCR	C7-C8-C9-C34
15	cA	851	BCR	C7-C8-C9-C34
15	aA	848	BCR	C21-C22-C23-C24
15	bA	848	BCR	C21-C22-C23-C24
15	cA	848	BCR	C21-C22-C23-C24
11	aB	816	CLA	C11-C12-C13-C14
11	bB	816	CLA	C11-C12-C13-C14
11	cB	816	CLA	C11-C12-C13-C14
12	bL	202	F6C	C3-C5-C6-C7
12	cL	202	F6C	C3-C5-C6-C7
11	aA	806	CLA	CBA-CGA-O2A-C1
11	bA	806	CLA	CBA-CGA-O2A-C1
11	cA	806	CLA	CBA-CGA-O2A-C1
16	aA	852	LHG	C15-C16-C17-C18
16	cA	852	LHG	C15-C16-C17-C18
16	bA	852	LHG	C15-C16-C17-C18
11	aA	808	CLA	C4B-C3B-CAB-CBB
11	aB	803	CLA	C4B-C3B-CAB-CBB
11	aB	809	CLA	C4B-C3B-CAB-CBB
11	aB	810	CLA	C4B-C3B-CAB-CBB
11	aB	811	CLA	C4B-C3B-CAB-CBB
11	aB	823	CLA	C4B-C3B-CAB-CBB
11	aB	826	CLA	C4B-C3B-CAB-CBB
11	aB	827	CLA	C4B-C3B-CAB-CBB
11	aB	831	CLA	C4B-C3B-CAB-CBB
11	aB	834	CLA	C4B-C3B-CAB-CBB
11	aB	839	CLA	C4B-C3B-CAB-CBB
11	aB	840	CLA	C4B-C3B-CAB-CBB
11	aK	101	CLA	C4B-C3B-CAB-CBB
11	aK	103	CLA	C4B-C3B-CAB-CBB
11	aL	206	CLA	C4B-C3B-CAB-CBB
11	bA	808	CLA	C4B-C3B-CAB-CBB
11	bB	803	CLA	C4B-C3B-CAB-CBB
11	bB	809	CLA	C4B-C3B-CAB-CBB
11	bB	810	CLA	C4B-C3B-CAB-CBB
11	bB	811	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
11	bB	823	CLA	C4B-C3B-CAB-CBB
11	bB	826	CLA	C4B-C3B-CAB-CBB
11	bB	827	CLA	C4B-C3B-CAB-CBB
11	bB	831	CLA	C4B-C3B-CAB-CBB
11	bB	839	CLA	C4B-C3B-CAB-CBB
11	bB	840	CLA	C4B-C3B-CAB-CBB
11	bK	101	CLA	C4B-C3B-CAB-CBB
11	bK	103	CLA	C4B-C3B-CAB-CBB
11	bL	206	CLA	C4B-C3B-CAB-CBB
11	cA	808	CLA	C4B-C3B-CAB-CBB
11	cB	803	CLA	C4B-C3B-CAB-CBB
11	cB	809	CLA	C4B-C3B-CAB-CBB
11	cB	810	CLA	C4B-C3B-CAB-CBB
11	cB	811	CLA	C4B-C3B-CAB-CBB
11	cB	823	CLA	C4B-C3B-CAB-CBB
11	cB	826	CLA	C4B-C3B-CAB-CBB
11	cB	827	CLA	C4B-C3B-CAB-CBB
11	cB	831	CLA	C4B-C3B-CAB-CBB
11	cB	839	CLA	C4B-C3B-CAB-CBB
11	cB	840	CLA	C4B-C3B-CAB-CBB
11	cK	101	CLA	C4B-C3B-CAB-CBB
11	cK	103	CLA	C4B-C3B-CAB-CBB
11	cL	206	CLA	C4B-C3B-CAB-CBB
11	aB	837	CLA	C5-C6-C7-C8
11	bB	837	CLA	C5-C6-C7-C8
11	cB	837	CLA	C5-C6-C7-C8
12	bL	202	F6C	CBD-CGD-O2D-CED
12	cL	202	F6C	CBD-CGD-O2D-CED
11	aA	834	CLA	C4-C3-C5-C6
11	bA	834	CLA	C4-C3-C5-C6
11	cA	834	CLA	C4-C3-C5-C6
12	aA	830	F6C	C4-C3-C5-C6
12	bA	830	F6C	C4-C3-C5-C6
12	cA	830	F6C	C4-C3-C5-C6
11	aA	835	CLA	C5-C6-C7-C8
12	aA	826	F6C	CBA-CGA-O2A-C1
12	bA	826	F6C	CBA-CGA-O2A-C1
12	cA	826	F6C	CBA-CGA-O2A-C1
11	aA	843	CLA	CAA-CBA-CGA-O2A
11	bA	843	CLA	CAA-CBA-CGA-O2A
11	cA	843	CLA	CAA-CBA-CGA-O2A
11	aA	813	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
11	bA	813	CLA	C6-C7-C8-C9
11	cA	813	CLA	C6-C7-C8-C9
16	aA	852	LHG	C2-C3-O3-P
16	bA	852	LHG	C2-C3-O3-P
16	cA	852	LHG	C2-C3-O3-P
11	aA	812	CLA	C3A-C2A-CAA-CBA
11	aA	813	CLA	C3A-C2A-CAA-CBA
11	aA	829	CLA	C3A-C2A-CAA-CBA
11	aA	843	CLA	C3A-C2A-CAA-CBA
11	aB	815	CLA	C3A-C2A-CAA-CBA
11	aB	832	CLA	C3A-C2A-CAA-CBA
11	aB	833	CLA	C3A-C2A-CAA-CBA
11	bA	812	CLA	C3A-C2A-CAA-CBA
11	bA	813	CLA	C3A-C2A-CAA-CBA
11	bA	829	CLA	C3A-C2A-CAA-CBA
11	bA	843	CLA	C3A-C2A-CAA-CBA
11	bB	815	CLA	C3A-C2A-CAA-CBA
11	bB	832	CLA	C3A-C2A-CAA-CBA
11	bB	833	CLA	C3A-C2A-CAA-CBA
11	cA	812	CLA	C3A-C2A-CAA-CBA
11	cA	813	CLA	C3A-C2A-CAA-CBA
11	cA	829	CLA	C3A-C2A-CAA-CBA
11	cA	843	CLA	C3A-C2A-CAA-CBA
11	cB	815	CLA	C3A-C2A-CAA-CBA
11	cB	832	CLA	C3A-C2A-CAA-CBA
11	cB	833	CLA	C3A-C2A-CAA-CBA
11	bA	835	CLA	C5-C6-C7-C8
11	cA	835	CLA	C5-C6-C7-C8
11	aA	819	CLA	C6-C7-C8-C9
11	bA	819	CLA	C6-C7-C8-C9
11	cA	819	CLA	C6-C7-C8-C9
11	aA	831	CLA	C5-C6-C7-C8
11	bA	831	CLA	C5-C6-C7-C8
11	cA	831	CLA	C5-C6-C7-C8
12	aL	202	F6C	CBD-CGD-O2D-CED
11	aB	816	CLA	O1A-CGA-O2A-C1
11	bB	816	CLA	O1A-CGA-O2A-C1
11	cB	816	CLA	O1A-CGA-O2A-C1
11	aB	803	CLA	C8-C10-C11-C12
11	bB	803	CLA	C8-C10-C11-C12
11	cB	803	CLA	C8-C10-C11-C12
11	cA	813	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
11	aA	834	CLA	C2-C3-C5-C6
11	cA	834	CLA	C2-C3-C5-C6
12	aA	830	F6C	C2-C3-C5-C6
12	bA	830	F6C	C2-C3-C5-C6
12	cA	830	F6C	C2-C3-C5-C6
17	aA	853	LMT	C5'-C4'-O1B-C1B
17	bA	853	LMT	C5'-C4'-O1B-C1B
17	cA	853	LMT	C5'-C4'-O1B-C1B
11	aA	811	CLA	C2A-CAA-CBA-CGA
11	aB	831	CLA	C2A-CAA-CBA-CGA
11	bA	811	CLA	C2A-CAA-CBA-CGA
11	bB	831	CLA	C2A-CAA-CBA-CGA
11	cA	811	CLA	C2A-CAA-CBA-CGA
11	cB	831	CLA	C2A-CAA-CBA-CGA
11	aB	805	CLA	O1A-CGA-O2A-C1
11	bB	805	CLA	O1A-CGA-O2A-C1
11	cB	805	CLA	O1A-CGA-O2A-C1
11	aA	808	CLA	C2B-C3B-CAB-CBB
11	aB	809	CLA	C2B-C3B-CAB-CBB
11	aB	810	CLA	C2B-C3B-CAB-CBB
11	aB	818	CLA	C2B-C3B-CAB-CBB
11	aL	206	CLA	C2B-C3B-CAB-CBB
11	bA	808	CLA	C2B-C3B-CAB-CBB
11	bB	809	CLA	C2B-C3B-CAB-CBB
11	bB	810	CLA	C2B-C3B-CAB-CBB
11	bB	818	CLA	C2B-C3B-CAB-CBB
11	bK	101	CLA	C2B-C3B-CAB-CBB
11	bL	206	CLA	C2B-C3B-CAB-CBB
11	cA	808	CLA	C2B-C3B-CAB-CBB
11	cB	809	CLA	C2B-C3B-CAB-CBB
11	cB	810	CLA	C2B-C3B-CAB-CBB
11	cB	818	CLA	C2B-C3B-CAB-CBB
11	cK	101	CLA	C2B-C3B-CAB-CBB
11	cL	206	CLA	C2B-C3B-CAB-CBB
11	cA	834	CLA	O1D-CGD-O2D-CED
12	aA	827	F6C	C3A-C2A-CAA-CBA
12	bA	827	F6C	C3A-C2A-CAA-CBA
12	cA	827	F6C	C3A-C2A-CAA-CBA
11	cA	822	CLA	C16-C17-C18-C20
18	aB	847	LMG	O6-C1-O1-C7
18	bB	847	LMG	O6-C1-O1-C7
18	cB	847	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
11	bA	834	CLA	O1D-CGD-O2D-CED
11	aA	807	CLA	C2-C1-O2A-CGA
11	bA	807	CLA	C2-C1-O2A-CGA
11	cA	807	CLA	C2-C1-O2A-CGA
11	bA	834	CLA	C2-C3-C5-C6
11	aA	821	CLA	C6-C7-C8-C9
11	aA	833	CLA	C11-C10-C8-C9
11	aA	839	CLA	C6-C7-C8-C9
11	aB	806	CLA	C6-C7-C8-C9
11	aB	825	CLA	C11-C12-C13-C14
11	aL	206	CLA	C11-C10-C8-C9
11	bA	821	CLA	C6-C7-C8-C9
11	bA	833	CLA	C11-C10-C8-C9
11	bA	839	CLA	C6-C7-C8-C9
11	bB	806	CLA	C6-C7-C8-C9
11	bB	825	CLA	C11-C12-C13-C14
11	bL	206	CLA	C11-C10-C8-C9
11	cA	821	CLA	C6-C7-C8-C9
11	cA	833	CLA	C11-C10-C8-C9
11	cA	839	CLA	C6-C7-C8-C9
11	cB	806	CLA	C6-C7-C8-C9
11	cB	825	CLA	C11-C12-C13-C14
11	cL	206	CLA	C11-C10-C8-C9
11	aB	817	CLA	CBD-CGD-O2D-CED
12	aA	830	F6C	C5-C6-C7-C8
12	cA	830	F6C	C5-C6-C7-C8
11	aB	836	CLA	C4-C3-C5-C6
11	bB	836	CLA	C4-C3-C5-C6
11	cB	836	CLA	C4-C3-C5-C6
11	aB	803	CLA	C2A-CAA-CBA-CGA
11	bB	803	CLA	C2A-CAA-CBA-CGA
11	cB	803	CLA	C2A-CAA-CBA-CGA
11	aA	822	CLA	C16-C17-C18-C20
11	bA	822	CLA	C16-C17-C18-C20
11	bB	817	CLA	CBD-CGD-O2D-CED
11	cB	817	CLA	CBD-CGD-O2D-CED
15	aA	849	BCR	C23-C24-C25-C26
15	aA	849	BCR	C23-C24-C25-C30
15	aA	850	BCR	C23-C24-C25-C26
15	aA	850	BCR	C23-C24-C25-C30
15	aA	851	BCR	C23-C24-C25-C26
15	aA	851	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
15	aB	842	BCR	C23-C24-C25-C26
15	aB	842	BCR	C23-C24-C25-C30
15	aB	846	BCR	C1-C6-C7-C8
15	aB	846	BCR	C23-C24-C25-C26
15	aB	846	BCR	C23-C24-C25-C30
15	aI	101	BCR	C23-C24-C25-C26
15	aI	101	BCR	C23-C24-C25-C30
15	aM	101	BCR	C23-C24-C25-C30
15	bA	849	BCR	C23-C24-C25-C26
15	bA	849	BCR	C23-C24-C25-C30
15	bA	850	BCR	C23-C24-C25-C26
15	bA	850	BCR	C23-C24-C25-C30
15	bA	851	BCR	C23-C24-C25-C26
15	bA	851	BCR	C23-C24-C25-C30
15	bB	842	BCR	C23-C24-C25-C26
15	bB	842	BCR	C23-C24-C25-C30
15	bB	843	BCR	C23-C24-C25-C26
15	bB	846	BCR	C1-C6-C7-C8
15	bB	846	BCR	C23-C24-C25-C30
15	bI	101	BCR	C23-C24-C25-C26
15	bI	101	BCR	C23-C24-C25-C30
15	bM	101	BCR	C23-C24-C25-C30
15	cA	849	BCR	C23-C24-C25-C30
15	cA	850	BCR	C23-C24-C25-C26
15	cA	850	BCR	C23-C24-C25-C30
15	cA	851	BCR	C23-C24-C25-C26
15	cA	851	BCR	C23-C24-C25-C30
15	cB	842	BCR	C23-C24-C25-C26
15	cB	842	BCR	C23-C24-C25-C30
15	cB	843	BCR	C23-C24-C25-C26
15	cB	846	BCR	C1-C6-C7-C8
15	cB	846	BCR	C23-C24-C25-C26
15	cB	846	BCR	C23-C24-C25-C30
15	cI	103	BCR	C23-C24-C25-C26
15	cI	103	BCR	C23-C24-C25-C30
15	cM	101	BCR	C23-C24-C25-C30
11	aB	812	CLA	C8-C10-C11-C12
12	bA	830	F6C	C5-C6-C7-C8
11	aA	834	CLA	O1D-CGD-O2D-CED
11	bB	812	CLA	C8-C10-C11-C12
11	cB	812	CLA	C8-C10-C11-C12
10	aA	801	CL0	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
10	bA	801	CL0	C13-C15-C16-C17
10	cA	801	CL0	C13-C15-C16-C17
11	aA	813	CLA	C4-C3-C5-C6
11	bA	813	CLA	C4-C3-C5-C6
11	aA	807	CLA	C12-C13-C15-C16
11	aA	812	CLA	C6-C7-C8-C10
11	aA	821	CLA	C6-C7-C8-C10
11	aA	825	CLA	C11-C10-C8-C7
11	aA	833	CLA	C11-C10-C8-C7
11	aA	833	CLA	C12-C13-C15-C16
11	aA	839	CLA	C6-C7-C8-C10
11	aA	839	CLA	C12-C13-C15-C16
11	aA	840	CLA	C6-C7-C8-C10
11	aB	806	CLA	C6-C7-C8-C10
11	aB	812	CLA	C12-C13-C15-C16
11	aL	206	CLA	C11-C10-C8-C7
11	bA	807	CLA	C12-C13-C15-C16
11	bA	812	CLA	C6-C7-C8-C10
11	bA	821	CLA	C6-C7-C8-C10
11	bA	825	CLA	C11-C10-C8-C7
11	bA	833	CLA	C11-C10-C8-C7
11	bA	833	CLA	C12-C13-C15-C16
11	bA	839	CLA	C6-C7-C8-C10
11	bA	839	CLA	C12-C13-C15-C16
11	bA	840	CLA	C6-C7-C8-C10
11	bB	806	CLA	C6-C7-C8-C10
11	bB	812	CLA	C12-C13-C15-C16
11	bL	206	CLA	C11-C10-C8-C7
11	cA	807	CLA	C12-C13-C15-C16
11	cA	812	CLA	C6-C7-C8-C10
11	cA	821	CLA	C6-C7-C8-C10
11	cA	825	CLA	C11-C10-C8-C7
11	cA	833	CLA	C11-C10-C8-C7
11	cA	833	CLA	C12-C13-C15-C16
11	cA	839	CLA	C6-C7-C8-C10
11	cA	839	CLA	C12-C13-C15-C16
11	cA	840	CLA	C6-C7-C8-C10
11	cB	806	CLA	C6-C7-C8-C10
11	cB	812	CLA	C12-C13-C15-C16
11	cL	206	CLA	C11-C10-C8-C7
13	aB	841	PQN	C16-C17-C18-C20
13	bB	841	PQN	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
13	cB	841	PQN	C16-C17-C18-C20
11	aA	822	CLA	C15-C16-C17-C18
11	bA	822	CLA	C15-C16-C17-C18
15	aB	848	BCR	C15-C16-C17-C18
15	aL	207	BCR	C9-C10-C11-C12
15	bB	848	BCR	C15-C16-C17-C18
15	bL	207	BCR	C9-C10-C11-C12
15	cB	848	BCR	C15-C16-C17-C18
15	cL	207	BCR	C9-C10-C11-C12
11	cA	822	CLA	C15-C16-C17-C18
11	aA	835	CLA	C2A-CAA-CBA-CGA
11	bA	835	CLA	C2A-CAA-CBA-CGA
11	cA	835	CLA	C2A-CAA-CBA-CGA
15	aB	842	BCR	C16-C17-C18-C36
15	bB	842	BCR	C16-C17-C18-C36
15	cB	842	BCR	C16-C17-C18-C36
11	aB	815	CLA	C3-C5-C6-C7
11	bB	815	CLA	C3-C5-C6-C7
11	cB	815	CLA	C3-C5-C6-C7
17	aA	853	LMT	C3'-C4'-O1B-C1B
17	bA	853	LMT	C3'-C4'-O1B-C1B
17	cA	853	LMT	C3'-C4'-O1B-C1B
11	bB	819	CLA	CBD-CGD-O2D-CED
11	cB	819	CLA	CBD-CGD-O2D-CED
11	aA	807	CLA	CAD-CBD-CGD-O2D
11	aA	813	CLA	CAD-CBD-CGD-O2D
11	aA	824	CLA	CAD-CBD-CGD-O2D
11	aA	825	CLA	CAD-CBD-CGD-O2D
11	aA	831	CLA	CAD-CBD-CGD-O2D
11	aB	830	CLA	CAD-CBD-CGD-O2D
11	aB	839	CLA	CAD-CBD-CGD-O2D
11	bA	807	CLA	CAD-CBD-CGD-O2D
11	bA	813	CLA	CAD-CBD-CGD-O2D
11	bA	824	CLA	CAD-CBD-CGD-O2D
11	bA	825	CLA	CAD-CBD-CGD-O2D
11	bA	831	CLA	CAD-CBD-CGD-O2D
11	bB	830	CLA	CAD-CBD-CGD-O2D
11	bB	839	CLA	CAD-CBD-CGD-O2D
11	cA	807	CLA	CAD-CBD-CGD-O2D
11	cA	813	CLA	CAD-CBD-CGD-O2D
11	cA	824	CLA	CAD-CBD-CGD-O2D
11	cA	825	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
11	cA	831	CLA	CAD-CBD-CGD-O2D
11	cB	830	CLA	CAD-CBD-CGD-O2D
11	cB	839	CLA	CAD-CBD-CGD-O2D
12	aA	827	F6C	C2B-C3B-CAB-CBB
12	aA	832	F6C	C2B-C3B-CAB-CBB
12	bA	827	F6C	C2B-C3B-CAB-CBB
12	bA	832	F6C	C2B-C3B-CAB-CBB
12	cA	827	F6C	C2B-C3B-CAB-CBB
12	cA	832	F6C	C2B-C3B-CAB-CBB
12	bA	827	F6C	C3-C5-C6-C7
11	aA	825	CLA	C8-C10-C11-C12
11	bA	825	CLA	C8-C10-C11-C12
11	cA	825	CLA	C8-C10-C11-C12
11	cB	808	CLA	C5-C6-C7-C8
11	aA	840	CLA	C16-C17-C18-C19
11	bA	840	CLA	C16-C17-C18-C19
11	cA	840	CLA	C16-C17-C18-C19
17	aA	853	LMT	C9-C10-C11-C12
17	bA	853	LMT	C9-C10-C11-C12
17	cA	853	LMT	C9-C10-C11-C12
11	aB	819	CLA	CBD-CGD-O2D-CED
11	aB	808	CLA	C5-C6-C7-C8
11	bB	808	CLA	C5-C6-C7-C8
12	aA	827	F6C	C3-C5-C6-C7
12	cA	827	F6C	C3-C5-C6-C7
11	aA	843	CLA	C2A-CAA-CBA-CGA
11	bA	843	CLA	C2A-CAA-CBA-CGA
11	bL	205	CLA	C2A-CAA-CBA-CGA
11	cA	843	CLA	C2A-CAA-CBA-CGA
18	aB	847	LMG	C11-C12-C13-C14
18	bB	847	LMG	C11-C12-C13-C14
18	cB	847	LMG	C11-C12-C13-C14
11	aA	806	CLA	CHA-CBD-CGD-O2D
11	aA	809	CLA	CHA-CBD-CGD-O1D
11	aA	809	CLA	CHA-CBD-CGD-O2D
11	aA	818	CLA	CHA-CBD-CGD-O1D
11	aA	823	CLA	CHA-CBD-CGD-O1D
11	aA	823	CLA	CHA-CBD-CGD-O2D
11	aB	801	CLA	CHA-CBD-CGD-O2D
11	aB	802	CLA	CHA-CBD-CGD-O1D
11	aB	802	CLA	CHA-CBD-CGD-O2D
11	aB	805	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
11	aB	805	CLA	CHA-CBD-CGD-O2D
11	bA	806	CLA	CHA-CBD-CGD-O2D
11	bA	809	CLA	CHA-CBD-CGD-O1D
11	bA	809	CLA	CHA-CBD-CGD-O2D
11	bA	818	CLA	CHA-CBD-CGD-O1D
11	bA	823	CLA	CHA-CBD-CGD-O1D
11	bA	823	CLA	CHA-CBD-CGD-O2D
11	bB	801	CLA	CHA-CBD-CGD-O2D
11	bB	802	CLA	CHA-CBD-CGD-O1D
11	bB	802	CLA	CHA-CBD-CGD-O2D
11	bB	805	CLA	CHA-CBD-CGD-O1D
11	bB	805	CLA	CHA-CBD-CGD-O2D
11	cA	806	CLA	CHA-CBD-CGD-O2D
11	cA	809	CLA	CHA-CBD-CGD-O1D
11	cA	809	CLA	CHA-CBD-CGD-O2D
11	cA	818	CLA	CHA-CBD-CGD-O1D
11	cA	823	CLA	CHA-CBD-CGD-O1D
11	cA	823	CLA	CHA-CBD-CGD-O2D
11	cB	801	CLA	CHA-CBD-CGD-O2D
11	cB	802	CLA	CHA-CBD-CGD-O1D
11	cB	802	CLA	CHA-CBD-CGD-O2D
11	cB	805	CLA	CHA-CBD-CGD-O1D
11	cB	805	CLA	CHA-CBD-CGD-O2D
12	aB	824	F6C	CHA-CBD-CGD-O1D
12	bB	824	F6C	CHA-CBD-CGD-O1D
12	cB	824	F6C	CHA-CBD-CGD-O1D
11	cB	812	CLA	C13-C15-C16-C17
12	aA	826	F6C	O1A-CGA-O2A-C1
12	bA	826	F6C	O1A-CGA-O2A-C1
12	cA	826	F6C	O1A-CGA-O2A-C1
17	bA	853	LMT	C4-C5-C6-C7
11	aB	812	CLA	C13-C15-C16-C17
11	bB	812	CLA	C13-C15-C16-C17
17	aA	853	LMT	C4-C5-C6-C7
17	cA	853	LMT	C4-C5-C6-C7
16	aA	852	LHG	O1-C1-C2-O2
16	bA	852	LHG	O1-C1-C2-O2
16	cA	852	LHG	O1-C1-C2-O2
17	bA	853	LMT	O1'-C1-C2-C3
17	aA	853	LMT	O1'-C1-C2-C3
17	cA	853	LMT	O1'-C1-C2-C3
11	aA	825	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
11	aA	831	CLA	C14-C13-C15-C16
11	aA	835	CLA	C14-C13-C15-C16
11	aB	806	CLA	C14-C13-C15-C16
11	aB	839	CLA	C14-C13-C15-C16
11	bA	825	CLA	C11-C10-C8-C9
11	bA	831	CLA	C14-C13-C15-C16
11	bA	835	CLA	C14-C13-C15-C16
11	bB	806	CLA	C14-C13-C15-C16
11	bB	839	CLA	C14-C13-C15-C16
11	cA	825	CLA	C11-C10-C8-C9
11	cA	831	CLA	C14-C13-C15-C16
11	cA	835	CLA	C14-C13-C15-C16
11	cB	806	CLA	C14-C13-C15-C16
11	cB	839	CLA	C14-C13-C15-C16
12	aA	844	F6C	C11-C10-C8-C9
12	bA	844	F6C	C11-C10-C8-C9
12	cA	844	F6C	C11-C10-C8-C9
11	aB	805	CLA	C10-C11-C12-C13
11	bB	805	CLA	C10-C11-C12-C13
11	aL	205	CLA	C2A-CAA-CBA-CGA
11	cL	205	CLA	C2A-CAA-CBA-CGA
11	cB	805	CLA	C10-C11-C12-C13
11	aA	806	CLA	O1A-CGA-O2A-C1
11	bA	806	CLA	O1A-CGA-O2A-C1
11	cA	806	CLA	O1A-CGA-O2A-C1
15	aL	207	BCR	C7-C8-C9-C34
15	bL	207	BCR	C7-C8-C9-C34
15	cL	207	BCR	C7-C8-C9-C34
15	aB	848	BCR	C7-C8-C9-C10
15	bB	848	BCR	C7-C8-C9-C10
15	cB	848	BCR	C7-C8-C9-C10
11	aK	103	CLA	C1A-C2A-CAA-CBA
11	bK	103	CLA	C1A-C2A-CAA-CBA
11	cK	103	CLA	C1A-C2A-CAA-CBA
11	aL	206	CLA	C10-C11-C12-C13
11	bL	206	CLA	C10-C11-C12-C13
11	cL	206	CLA	C10-C11-C12-C13
11	aB	827	CLA	CBA-CGA-O2A-C1
11	bB	827	CLA	CBA-CGA-O2A-C1
11	cB	827	CLA	CBA-CGA-O2A-C1
16	bA	852	LHG	C24-C23-O8-C6
15	aB	842	BCR	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
15	bB	842	BCR	C15-C16-C17-C18
15	cB	842	BCR	C15-C16-C17-C18
11	aA	828	CLA	C4-C3-C5-C6
11	bA	828	CLA	C4-C3-C5-C6
11	cA	828	CLA	C4-C3-C5-C6
11	aA	822	CLA	C2-C3-C5-C6
11	bA	822	CLA	C2-C3-C5-C6
11	cA	822	CLA	C2-C3-C5-C6
11	aA	819	CLA	C4B-C3B-CAB-CBB
11	aA	839	CLA	C4B-C3B-CAB-CBB
11	aA	842	CLA	C4B-C3B-CAB-CBB
11	aA	843	CLA	C4B-C3B-CAB-CBB
11	aB	814	CLA	C4B-C3B-CAB-CBB
11	aB	818	CLA	C4B-C3B-CAB-CBB
11	aB	821	CLA	C4B-C3B-CAB-CBB
11	aB	833	CLA	C4B-C3B-CAB-CBB
11	aB	836	CLA	C4B-C3B-CAB-CBB
11	bA	819	CLA	C4B-C3B-CAB-CBB
11	bA	839	CLA	C4B-C3B-CAB-CBB
11	bA	842	CLA	C4B-C3B-CAB-CBB
11	bA	843	CLA	C4B-C3B-CAB-CBB
11	bB	814	CLA	C4B-C3B-CAB-CBB
11	bB	818	CLA	C4B-C3B-CAB-CBB
11	bB	821	CLA	C4B-C3B-CAB-CBB
11	bB	833	CLA	C4B-C3B-CAB-CBB
11	bB	836	CLA	C4B-C3B-CAB-CBB
11	cA	819	CLA	C4B-C3B-CAB-CBB
11	cA	839	CLA	C4B-C3B-CAB-CBB
11	cA	842	CLA	C4B-C3B-CAB-CBB
11	cA	843	CLA	C4B-C3B-CAB-CBB
11	cB	814	CLA	C4B-C3B-CAB-CBB
11	cB	818	CLA	C4B-C3B-CAB-CBB
11	cB	821	CLA	C4B-C3B-CAB-CBB
11	cB	833	CLA	C4B-C3B-CAB-CBB
11	cB	836	CLA	C4B-C3B-CAB-CBB
11	aB	805	CLA	C16-C17-C18-C19
11	bB	805	CLA	C16-C17-C18-C19
11	cB	805	CLA	C16-C17-C18-C19
16	aA	852	LHG	C24-C23-O8-C6
16	cA	852	LHG	C24-C23-O8-C6
11	aA	829	CLA	O1D-CGD-O2D-CED
11	cA	829	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	bA	829	CLA	O1D-CGD-O2D-CED
11	aA	805	CLA	CAD-CBD-CGD-O1D
11	aA	806	CLA	CAD-CBD-CGD-O1D
11	aB	802	CLA	CAD-CBD-CGD-O1D
11	aB	805	CLA	CAD-CBD-CGD-O1D
11	bA	805	CLA	CAD-CBD-CGD-O1D
11	bA	806	CLA	CAD-CBD-CGD-O1D
11	bB	802	CLA	CAD-CBD-CGD-O1D
11	bB	805	CLA	CAD-CBD-CGD-O1D
11	cA	805	CLA	CAD-CBD-CGD-O1D
11	cA	806	CLA	CAD-CBD-CGD-O1D
11	cB	802	CLA	CAD-CBD-CGD-O1D
11	cB	805	CLA	CAD-CBD-CGD-O1D
11	aB	801	CLA	CBA-CGA-O2A-C1
11	bB	801	CLA	CBA-CGA-O2A-C1
11	cB	801	CLA	CBA-CGA-O2A-C1
11	aA	829	CLA	C4-C3-C5-C6
11	bA	829	CLA	C4-C3-C5-C6
11	cA	829	CLA	C4-C3-C5-C6
11	aA	821	CLA	C11-C10-C8-C7
11	aA	831	CLA	C12-C13-C15-C16
11	aA	835	CLA	C12-C13-C15-C16
11	aB	803	CLA	C11-C10-C8-C7
11	aB	839	CLA	C12-C13-C15-C16
11	bA	821	CLA	C11-C10-C8-C7
11	bA	831	CLA	C12-C13-C15-C16
11	bA	835	CLA	C12-C13-C15-C16
11	bB	803	CLA	C11-C10-C8-C7
11	bB	839	CLA	C12-C13-C15-C16
11	cA	821	CLA	C11-C10-C8-C7
11	cA	831	CLA	C12-C13-C15-C16
11	cA	835	CLA	C12-C13-C15-C16
11	cB	803	CLA	C11-C10-C8-C7
11	cB	839	CLA	C12-C13-C15-C16
12	aA	826	F6C	C11-C10-C8-C7
12	aA	844	F6C	C12-C13-C15-C16
12	aL	202	F6C	C11-C10-C8-C7
12	bA	826	F6C	C11-C10-C8-C7
12	bA	844	F6C	C12-C13-C15-C16
12	bL	202	F6C	C11-C10-C8-C7
12	cA	826	F6C	C11-C10-C8-C7
12	cA	844	F6C	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
12	cL	202	F6C	C11-C10-C8-C7
16	aA	852	LHG	C11-C12-C13-C14
16	bA	852	LHG	C11-C12-C13-C14
16	cA	852	LHG	C11-C12-C13-C14
11	aB	825	CLA	C10-C11-C12-C13
11	cB	825	CLA	C10-C11-C12-C13
11	bB	825	CLA	C10-C11-C12-C13
12	aA	832	F6C	C1B-C2B-CMB-OMB
12	aL	202	F6C	C1B-C2B-CMB-OMB
12	bA	832	F6C	C1B-C2B-CMB-OMB
12	bL	202	F6C	C1B-C2B-CMB-OMB
12	cA	832	F6C	C1B-C2B-CMB-OMB
12	cL	202	F6C	C1B-C2B-CMB-OMB
18	aB	847	LMG	C37-C38-C39-C40
18	bB	847	LMG	C37-C38-C39-C40
11	aB	827	CLA	O1A-CGA-O2A-C1
11	bB	827	CLA	O1A-CGA-O2A-C1
11	cB	827	CLA	O1A-CGA-O2A-C1
18	cB	847	LMG	C37-C38-C39-C40
11	aA	802	CLA	C8-C10-C11-C12
11	bA	802	CLA	C8-C10-C11-C12
11	cA	802	CLA	C8-C10-C11-C12
12	aA	827	F6C	O1A-CGA-O2A-C1
12	bA	827	F6C	O1A-CGA-O2A-C1
12	cA	827	F6C	O1A-CGA-O2A-C1
12	aB	824	F6C	C4-C3-C5-C6
12	bB	824	F6C	C4-C3-C5-C6
12	cB	824	F6C	C4-C3-C5-C6
12	aA	827	F6C	CBA-CGA-O2A-C1
12	bA	827	F6C	CBA-CGA-O2A-C1
12	cA	827	F6C	CBA-CGA-O2A-C1
11	aA	812	CLA	C6-C7-C8-C9
11	bA	812	CLA	C6-C7-C8-C9
11	cA	812	CLA	C6-C7-C8-C9
12	aA	844	F6C	C14-C13-C15-C16
12	bA	844	F6C	C14-C13-C15-C16
11	aB	801	CLA	O1A-CGA-O2A-C1
11	cB	801	CLA	O1A-CGA-O2A-C1
11	bA	813	CLA	CAA-CBA-CGA-O2A
11	aA	805	CLA	C2B-C3B-CAB-CBB
11	aA	806	CLA	C2B-C3B-CAB-CBB
11	aA	816	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
11	aA	819	CLA	C2B-C3B-CAB-CBB
11	aA	839	CLA	C2B-C3B-CAB-CBB
11	aB	803	CLA	C2B-C3B-CAB-CBB
11	aB	812	CLA	C2B-C3B-CAB-CBB
11	aB	817	CLA	C2B-C3B-CAB-CBB
11	aB	821	CLA	C2B-C3B-CAB-CBB
11	aB	823	CLA	C2B-C3B-CAB-CBB
11	aB	826	CLA	C2B-C3B-CAB-CBB
11	aB	827	CLA	C2B-C3B-CAB-CBB
11	bA	805	CLA	C2B-C3B-CAB-CBB
11	bA	806	CLA	C2B-C3B-CAB-CBB
11	bA	816	CLA	C2B-C3B-CAB-CBB
11	bA	819	CLA	C2B-C3B-CAB-CBB
11	bA	839	CLA	C2B-C3B-CAB-CBB
11	bB	803	CLA	C2B-C3B-CAB-CBB
11	bB	812	CLA	C2B-C3B-CAB-CBB
11	bB	817	CLA	C2B-C3B-CAB-CBB
11	bB	821	CLA	C2B-C3B-CAB-CBB
11	bB	823	CLA	C2B-C3B-CAB-CBB
11	bB	826	CLA	C2B-C3B-CAB-CBB
11	bB	827	CLA	C2B-C3B-CAB-CBB
11	cA	805	CLA	C2B-C3B-CAB-CBB
11	cA	806	CLA	C2B-C3B-CAB-CBB
11	cA	816	CLA	C2B-C3B-CAB-CBB
11	cA	819	CLA	C2B-C3B-CAB-CBB
11	cA	839	CLA	C2B-C3B-CAB-CBB
11	cB	803	CLA	C2B-C3B-CAB-CBB
11	cB	812	CLA	C2B-C3B-CAB-CBB
11	cB	821	CLA	C2B-C3B-CAB-CBB
11	cB	823	CLA	C2B-C3B-CAB-CBB
11	cB	826	CLA	C2B-C3B-CAB-CBB
11	cB	827	CLA	C2B-C3B-CAB-CBB
11	bB	801	CLA	O1A-CGA-O2A-C1
11	aA	813	CLA	CAA-CBA-CGA-O2A
11	cA	813	CLA	CAA-CBA-CGA-O2A
11	aB	830	CLA	C1-C2-C3-C4
11	bB	830	CLA	C1-C2-C3-C4
11	cB	830	CLA	C1-C2-C3-C4
11	aA	819	CLA	C2A-CAA-CBA-CGA
11	bA	819	CLA	C2A-CAA-CBA-CGA
11	cA	819	CLA	C2A-CAA-CBA-CGA
11	aA	821	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
11	bA	821	CLA	C5-C6-C7-C8
11	cA	821	CLA	C5-C6-C7-C8
11	aA	817	CLA	C2-C1-O2A-CGA
11	bA	817	CLA	C2-C1-O2A-CGA
11	cA	817	CLA	C2-C1-O2A-CGA
11	aA	820	CLA	C4-C3-C5-C6
11	bA	820	CLA	C4-C3-C5-C6
11	cA	820	CLA	C4-C3-C5-C6
18	aB	847	LMG	C30-C31-C32-C33
18	bB	847	LMG	C30-C31-C32-C33
15	aB	843	BCR	C23-C24-C25-C26
15	aB	844	BCR	C23-C24-C25-C26
15	aB	846	BCR	C5-C6-C7-C8
15	aM	101	BCR	C23-C24-C25-C26
15	bB	843	BCR	C23-C24-C25-C30
15	bB	844	BCR	C23-C24-C25-C26
15	bB	846	BCR	C5-C6-C7-C8
15	bB	846	BCR	C23-C24-C25-C26
15	bM	101	BCR	C23-C24-C25-C26
15	cB	844	BCR	C23-C24-C25-C26
15	cB	846	BCR	C5-C6-C7-C8
15	cM	101	BCR	C23-C24-C25-C26
11	aA	813	CLA	C2-C3-C5-C6
11	bA	813	CLA	C2-C3-C5-C6
11	cA	813	CLA	C2-C3-C5-C6
18	cB	847	LMG	C30-C31-C32-C33
11	bA	822	CLA	C10-C11-C12-C13
11	aA	822	CLA	C10-C11-C12-C13
11	cA	822	CLA	C10-C11-C12-C13
11	aB	801	CLA	C8-C10-C11-C12
11	bB	801	CLA	C8-C10-C11-C12
11	cB	801	CLA	C8-C10-C11-C12
16	aA	852	LHG	C25-C26-C27-C28
16	bA	852	LHG	C25-C26-C27-C28
18	aB	847	LMG	O1-C7-C8-C9
18	bB	847	LMG	O1-C7-C8-C9
18	cB	847	LMG	O1-C7-C8-C9
16	aA	852	LHG	C26-C27-C28-C29
16	bA	852	LHG	C26-C27-C28-C29
16	cA	852	LHG	C26-C27-C28-C29
11	aA	818	CLA	C2-C3-C5-C6
11	bA	818	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
11	cA	818	CLA	C2-C3-C5-C6
16	cA	852	LHG	C25-C26-C27-C28
11	aB	801	CLA	CAA-CBA-CGA-O2A
11	bB	801	CLA	CAA-CBA-CGA-O2A
11	cB	801	CLA	CAA-CBA-CGA-O2A
11	aA	807	CLA	C14-C13-C15-C16
11	aA	828	CLA	C6-C7-C8-C9
11	aA	840	CLA	C6-C7-C8-C9
11	aB	803	CLA	C11-C10-C8-C9
11	aB	816	CLA	C11-C10-C8-C9
11	bA	807	CLA	C14-C13-C15-C16
11	bA	828	CLA	C6-C7-C8-C9
11	bA	840	CLA	C6-C7-C8-C9
11	bB	803	CLA	C11-C10-C8-C9
11	bB	816	CLA	C11-C10-C8-C9
11	cA	807	CLA	C14-C13-C15-C16
11	cA	828	CLA	C6-C7-C8-C9
11	cA	840	CLA	C6-C7-C8-C9
11	cB	803	CLA	C11-C10-C8-C9
11	cB	816	CLA	C11-C10-C8-C9
12	cA	844	F6C	C14-C13-C15-C16
11	aB	825	CLA	C16-C17-C18-C20
11	bB	825	CLA	C16-C17-C18-C20
11	cB	825	CLA	C16-C17-C18-C20
11	aA	806	CLA	C15-C16-C17-C18
11	bA	806	CLA	C15-C16-C17-C18
11	cA	806	CLA	C15-C16-C17-C18
11	aB	840	CLA	C2A-CAA-CBA-CGA
11	bB	840	CLA	C2A-CAA-CBA-CGA
11	cB	840	CLA	C2A-CAA-CBA-CGA
16	aA	852	LHG	C31-C32-C33-C34
16	cA	852	LHG	C31-C32-C33-C34
16	bA	852	LHG	C31-C32-C33-C34
11	cA	819	CLA	O1D-CGD-O2D-CED
11	bA	819	CLA	O1D-CGD-O2D-CED
11	aB	823	CLA	C2-C3-C5-C6
11	bB	823	CLA	C2-C3-C5-C6
11	cB	823	CLA	C2-C3-C5-C6
11	aB	815	CLA	CAA-CBA-CGA-O1A
11	bB	815	CLA	CAA-CBA-CGA-O1A
11	bA	828	CLA	C5-C6-C7-C8
11	aA	819	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	cB	815	CLA	CAA-CBA-CGA-O1A
11	aA	828	CLA	C5-C6-C7-C8
11	cA	828	CLA	C5-C6-C7-C8
11	aA	805	CLA	C4B-C3B-CAB-CBB
11	aA	806	CLA	C4B-C3B-CAB-CBB
11	aA	816	CLA	C4B-C3B-CAB-CBB
11	aA	828	CLA	C4B-C3B-CAB-CBB
11	aB	812	CLA	C4B-C3B-CAB-CBB
11	aB	817	CLA	C4B-C3B-CAB-CBB
11	bA	805	CLA	C4B-C3B-CAB-CBB
11	bA	806	CLA	C4B-C3B-CAB-CBB
11	bA	816	CLA	C4B-C3B-CAB-CBB
11	bA	828	CLA	C4B-C3B-CAB-CBB
11	bB	812	CLA	C4B-C3B-CAB-CBB
11	bB	817	CLA	C4B-C3B-CAB-CBB
11	cA	805	CLA	C4B-C3B-CAB-CBB
11	cA	806	CLA	C4B-C3B-CAB-CBB
11	cA	816	CLA	C4B-C3B-CAB-CBB
11	cA	828	CLA	C4B-C3B-CAB-CBB
11	cB	812	CLA	C4B-C3B-CAB-CBB
11	cB	817	CLA	C4B-C3B-CAB-CBB
11	aA	822	CLA	C2A-CAA-CBA-CGA
11	bA	822	CLA	C2A-CAA-CBA-CGA
11	cA	822	CLA	C2A-CAA-CBA-CGA
15	aA	848	BCR	C19-C20-C21-C22
15	bA	848	BCR	C19-C20-C21-C22
15	cA	848	BCR	C19-C20-C21-C22
11	cB	819	CLA	O1D-CGD-O2D-CED
11	aB	808	CLA	C4-C3-C5-C6
11	bB	808	CLA	C4-C3-C5-C6
11	cB	808	CLA	C4-C3-C5-C6
12	aA	827	F6C	C4-C3-C5-C6
12	bA	827	F6C	C4-C3-C5-C6
12	cA	827	F6C	C4-C3-C5-C6
18	bB	847	LMG	C32-C33-C34-C35
18	cB	847	LMG	C32-C33-C34-C35
11	aB	828	CLA	C2-C3-C5-C6
11	bB	828	CLA	C2-C3-C5-C6
11	cB	828	CLA	C2-C3-C5-C6
18	aB	847	LMG	C32-C33-C34-C35
11	aB	813	CLA	O1D-CGD-O2D-CED
10	aA	801	CL0	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
10	bA	801	CL0	CAA-CBA-CGA-O2A
10	cA	801	CL0	CAA-CBA-CGA-O2A
11	aB	830	CLA	C2-C1-O2A-CGA
11	bB	830	CLA	C2-C1-O2A-CGA
11	cB	830	CLA	C2-C1-O2A-CGA
12	aA	832	F6C	C2-C1-O2A-CGA
12	bA	832	F6C	C2-C1-O2A-CGA
12	cA	832	F6C	C2-C1-O2A-CGA
11	aB	819	CLA	O1D-CGD-O2D-CED
18	aB	847	LMG	C2-C1-O1-C7
18	bB	847	LMG	C2-C1-O1-C7
11	aB	832	CLA	CAA-CBA-CGA-O1A
11	bB	832	CLA	CAA-CBA-CGA-O1A
11	cB	832	CLA	CAA-CBA-CGA-O1A
11	aA	823	CLA	C2A-CAA-CBA-CGA
11	bA	823	CLA	C2A-CAA-CBA-CGA
11	cA	823	CLA	C2A-CAA-CBA-CGA
11	bB	819	CLA	O1D-CGD-O2D-CED
11	aA	815	CLA	C3A-C2A-CAA-CBA
11	aB	817	CLA	C3A-C2A-CAA-CBA
11	bA	815	CLA	C3A-C2A-CAA-CBA
11	bB	817	CLA	C3A-C2A-CAA-CBA
11	cA	815	CLA	C3A-C2A-CAA-CBA
11	cB	817	CLA	C3A-C2A-CAA-CBA
11	aB	813	CLA	C4-C3-C5-C6
11	bB	813	CLA	C4-C3-C5-C6
11	cB	813	CLA	C4-C3-C5-C6
11	aA	828	CLA	C2-C3-C5-C6
11	bB	813	CLA	O1D-CGD-O2D-CED
15	aA	851	BCR	C11-C10-C9-C34
15	bA	851	BCR	C11-C10-C9-C34
15	cA	851	BCR	C11-C10-C9-C34
11	cB	813	CLA	O1D-CGD-O2D-CED
11	aB	813	CLA	CBA-CGA-O2A-C1
11	bB	813	CLA	CBA-CGA-O2A-C1
11	cB	813	CLA	CBA-CGA-O2A-C1
12	aA	832	F6C	C1A-C2A-CAA-CBA
12	bA	832	F6C	C1A-C2A-CAA-CBA
12	cA	832	F6C	C1A-C2A-CAA-CBA
11	aB	834	CLA	CAA-CBA-CGA-O1A
11	bB	834	CLA	CAA-CBA-CGA-O1A
11	cB	834	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
11	aA	802	CLA	C1A-C2A-CAA-CBA
11	aA	812	CLA	C1A-C2A-CAA-CBA
11	aA	813	CLA	C1A-C2A-CAA-CBA
11	aA	843	CLA	C1A-C2A-CAA-CBA
11	aB	815	CLA	C1A-C2A-CAA-CBA
11	aB	816	CLA	C1A-C2A-CAA-CBA
11	aB	834	CLA	C1A-C2A-CAA-CBA
11	bA	802	CLA	C1A-C2A-CAA-CBA
11	bA	812	CLA	C1A-C2A-CAA-CBA
11	bA	813	CLA	C1A-C2A-CAA-CBA
11	bA	843	CLA	C1A-C2A-CAA-CBA
11	bB	815	CLA	C1A-C2A-CAA-CBA
11	bB	816	CLA	C1A-C2A-CAA-CBA
11	bB	833	CLA	C1A-C2A-CAA-CBA
11	bB	834	CLA	C1A-C2A-CAA-CBA
11	cA	802	CLA	C1A-C2A-CAA-CBA
11	cA	812	CLA	C1A-C2A-CAA-CBA
11	cA	813	CLA	C1A-C2A-CAA-CBA
11	cA	843	CLA	C1A-C2A-CAA-CBA
11	cB	815	CLA	C1A-C2A-CAA-CBA
11	cB	816	CLA	C1A-C2A-CAA-CBA
11	cB	834	CLA	C1A-C2A-CAA-CBA
11	aA	820	CLA	C11-C12-C13-C15
11	aA	822	CLA	C6-C7-C8-C10
11	aL	205	CLA	C12-C13-C15-C16
11	bA	820	CLA	C11-C12-C13-C15
11	bA	822	CLA	C6-C7-C8-C10
11	bA	828	CLA	C2-C3-C5-C6
11	bL	205	CLA	C12-C13-C15-C16
11	cA	820	CLA	C11-C12-C13-C15
11	cA	822	CLA	C6-C7-C8-C10
11	cA	828	CLA	C2-C3-C5-C6
11	cL	205	CLA	C12-C13-C15-C16
11	aA	802	CLA	C3-C5-C6-C7
11	bA	802	CLA	C3-C5-C6-C7
11	cA	802	CLA	C3-C5-C6-C7
11	aB	810	CLA	CAA-CBA-CGA-O2A
11	aB	832	CLA	CAA-CBA-CGA-O2A
11	aB	834	CLA	CAA-CBA-CGA-O2A
11	bB	810	CLA	CAA-CBA-CGA-O2A
11	bB	832	CLA	CAA-CBA-CGA-O2A
11	cB	810	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
11	cB	832	CLA	CAA-CBA-CGA-O2A
11	aB	808	CLA	C8-C10-C11-C12
11	bB	808	CLA	C8-C10-C11-C12
11	cA	831	CLA	C10-C11-C12-C13
11	aB	815	CLA	C5-C6-C7-C8
11	bA	831	CLA	C10-C11-C12-C13
11	cB	808	CLA	C8-C10-C11-C12
11	cB	815	CLA	C5-C6-C7-C8
12	aB	824	F6C	C2-C3-C5-C6
12	bB	824	F6C	C2-C3-C5-C6
12	cB	824	F6C	C2-C3-C5-C6
11	aA	828	CLA	C2B-C3B-CAB-CBB
11	aA	842	CLA	C2B-C3B-CAB-CBB
11	aA	843	CLA	C2B-C3B-CAB-CBB
11	aB	814	CLA	C2B-C3B-CAB-CBB
11	aB	833	CLA	C2B-C3B-CAB-CBB
11	aB	836	CLA	C2B-C3B-CAB-CBB
11	bA	842	CLA	C2B-C3B-CAB-CBB
11	bA	843	CLA	C2B-C3B-CAB-CBB
11	bB	814	CLA	C2B-C3B-CAB-CBB
11	bB	833	CLA	C2B-C3B-CAB-CBB
11	bB	836	CLA	C2B-C3B-CAB-CBB
11	cA	828	CLA	C2B-C3B-CAB-CBB
11	cA	842	CLA	C2B-C3B-CAB-CBB
11	cA	843	CLA	C2B-C3B-CAB-CBB
11	cB	814	CLA	C2B-C3B-CAB-CBB
11	cB	817	CLA	C2B-C3B-CAB-CBB
11	cB	833	CLA	C2B-C3B-CAB-CBB
11	cB	836	CLA	C2B-C3B-CAB-CBB
11	bB	834	CLA	CAA-CBA-CGA-O2A
11	cB	834	CLA	CAA-CBA-CGA-O2A
11	aA	831	CLA	C10-C11-C12-C13
11	bB	815	CLA	C5-C6-C7-C8
11	bA	819	CLA	CBD-CGD-O2D-CED
15	aA	851	BCR	C11-C10-C9-C8
15	aA	851	BCR	C16-C17-C18-C19
15	aB	844	BCR	C11-C10-C9-C8
15	aB	844	BCR	C20-C21-C22-C23
15	aB	846	BCR	C12-C13-C14-C15
15	bA	851	BCR	C11-C10-C9-C8
15	bA	851	BCR	C16-C17-C18-C19
15	bB	844	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
15	bB	844	BCR	C20-C21-C22-C23
15	bB	846	BCR	C12-C13-C14-C15
15	cA	851	BCR	C11-C10-C9-C8
15	cA	851	BCR	C16-C17-C18-C19
15	cB	844	BCR	C11-C10-C9-C8
15	cB	844	BCR	C20-C21-C22-C23
15	cB	846	BCR	C12-C13-C14-C15
18	cB	847	LMG	C2-C1-O1-C7
11	bA	836	CLA	CAA-CBA-CGA-O2A
11	cA	819	CLA	CBD-CGD-O2D-CED
11	aA	804	CLA	C2A-CAA-CBA-CGA
11	bA	804	CLA	C2A-CAA-CBA-CGA
11	cA	804	CLA	C2A-CAA-CBA-CGA
11	aB	835	CLA	CAA-CBA-CGA-O1A
11	bB	835	CLA	CAA-CBA-CGA-O1A
11	cB	835	CLA	CAA-CBA-CGA-O1A
11	aA	836	CLA	CAA-CBA-CGA-O2A
11	aA	840	CLA	C4-C3-C5-C6
11	aB	812	CLA	C4-C3-C5-C6
11	bA	840	CLA	C4-C3-C5-C6
11	bB	812	CLA	C4-C3-C5-C6
11	cA	840	CLA	C4-C3-C5-C6
11	cB	812	CLA	C4-C3-C5-C6
11	aA	812	CLA	C2-C1-O2A-CGA
11	aB	813	CLA	C2-C1-O2A-CGA
11	bA	812	CLA	C2-C1-O2A-CGA
11	bB	813	CLA	C2-C1-O2A-CGA
11	cA	812	CLA	C2-C1-O2A-CGA
11	cB	813	CLA	C2-C1-O2A-CGA
11	aB	808	CLA	C2-C3-C5-C6
11	aB	813	CLA	C2-C3-C5-C6
11	bB	808	CLA	C2-C3-C5-C6
11	bB	813	CLA	C2-C3-C5-C6
11	cB	808	CLA	C2-C3-C5-C6
11	cB	813	CLA	C2-C3-C5-C6
11	aL	205	CLA	C13-C15-C16-C17
11	bL	205	CLA	C13-C15-C16-C17
11	cL	205	CLA	C13-C15-C16-C17
11	cA	836	CLA	CAA-CBA-CGA-O2A
12	aL	202	F6C	C6-C7-C8-C9
12	bL	202	F6C	C6-C7-C8-C9
12	cL	202	F6C	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
11	aA	819	CLA	CBD-CGD-O2D-CED
11	aB	810	CLA	CAA-CBA-CGA-O1A
11	aB	826	CLA	CAA-CBA-CGA-O2A
11	bB	826	CLA	CAA-CBA-CGA-O2A
11	cB	826	CLA	CAA-CBA-CGA-O2A
11	aA	829	CLA	C16-C17-C18-C19
11	bA	829	CLA	C16-C17-C18-C19
11	cA	829	CLA	C16-C17-C18-C19
11	bB	810	CLA	CAA-CBA-CGA-O1A
11	aB	813	CLA	O1A-CGA-O2A-C1
11	bB	813	CLA	O1A-CGA-O2A-C1
11	cB	813	CLA	O1A-CGA-O2A-C1
15	aB	843	BCR	C23-C24-C25-C30
15	aB	844	BCR	C23-C24-C25-C30
15	bB	844	BCR	C23-C24-C25-C30
15	cB	843	BCR	C23-C24-C25-C30
15	cB	844	BCR	C23-C24-C25-C30
11	aA	819	CLA	CAA-CBA-CGA-O2A
11	bA	819	CLA	CAA-CBA-CGA-O2A
11	cA	819	CLA	CAA-CBA-CGA-O2A
11	bB	804	CLA	O1D-CGD-O2D-CED
11	aB	835	CLA	CAA-CBA-CGA-O2A
11	bB	835	CLA	CAA-CBA-CGA-O2A
11	cB	810	CLA	CAA-CBA-CGA-O1A
11	cB	835	CLA	CAA-CBA-CGA-O2A
15	aB	848	BCR	C17-C18-C19-C20
15	bB	848	BCR	C17-C18-C19-C20
15	cB	848	BCR	C17-C18-C19-C20
11	aA	820	CLA	C2-C3-C5-C6
11	bA	820	CLA	C2-C3-C5-C6
11	cA	820	CLA	C2-C3-C5-C6
11	aA	836	CLA	CAA-CBA-CGA-O1A
11	bA	836	CLA	CAA-CBA-CGA-O1A
11	cA	836	CLA	CAA-CBA-CGA-O1A
15	aL	203	BCR	C14-C15-C16-C17
15	bL	203	BCR	C14-C15-C16-C17
15	cL	203	BCR	C14-C15-C16-C17
11	aB	804	CLA	O1D-CGD-O2D-CED
11	cB	804	CLA	O1D-CGD-O2D-CED
11	aA	842	CLA	CAA-CBA-CGA-O2A
11	bA	842	CLA	CAA-CBA-CGA-O2A
11	cA	842	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
11	aA	809	CLA	C4B-C3B-CAB-CBB
11	aB	804	CLA	C4B-C3B-CAB-CBB
11	aB	808	CLA	C4B-C3B-CAB-CBB
11	bA	809	CLA	C4B-C3B-CAB-CBB
11	bB	804	CLA	C4B-C3B-CAB-CBB
11	bB	808	CLA	C4B-C3B-CAB-CBB
11	cA	809	CLA	C4B-C3B-CAB-CBB
11	cB	804	CLA	C4B-C3B-CAB-CBB
11	cB	808	CLA	C4B-C3B-CAB-CBB
10	bA	801	CL0	C16-C17-C18-C20
10	cA	801	CL0	C16-C17-C18-C20
11	aB	806	CLA	C12-C13-C15-C16
11	aB	812	CLA	C2-C3-C5-C6
11	bB	806	CLA	C12-C13-C15-C16
11	bB	812	CLA	C2-C3-C5-C6
11	cB	806	CLA	C12-C13-C15-C16
11	cB	812	CLA	C2-C3-C5-C6
12	aA	844	F6C	C11-C10-C8-C7
12	bA	844	F6C	C11-C10-C8-C7
12	cA	844	F6C	C11-C10-C8-C7
12	aA	826	F6C	C3-C5-C6-C7
12	bA	826	F6C	C3-C5-C6-C7
12	cA	826	F6C	C3-C5-C6-C7
10	aA	801	CL0	C16-C17-C18-C20
11	aA	807	CLA	C15-C16-C17-C18
11	bA	807	CLA	C15-C16-C17-C18
11	cA	807	CLA	C15-C16-C17-C18
11	aB	819	CLA	O1A-CGA-O2A-C1
11	bB	819	CLA	O1A-CGA-O2A-C1
11	cB	819	CLA	O1A-CGA-O2A-C1
11	aB	813	CLA	C2A-CAA-CBA-CGA
11	aB	823	CLA	C2A-CAA-CBA-CGA
11	bB	813	CLA	C2A-CAA-CBA-CGA
11	bB	823	CLA	C2A-CAA-CBA-CGA
11	cB	813	CLA	C2A-CAA-CBA-CGA
11	aB	817	CLA	O1D-CGD-O2D-CED
11	aB	825	CLA	C15-C16-C17-C18
11	bB	825	CLA	C15-C16-C17-C18
11	cB	825	CLA	C15-C16-C17-C18
15	aA	847	BCR	C16-C17-C18-C36
15	aA	850	BCR	C16-C17-C18-C36
15	aA	851	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
15	aB	842	BCR	C20-C21-C22-C37
15	aB	844	BCR	C11-C10-C9-C34
15	aL	203	BCR	C20-C21-C22-C37
15	aL	208	BCR	C35-C13-C14-C15
15	bA	847	BCR	C16-C17-C18-C36
15	bA	850	BCR	C16-C17-C18-C36
15	bA	851	BCR	C16-C17-C18-C36
15	bB	842	BCR	C20-C21-C22-C37
15	bB	844	BCR	C11-C10-C9-C34
15	bL	203	BCR	C20-C21-C22-C37
15	bL	208	BCR	C35-C13-C14-C15
15	cA	847	BCR	C16-C17-C18-C36
15	cA	850	BCR	C16-C17-C18-C36
15	cA	851	BCR	C16-C17-C18-C36
15	cB	842	BCR	C20-C21-C22-C37
15	cB	844	BCR	C11-C10-C9-C34
15	cL	203	BCR	C20-C21-C22-C37
15	cL	208	BCR	C35-C13-C14-C15
11	aB	839	CLA	C4-C3-C5-C6
11	bB	839	CLA	C4-C3-C5-C6
11	cB	839	CLA	C4-C3-C5-C6
12	aA	832	F6C	C2A-CAA-CBA-CGA
12	bA	832	F6C	C2A-CAA-CBA-CGA
12	cA	832	F6C	C2A-CAA-CBA-CGA
11	aA	821	CLA	C11-C10-C8-C9
11	aB	817	CLA	C6-C7-C8-C9
11	aL	205	CLA	C14-C13-C15-C16
11	bA	821	CLA	C11-C10-C8-C9
11	bB	817	CLA	C6-C7-C8-C9
11	bL	205	CLA	C14-C13-C15-C16
11	cA	821	CLA	C11-C10-C8-C9
11	cB	817	CLA	C6-C7-C8-C9
11	cL	205	CLA	C14-C13-C15-C16
12	aA	826	F6C	C11-C10-C8-C9
12	aL	202	F6C	C11-C10-C8-C9
12	bA	826	F6C	C11-C10-C8-C9
12	bL	202	F6C	C11-C10-C8-C9
12	cA	826	F6C	C11-C10-C8-C9
12	cL	202	F6C	C11-C10-C8-C9
11	bB	817	CLA	O1D-CGD-O2D-CED
11	cB	817	CLA	O1D-CGD-O2D-CED
11	aA	842	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
11	bA	842	CLA	CAA-CBA-CGA-O1A
11	cA	842	CLA	CAA-CBA-CGA-O1A
11	aB	809	CLA	C3A-C2A-CAA-CBA
11	aB	834	CLA	C3A-C2A-CAA-CBA
11	bB	809	CLA	C3A-C2A-CAA-CBA
11	bB	834	CLA	C3A-C2A-CAA-CBA
11	cB	809	CLA	C3A-C2A-CAA-CBA
11	cB	834	CLA	C3A-C2A-CAA-CBA
11	aA	804	CLA	CAA-CBA-CGA-O2A
11	bA	804	CLA	CAA-CBA-CGA-O2A
11	cA	804	CLA	CAA-CBA-CGA-O2A
11	aA	814	CLA	CAD-CBD-CGD-O2D
11	aA	815	CLA	CAD-CBD-CGD-O2D
11	aA	820	CLA	CAD-CBD-CGD-O2D
11	aA	821	CLA	CAD-CBD-CGD-O2D
11	aA	838	CLA	CAD-CBD-CGD-O2D
11	aB	812	CLA	CAD-CBD-CGD-O2D
11	aB	828	CLA	CAD-CBD-CGD-O2D
11	aB	832	CLA	CAD-CBD-CGD-O2D
11	aB	836	CLA	CAD-CBD-CGD-O2D
11	bA	814	CLA	CAD-CBD-CGD-O2D
11	bA	815	CLA	CAD-CBD-CGD-O2D
11	bA	820	CLA	CAD-CBD-CGD-O2D
11	bA	821	CLA	CAD-CBD-CGD-O2D
11	bA	838	CLA	CAD-CBD-CGD-O2D
11	bB	812	CLA	CAD-CBD-CGD-O2D
11	bB	828	CLA	CAD-CBD-CGD-O2D
11	bB	832	CLA	CAD-CBD-CGD-O2D
11	bB	836	CLA	CAD-CBD-CGD-O2D
11	cA	814	CLA	CAD-CBD-CGD-O2D
11	cA	815	CLA	CAD-CBD-CGD-O2D
11	cA	820	CLA	CAD-CBD-CGD-O2D
11	cA	821	CLA	CAD-CBD-CGD-O2D
11	cA	838	CLA	CAD-CBD-CGD-O2D
11	cB	812	CLA	CAD-CBD-CGD-O2D
11	cB	828	CLA	CAD-CBD-CGD-O2D
11	cB	832	CLA	CAD-CBD-CGD-O2D
11	cB	836	CLA	CAD-CBD-CGD-O2D
12	aA	827	F6C	CAD-CBD-CGD-O2D
12	aL	202	F6C	CAD-CBD-CGD-O2D
12	bA	827	F6C	CAD-CBD-CGD-O2D
12	bL	202	F6C	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
12	cA	827	F6C	CAD-CBD-CGD-O2D
12	cL	202	F6C	CAD-CBD-CGD-O2D
11	cB	823	CLA	C2A-CAA-CBA-CGA
11	cB	837	CLA	CAA-CBA-CGA-O2A
15	aI	101	BCR	C6-C7-C8-C9
15	aK	102	BCR	C22-C23-C24-C25
15	bI	101	BCR	C6-C7-C8-C9
15	cI	103	BCR	C6-C7-C8-C9
15	cK	102	BCR	C22-C23-C24-C25
11	aB	839	CLA	C2-C3-C5-C6
11	bB	839	CLA	C2-C3-C5-C6
11	cB	839	CLA	C2-C3-C5-C6
11	aB	837	CLA	CAA-CBA-CGA-O2A
11	bB	837	CLA	CAA-CBA-CGA-O2A
15	aA	848	BCR	C7-C8-C9-C10
15	aA	849	BCR	C7-C8-C9-C10
15	aB	844	BCR	C17-C18-C19-C20
15	aL	203	BCR	C7-C8-C9-C10
15	bA	848	BCR	C7-C8-C9-C10
15	bA	849	BCR	C7-C8-C9-C10
15	bB	844	BCR	C17-C18-C19-C20
15	bL	203	BCR	C7-C8-C9-C10
15	cA	848	BCR	C7-C8-C9-C10
15	cA	849	BCR	C7-C8-C9-C10
15	cB	844	BCR	C17-C18-C19-C20
15	cL	203	BCR	C7-C8-C9-C10
16	aA	852	LHG	C4-C5-C6-O8
16	bA	852	LHG	C4-C5-C6-O8
16	cA	852	LHG	C4-C5-C6-O8
11	aA	828	CLA	CAA-CBA-CGA-O2A
11	bA	828	CLA	CAA-CBA-CGA-O2A
11	cA	828	CLA	CAA-CBA-CGA-O2A
16	bA	852	LHG	O8-C23-C24-C25
11	aA	843	CLA	CAA-CBA-CGA-O1A
11	bA	843	CLA	CAA-CBA-CGA-O1A
11	cA	843	CLA	CAA-CBA-CGA-O1A
11	aB	822	CLA	CAA-CBA-CGA-O1A
11	bB	822	CLA	CAA-CBA-CGA-O1A
11	cB	822	CLA	CAA-CBA-CGA-O1A
11	aB	823	CLA	O2A-C1-C2-C3
11	bB	823	CLA	O2A-C1-C2-C3
11	cB	823	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
12	aA	827	F6C	C4B-C3B-CAB-CBB
12	aA	832	F6C	C4B-C3B-CAB-CBB
12	bA	827	F6C	C4B-C3B-CAB-CBB
12	bA	832	F6C	C4B-C3B-CAB-CBB
12	cA	827	F6C	C4B-C3B-CAB-CBB
12	cA	832	F6C	C4B-C3B-CAB-CBB
11	cB	819	CLA	CBA-CGA-O2A-C1
12	aA	844	F6C	CAA-CBA-CGA-O2A
12	bA	844	F6C	CAA-CBA-CGA-O2A
12	cA	844	F6C	CAA-CBA-CGA-O2A
16	aA	852	LHG	O8-C23-C24-C25
16	cA	852	LHG	O8-C23-C24-C25
11	aA	804	CLA	CAA-CBA-CGA-O1A
11	aB	822	CLA	CAA-CBA-CGA-O2A
11	bA	804	CLA	CAA-CBA-CGA-O1A
11	bB	822	CLA	CAA-CBA-CGA-O2A
11	cA	804	CLA	CAA-CBA-CGA-O1A
11	cB	822	CLA	CAA-CBA-CGA-O2A
11	aB	816	CLA	C10-C11-C12-C13
11	bB	816	CLA	C10-C11-C12-C13
11	cB	816	CLA	C10-C11-C12-C13
11	aA	804	CLA	CHA-CBD-CGD-O1D
11	aA	804	CLA	CHA-CBD-CGD-O2D
11	aA	811	CLA	CHA-CBD-CGD-O1D
11	aA	811	CLA	CHA-CBD-CGD-O2D
11	aA	825	CLA	CHA-CBD-CGD-O2D
11	aA	840	CLA	CHA-CBD-CGD-O2D
11	aB	804	CLA	CHA-CBD-CGD-O2D
11	aB	808	CLA	CHA-CBD-CGD-O1D
11	aB	808	CLA	CHA-CBD-CGD-O2D
11	aB	814	CLA	CHA-CBD-CGD-O2D
11	aB	820	CLA	CHA-CBD-CGD-O1D
11	aB	820	CLA	CHA-CBD-CGD-O2D
11	aB	826	CLA	CHA-CBD-CGD-O1D
11	aB	826	CLA	CHA-CBD-CGD-O2D
11	aB	836	CLA	CHA-CBD-CGD-O2D
11	bA	804	CLA	CHA-CBD-CGD-O1D
11	bA	804	CLA	CHA-CBD-CGD-O2D
11	bA	811	CLA	CHA-CBD-CGD-O1D
11	bA	811	CLA	CHA-CBD-CGD-O2D
11	bA	825	CLA	CHA-CBD-CGD-O2D
11	bA	840	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
11	bB	804	CLA	CHA-CBD-CGD-O2D
11	bB	808	CLA	CHA-CBD-CGD-O1D
11	bB	808	CLA	CHA-CBD-CGD-O2D
11	bB	814	CLA	CHA-CBD-CGD-O2D
11	bB	820	CLA	CHA-CBD-CGD-O1D
11	bB	820	CLA	CHA-CBD-CGD-O2D
11	bB	826	CLA	CHA-CBD-CGD-O1D
11	bB	826	CLA	CHA-CBD-CGD-O2D
11	bB	836	CLA	CHA-CBD-CGD-O2D
11	cA	804	CLA	CHA-CBD-CGD-O1D
11	cA	804	CLA	CHA-CBD-CGD-O2D
11	cA	811	CLA	CHA-CBD-CGD-O1D
11	cA	811	CLA	CHA-CBD-CGD-O2D
11	cA	825	CLA	CHA-CBD-CGD-O2D
11	cA	840	CLA	CHA-CBD-CGD-O2D
11	cB	804	CLA	CHA-CBD-CGD-O2D
11	cB	808	CLA	CHA-CBD-CGD-O1D
11	cB	814	CLA	CHA-CBD-CGD-O2D
11	cB	820	CLA	CHA-CBD-CGD-O1D
11	cB	820	CLA	CHA-CBD-CGD-O2D
11	cB	826	CLA	CHA-CBD-CGD-O1D
11	cB	826	CLA	CHA-CBD-CGD-O2D
11	cB	836	CLA	CHA-CBD-CGD-O2D
12	aA	826	F6C	CHA-CBD-CGD-O1D
12	aA	826	F6C	CHA-CBD-CGD-O2D
12	aA	832	F6C	CHA-CBD-CGD-O2D
12	bA	826	F6C	CHA-CBD-CGD-O1D
12	bA	826	F6C	CHA-CBD-CGD-O2D
12	bA	832	F6C	CHA-CBD-CGD-O2D
12	cA	826	F6C	CHA-CBD-CGD-O1D
12	cA	826	F6C	CHA-CBD-CGD-O2D
12	cA	832	F6C	CHA-CBD-CGD-O2D
15	aA	851	BCR	C13-C14-C15-C16
15	bA	851	BCR	C13-C14-C15-C16
15	cA	851	BCR	C13-C14-C15-C16
11	bA	821	CLA	CAA-CBA-CGA-O2A
11	cA	821	CLA	CAA-CBA-CGA-O2A
11	aB	819	CLA	CBA-CGA-O2A-C1
11	bB	819	CLA	CBA-CGA-O2A-C1
11	aA	821	CLA	CAA-CBA-CGA-O2A
11	bB	806	CLA	CAA-CBA-CGA-O2A
11	cA	825	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
18	aB	847	LMG	O7-C8-C9-O8
18	bB	847	LMG	O7-C8-C9-O8
18	cB	847	LMG	O7-C8-C9-O8
11	aA	825	CLA	CAA-CBA-CGA-O2A
11	bA	825	CLA	CAA-CBA-CGA-O2A
11	aA	803	CLA	C2A-CAA-CBA-CGA
11	cA	803	CLA	C2A-CAA-CBA-CGA
11	aA	838	CLA	CAA-CBA-CGA-O2A
11	aB	806	CLA	CAA-CBA-CGA-O2A
11	bA	838	CLA	CAA-CBA-CGA-O2A
11	cA	838	CLA	CAA-CBA-CGA-O2A
11	cB	806	CLA	CAA-CBA-CGA-O2A
18	cB	847	LMG	C31-C32-C33-C34
11	aL	205	CLA	C11-C10-C8-C7
11	bL	205	CLA	C11-C10-C8-C7
11	cL	205	CLA	C11-C10-C8-C7
12	aA	844	F6C	C3A-C2A-CAA-CBA
12	bA	844	F6C	C3A-C2A-CAA-CBA
12	cA	844	F6C	C3A-C2A-CAA-CBA
18	aB	847	LMG	C31-C32-C33-C34
18	bB	847	LMG	C31-C32-C33-C34
11	aA	806	CLA	C11-C12-C13-C14
11	aA	820	CLA	C11-C12-C13-C14
11	bA	806	CLA	C11-C12-C13-C14
11	cA	806	CLA	C11-C12-C13-C14
11	cA	820	CLA	C11-C12-C13-C14
11	aA	821	CLA	C2B-C3B-CAB-CBB
11	bA	821	CLA	C2B-C3B-CAB-CBB
11	bA	828	CLA	C2B-C3B-CAB-CBB
11	cA	821	CLA	C2B-C3B-CAB-CBB
11	aB	820	CLA	CAA-CBA-CGA-O2A
11	bB	820	CLA	CAA-CBA-CGA-O2A
11	cB	820	CLA	CAA-CBA-CGA-O2A
11	aA	834	CLA	O1A-CGA-O2A-C1
11	bA	834	CLA	O1A-CGA-O2A-C1
11	cA	834	CLA	O1A-CGA-O2A-C1
11	aA	818	CLA	C2A-CAA-CBA-CGA
11	aA	821	CLA	C2A-CAA-CBA-CGA
11	bA	803	CLA	C2A-CAA-CBA-CGA
11	bA	818	CLA	C2A-CAA-CBA-CGA
11	bA	821	CLA	C2A-CAA-CBA-CGA
11	cA	818	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
11	cA	821	CLA	C2A-CAA-CBA-CGA
11	aB	838	CLA	CAA-CBA-CGA-O2A
11	bB	838	CLA	CAA-CBA-CGA-O2A
11	cB	838	CLA	CAA-CBA-CGA-O2A
11	bB	818	CLA	C10-C11-C12-C13
12	aA	830	F6C	C16-C17-C18-C19
12	bA	830	F6C	C16-C17-C18-C19
12	cA	830	F6C	C16-C17-C18-C19
11	bB	828	CLA	C4-C3-C5-C6
16	aA	852	LHG	O1-C1-C2-C3
16	bA	852	LHG	O1-C1-C2-C3
16	cA	852	LHG	O1-C1-C2-C3
11	aB	821	CLA	CAA-CBA-CGA-O2A
11	bB	821	CLA	CAA-CBA-CGA-O2A
11	cB	821	CLA	CAA-CBA-CGA-O2A
11	aA	815	CLA	C1A-C2A-CAA-CBA
11	aA	829	CLA	C1A-C2A-CAA-CBA
11	aB	831	CLA	C1A-C2A-CAA-CBA
11	aB	833	CLA	C1A-C2A-CAA-CBA
11	aL	206	CLA	C1A-C2A-CAA-CBA
11	bA	815	CLA	C1A-C2A-CAA-CBA
11	bA	829	CLA	C1A-C2A-CAA-CBA
11	bB	831	CLA	C1A-C2A-CAA-CBA
11	bL	206	CLA	C1A-C2A-CAA-CBA
11	cA	815	CLA	C1A-C2A-CAA-CBA
11	cA	829	CLA	C1A-C2A-CAA-CBA
11	cB	831	CLA	C1A-C2A-CAA-CBA
11	cB	833	CLA	C1A-C2A-CAA-CBA
11	cL	206	CLA	C1A-C2A-CAA-CBA
11	bB	837	CLA	CAA-CBA-CGA-O1A
11	cB	837	CLA	CAA-CBA-CGA-O1A
11	cA	807	CLA	CAA-CBA-CGA-O2A
11	aB	837	CLA	CAA-CBA-CGA-O1A
11	aA	807	CLA	CAA-CBA-CGA-O2A
11	aL	204	CLA	CAA-CBA-CGA-O2A
11	bA	807	CLA	CAA-CBA-CGA-O2A
11	bL	204	CLA	CAA-CBA-CGA-O2A
11	cL	204	CLA	CAA-CBA-CGA-O2A
11	aB	818	CLA	C10-C11-C12-C13
11	cB	818	CLA	C10-C11-C12-C13
11	aB	812	CLA	C2A-CAA-CBA-CGA
11	bB	812	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
11	cB	812	CLA	C2A-CAA-CBA-CGA
11	aA	838	CLA	CBD-CGD-O2D-CED
11	bA	838	CLA	CBD-CGD-O2D-CED
11	cA	838	CLA	CBD-CGD-O2D-CED
11	aA	837	CLA	CAA-CBA-CGA-O1A
11	cA	837	CLA	CAA-CBA-CGA-O1A
11	aA	802	CLA	C4-C3-C5-C6
11	aB	828	CLA	C4-C3-C5-C6
11	bA	802	CLA	C4-C3-C5-C6
11	cA	802	CLA	C4-C3-C5-C6
11	cB	828	CLA	C4-C3-C5-C6
11	aB	817	CLA	CAA-CBA-CGA-O2A
11	cB	817	CLA	CAA-CBA-CGA-O2A
15	bK	102	BCR	C22-C23-C24-C25
11	bA	837	CLA	CAA-CBA-CGA-O1A
11	aA	821	CLA	C4B-C3B-CAB-CBB
11	aB	838	CLA	C4B-C3B-CAB-CBB
11	bA	821	CLA	C4B-C3B-CAB-CBB
11	bB	838	CLA	C4B-C3B-CAB-CBB
11	cA	821	CLA	C4B-C3B-CAB-CBB
11	cB	838	CLA	C4B-C3B-CAB-CBB
11	aA	825	CLA	CAA-CBA-CGA-O1A
11	bA	821	CLA	CAA-CBA-CGA-O1A
11	bA	825	CLA	CAA-CBA-CGA-O1A
11	cA	821	CLA	CAA-CBA-CGA-O1A
11	cA	825	CLA	CAA-CBA-CGA-O1A
12	aA	844	F6C	CAA-CBA-CGA-O1A
11	bB	817	CLA	CAA-CBA-CGA-O2A
11	cK	103	CLA	CAA-CBA-CGA-O2A
11	bA	823	CLA	CAA-CBA-CGA-O2A
15	aA	851	BCR	C1-C6-C7-C8
15	aA	851	BCR	C5-C6-C7-C8
15	bA	851	BCR	C1-C6-C7-C8
15	bA	851	BCR	C5-C6-C7-C8
15	cA	851	BCR	C1-C6-C7-C8
15	cA	851	BCR	C5-C6-C7-C8
11	aA	821	CLA	CAA-CBA-CGA-O1A
12	bA	844	F6C	CAA-CBA-CGA-O1A
12	cA	844	F6C	CAA-CBA-CGA-O1A
16	aA	852	LHG	O9-C7-C8-C9
16	bA	852	LHG	O9-C7-C8-C9
16	cA	852	LHG	O9-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
11	aK	103	CLA	CAA-CBA-CGA-O2A
11	bK	103	CLA	CAA-CBA-CGA-O2A
11	cA	823	CLA	CAA-CBA-CGA-O2A
15	aB	842	BCR	C18-C19-C20-C21
15	bB	842	BCR	C18-C19-C20-C21
15	cB	842	BCR	C18-C19-C20-C21
11	bA	814	CLA	O1A-CGA-O2A-C1
11	cA	814	CLA	O1A-CGA-O2A-C1
11	aA	823	CLA	CAA-CBA-CGA-O2A
11	aB	811	CLA	CAA-CBA-CGA-O2A
11	bB	811	CLA	CAA-CBA-CGA-O2A
11	cB	811	CLA	CAA-CBA-CGA-O2A
11	aB	837	CLA	C4-C3-C5-C6
11	bB	837	CLA	C4-C3-C5-C6
11	cB	837	CLA	C4-C3-C5-C6
12	bA	827	F6C	C2-C3-C5-C6
11	aB	813	CLA	C5-C6-C7-C8
11	cB	813	CLA	C5-C6-C7-C8
11	aA	823	CLA	CAA-CBA-CGA-O1A
11	aB	811	CLA	CAA-CBA-CGA-O1A
11	bA	823	CLA	CAA-CBA-CGA-O1A
11	cA	805	CLA	CAA-CBA-CGA-O2A
11	cA	823	CLA	CAA-CBA-CGA-O1A
11	aA	816	CLA	CAD-CBD-CGD-O1D
11	aA	840	CLA	CAD-CBD-CGD-O1D
11	aB	801	CLA	CAD-CBD-CGD-O1D
11	aB	829	CLA	CAD-CBD-CGD-O1D
11	aB	833	CLA	CAD-CBD-CGD-O1D
11	aB	834	CLA	CAD-CBD-CGD-O1D
11	bA	816	CLA	CAD-CBD-CGD-O1D
11	bA	840	CLA	CAD-CBD-CGD-O1D
11	bB	801	CLA	CAD-CBD-CGD-O1D
11	bB	829	CLA	CAD-CBD-CGD-O1D
11	bB	833	CLA	CAD-CBD-CGD-O1D
11	bB	834	CLA	CAD-CBD-CGD-O1D
11	cA	816	CLA	CAD-CBD-CGD-O1D
11	cA	840	CLA	CAD-CBD-CGD-O1D
11	cB	801	CLA	CAD-CBD-CGD-O1D
11	cB	829	CLA	CAD-CBD-CGD-O1D
11	cB	833	CLA	CAD-CBD-CGD-O1D
12	aA	830	F6C	CAD-CBD-CGD-O1D
12	bA	830	F6C	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
12	cA	830	F6C	CAD-CBD-CGD-O1D
11	aA	814	CLA	O1A-CGA-O2A-C1
11	aA	828	CLA	CAA-CBA-CGA-O1A
11	bA	828	CLA	CAA-CBA-CGA-O1A
11	cA	828	CLA	CAA-CBA-CGA-O1A
11	aA	824	CLA	CAA-CBA-CGA-O2A
11	bB	813	CLA	C5-C6-C7-C8
11	bA	820	CLA	C11-C12-C13-C14
13	aA	845	PQN	C19-C18-C20-C21
13	bA	845	PQN	C19-C18-C20-C21
13	cA	845	PQN	C19-C18-C20-C21
11	aA	805	CLA	CAA-CBA-CGA-O2A
11	bA	805	CLA	CAA-CBA-CGA-O2A
11	bA	824	CLA	CAA-CBA-CGA-O2A
11	cA	824	CLA	CAA-CBA-CGA-O2A
11	cA	814	CLA	C13-C15-C16-C17
13	cA	845	PQN	C18-C20-C21-C22
11	aB	820	CLA	CAA-CBA-CGA-O1A
11	bB	811	CLA	CAA-CBA-CGA-O1A
11	bB	820	CLA	CAA-CBA-CGA-O1A
11	cB	820	CLA	CAA-CBA-CGA-O1A
11	aA	803	CLA	CAA-CBA-CGA-O2A
11	bA	803	CLA	CAA-CBA-CGA-O2A
11	cA	803	CLA	CAA-CBA-CGA-O2A
11	aA	814	CLA	C13-C15-C16-C17
11	bA	814	CLA	C13-C15-C16-C17
13	aA	845	PQN	C18-C20-C21-C22
13	bA	845	PQN	C18-C20-C21-C22
11	cB	811	CLA	CAA-CBA-CGA-O1A
16	aA	852	LHG	C23-C24-C25-C26
16	cA	852	LHG	C23-C24-C25-C26
11	aL	204	CLA	CAA-CBA-CGA-O1A
11	bL	204	CLA	CAA-CBA-CGA-O1A
18	aB	847	LMG	C4-C5-C6-O5
11	aA	806	CLA	C11-C12-C13-C15
11	aA	822	CLA	C11-C12-C13-C15
11	aB	816	CLA	C6-C7-C8-C10
11	bA	806	CLA	C11-C12-C13-C15
11	bA	822	CLA	C11-C12-C13-C15
11	bB	816	CLA	C6-C7-C8-C10
11	cA	806	CLA	C11-C12-C13-C15
11	cA	822	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
11	cB	816	CLA	C6-C7-C8-C10
12	aA	827	F6C	C2-C3-C5-C6
12	cA	827	F6C	C2-C3-C5-C6
16	bA	852	LHG	C23-C24-C25-C26
11	aA	807	CLA	CAA-CBA-CGA-O1A
11	aB	821	CLA	CAA-CBA-CGA-O1A
11	bB	806	CLA	CAA-CBA-CGA-O1A
11	cA	807	CLA	CAA-CBA-CGA-O1A
11	cB	806	CLA	CAA-CBA-CGA-O1A
11	cL	204	CLA	CAA-CBA-CGA-O1A
11	aA	829	CLA	CAA-CBA-CGA-O2A
11	aA	840	CLA	CAA-CBA-CGA-O2A
11	aB	807	CLA	CAA-CBA-CGA-O2A
11	aB	809	CLA	CAA-CBA-CGA-O2A
11	bA	829	CLA	CAA-CBA-CGA-O2A
11	bA	840	CLA	CAA-CBA-CGA-O2A
11	bB	807	CLA	CAA-CBA-CGA-O2A
11	bB	809	CLA	CAA-CBA-CGA-O2A
11	cA	829	CLA	CAA-CBA-CGA-O2A
11	cA	840	CLA	CAA-CBA-CGA-O2A
11	cB	807	CLA	CAA-CBA-CGA-O2A
11	cB	809	CLA	CAA-CBA-CGA-O2A
18	bB	847	LMG	C4-C5-C6-O5
11	aA	817	CLA	O2A-C1-C2-C3
11	bA	817	CLA	O2A-C1-C2-C3
11	cA	817	CLA	O2A-C1-C2-C3
15	aL	208	BCR	C17-C18-C19-C20
15	bL	208	BCR	C17-C18-C19-C20
15	cL	208	BCR	C17-C18-C19-C20
11	aA	838	CLA	CAA-CBA-CGA-O1A
11	aB	806	CLA	CAA-CBA-CGA-O1A
11	bA	807	CLA	CAA-CBA-CGA-O1A
11	bA	838	CLA	CAA-CBA-CGA-O1A
11	bB	809	CLA	CAA-CBA-CGA-O1A
11	bB	821	CLA	CAA-CBA-CGA-O1A
11	cA	838	CLA	CAA-CBA-CGA-O1A
15	aA	851	BCR	C15-C16-C17-C18
15	bA	851	BCR	C15-C16-C17-C18
15	cA	851	BCR	C15-C16-C17-C18
11	aA	829	CLA	C16-C17-C18-C20
11	bA	829	CLA	C16-C17-C18-C20
11	cA	829	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
17	aA	853	LMT	C2-C1-O1'-C1'
17	bA	853	LMT	C2-C1-O1'-C1'
17	cA	853	LMT	C2-C1-O1'-C1'
11	aB	805	CLA	CAA-CBA-CGA-O2A
11	cB	805	CLA	CAA-CBA-CGA-O2A
11	aA	824	CLA	CAA-CBA-CGA-O1A
11	aB	809	CLA	CAA-CBA-CGA-O1A
11	bA	824	CLA	CAA-CBA-CGA-O1A
11	cA	824	CLA	CAA-CBA-CGA-O1A
11	cB	809	CLA	CAA-CBA-CGA-O1A
11	cB	821	CLA	CAA-CBA-CGA-O1A
16	aA	852	LHG	O10-C23-C24-C25
16	bA	852	LHG	O10-C23-C24-C25
16	cA	852	LHG	O10-C23-C24-C25
18	cB	847	LMG	C4-C5-C6-O5
11	aA	837	CLA	CAA-CBA-CGA-O2A
11	bA	837	CLA	CAA-CBA-CGA-O2A
11	cA	837	CLA	CAA-CBA-CGA-O2A
11	aB	816	CLA	CAA-CBA-CGA-O2A
11	bB	805	CLA	CAA-CBA-CGA-O2A
11	bB	816	CLA	CAA-CBA-CGA-O2A
11	cB	816	CLA	CAA-CBA-CGA-O2A
16	aA	852	LHG	O7-C7-C8-C9
16	bA	852	LHG	O7-C7-C8-C9
16	cA	852	LHG	O7-C7-C8-C9
11	aA	807	CLA	C8-C10-C11-C12
11	aB	818	CLA	C15-C16-C17-C18
11	bA	807	CLA	C8-C10-C11-C12
11	bB	818	CLA	C15-C16-C17-C18
11	cA	807	CLA	C8-C10-C11-C12
11	cB	818	CLA	C15-C16-C17-C18
11	aA	805	CLA	CAA-CBA-CGA-O1A
11	bA	805	CLA	CAA-CBA-CGA-O1A
11	cA	805	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

240 monomers are involved in 402 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	cA	834	CLA	1	0
11	cB	823	CLA	5	0
11	cA	835	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	bL	203	BCR	3	0
11	aB	823	CLA	6	0
17	aA	853	LMT	2	0
11	bB	817	CLA	1	0
11	bB	833	CLA	1	0
11	bB	808	CLA	4	0
11	cA	840	CLA	2	0
15	cB	848	BCR	3	0
11	aB	838	CLA	2	0
13	bB	841	PQN	2	0
11	cB	813	CLA	1	0
15	aB	848	BCR	2	0
16	cA	852	LHG	1	0
11	bA	813	CLA	1	0
11	cB	816	CLA	3	0
11	cB	839	CLA	1	0
11	bB	813	CLA	1	0
11	cA	813	CLA	2	0
11	cA	804	CLA	1	0
11	cL	205	CLA	3	0
11	bA	812	CLA	1	0
15	aI	101	BCR	2	0
11	cB	837	CLA	3	0
11	cA	803	CLA	2	0
11	cA	822	CLA	5	0
15	bL	207	BCR	2	0
11	cB	805	CLA	3	0
11	cA	809	CLA	2	0
11	cB	838	CLA	2	0
11	aA	840	CLA	3	0
11	bA	840	CLA	2	0
11	aA	821	CLA	2	0
11	aB	817	CLA	2	0
11	aA	831	CLA	1	0
15	bA	847	BCR	4	0
11	bA	838	CLA	2	0
11	cA	807	CLA	1	0
11	cA	838	CLA	2	0
15	bB	846	BCR	1	0
11	aB	802	CLA	4	0
11	aB	815	CLA	3	0
11	aL	206	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	cB	825	CLA	1	0
11	cA	814	CLA	3	0
11	cA	833	CLA	2	0
11	bA	829	CLA	4	0
11	bB	826	CLA	1	0
17	cA	853	LMT	2	0
11	cA	802	CLA	1	0
15	aB	845	BCR	2	0
15	aB	843	BCR	1	0
11	cB	834	CLA	1	0
11	cB	840	CLA	1	0
11	bA	804	CLA	1	0
15	bB	843	BCR	1	0
11	cB	804	CLA	4	0
11	cB	807	CLA	1	0
11	cA	828	CLA	1	0
11	bA	821	CLA	2	0
11	aA	818	CLA	2	0
11	aA	823	CLA	1	0
11	cA	806	CLA	5	0
11	aB	804	CLA	4	0
11	aA	822	CLA	4	0
11	cA	836	CLA	2	0
11	bA	803	CLA	1	0
11	cB	808	CLA	3	0
15	aB	842	BCR	1	0
11	bA	809	CLA	2	0
15	cL	203	BCR	2	0
11	aB	813	CLA	1	0
15	aA	848	BCR	3	0
11	cB	836	CLA	2	0
15	bB	848	BCR	2	0
11	cB	802	CLA	3	0
11	cB	815	CLA	2	0
11	cA	825	CLA	2	0
15	cB	845	BCR	2	0
11	cL	204	CLA	1	0
11	bA	823	CLA	2	0
11	aB	808	CLA	4	0
15	aL	207	BCR	2	0
11	bB	838	CLA	1	0
11	cB	803	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	aB	801	CLA	3	0
12	cB	824	F6C	1	0
11	aA	839	CLA	3	0
15	aB	846	BCR	2	0
13	cA	845	PQN	1	0
11	aB	812	CLA	3	0
11	aA	824	CLA	2	0
11	aA	820	CLA	3	0
11	aB	810	CLA	1	0
15	bK	102	BCR	2	0
15	cB	842	BCR	1	0
11	aB	832	CLA	1	0
11	aA	829	CLA	3	0
17	bA	853	LMT	2	0
11	aA	802	CLA	1	0
11	cA	818	CLA	2	0
18	bB	847	LMG	1	0
11	bB	819	CLA	1	0
11	bA	819	CLA	2	0
11	aB	807	CLA	1	0
11	cK	103	CLA	1	0
11	cA	821	CLA	2	0
11	cB	832	CLA	1	0
15	cB	846	BCR	2	0
15	cA	851	BCR	7	0
11	cB	812	CLA	5	0
11	bB	829	CLA	1	0
11	aB	837	CLA	2	0
11	bA	831	CLA	1	0
11	bB	804	CLA	3	0
13	cB	841	PQN	1	0
15	aL	208	BCR	3	0
11	bA	839	CLA	3	0
11	aB	827	CLA	3	0
11	aA	825	CLA	3	0
11	cB	828	CLA	3	0
11	aB	826	CLA	1	0
11	cA	820	CLA	4	0
12	aB	824	F6C	1	0
11	aA	833	CLA	2	0
11	bB	828	CLA	2	0
11	bB	836	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	bA	849	BCR	3	0
11	bB	815	CLA	1	0
11	cB	827	CLA	3	0
15	cL	207	BCR	2	0
11	cA	824	CLA	2	0
18	aB	847	LMG	1	0
15	aA	849	BCR	2	0
15	cA	850	BCR	1	0
11	bB	805	CLA	3	0
11	cA	812	CLA	1	0
11	bB	825	CLA	1	0
11	cB	801	CLA	2	0
11	aB	803	CLA	1	0
11	bA	818	CLA	2	0
15	bA	851	BCR	7	0
15	aL	203	BCR	2	0
11	cB	829	CLA	1	0
11	bL	206	CLA	3	0
11	bB	834	CLA	1	0
11	aA	806	CLA	4	0
11	bB	801	CLA	2	0
15	bB	845	BCR	1	0
15	bB	844	BCR	1	0
15	bA	848	BCR	3	0
11	aB	833	CLA	1	0
11	aA	803	CLA	3	0
11	bA	814	CLA	3	0
11	bA	843	CLA	2	0
11	cL	206	CLA	1	0
15	aA	851	BCR	7	0
11	cA	839	CLA	3	0
18	cB	847	LMG	1	0
11	aB	840	CLA	1	0
11	cB	818	CLA	1	0
11	bB	832	CLA	1	0
11	bA	833	CLA	3	0
11	bL	205	CLA	3	0
11	aB	818	CLA	1	0
11	aA	819	CLA	1	0
11	bL	204	CLA	2	0
11	aA	813	CLA	3	0
11	bA	820	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	cB	821	CLA	1	0
11	cB	810	CLA	1	0
15	bB	842	BCR	1	0
11	bB	810	CLA	1	0
11	aK	103	CLA	1	0
16	aA	852	LHG	1	0
11	cB	833	CLA	1	0
15	aA	850	BCR	1	0
15	bA	850	BCR	1	0
11	aL	205	CLA	3	0
11	bB	806	CLA	3	0
11	cB	817	CLA	1	0
11	bK	103	CLA	1	0
11	bB	802	CLA	4	0
13	aB	841	PQN	3	0
15	aB	844	BCR	1	0
15	aA	847	BCR	3	0
11	aA	838	CLA	2	0
11	aB	805	CLA	2	0
11	bB	812	CLA	3	0
16	bA	852	LHG	1	0
11	bB	823	CLA	4	0
11	cA	843	CLA	2	0
15	cA	847	BCR	2	0
11	aA	828	CLA	2	0
11	bA	828	CLA	1	0
15	cA	848	BCR	3	0
13	bA	845	PQN	1	0
11	bA	825	CLA	2	0
11	bB	837	CLA	2	0
15	aK	102	BCR	2	0
11	bA	806	CLA	5	0
11	cA	823	CLA	1	0
11	aB	806	CLA	3	0
11	bB	840	CLA	1	0
11	bB	807	CLA	1	0
15	bM	101	BCR	2	0
11	aB	836	CLA	2	0
15	cB	844	BCR	2	0
11	bB	816	CLA	4	0
11	bA	824	CLA	2	0
11	aA	809	CLA	2	0

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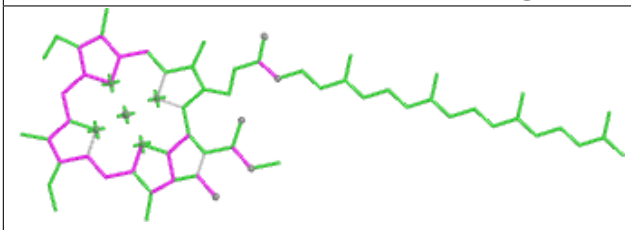
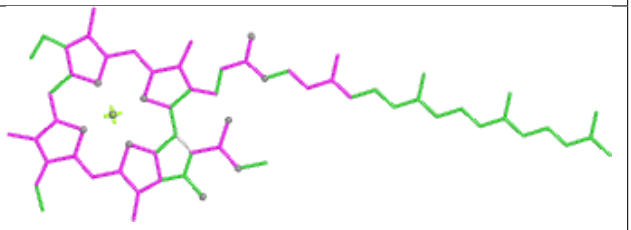
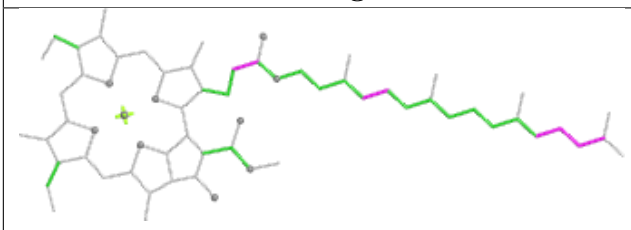
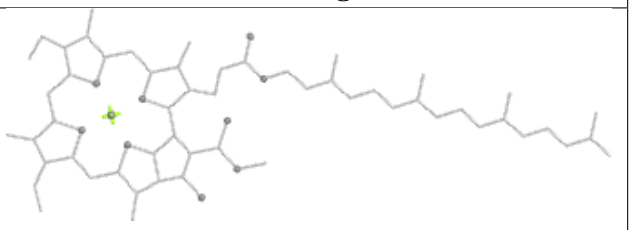
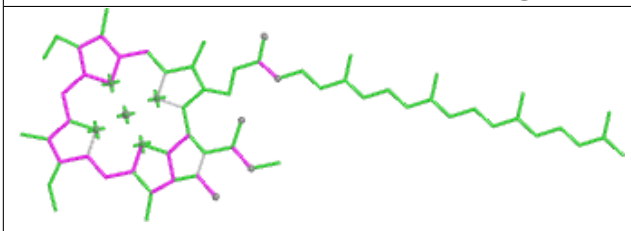
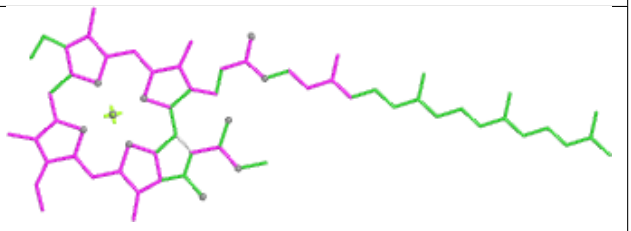
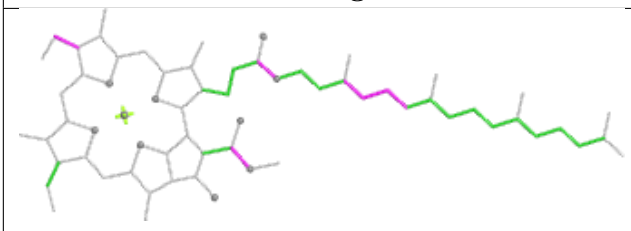
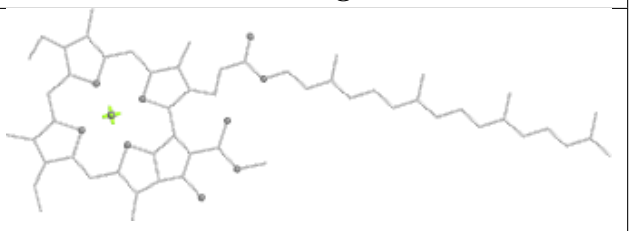
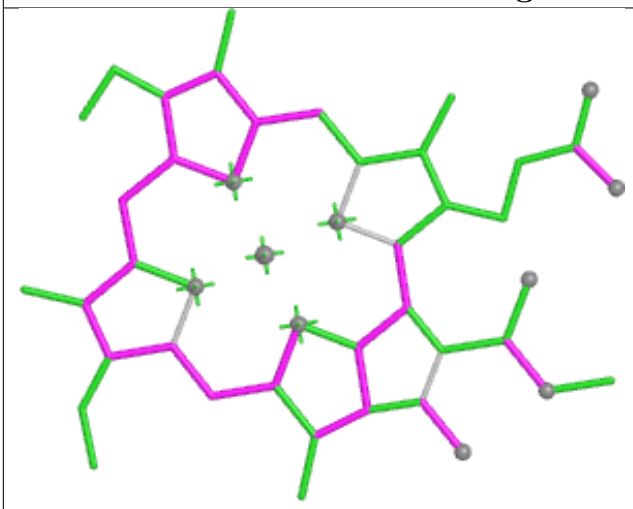
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	aL	204	CLA	1	0
11	cB	806	CLA	3	0
11	aB	828	CLA	2	0
11	cB	826	CLA	1	0
11	aB	834	CLA	1	0
11	bB	818	CLA	1	0
11	aA	804	CLA	1	0
11	aA	812	CLA	1	0
11	aA	814	CLA	3	0
11	bB	839	CLA	1	0
11	aA	843	CLA	2	0
11	bB	821	CLA	1	0
11	aB	825	CLA	1	0
15	bL	208	BCR	2	0
15	cA	849	BCR	2	0
11	bB	827	CLA	3	0
11	bA	836	CLA	2	0
11	aA	836	CLA	2	0
11	aB	839	CLA	1	0
15	cK	102	BCR	2	0
15	cL	208	BCR	5	0
11	cA	829	CLA	5	0
11	bA	810	CLA	1	0
11	bA	822	CLA	4	0
11	cA	819	CLA	3	0
11	cA	831	CLA	1	0
11	aB	816	CLA	4	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 then 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.

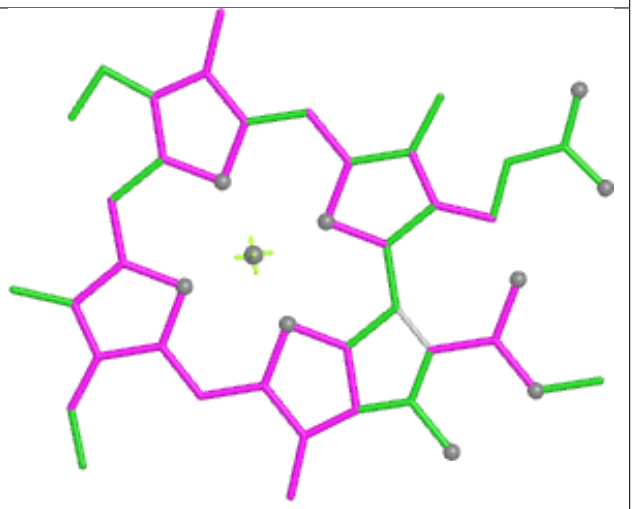
Ligand CL0 bA 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA cA 834	
 Bond lengths	 Bond angles
 Torsions	 Rings

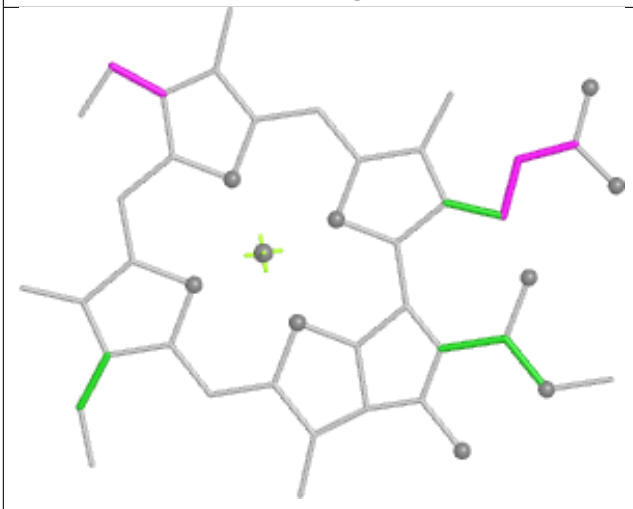
Ligand CLA aB 811



Bond lengths



Bond angles

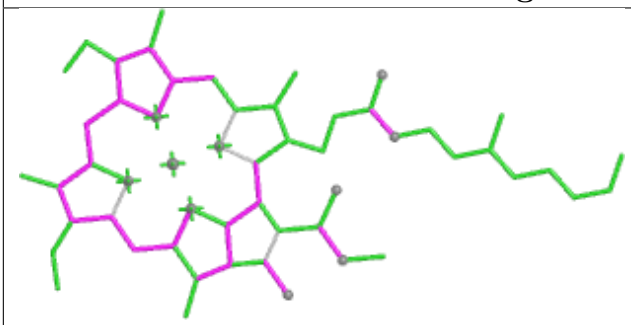


Torsions

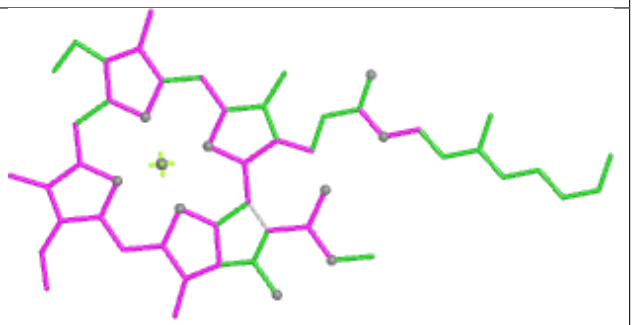


Rings

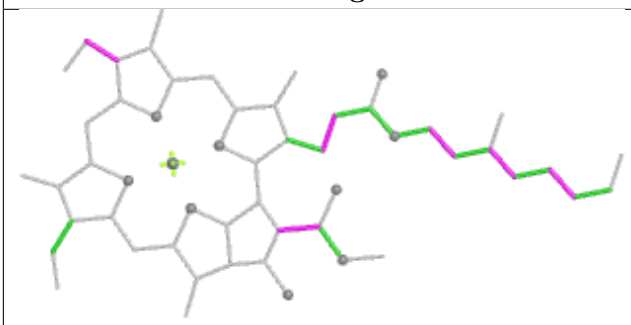
Ligand CLA cB 823



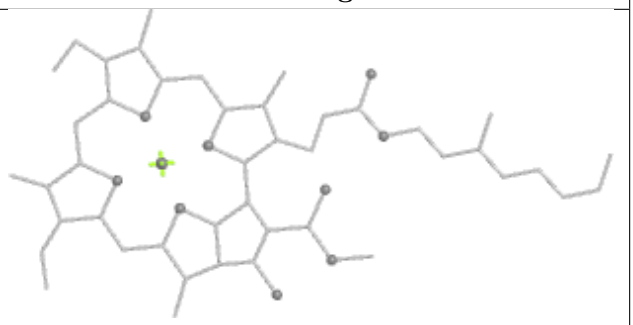
Bond lengths



Bond angles

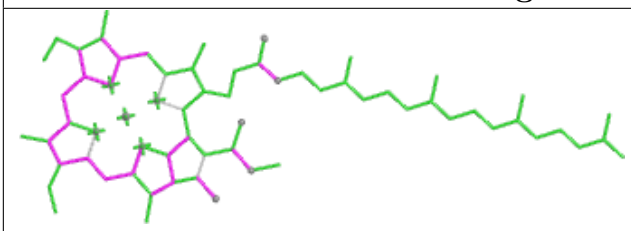


Torsions



Rings

Ligand CLA cA 835



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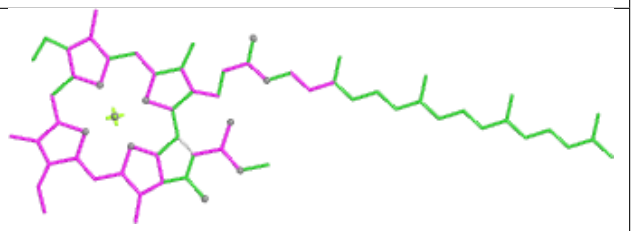
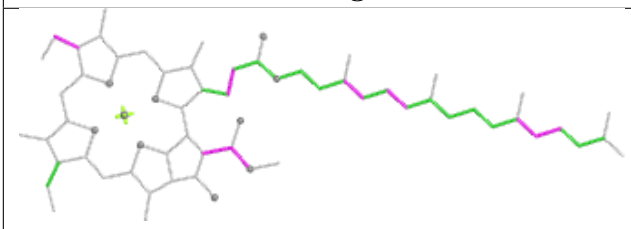


Bond angles



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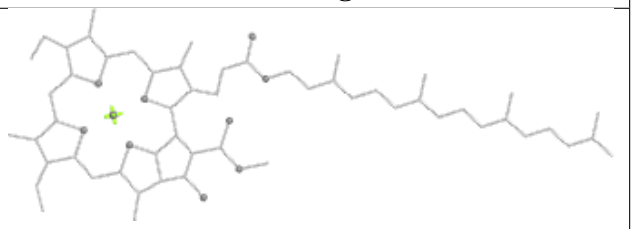
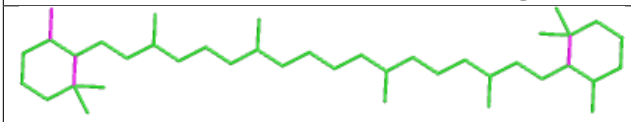


Rings

Ligand BCR bL 203



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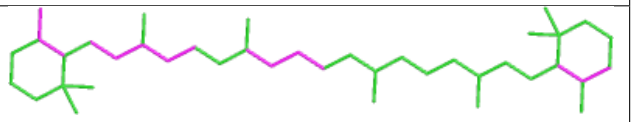
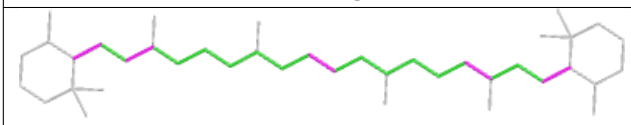
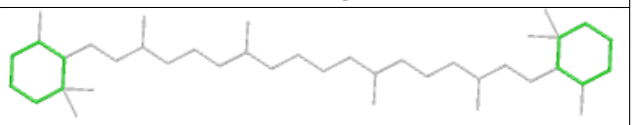


Bond angles

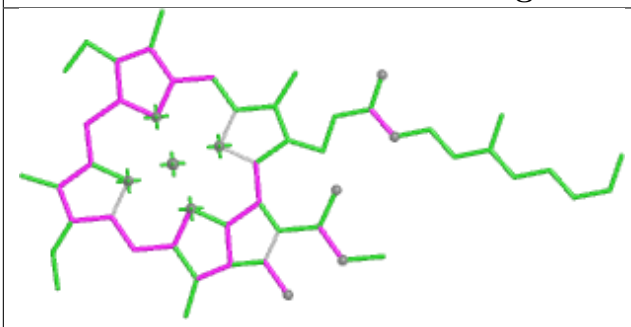


Torsions



Rings

Ligand CLA aB 823



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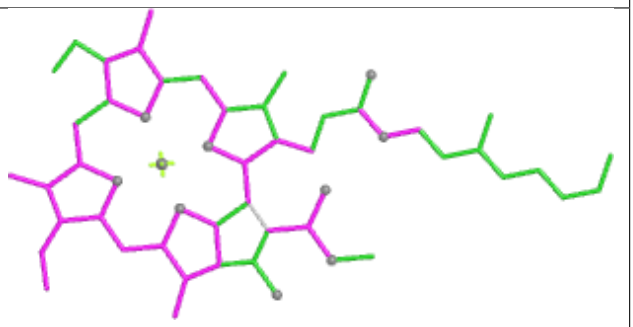
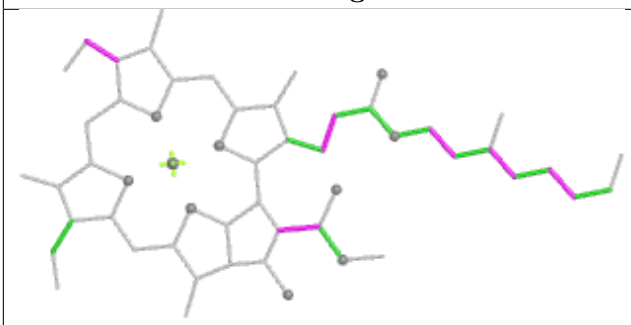
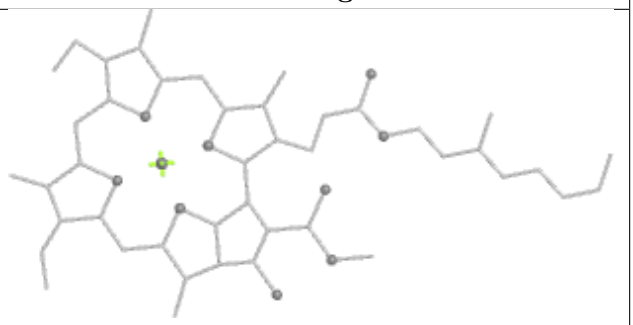


Bond angles

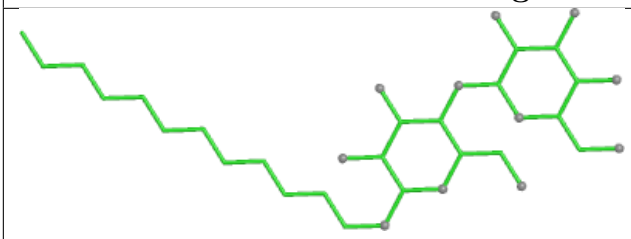


Torsions

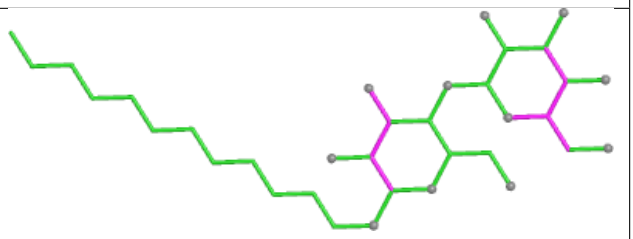


Rings

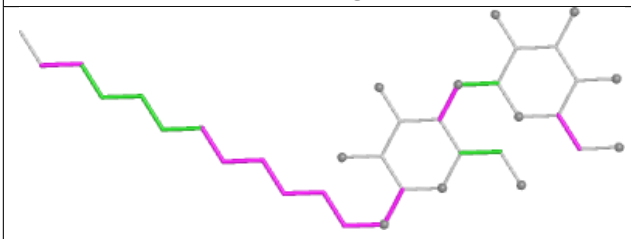
Ligand LMT aA 853



Bond lengths



Bond angles



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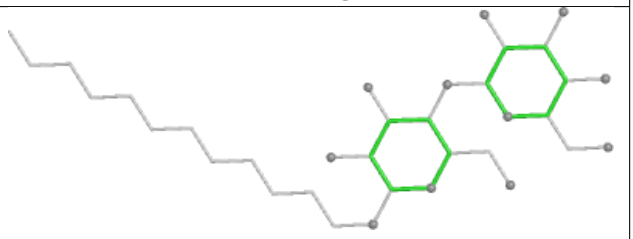
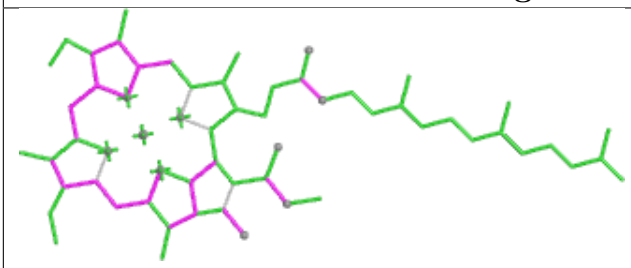


Rings

Ligand CLA bB 817



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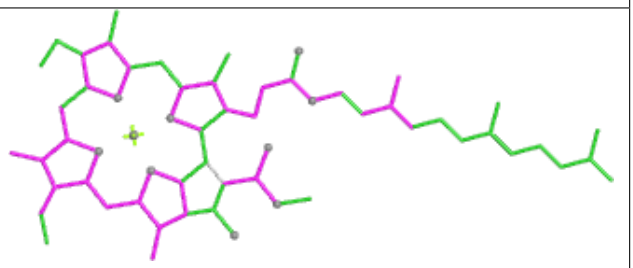
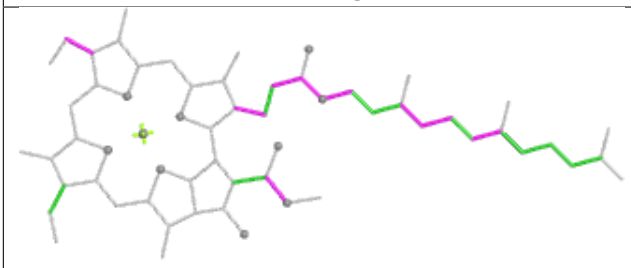


Bond angles



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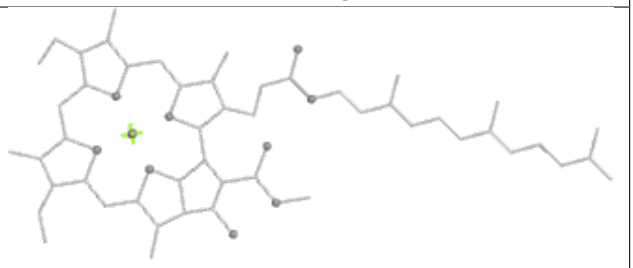
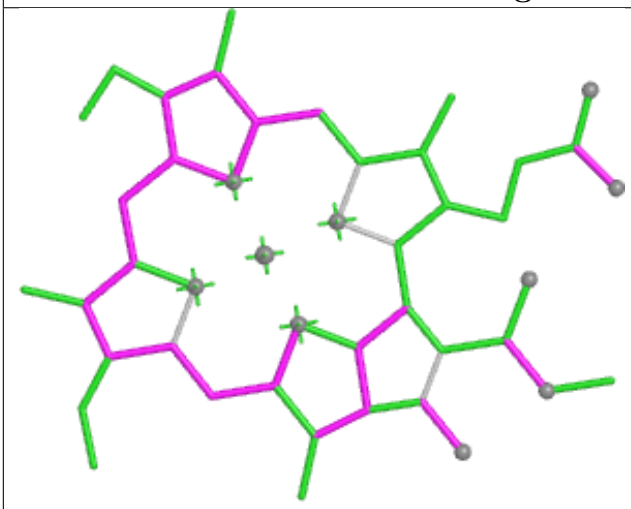


Rings

Ligand CLA bB 833



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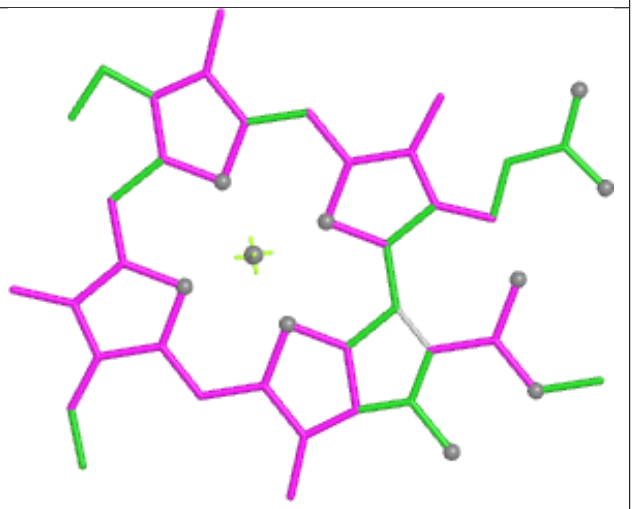
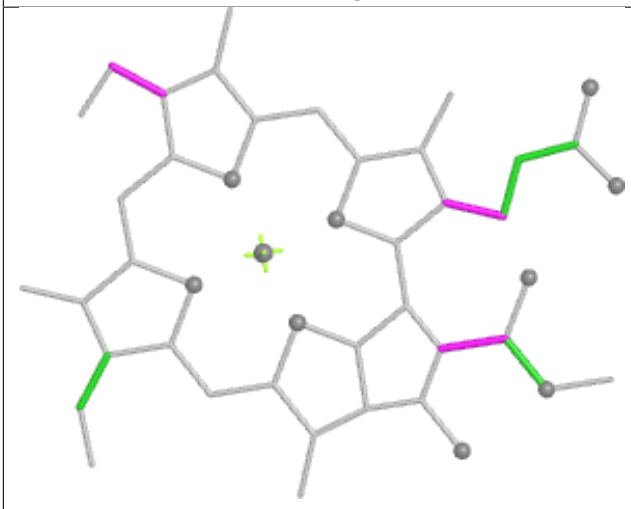


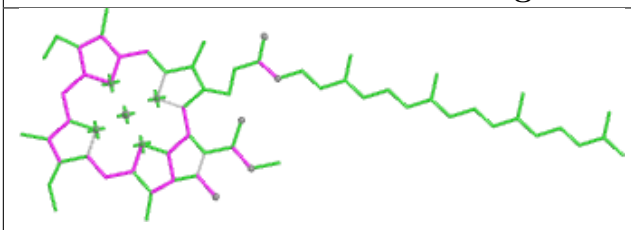
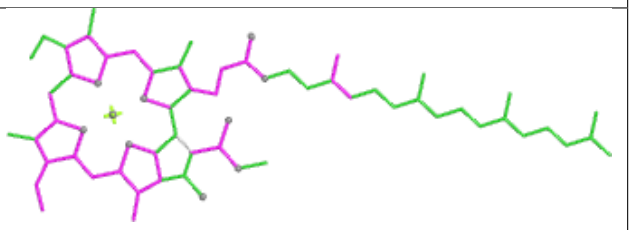
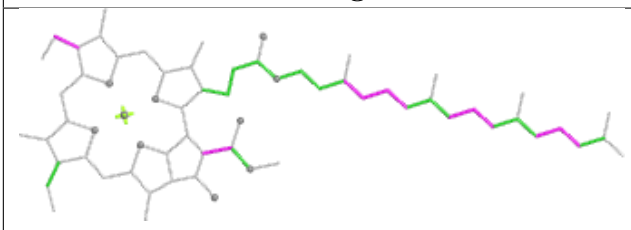
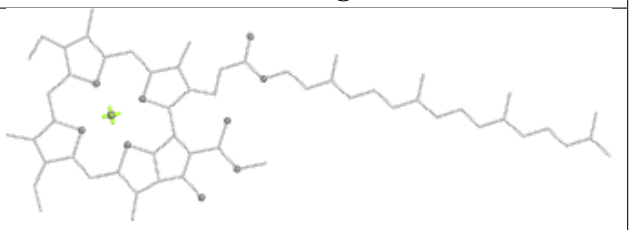
Bond angles

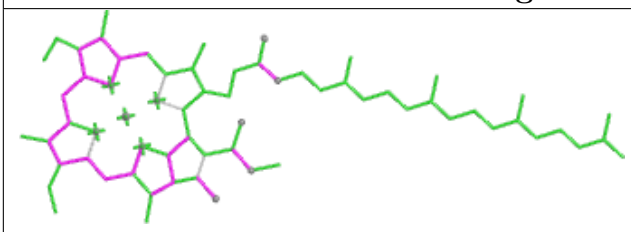
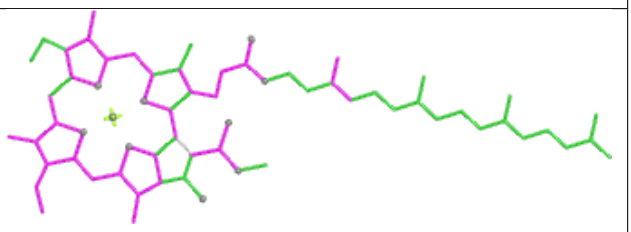
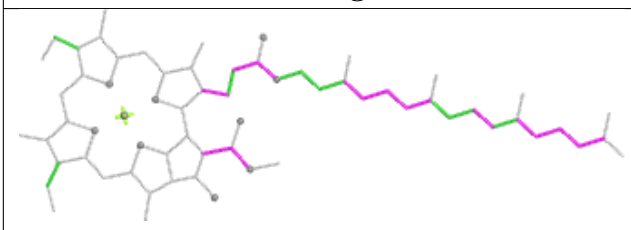
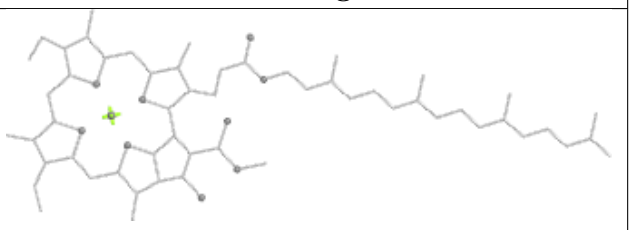


Torsions

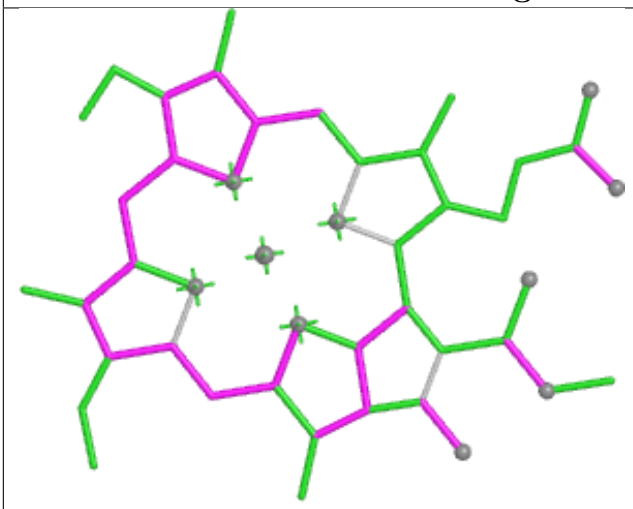


Rings

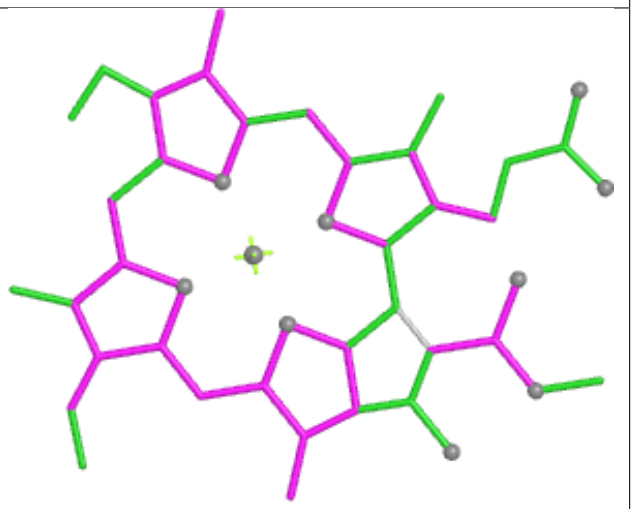
Ligand CLA bB 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA cA 840	
	
Bond lengths	Bond angles
	
Torsions	Rings

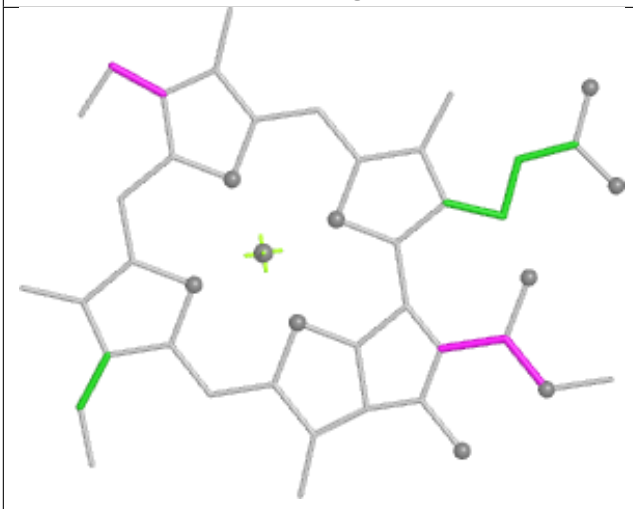
Ligand CLA bA 816



Bond lengths



Bond angles

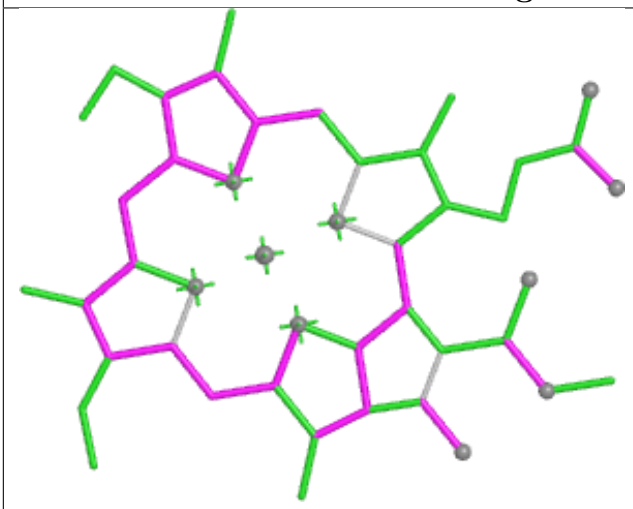


Torsions



Rings

Ligand CLA cA 842



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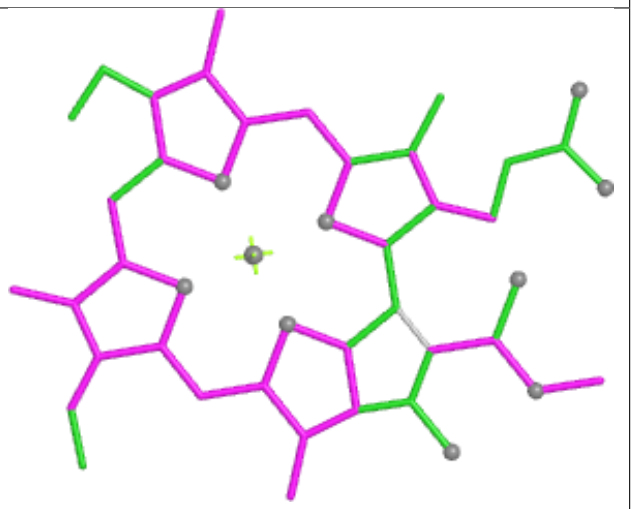
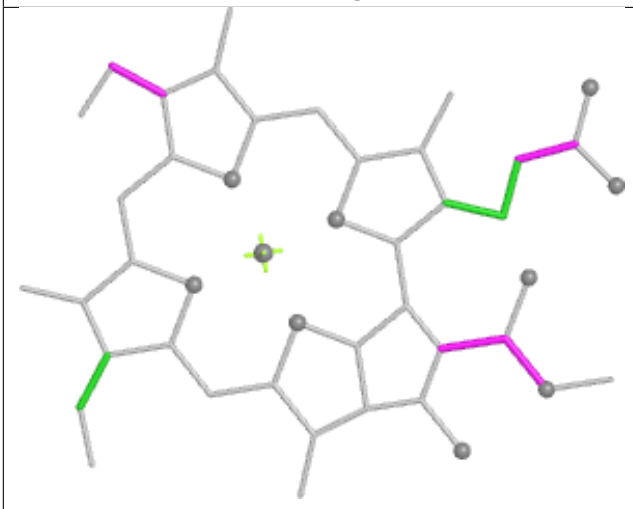


Bond angles

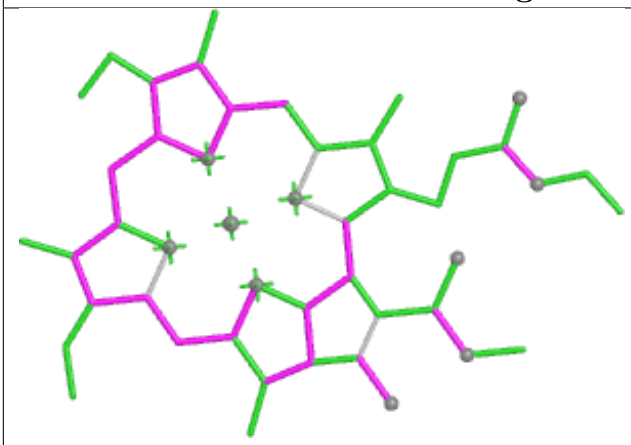


Torsions



Rings

Ligand CLA aB 819



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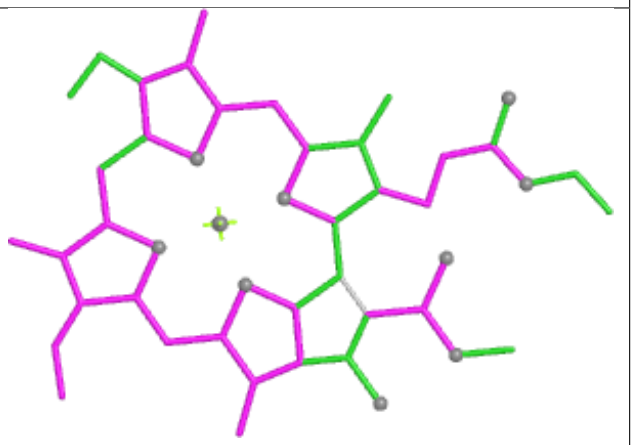
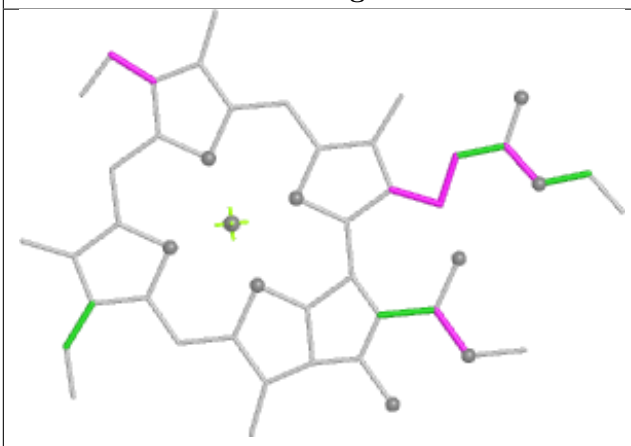
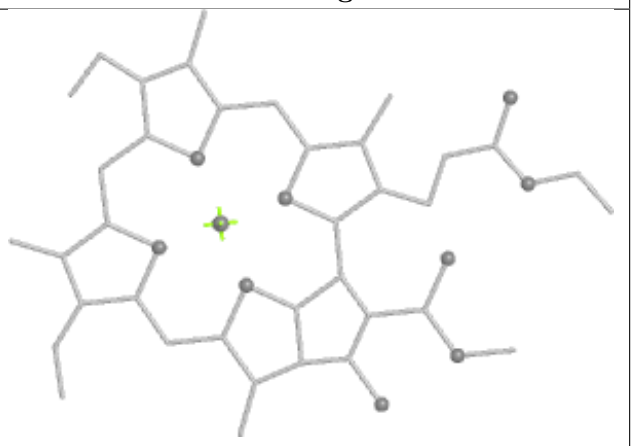


Bond angles



Torsions

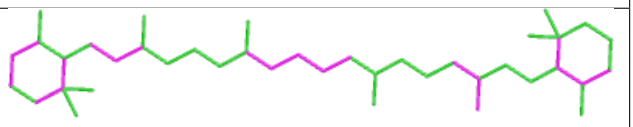


Rings

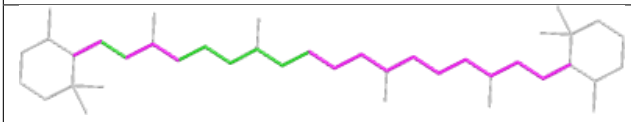
Ligand BCR cB 848



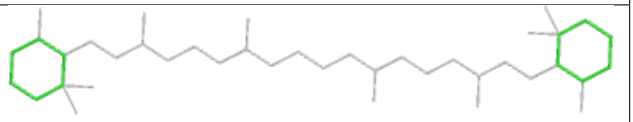
Bond lengths



Bond angles

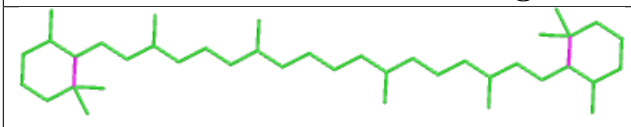


Torsions



Rings

Ligand BCR cB 843



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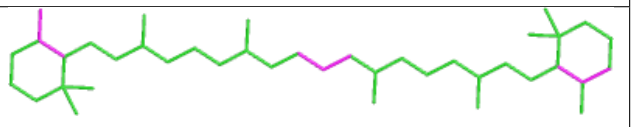
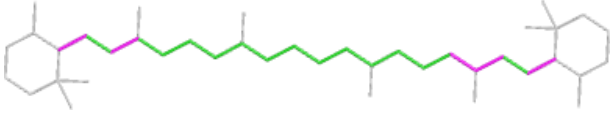


Bond angles



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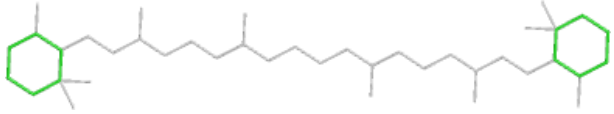
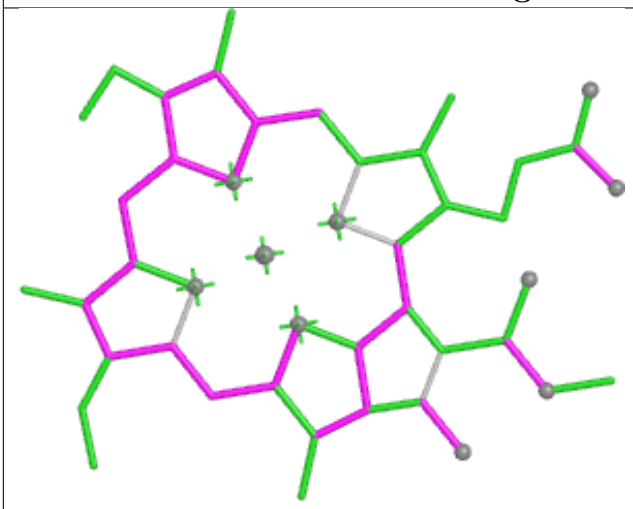


Rings

Ligand CLA bA 837



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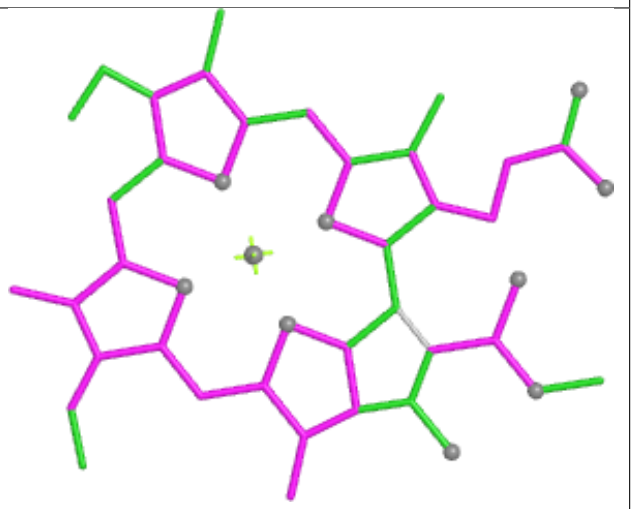
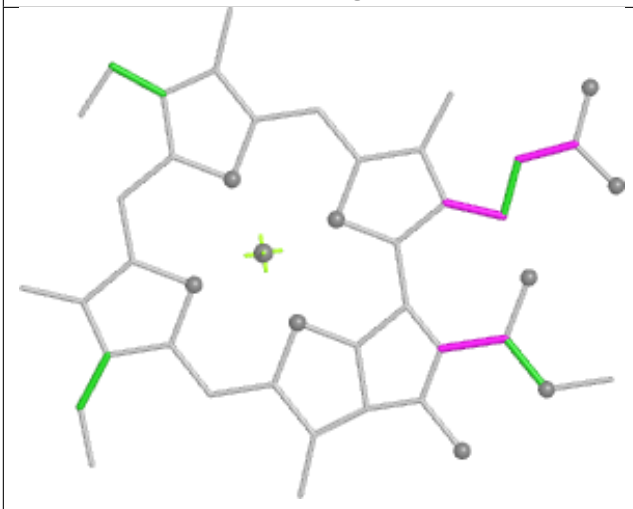


Bond angles

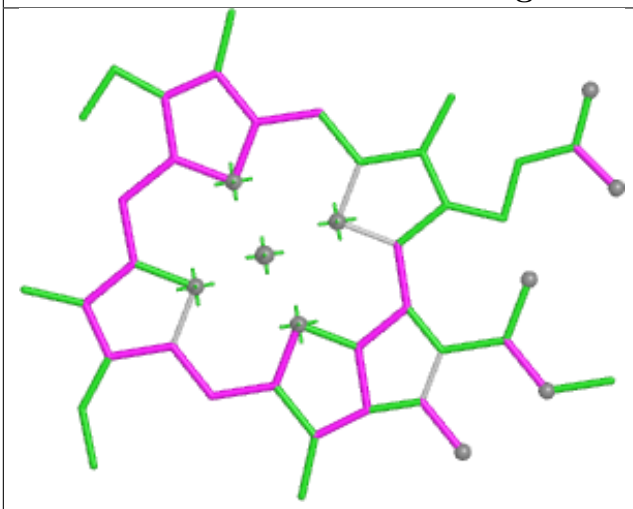


Torsions

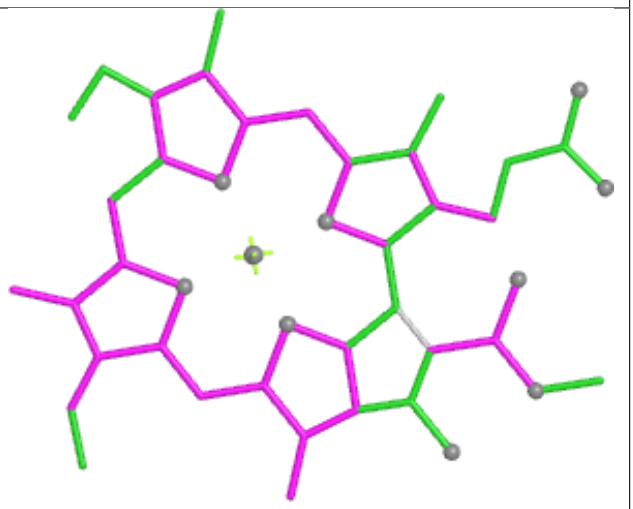


Rings

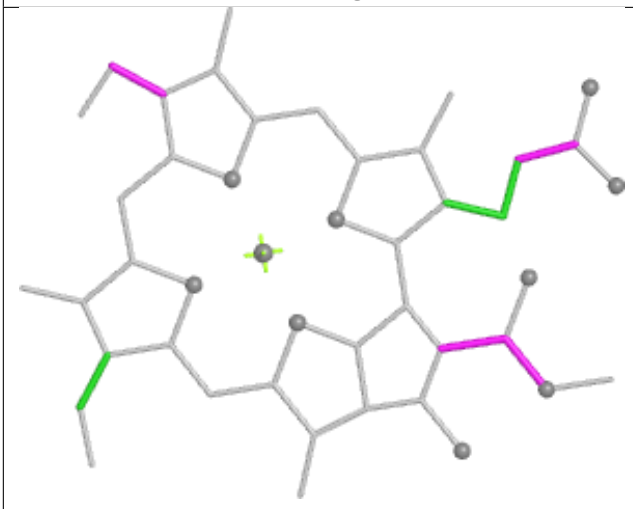
Ligand CLA cA 805



Bond lengths



Bond angles

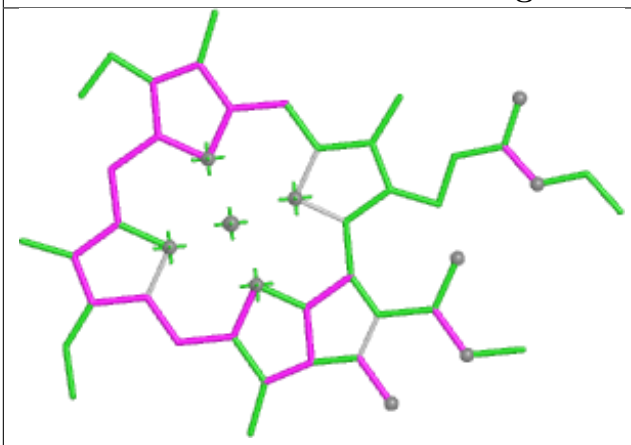


Torsions

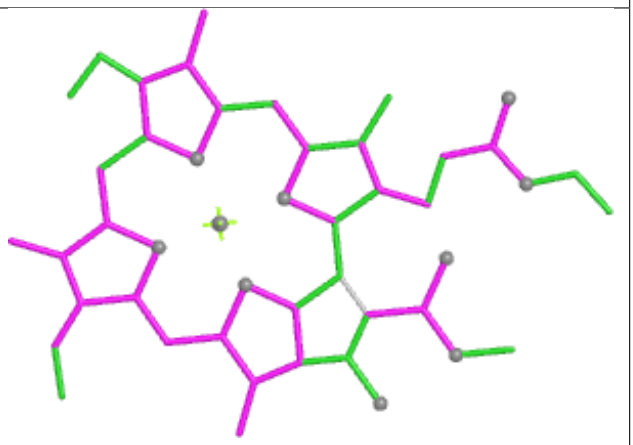


Rings

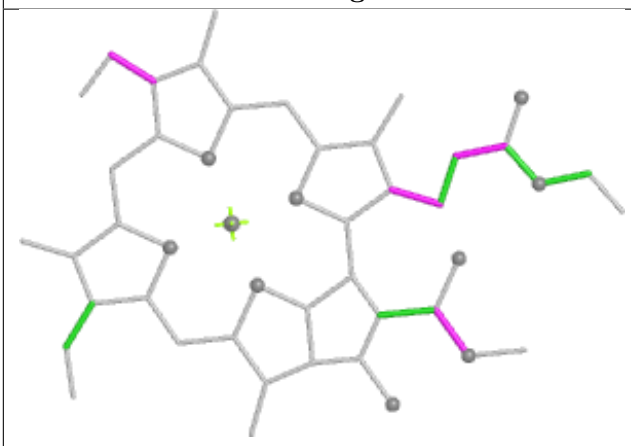
Ligand CLA aB 838



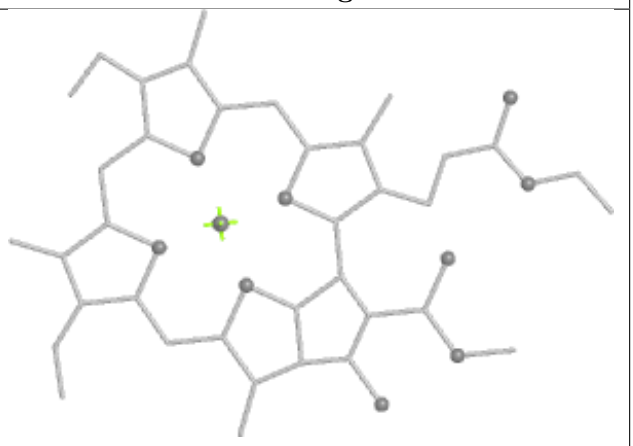
Bond lengths



Bond angles

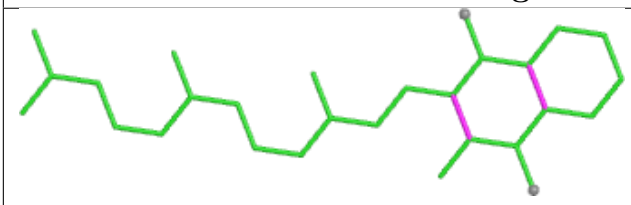


Torsions



Rings

Ligand PQN bB 841



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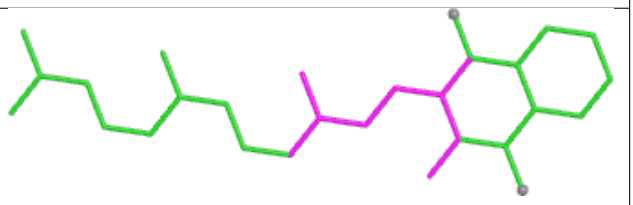
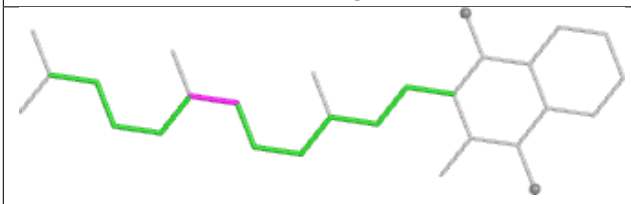


Bond angles



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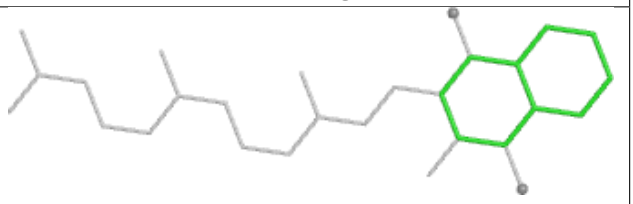
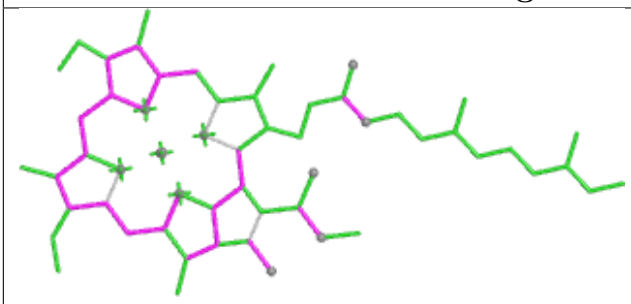


Rings

Ligand CLA cB 813



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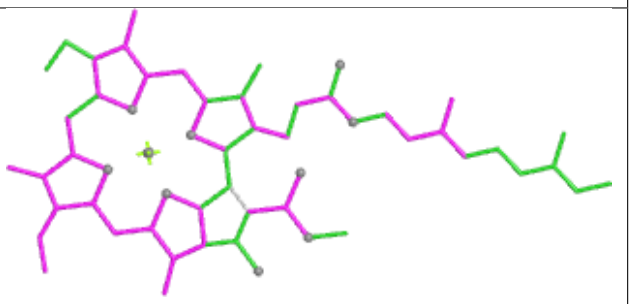
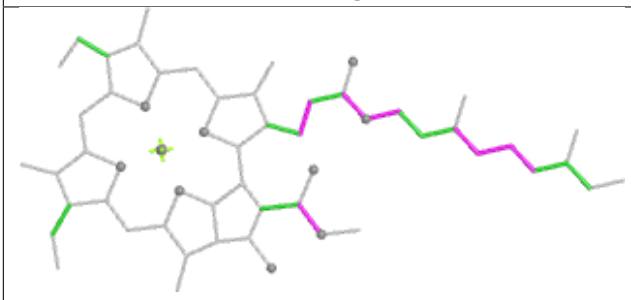


Bond angles



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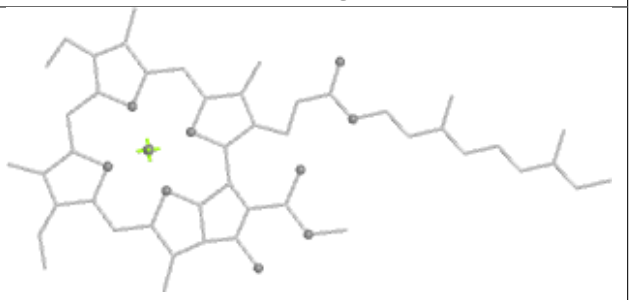
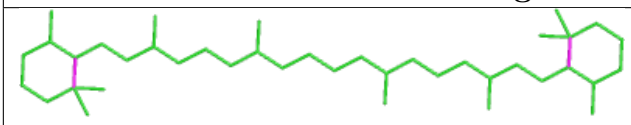


Rings

Ligand BCR aB 848



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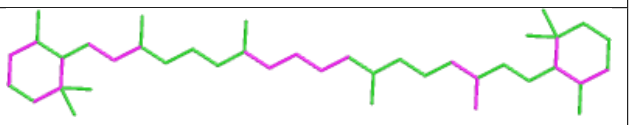
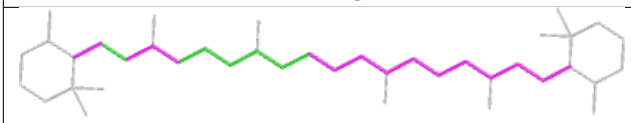


Bond angles



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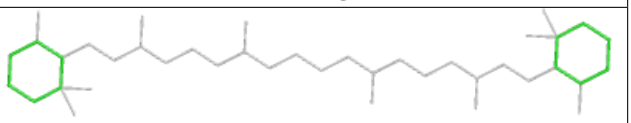
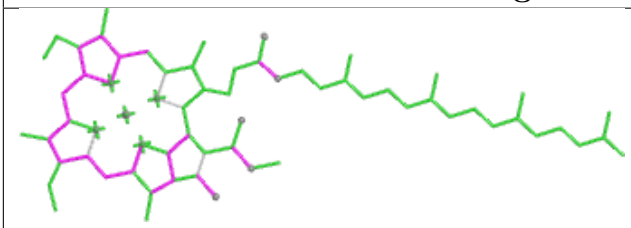


Rings

Ligand CLA bA 802



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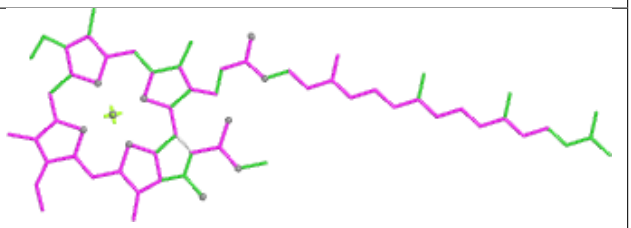
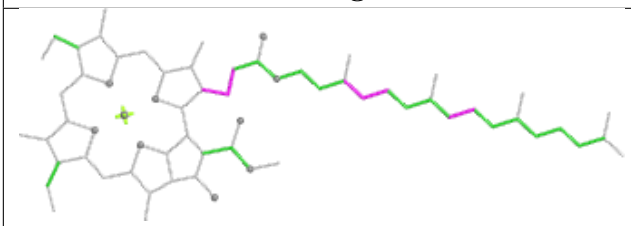


Bond angles



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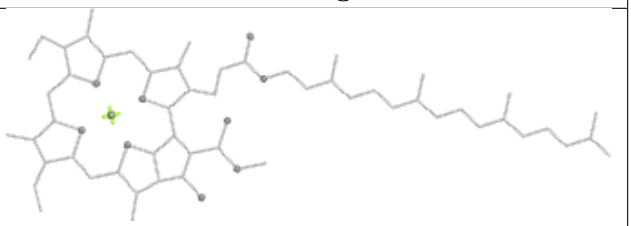
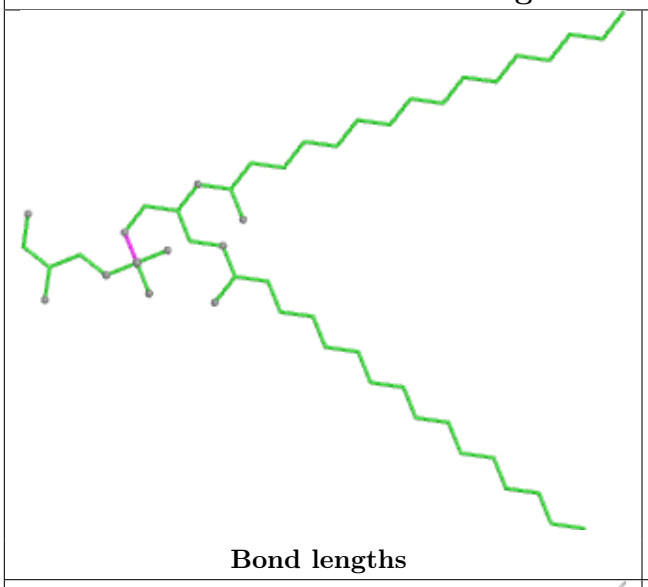


Rings

Ligand LHG cA 852



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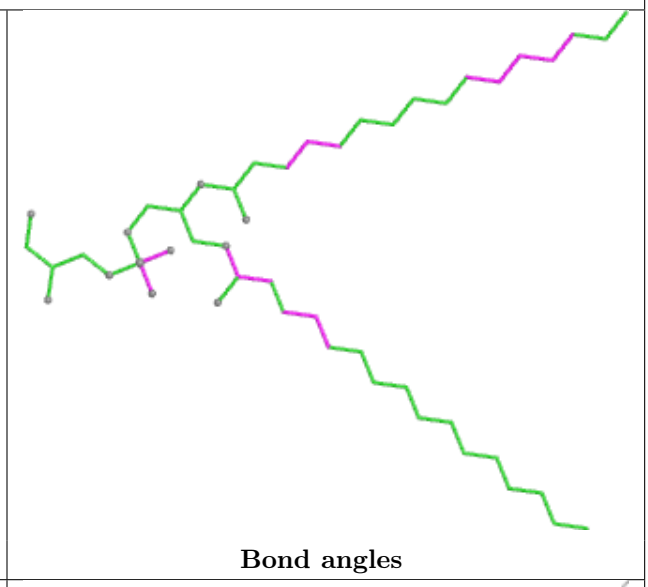
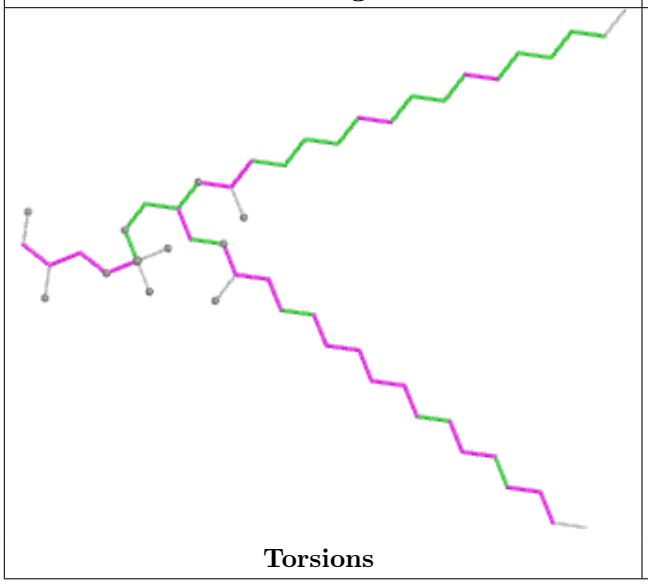


Bond angles



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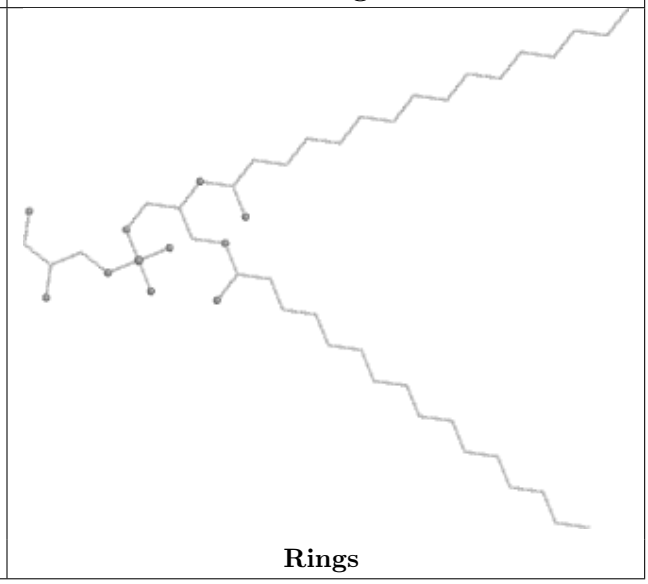
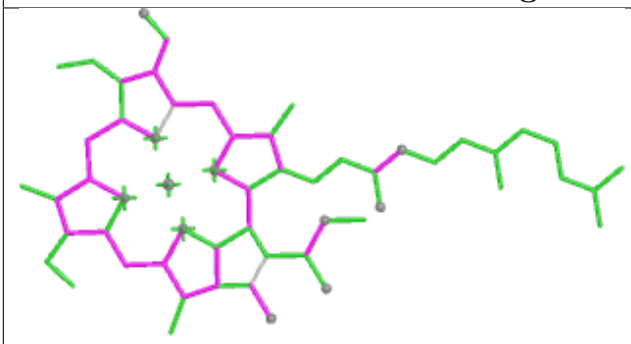


Rings

Ligand F6C cA 827



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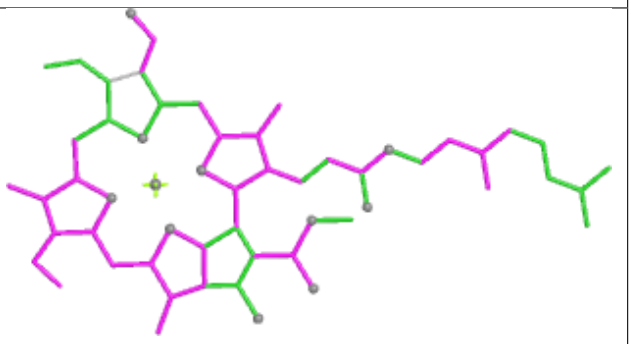
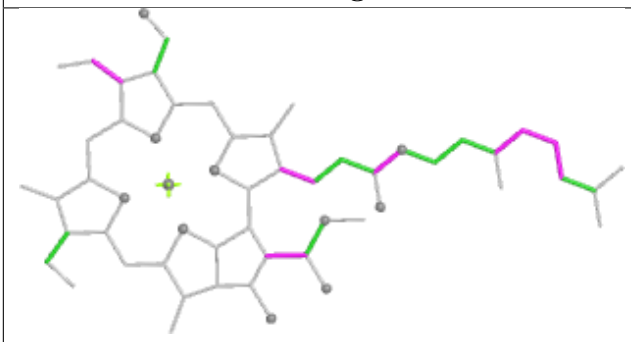


Bond angles



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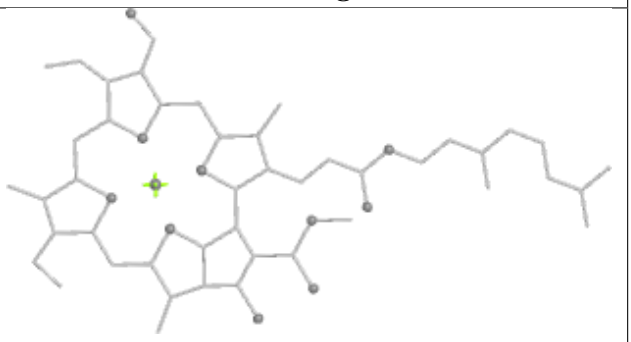
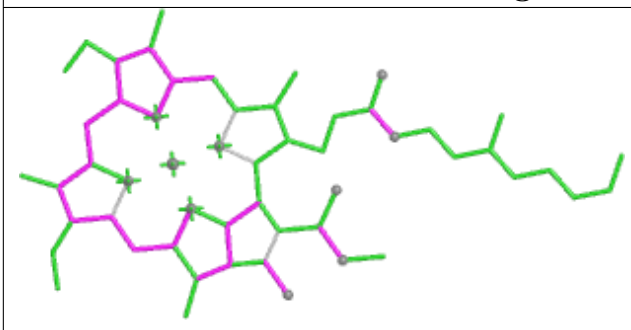


Rings

Ligand CLA bA 813



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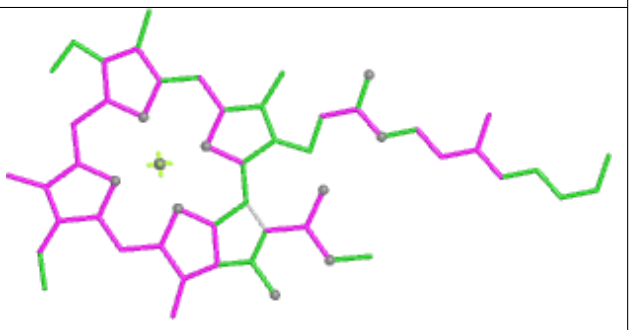
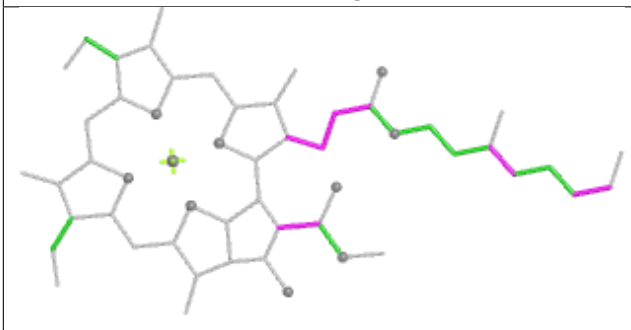


Bond angles



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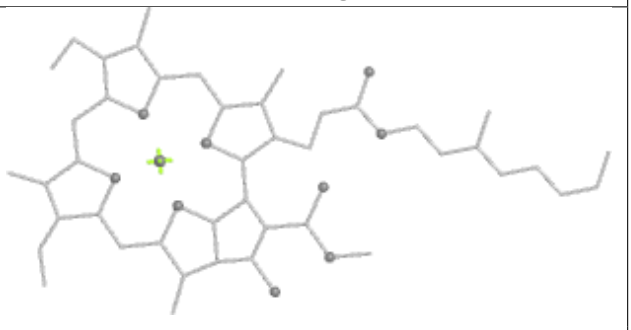
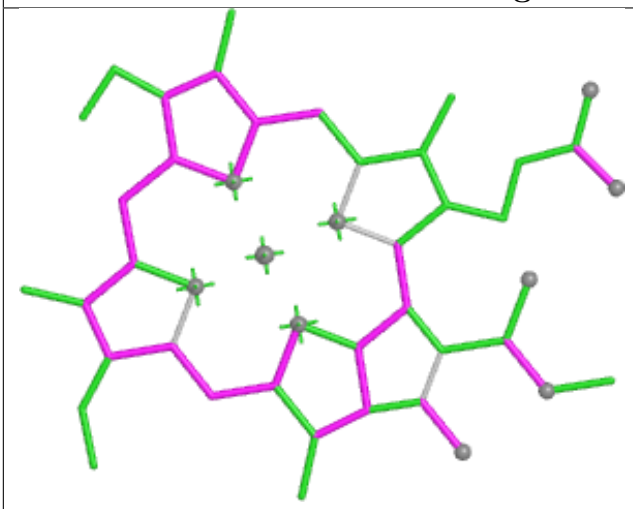


Rings

Ligand CLA bA 805



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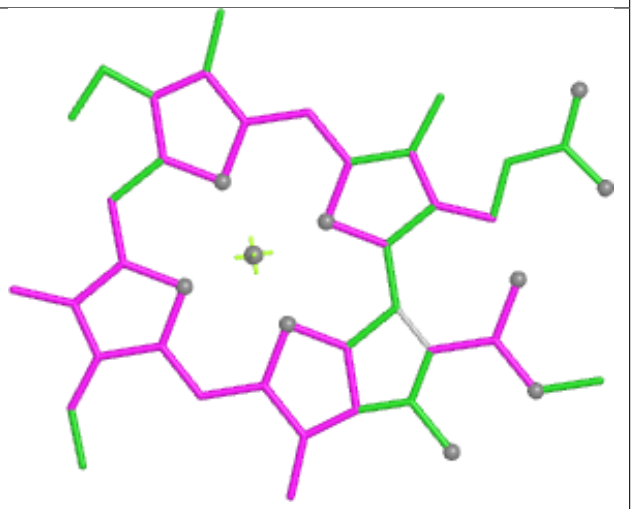
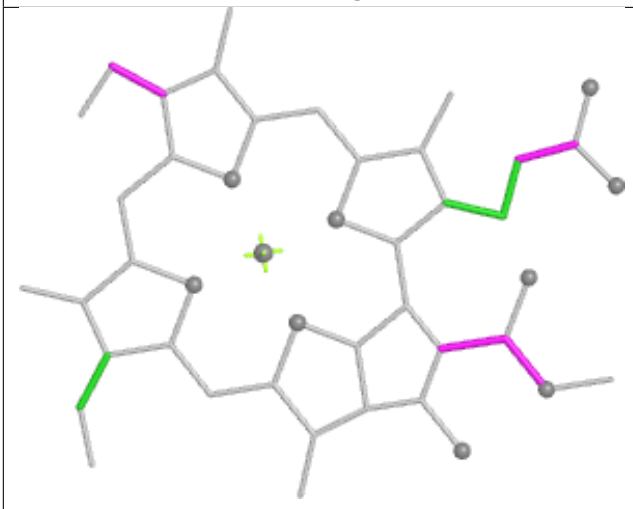


Bond angles

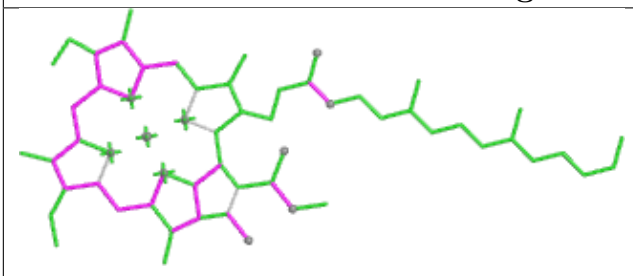


Torsions



Rings

Ligand CLA cB 816



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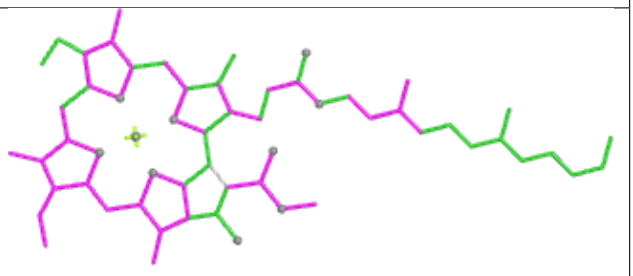
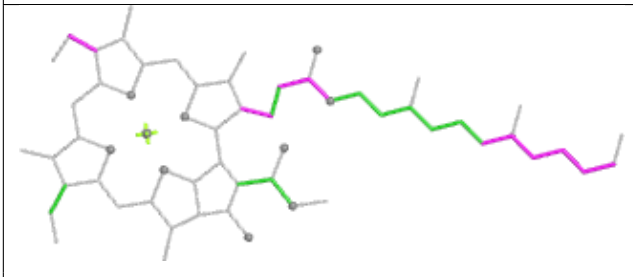


Bond angles



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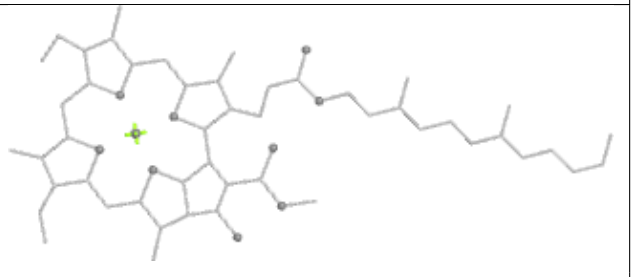
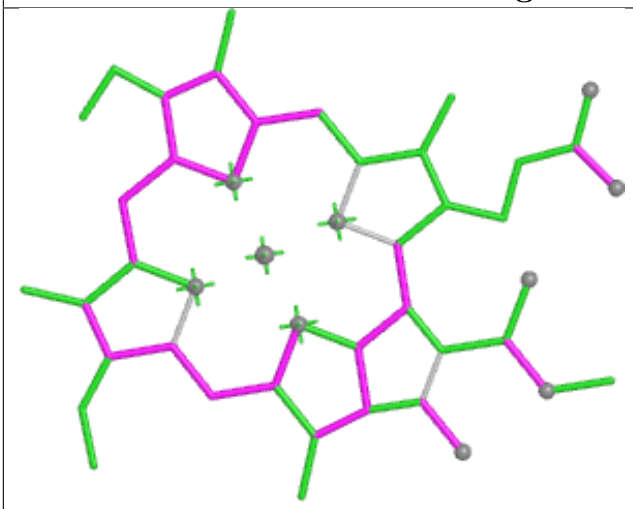


Rings

Ligand CLA cA 815



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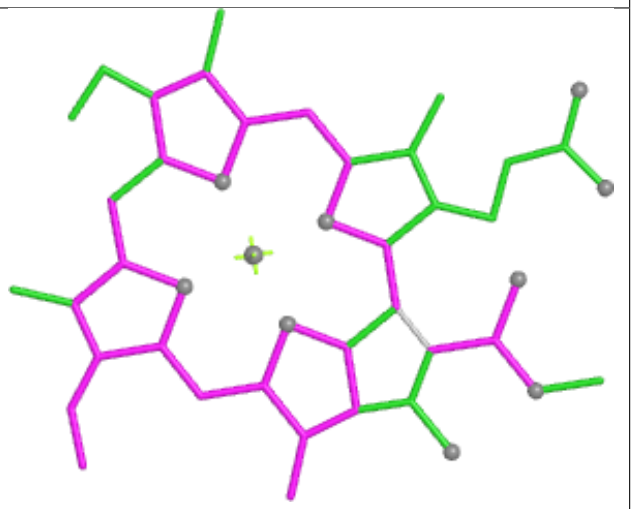
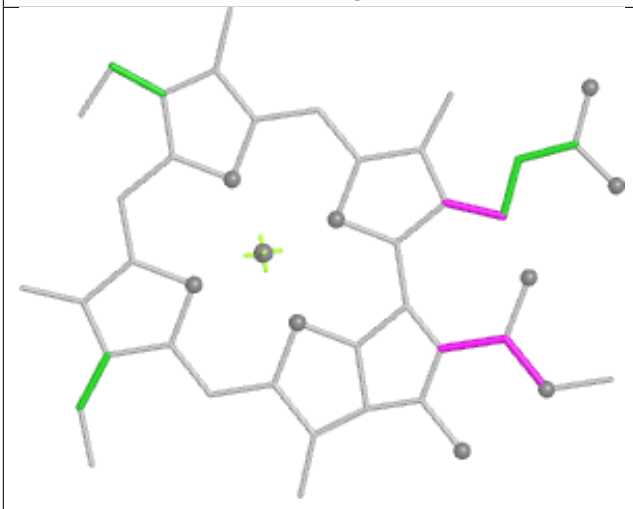


Bond angles

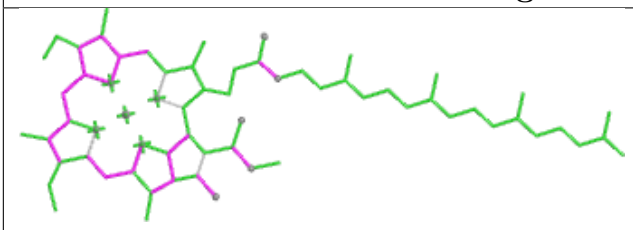


Torsions



Rings

Ligand CLA cB 839



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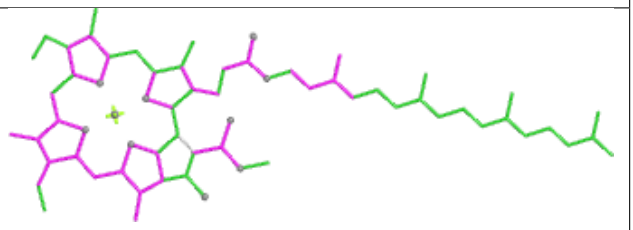
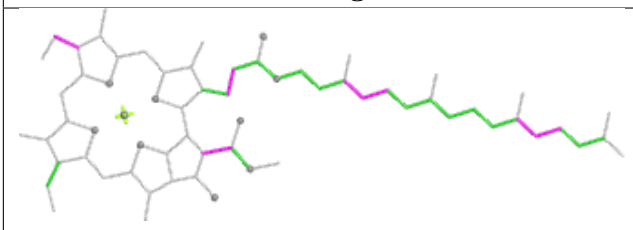


Bond angles



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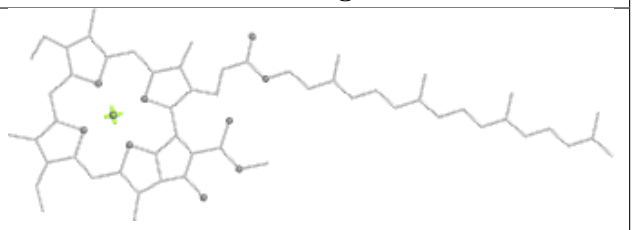
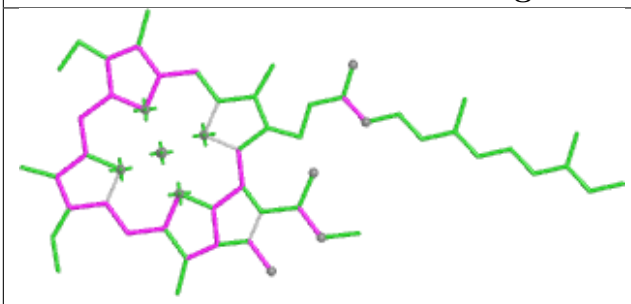
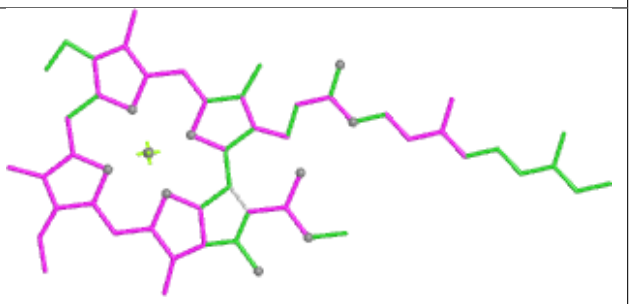
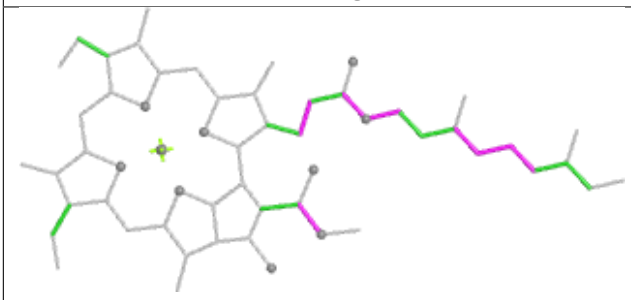
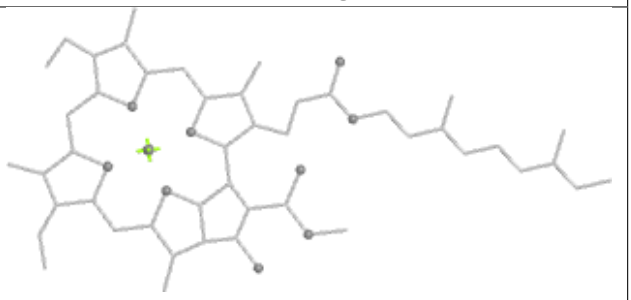
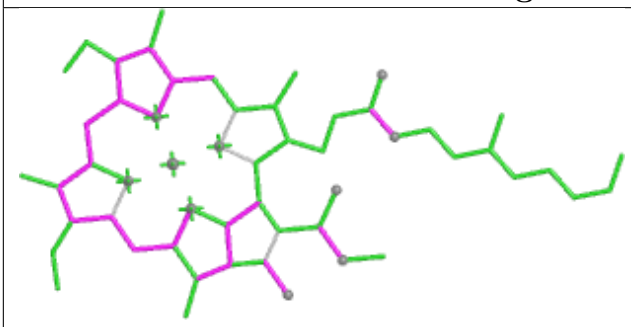
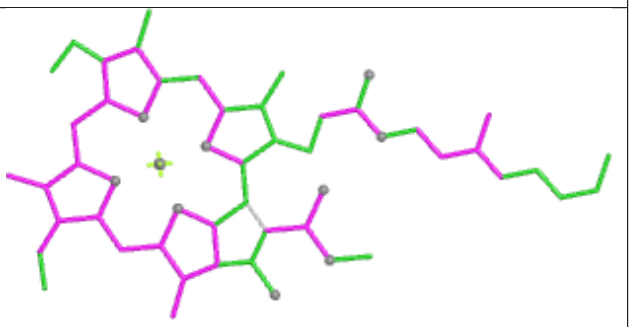
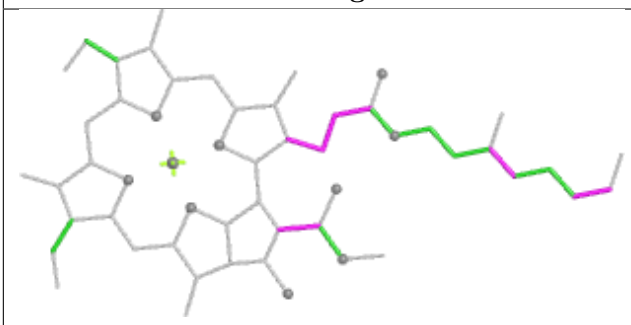
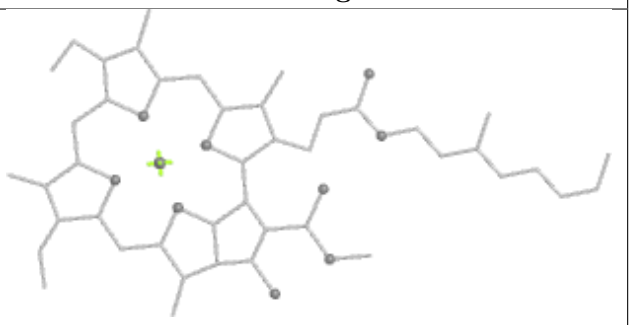
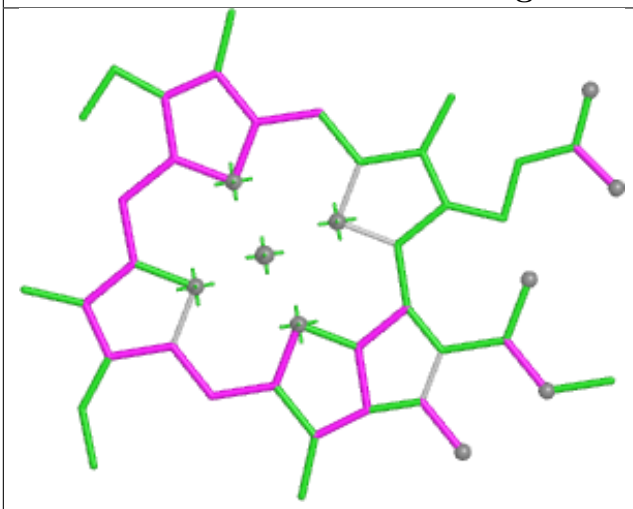


Rings

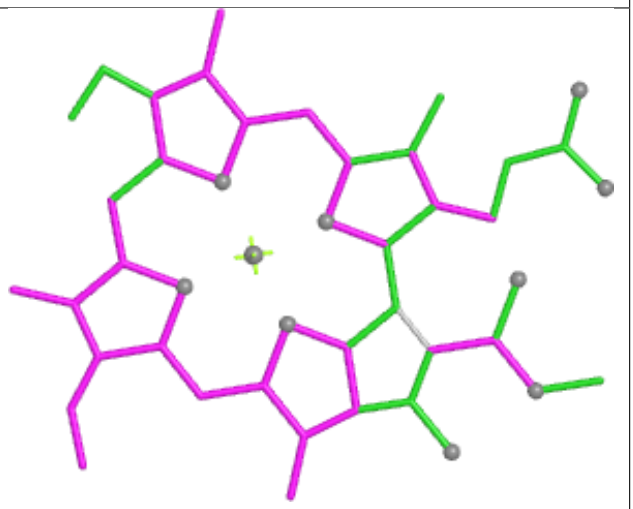
Ligand CLA bB 813	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA cA 813	
	
Bond lengths	Bond angles
	
Torsions	Rings

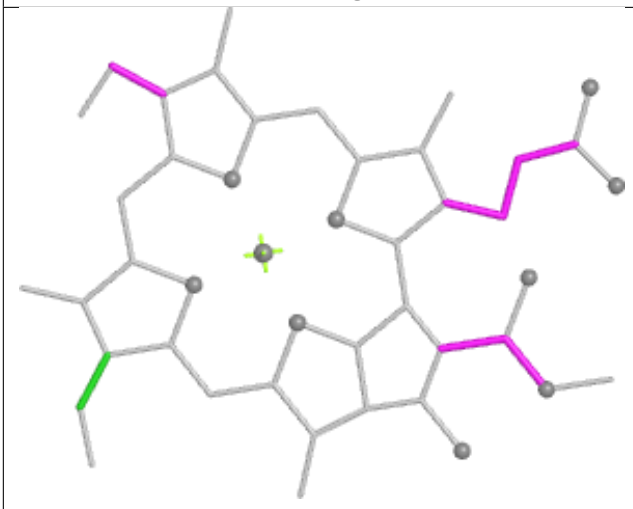
Ligand CLA cA 804



Bond lengths



Bond angles

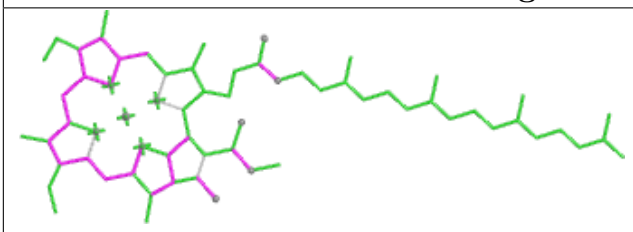


Torsions

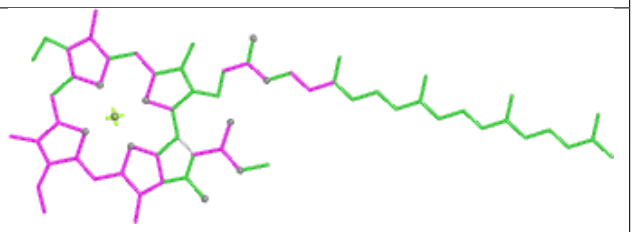


Rings

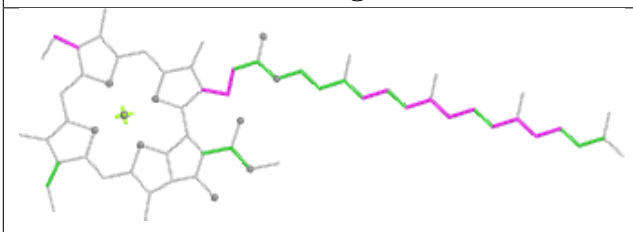
Ligand CLA cL 205



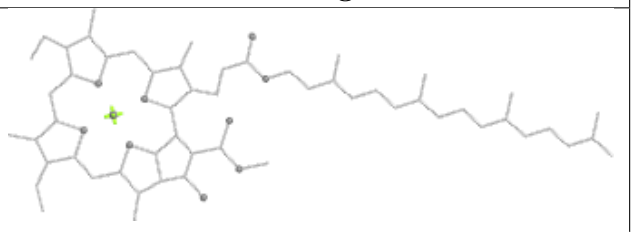
Bond lengths



Bond angles

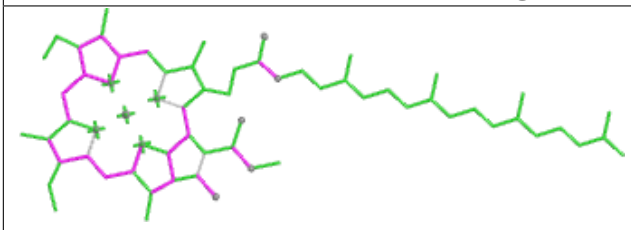


Torsions



Rings

Ligand CLA bA 812



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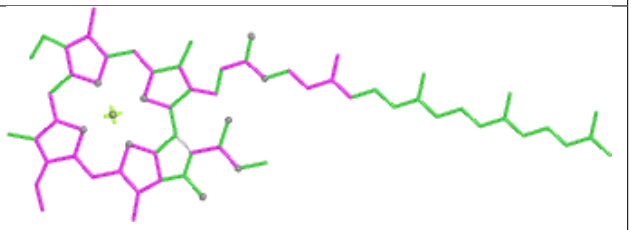
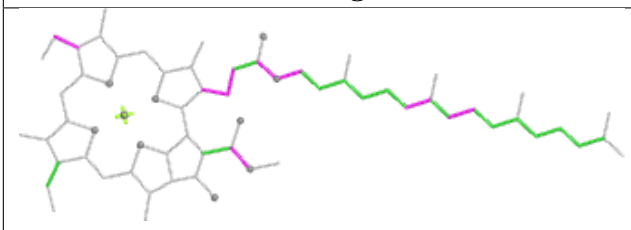


Bond angles



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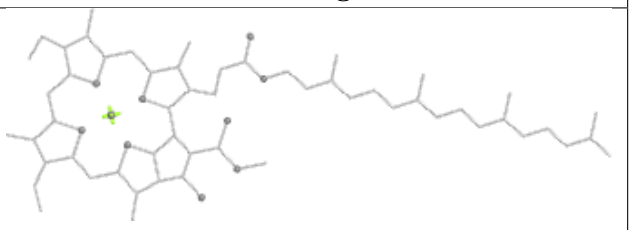
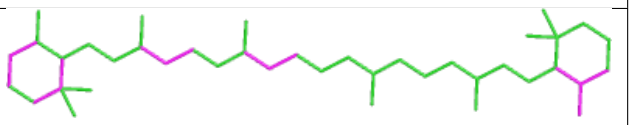


Rings

Ligand BCR aI 101



Bond lengths



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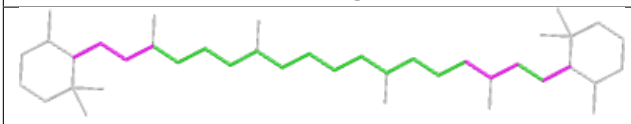

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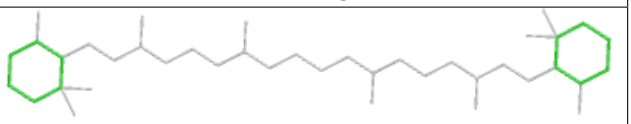
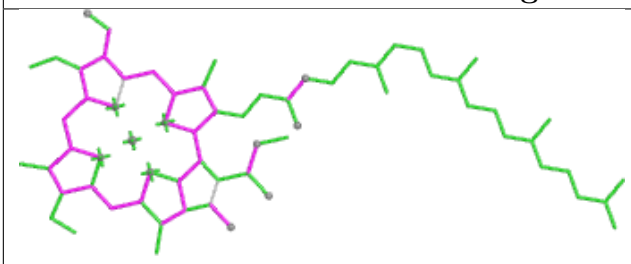


Rings

Ligand F6C bL 202



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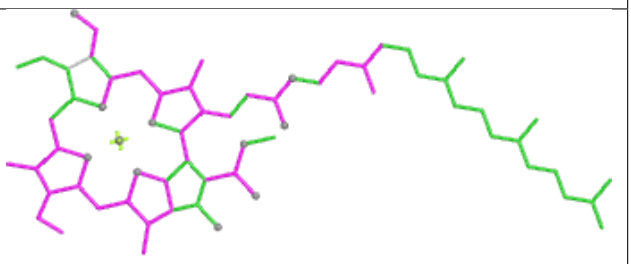
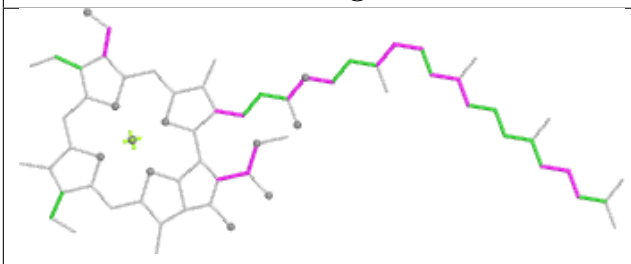


Bond angles



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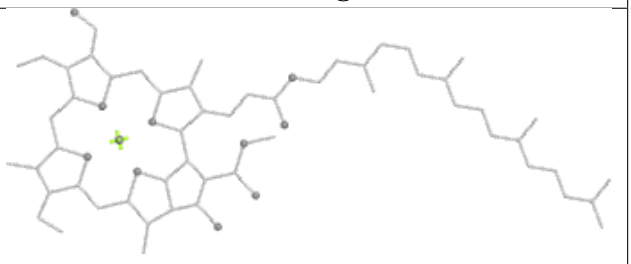
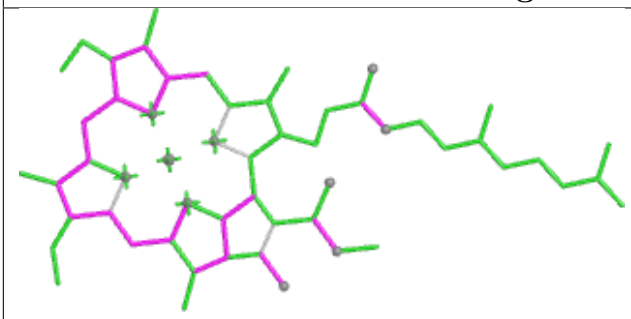


Rings

Ligand CLA cB 837



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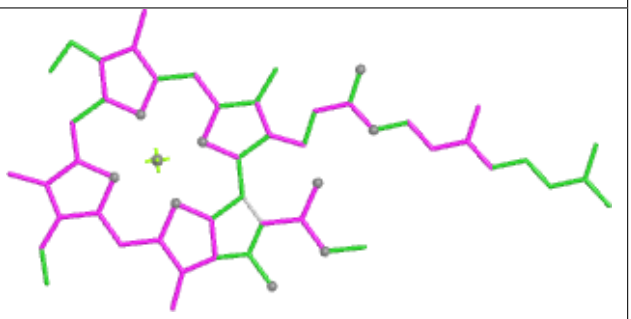

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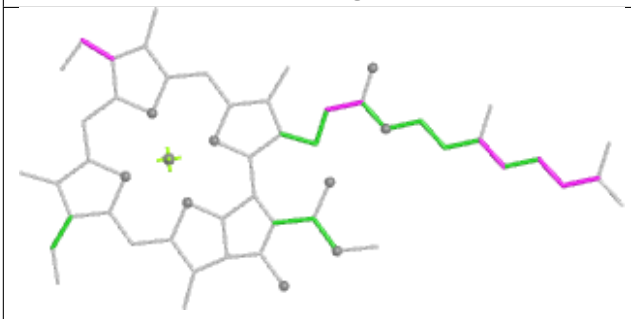

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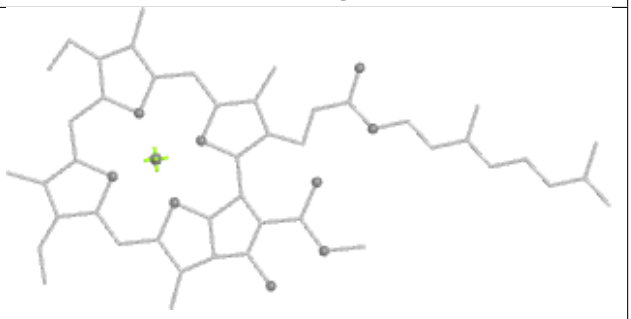
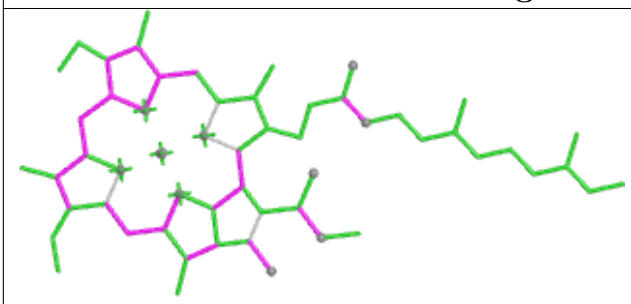


Rings

Ligand CLA cA 803



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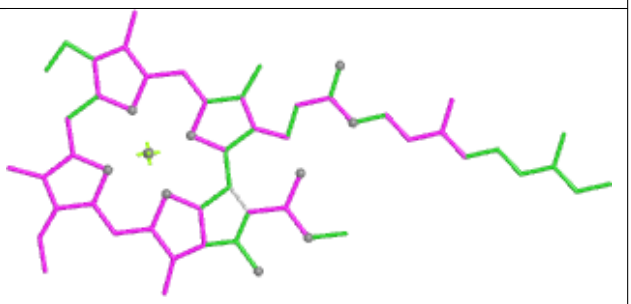

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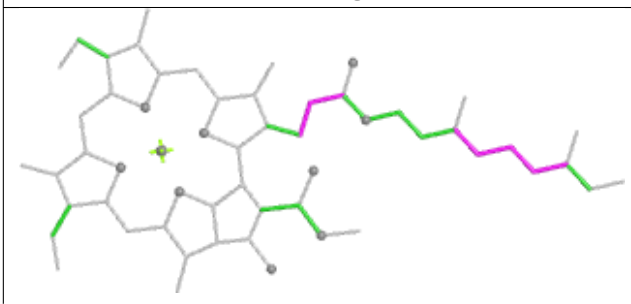

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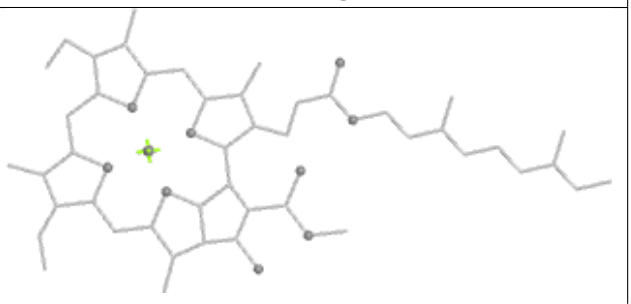
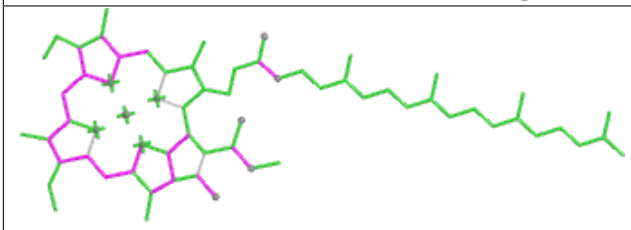


Rings

Ligand CLA cA 822



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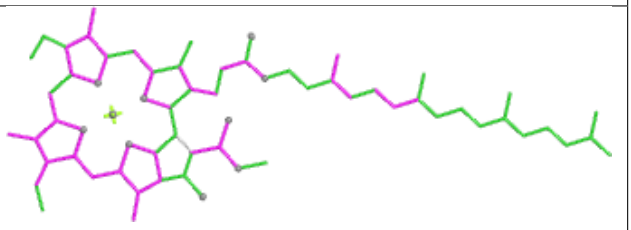
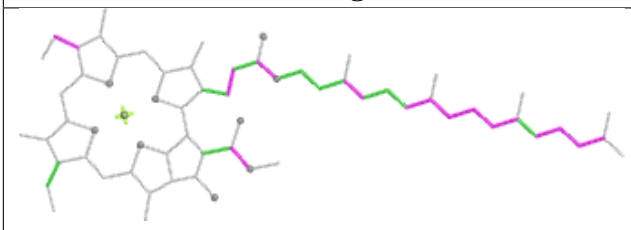


Bond angles



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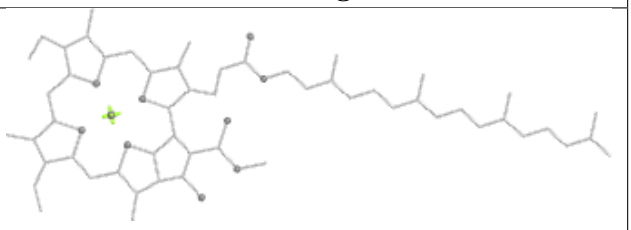
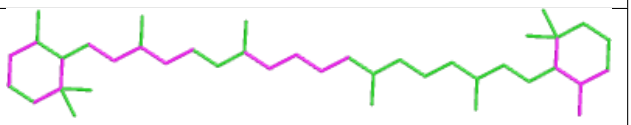


Rings

Ligand BCR bL 207



Bond lengths



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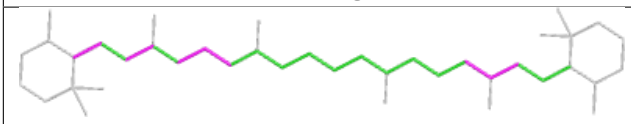

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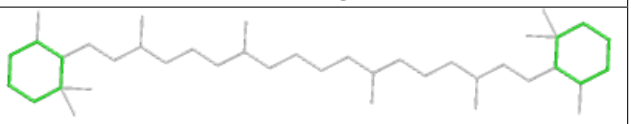
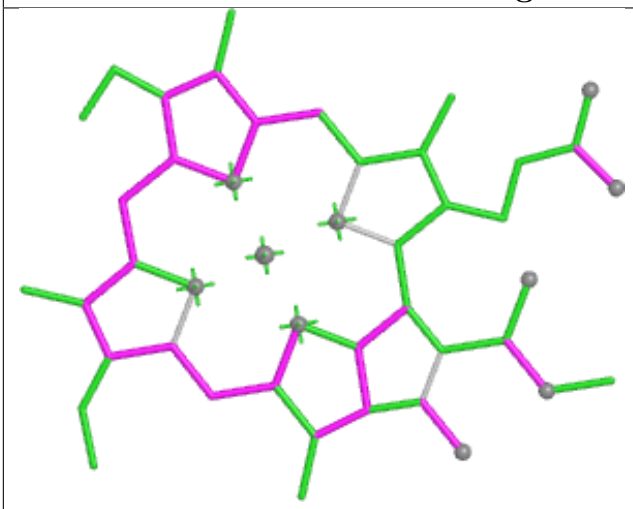


Rings

Ligand CLA cA 811



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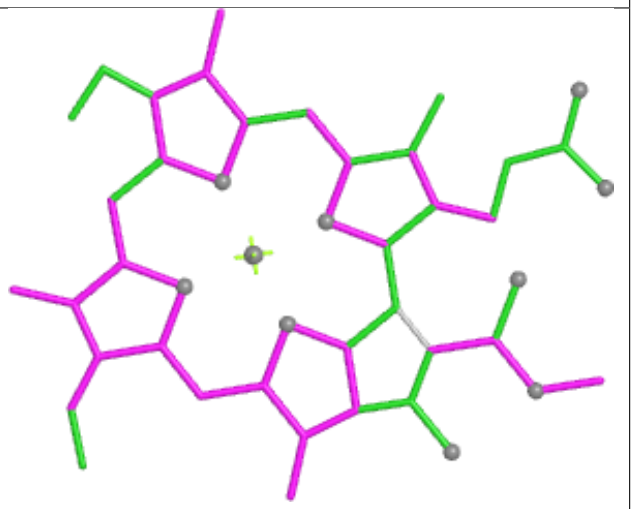
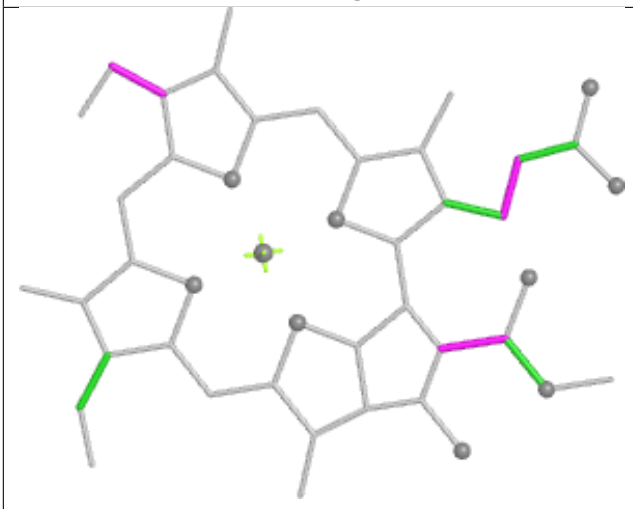


Bond angles

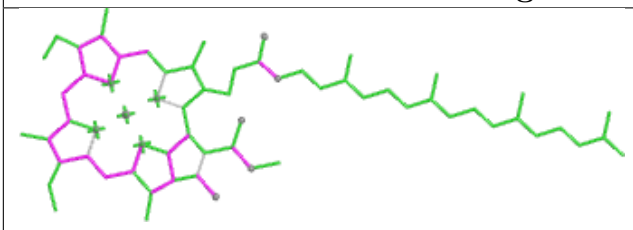


Torsions



Rings

Ligand CLA cB 805



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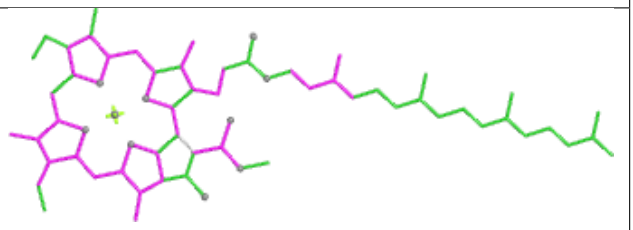
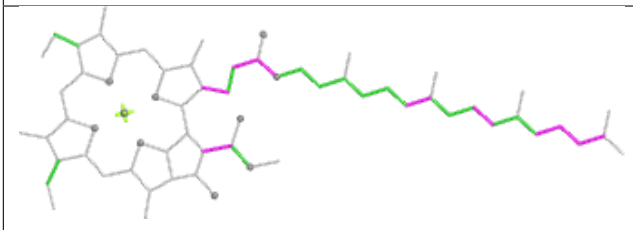


Bond angles



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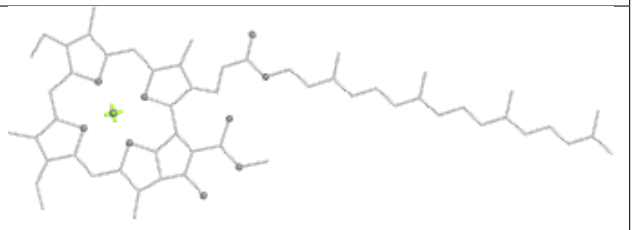
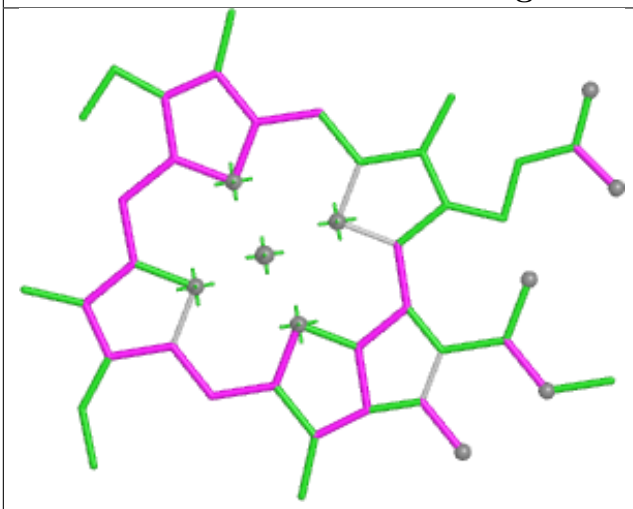


Rings

Ligand CLA cA 809



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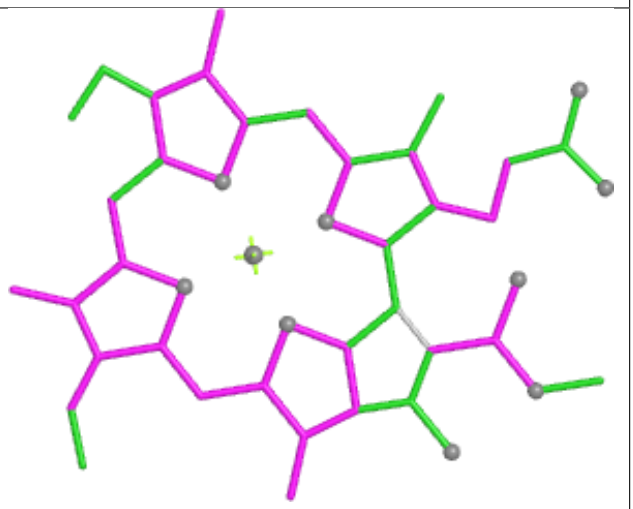
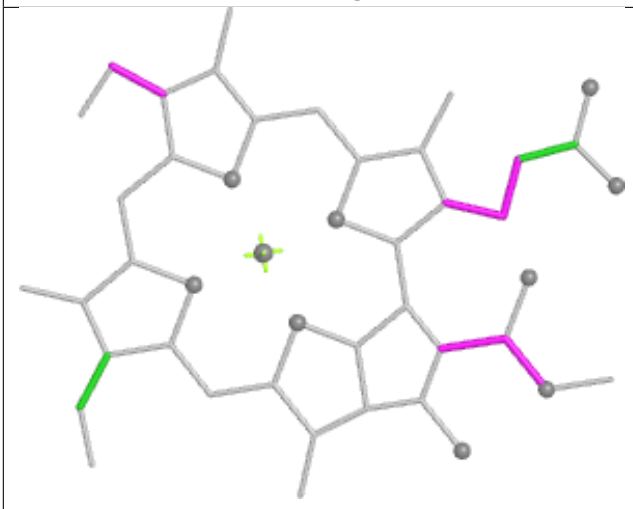


Bond angles

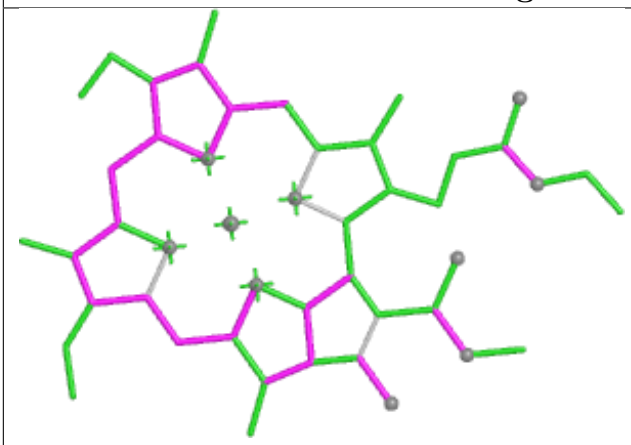


Torsions



Rings

Ligand CLA cB 838



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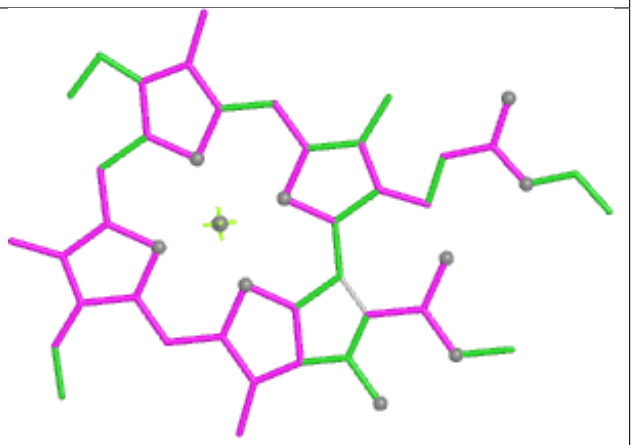
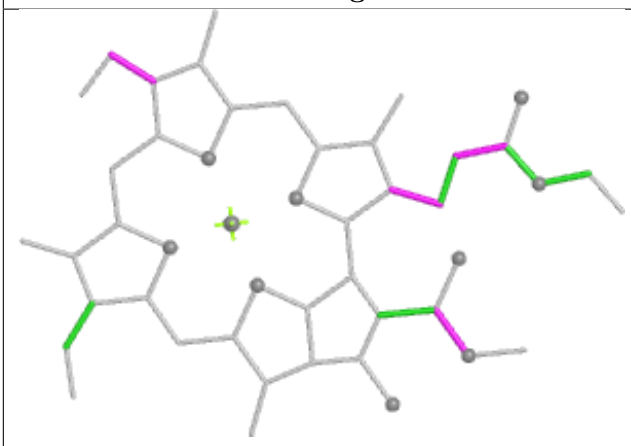


Bond angles



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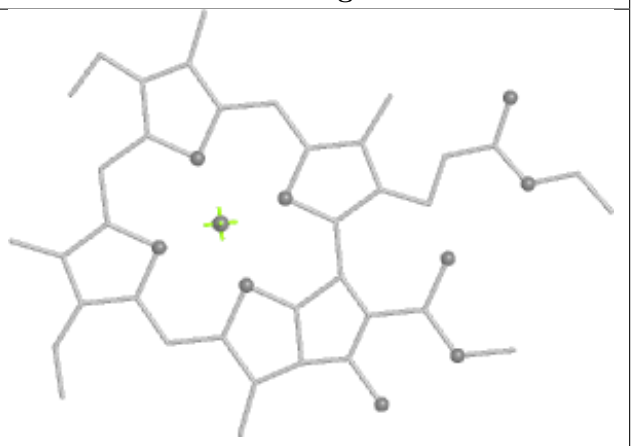
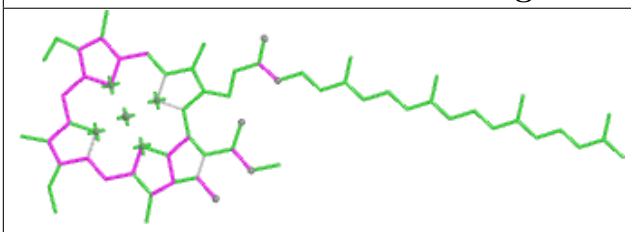


Rings

Ligand CLA aA 840



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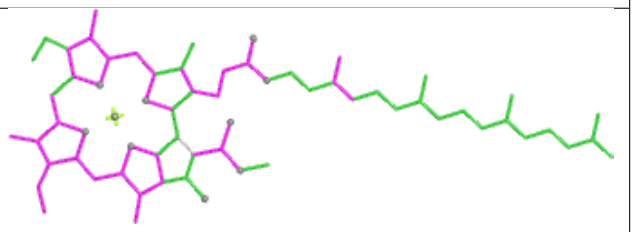
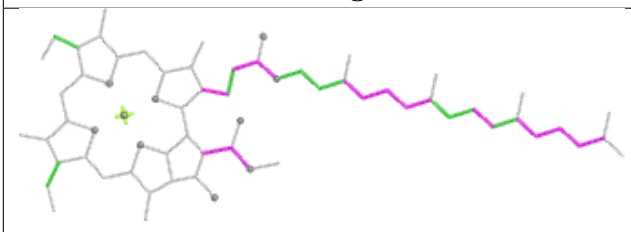


Bond angles



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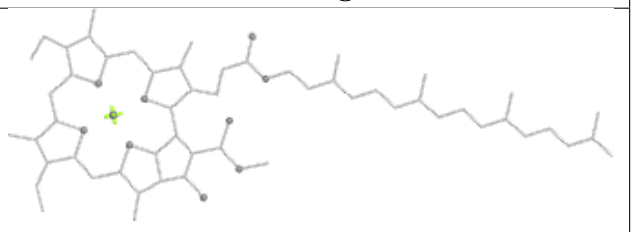
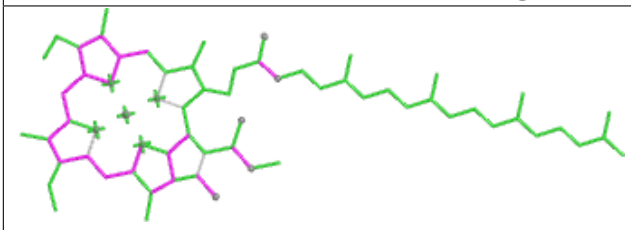
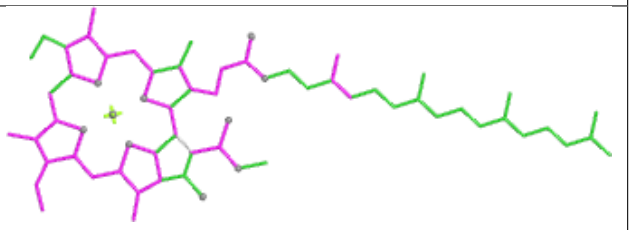
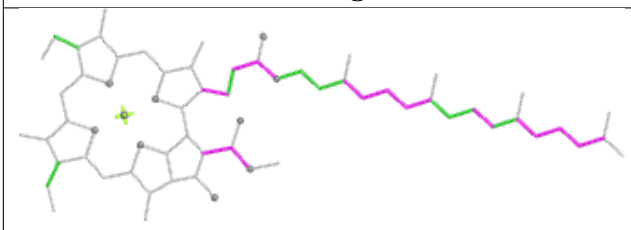
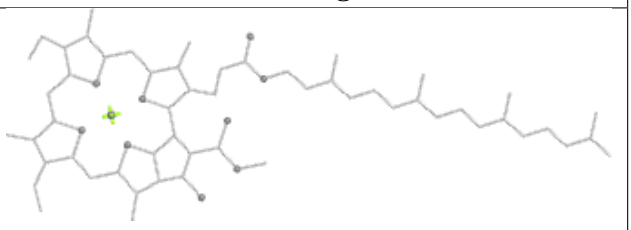
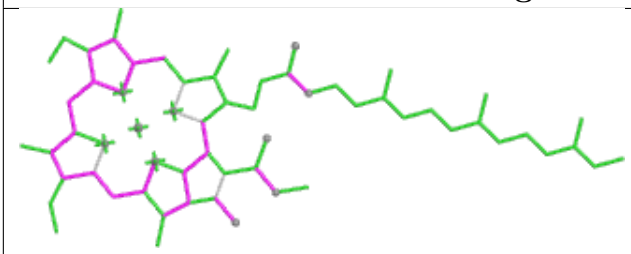
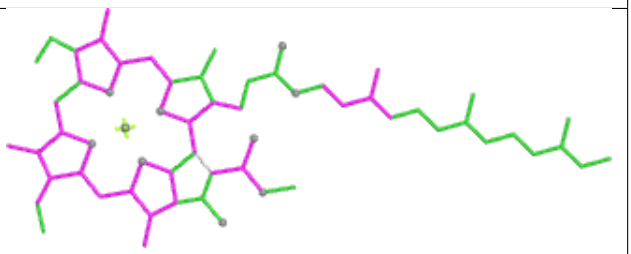
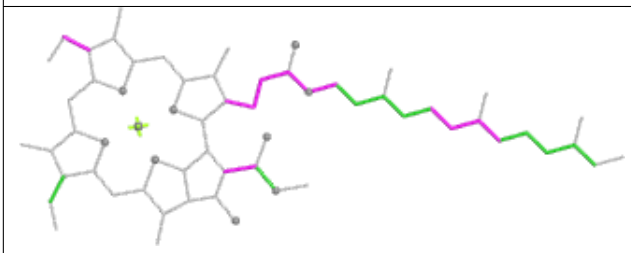
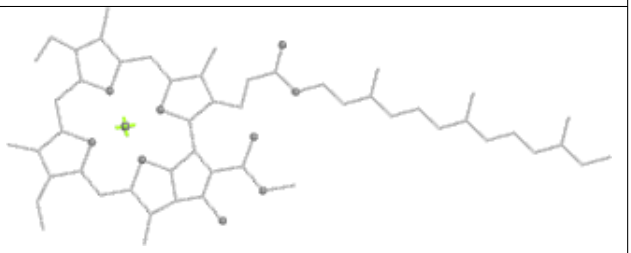
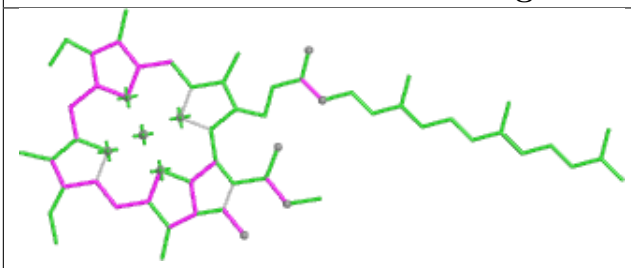


Rings

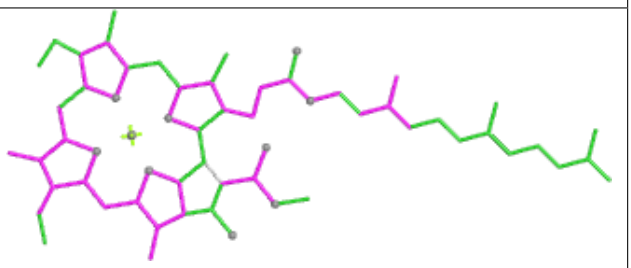
Ligand CLA bA 840	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA aA 821	
 Bond lengths	 Bond angles
 Torsions	 Rings

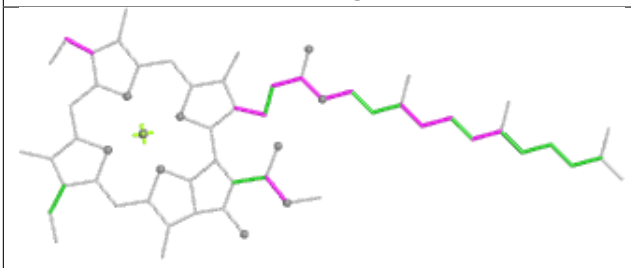
Ligand CLA aB 817



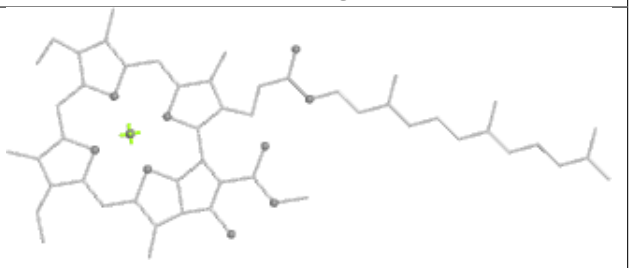
Bond lengths



Bond angles

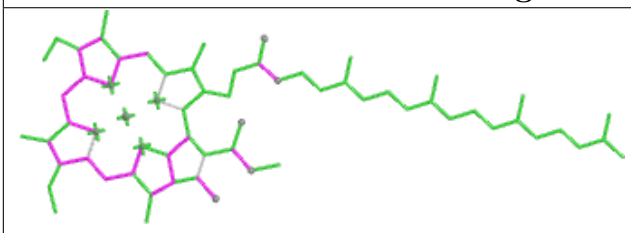


Torsions

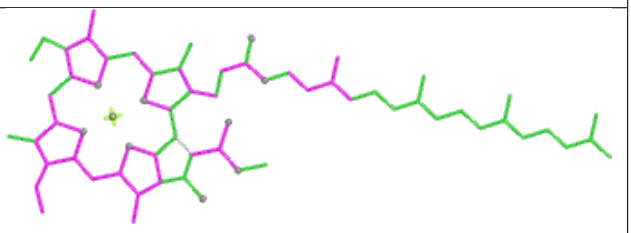


Rings

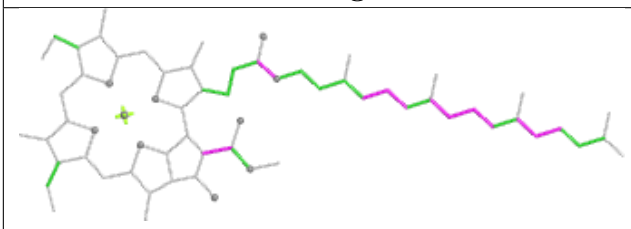
Ligand CLA aA 831



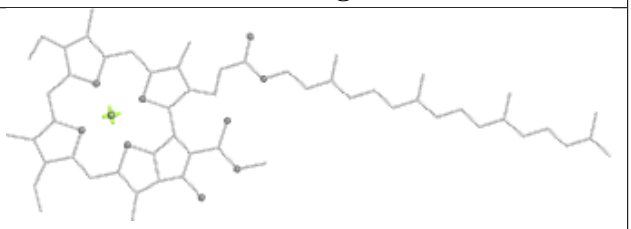
Bond lengths



Bond angles



Torsions

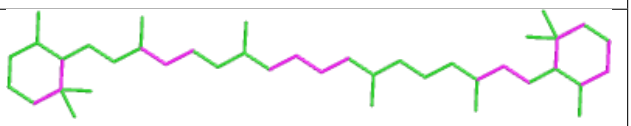


Rings

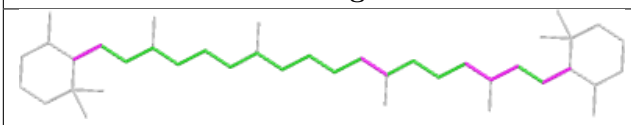
Ligand BCR bA 847



Bond lengths



Bond angles



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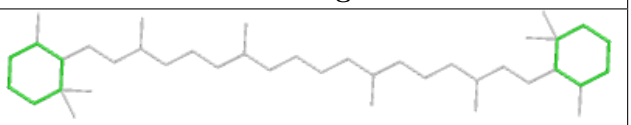
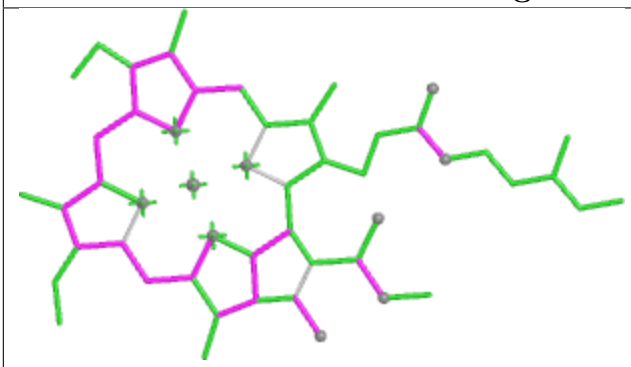


Rings

Ligand CLA bA 838



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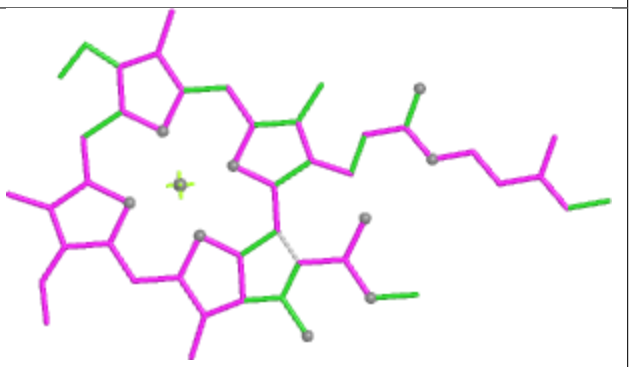

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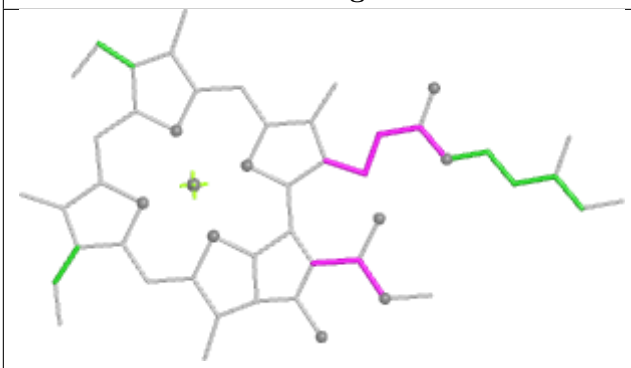

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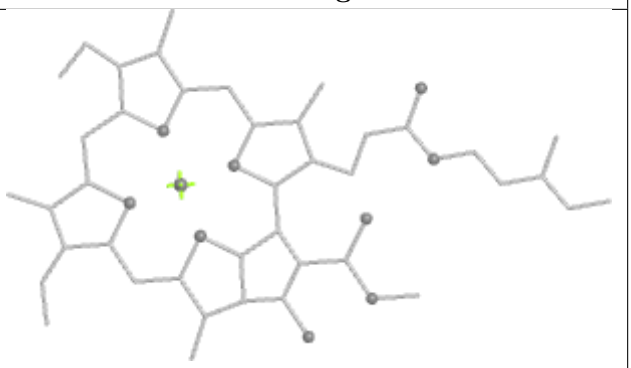
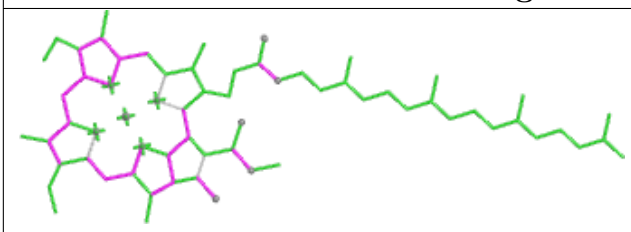


Rings

Ligand CLA cA 807



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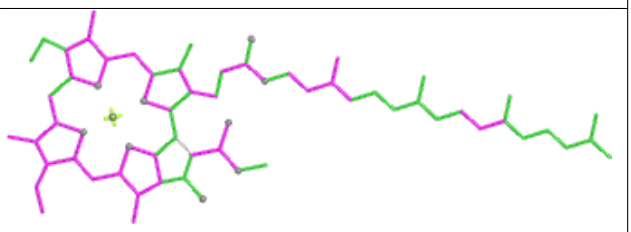
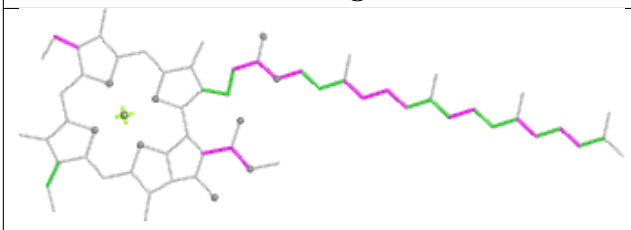


Bond angles



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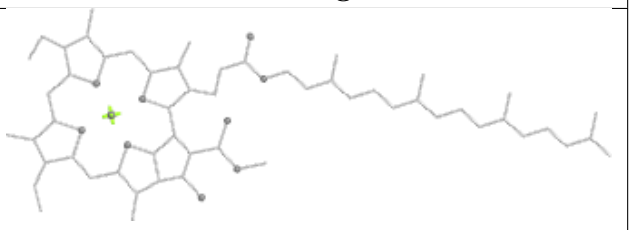
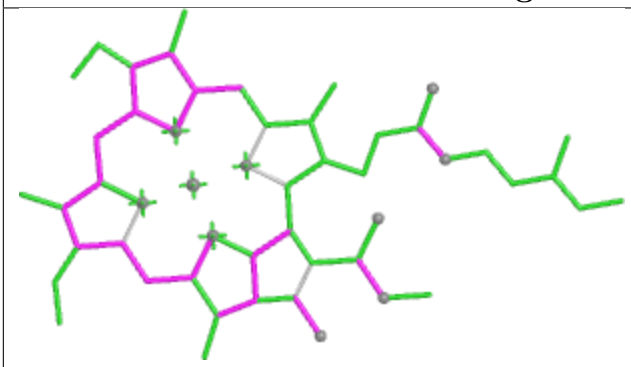


Rings

Ligand CLA cA 838



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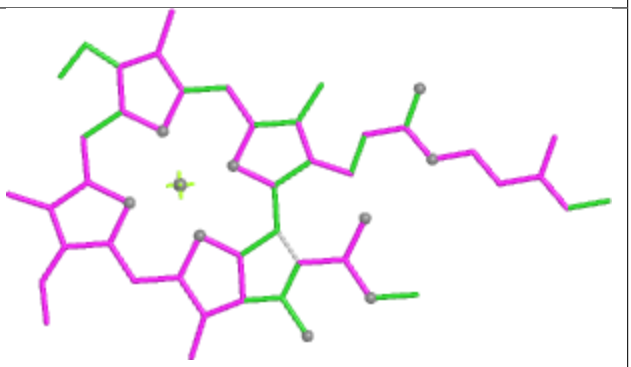
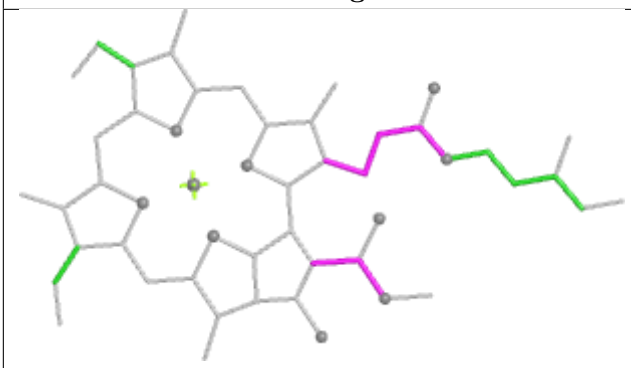


Bond angles



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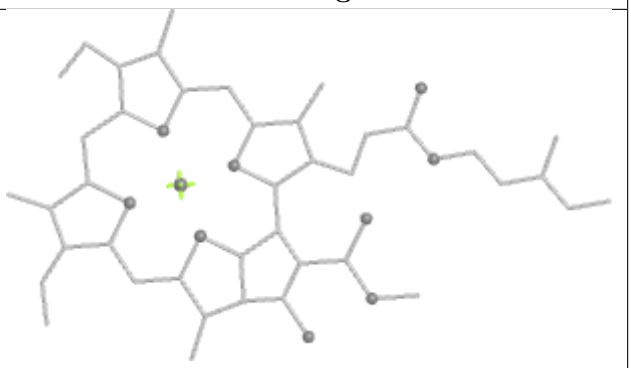
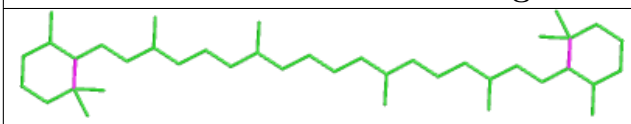


Rings

Ligand BCR bB 846



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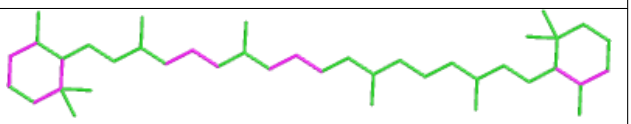

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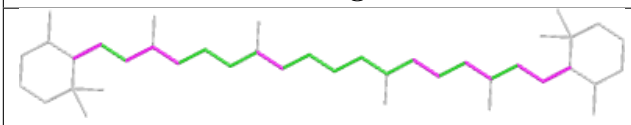

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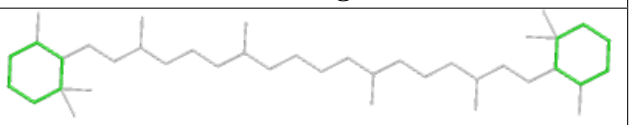
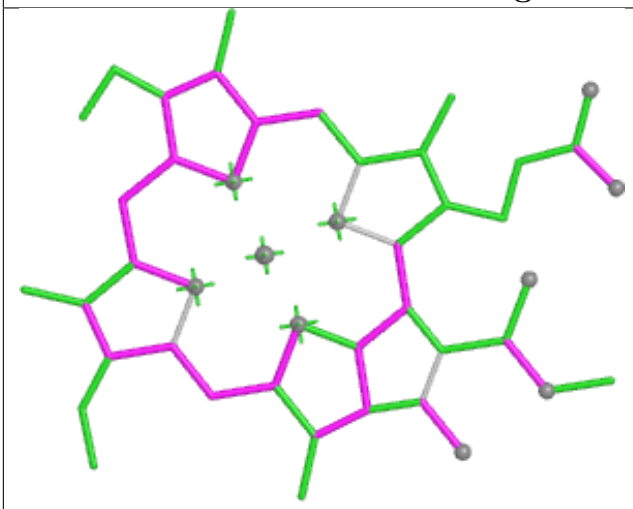


Rings

Ligand CLA bB 814



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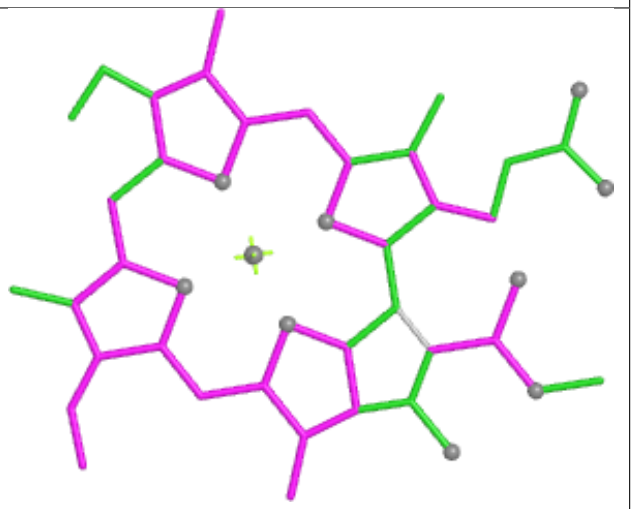

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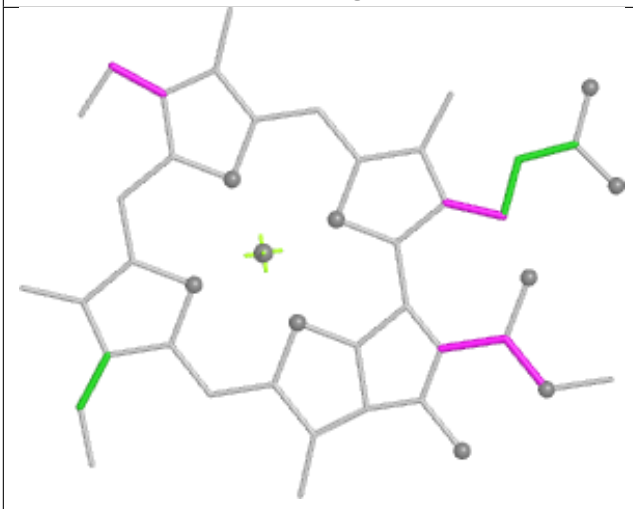
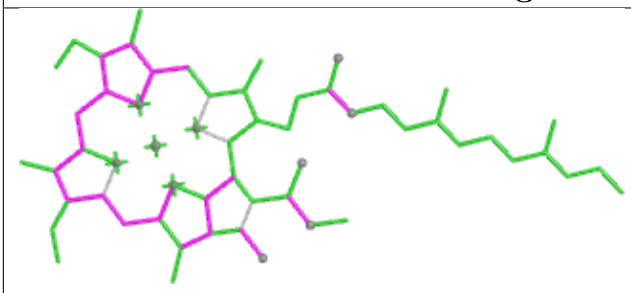
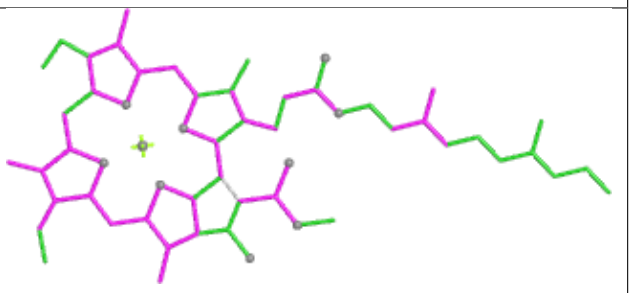
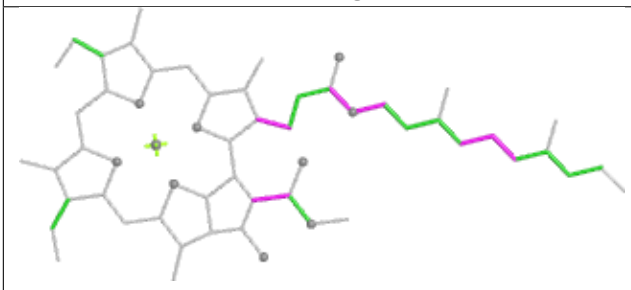
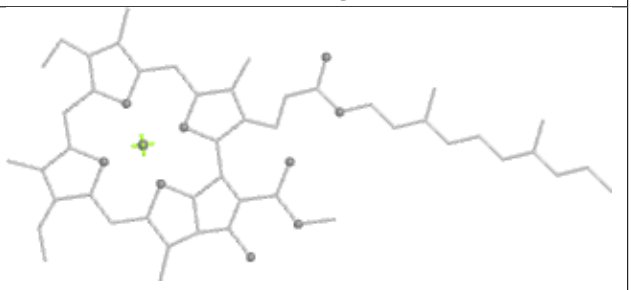


Torsions



Rings

Ligand CLA aB 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

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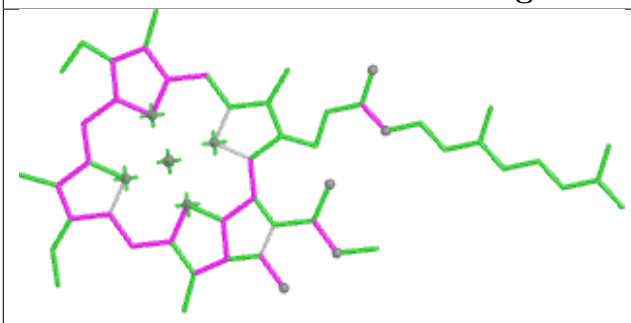
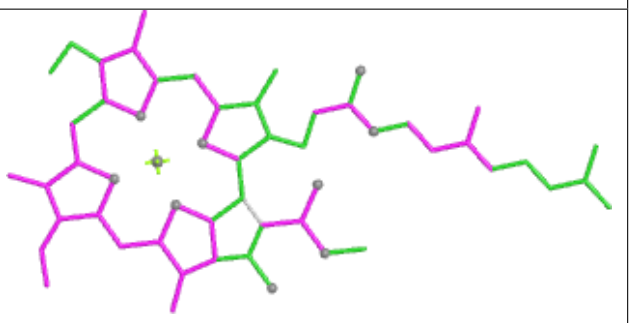
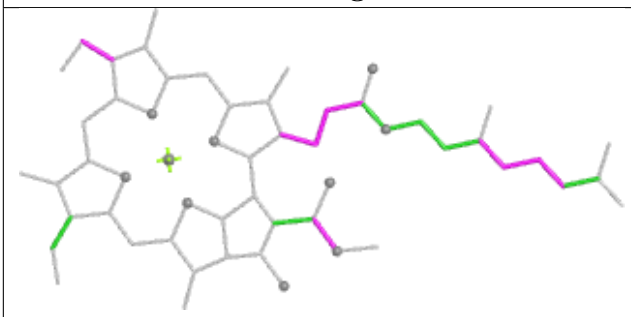
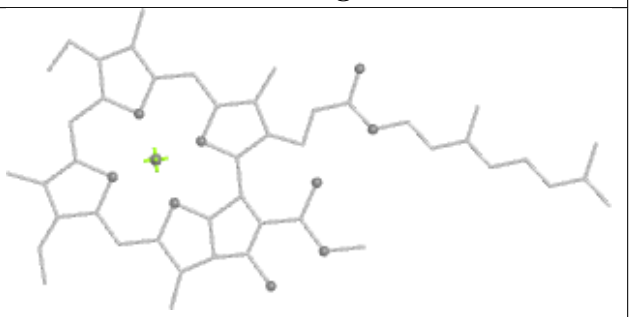
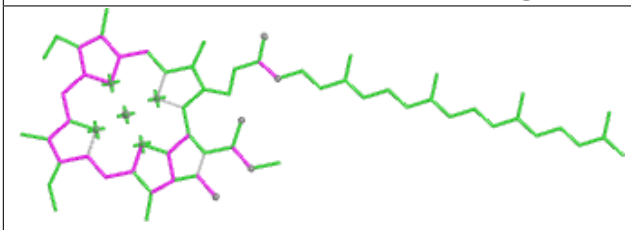
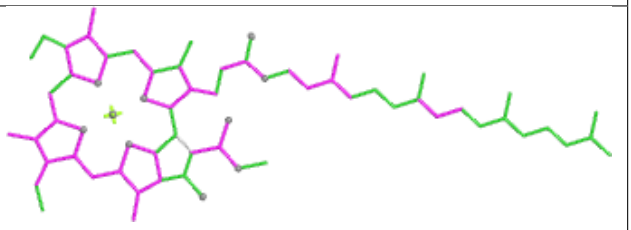
 Bond lengths	 Bond angles
 Torsions	 Rings

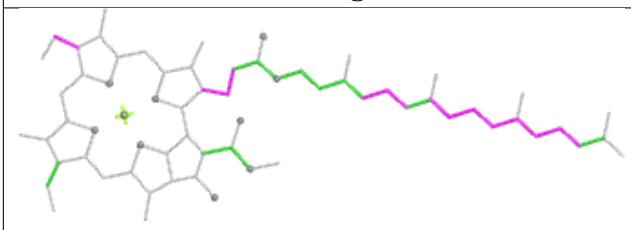
Ligand CLA aL 206



Bond lengths



Bond angles



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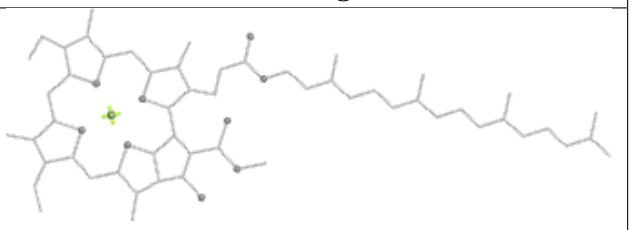
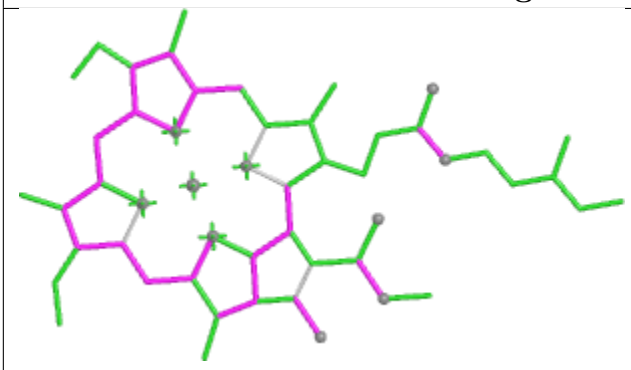


Rings

Ligand CLA aA 808



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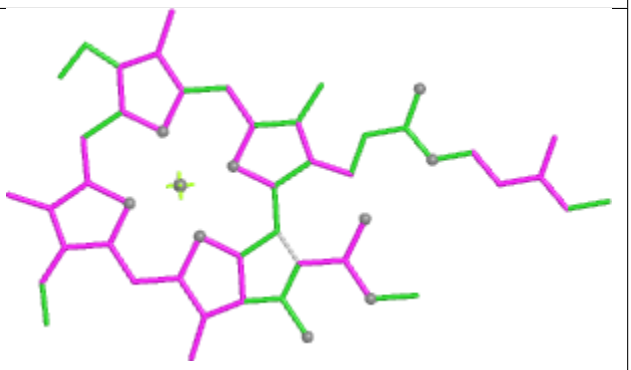

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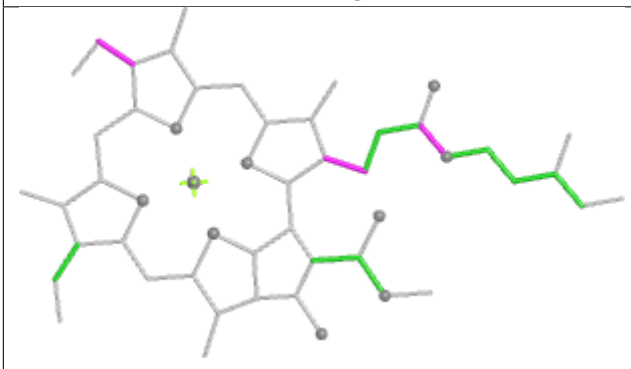

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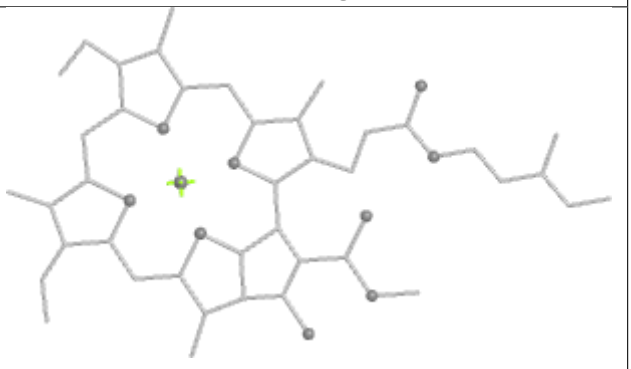
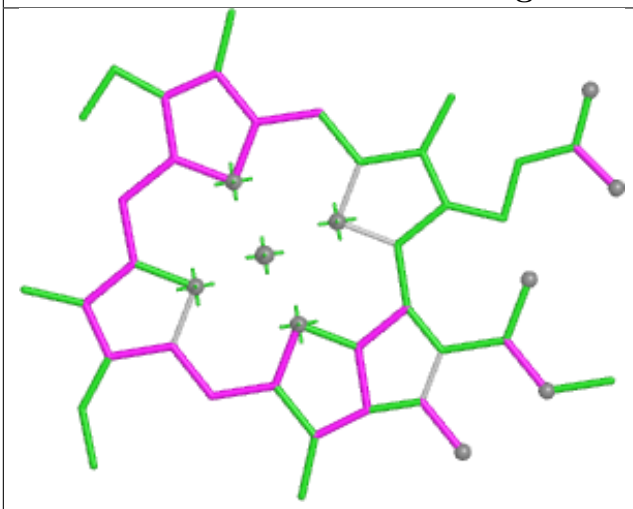


Rings

Ligand CLA cA 810



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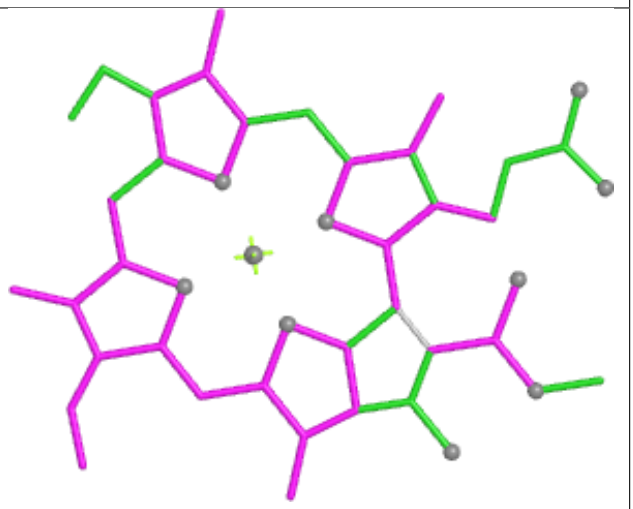
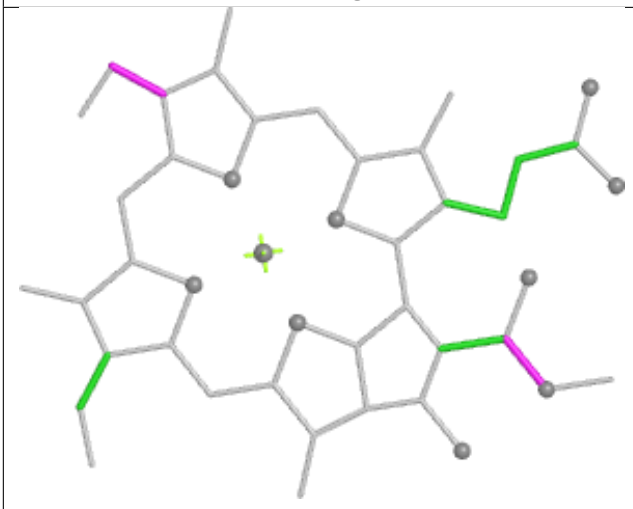


Bond angles

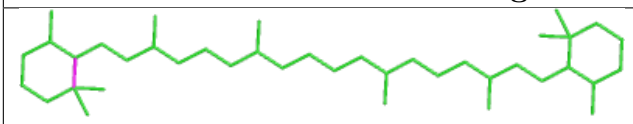


Torsions



Rings

Ligand BCR cM 101



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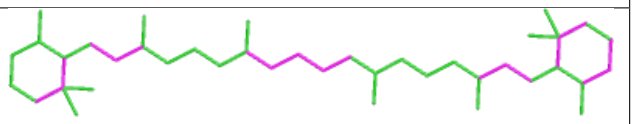
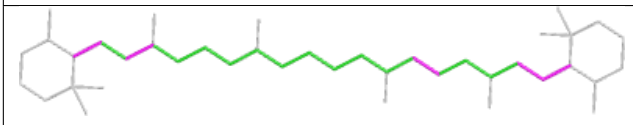


Bond angles



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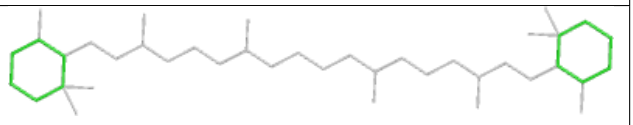
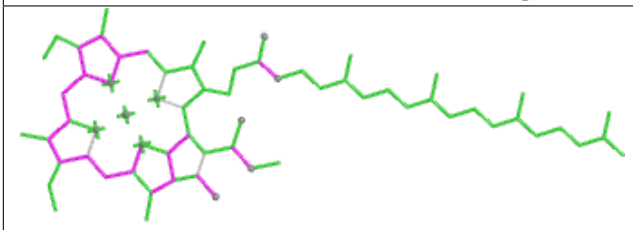


Rings

Ligand CLA cB 825



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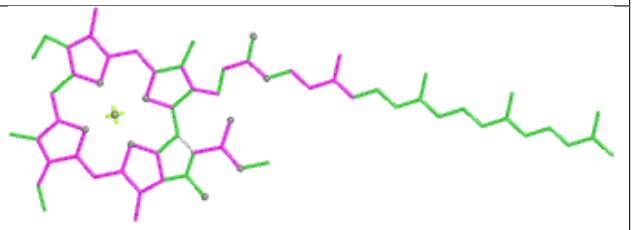
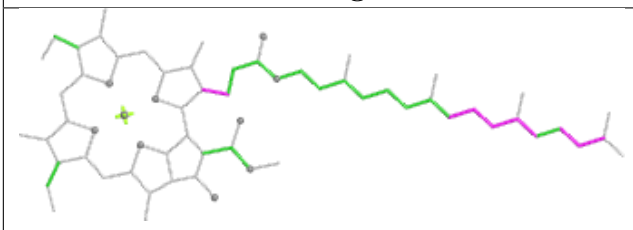


Bond angles



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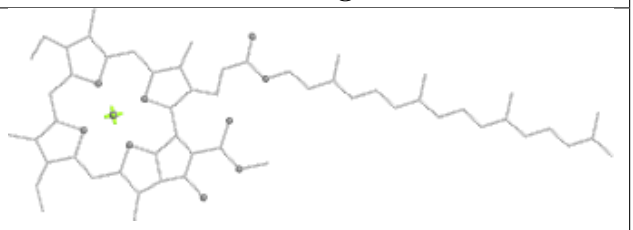
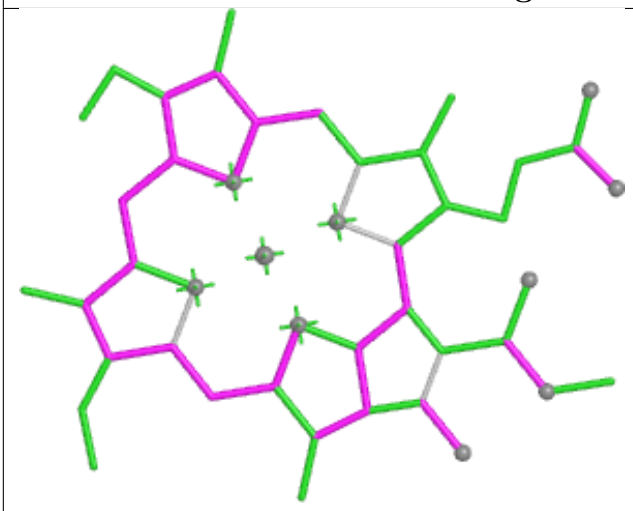


Rings

Ligand CLA aA 842



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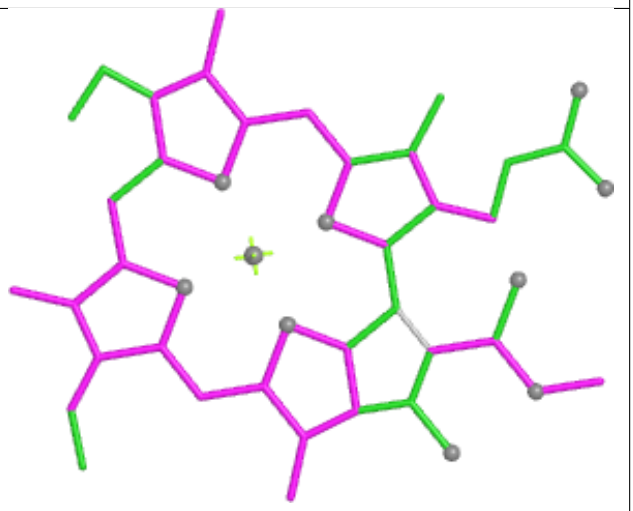
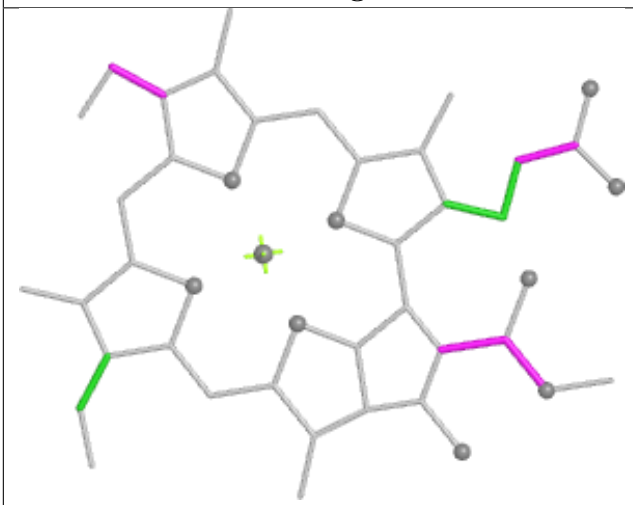


Bond angles



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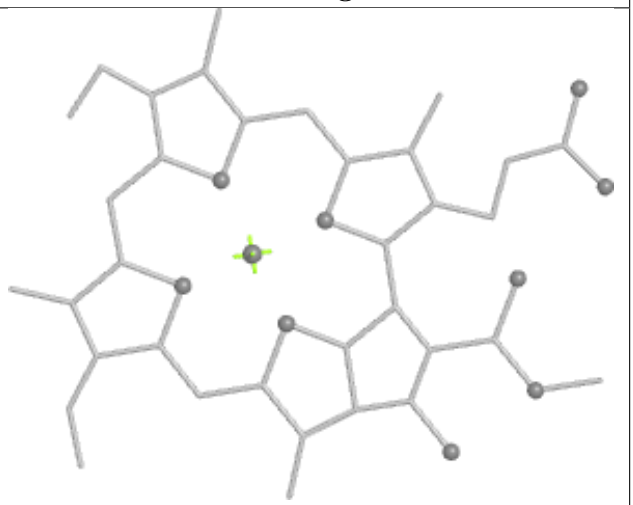
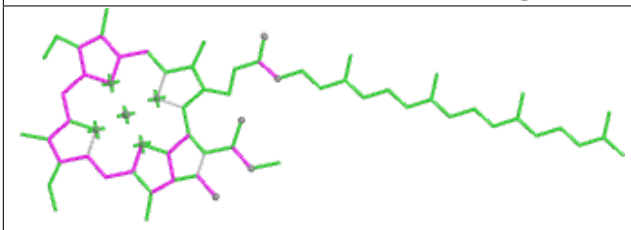
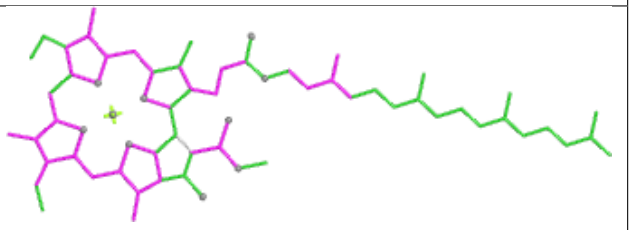


Rings

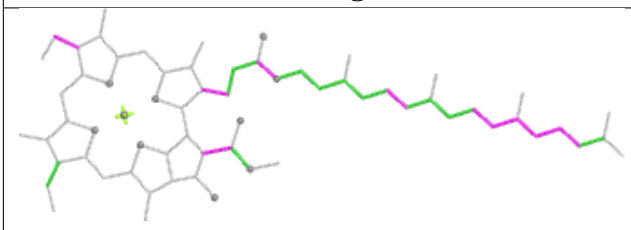
Ligand CLA cA 814



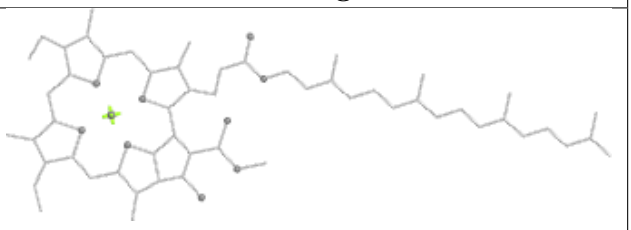
Bond lengths



Bond angles

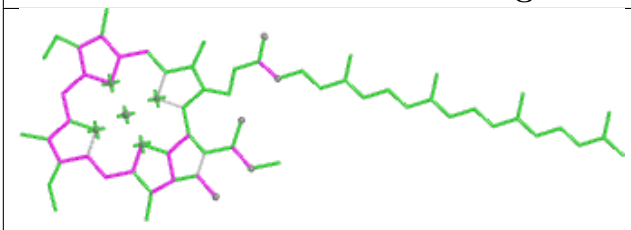


Torsions

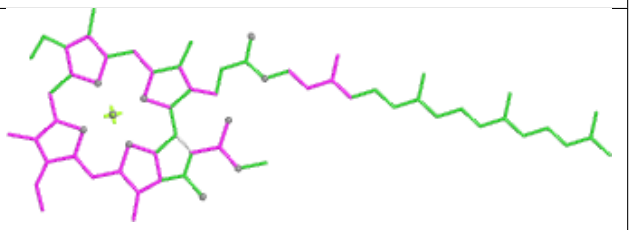


Rings

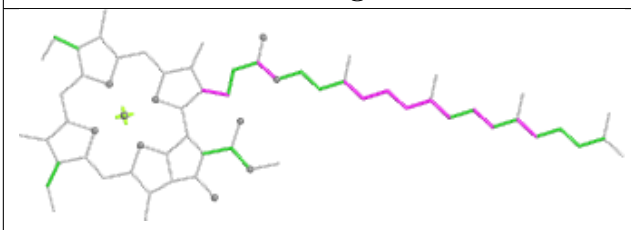
Ligand CLA cA 833



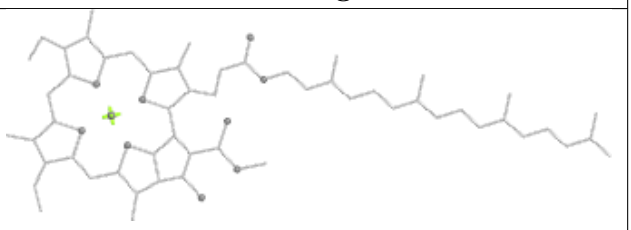
Bond lengths



Bond angles

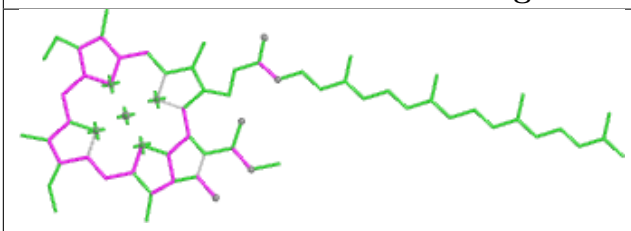


Torsions



Rings

Ligand CLA bA 829



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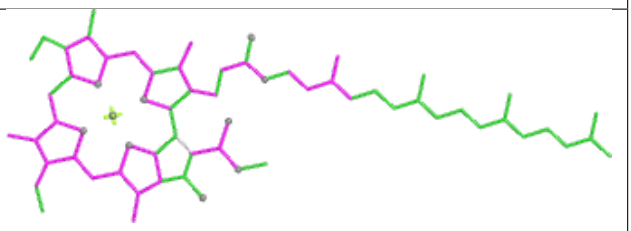
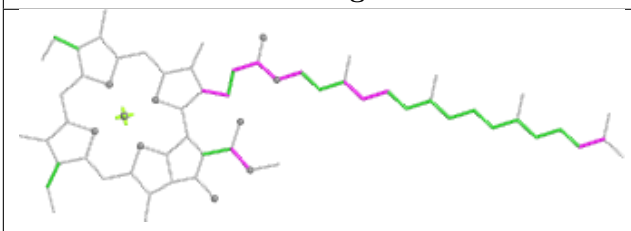


Bond angles



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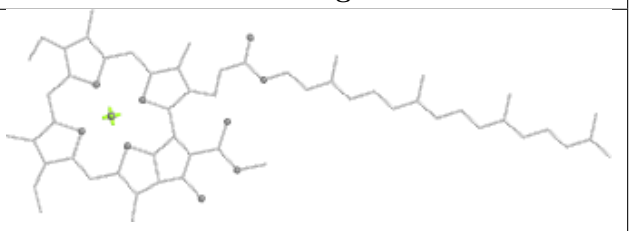
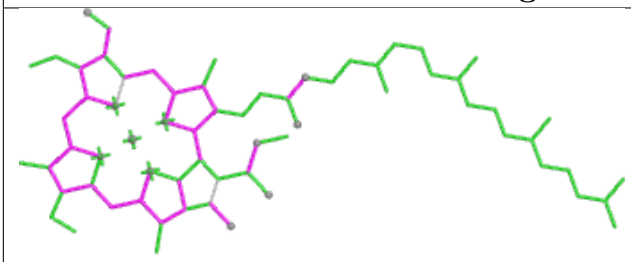
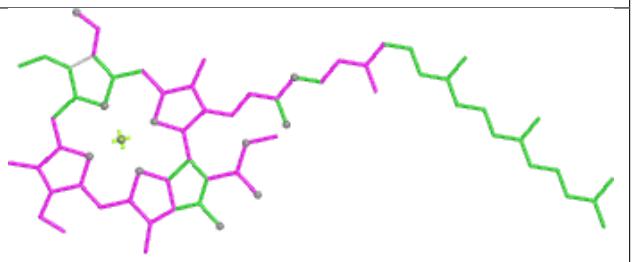


Rings

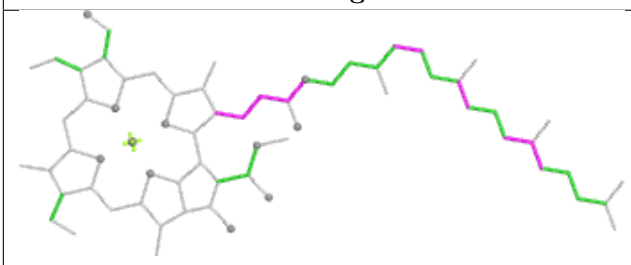
Ligand F6C aA 844



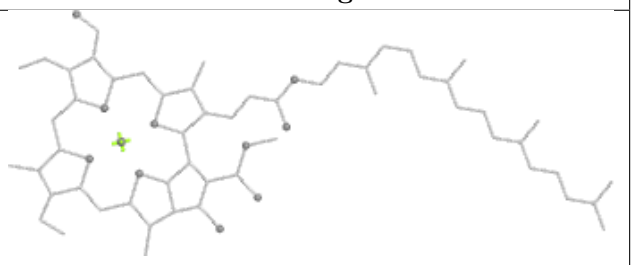
Bond lengths



Bond angles

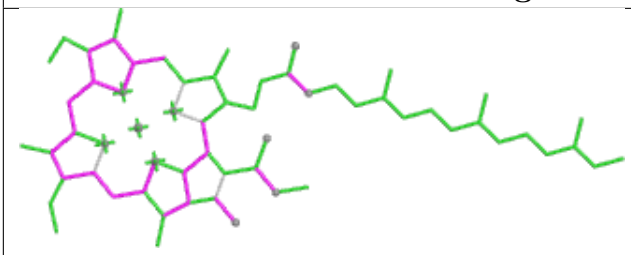


Torsions

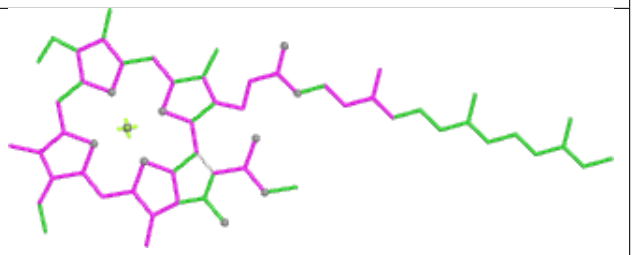


Rings

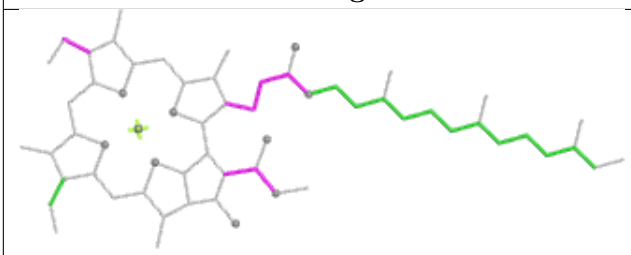
Ligand CLA bB 826



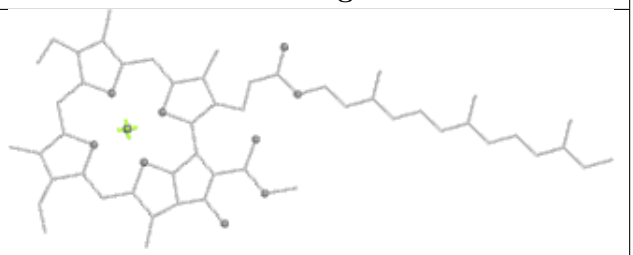
Bond lengths



Bond angles

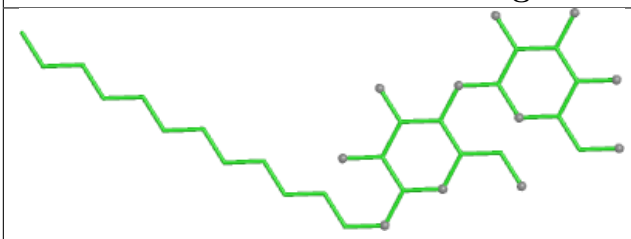


Torsions



Rings

Ligand LMT cA 853



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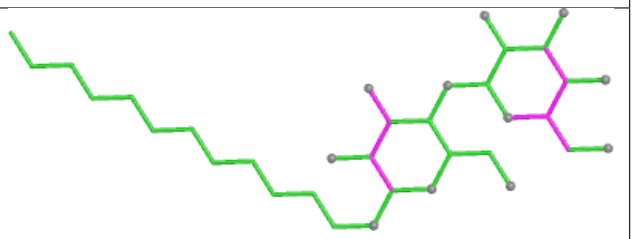
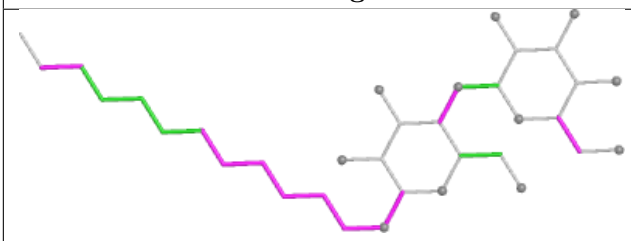


Bond angles



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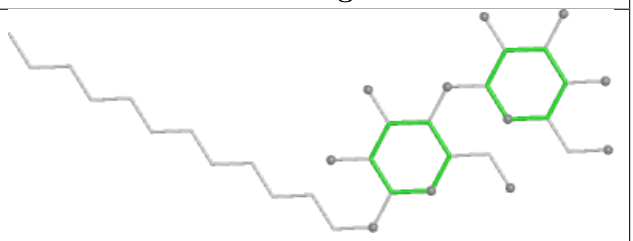
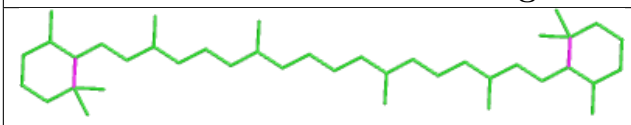


Rings

Ligand BCR bI 101



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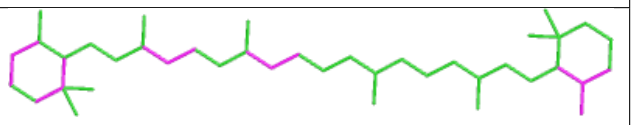
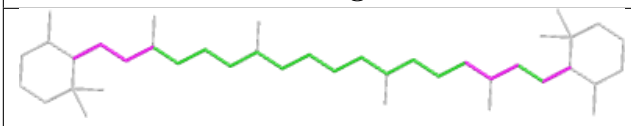


Bond angles



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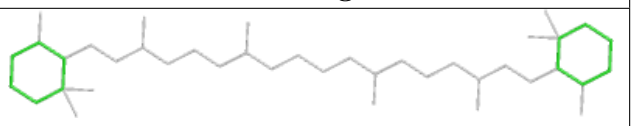
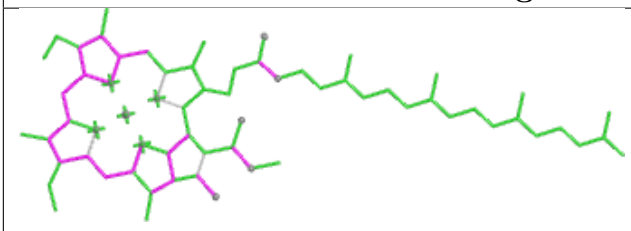


Rings

Ligand CLA cA 802



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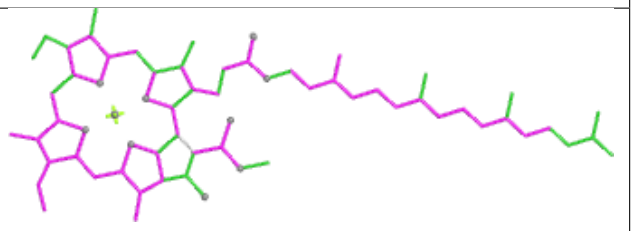
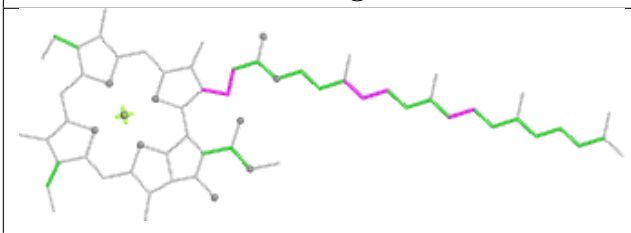


Bond angles



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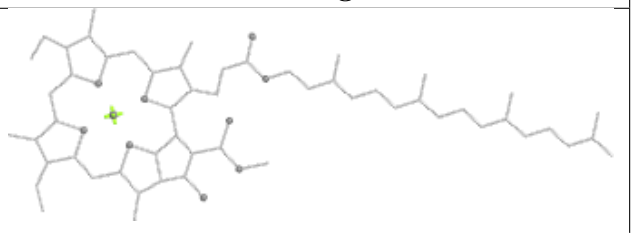
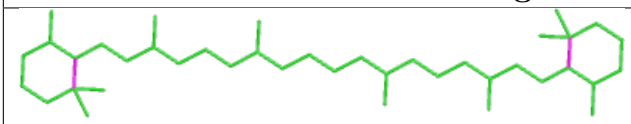
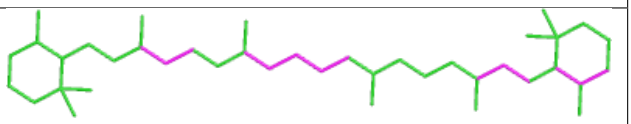
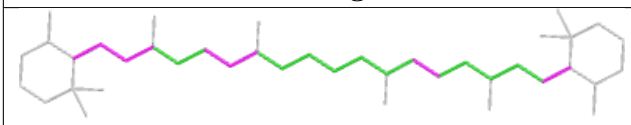
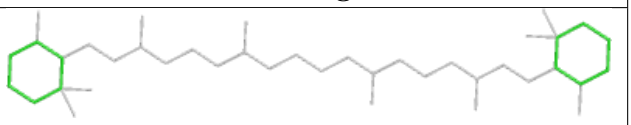
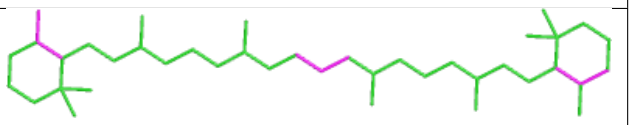
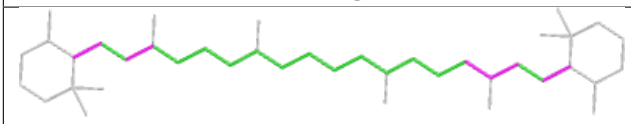
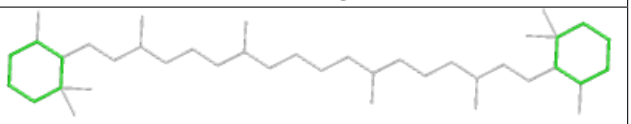
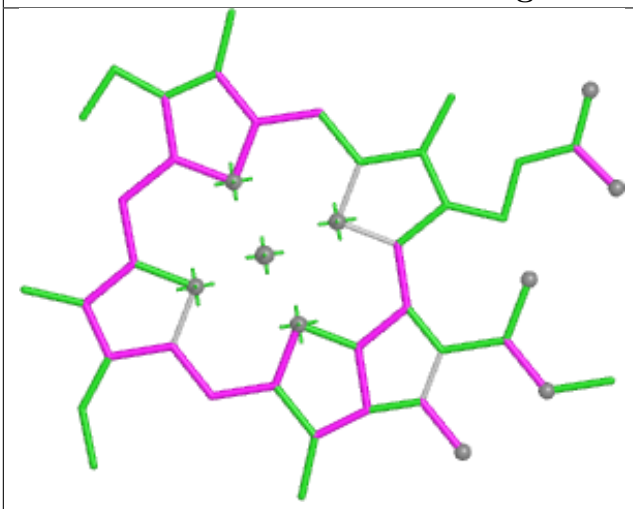


Rings

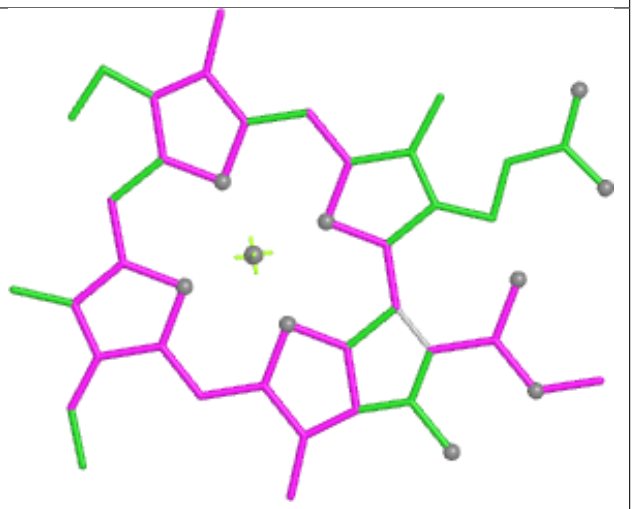
Ligand BCR aB 845	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR aB 843	
	
Bond lengths	Bond angles
	
Torsions	Rings

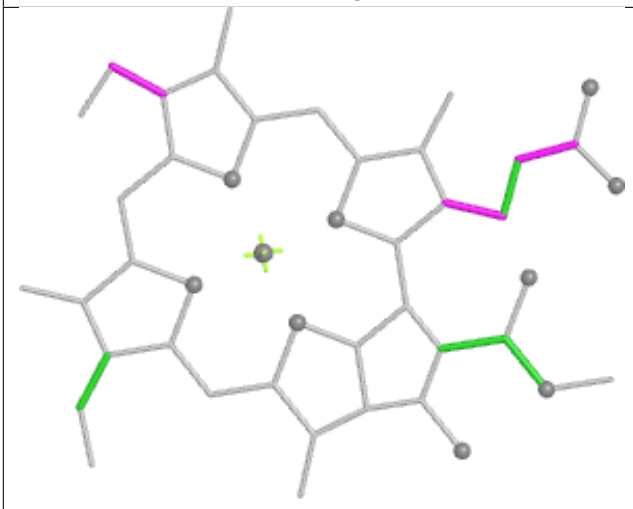
Ligand CLA cB 834



Bond lengths



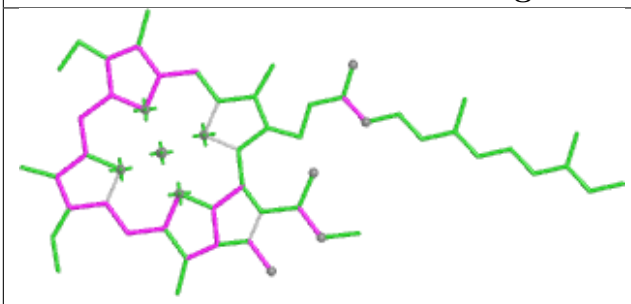
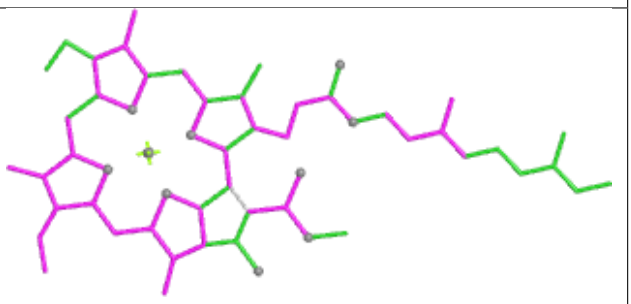
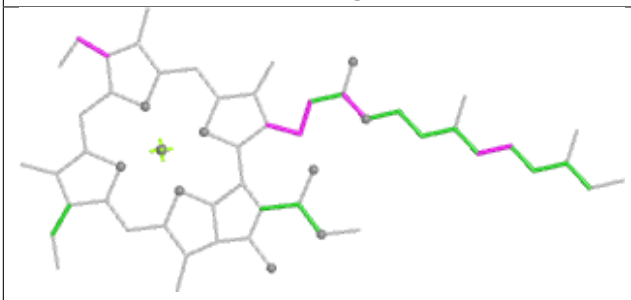
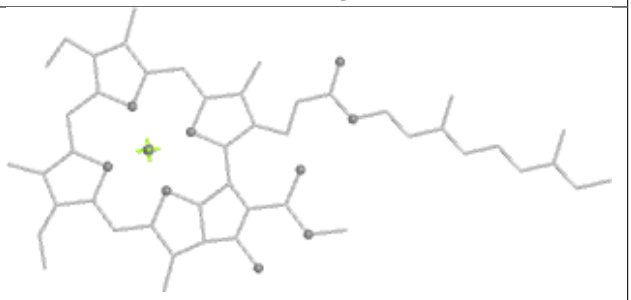
Bond angles



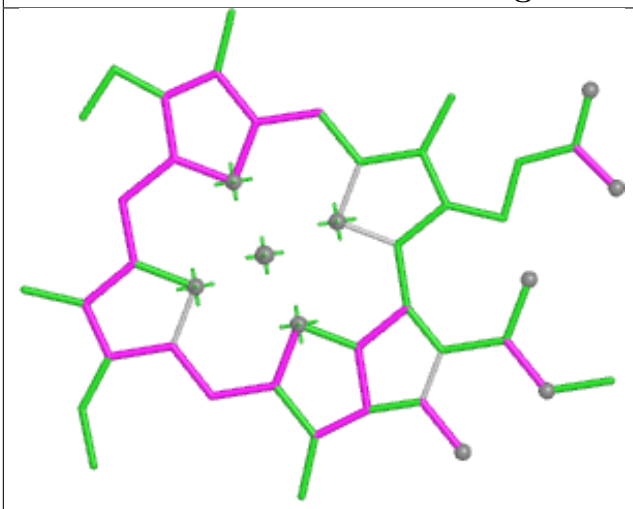
Torsions



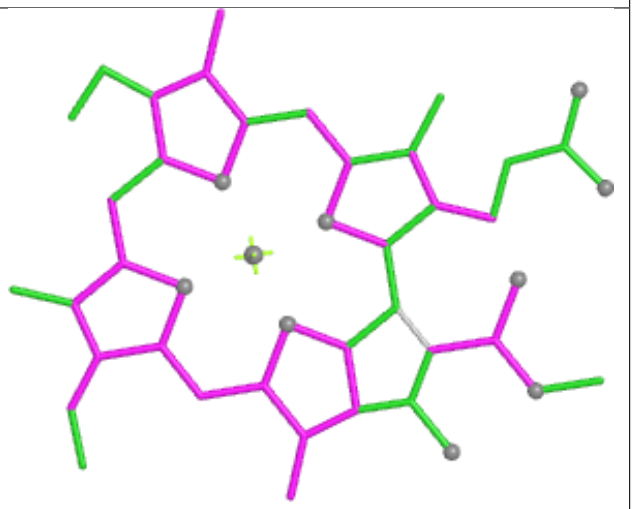
Rings

Ligand CLA bB 831	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

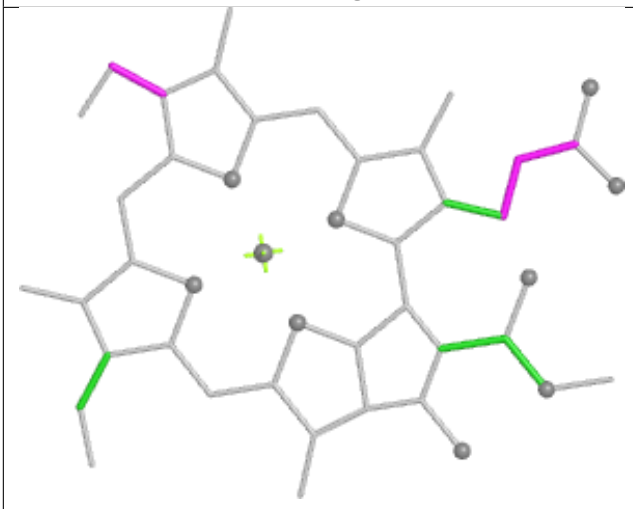
Ligand CLA bB 811



Bond lengths



Bond angles

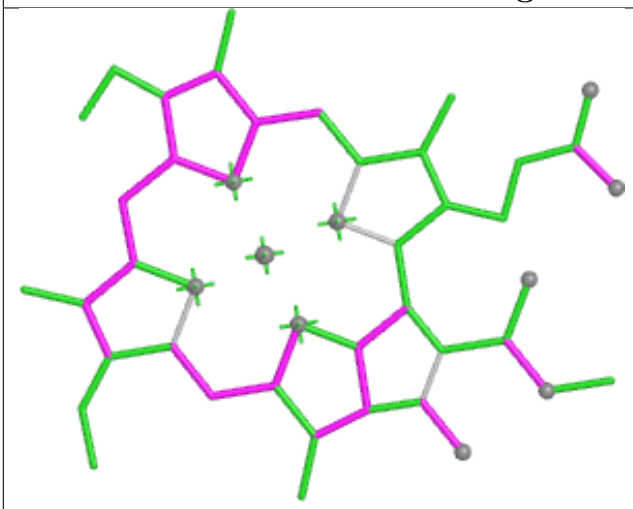


Torsions

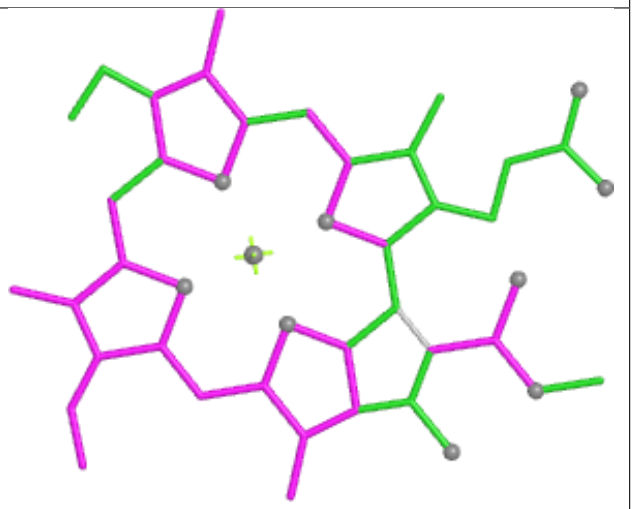


Rings

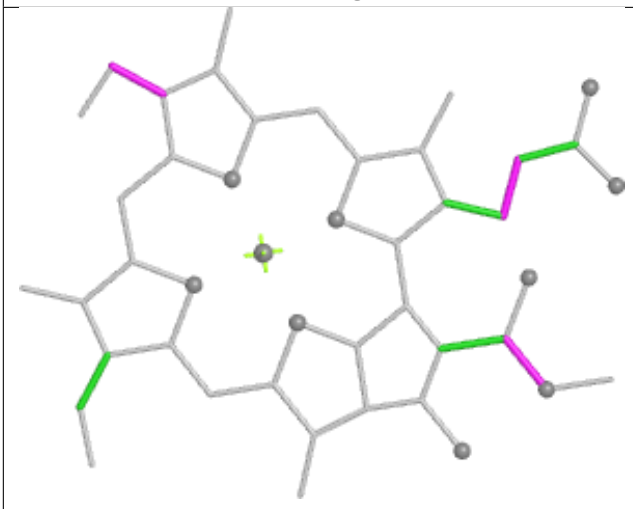
Ligand CLA cB 840



Bond lengths



Bond angles

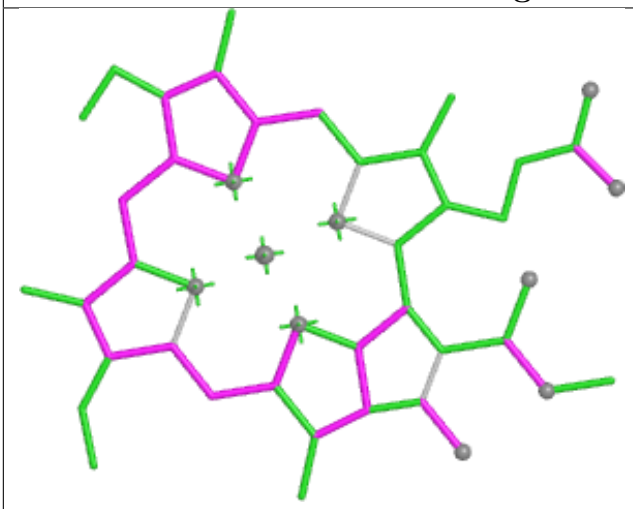


Torsions

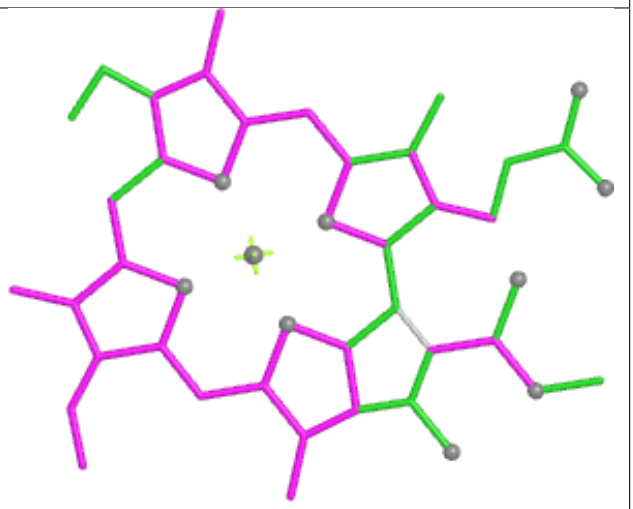


Rings

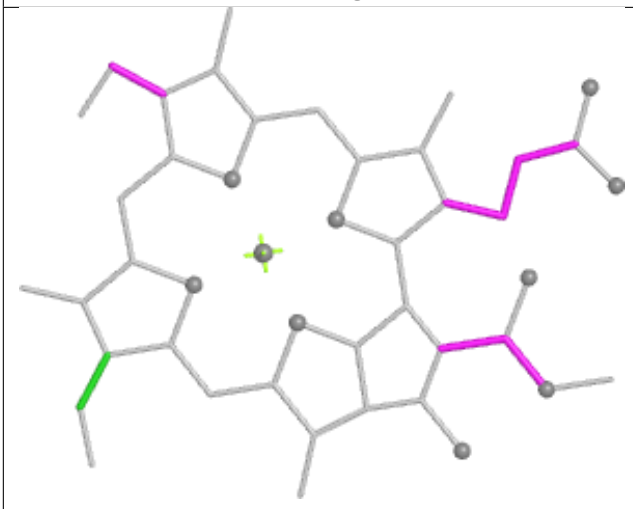
Ligand CLA bA 804



Bond lengths



Bond angles

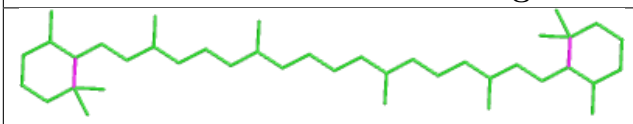


Torsions

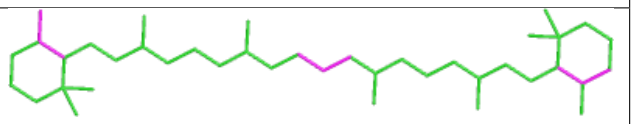


Rings

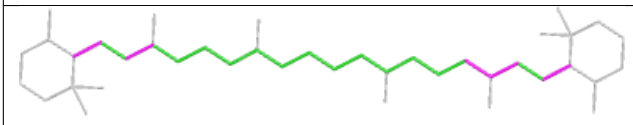
Ligand BCR bB 843



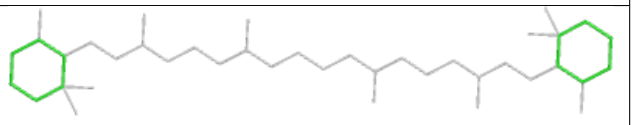
Bond lengths



Bond angles

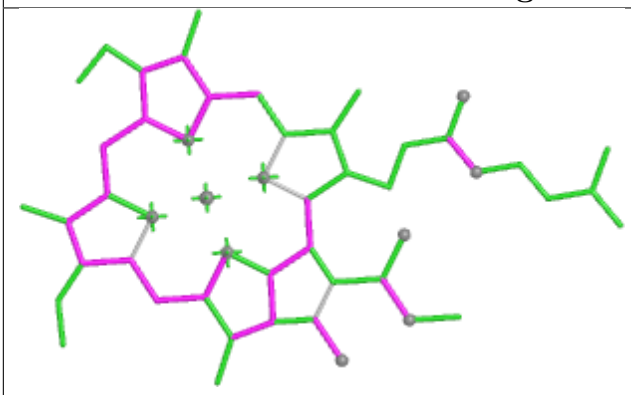


Torsions

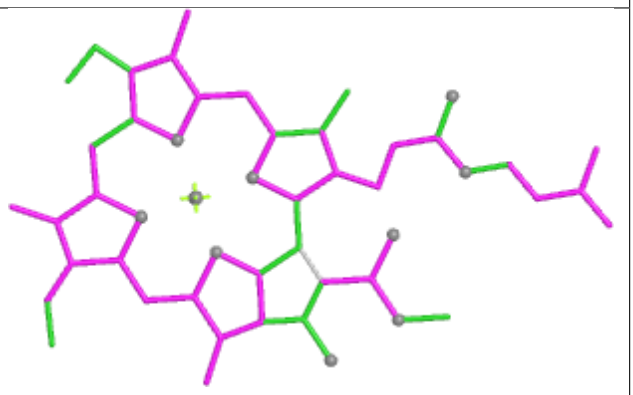


Rings

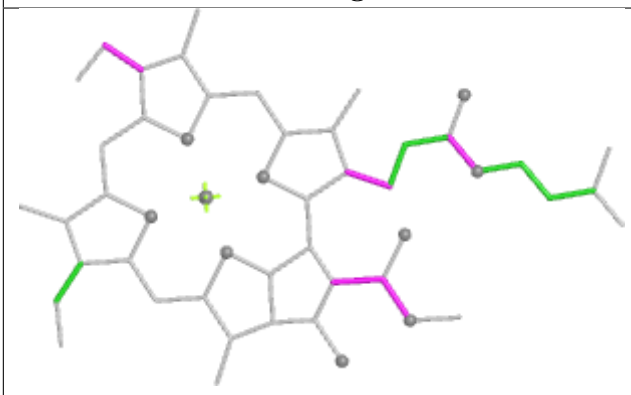
Ligand CLA cB 804



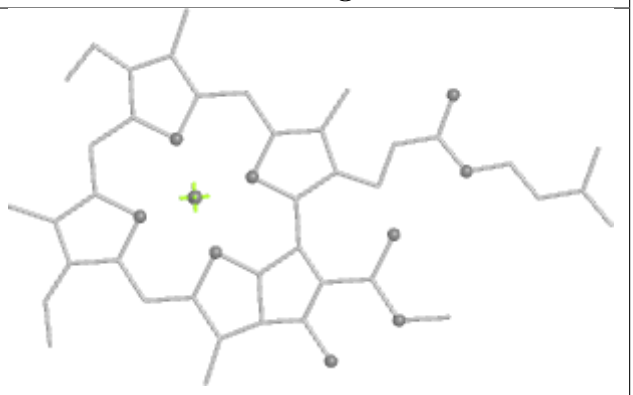
Bond lengths



Bond angles

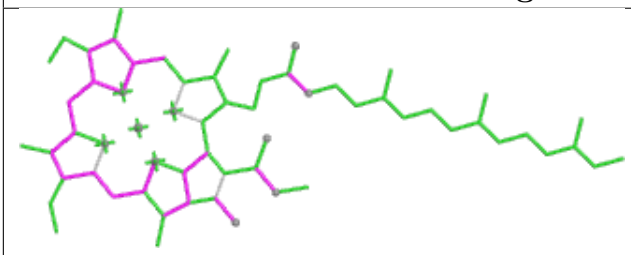


Torsions



Rings

Ligand CLA cB 807



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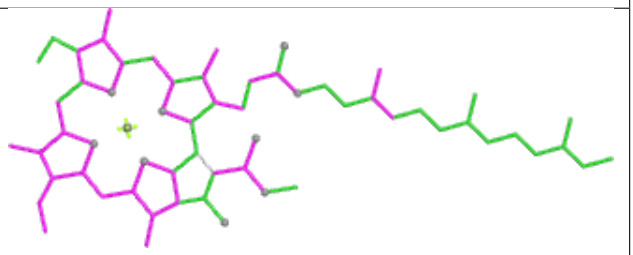
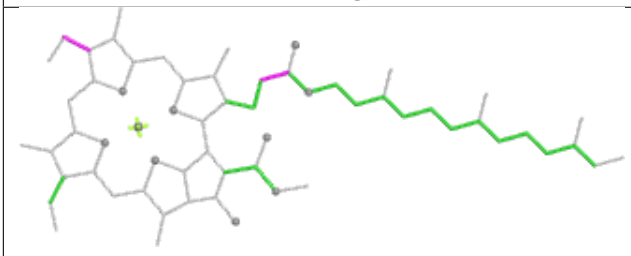


Bond angles



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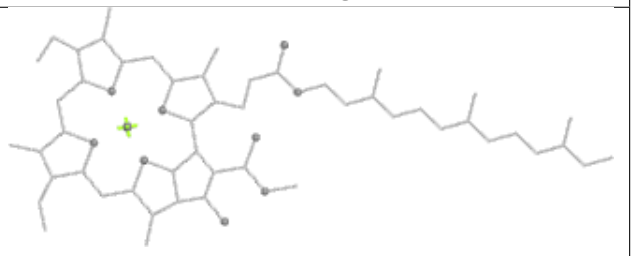
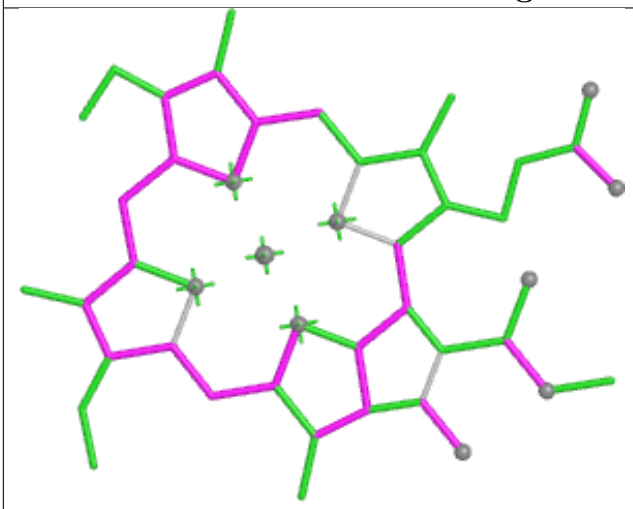


Rings

Ligand CLA aB 835



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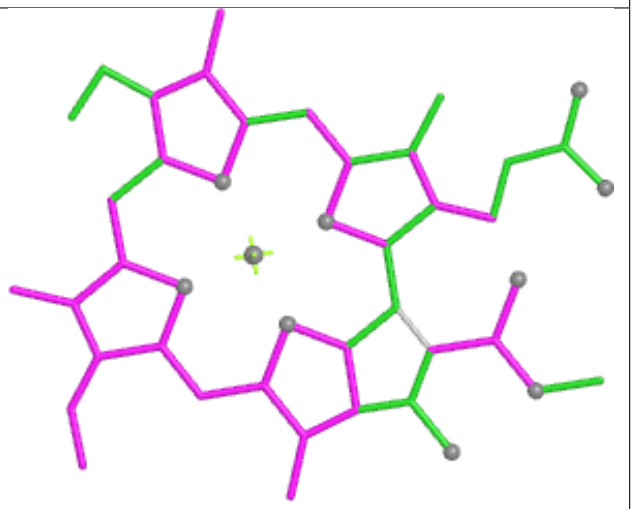
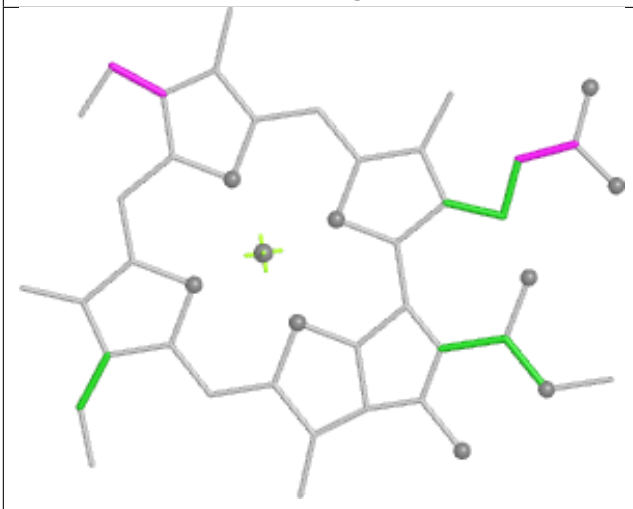


Bond angles

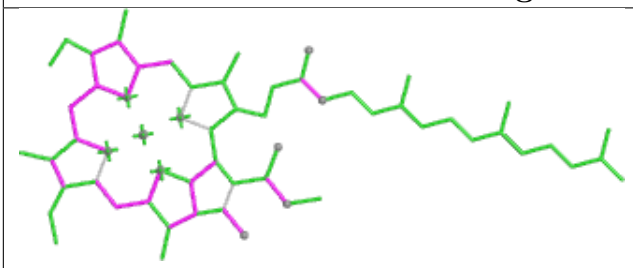


Torsions



Rings

Ligand CLA cA 828



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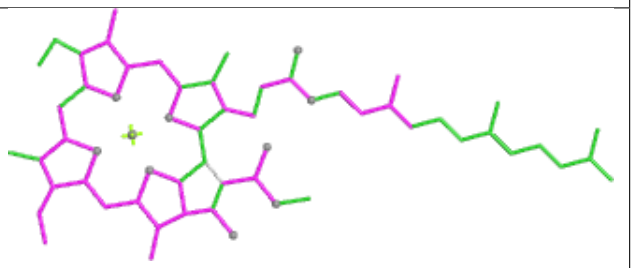
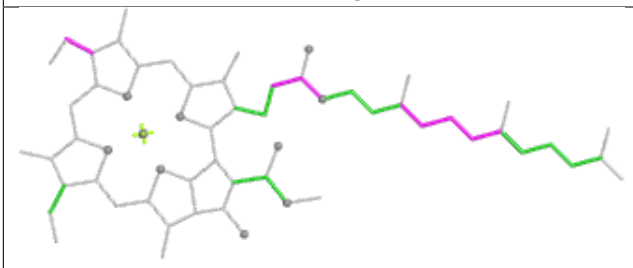


Bond angles



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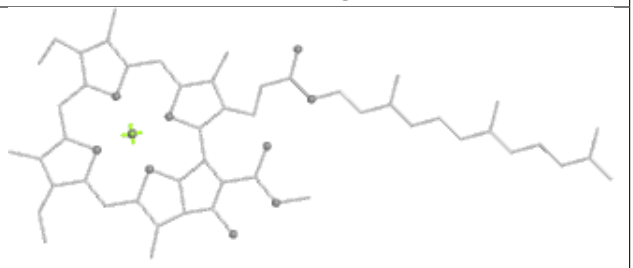
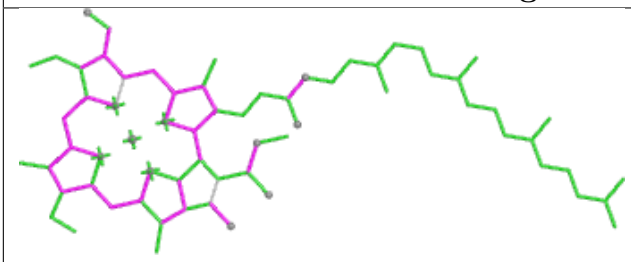


Rings

Ligand F6C cA 830



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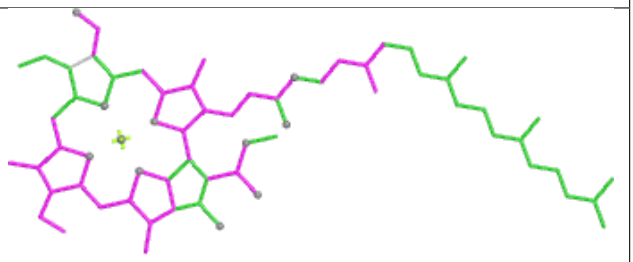
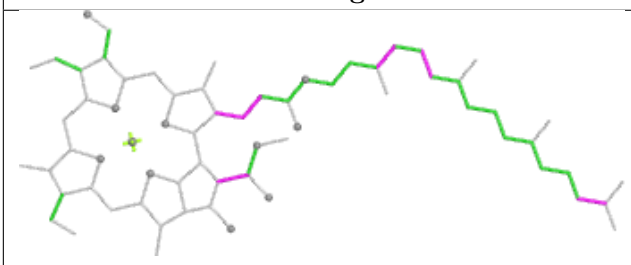


Bond angles



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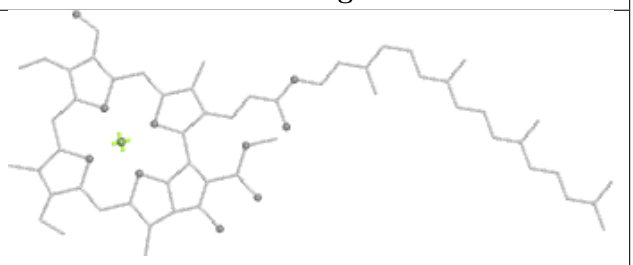
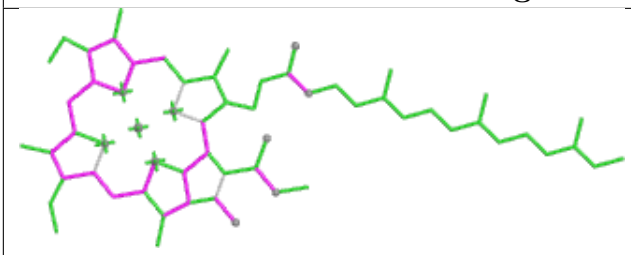


Rings

Ligand CLA bA 821



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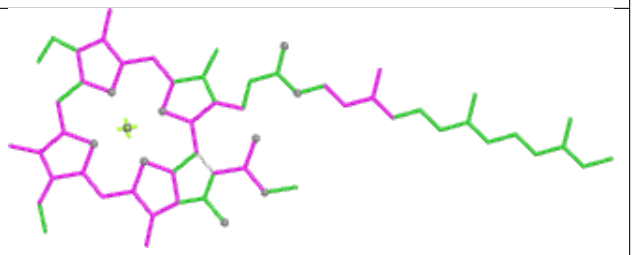
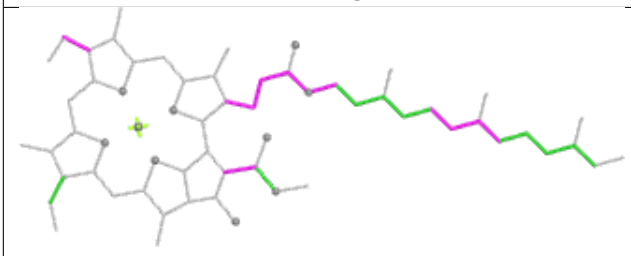


Bond angles



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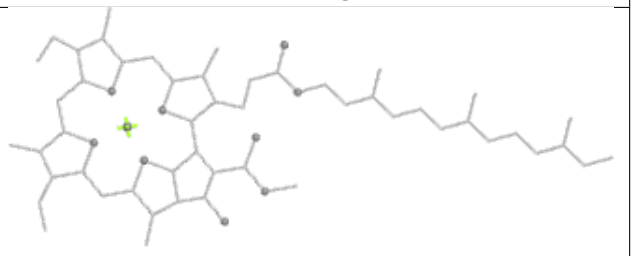
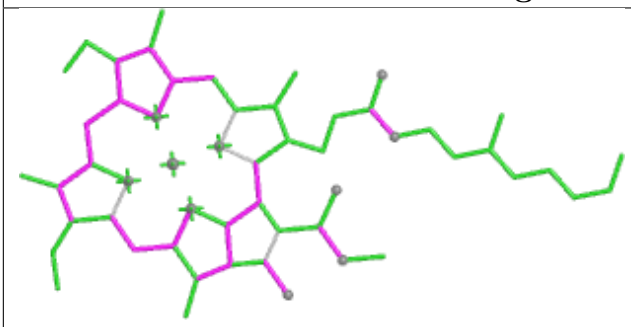


Rings

Ligand CLA aA 818



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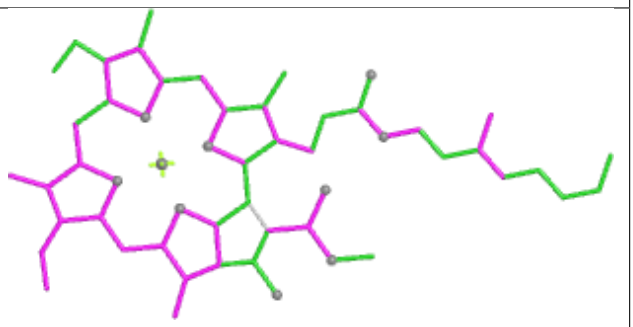
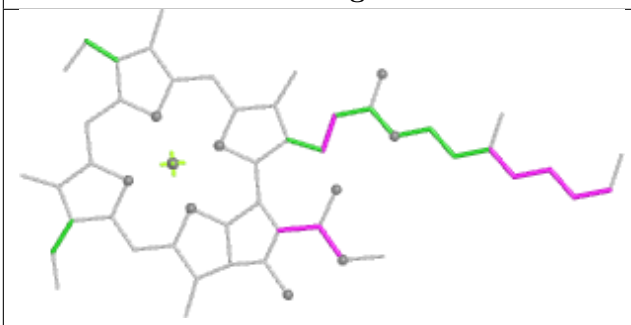


Bond angles



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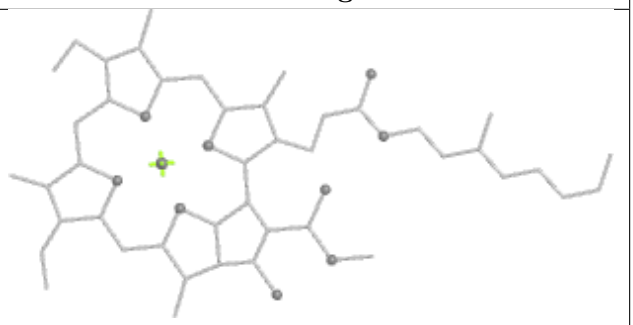
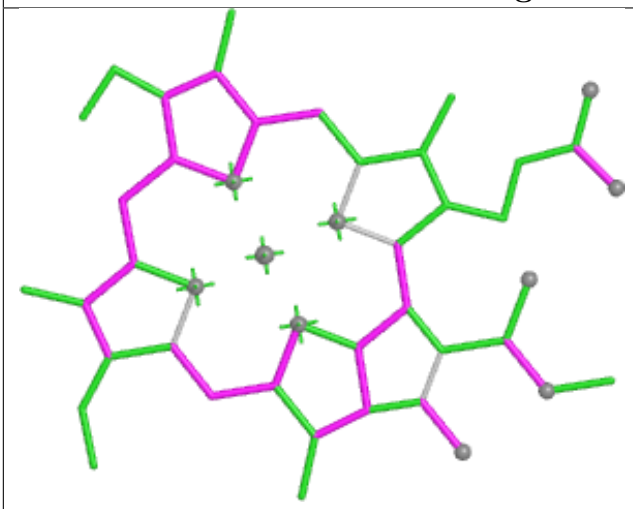


Rings

Ligand CLA aA 823



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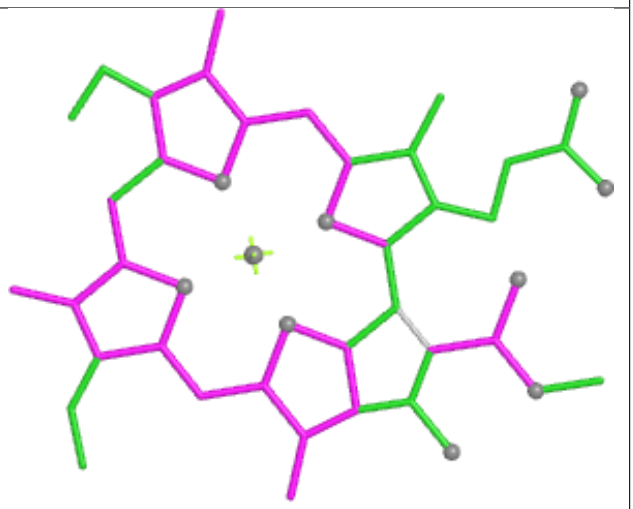
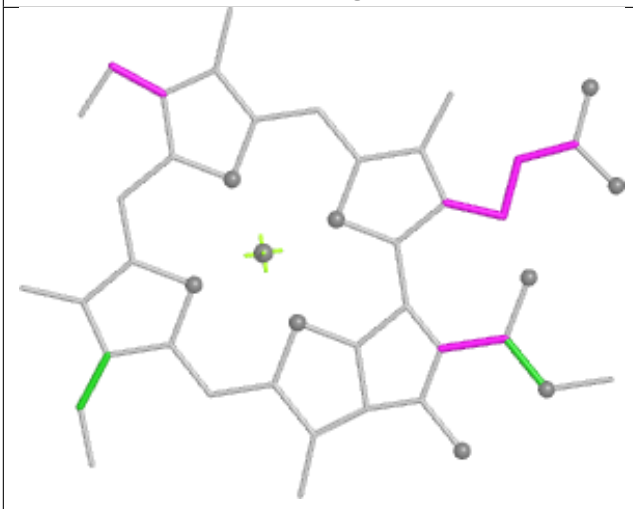


Bond angles

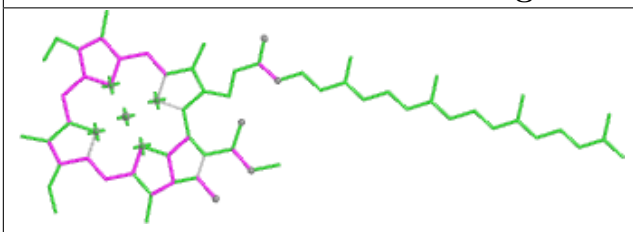


Torsions



Rings

Ligand CLA cA 806



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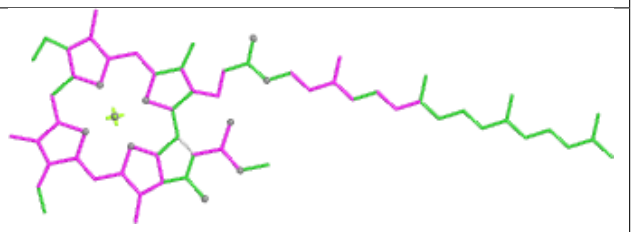

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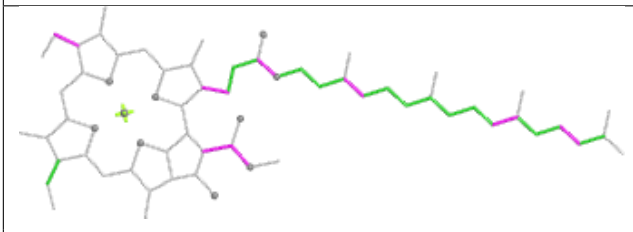

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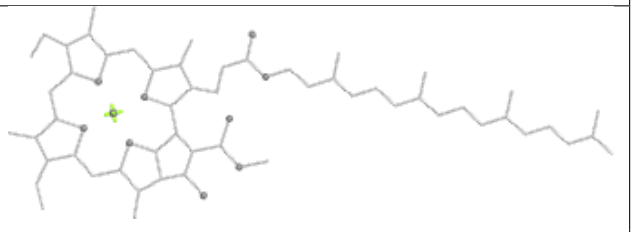
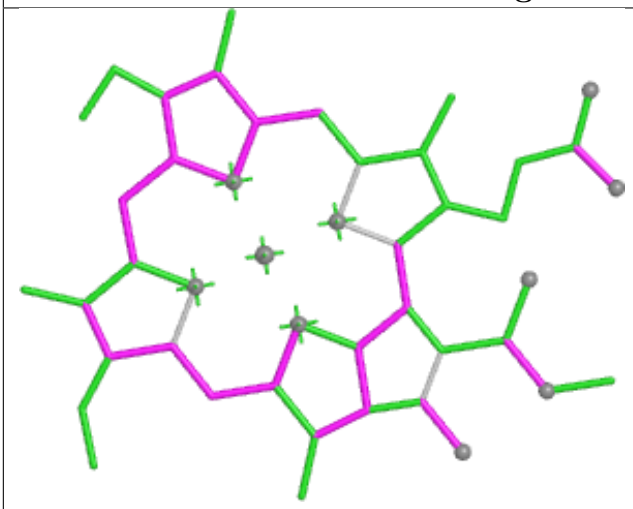


Rings

Ligand CLA aA 815



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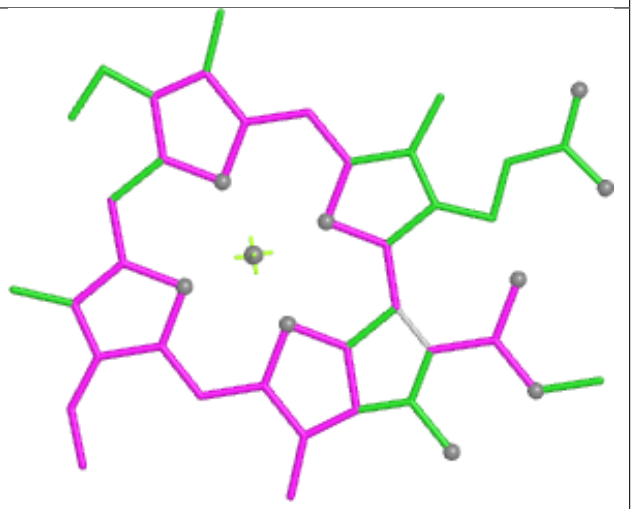
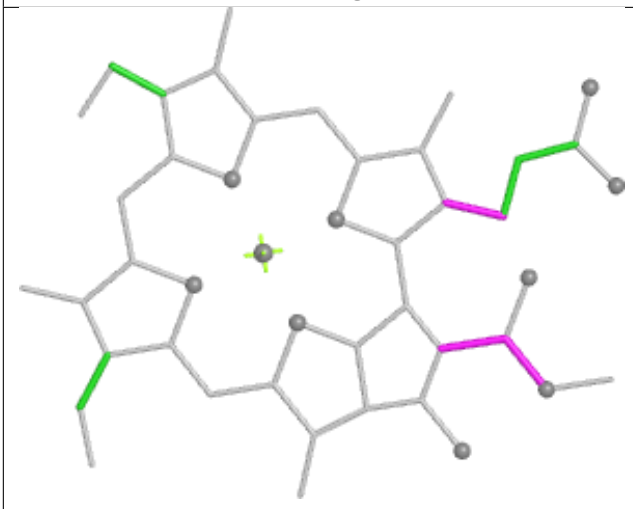


Bond angles

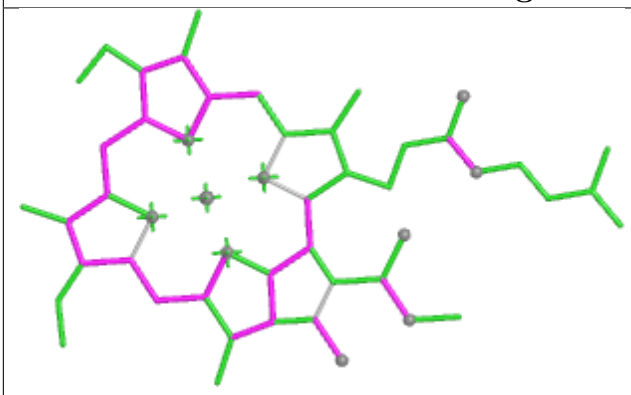


Torsions



Rings

Ligand CLA aB 804



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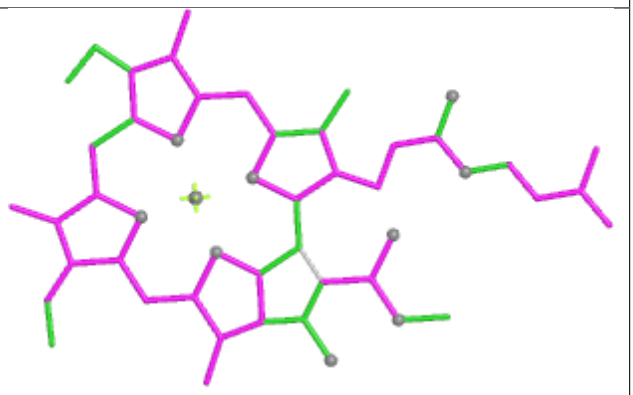
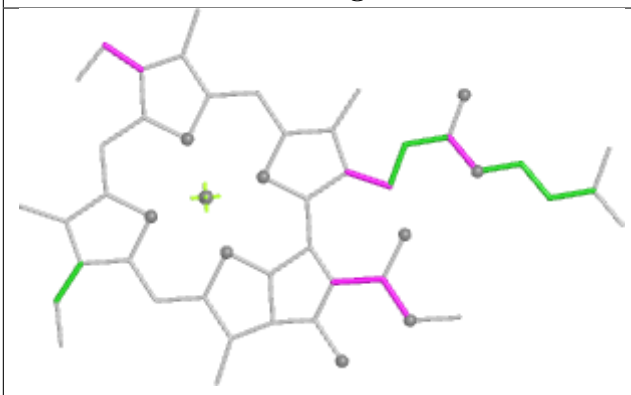


Bond angles



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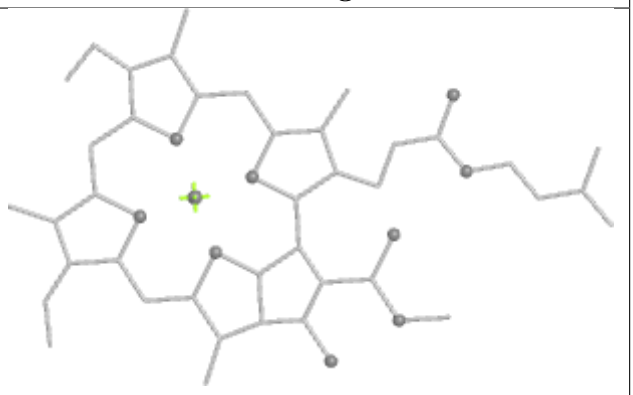
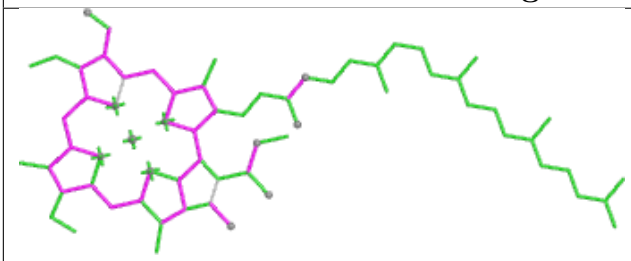


Rings

Ligand F6C aL 202



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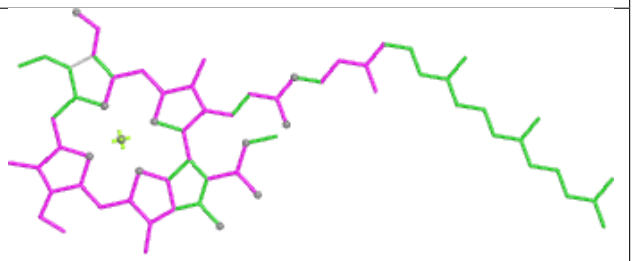

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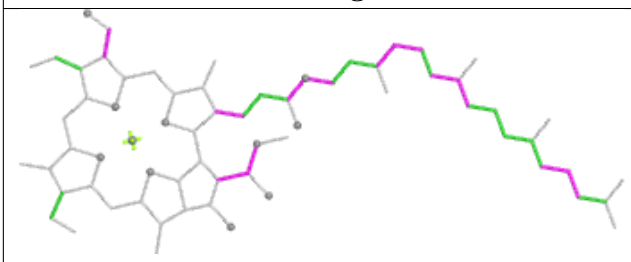

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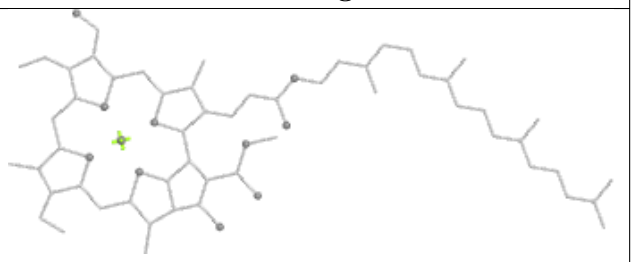
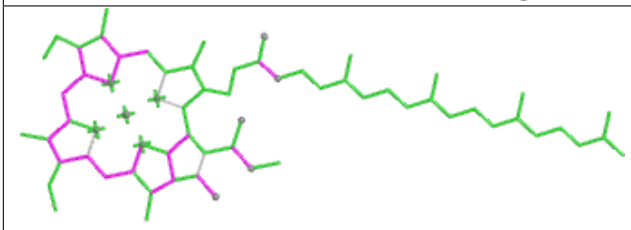


Rings

Ligand CLA aA 822



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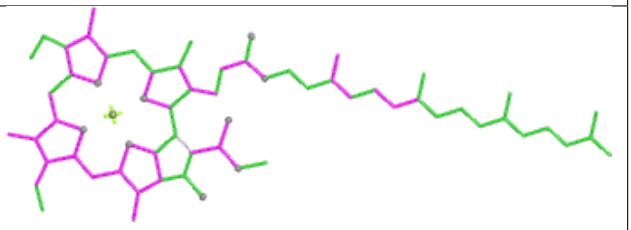
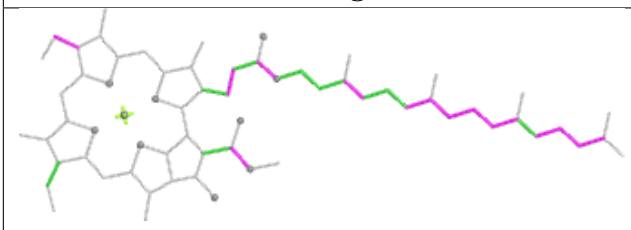


Bond angles



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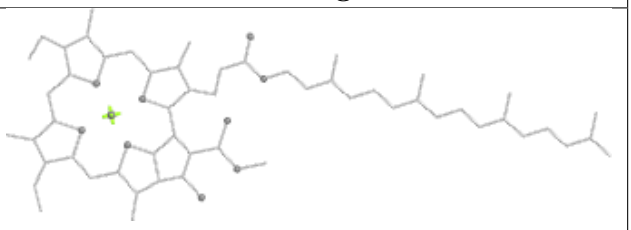
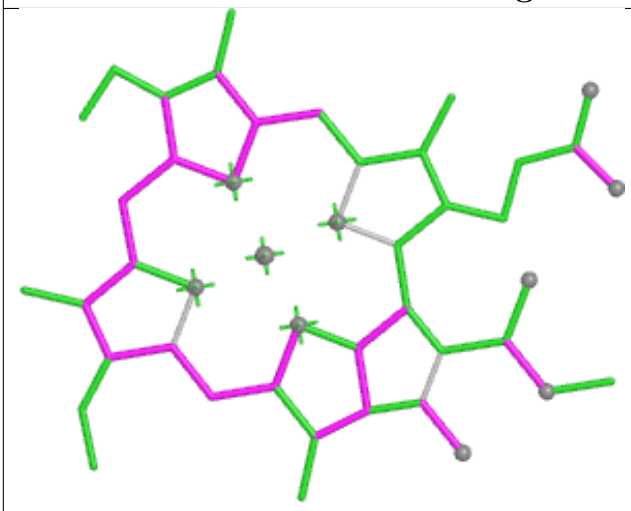


Rings

Ligand CLA cA 836



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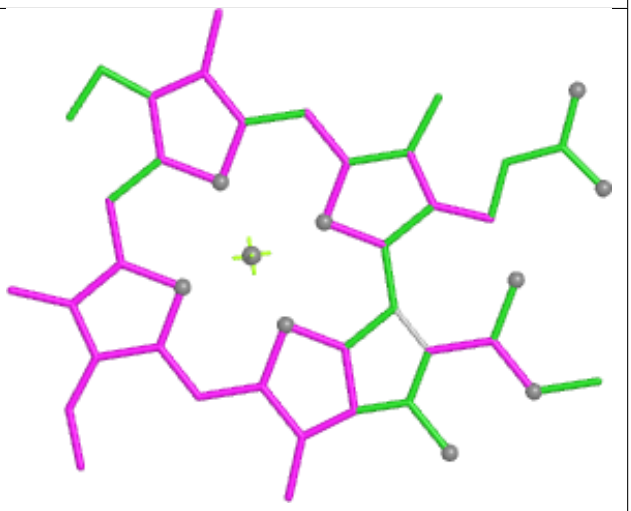
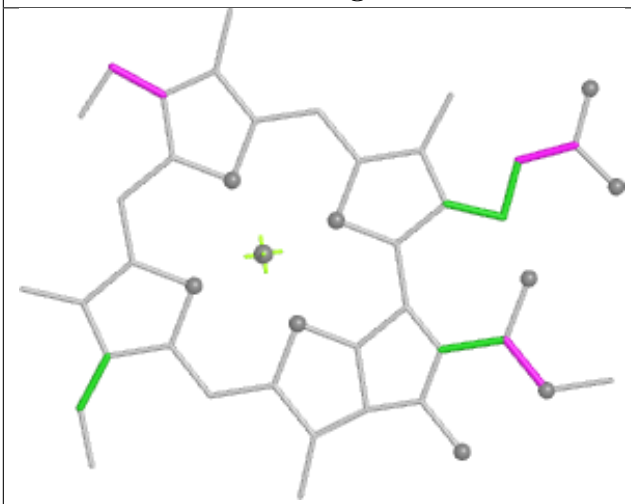


Bond angles



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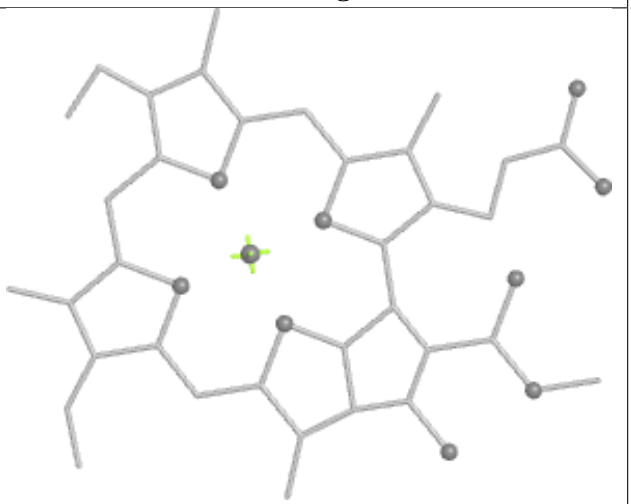
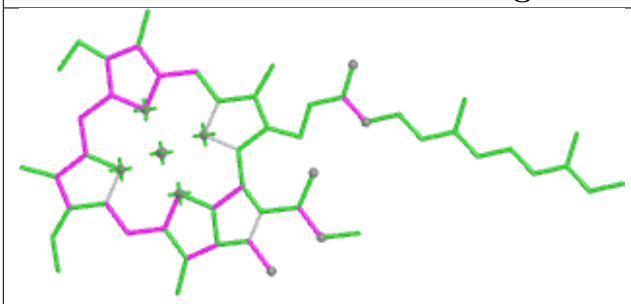
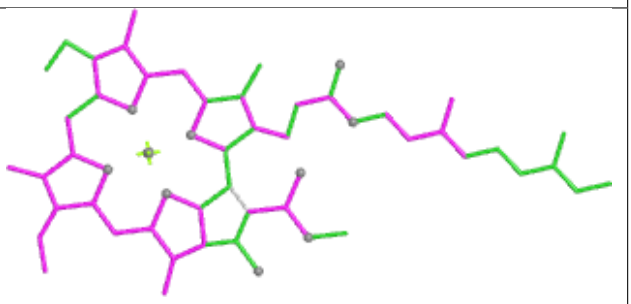
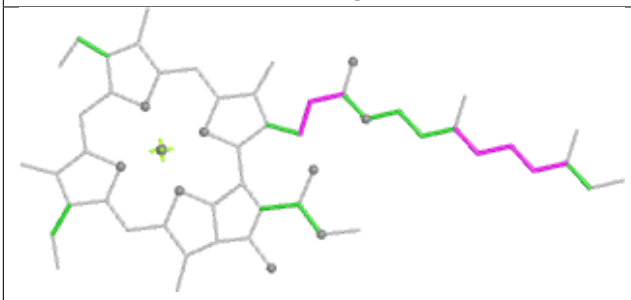
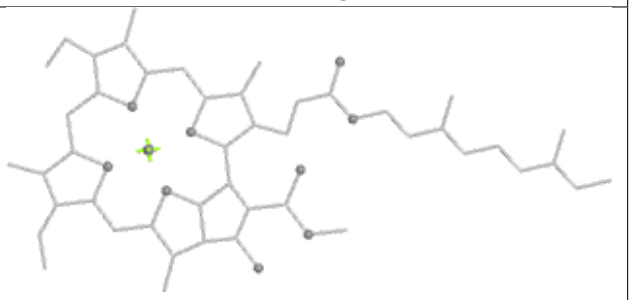


Rings

Ligand CLA bA 803	
	
Bond lengths	Bond angles
	
Torsions	Rings

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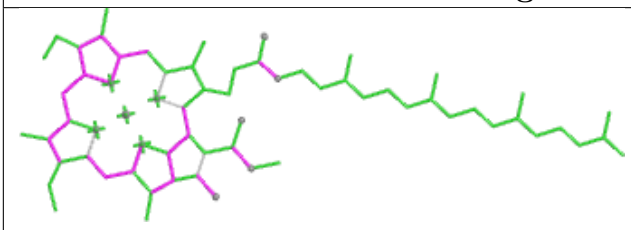
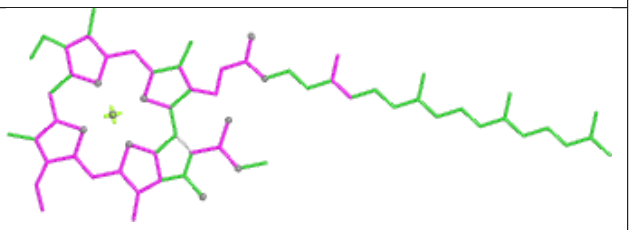
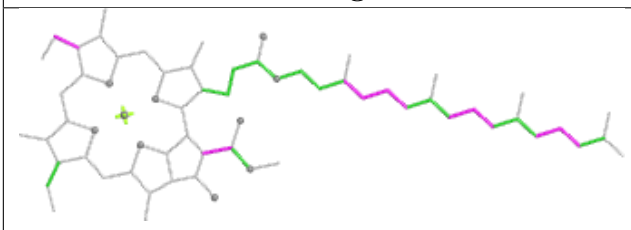
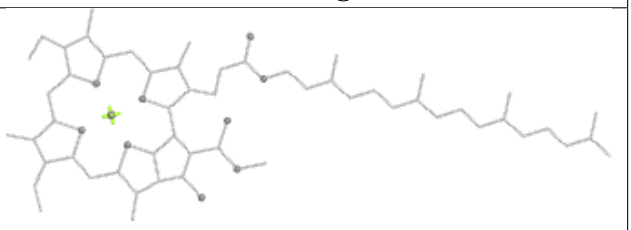
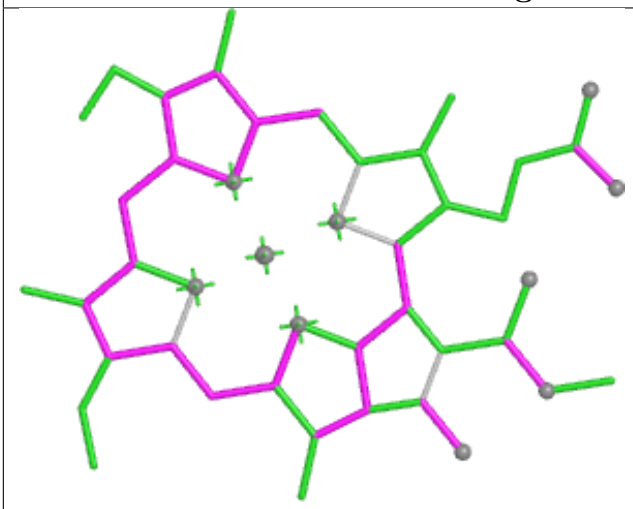
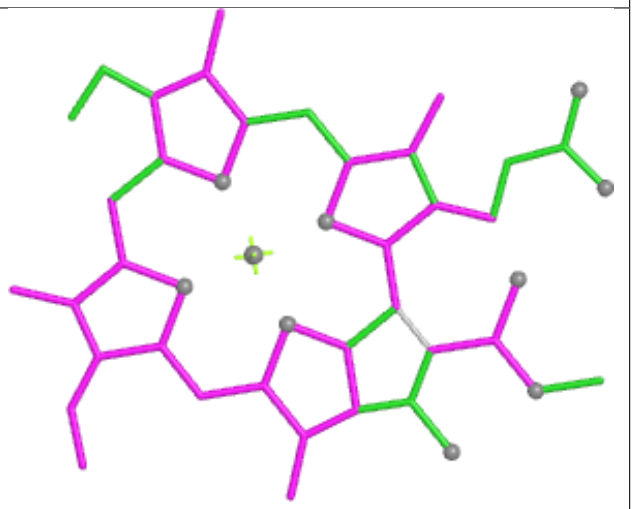
	
Bond lengths	Bond angles
	
Torsions	Rings

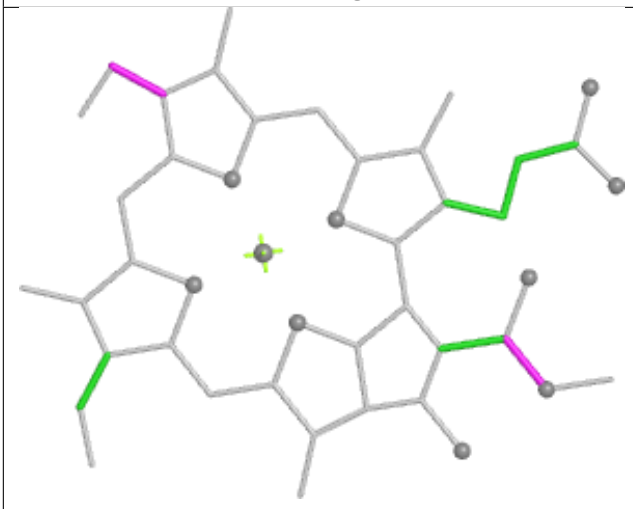
Ligand CLA aA 810



Bond lengths



Bond angles

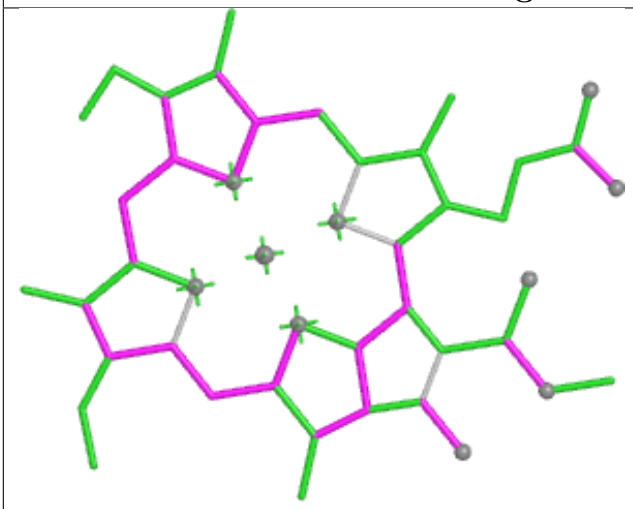


Torsions



Rings

Ligand CLA aB 829



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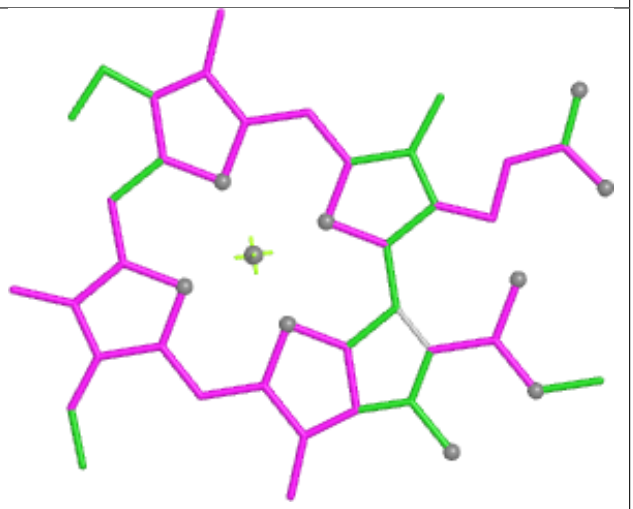

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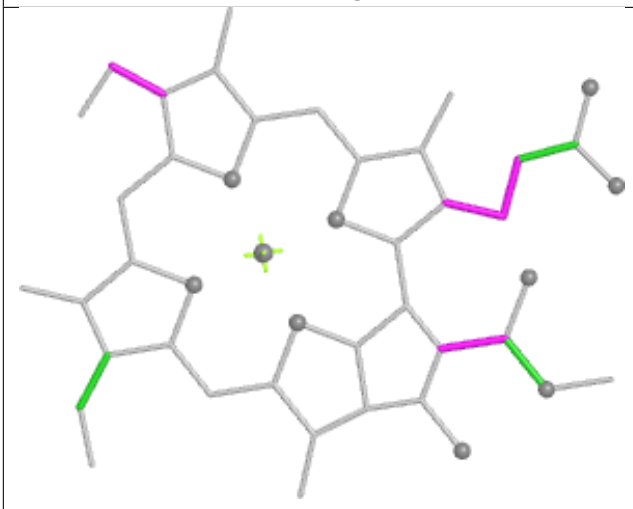
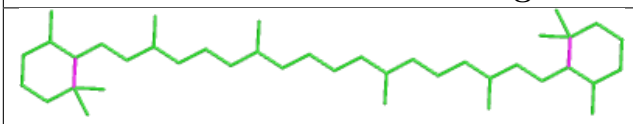


Torsions



Rings

Ligand BCR aB 842



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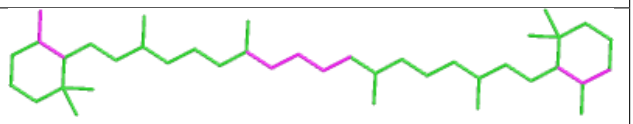
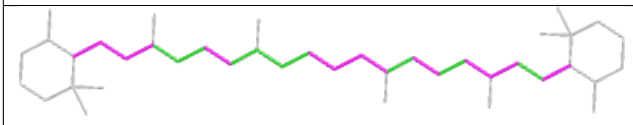


Bond angles



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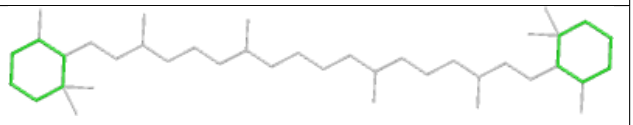
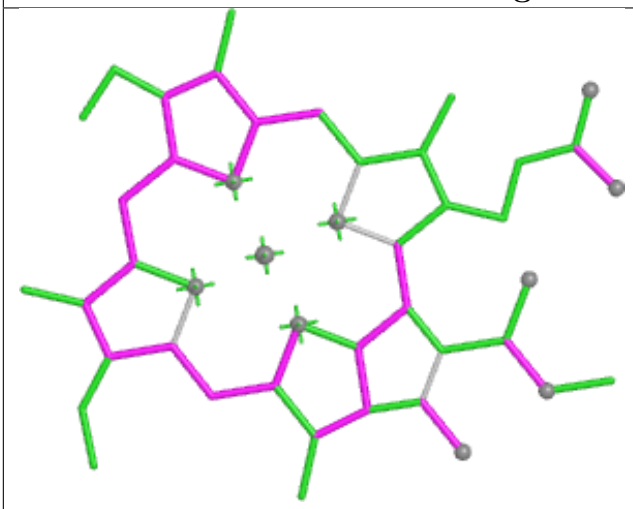


Rings

Ligand CLA bA 809



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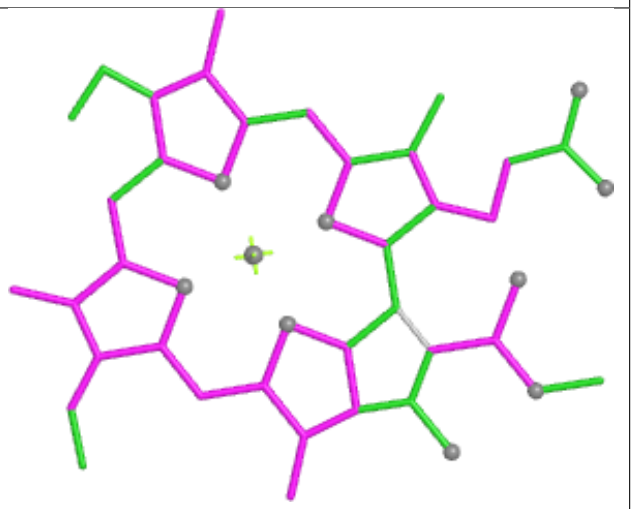

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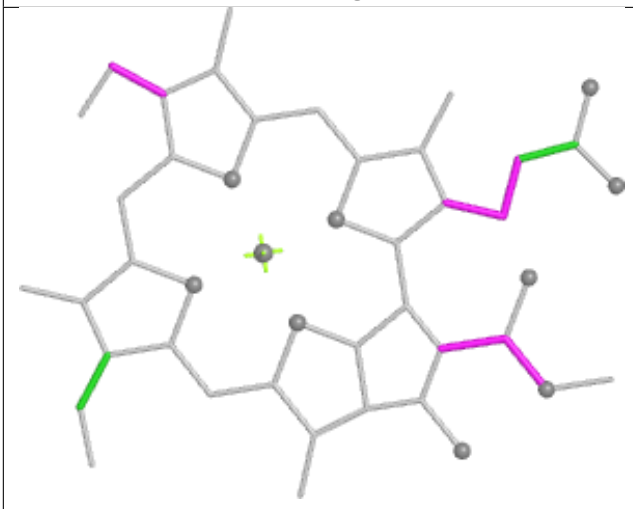
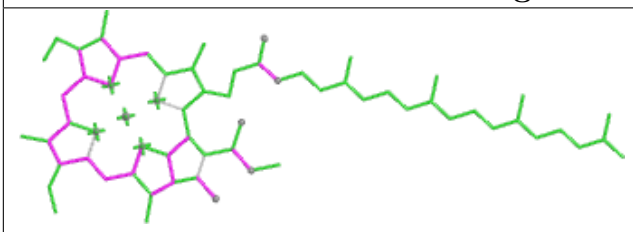


Torsions



Rings

Ligand CLA bA 835



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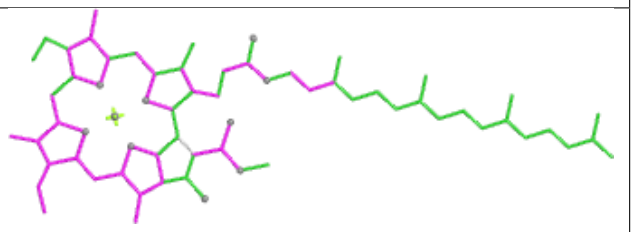
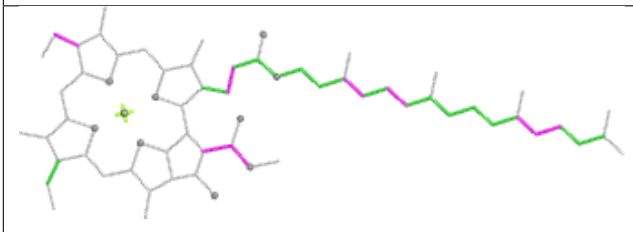


Bond angles



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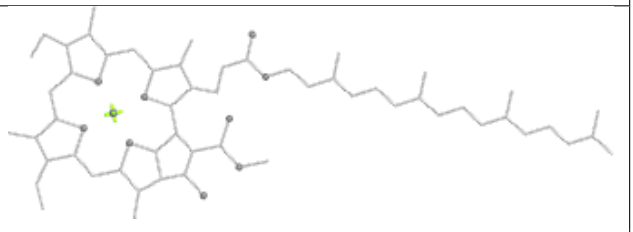
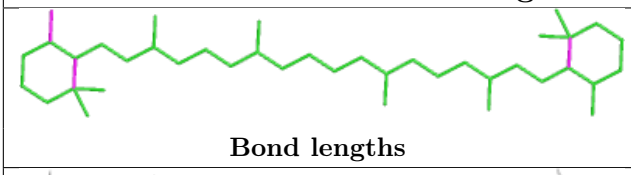


Rings

Ligand BCR cL 203



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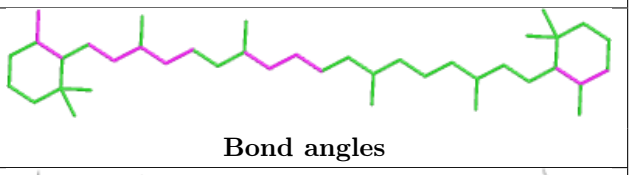

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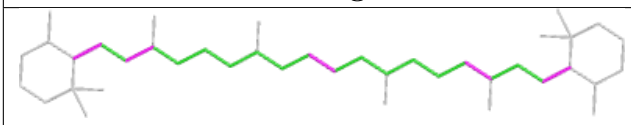

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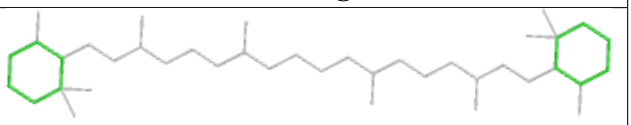
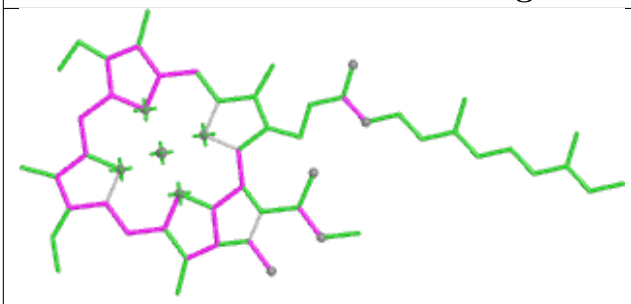


Rings

Ligand CLA aB 813



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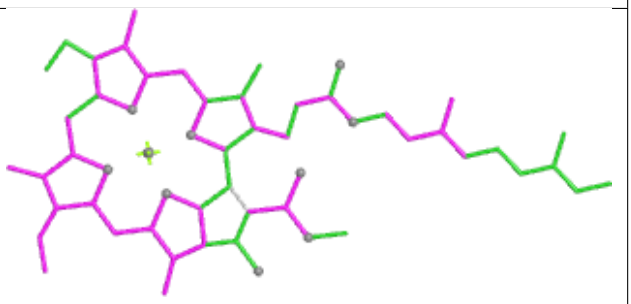

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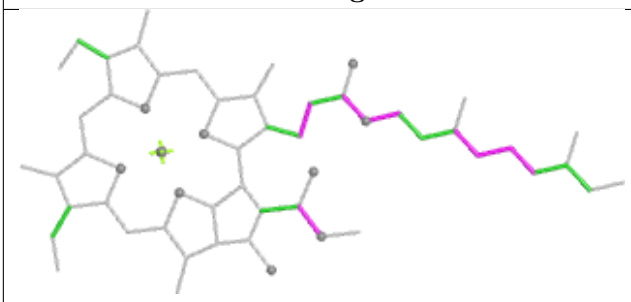

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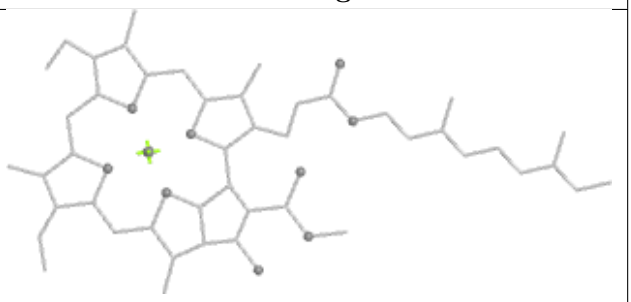
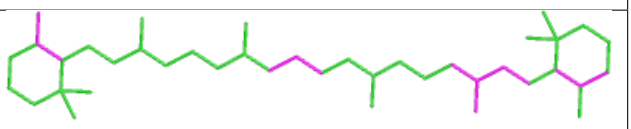


Rings

Ligand BCR aA 848



Bond lengths



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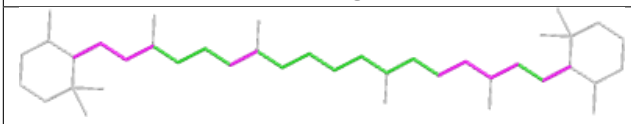

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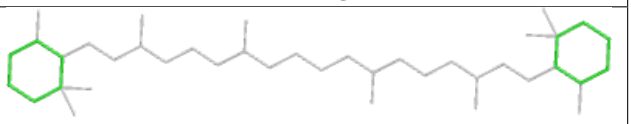
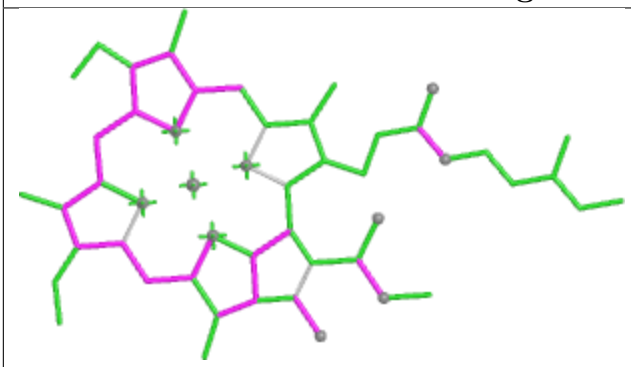


Rings

Ligand CLA cB 836



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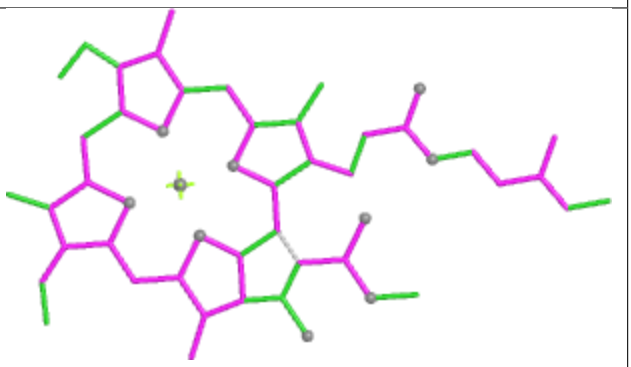
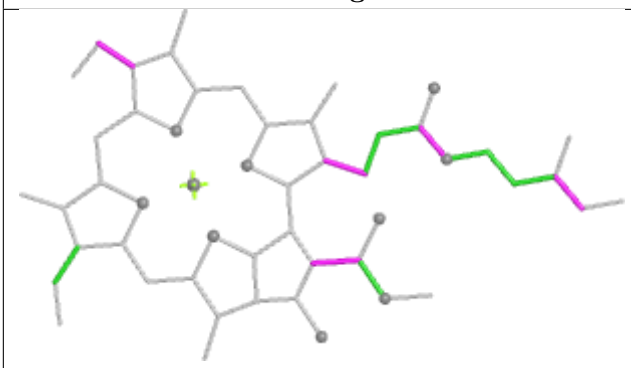


Bond angles



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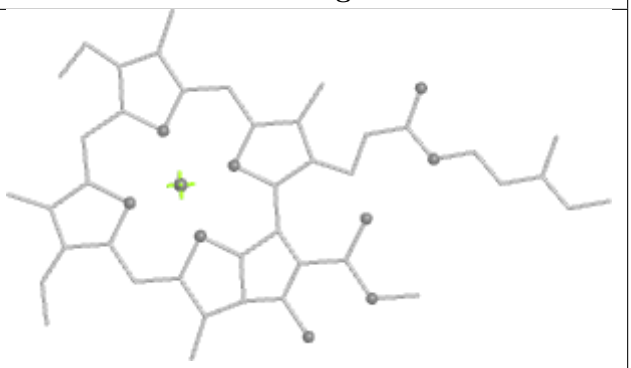
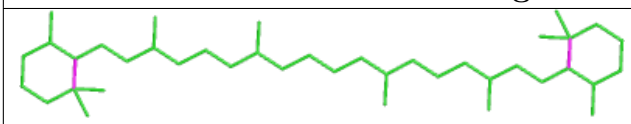


Rings

Ligand BCR bB 848



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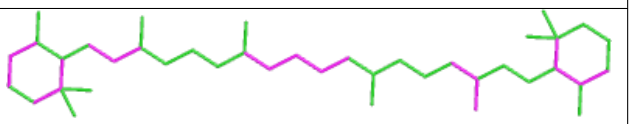
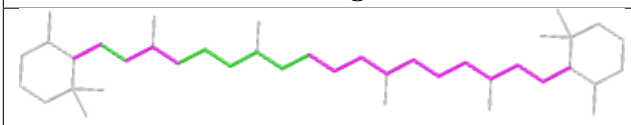


Bond angles



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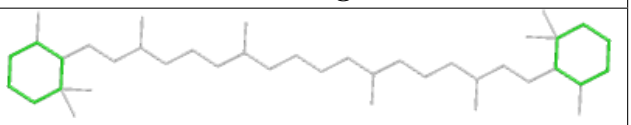
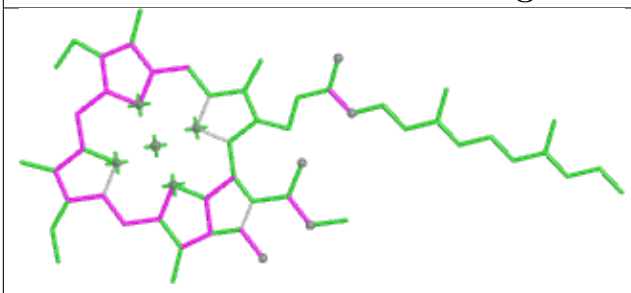
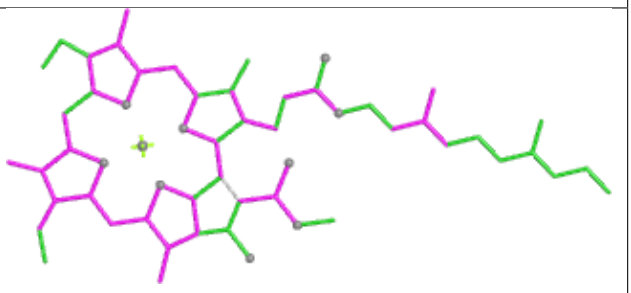
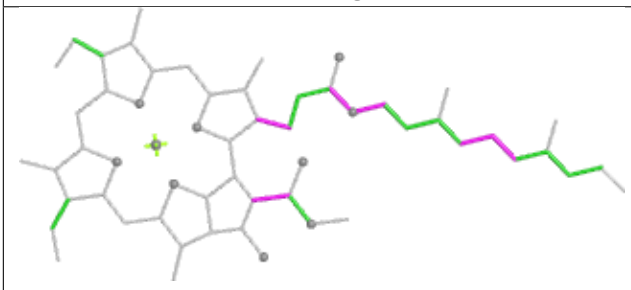
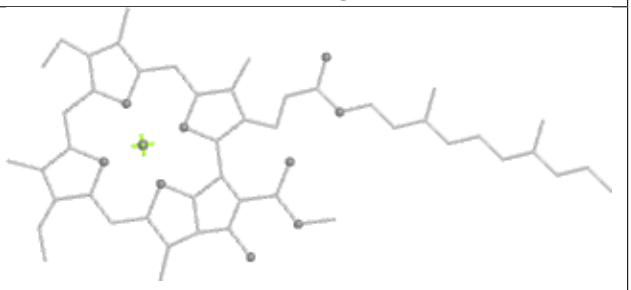


Rings

Ligand CLA cB 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

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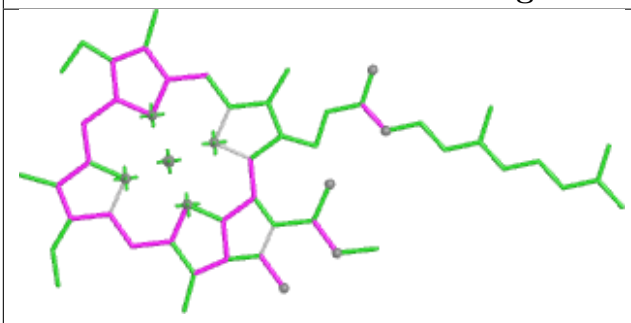
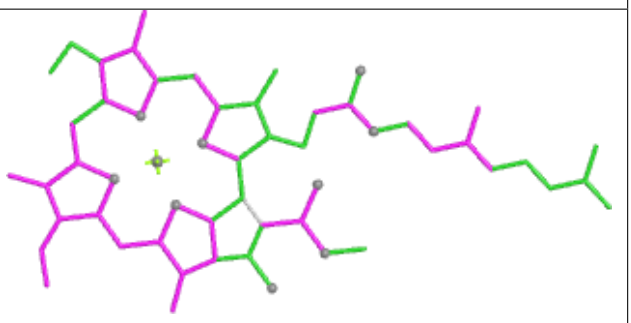
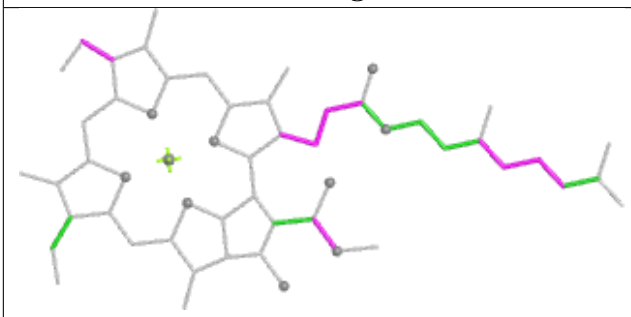
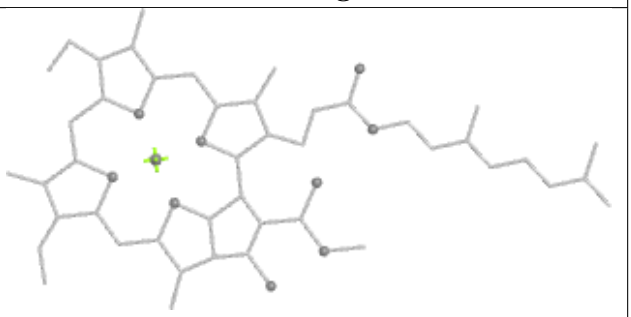
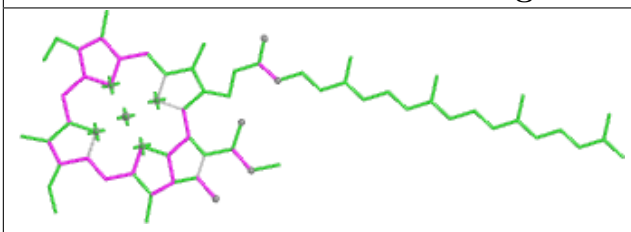
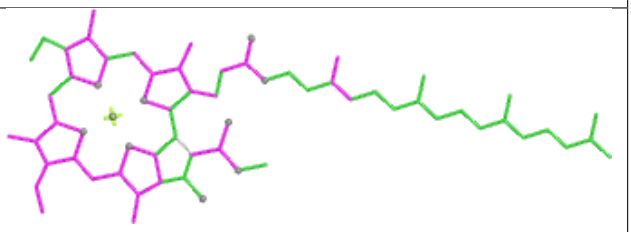
 Bond lengths	 Bond angles
 Torsions	 Rings

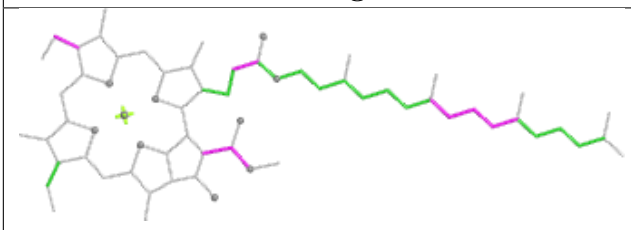
Ligand CLA cA 825



Bond lengths



Bond angles



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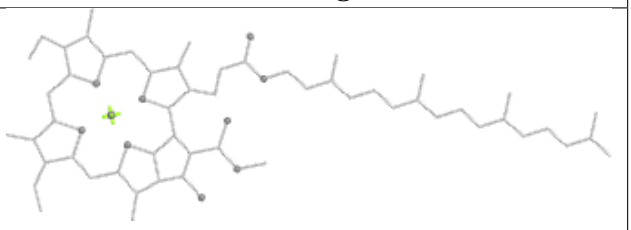
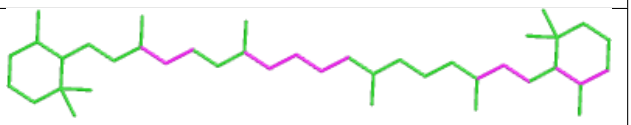


Rings

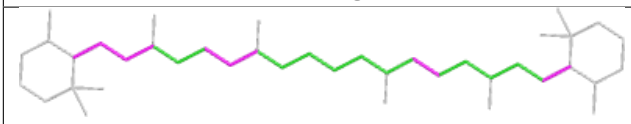
Ligand BCR cB 845



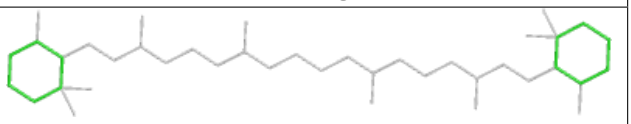
Bond lengths



Bond angles

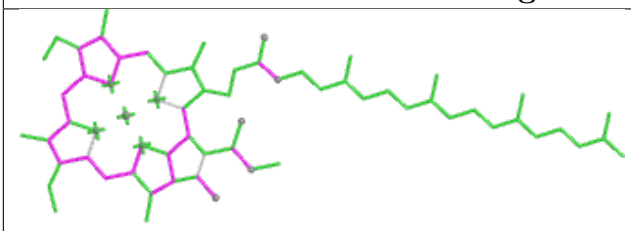


Torsions

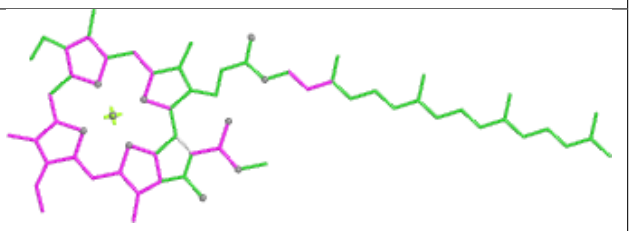


Rings

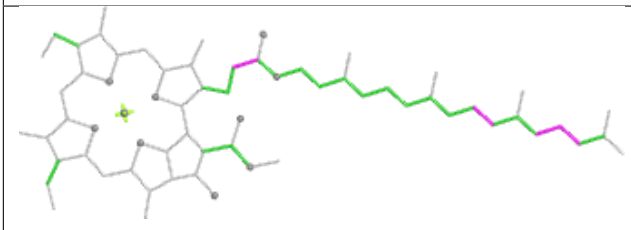
Ligand CLA cL 204



Bond lengths



Bond angles



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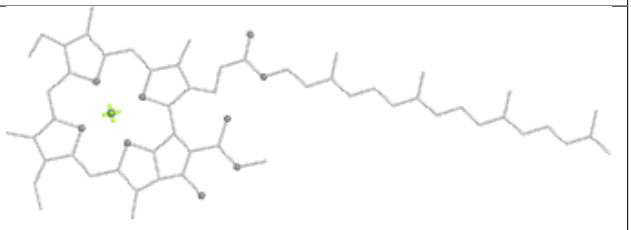
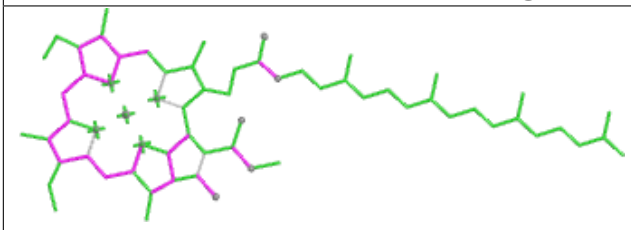
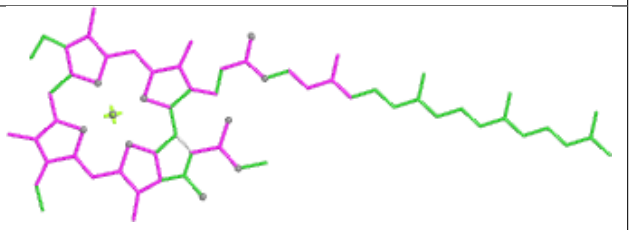


Rings

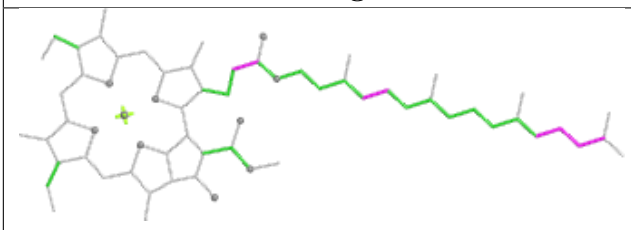
Ligand CL0 aA 801



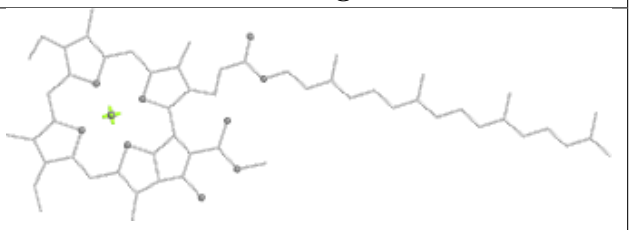
Bond lengths



Bond angles

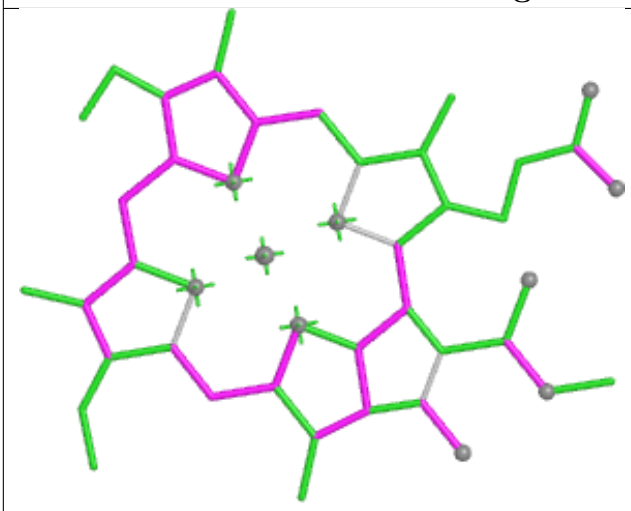


Torsions



Rings

Ligand CLA bA 823



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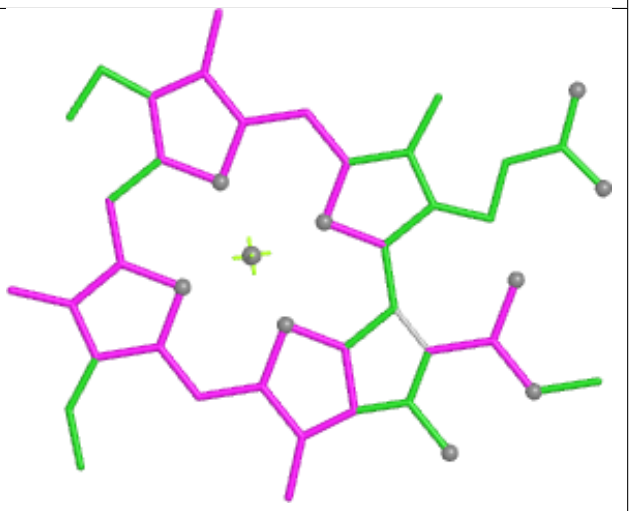

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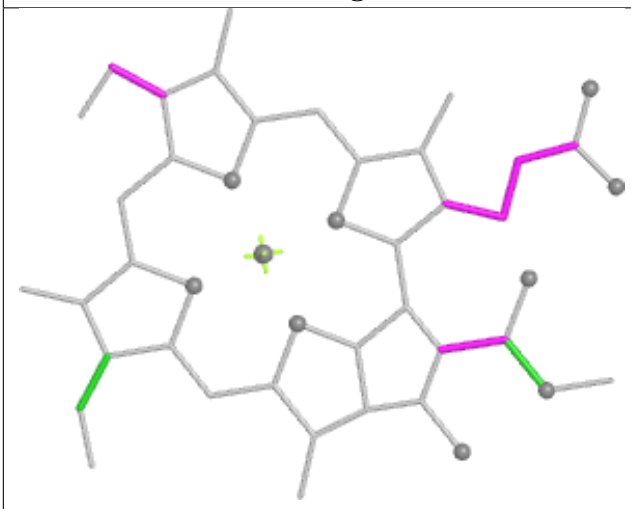

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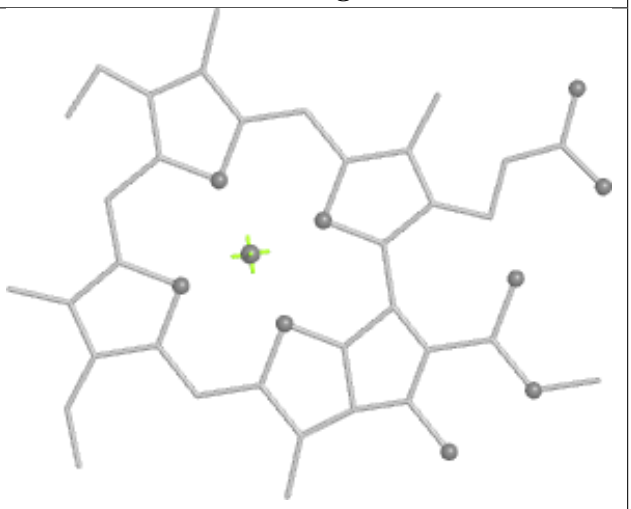
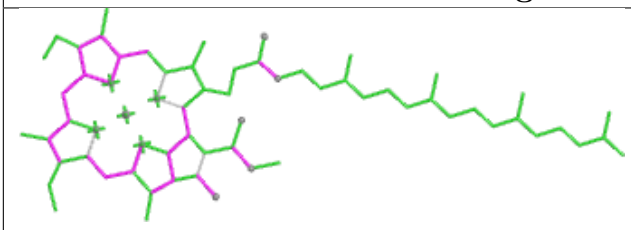
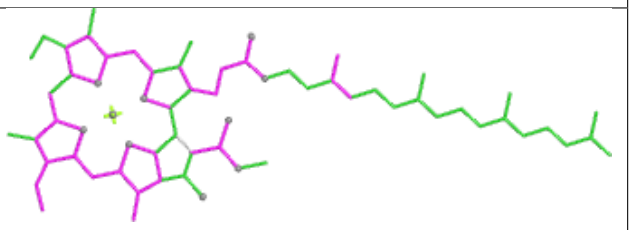
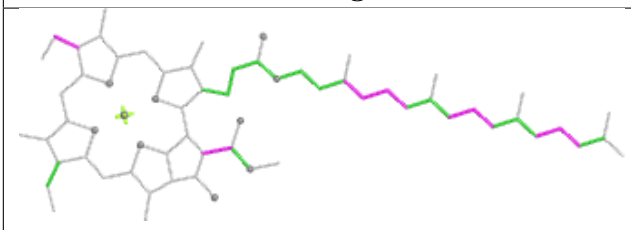
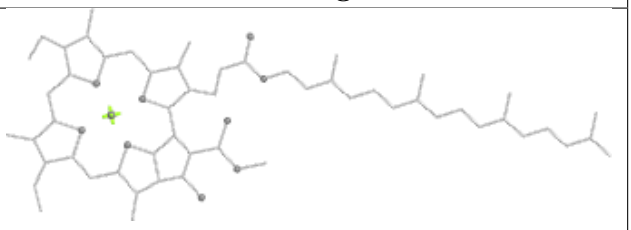
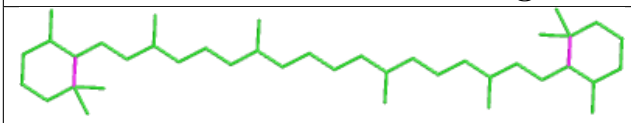
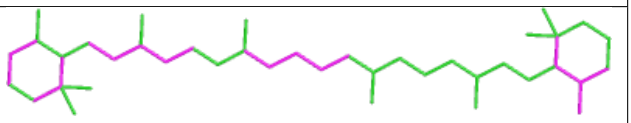
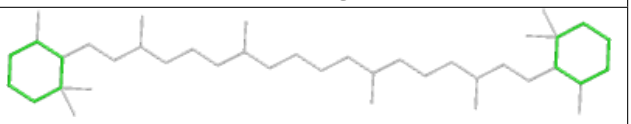
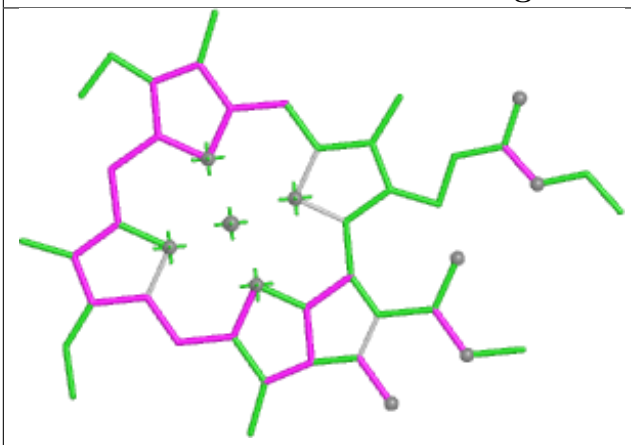


Rings

Ligand CLA aB 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR aL 207	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA bB 838



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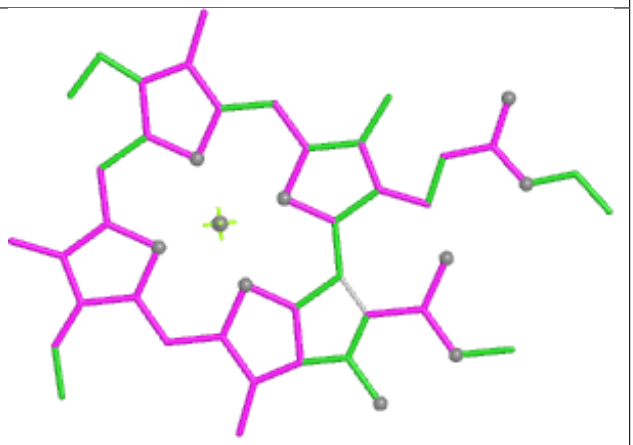
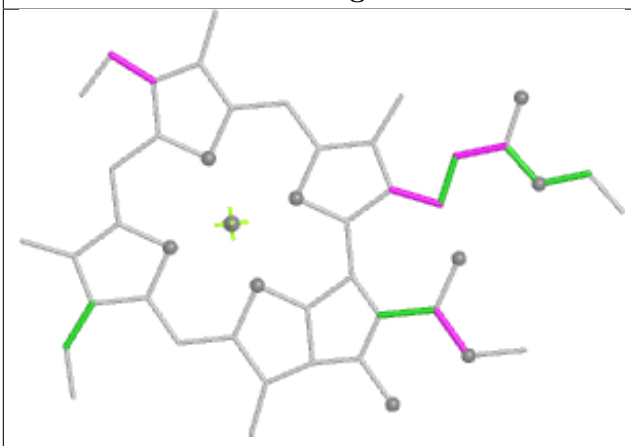


Bond angles



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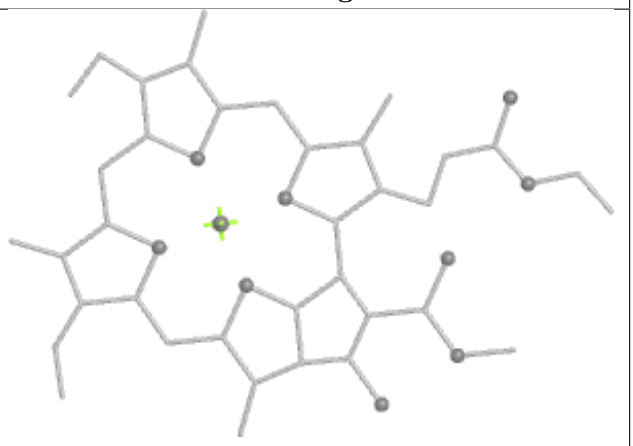
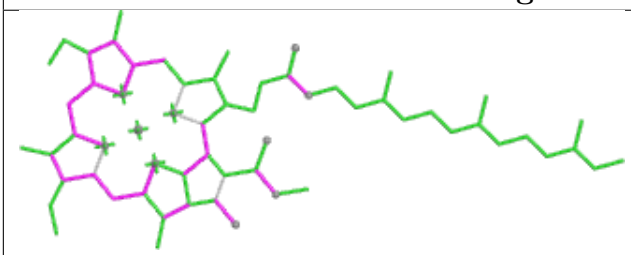


Rings

Ligand CLA cB 803



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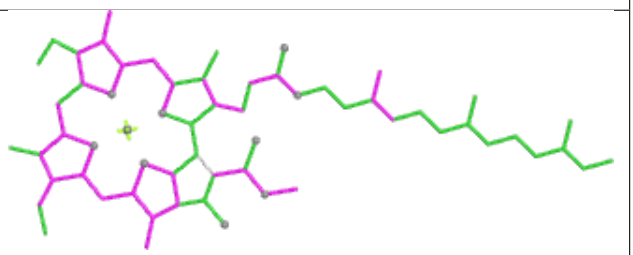
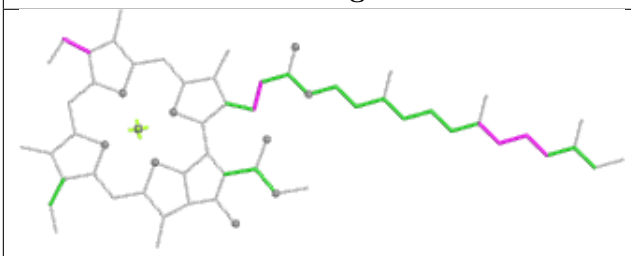


Bond angles



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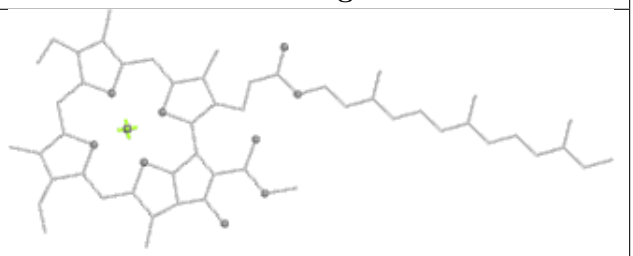
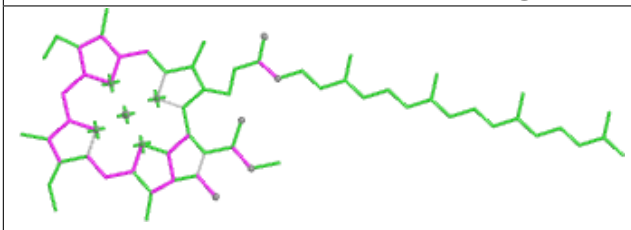


Rings

Ligand CLA aB 801



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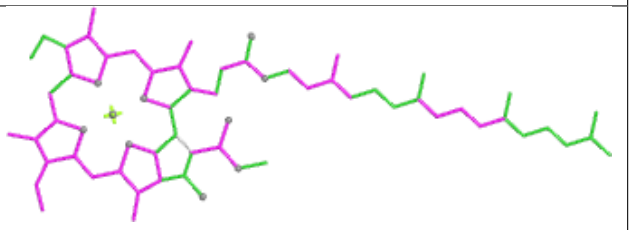
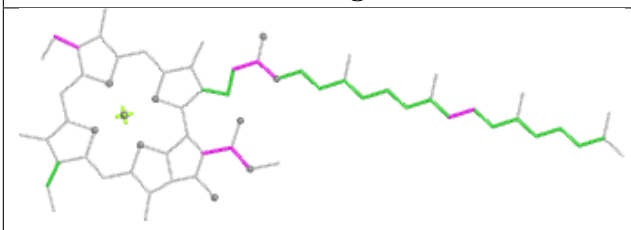


Bond angles



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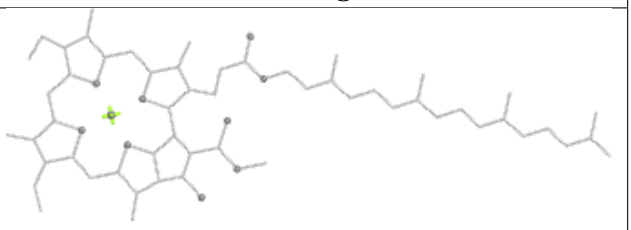
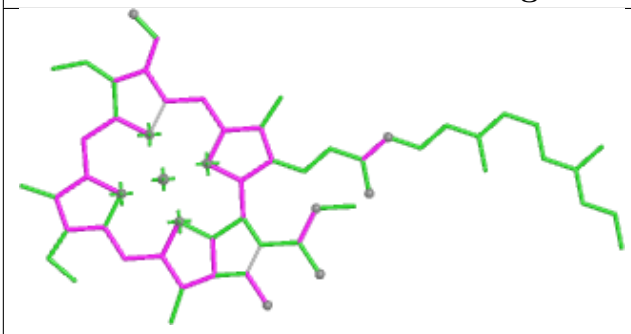


Rings

Ligand F6C cB 824



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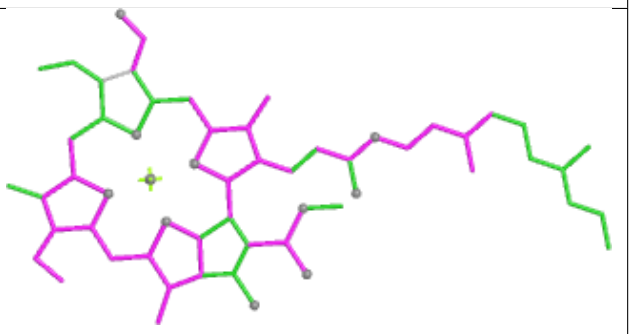
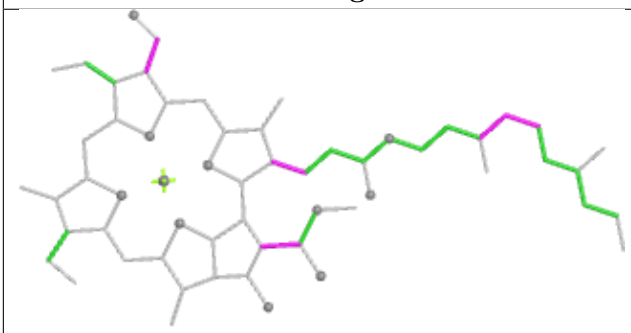


Bond angles



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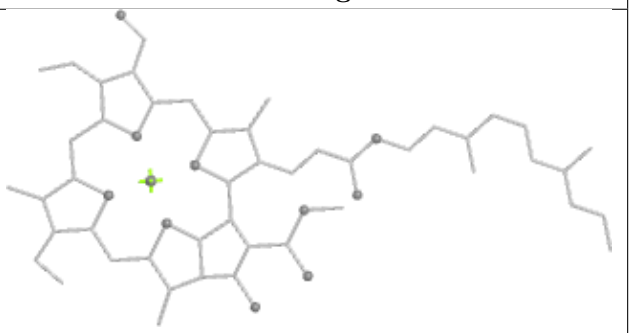
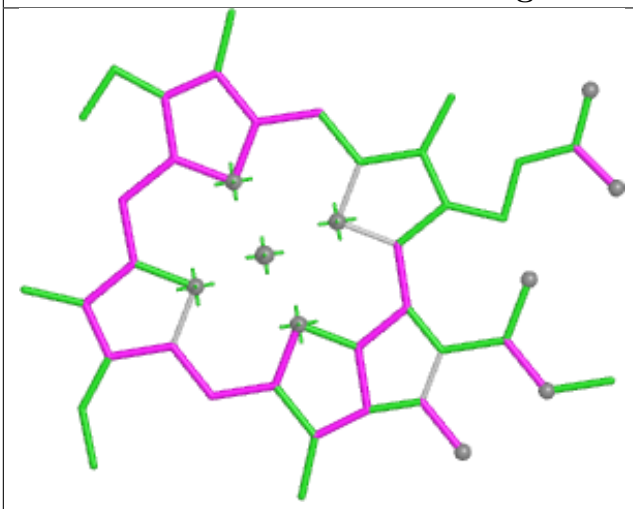


Rings

Ligand CLA cB 835



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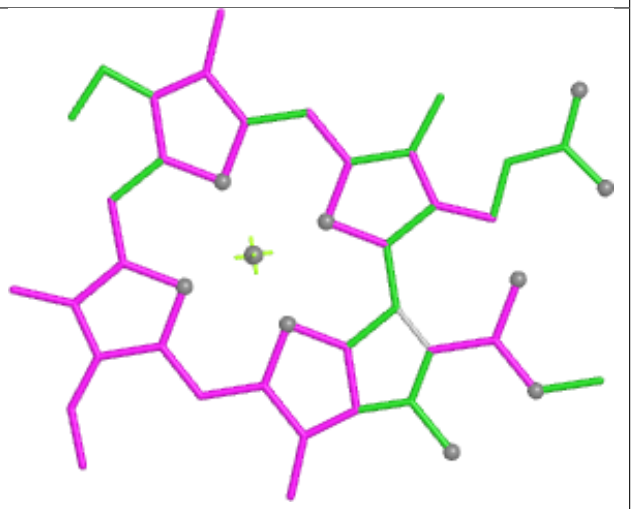
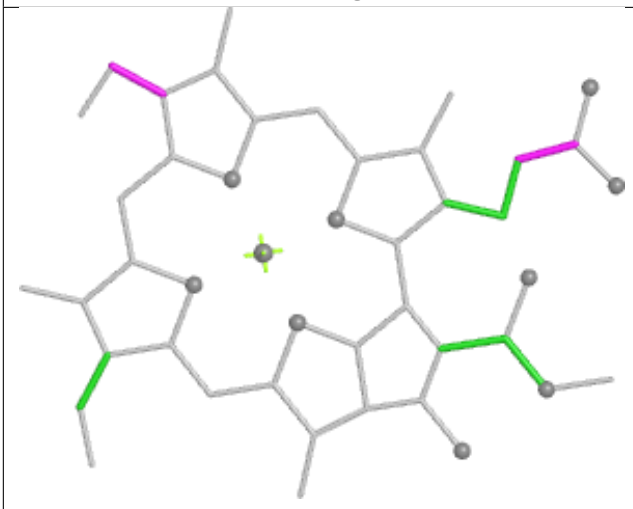


Bond angles

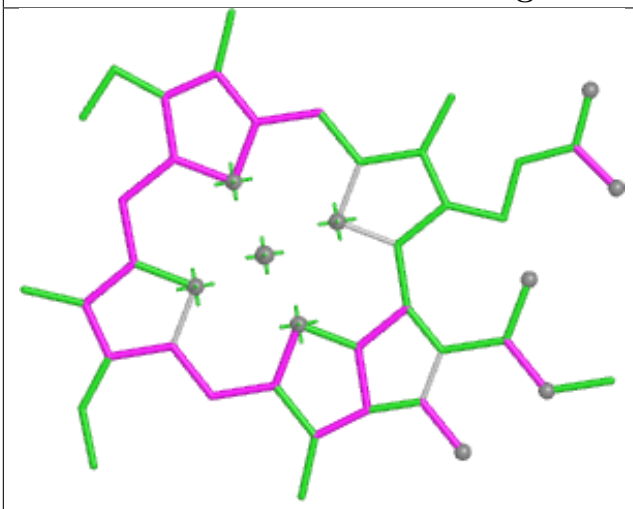


Torsions



Rings

Ligand CLA cB 811



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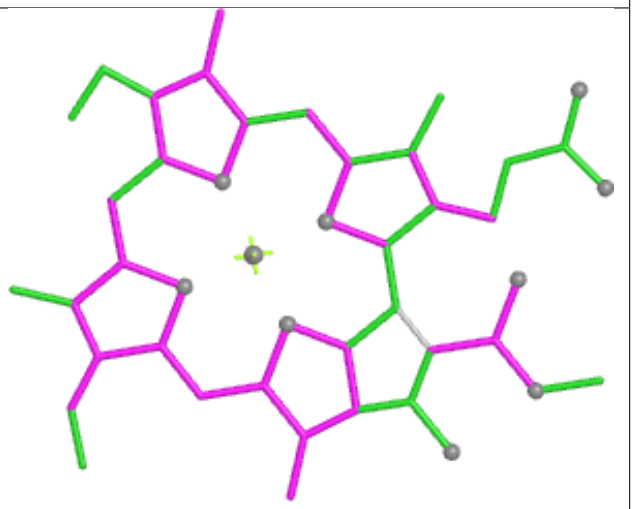
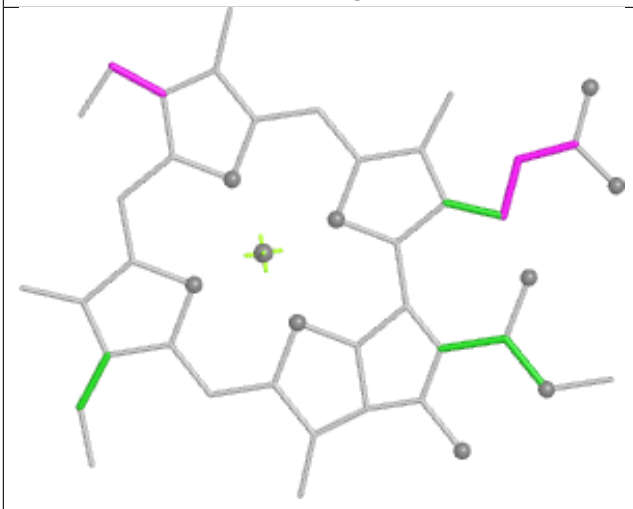


Bond angles

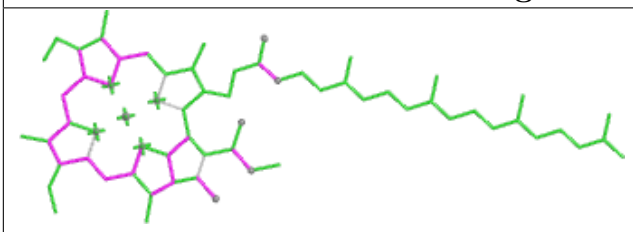


Torsions



Rings

Ligand CLA aA 839



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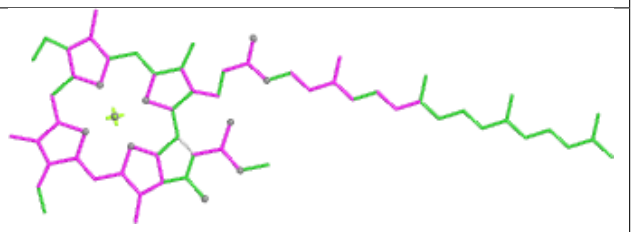
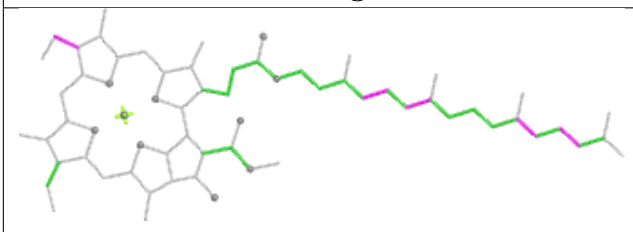


Bond angles



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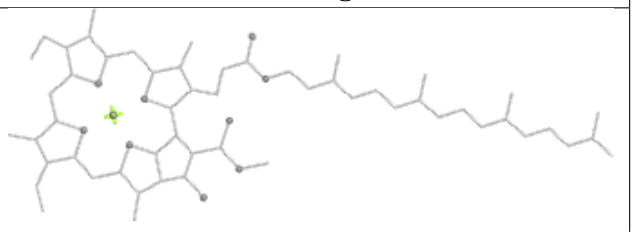
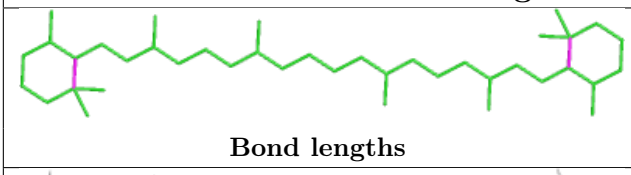


Rings

Ligand BCR aB 846



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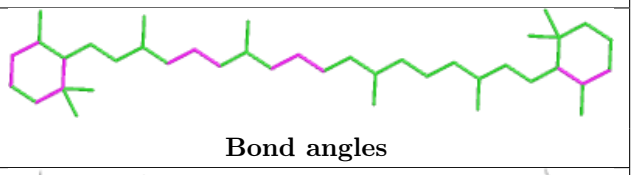

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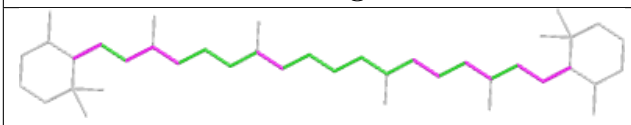

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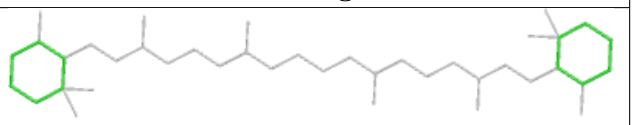
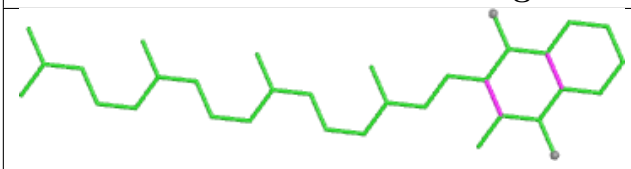


Rings

Ligand PQN cA 845



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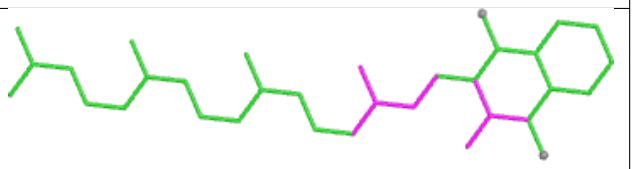

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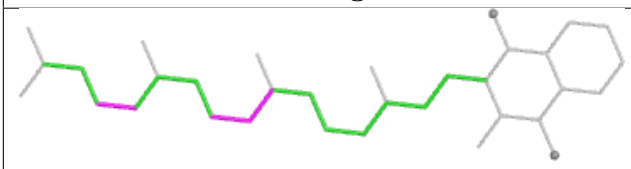

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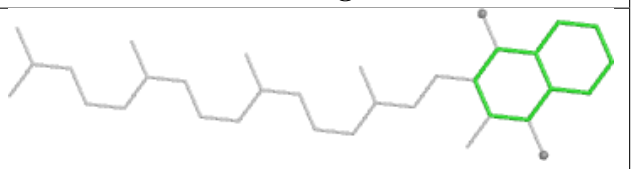
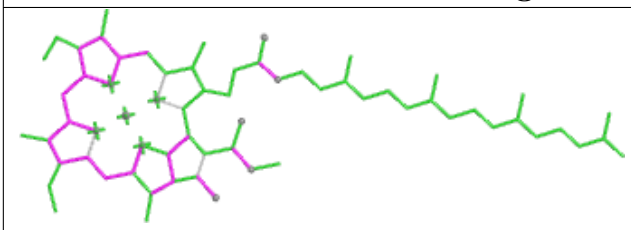


Rings

Ligand CLA aB 812



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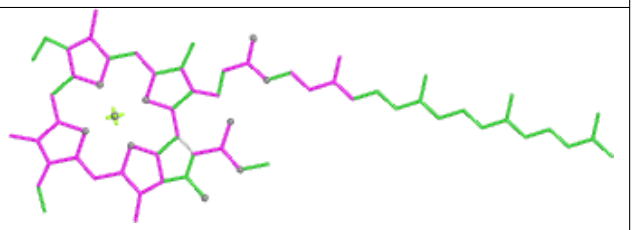
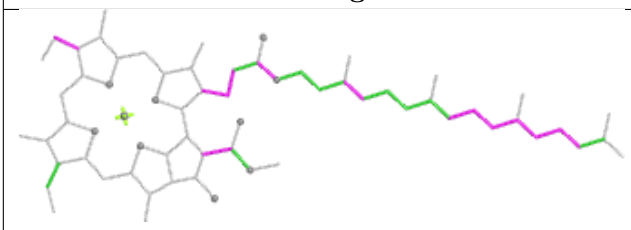


Bond angles



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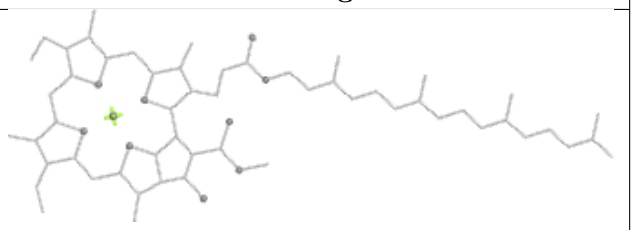
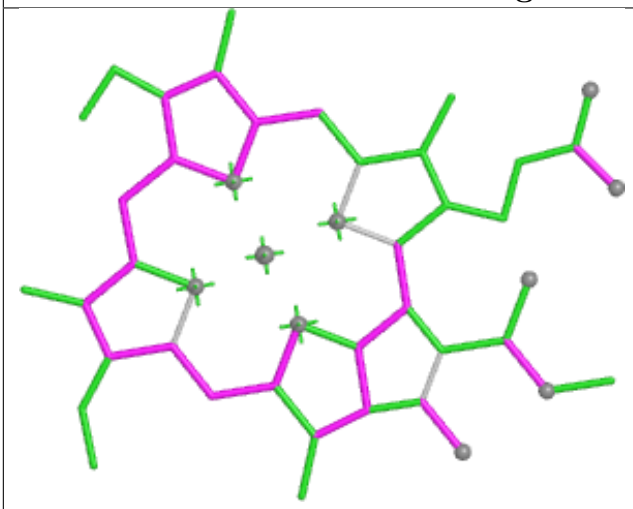


Rings

Ligand CLA cA 816



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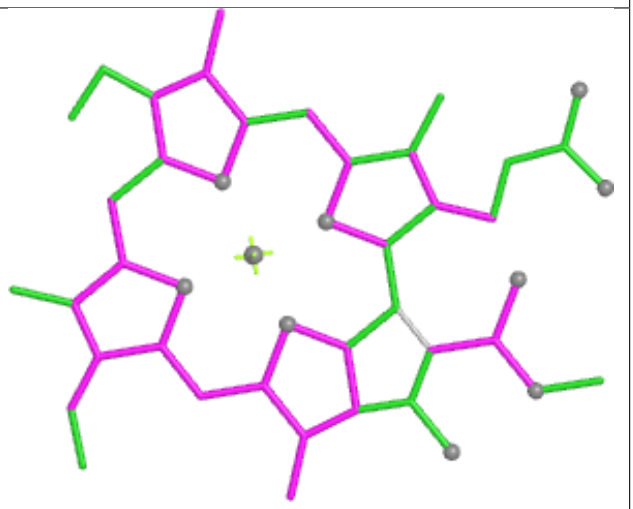
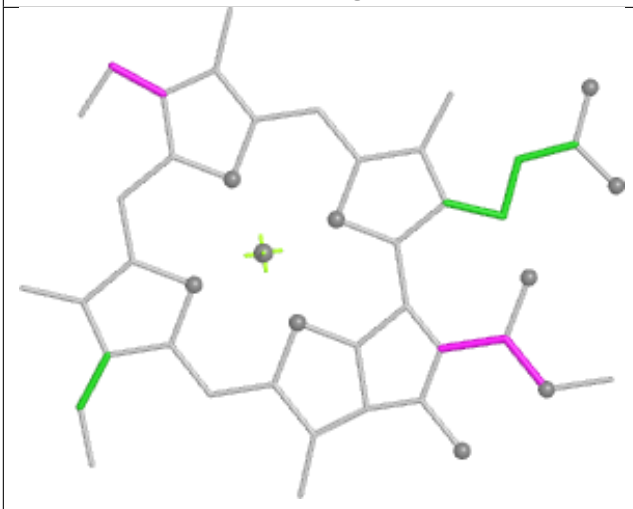


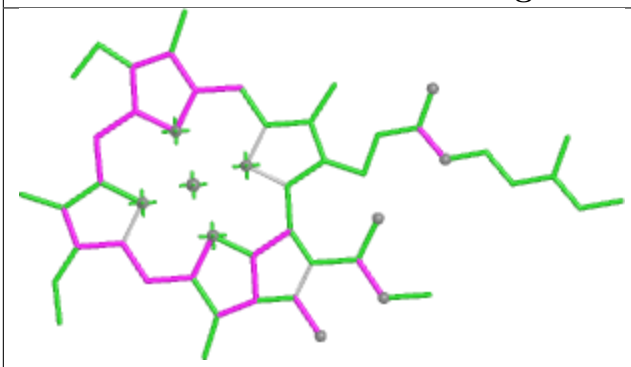
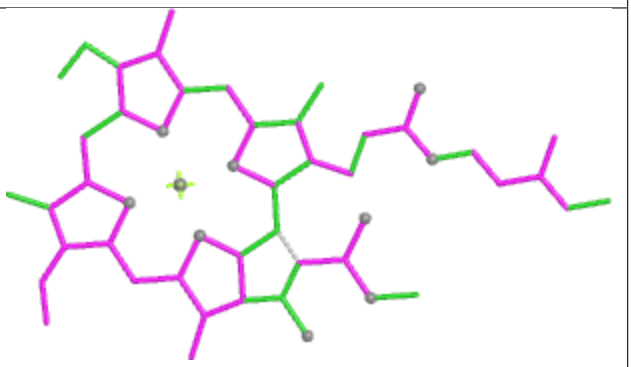
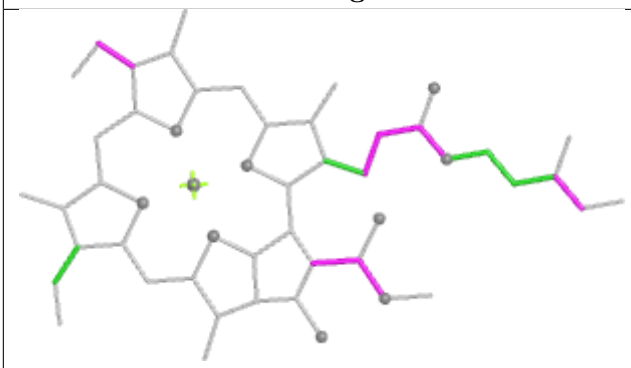
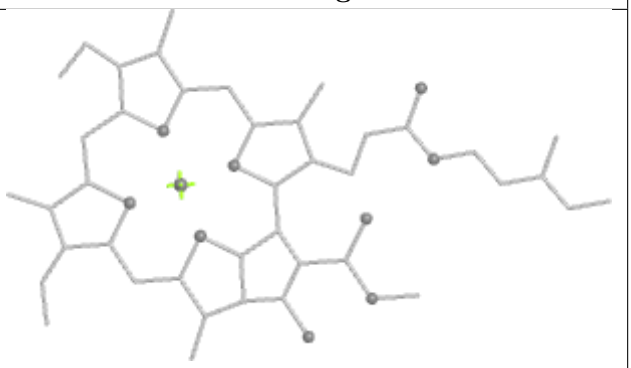
Bond angles

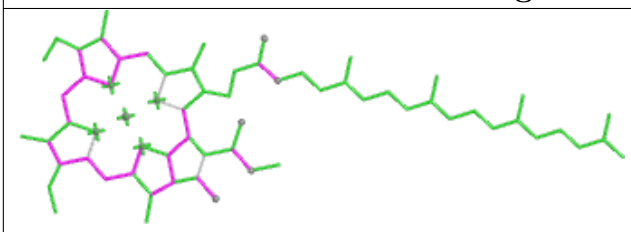
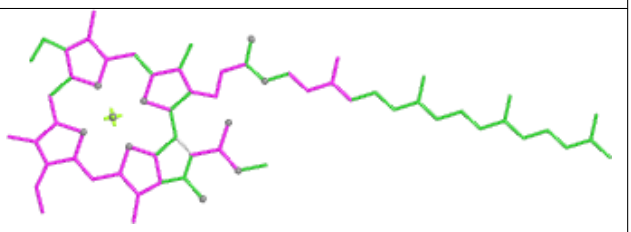
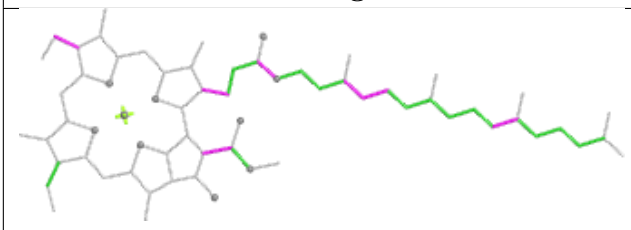
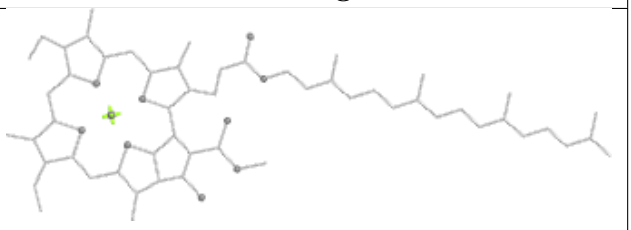


Torsions

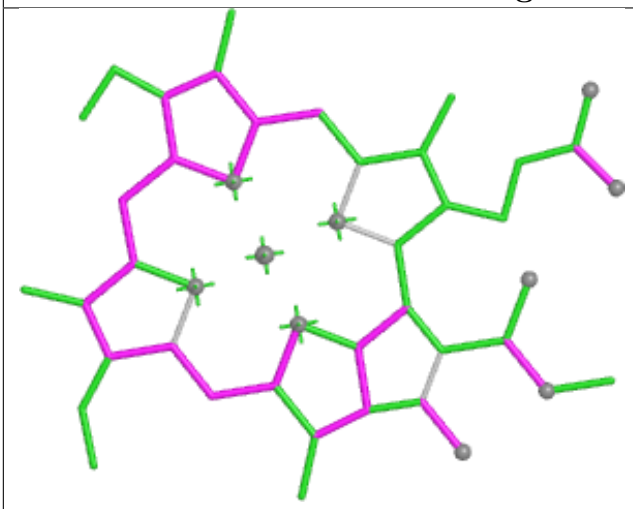


Rings

Ligand CLA aA 824	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA aA 820	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA aB 810



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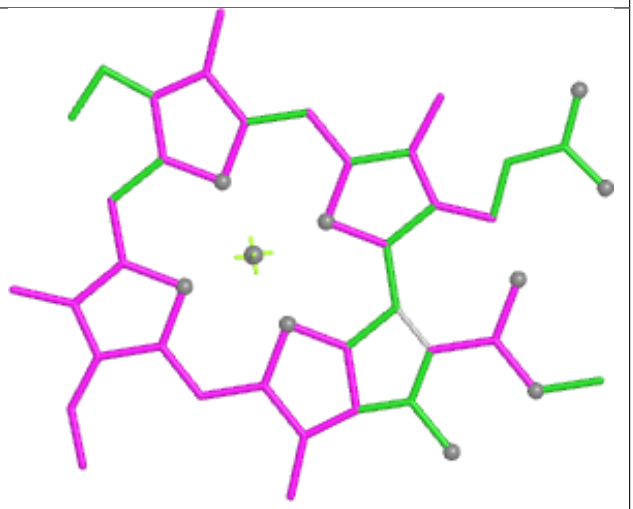
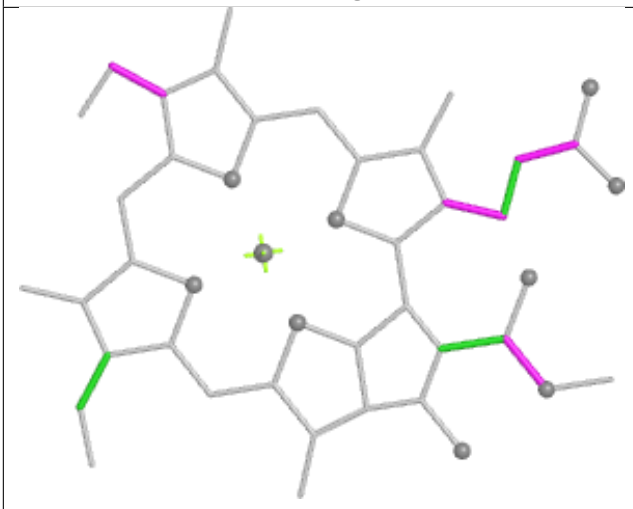


Bond angles

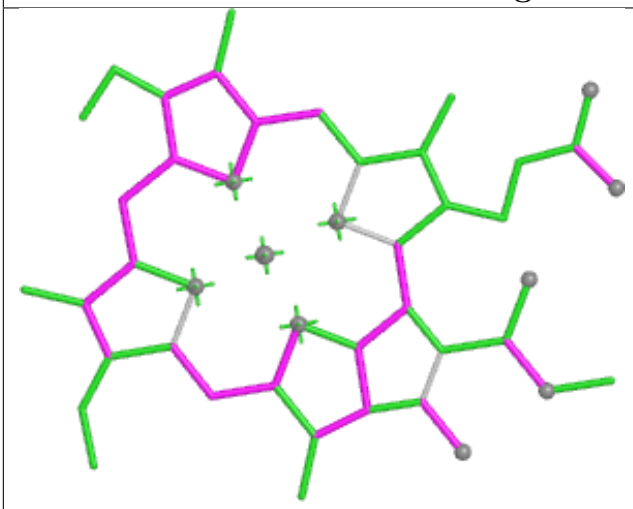


Torsions



Rings

Ligand CLA bB 820



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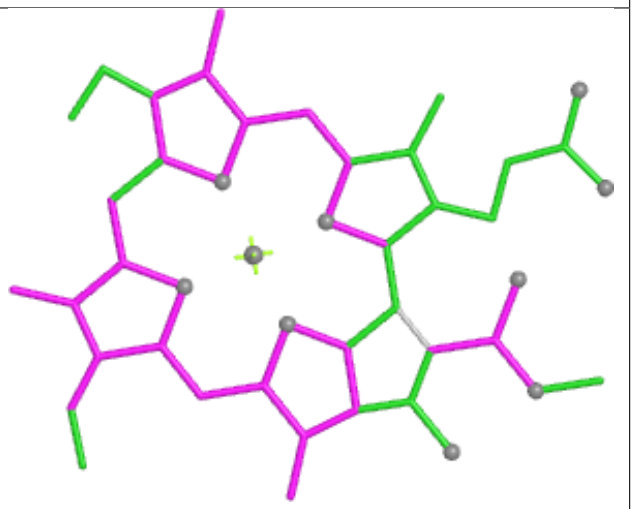
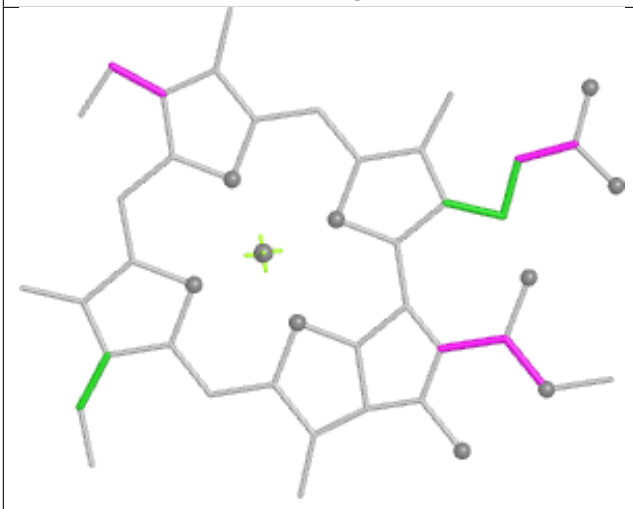


Bond angles

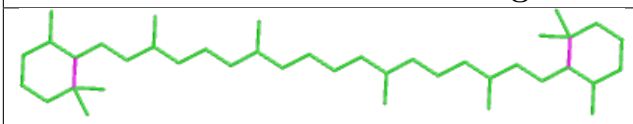


Torsions



Rings

Ligand BCR bK 102



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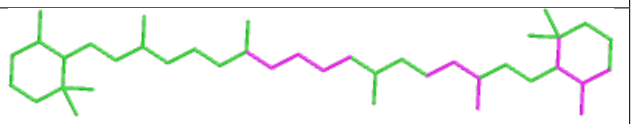
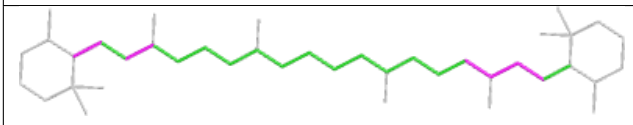
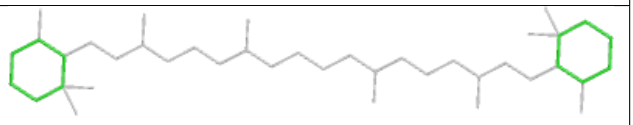


Bond angles

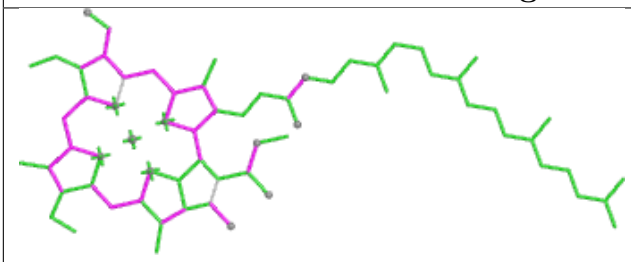


Torsions



Rings

Ligand F6C cA 826



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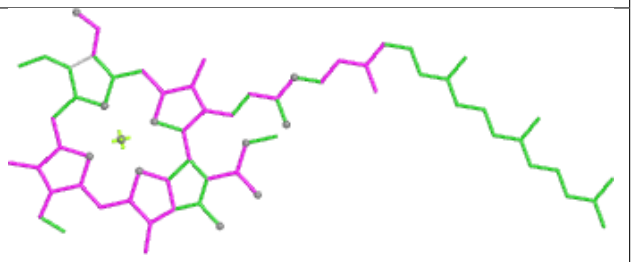
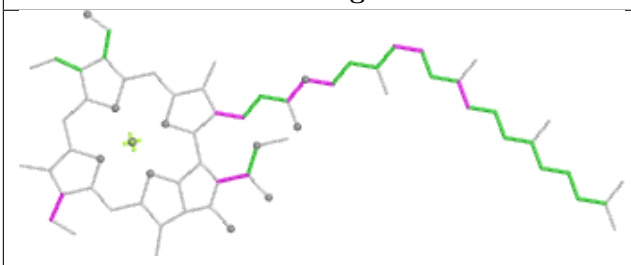


Bond angles



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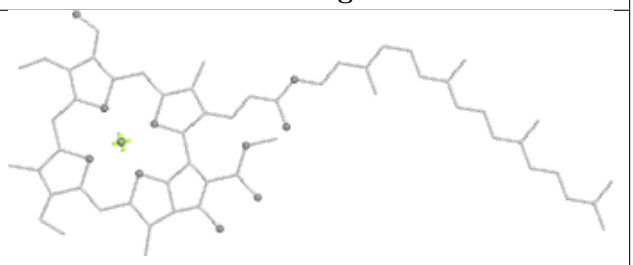
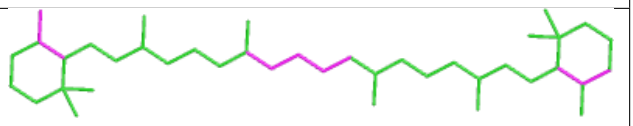


Rings

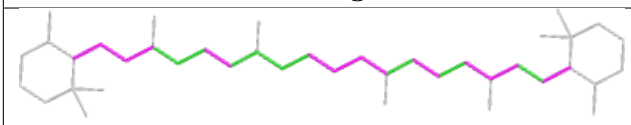
Ligand BCR cB 842



Bond lengths



Bond angles



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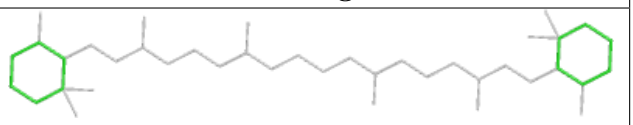
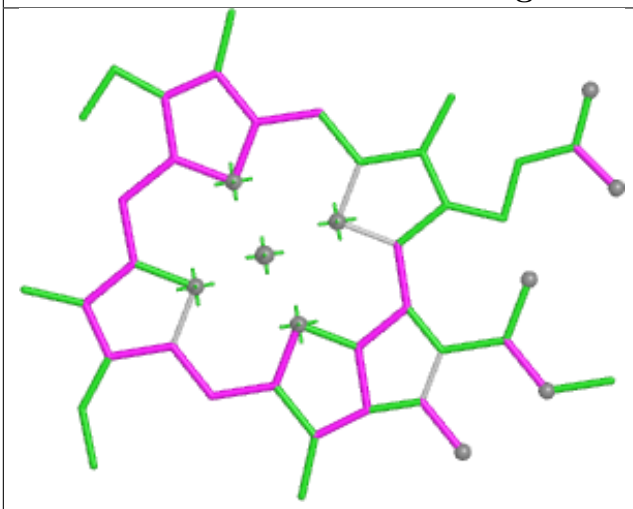


Rings

Ligand CLA aB 832



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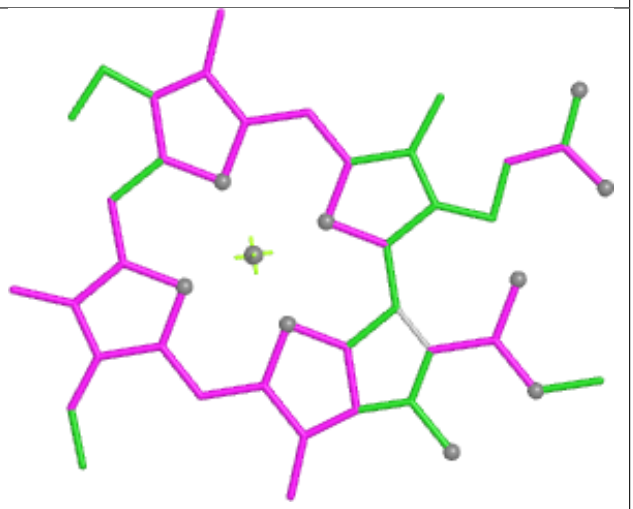
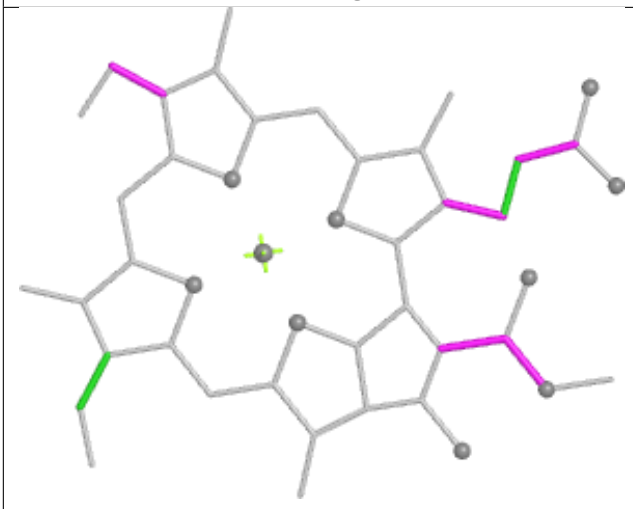


Bond angles

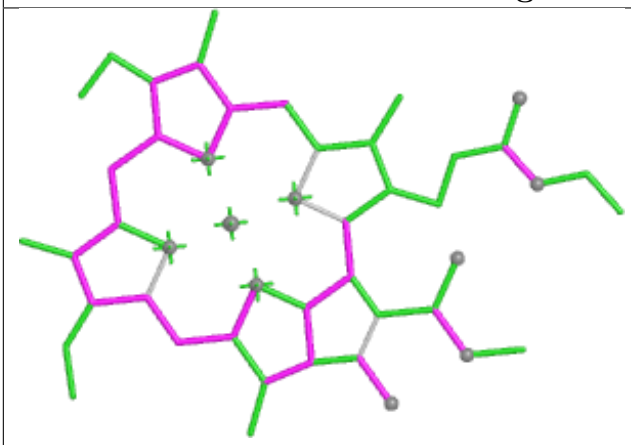


Torsions

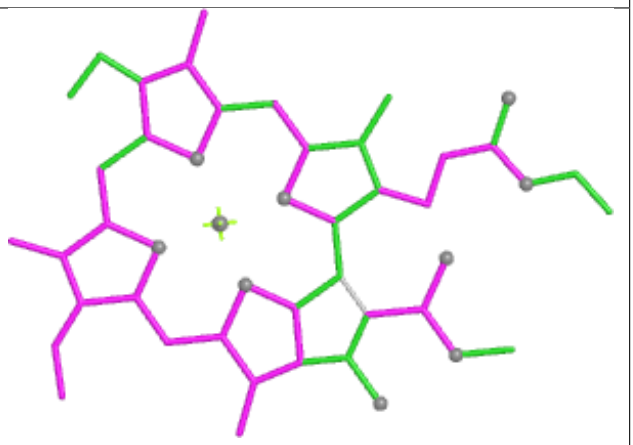


Rings

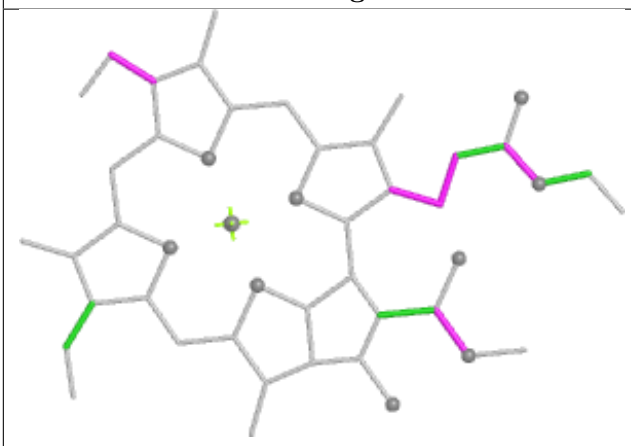
Ligand CLA cB 819



Bond lengths



Bond angles



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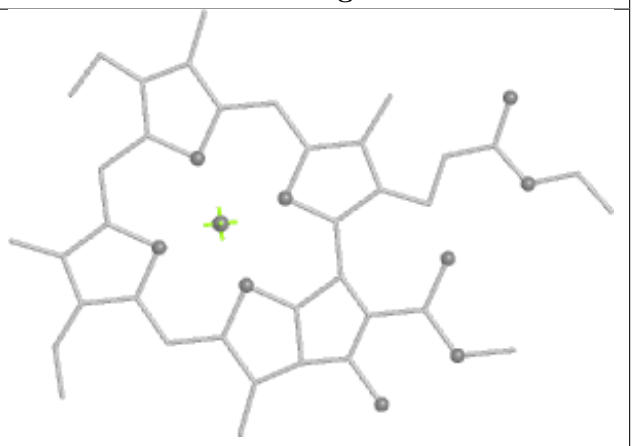
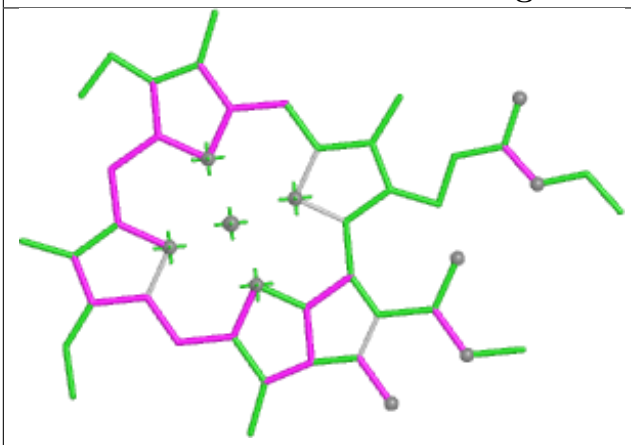


Rings

Ligand CLA aB 809



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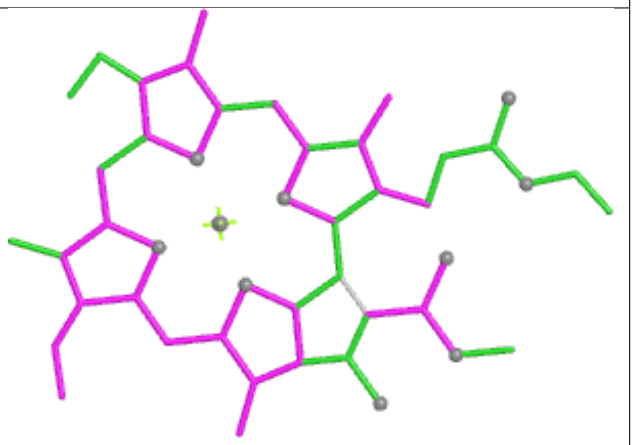
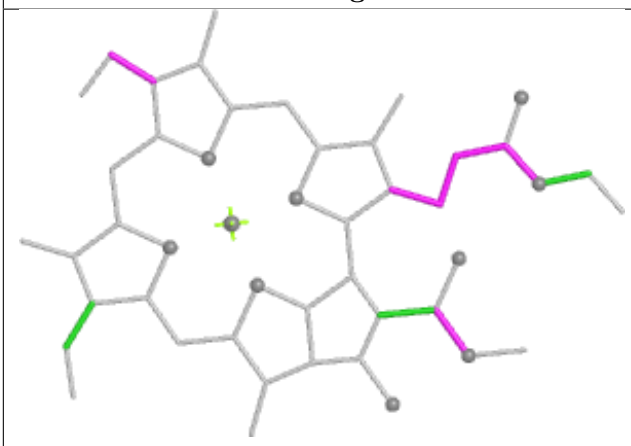


Bond angles



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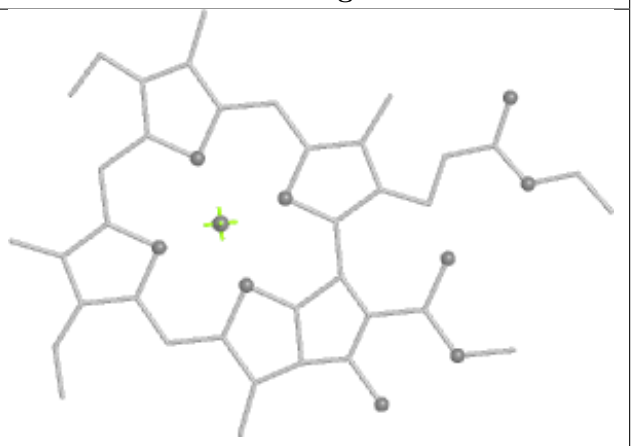
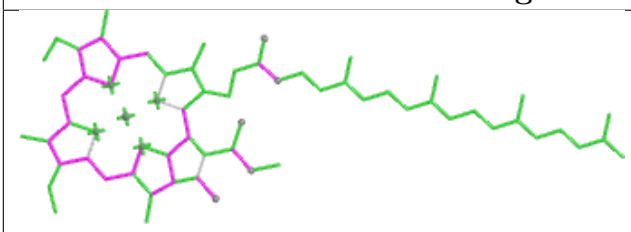


Rings

Ligand CLA aA 829



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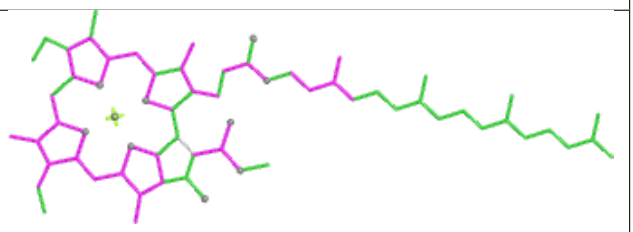
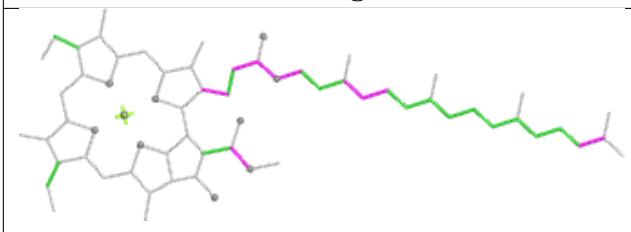


Bond angles



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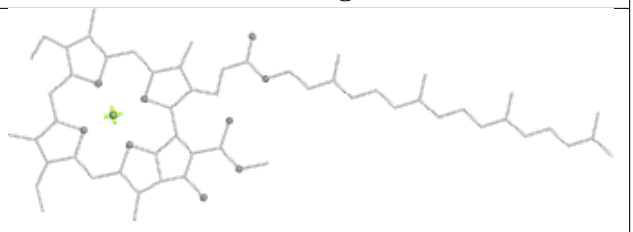
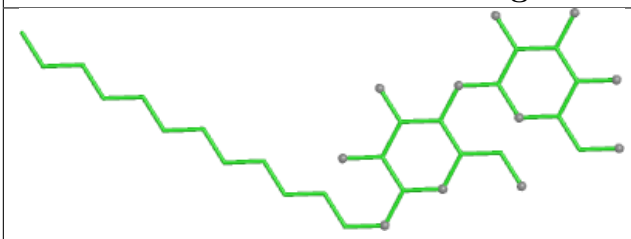


Rings

Ligand LMT bA 853



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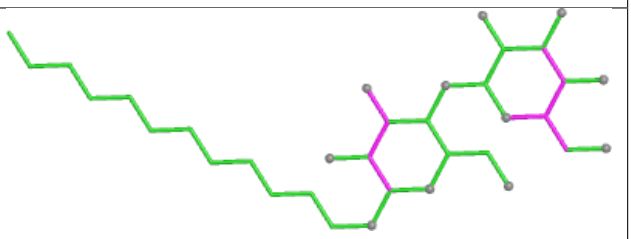
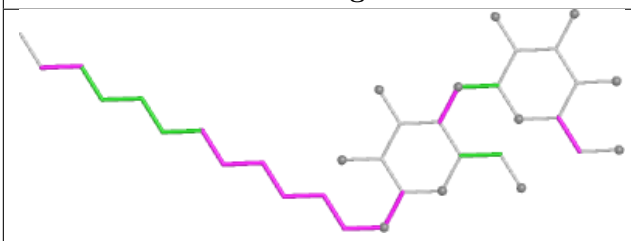


Bond angles



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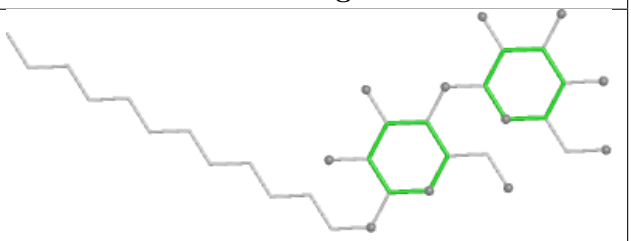
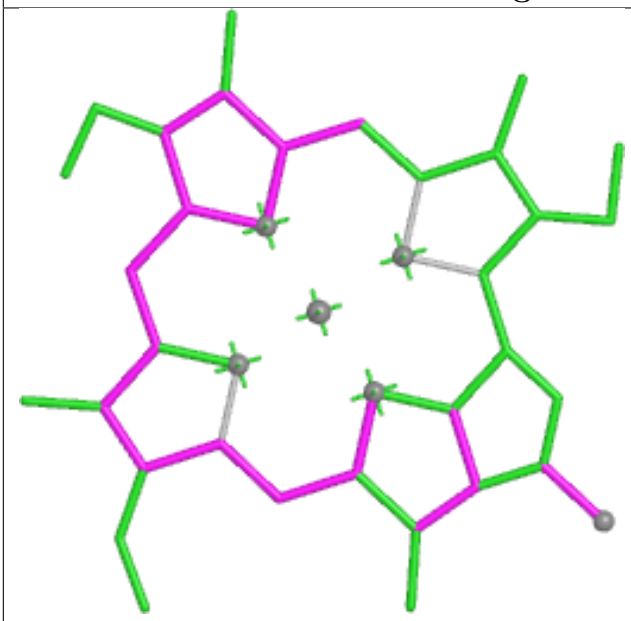


Rings

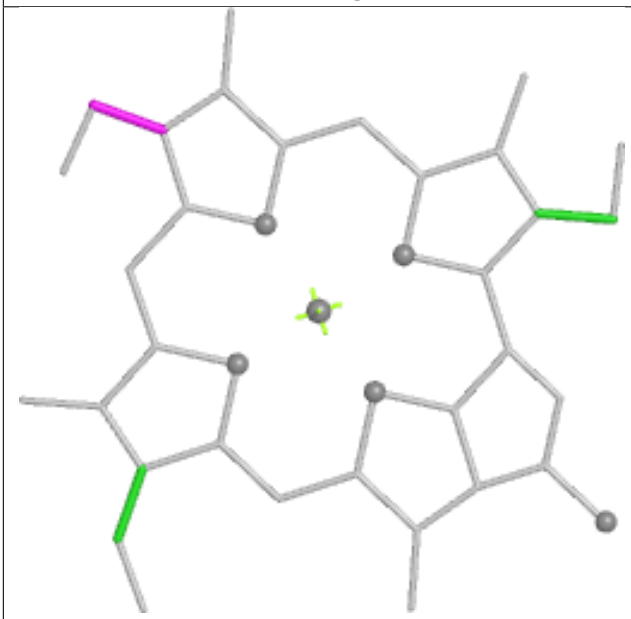
Ligand CLA bK 101



Bond lengths



Bond angles



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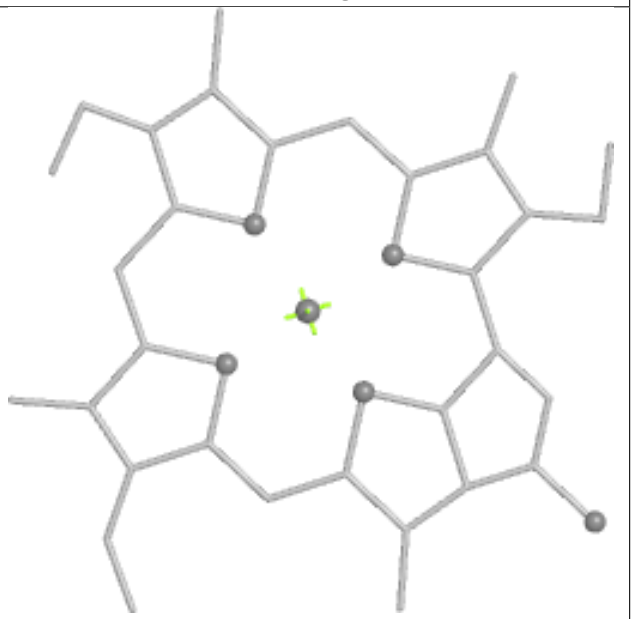
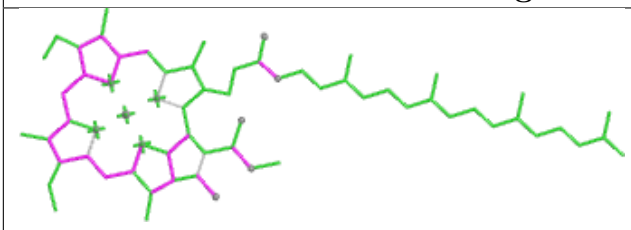
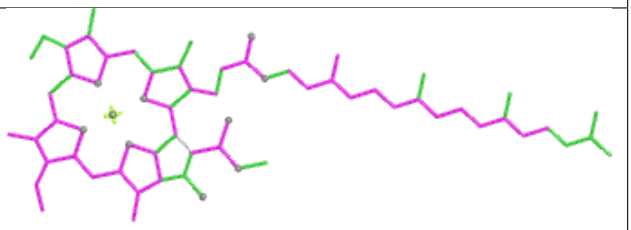


Rings

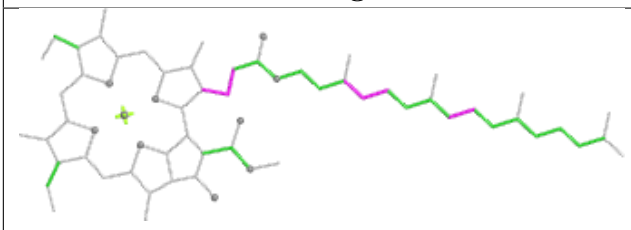
Ligand CLA aA 802



Bond lengths



Bond angles



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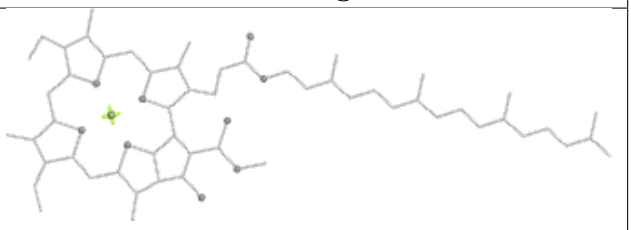
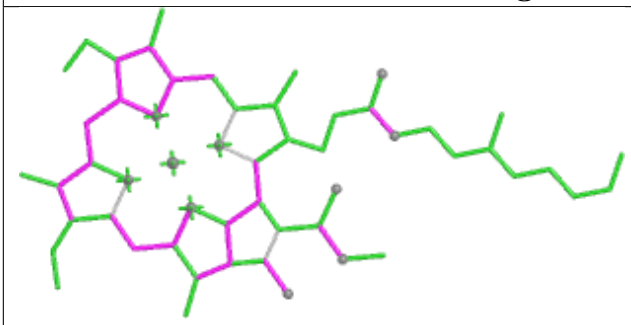


Rings

Ligand CLA cA 818



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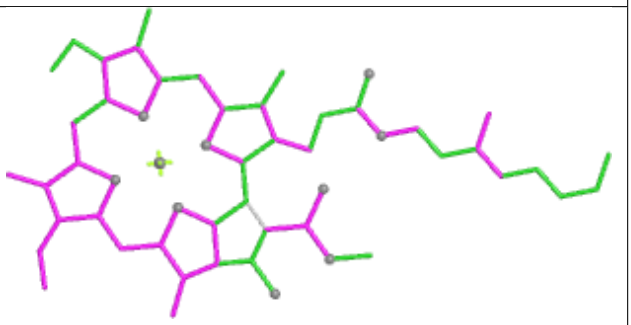
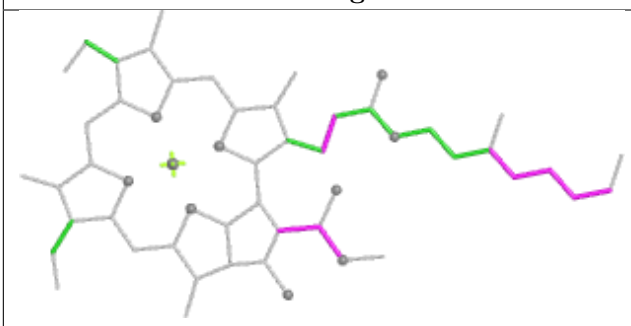
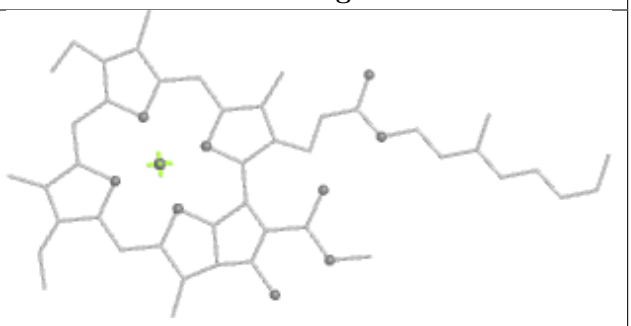


Bond angles

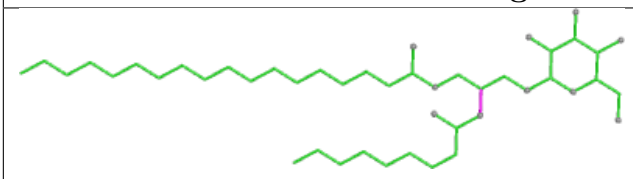


Torsions

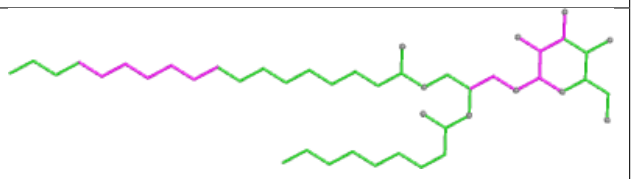


Rings

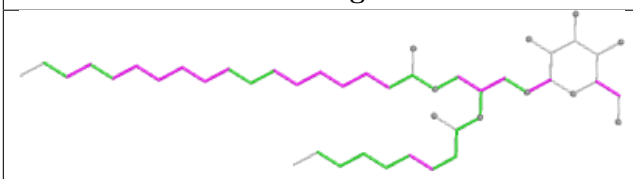
Ligand LMG bB 847



Bond lengths



Bond angles



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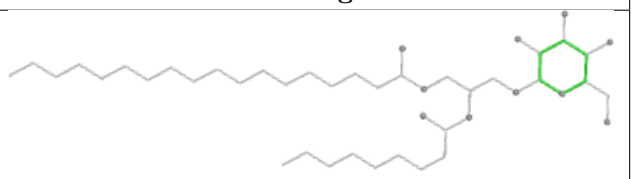
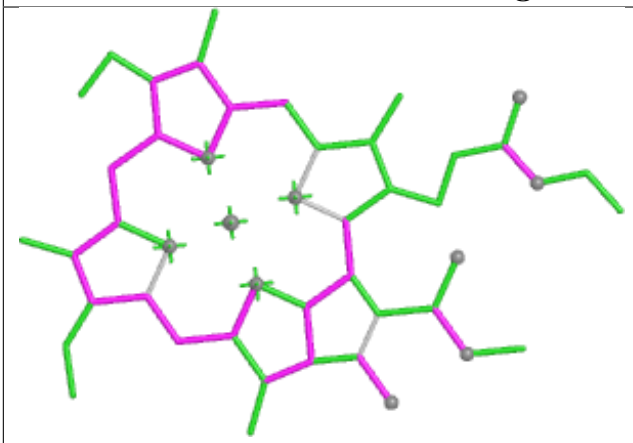
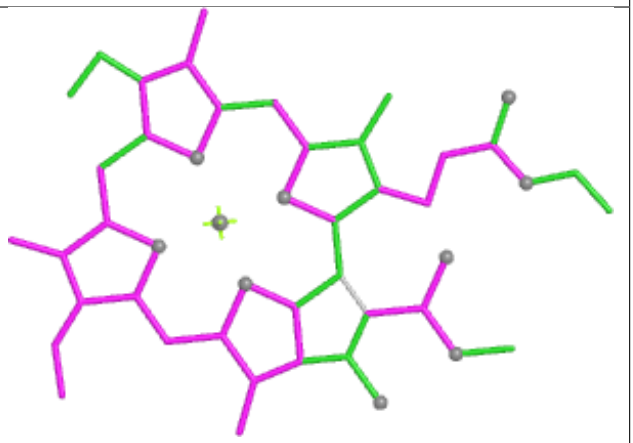


Rings

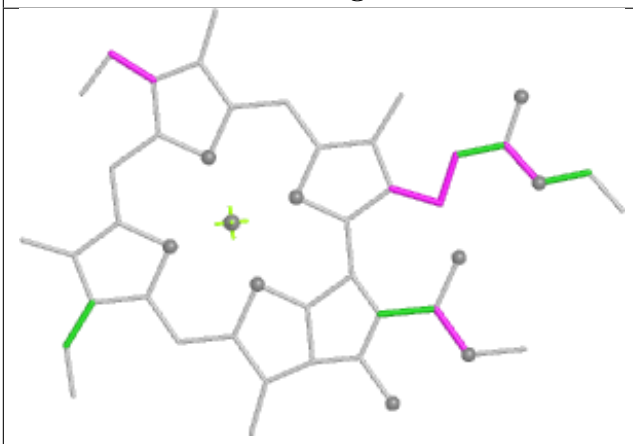
Ligand CLA bB 819



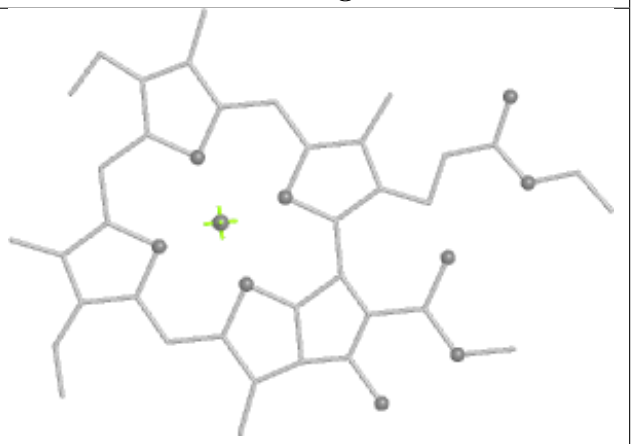
Bond lengths



Bond angles

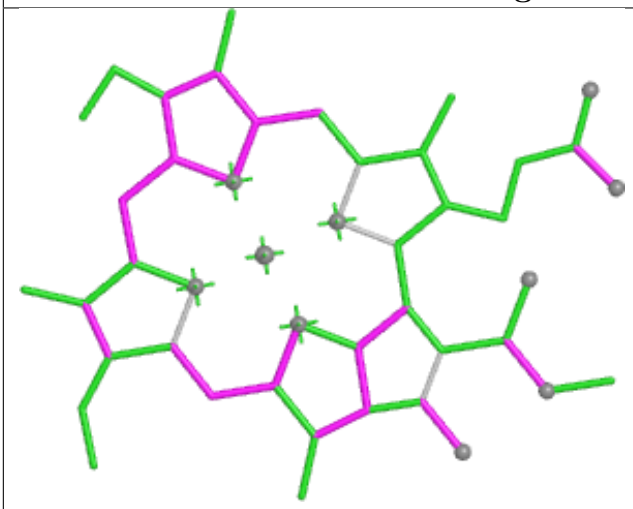


Torsions



Rings

Ligand CLA bB 822



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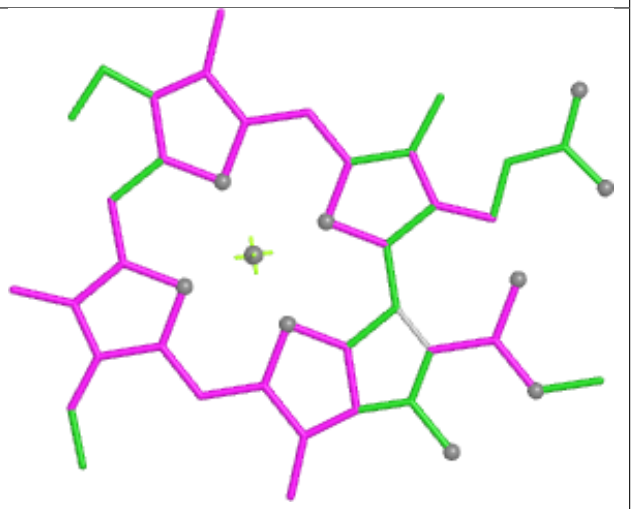

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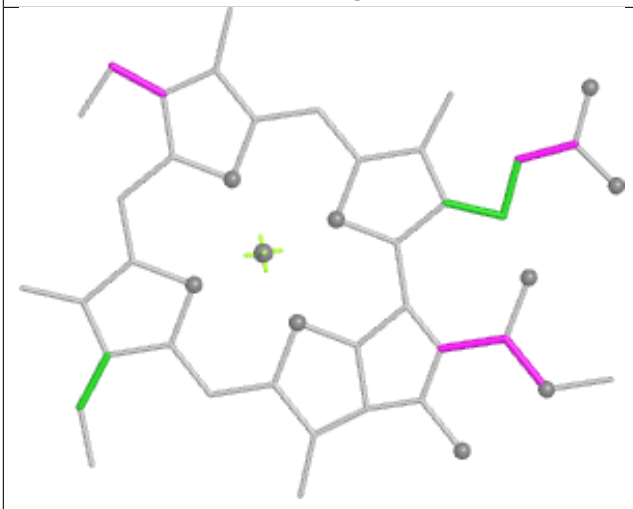
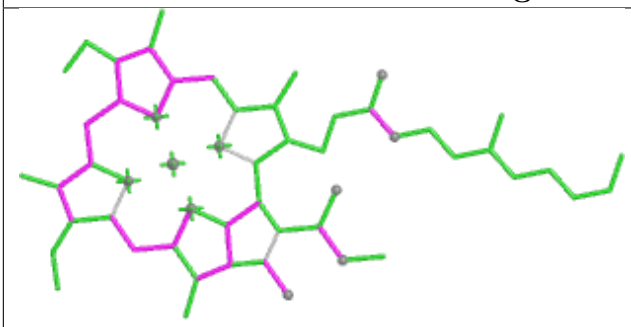


Torsions



Rings

Ligand CLA bA 819



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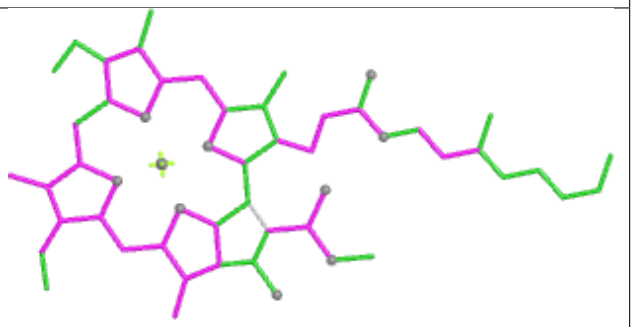
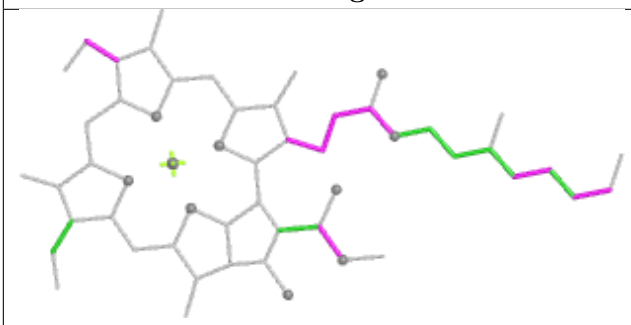


Bond angles



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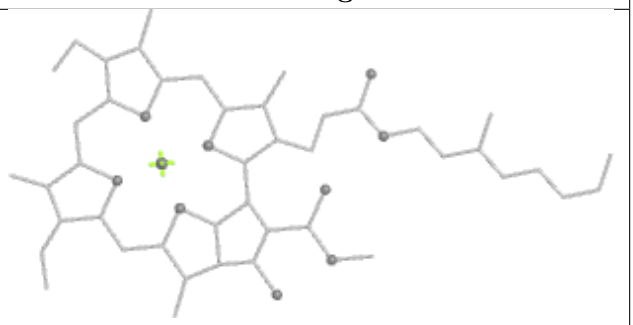
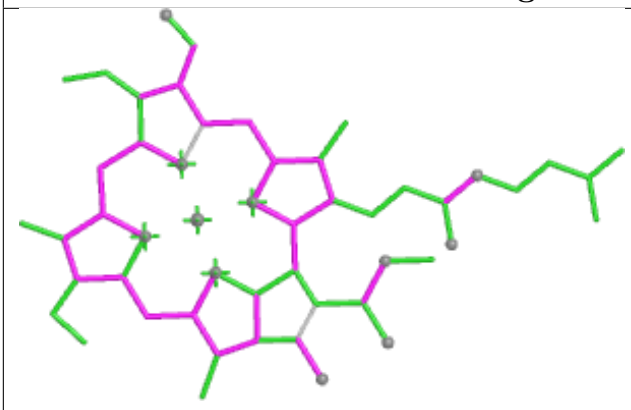


Rings

Ligand F6C bA 832



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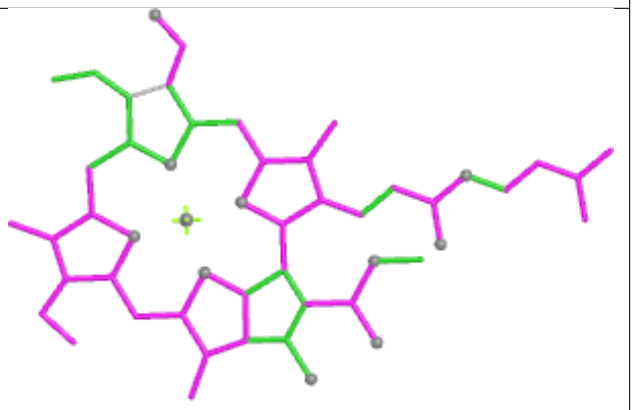
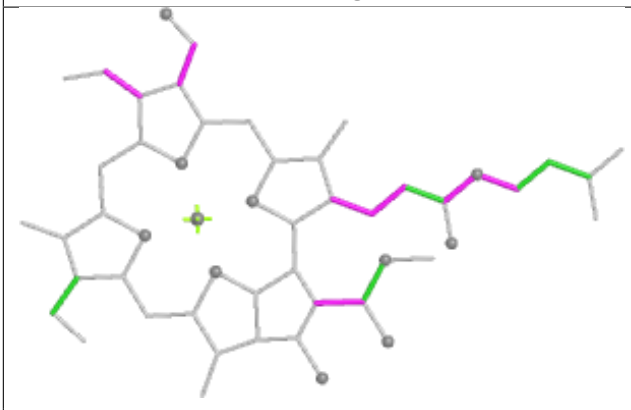


Bond angles



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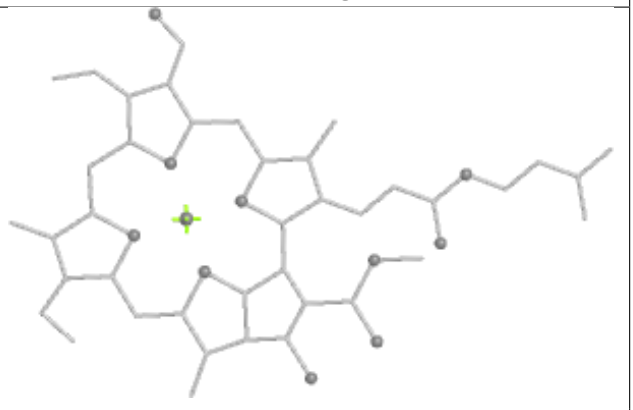
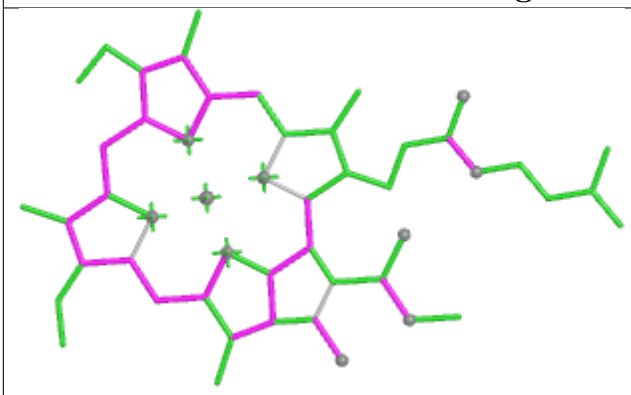


Rings

Ligand CLA aA 841



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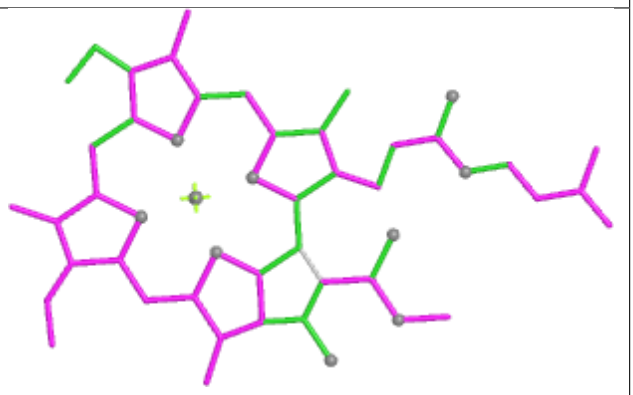
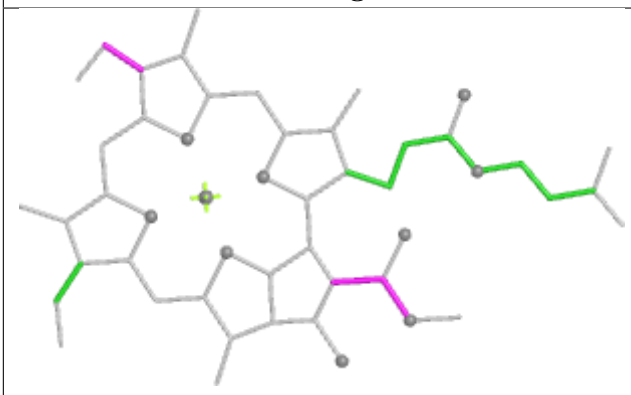


Bond angles



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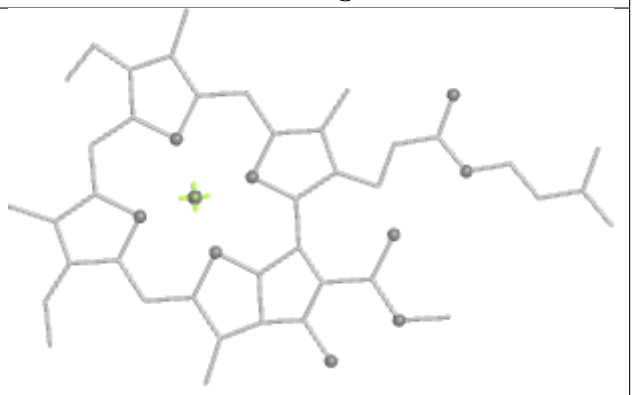
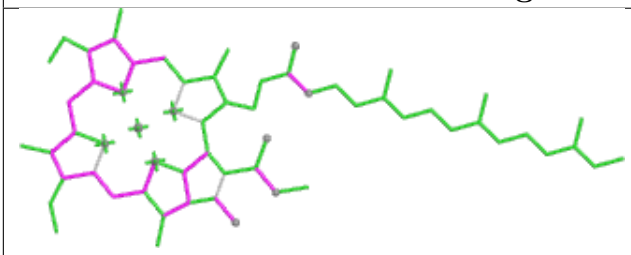


Rings

Ligand CLA aB 807



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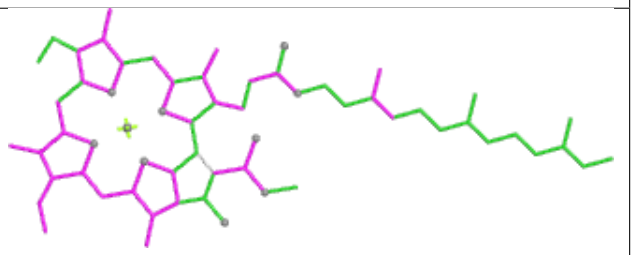

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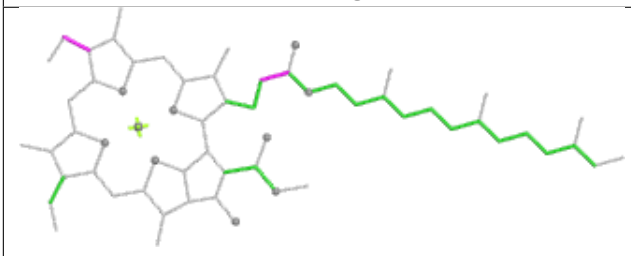

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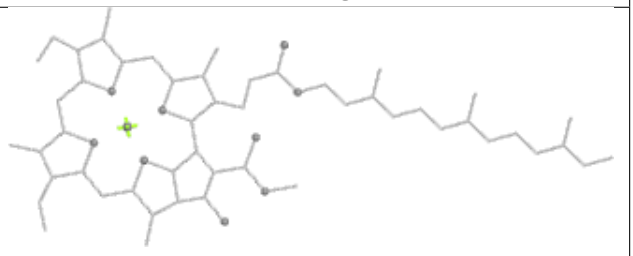
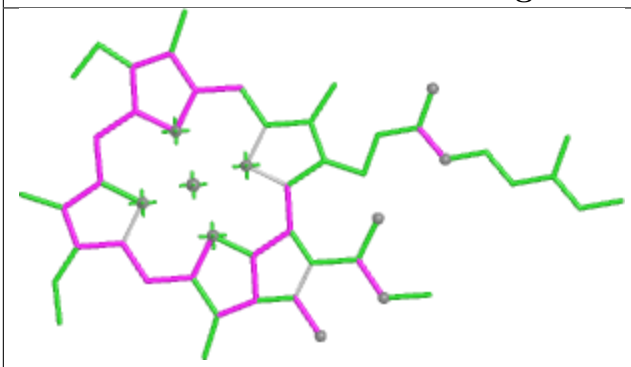


Rings

Ligand CLA cK 103



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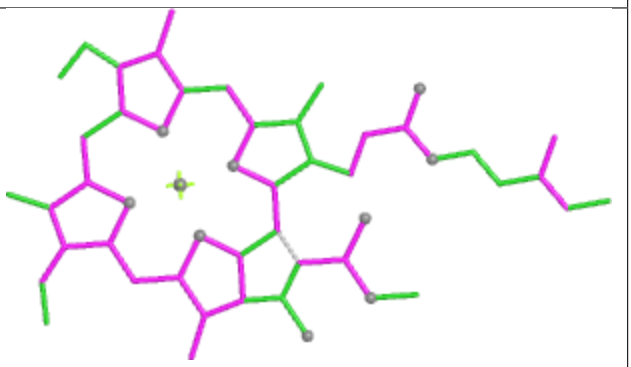

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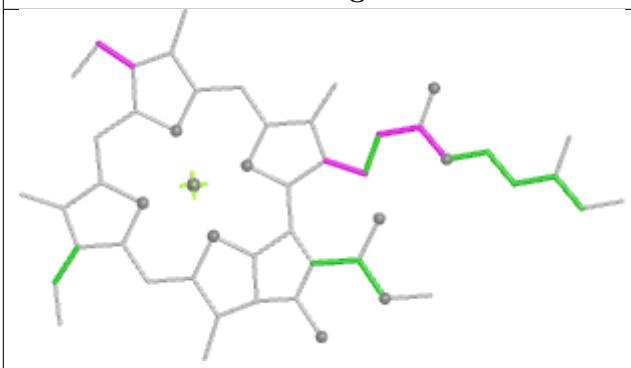

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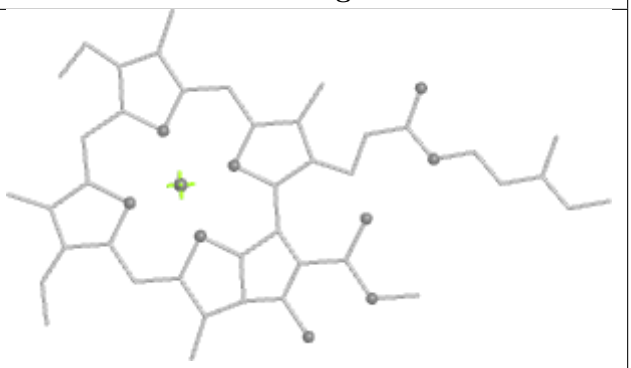
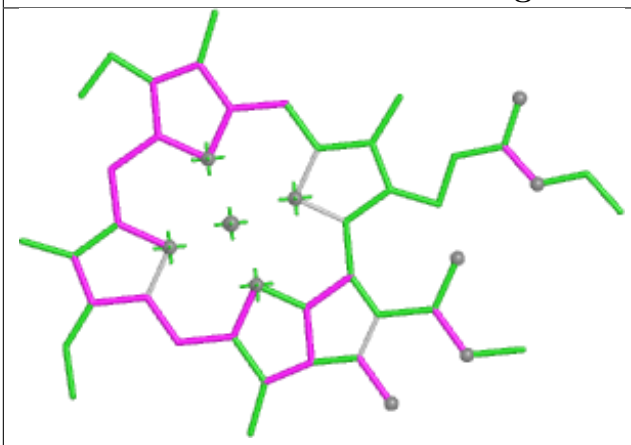


Rings

Ligand CLA bB 809



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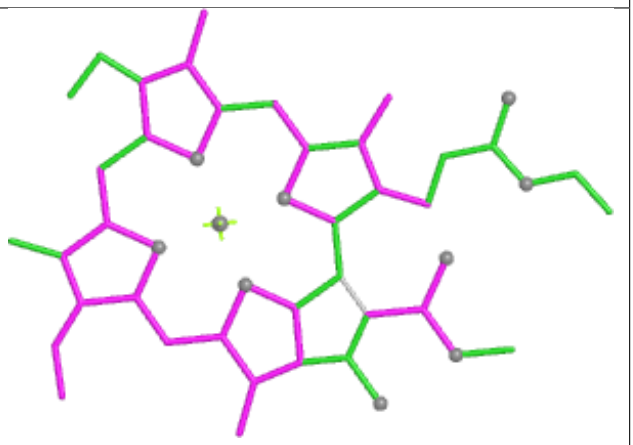

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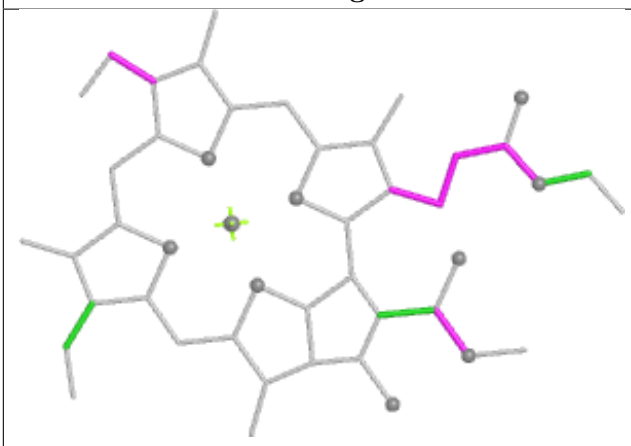

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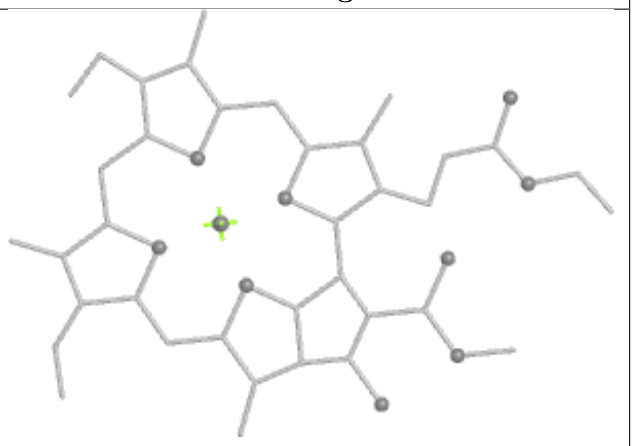
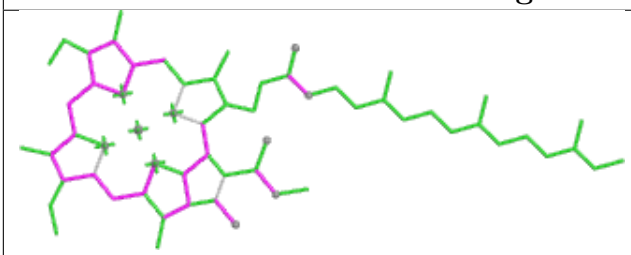


Rings

Ligand CLA cA 821



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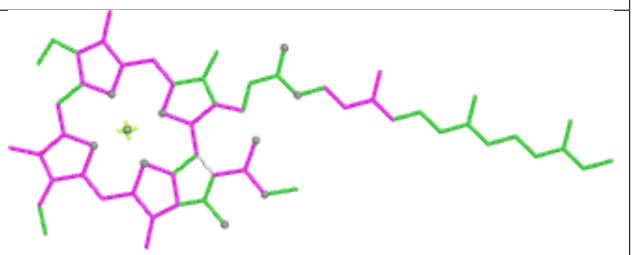
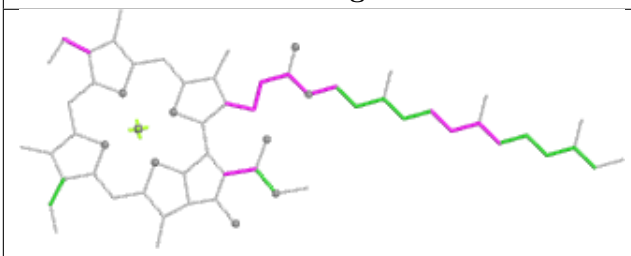


Bond angles



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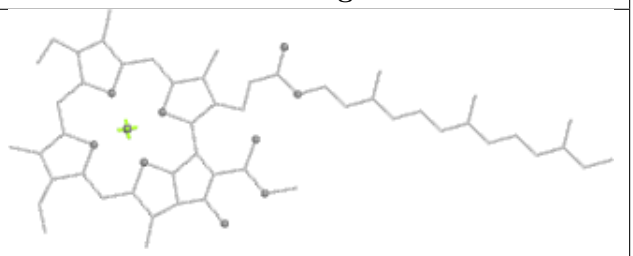

Rings

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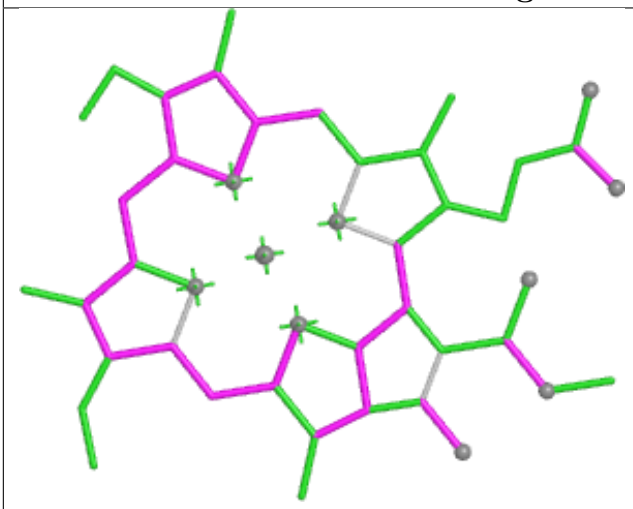

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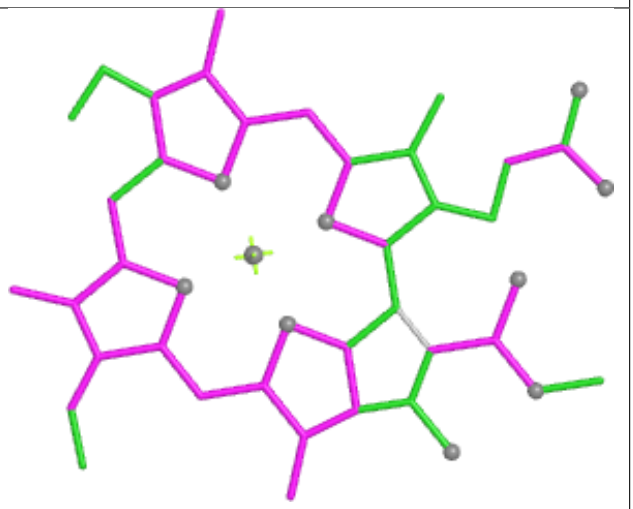
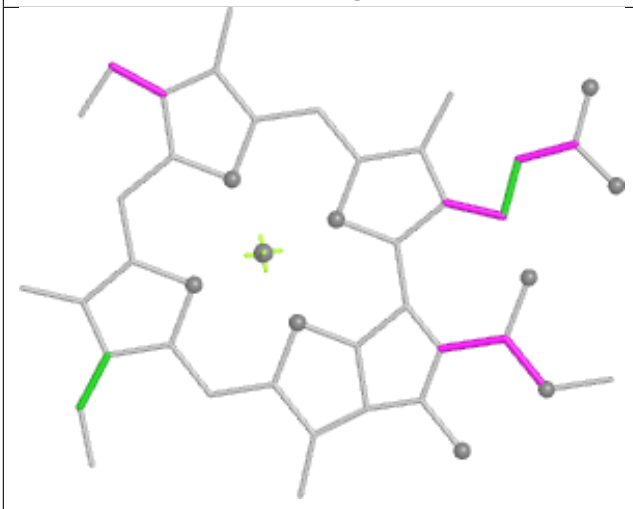


Bond angles

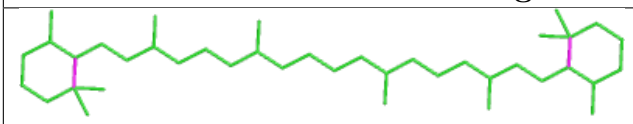


Torsions



Rings

Ligand BCR cB 846



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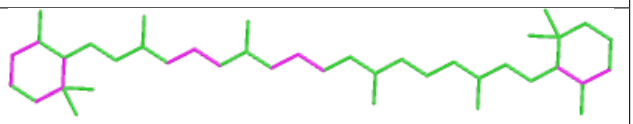

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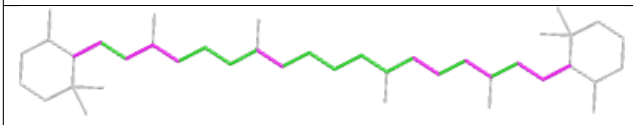

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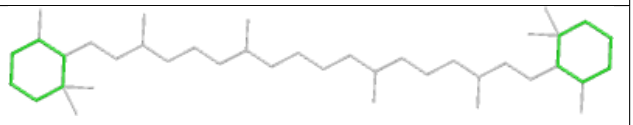
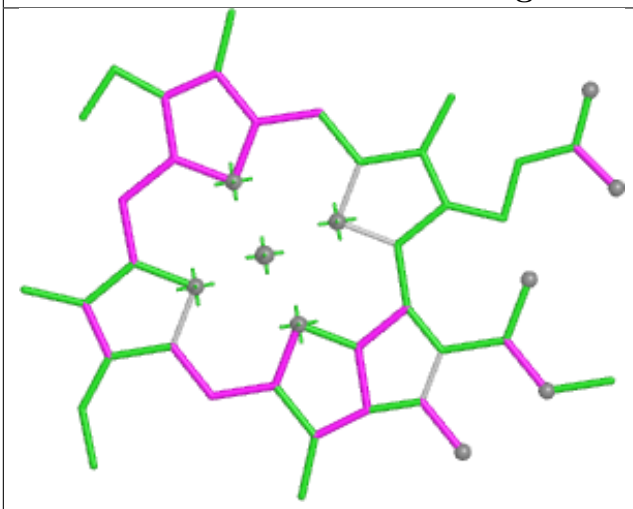


Rings

Ligand CLA aB 822



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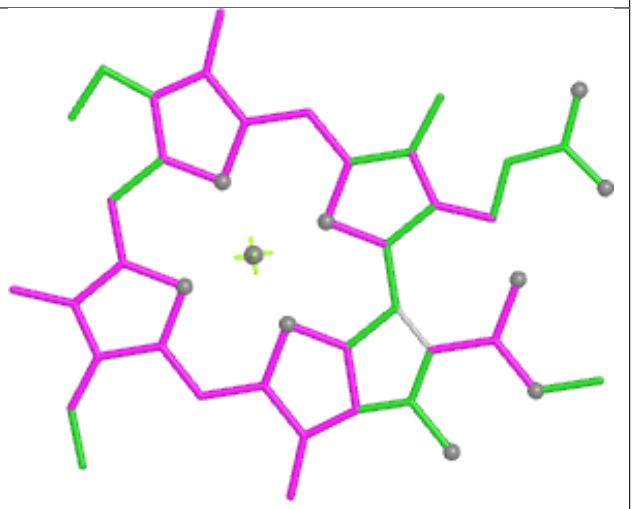
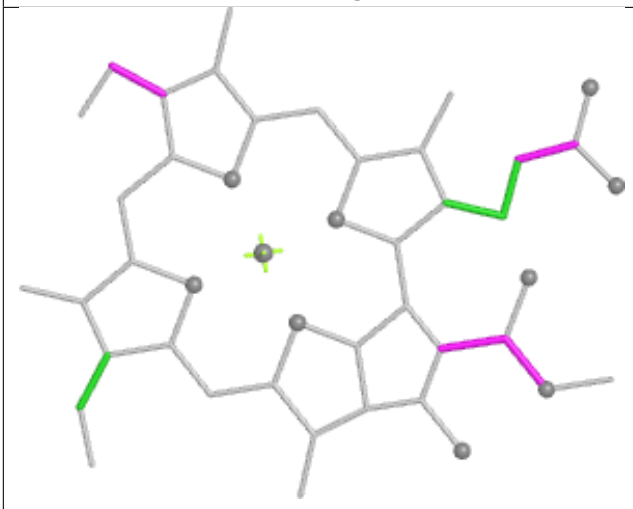


Bond angles

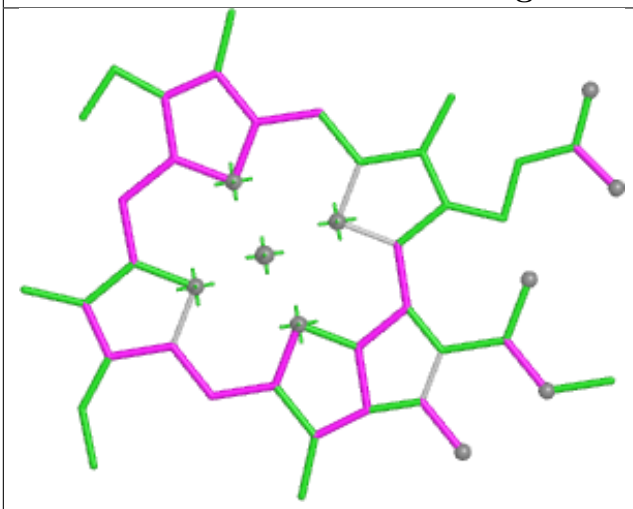


Torsions



Rings

Ligand CLA aB 814



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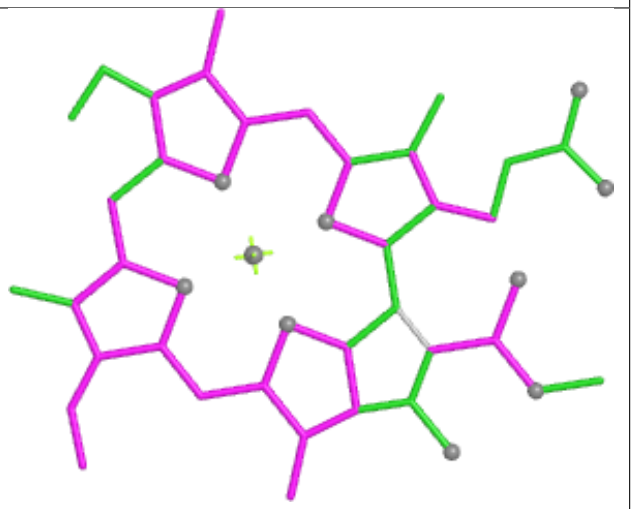
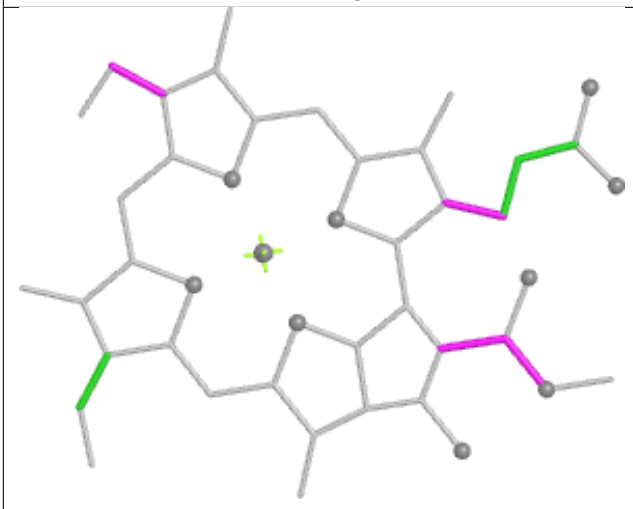


Bond angles

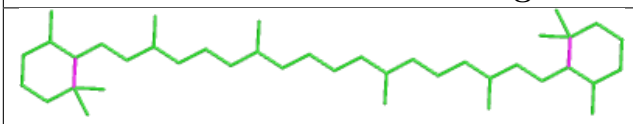


Torsions



Rings

Ligand BCR cA 851



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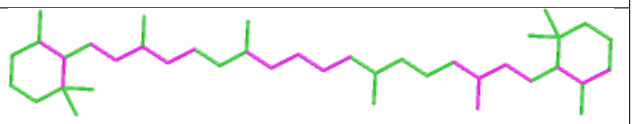
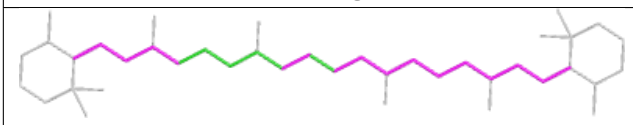
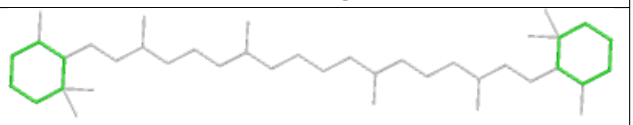


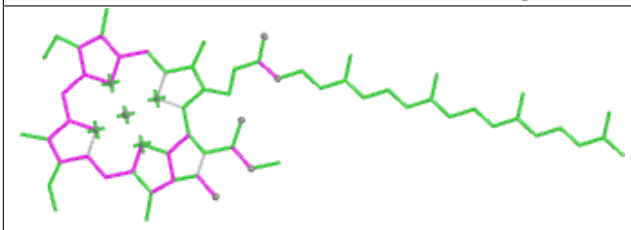
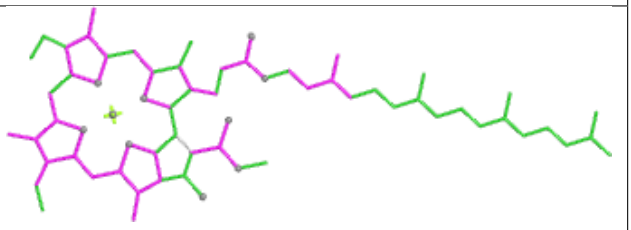
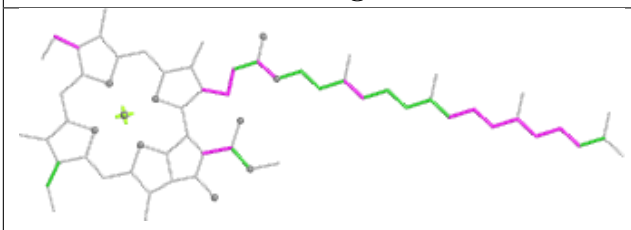
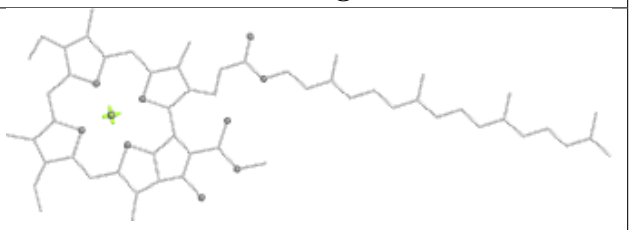
Bond angles



Torsions



Rings

Ligand CLA cB 812	
 Bond lengths	 Bond angles
 Torsions	 Rings

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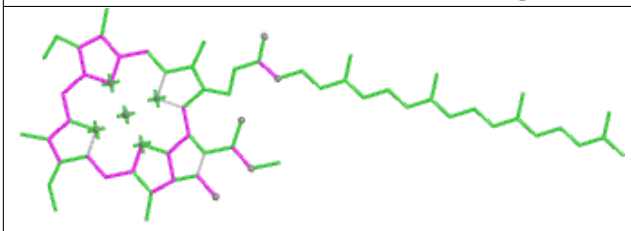
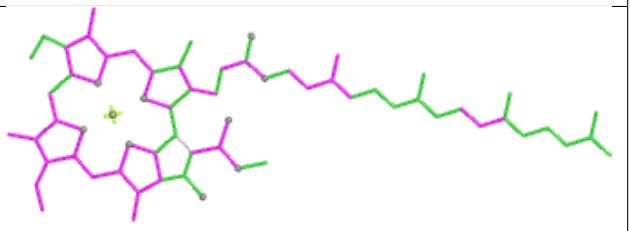
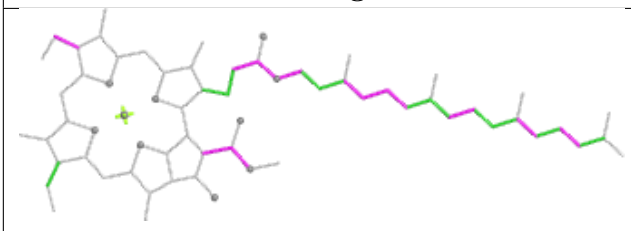
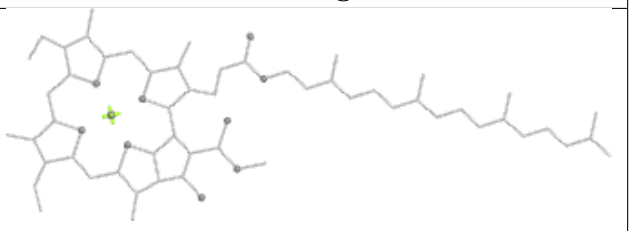
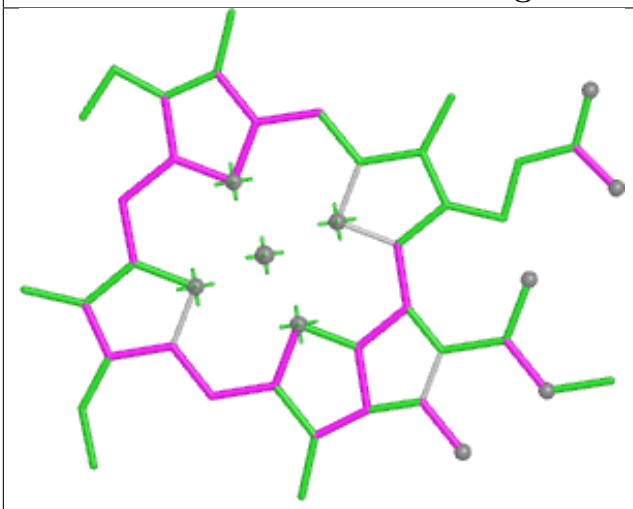
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA bB 829



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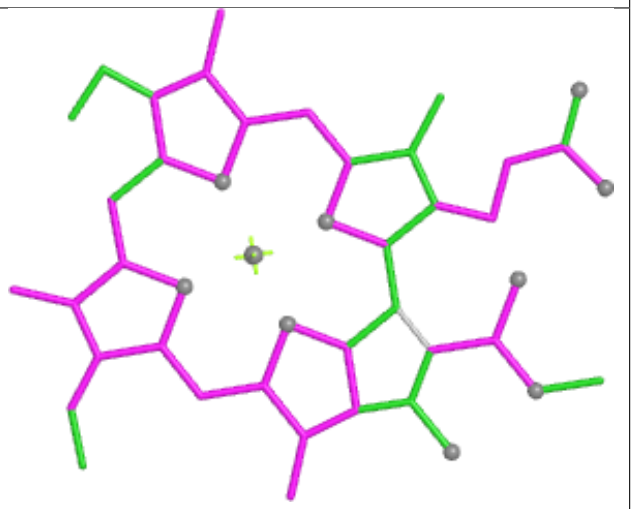
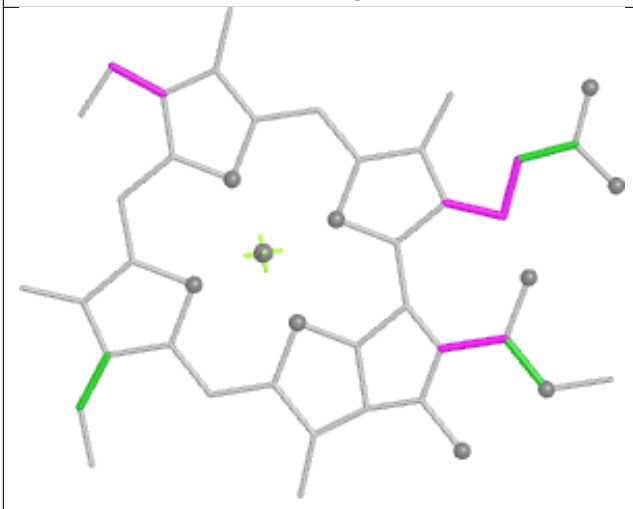


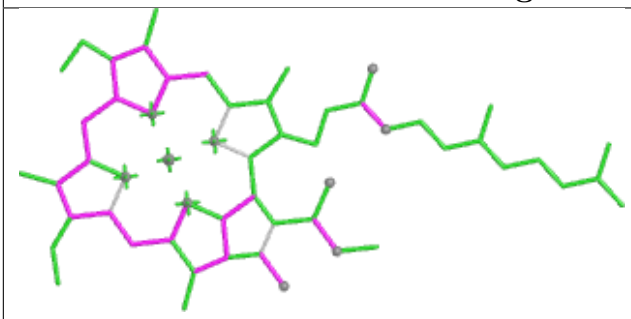
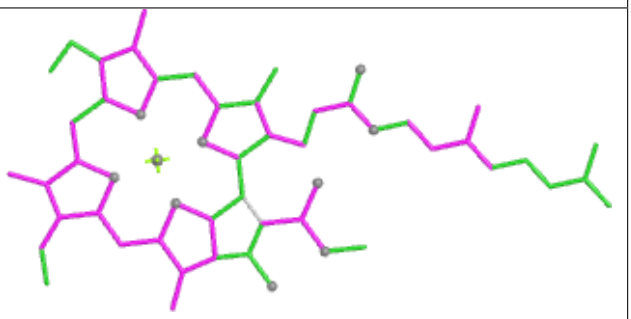
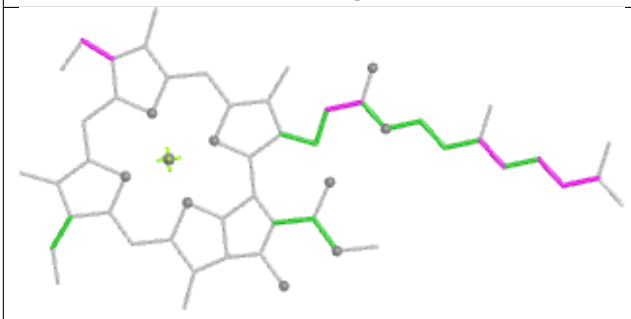
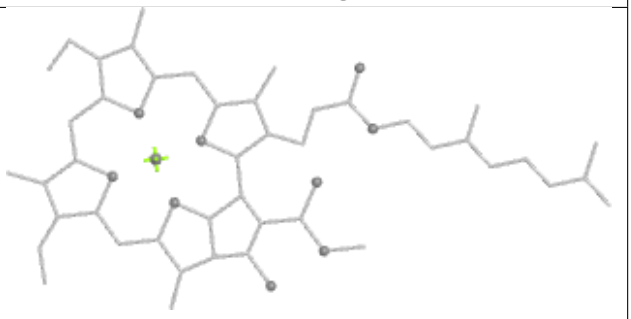
Bond angles



Torsions



Rings

Ligand CLA aB 837	
	
Bond lengths	Bond angles
	
Torsions	Rings

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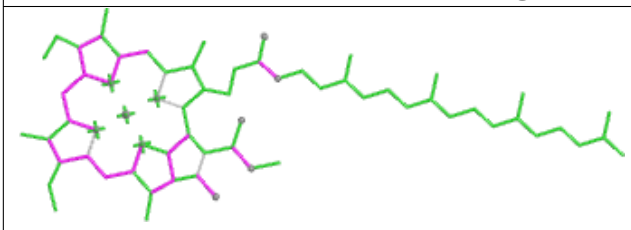
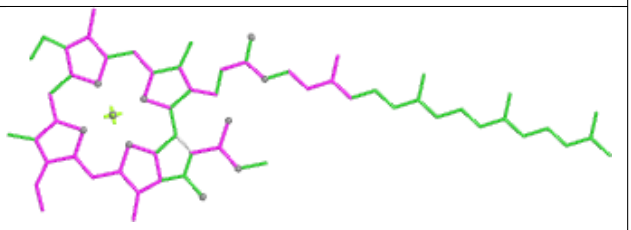
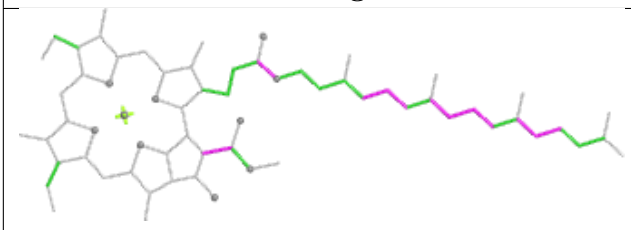
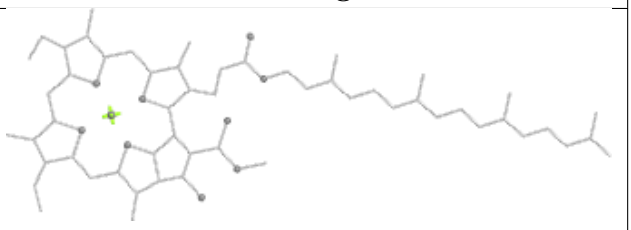
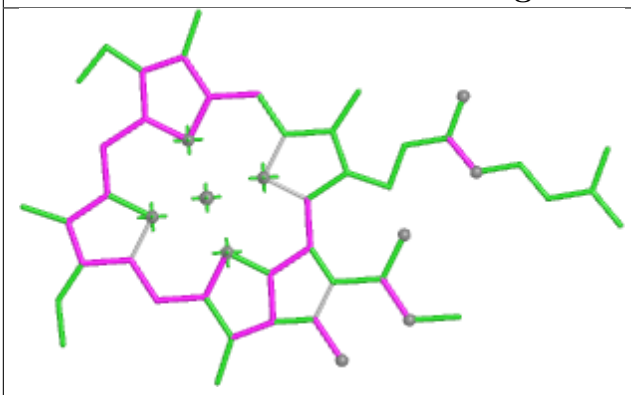
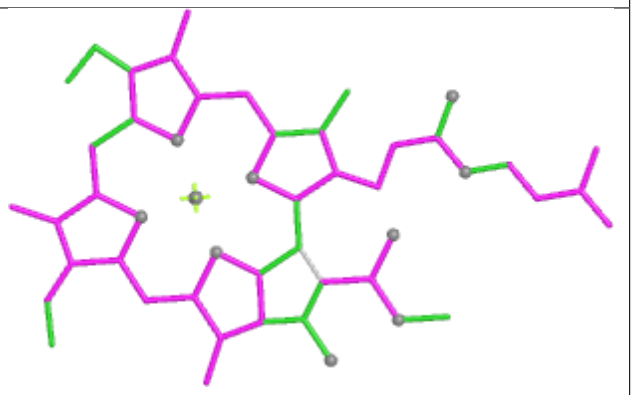
	
Bond lengths	Bond angles
	
Torsions	Rings

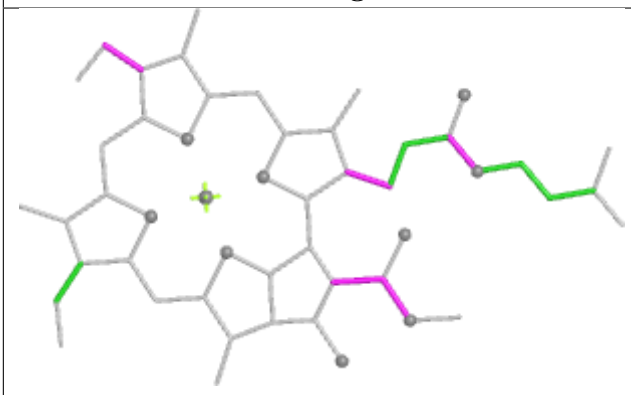
Ligand CLA bB 804



Bond lengths



Bond angles



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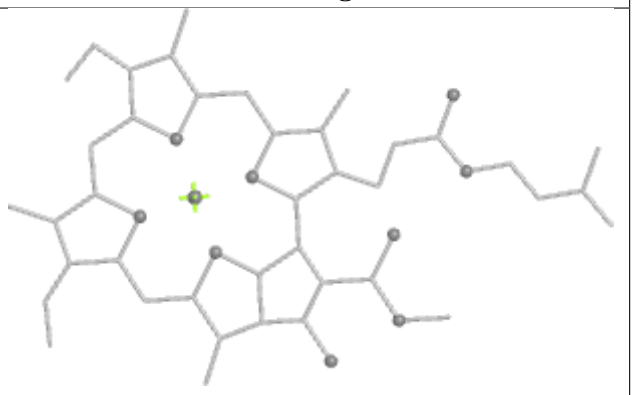
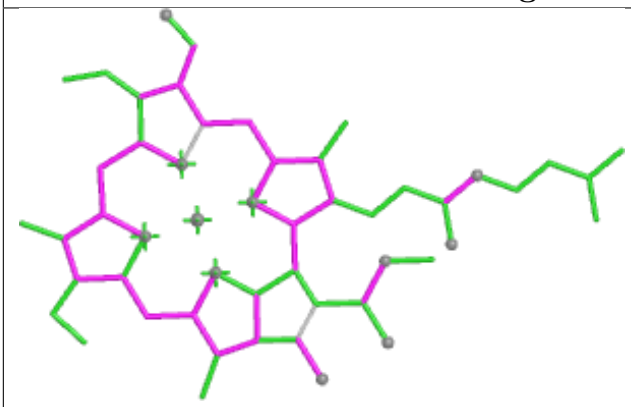


Rings

Ligand F6C aA 832



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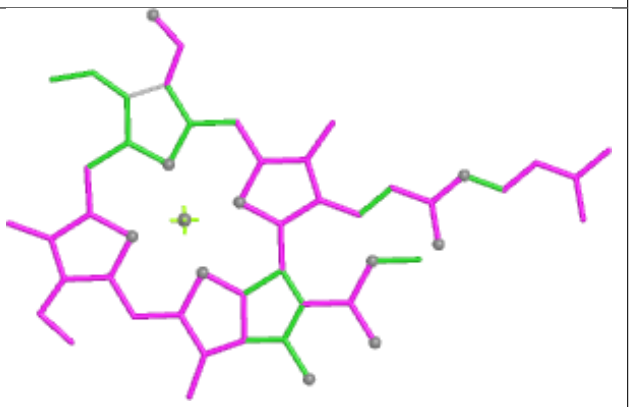

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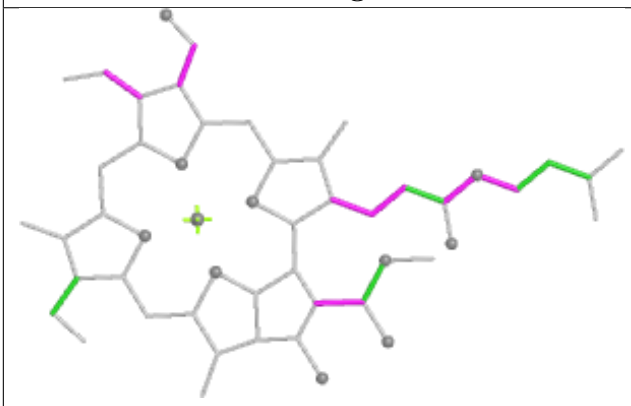

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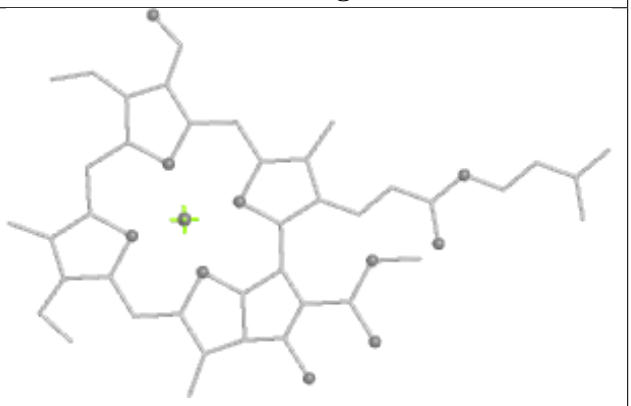
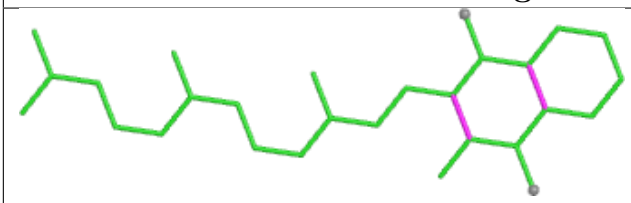


Rings

Ligand PQN cB 841



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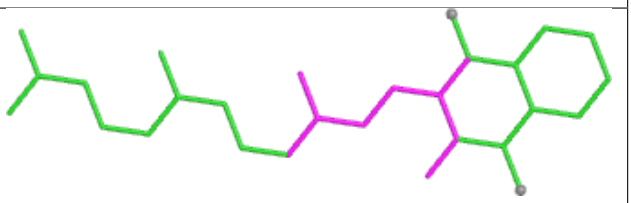

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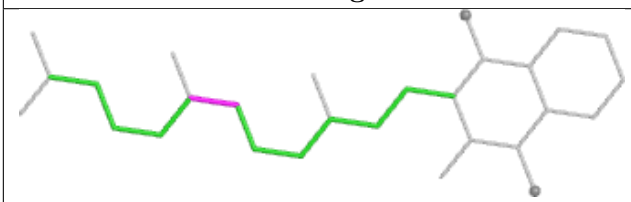

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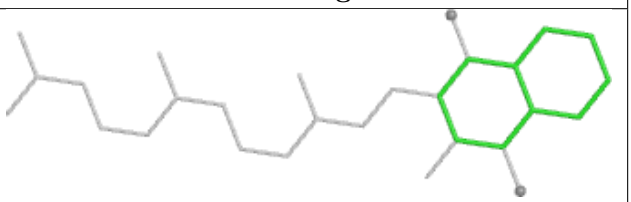
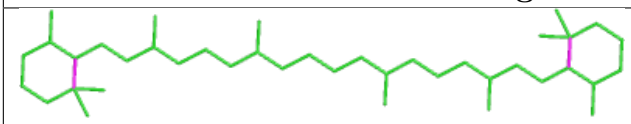


Rings

Ligand BCR aL 208



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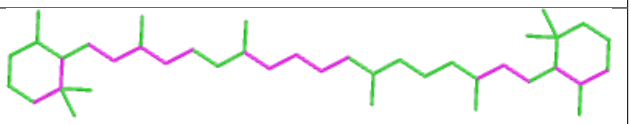
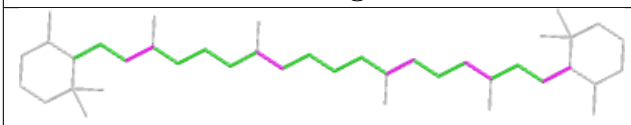


Bond angles



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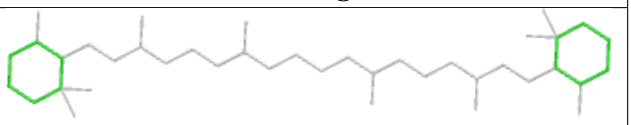
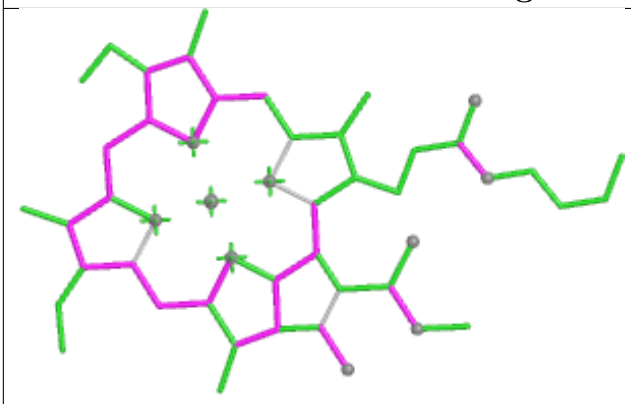


Rings

Ligand CLA cA 817



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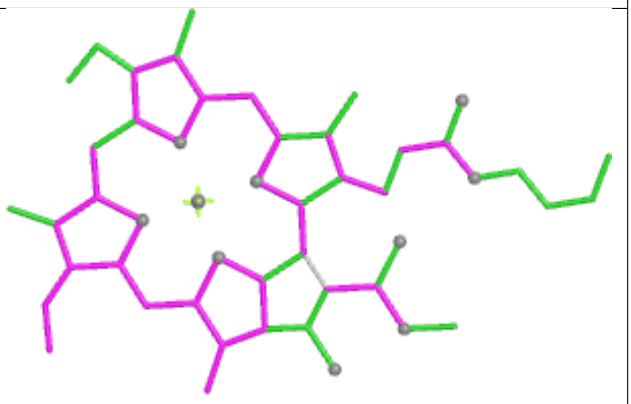
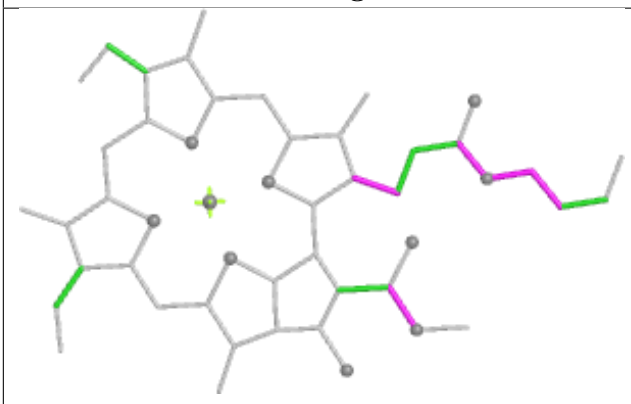


Bond angles



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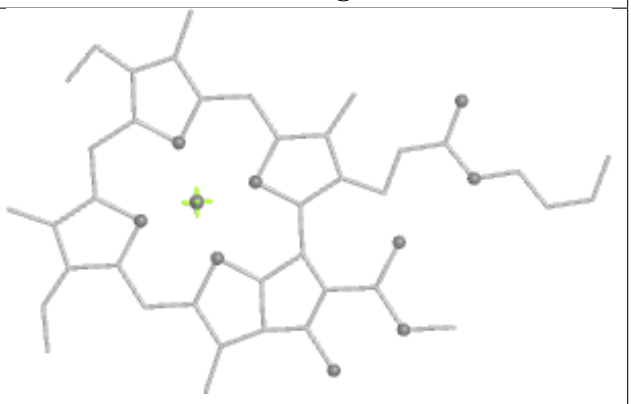
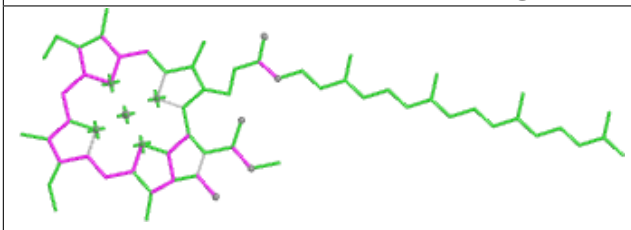


Rings

Ligand CLA bA 839



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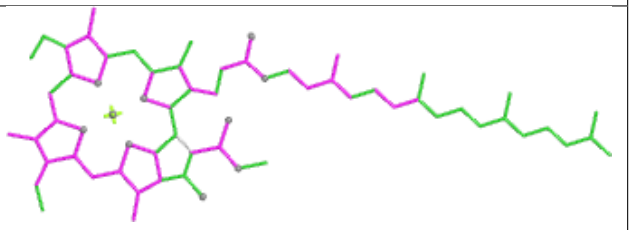

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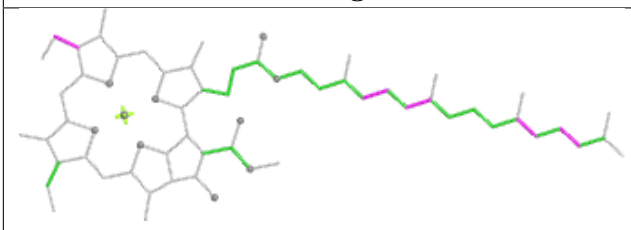

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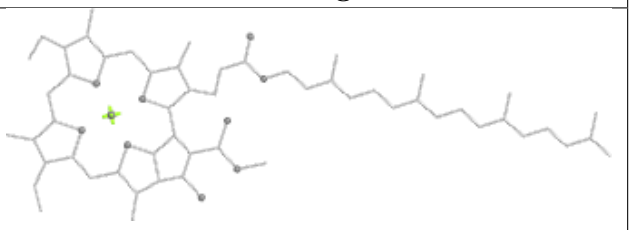
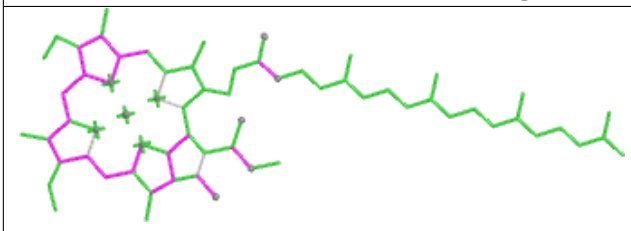


Rings

Ligand CLA aB 827



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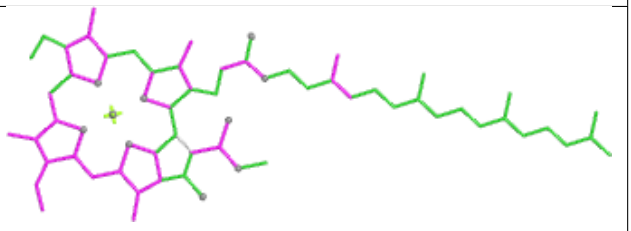
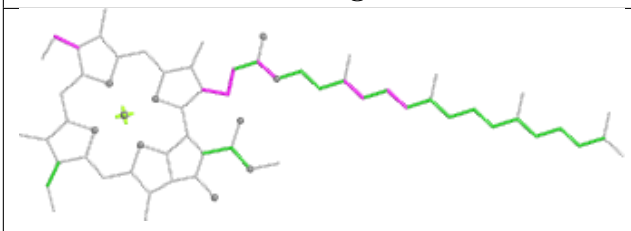


Bond angles



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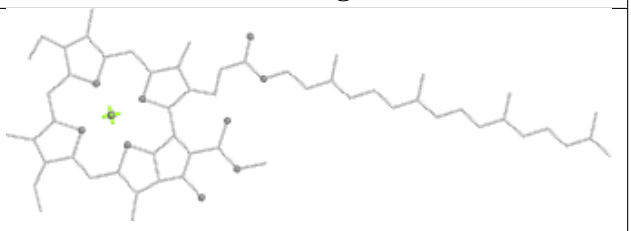
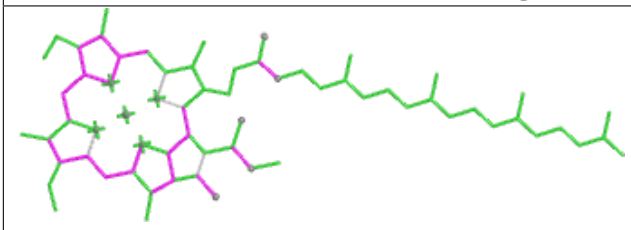


Rings

Ligand CLA aA 825



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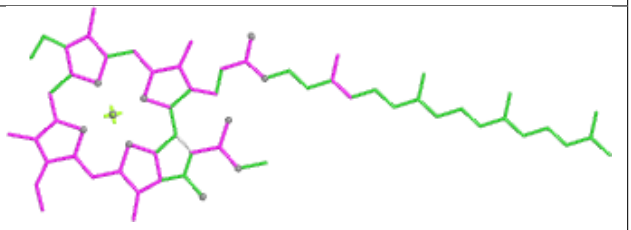
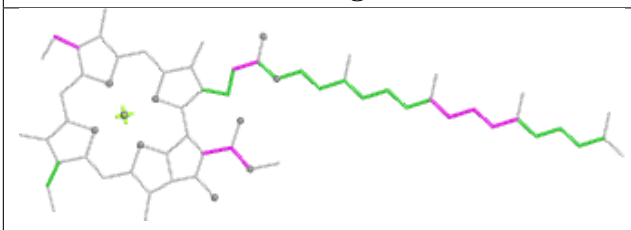


Bond angles



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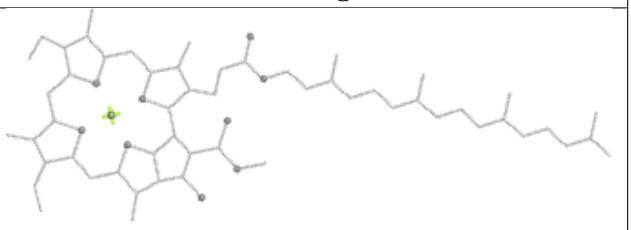
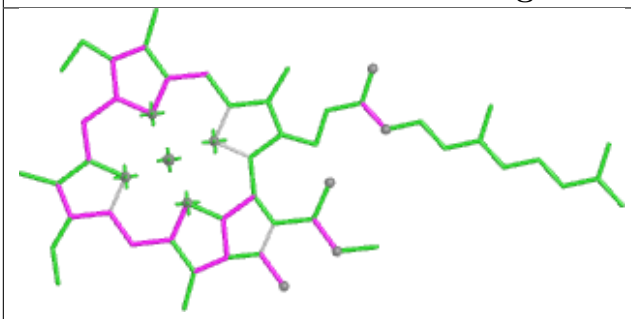
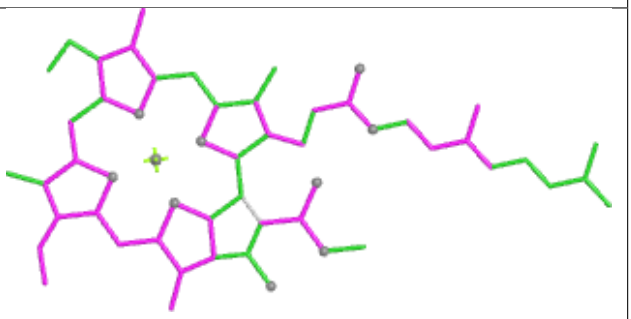
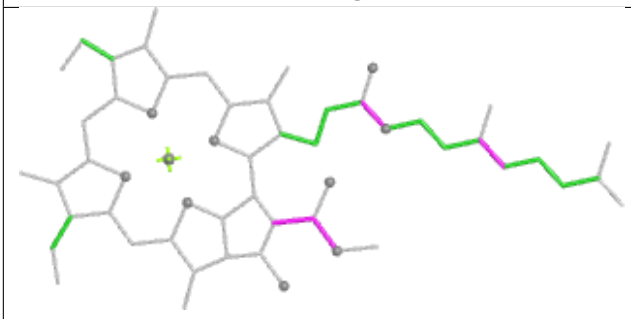
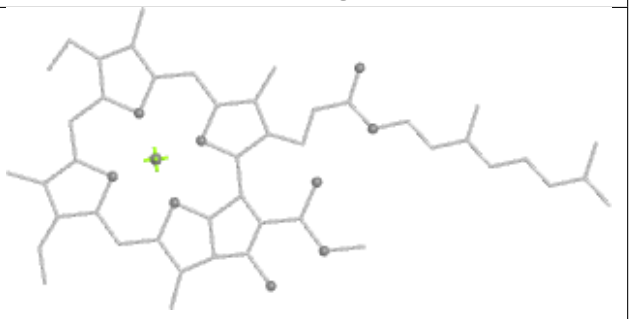
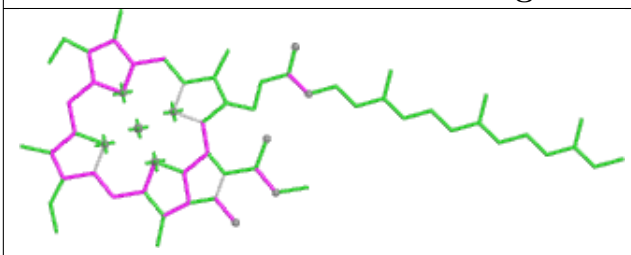
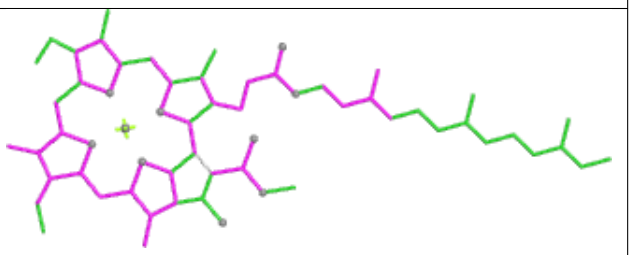
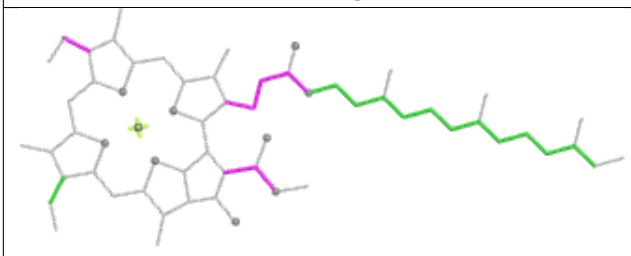
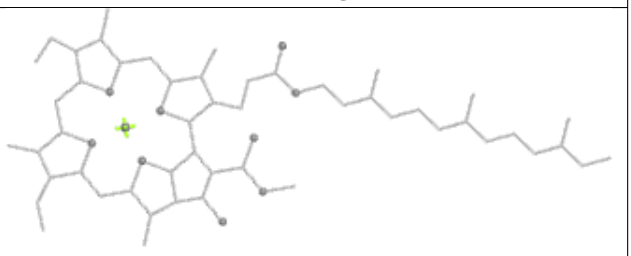
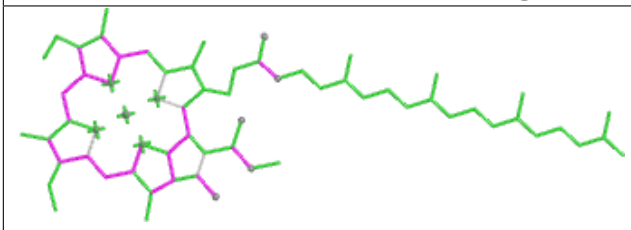


Rings

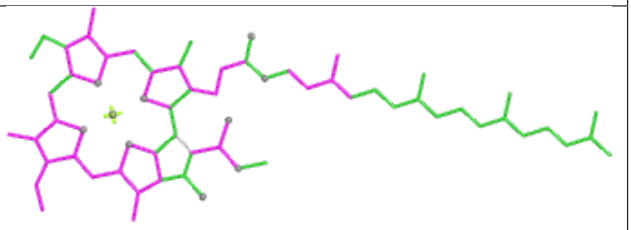
Ligand CLA cB 828	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA aB 826	
	
Bond lengths	Bond angles
	
Torsions	Rings

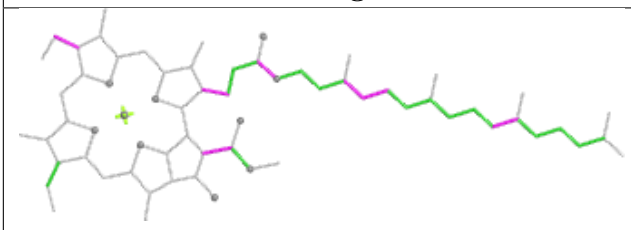
Ligand CLA cA 820



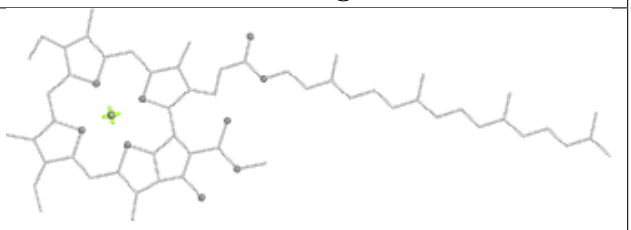
Bond lengths



Bond angles

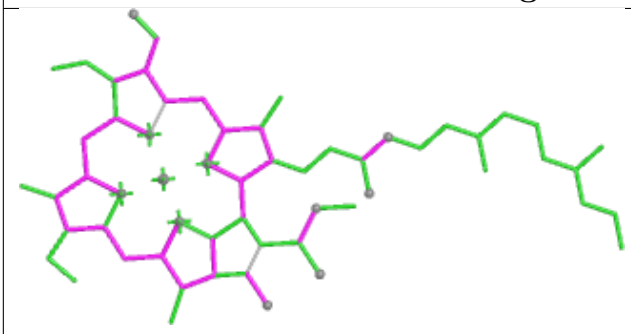


Torsions

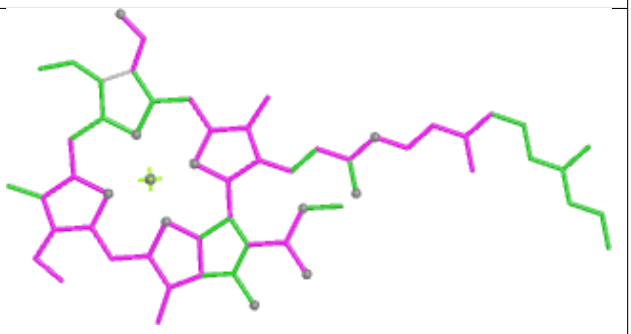


Rings

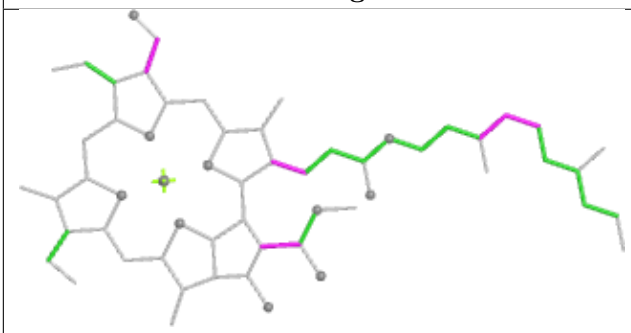
Ligand F6C aB 824



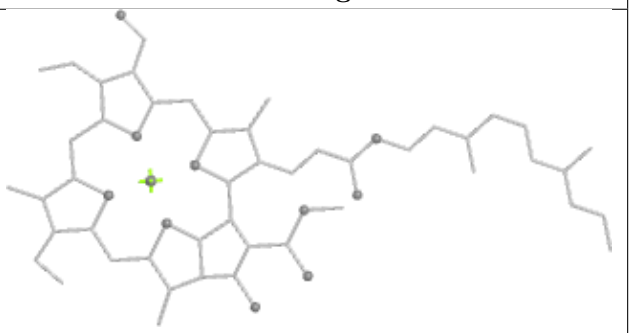
Bond lengths



Bond angles

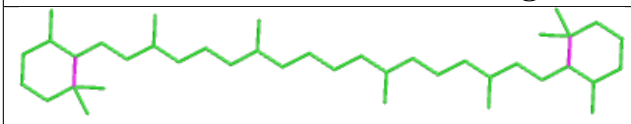


Torsions



Rings

Ligand BCR cI 103



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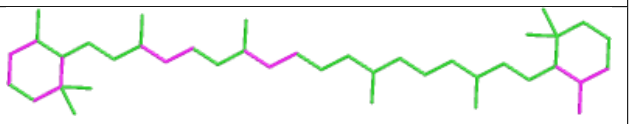
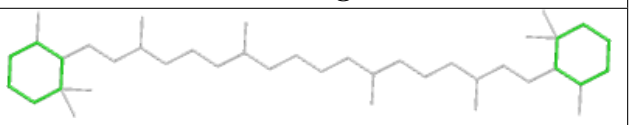


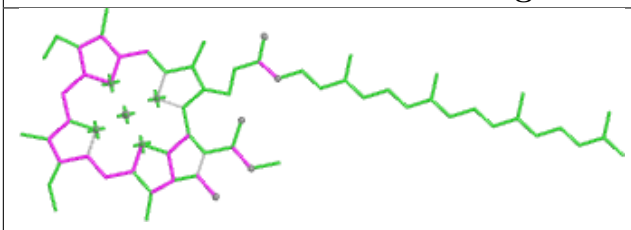
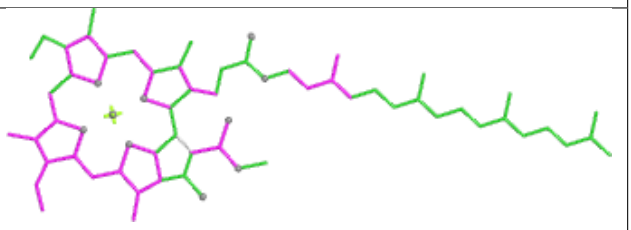
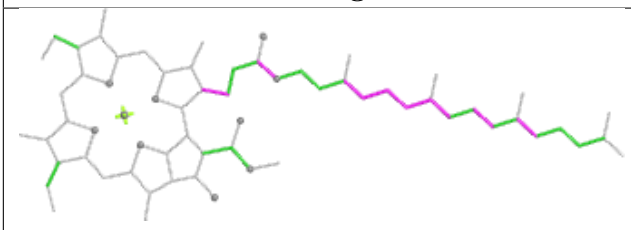
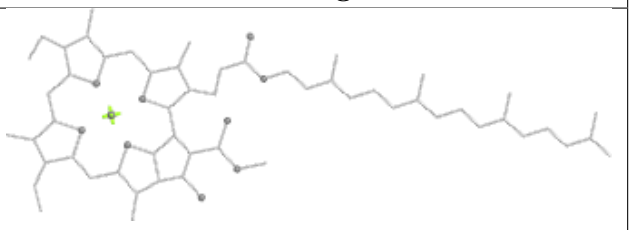
Bond angles

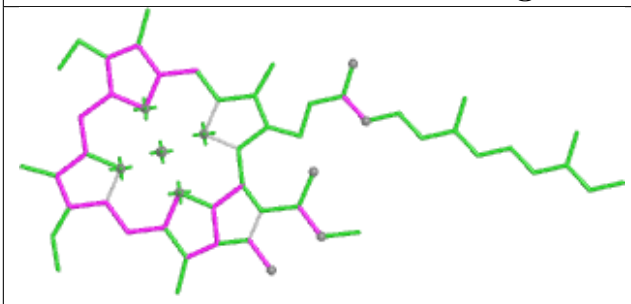
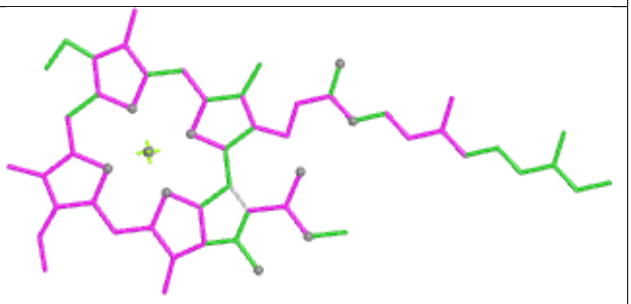
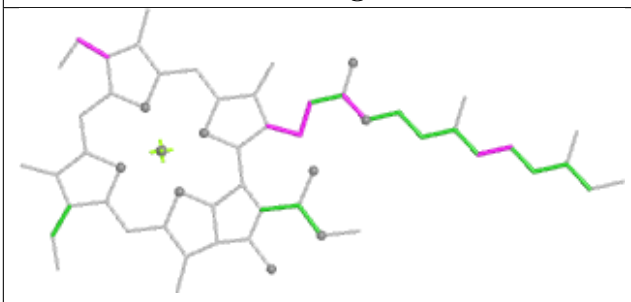
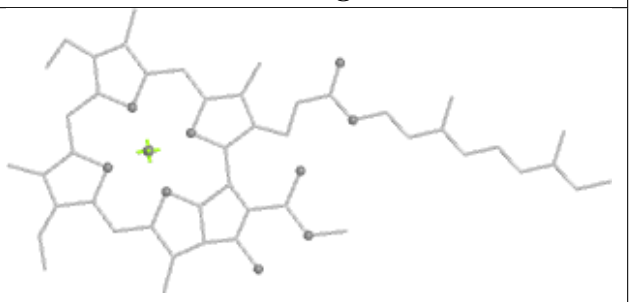


Torsions

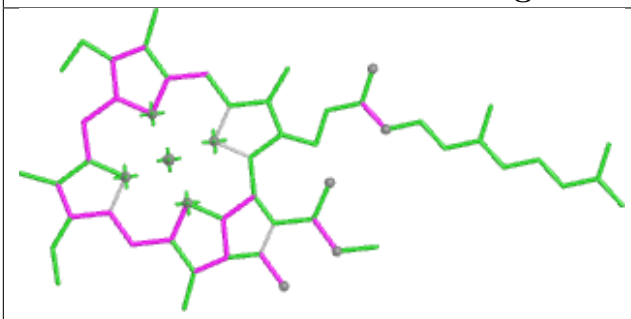


Rings

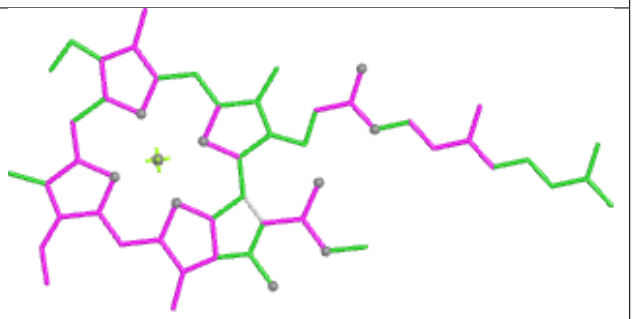
Ligand CLA aA 833	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA cB 831	
	
Bond lengths	Bond angles
	
Torsions	Rings

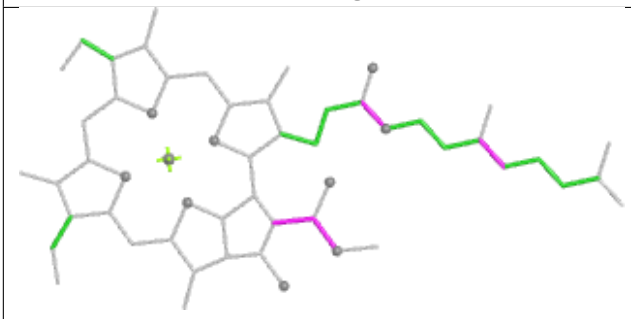
Ligand CLA bB 828



Bond lengths



Bond angles



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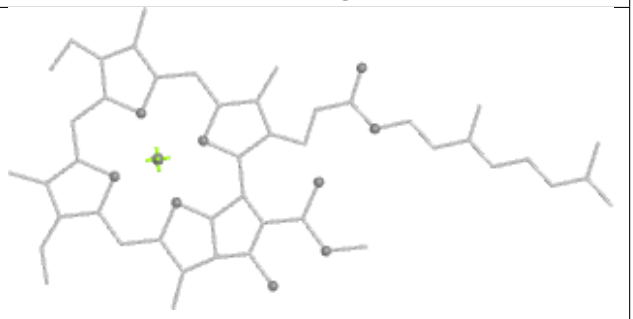
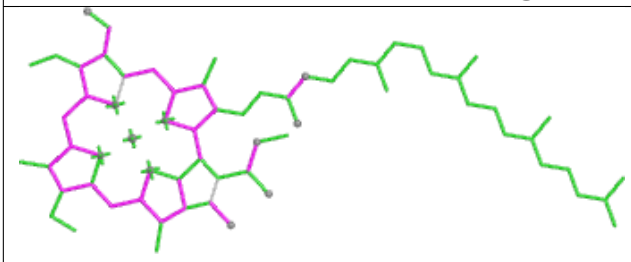


Rings

Ligand F6C bA 844



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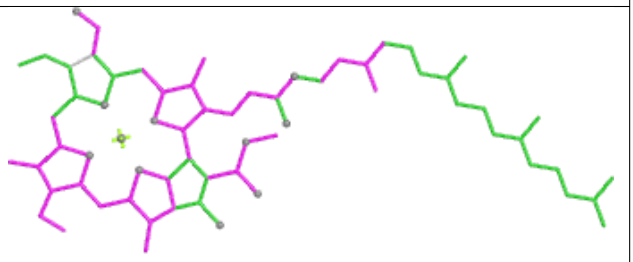
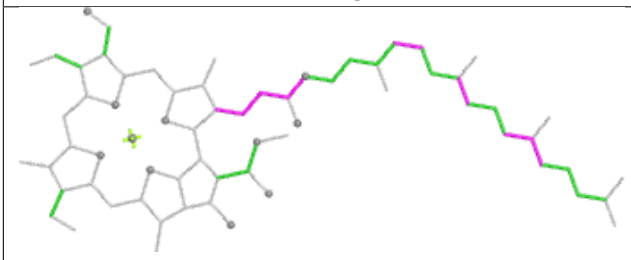


Bond angles



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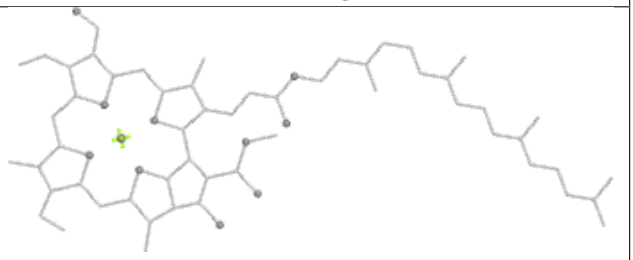
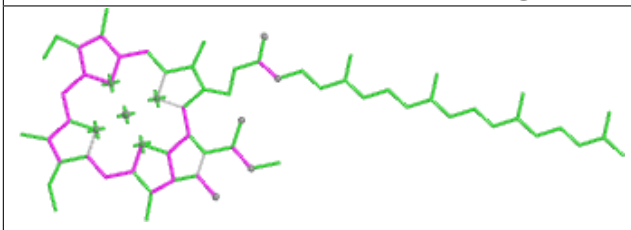


Rings

Ligand CLA aA 807



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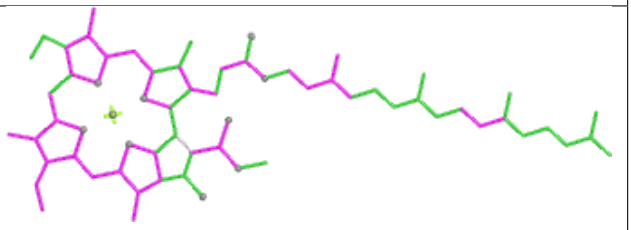
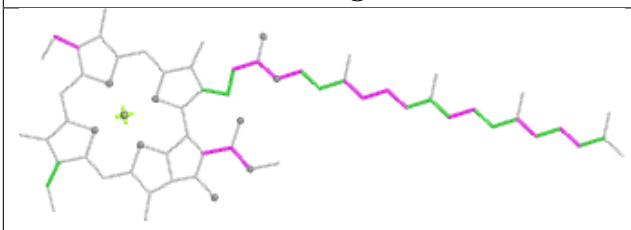


Bond angles



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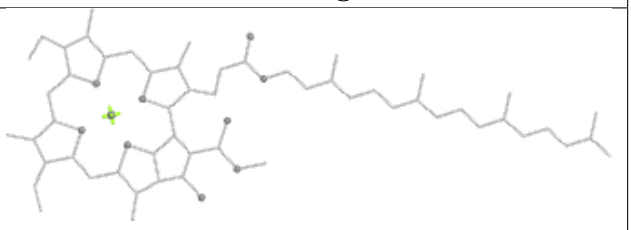
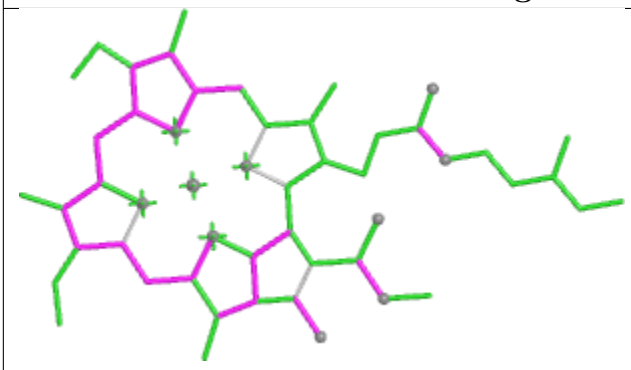


Rings

Ligand CLA bB 836



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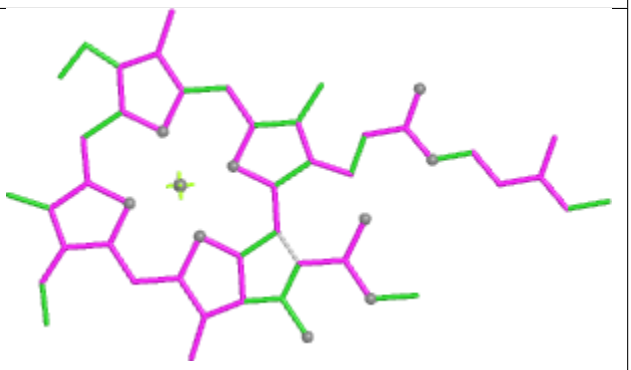
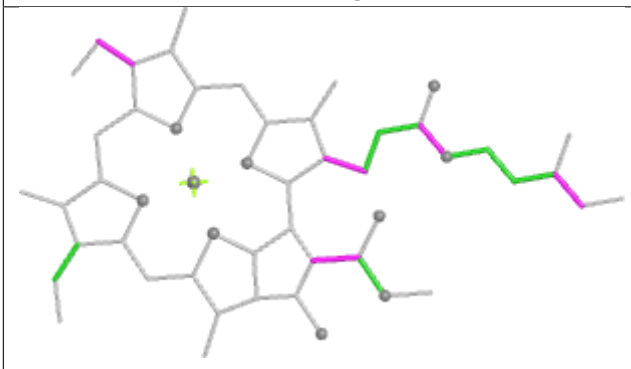


Bond angles



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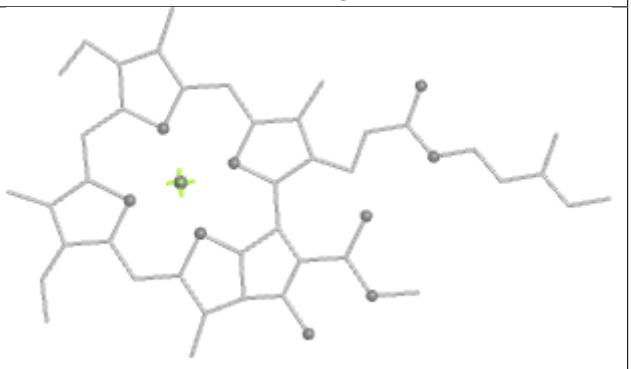
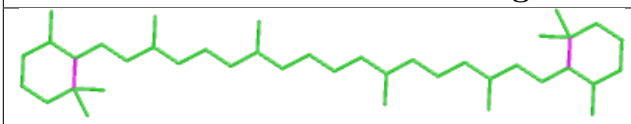


Rings

Ligand BCR bA 849



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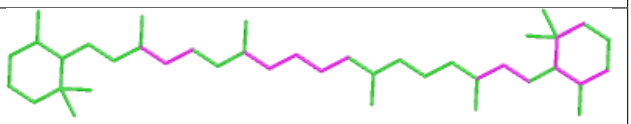
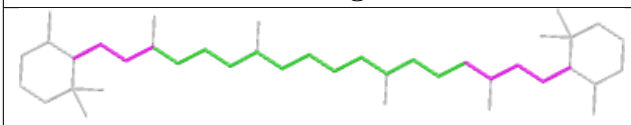


Bond angles



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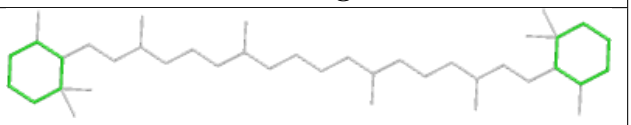
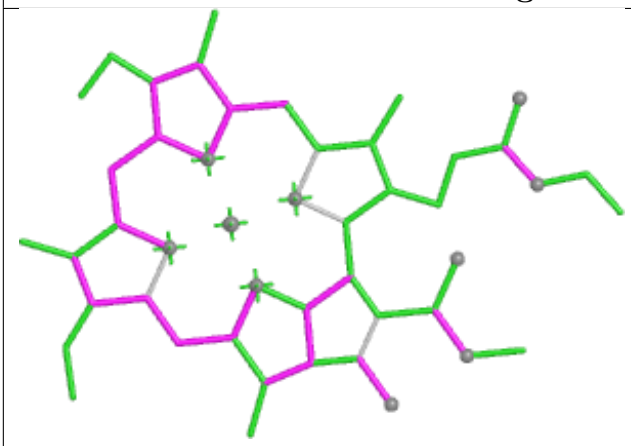


Rings

Ligand CLA cB 809



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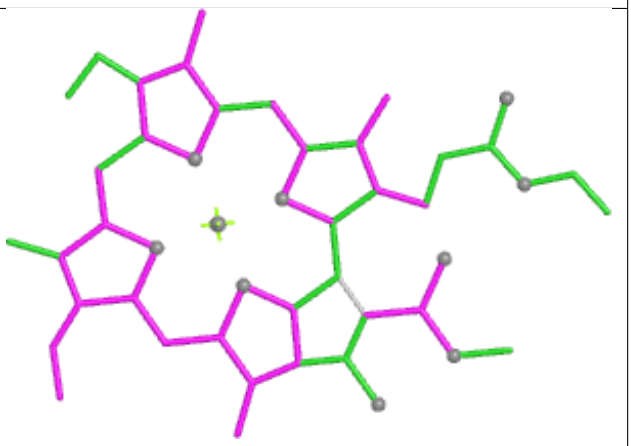
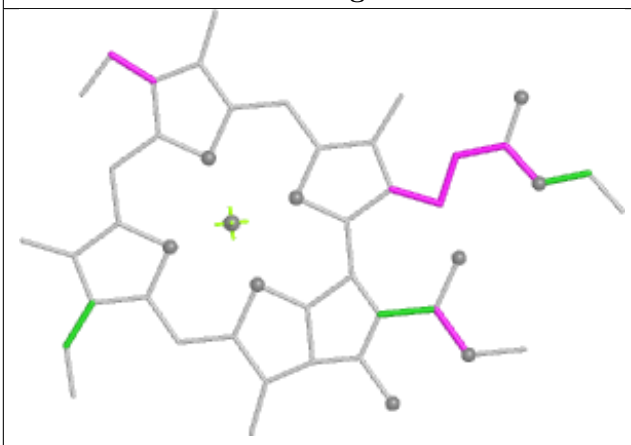


Bond angles



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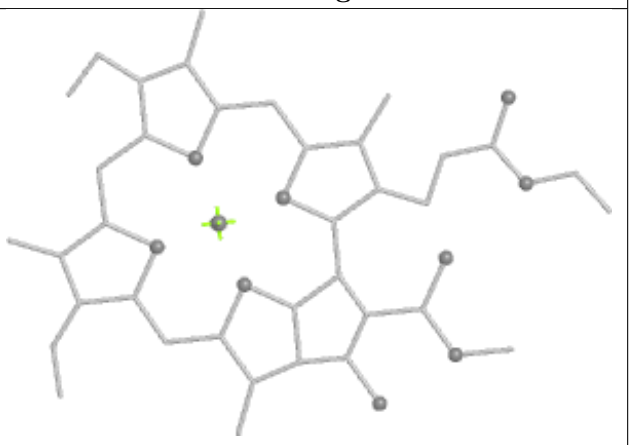
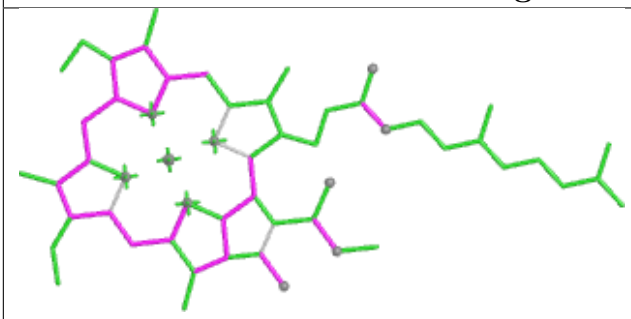


Rings

Ligand CLA bB 815



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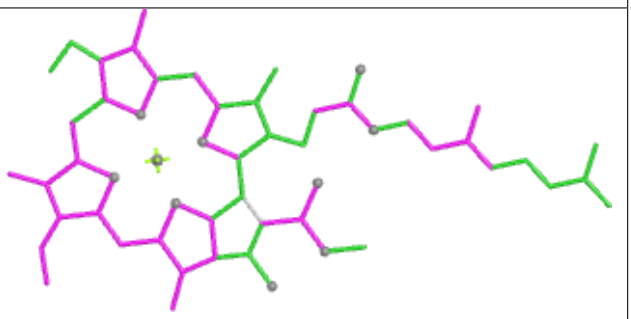
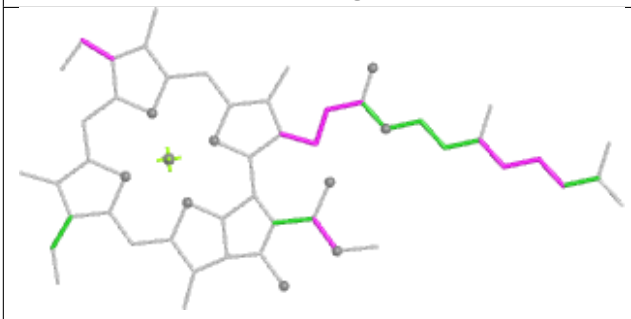


Bond angles



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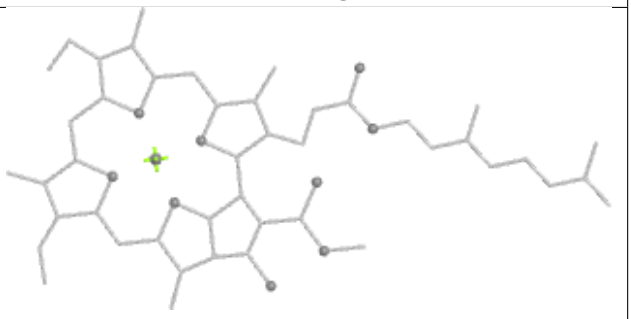
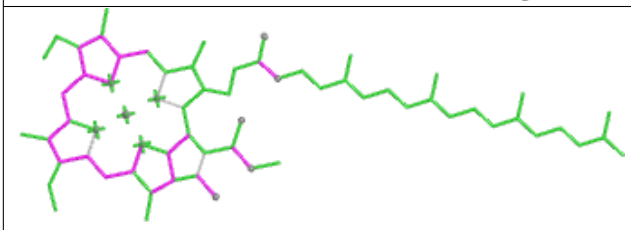


Rings

Ligand CLA cB 827



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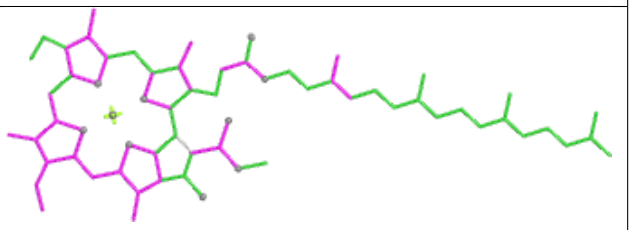
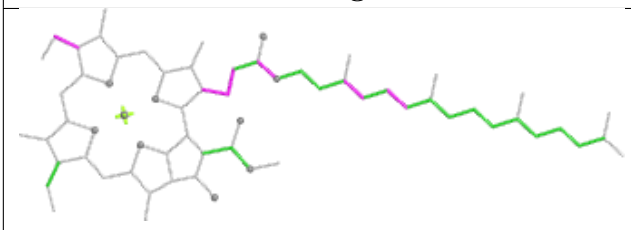


Bond angles



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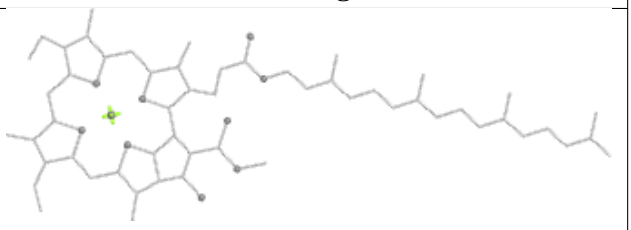
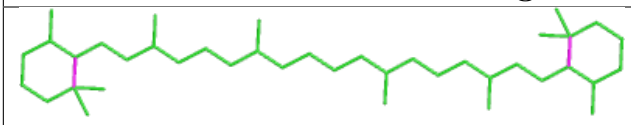


Rings

Ligand BCR cL 207



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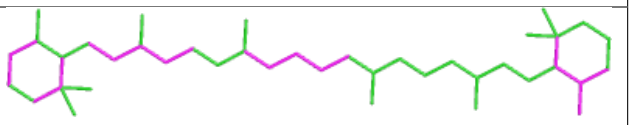
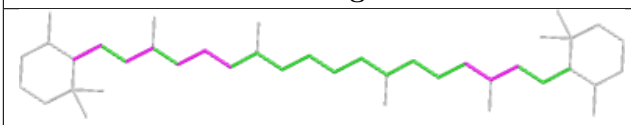


Bond angles



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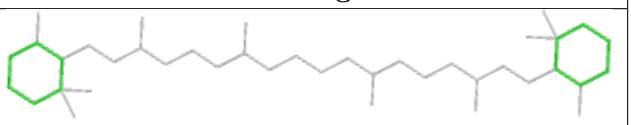
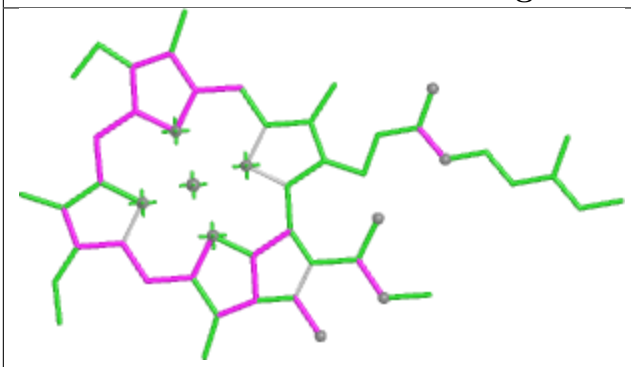


Rings

Ligand CLA cA 824



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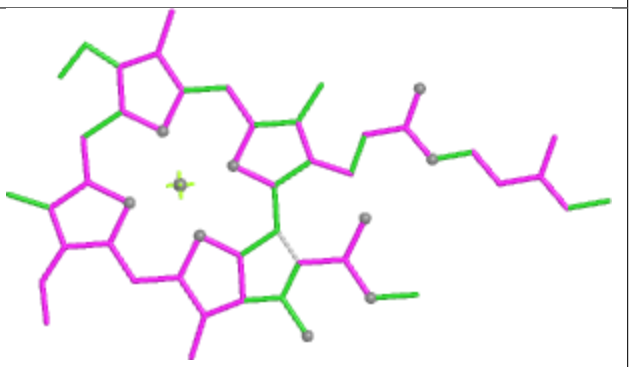
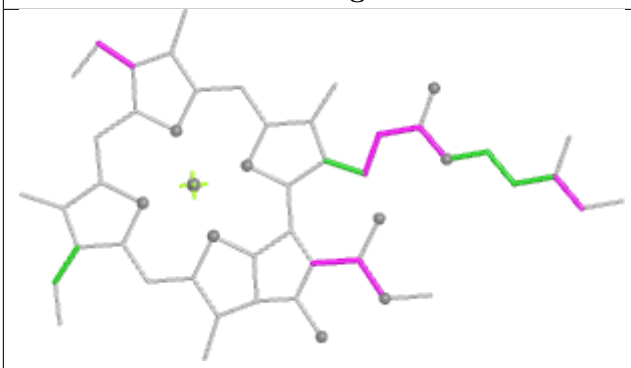


Bond angles



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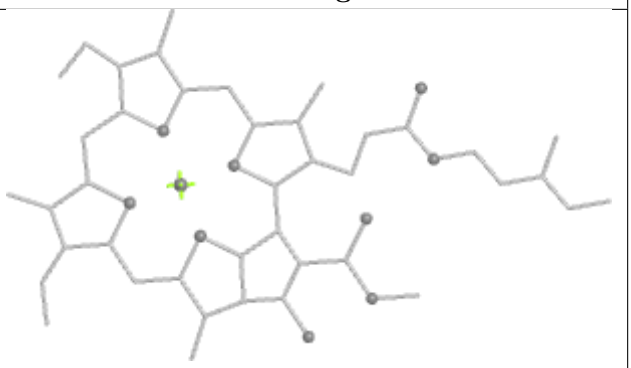
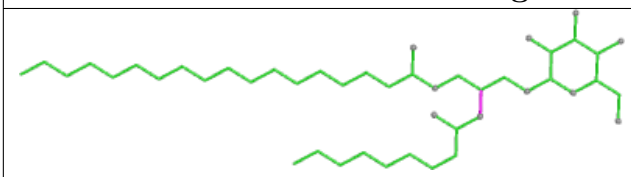
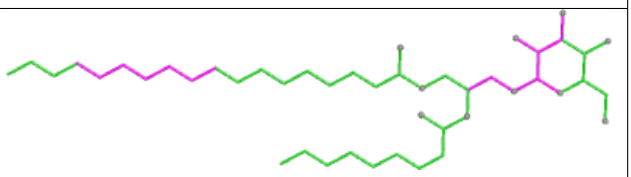


Rings

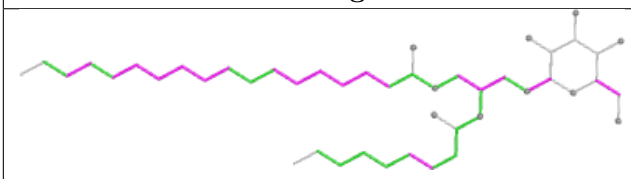
Ligand LMG aB 847



Bond lengths



Bond angles



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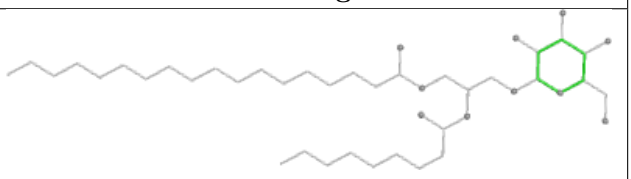
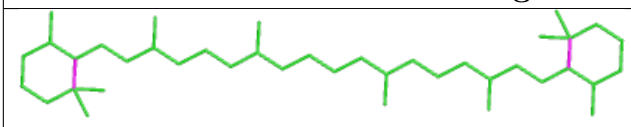
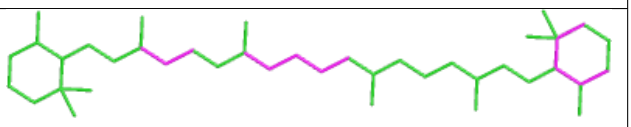


Rings

Ligand BCR aA 849



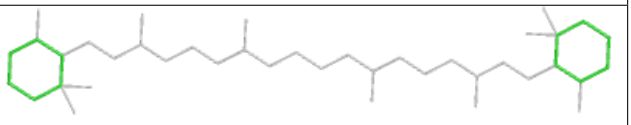
Bond lengths



Bond angles

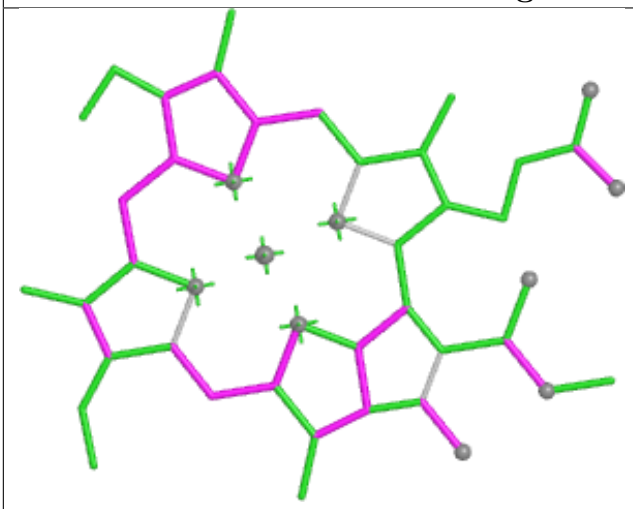


Torsions

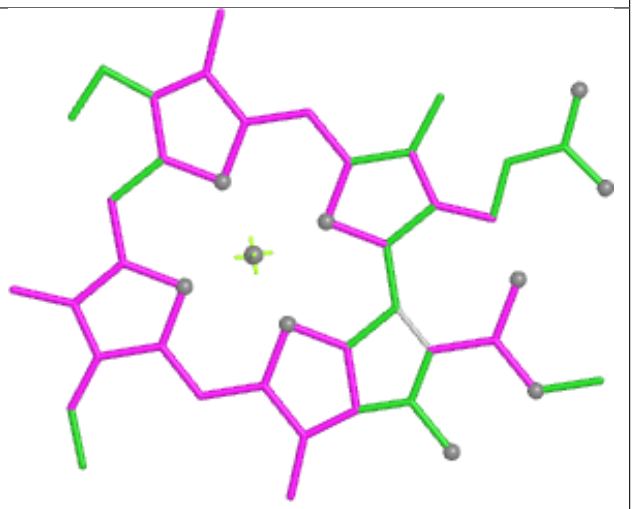


Rings

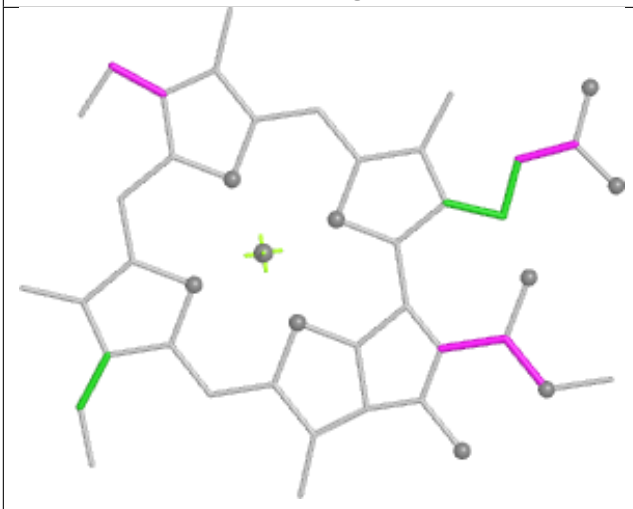
Ligand CLA cB 822



Bond lengths



Bond angles

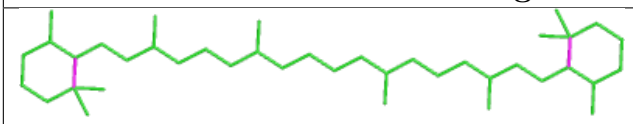


Torsions



Rings

Ligand BCR cA 850



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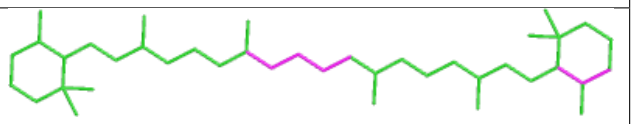
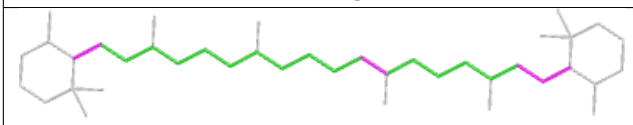


Bond angles



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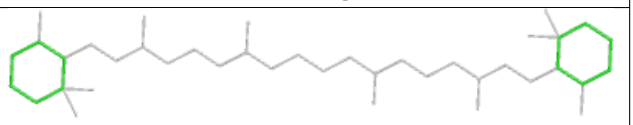
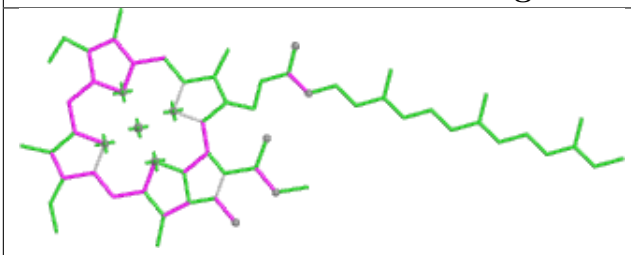
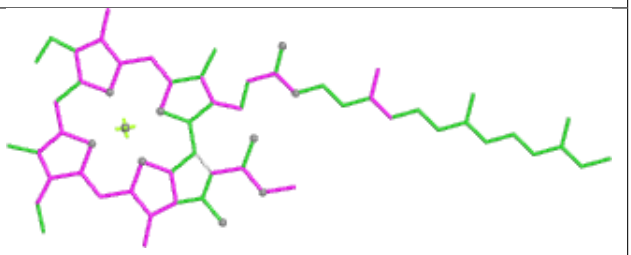
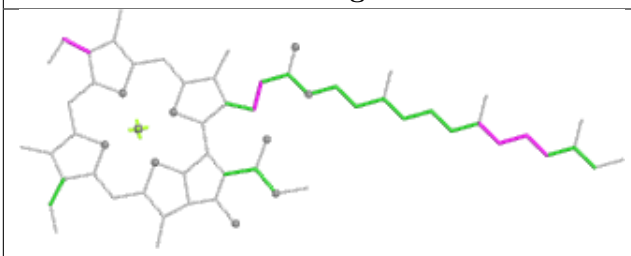
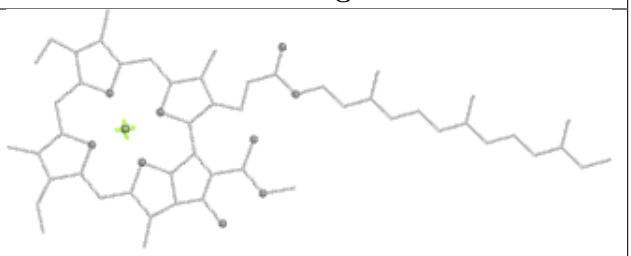
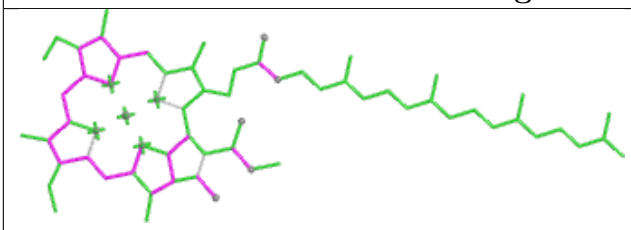
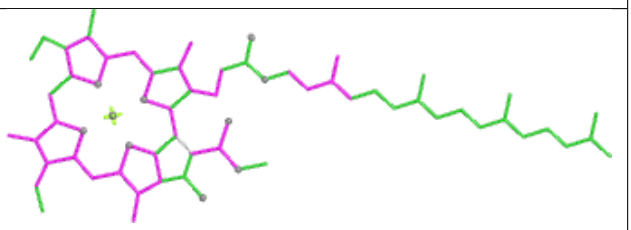
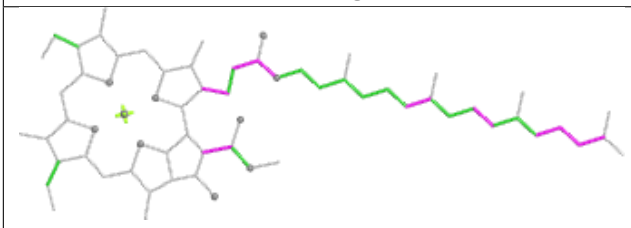
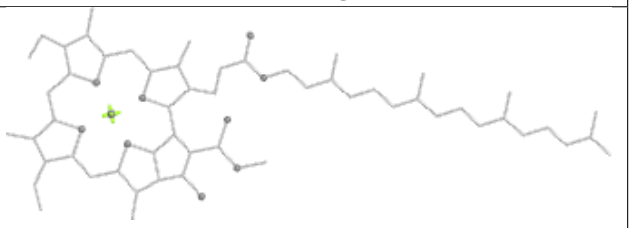
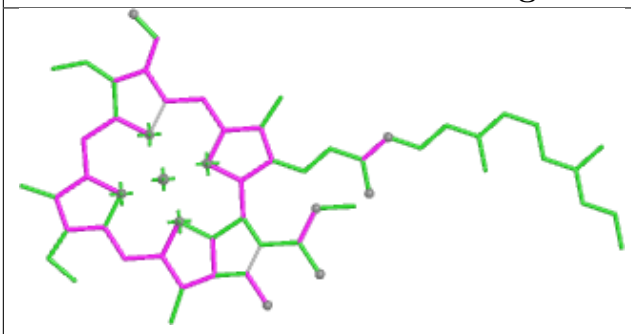


Rings

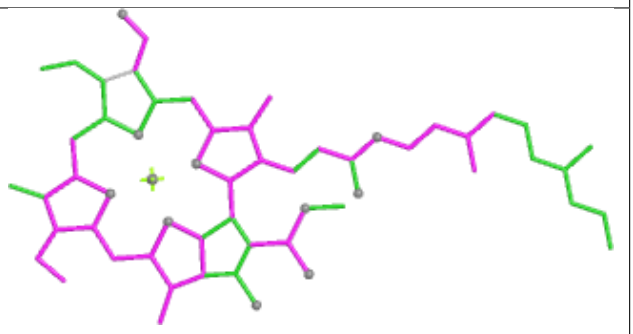
Ligand CLA bB 803	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA bB 805	
	
Bond lengths	Bond angles
	
Torsions	Rings

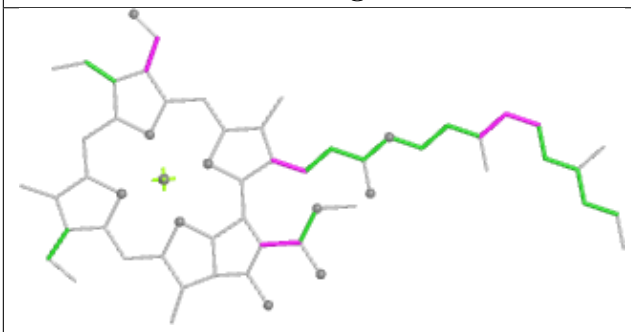
Ligand F6C bB 824



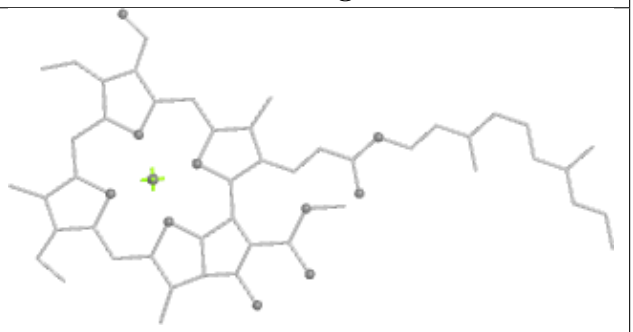
Bond lengths



Bond angles

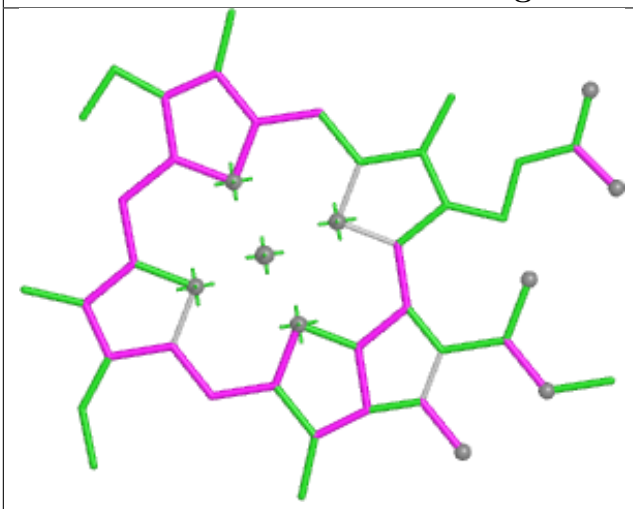


Torsions



Rings

Ligand CLA bB 835



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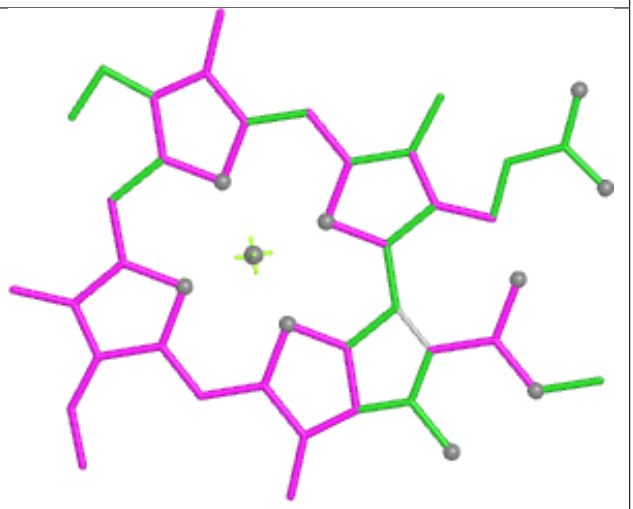
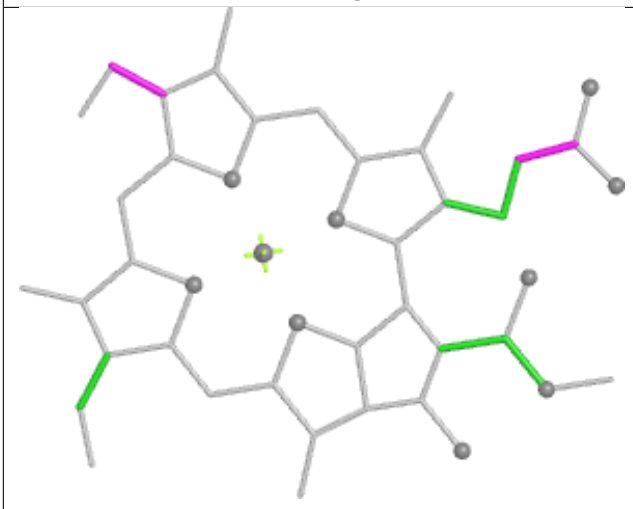


Bond angles

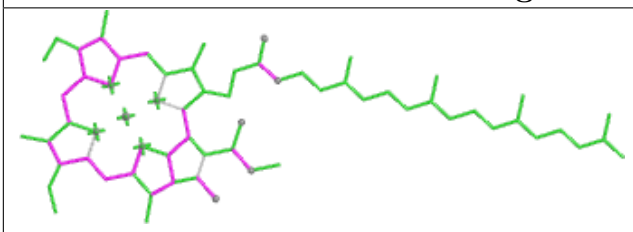


Torsions



Rings

Ligand CLA cA 812



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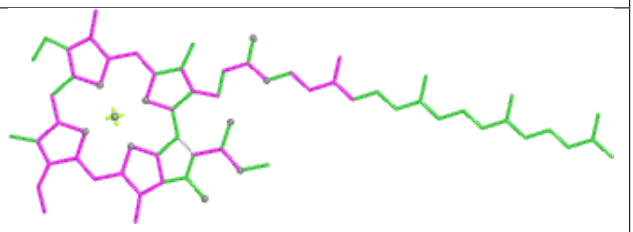
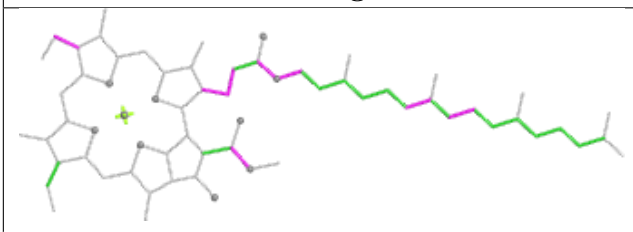


Bond angles



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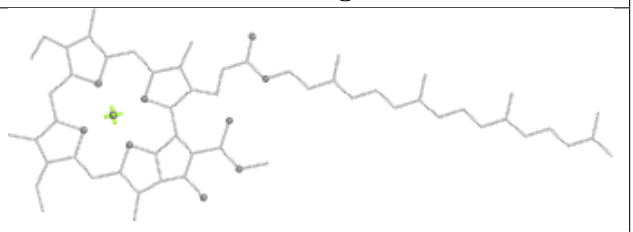
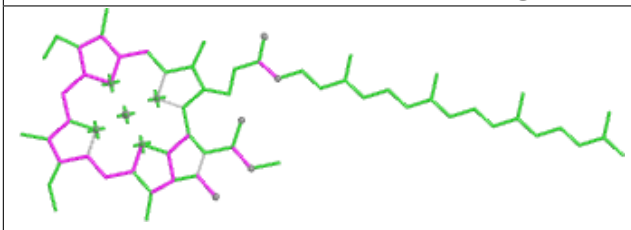


Rings

Ligand CLA bB 825



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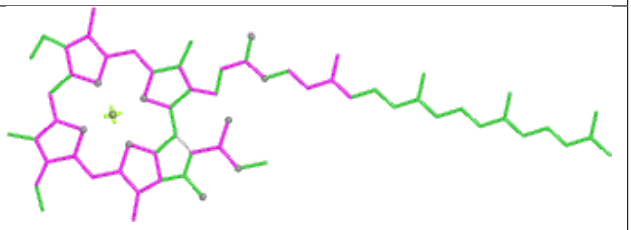
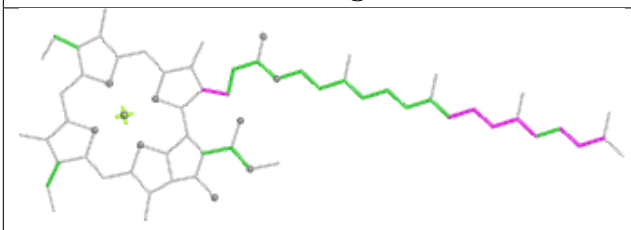


Bond angles



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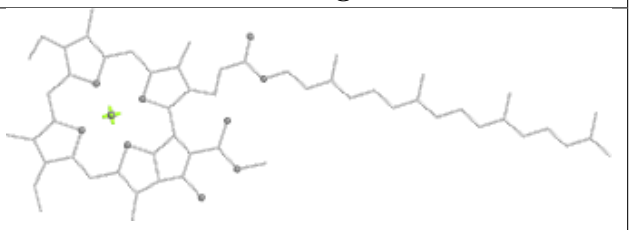
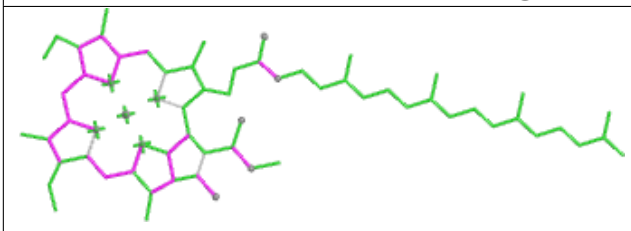


Rings

Ligand CLA cB 801



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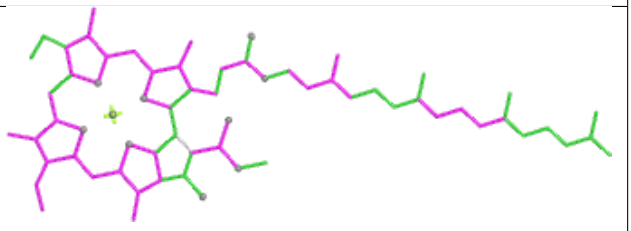
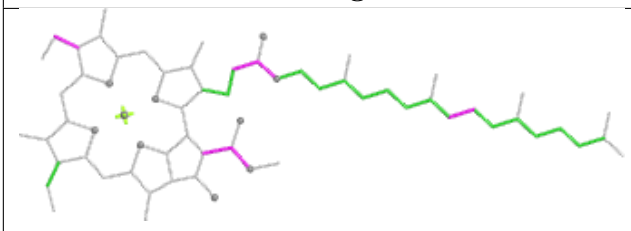


Bond angles



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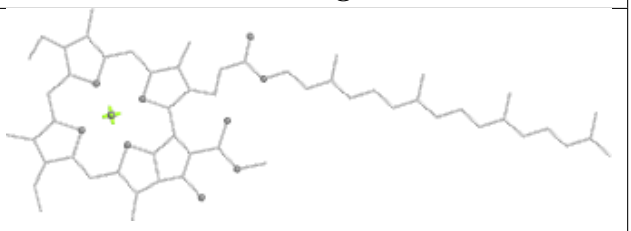
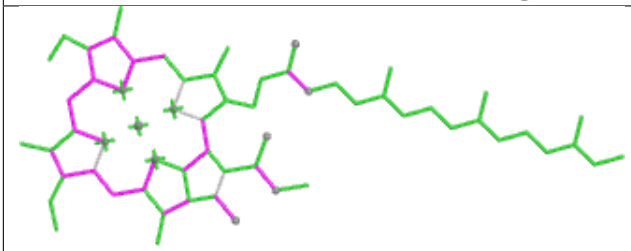


Rings

Ligand CLA aB 803



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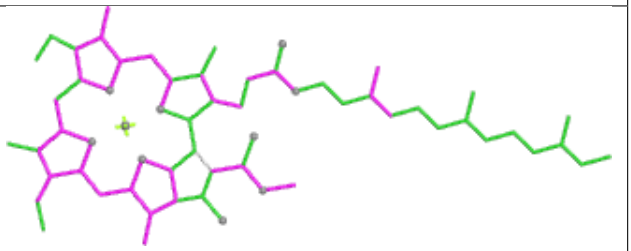
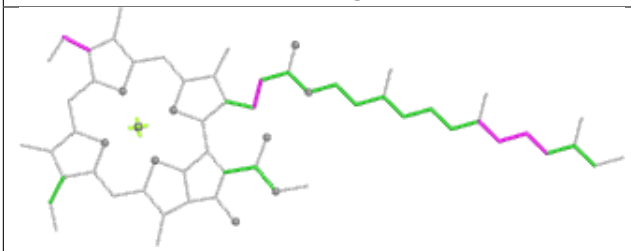


Bond angles



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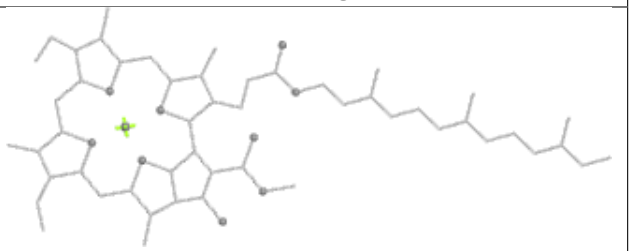
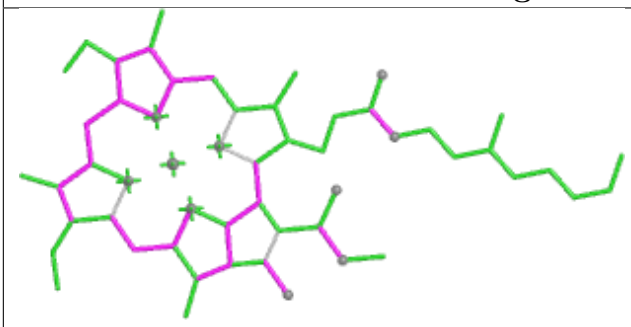


Rings

Ligand CLA bA 818



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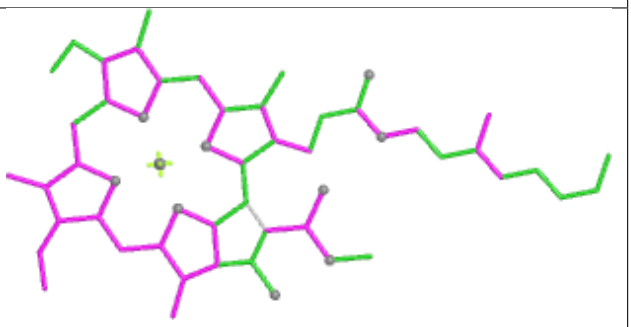
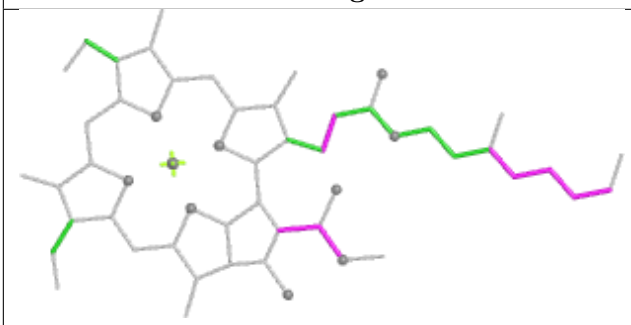


Bond angles



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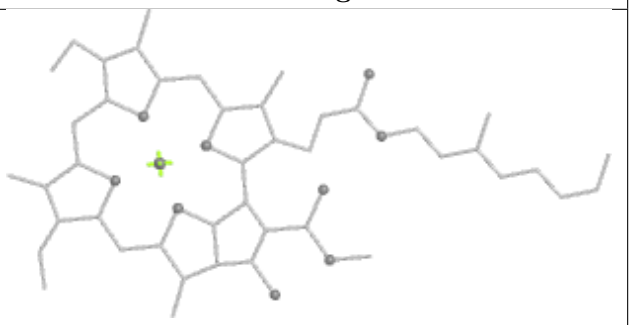
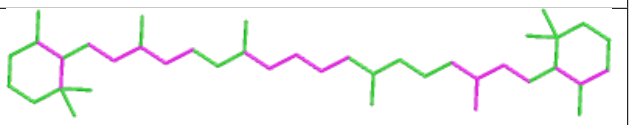


Rings

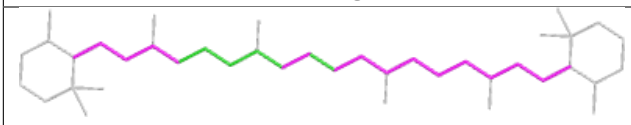
Ligand BCR bA 851



Bond lengths



Bond angles



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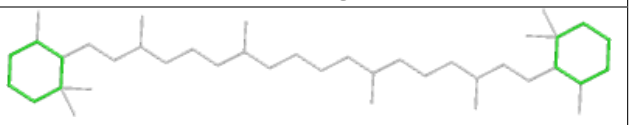
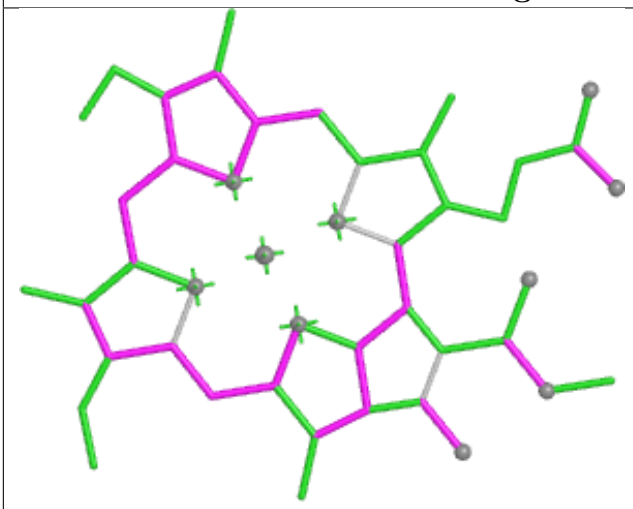


Rings

Ligand CLA bA 815



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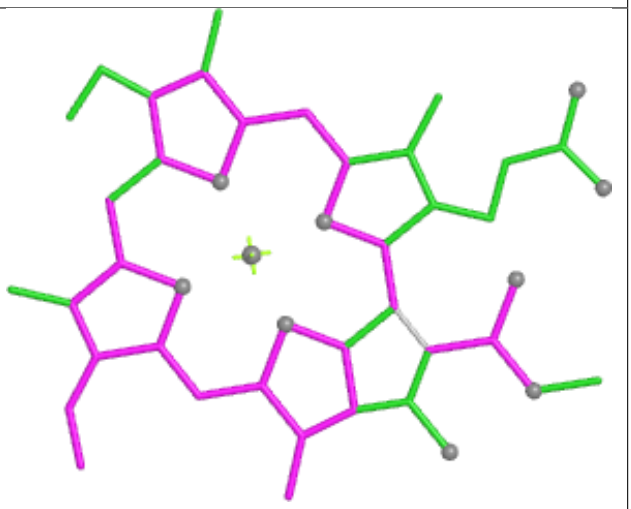
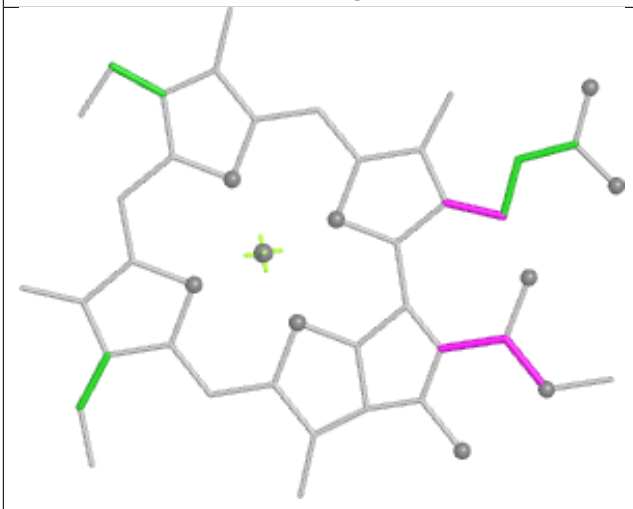


Bond angles

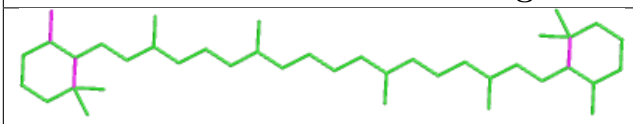


Torsions

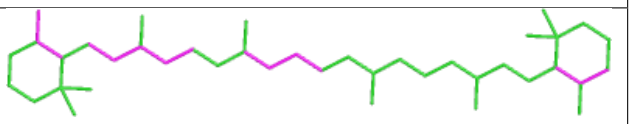


Rings

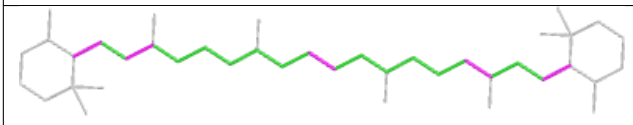
Ligand BCR aL 203



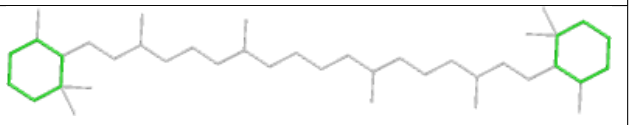
Bond lengths



Bond angles

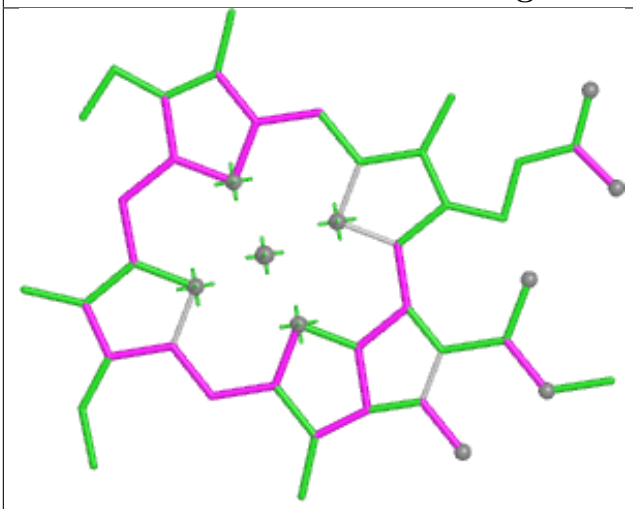


Torsions



Rings

Ligand CLA cB 829



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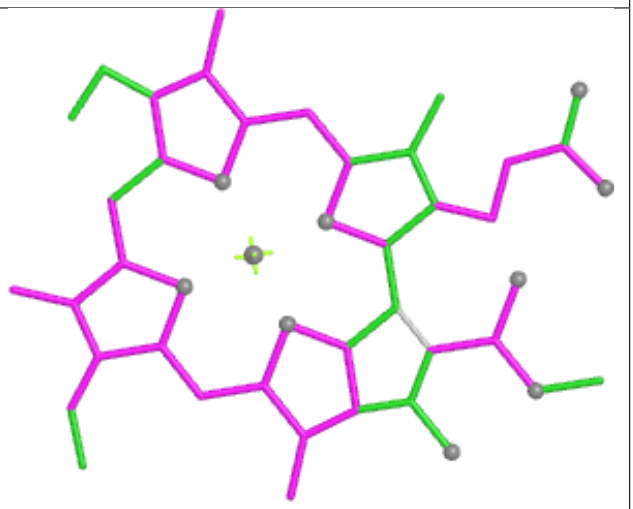
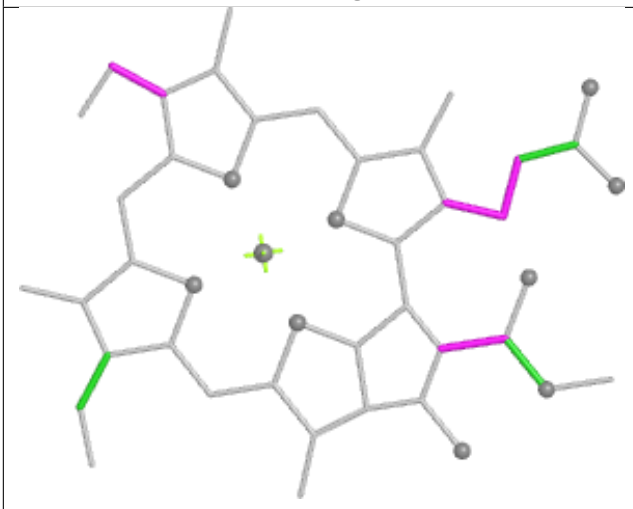


Bond angles

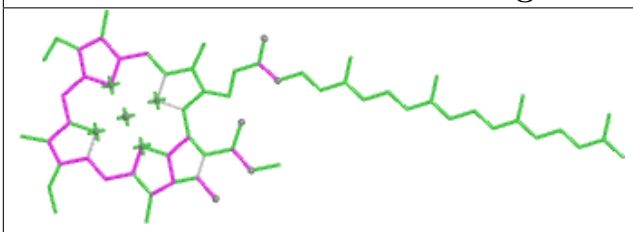


Torsions

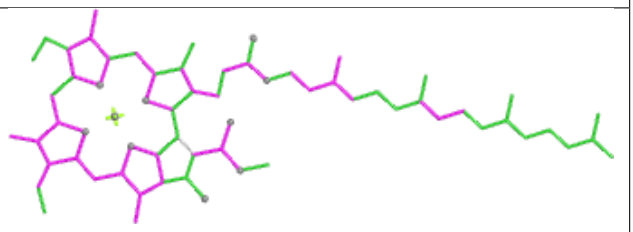


Rings

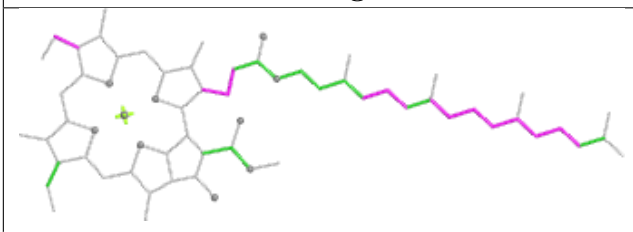
Ligand CLA bL 206



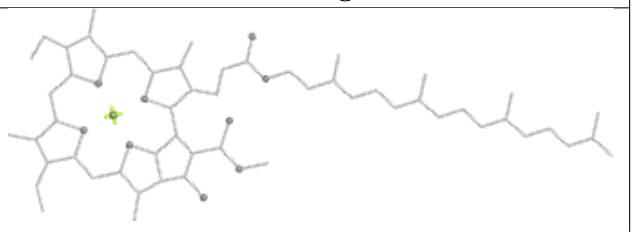
Bond lengths



Bond angles

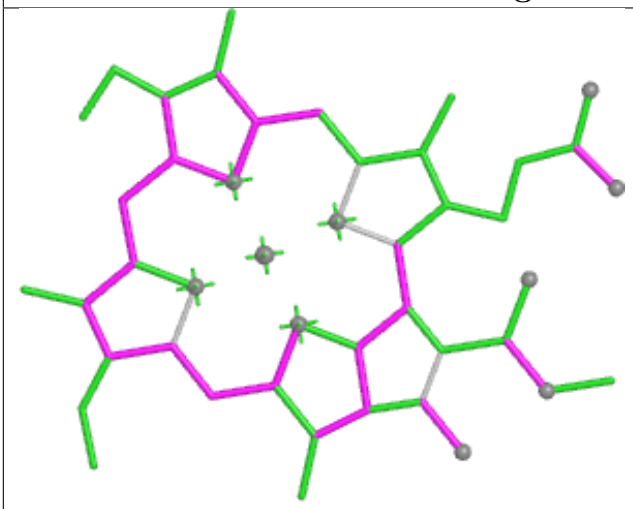


Torsions

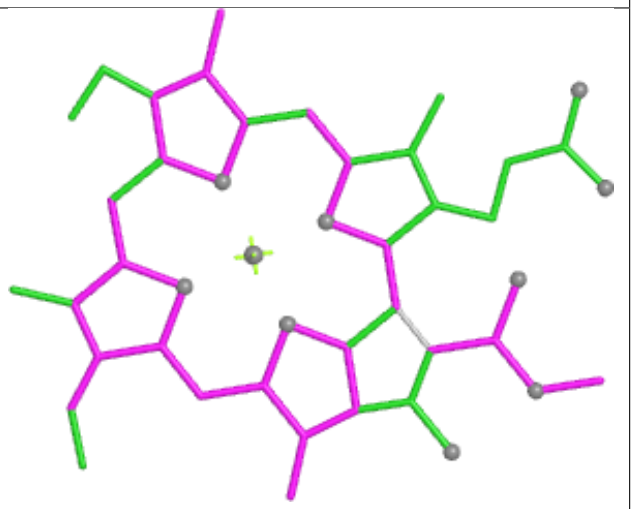


Rings

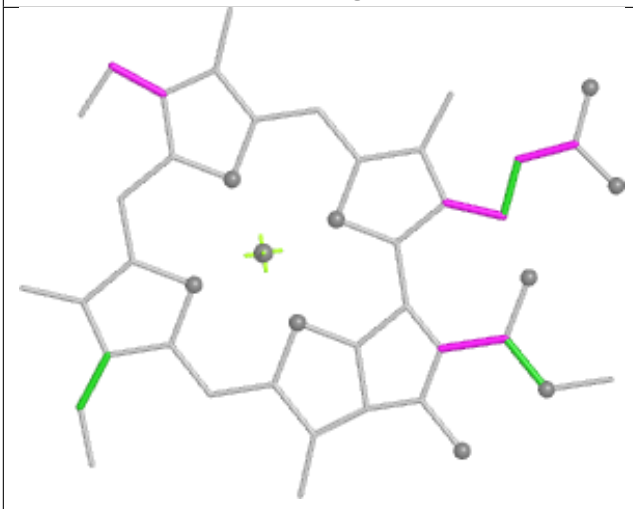
Ligand CLA bB 834



Bond lengths



Bond angles

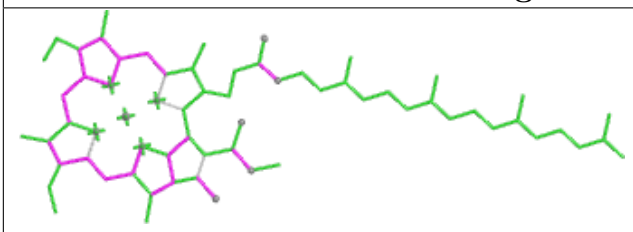


Torsions



Rings

Ligand CLA aA 806



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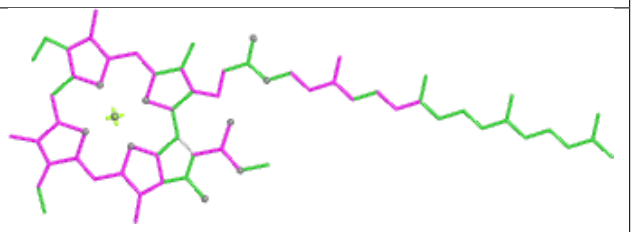
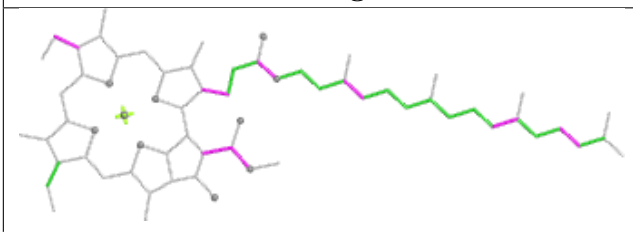


Bond angles



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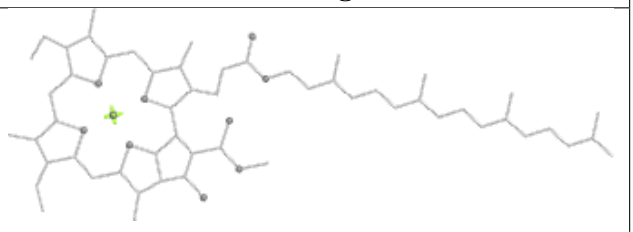
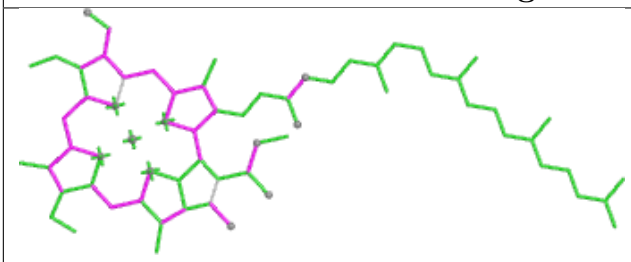


Rings

Ligand F6C bA 826



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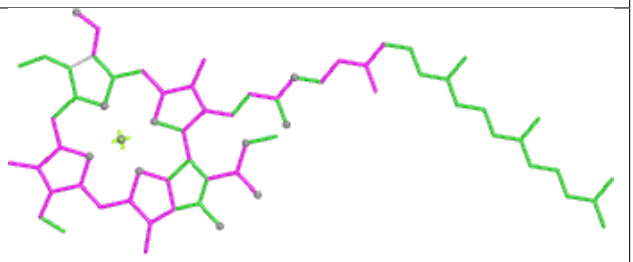
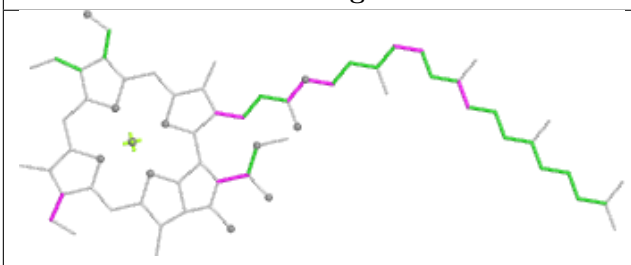
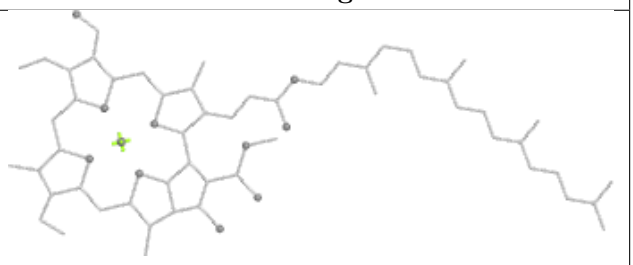


Bond angles

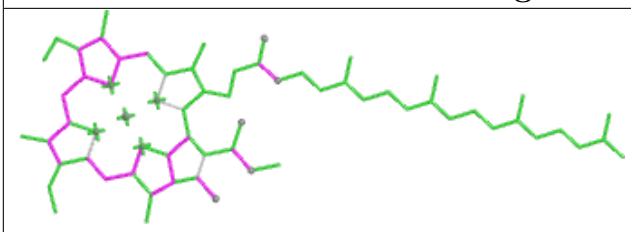


Torsions



Rings

Ligand CLA bB 801



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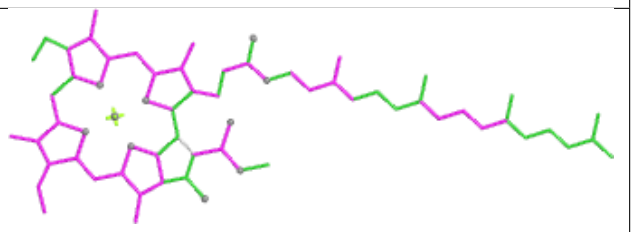
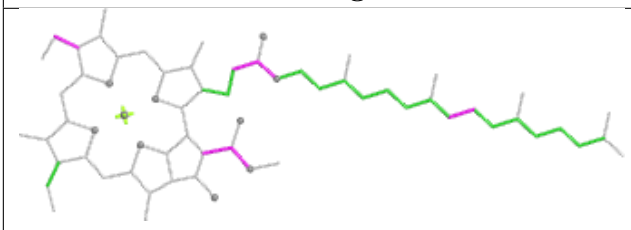


Bond angles



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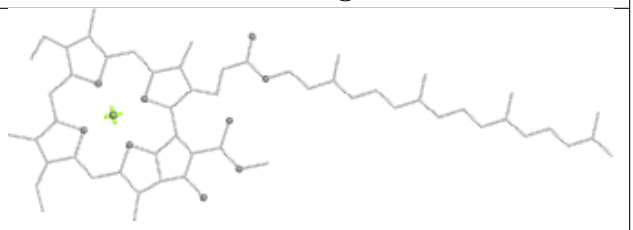
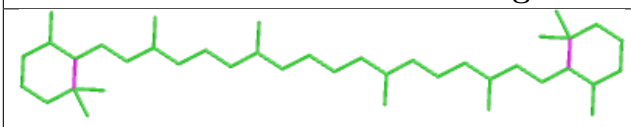


Rings

Ligand BCR bB 845



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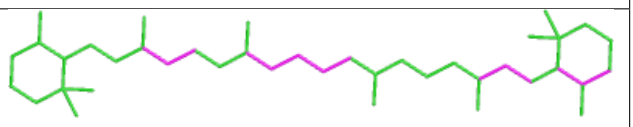
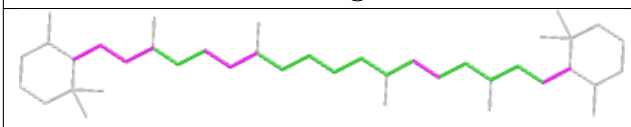


Bond angles



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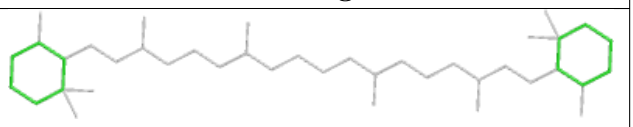
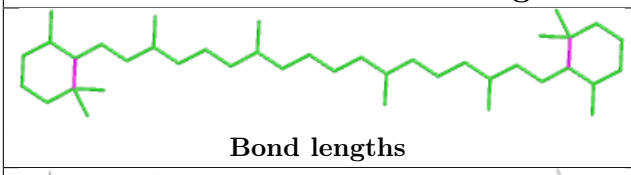


Rings

Ligand BCR bB 844



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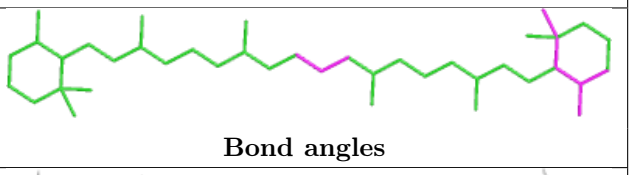
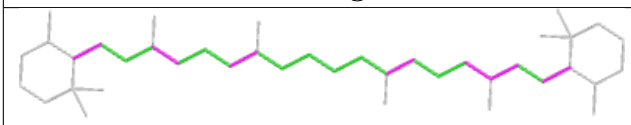
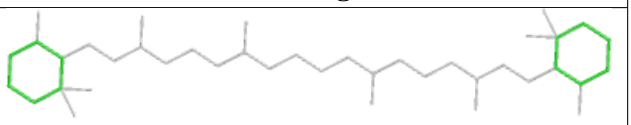


Bond angles

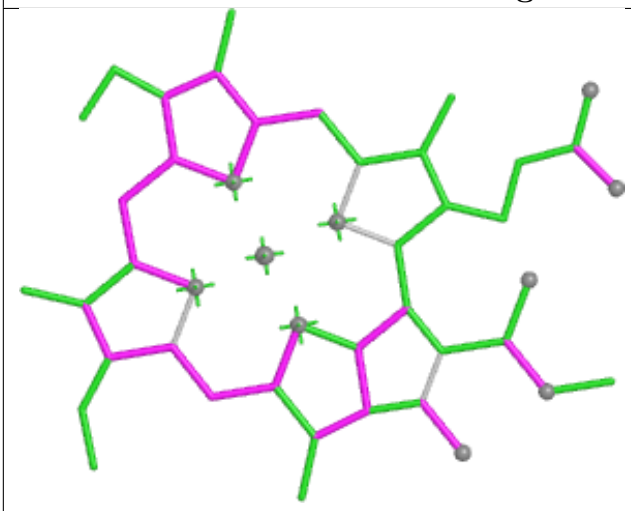


Torsions



Rings

Ligand CLA cB 814



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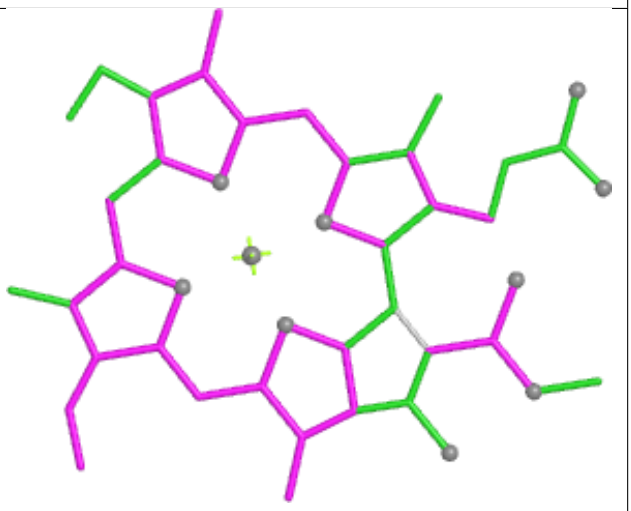
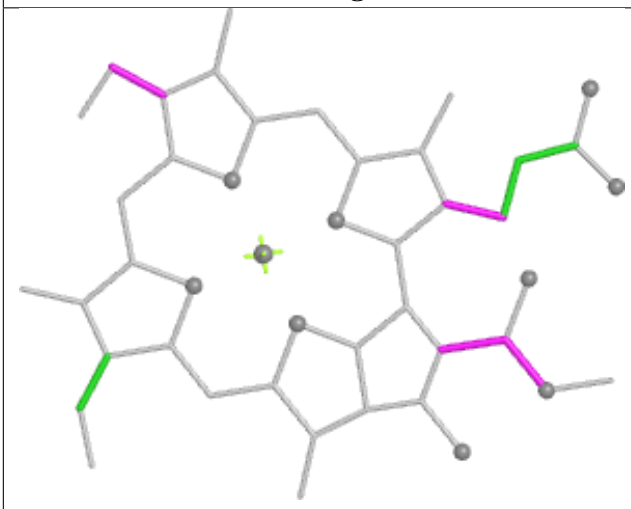


Bond angles



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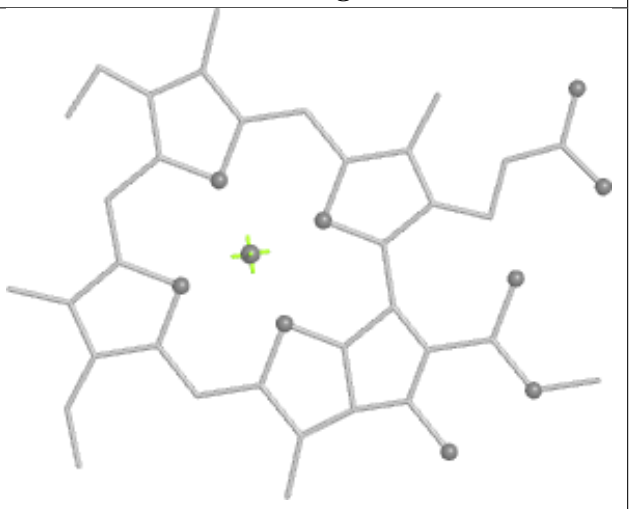
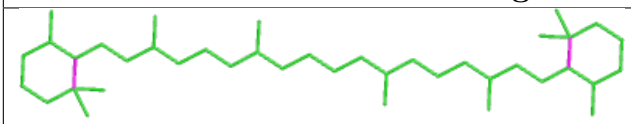


Rings

Ligand BCR bA 848



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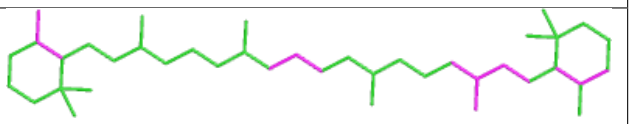
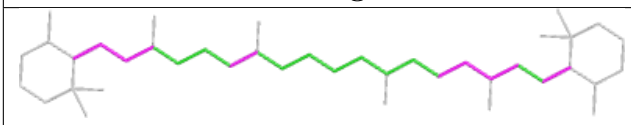


Bond angles



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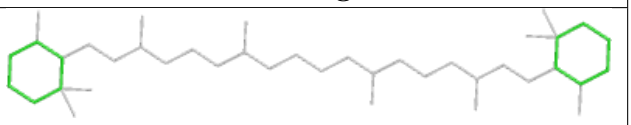
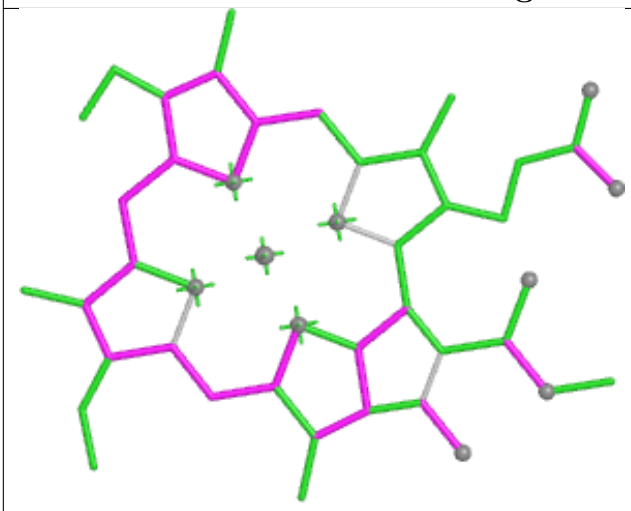
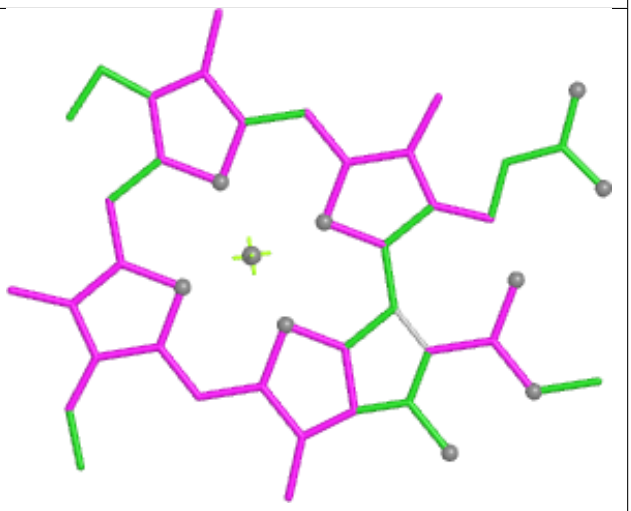


Rings

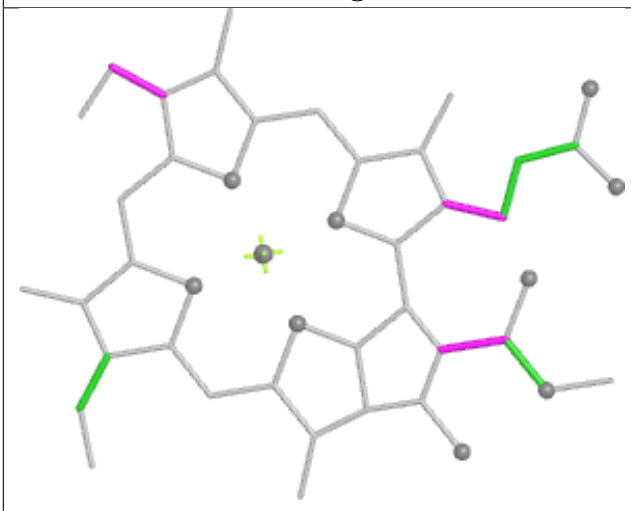
Ligand CLA aB 833



Bond lengths



Bond angles



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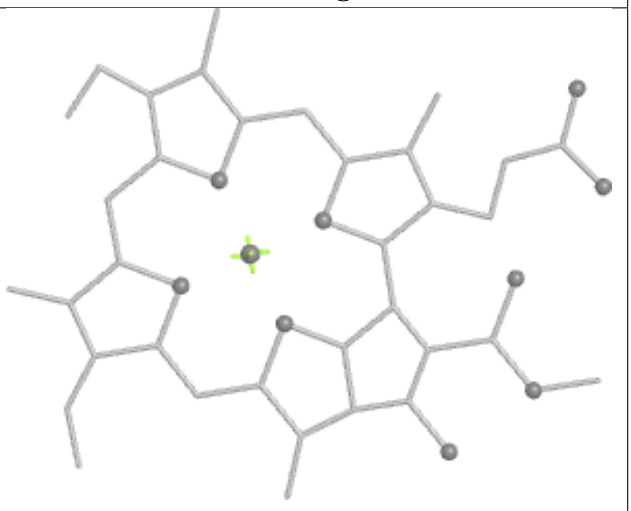
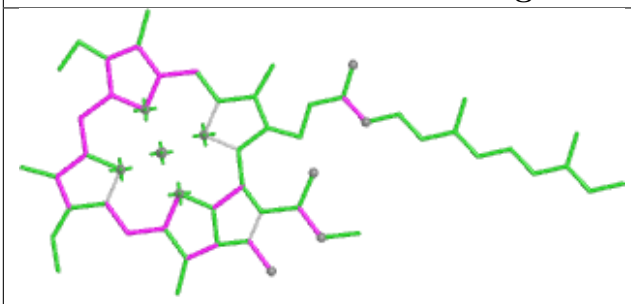
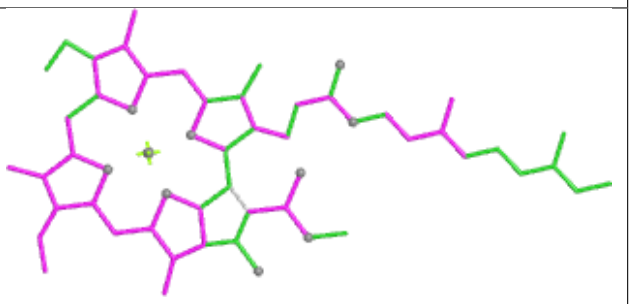
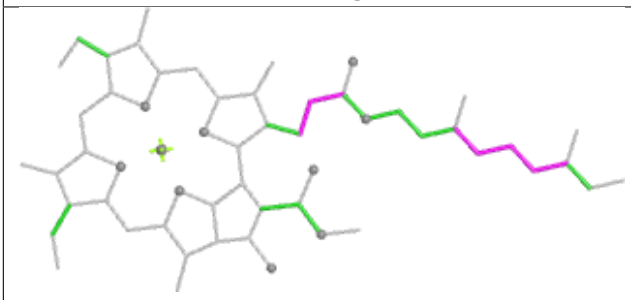
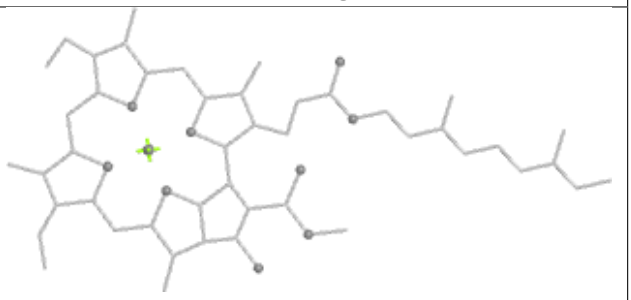
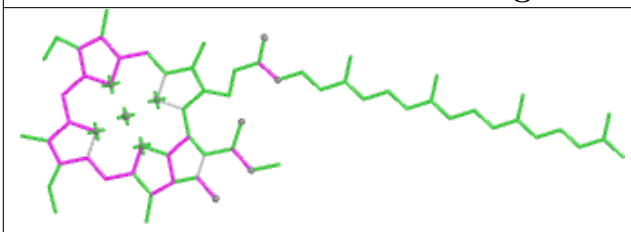
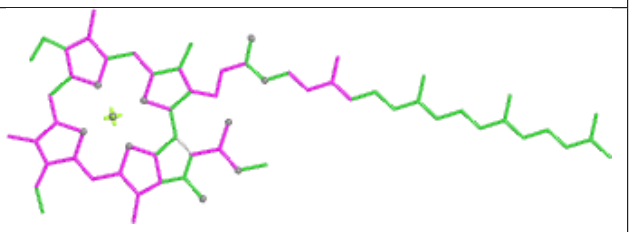
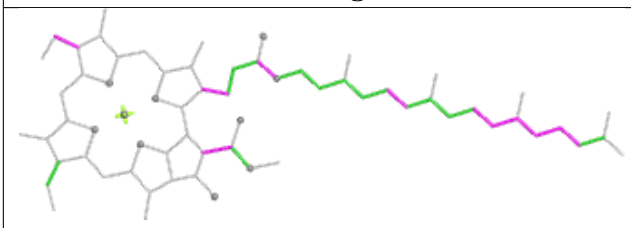
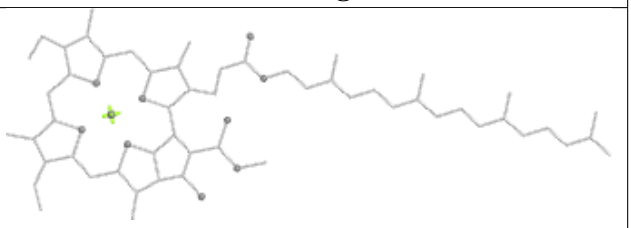
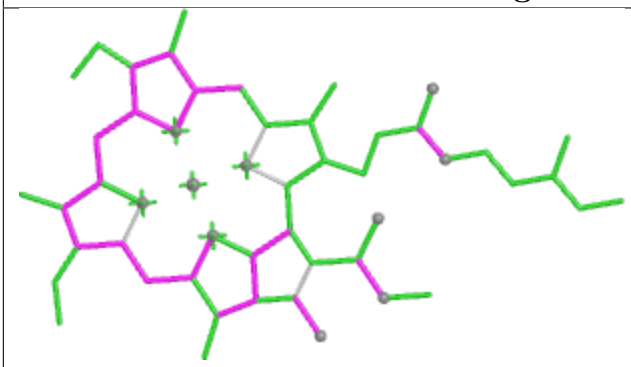


Rings

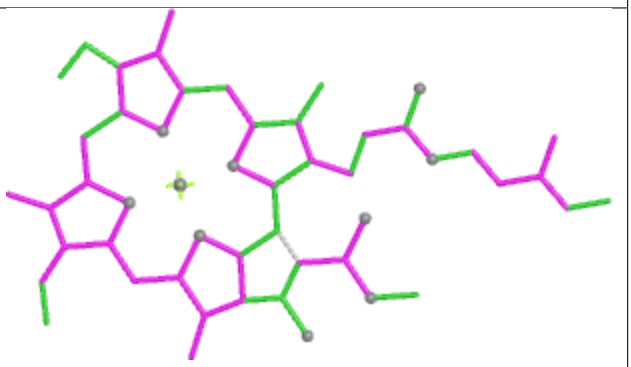
Ligand CLA aA 803	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA bA 814	
	
Bond lengths	Bond angles
	
Torsions	Rings

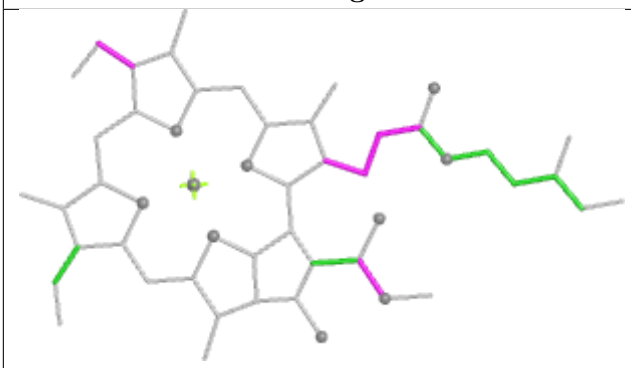
Ligand CLA bA 843



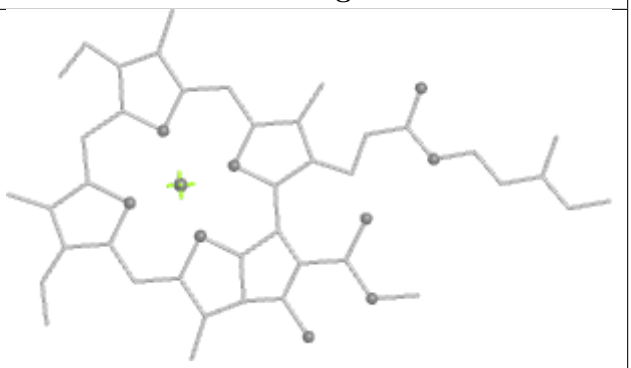
Bond lengths



Bond angles

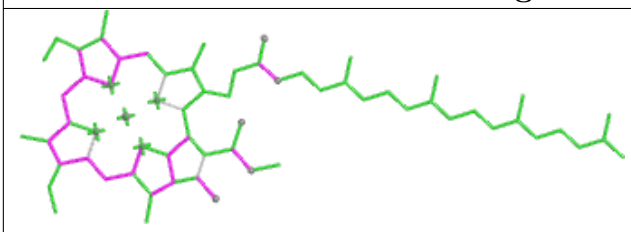


Torsions

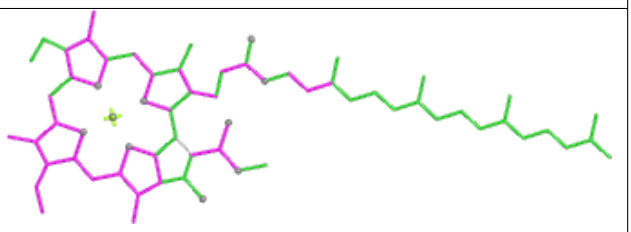


Rings

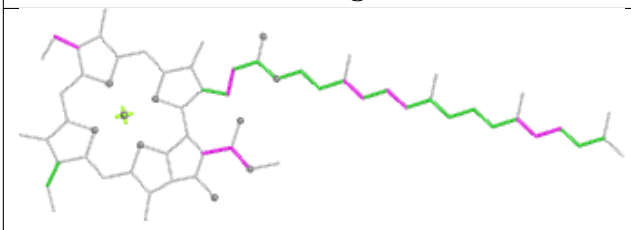
Ligand CLA aA 835



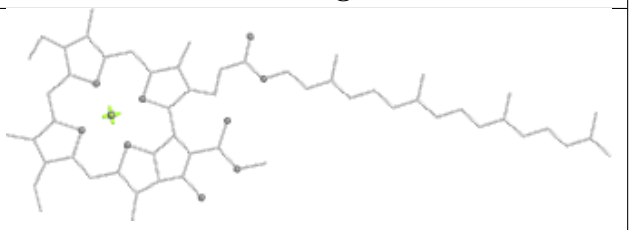
Bond lengths



Bond angles

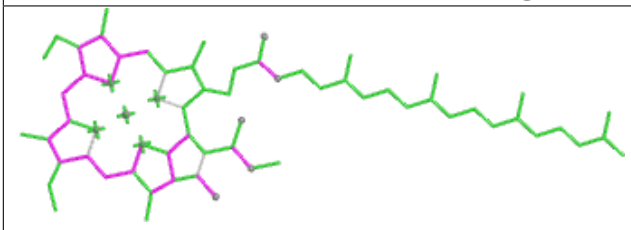


Torsions

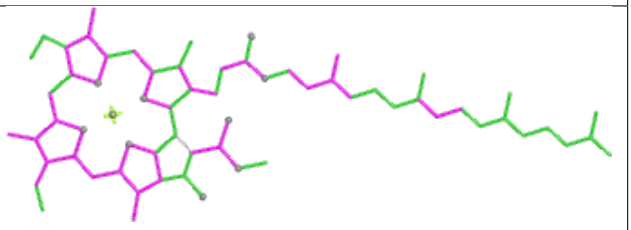


Rings

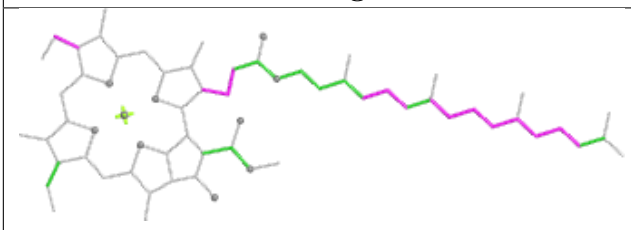
Ligand CLA cL 206



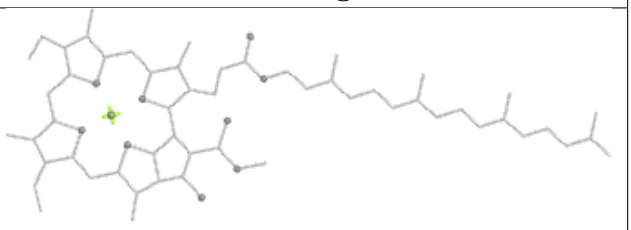
Bond lengths



Bond angles



Torsions

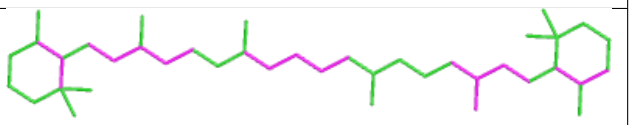


Rings

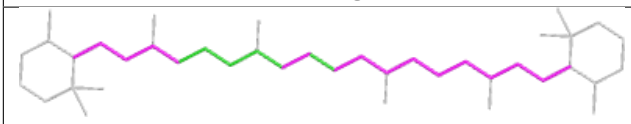
Ligand BCR aA 851



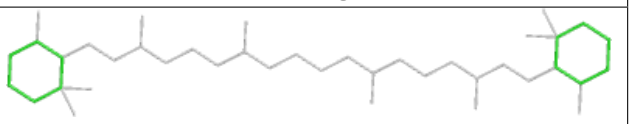
Bond lengths



Bond angles

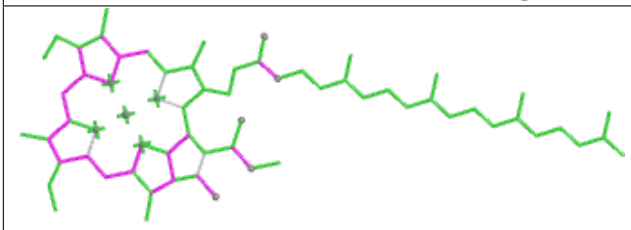


Torsions

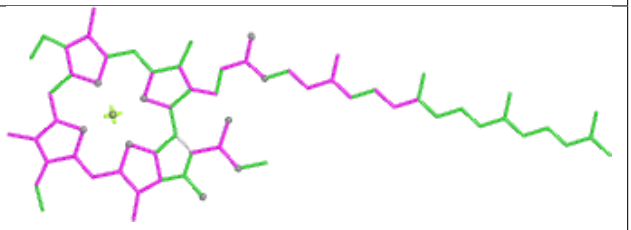


Rings

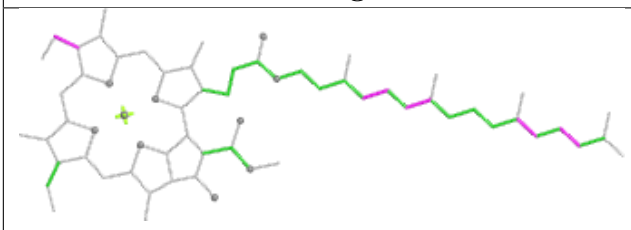
Ligand CLA cA 839



Bond lengths



Bond angles



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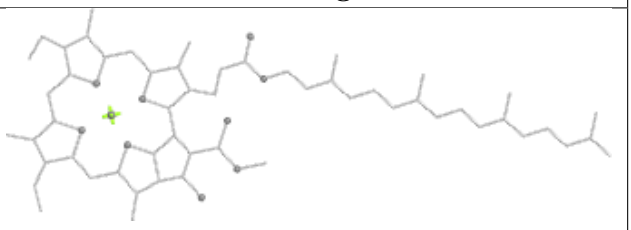
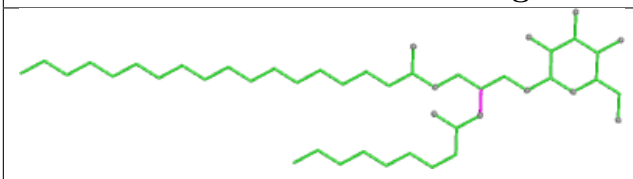
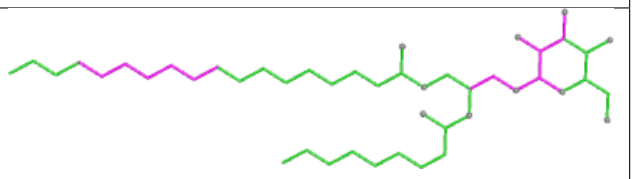


Rings

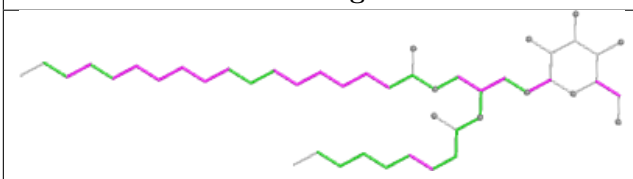
Ligand LMG cB 847



Bond lengths



Bond angles



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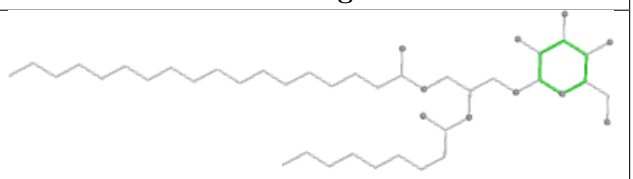
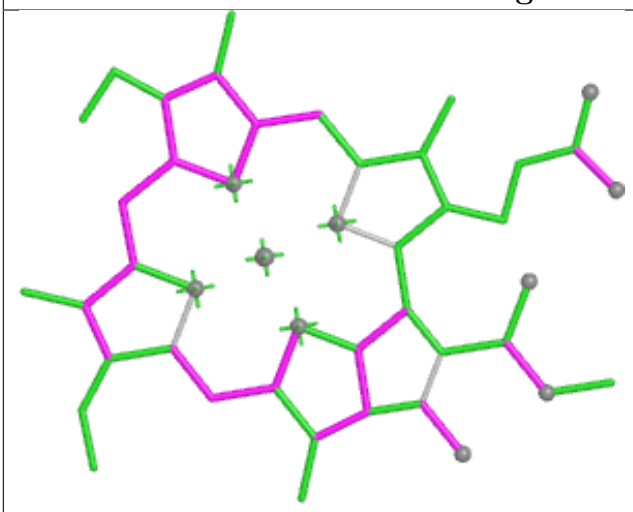


Rings

Ligand CLA aB 840



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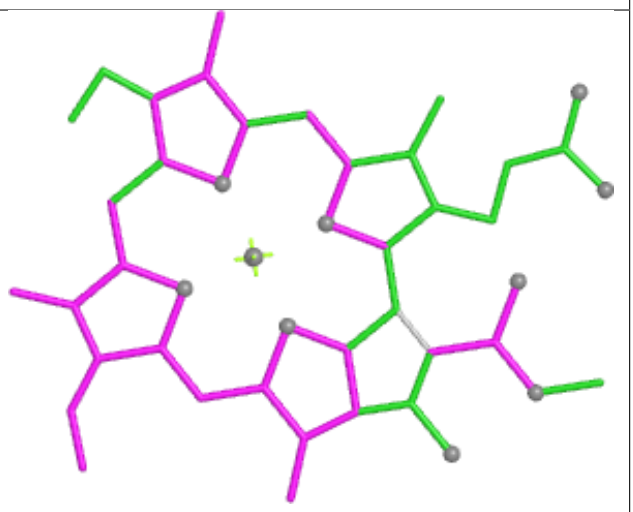
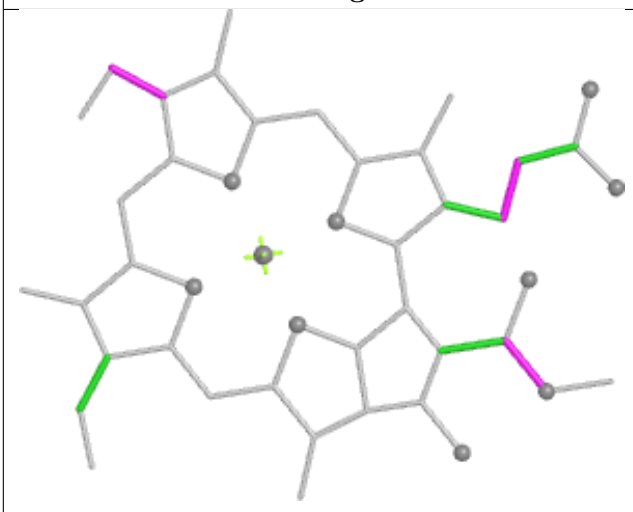


Bond angles

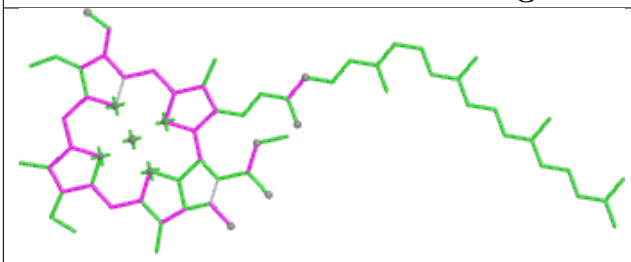


Torsions



Rings

Ligand F6C bA 830



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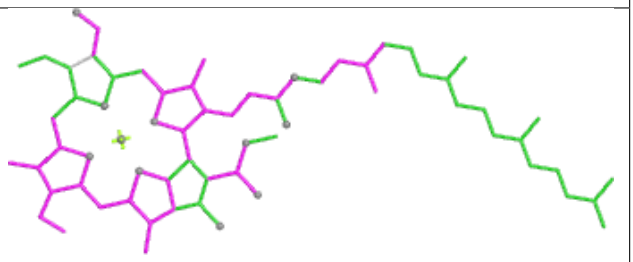
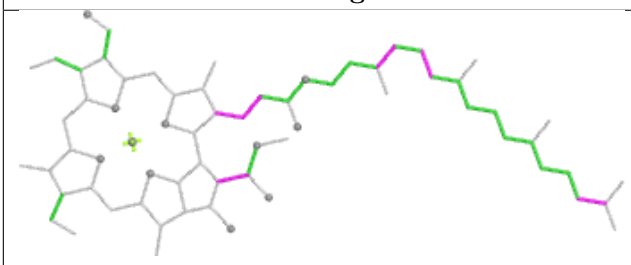
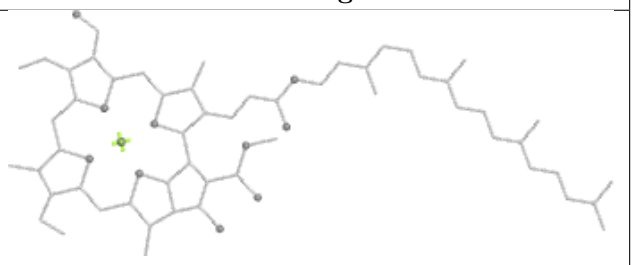


Bond angles

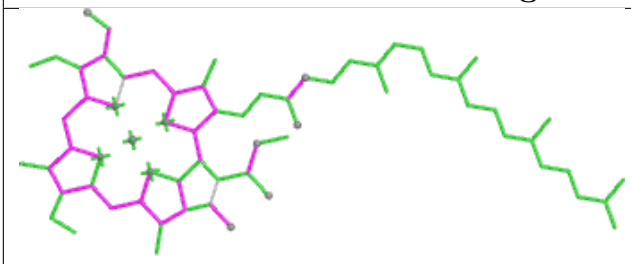


Torsions



Rings

Ligand F6C cA 844



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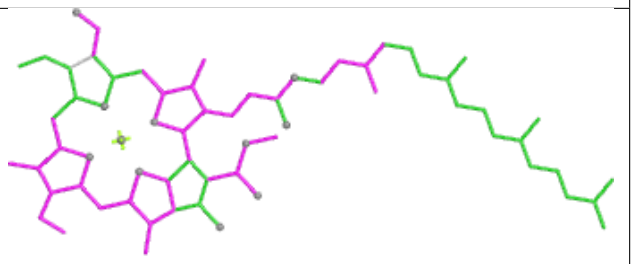
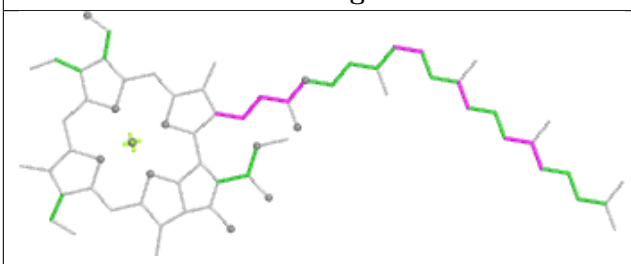


Bond angles



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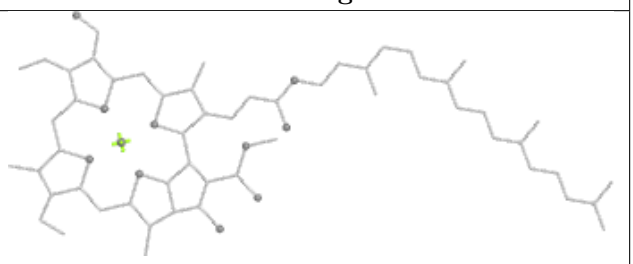
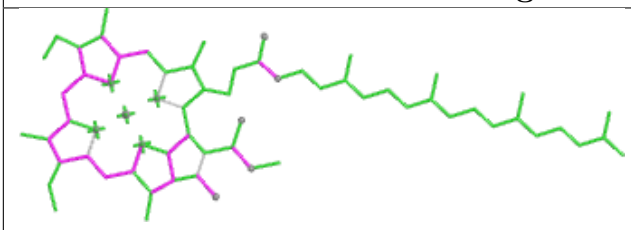


Rings

Ligand CLA cB 818



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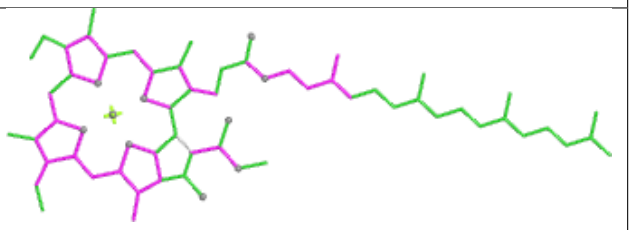
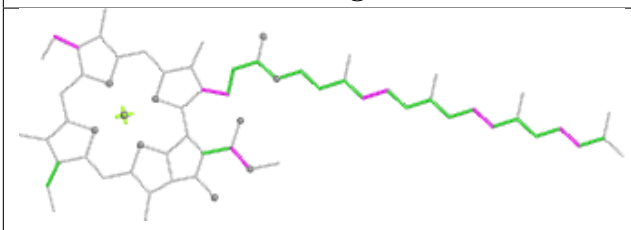


Bond angles



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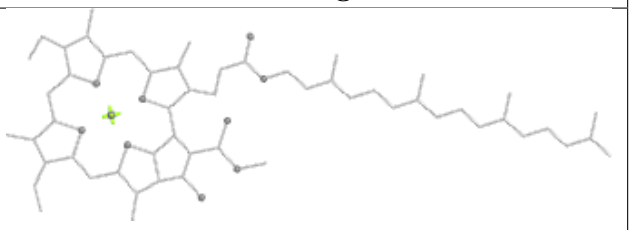
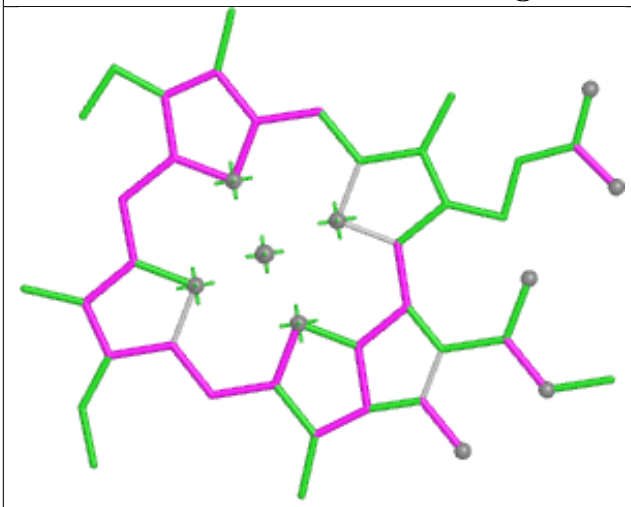


Rings

Ligand CLA bB 832



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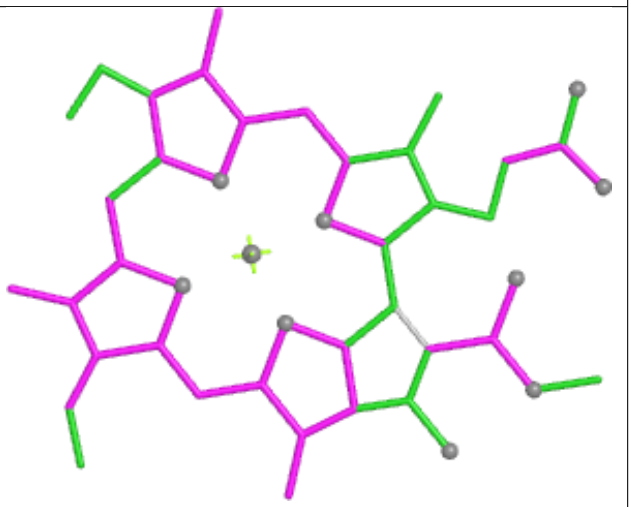
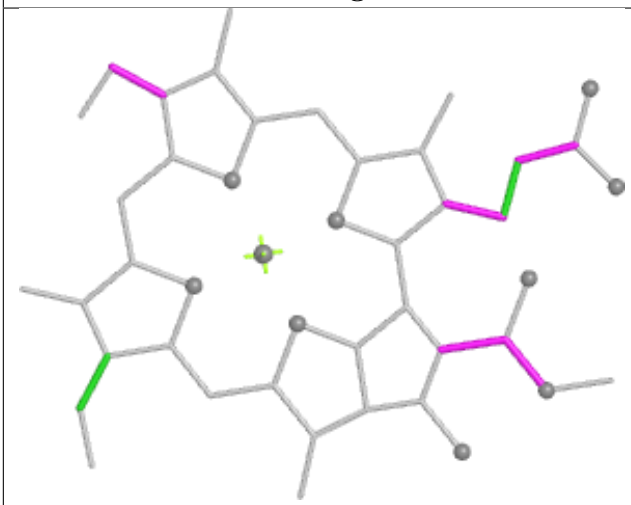


Bond angles



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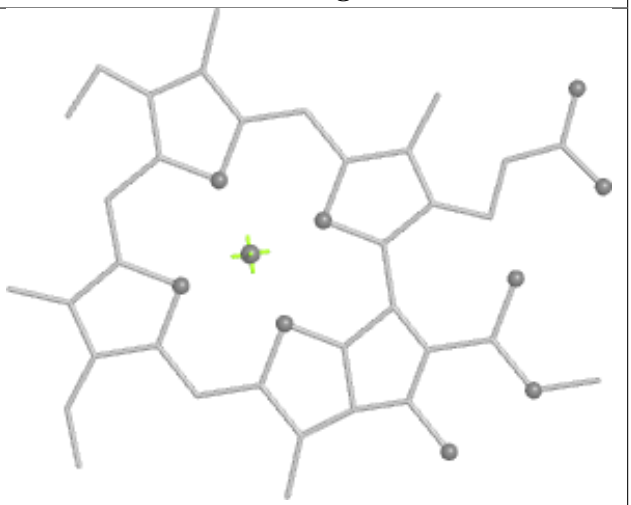
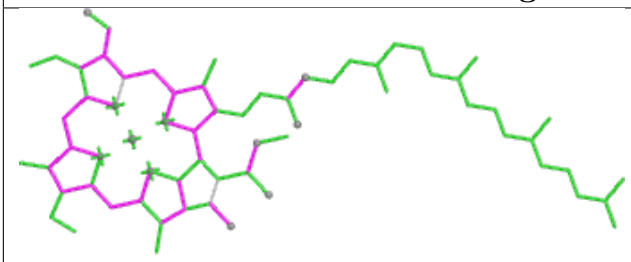


Rings

Ligand F6C aA 830



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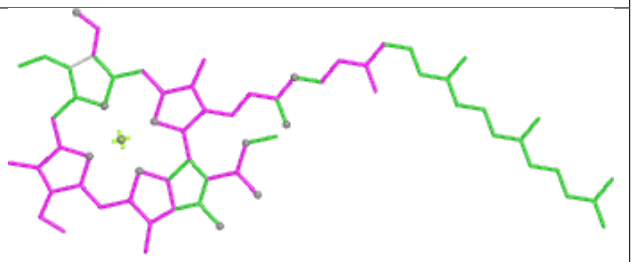
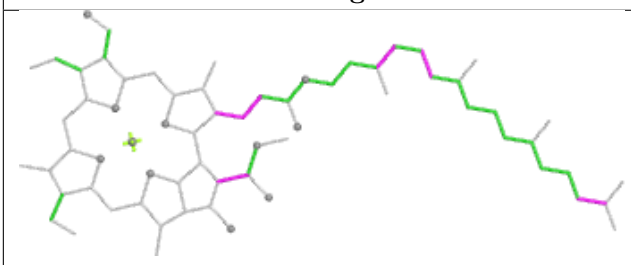


Bond angles



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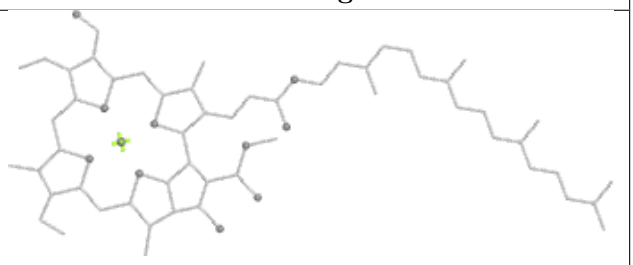
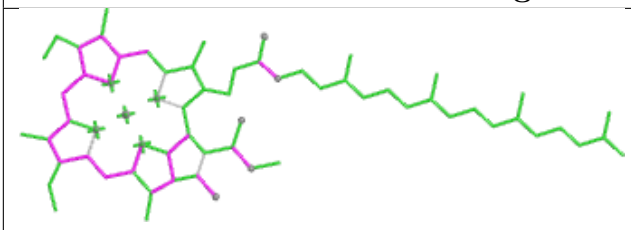


Rings

Ligand CLA bA 833



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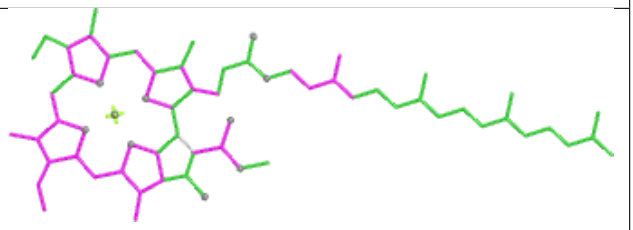
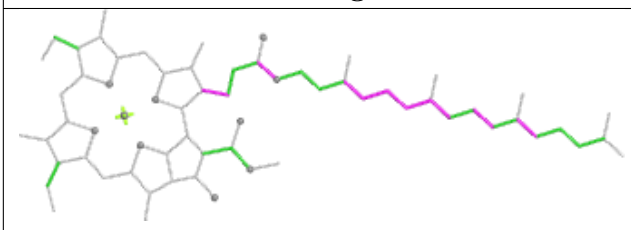


Bond angles



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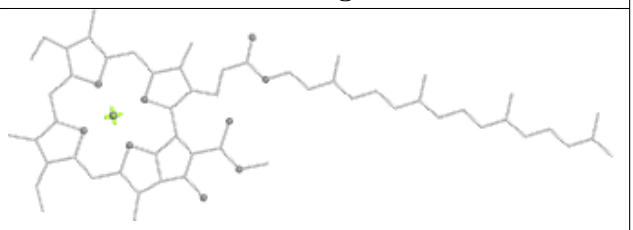
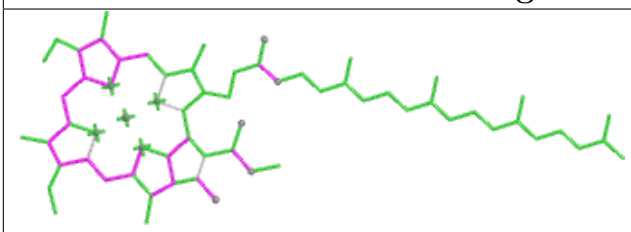


Rings

Ligand CLA bL 205



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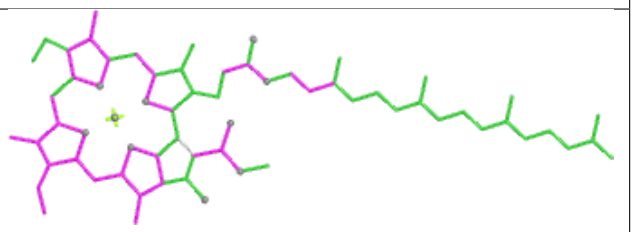
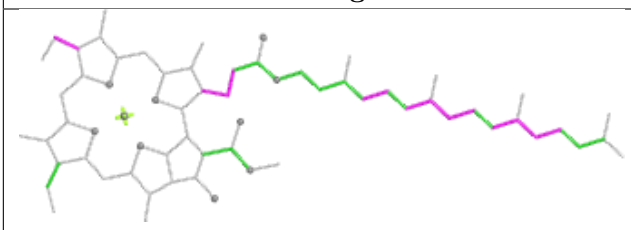


Bond angles



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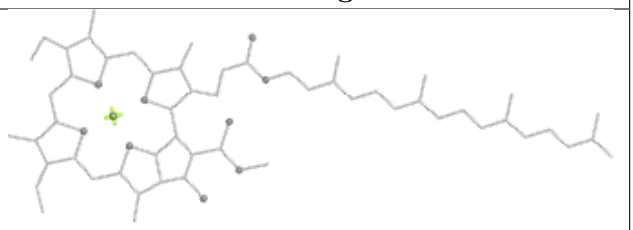
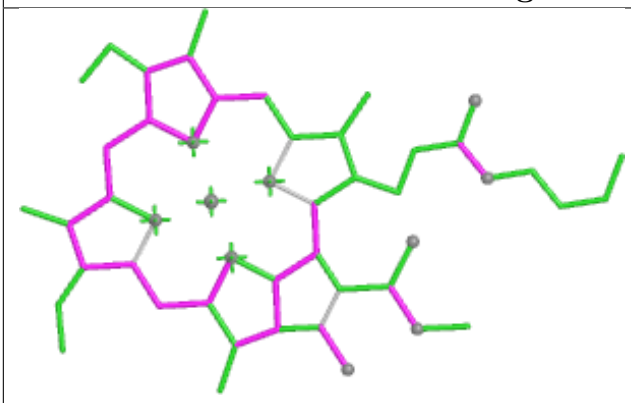


Rings

Ligand CLA cB 830



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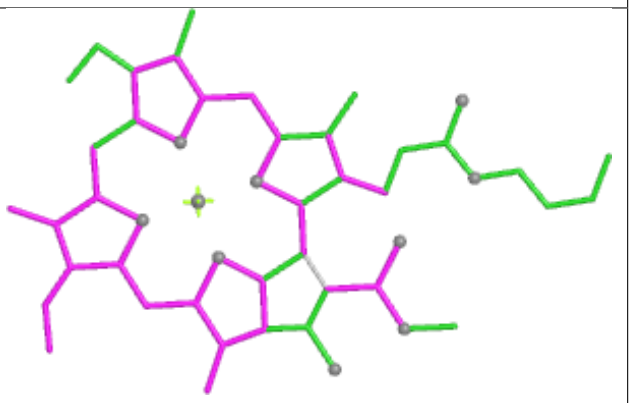
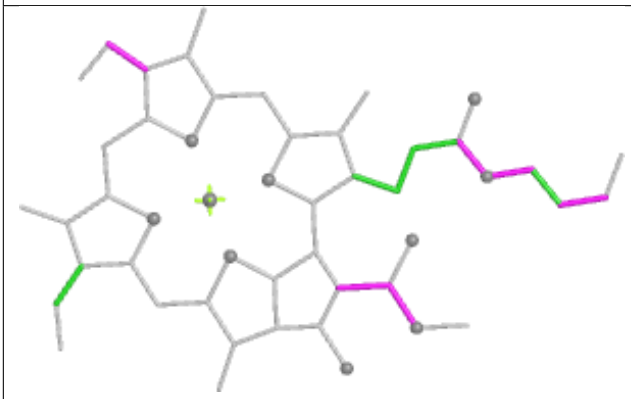


Bond angles



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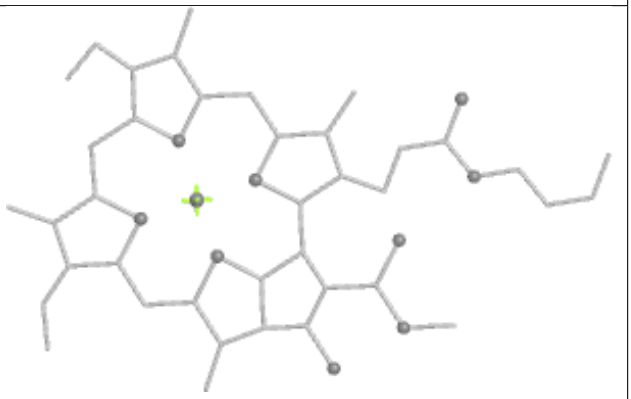
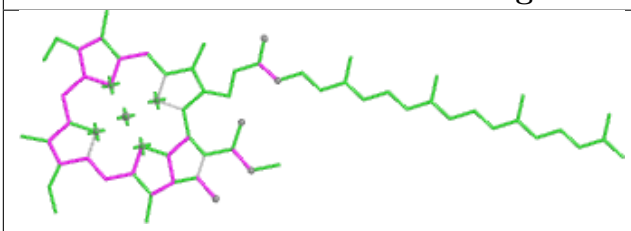


Rings

Ligand CLA aB 818



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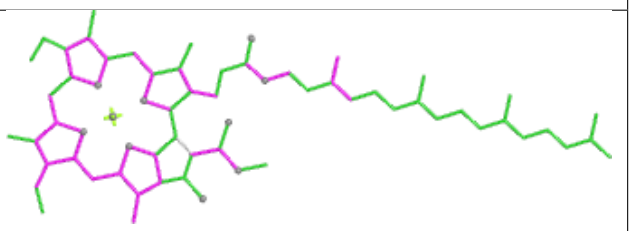
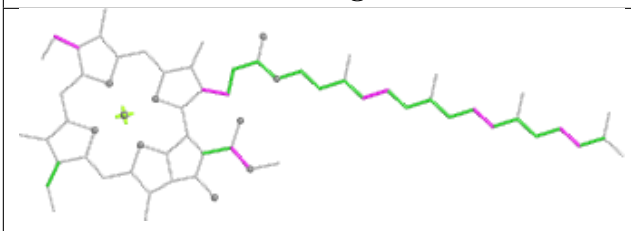
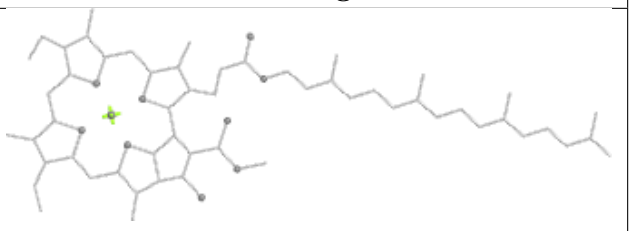


Bond angles

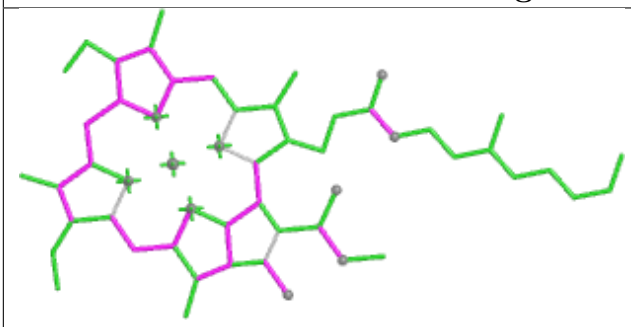


Torsions

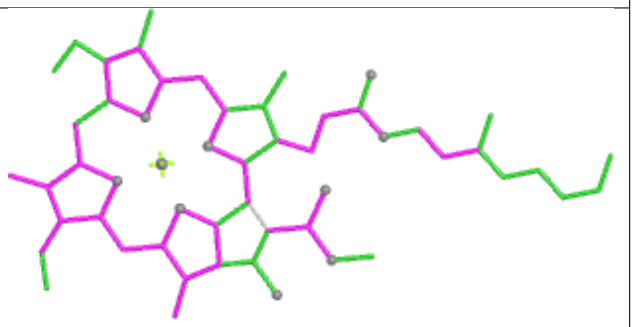


Rings

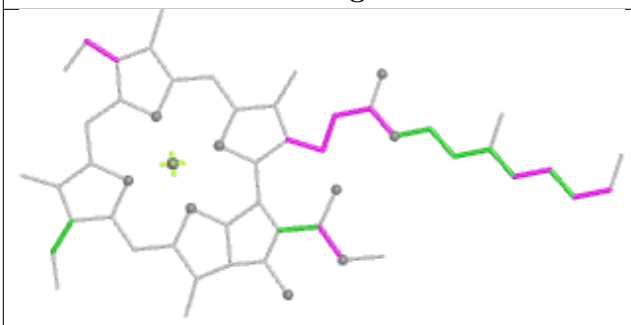
Ligand CLA aA 819



Bond lengths



Bond angles



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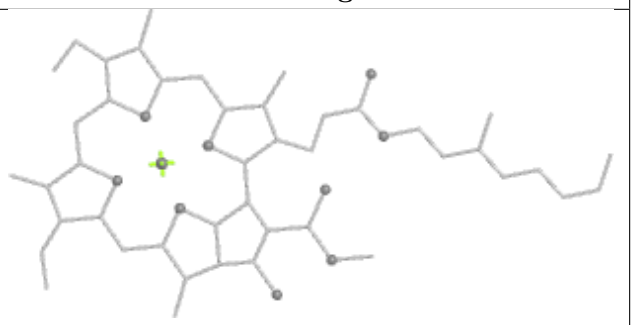
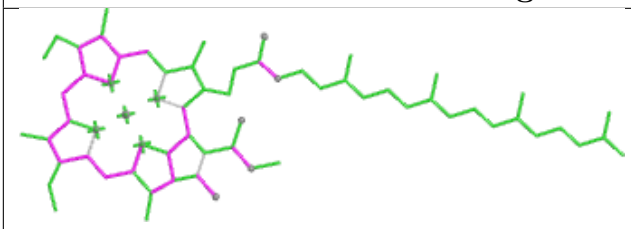
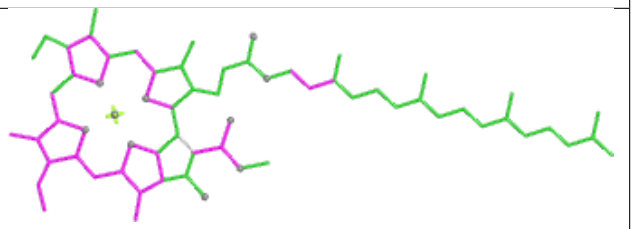


Rings

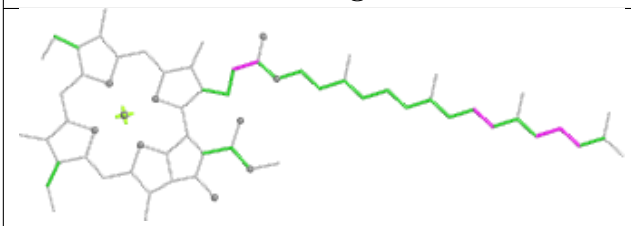
Ligand CLA bL 204



Bond lengths



Bond angles



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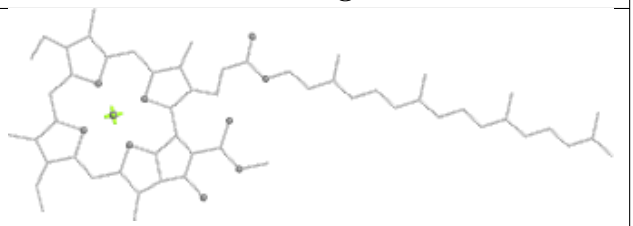
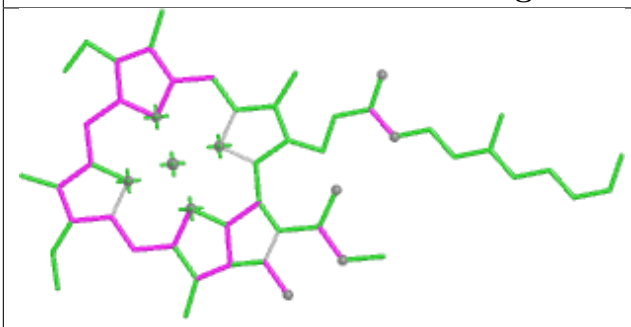
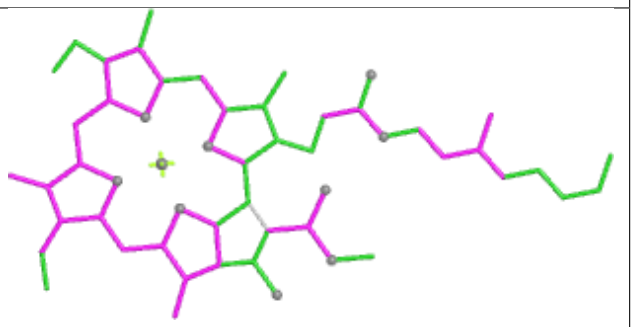


Rings

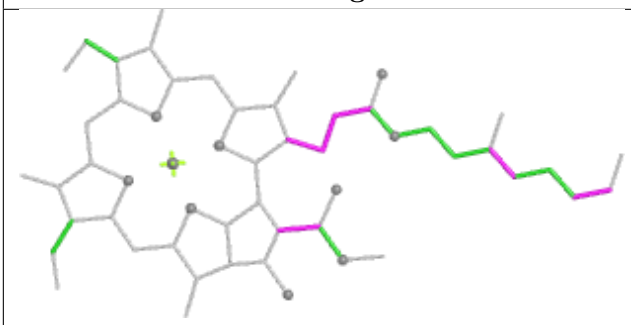
Ligand CLA aA 813



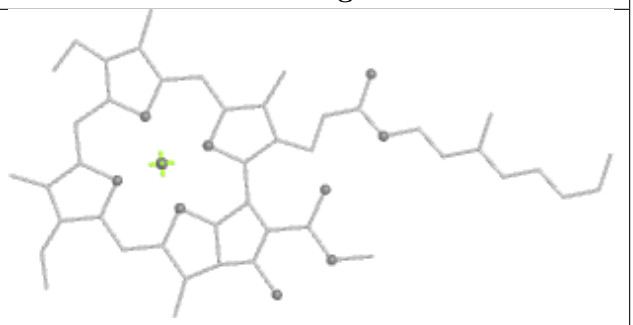
Bond lengths



Bond angles

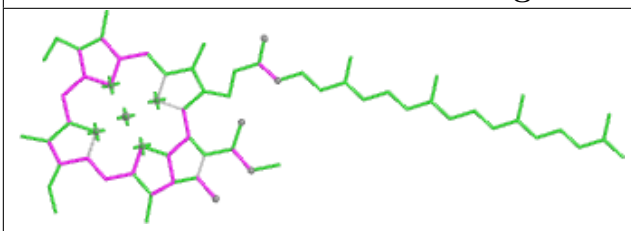


Torsions



Rings

Ligand CLA bA 820



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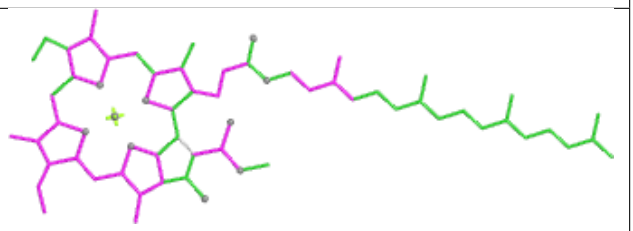
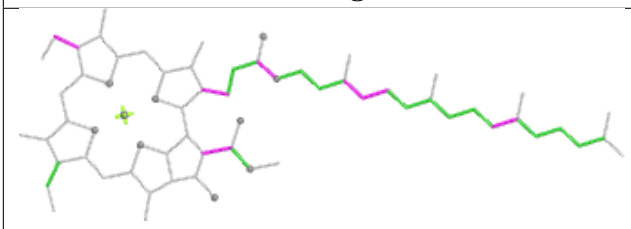


Bond angles



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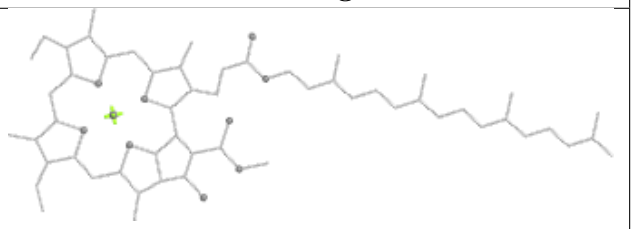
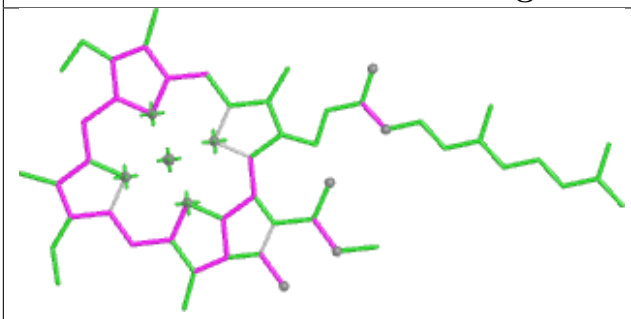


Rings

Ligand CLA cB 821



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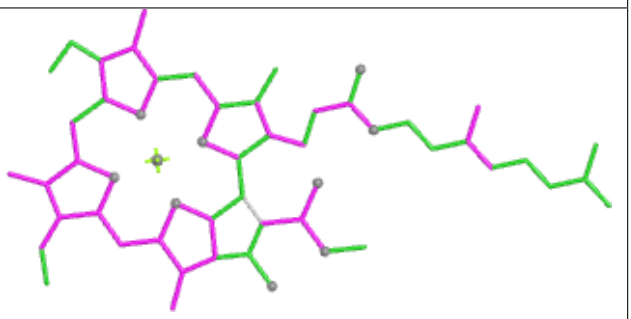
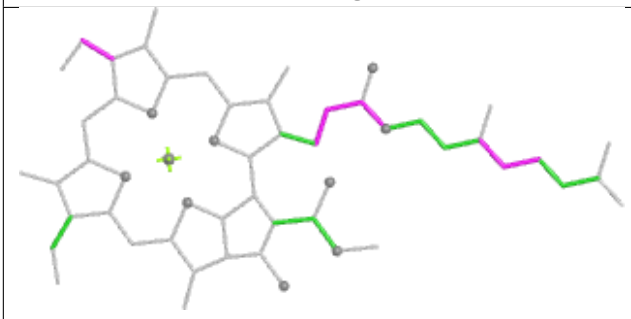


Bond angles



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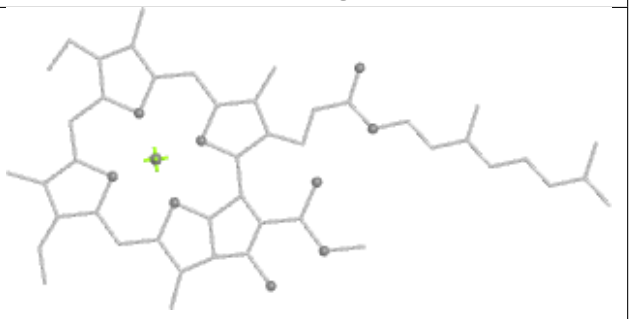
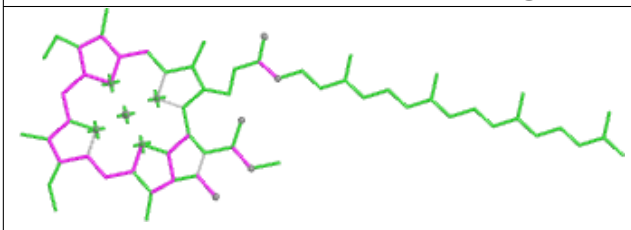


Rings

Ligand CL0 cA 801



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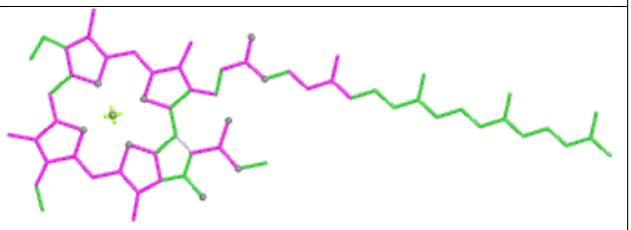
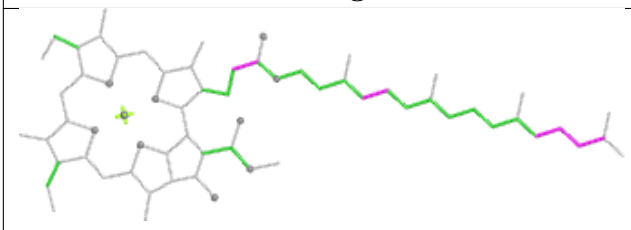
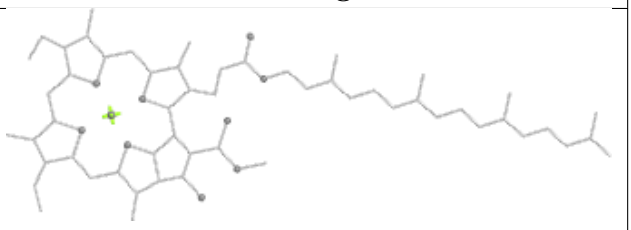


Bond angles

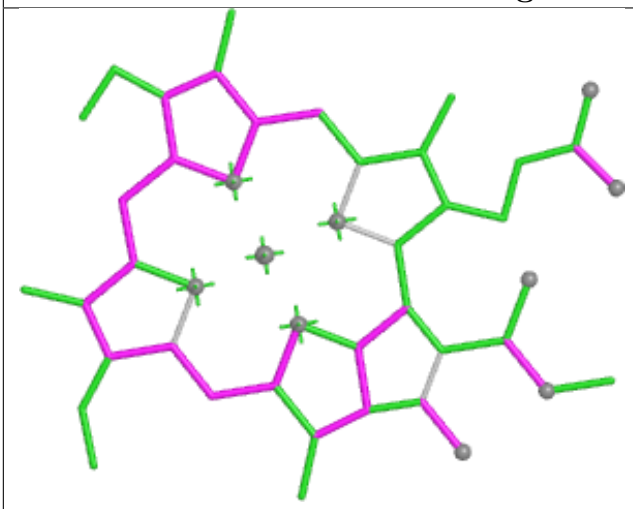


Torsions



Rings

Ligand CLA cB 810



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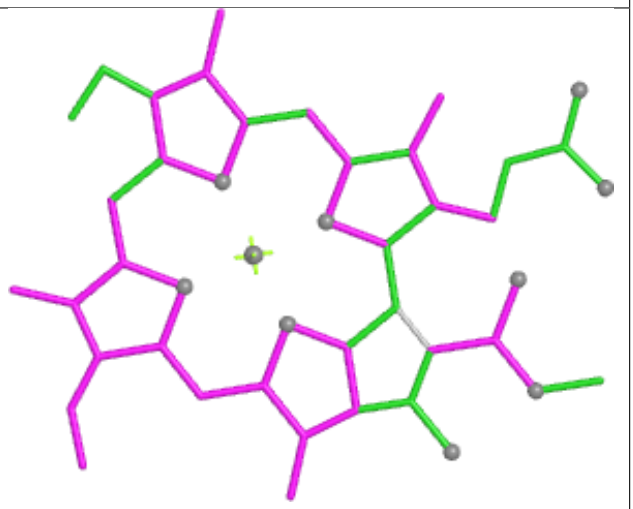
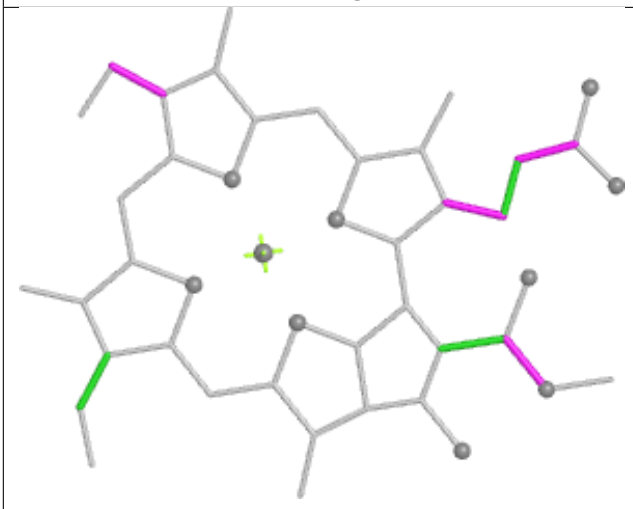


Bond angles

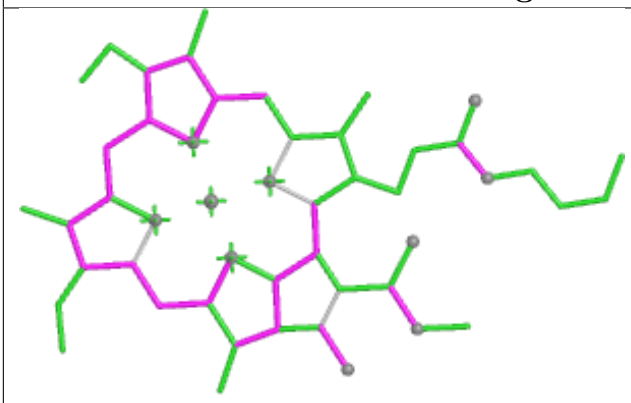


Torsions



Rings

Ligand CLA aB 830



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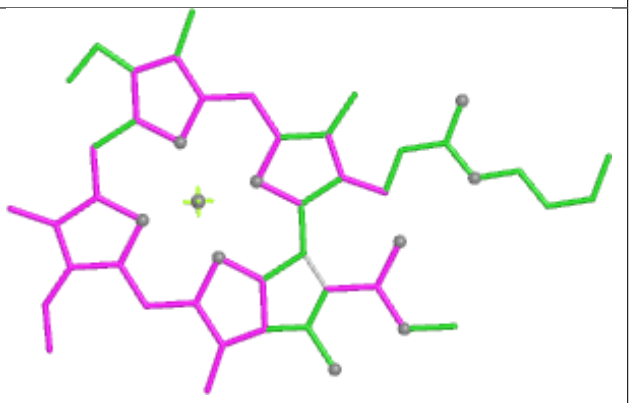
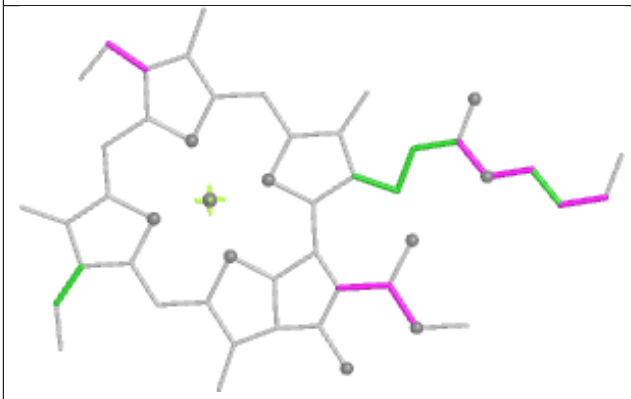


Bond angles



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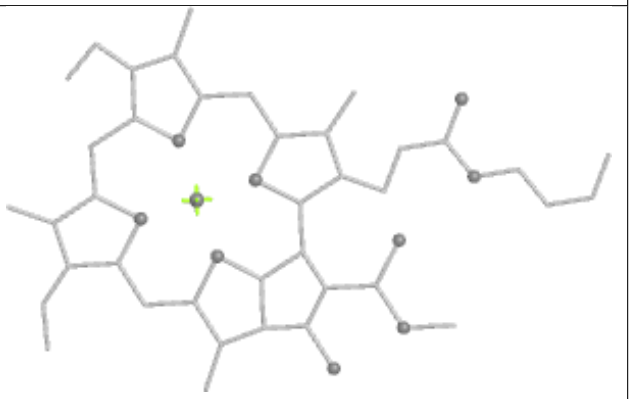
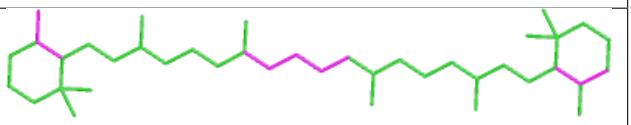


Rings

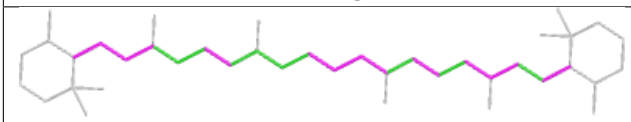
Ligand BCR bB 842



Bond lengths



Bond angles



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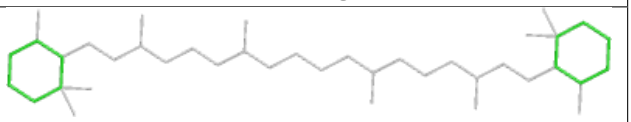
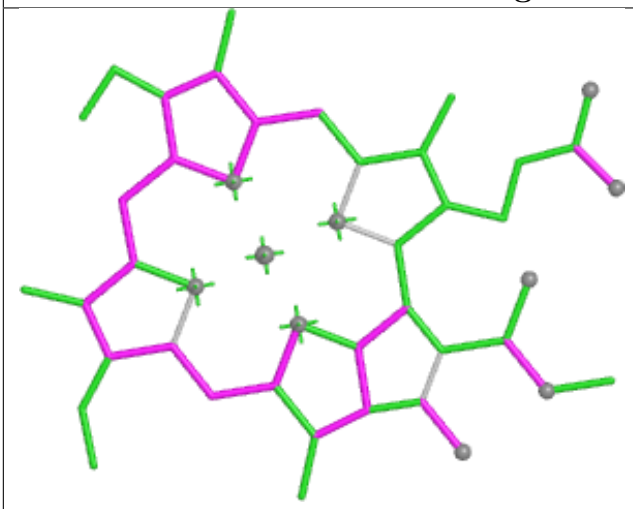


Rings

Ligand CLA bB 810



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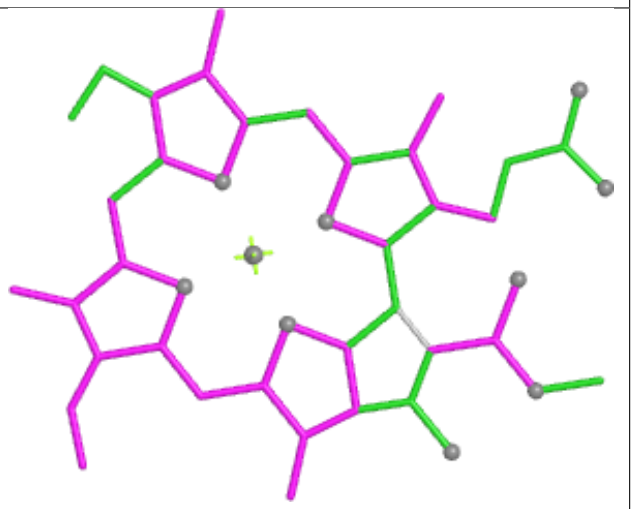
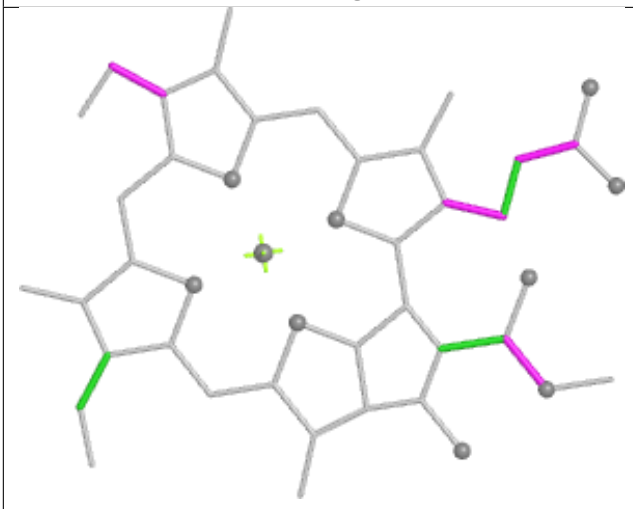


Bond angles

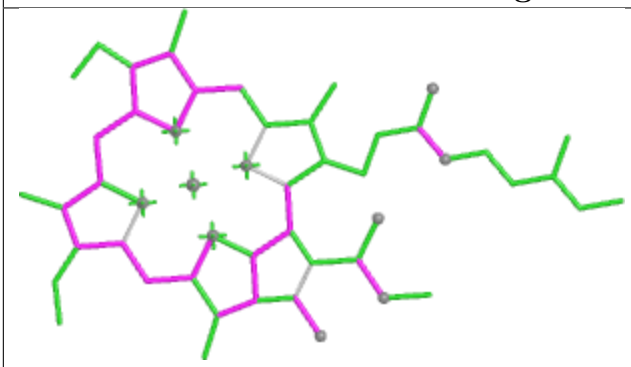


Torsions



Rings

Ligand CLA aK 103



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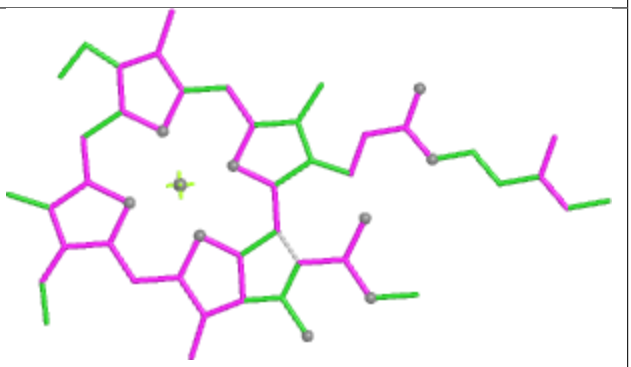
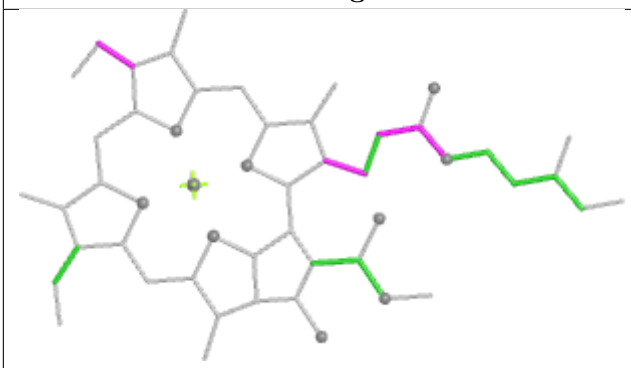


Bond angles



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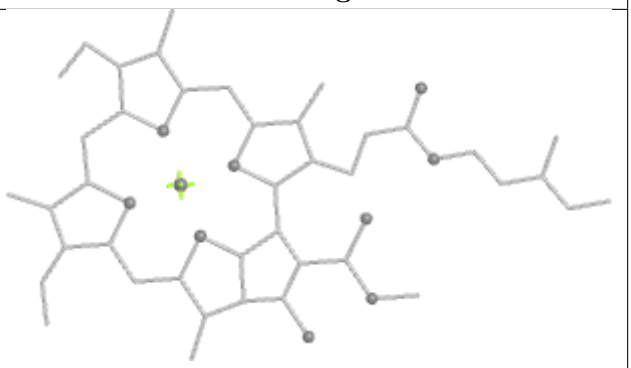
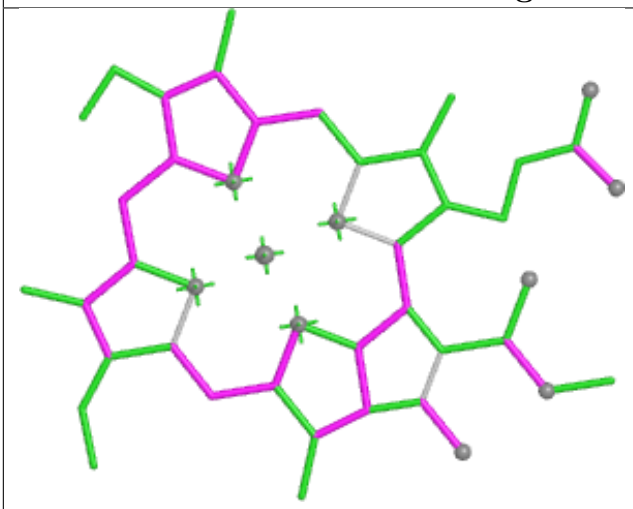


Rings

Ligand CLA aB 820



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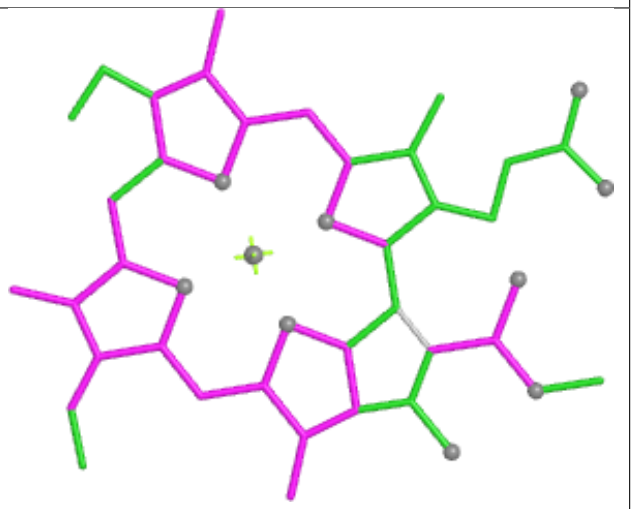
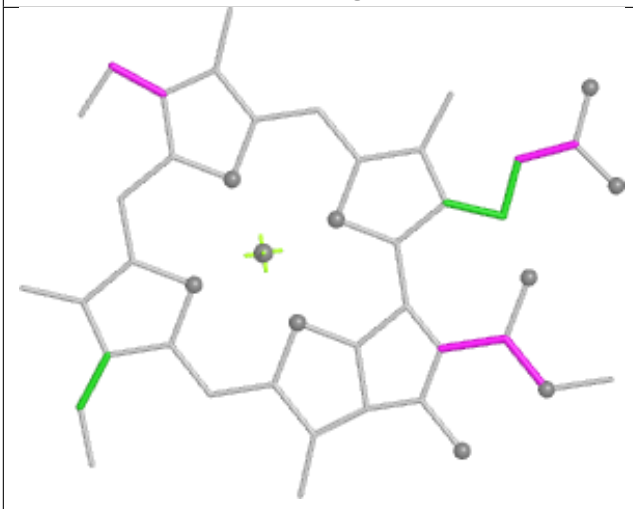


Bond angles

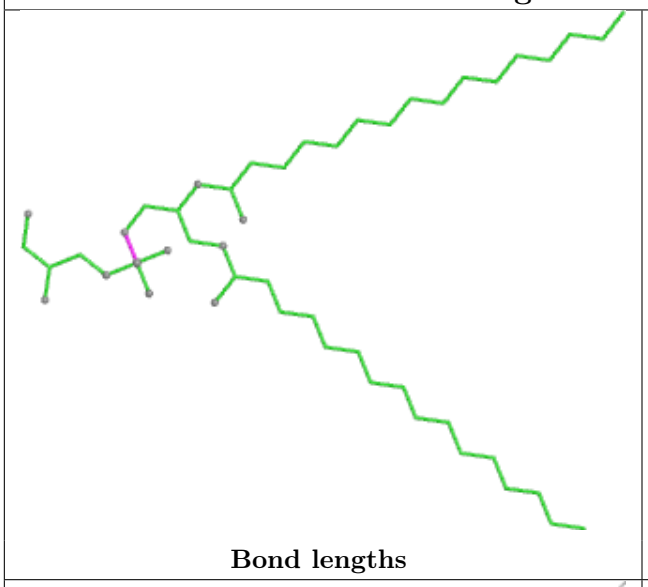


Torsions



Rings

Ligand LHG aA 852



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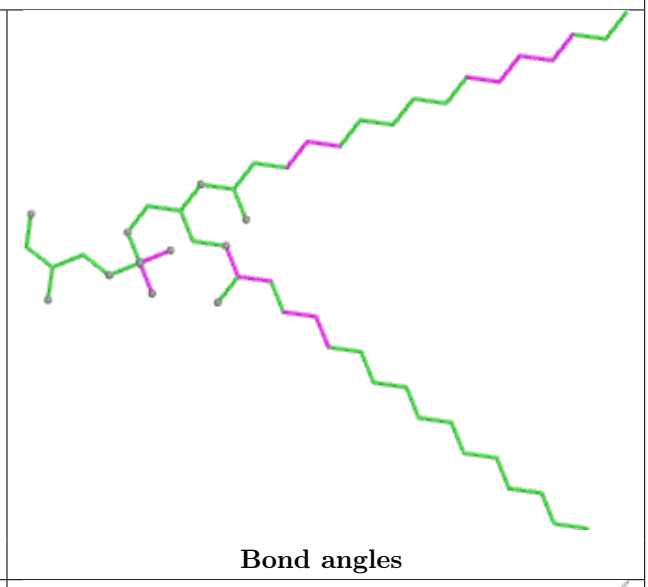
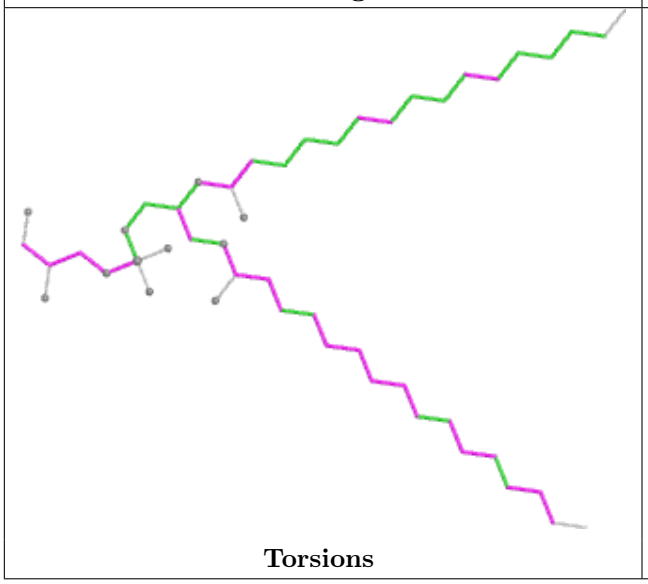
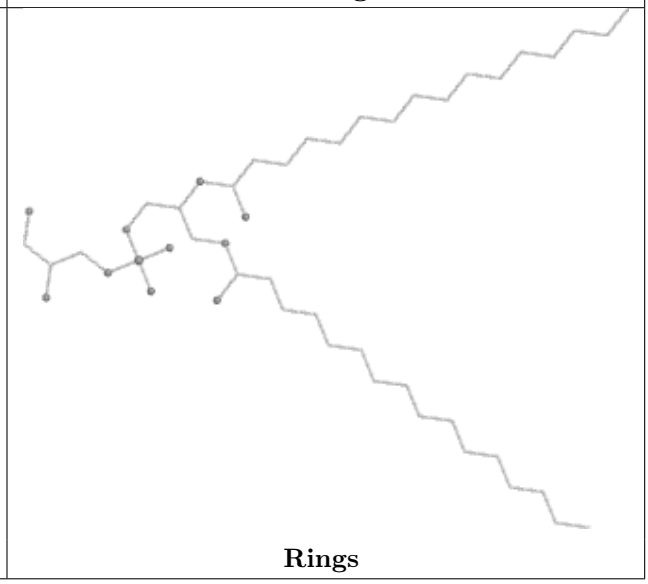


Bond angles

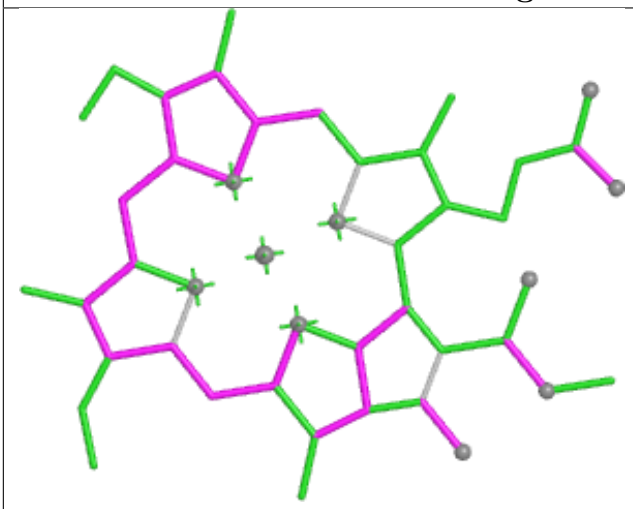


Torsions



Rings

Ligand CLA cB 833



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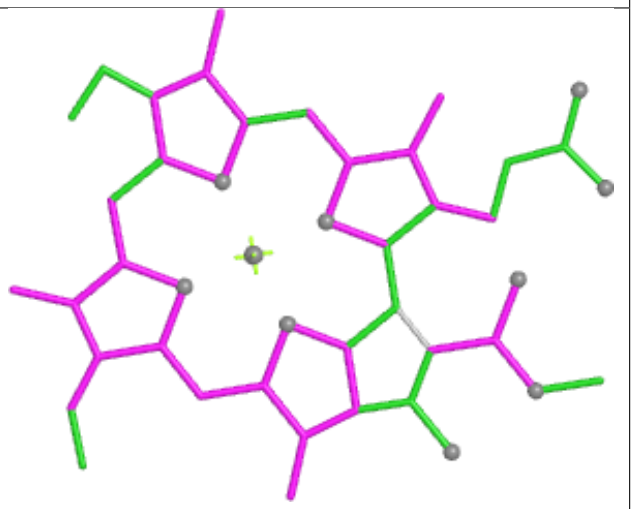
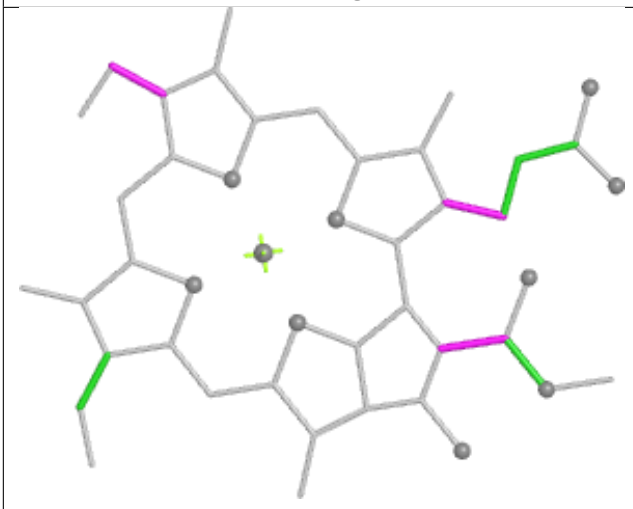


Bond angles

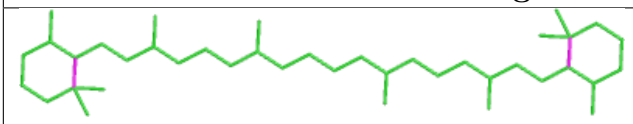


Torsions



Rings

Ligand BCR aA 850



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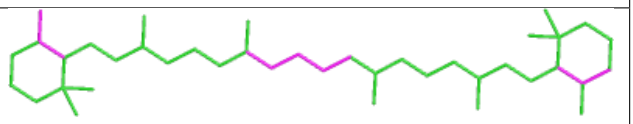
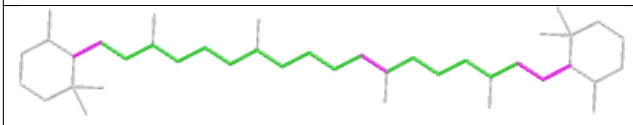


Bond angles



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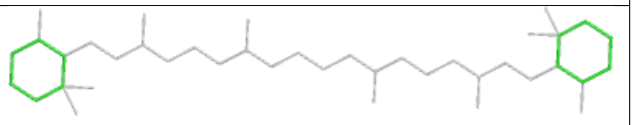
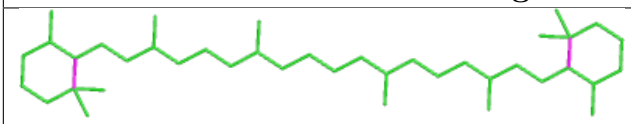


Rings

Ligand BCR bA 850



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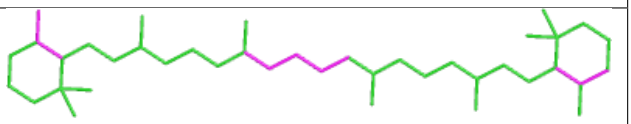
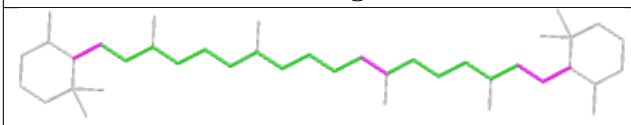


Bond angles



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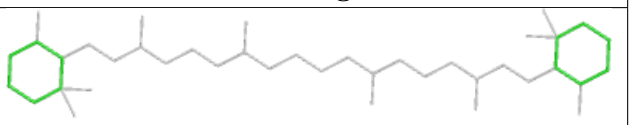
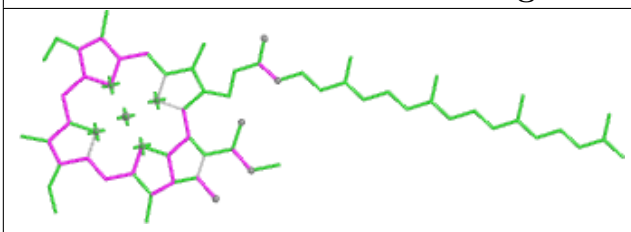


Rings

Ligand CLA aL 205



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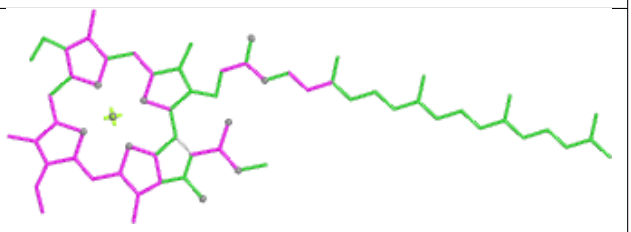
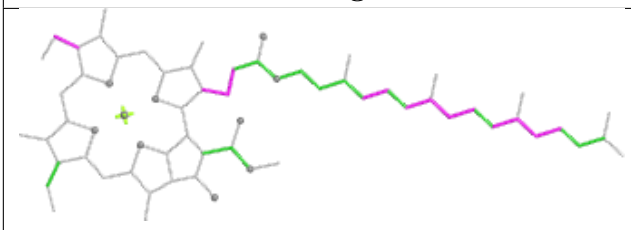


Bond angles



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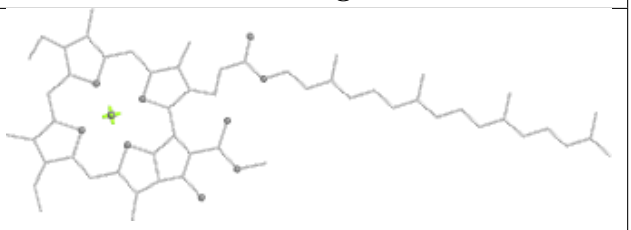
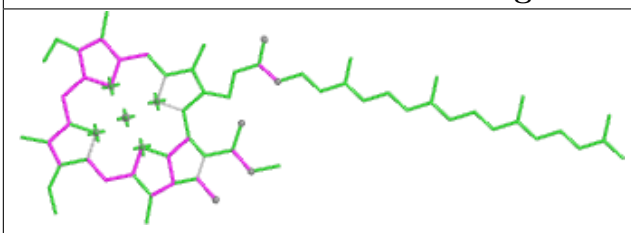
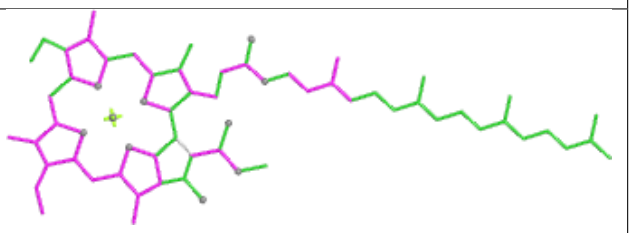


Rings

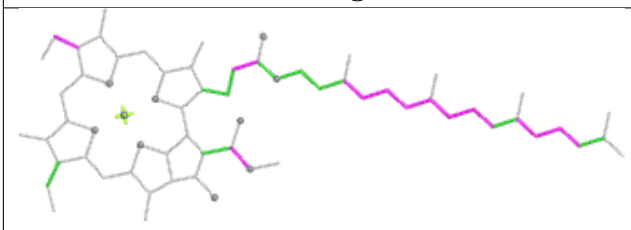
Ligand CLA bB 806



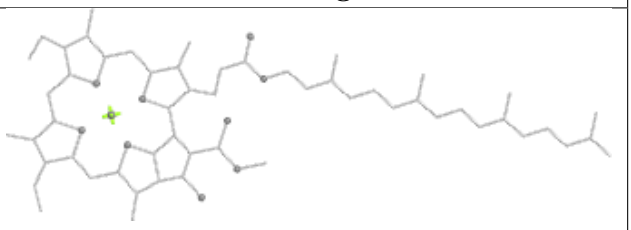
Bond lengths



Bond angles

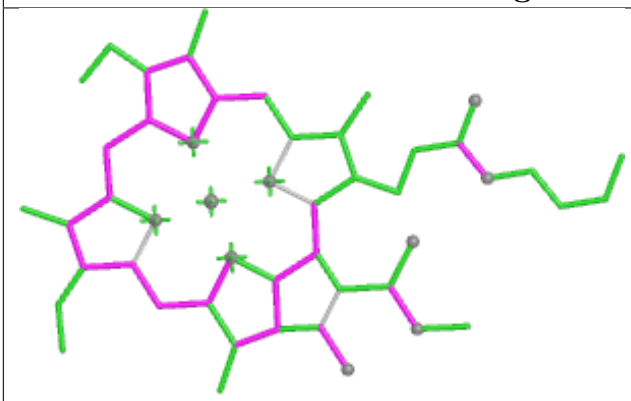


Torsions

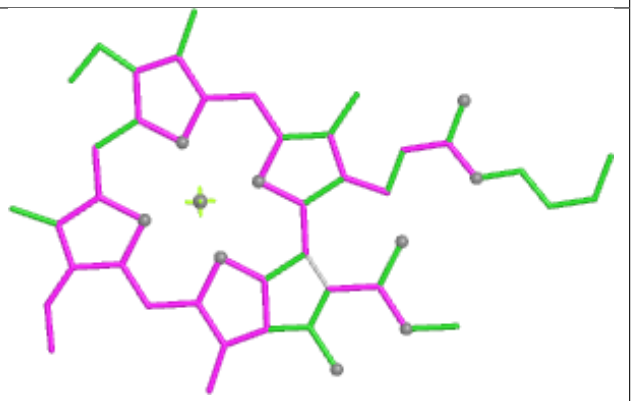


Rings

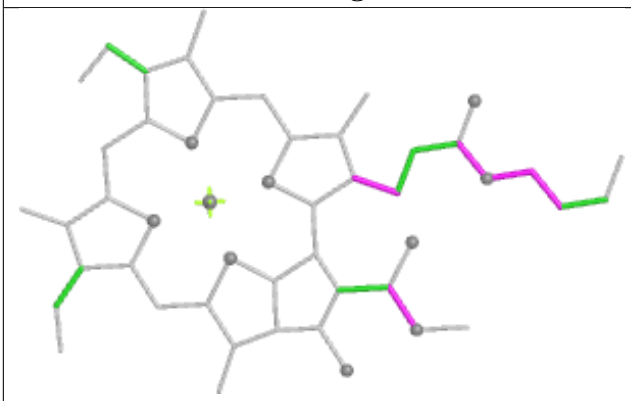
Ligand CLA bA 817



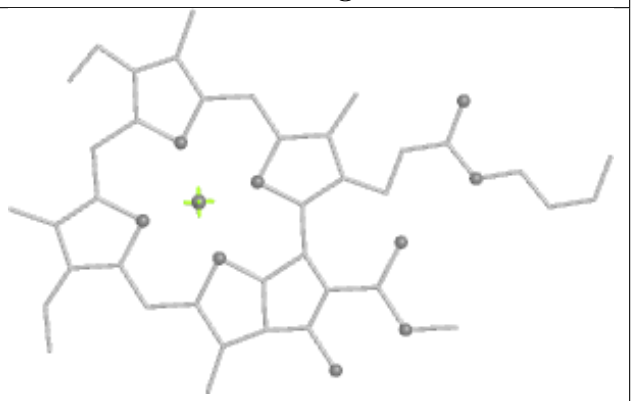
Bond lengths



Bond angles

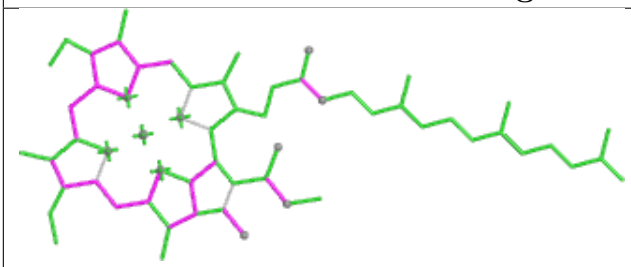


Torsions



Rings

Ligand CLA cB 817



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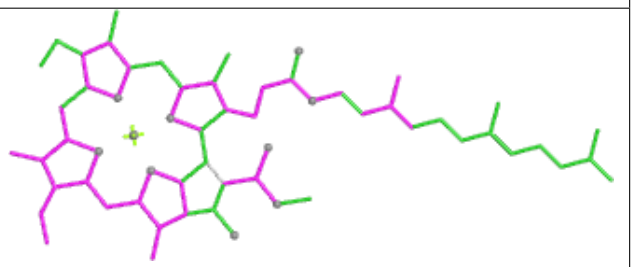

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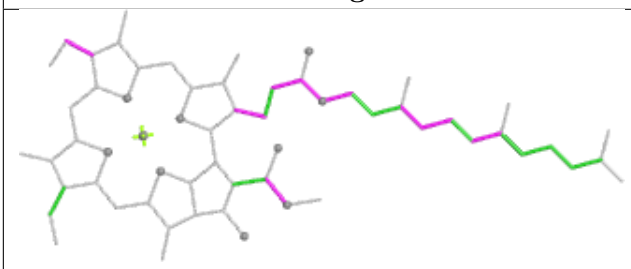

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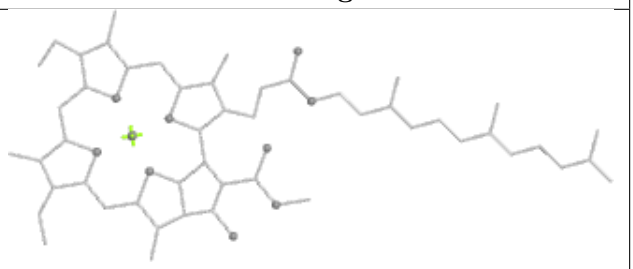
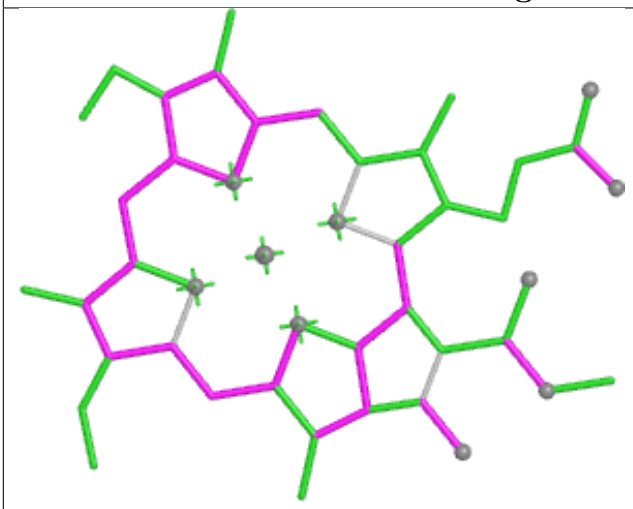


Rings

Ligand CLA aA 837



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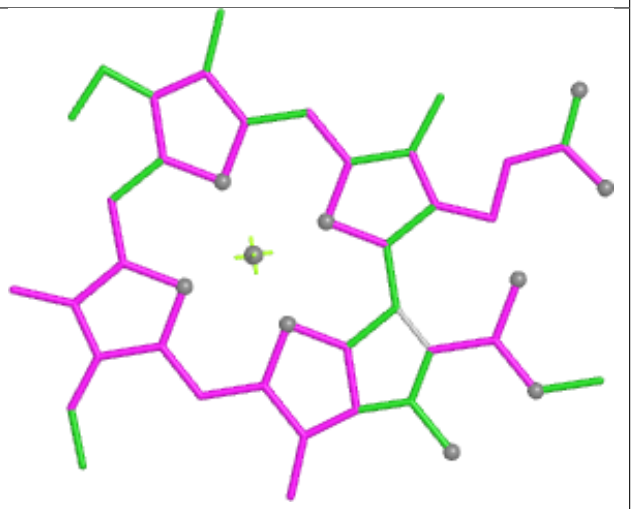

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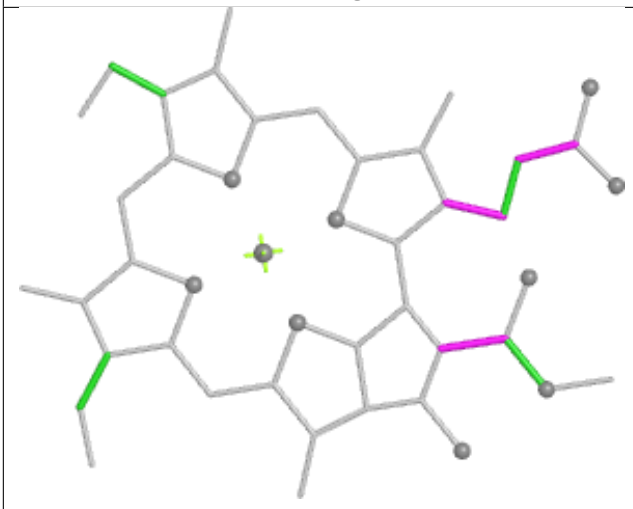
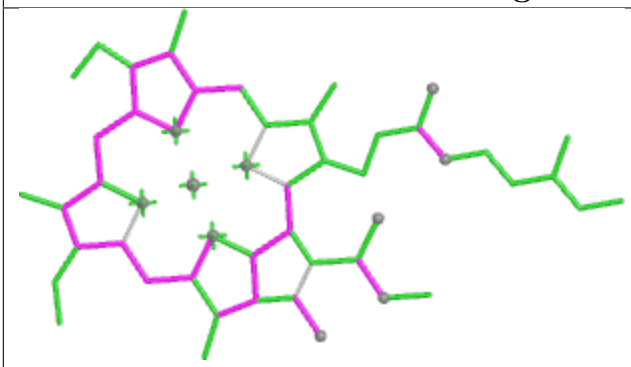


Torsions



Rings

Ligand CLA bK 103



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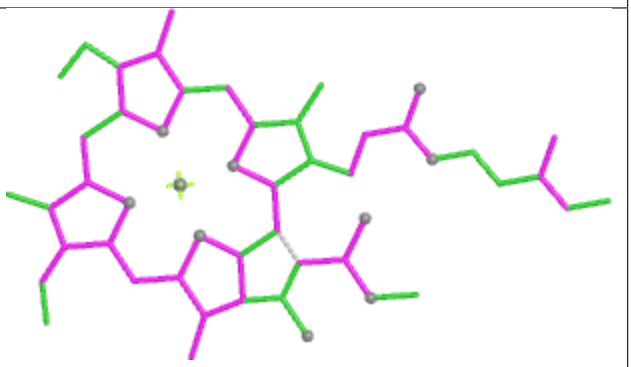
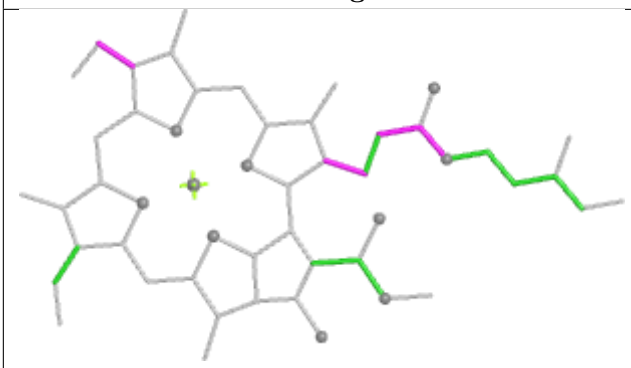


Bond angles



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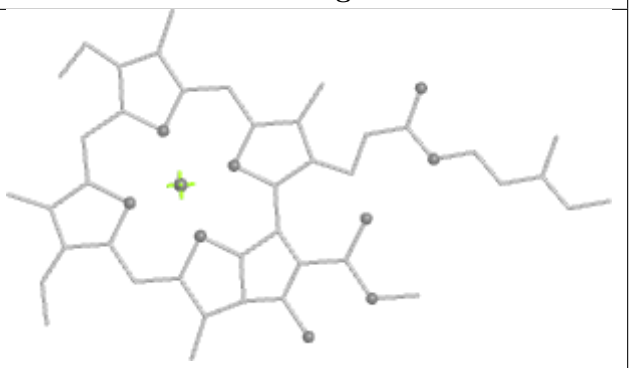
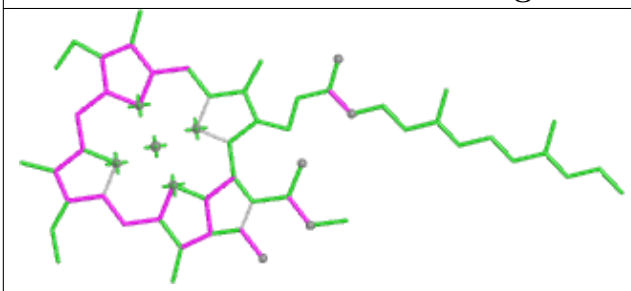


Rings

Ligand CLA bB 802



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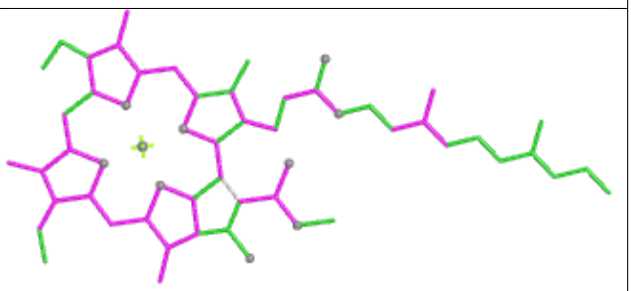
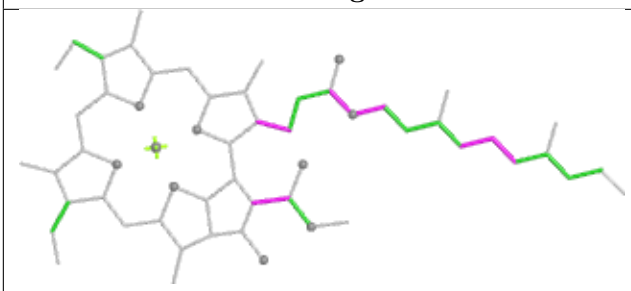


Bond angles



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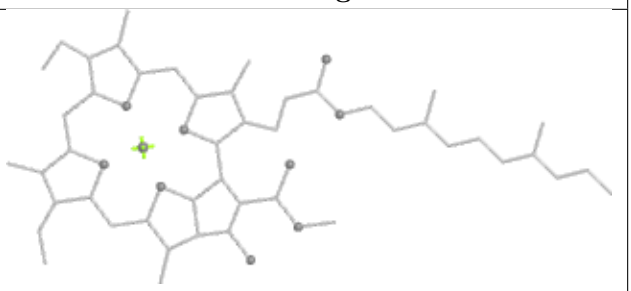
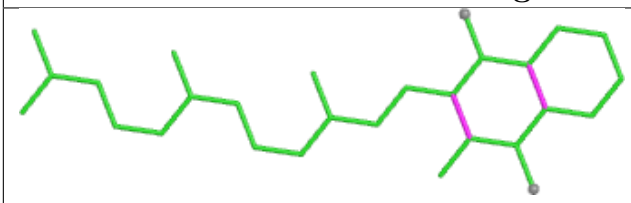
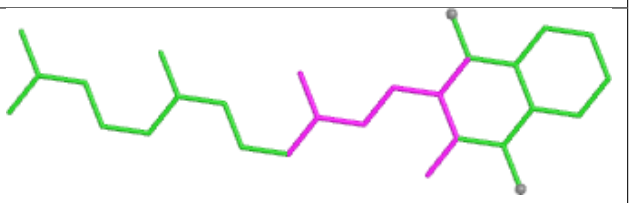
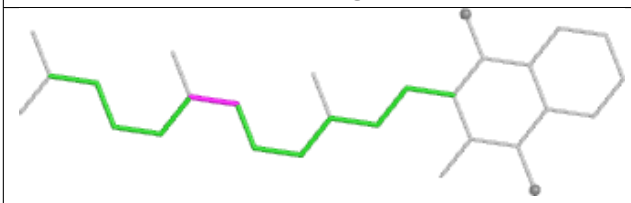
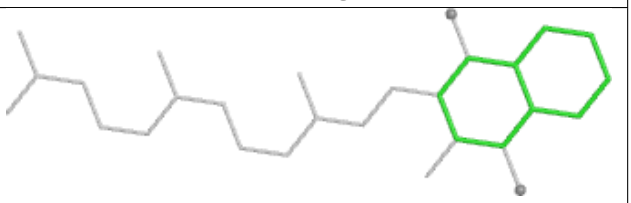
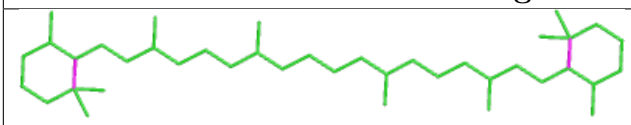
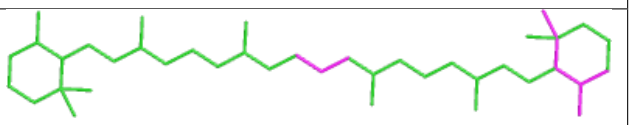
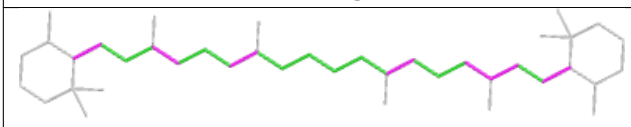
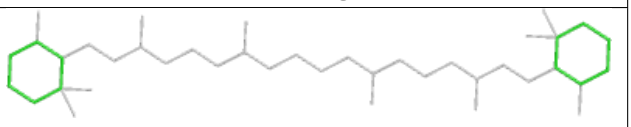
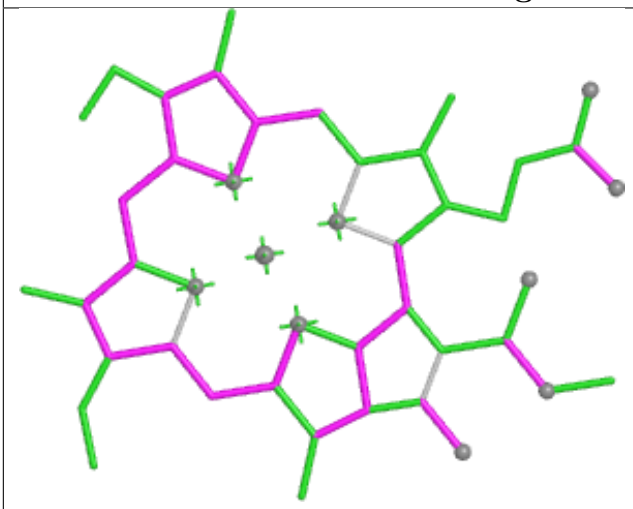


Rings

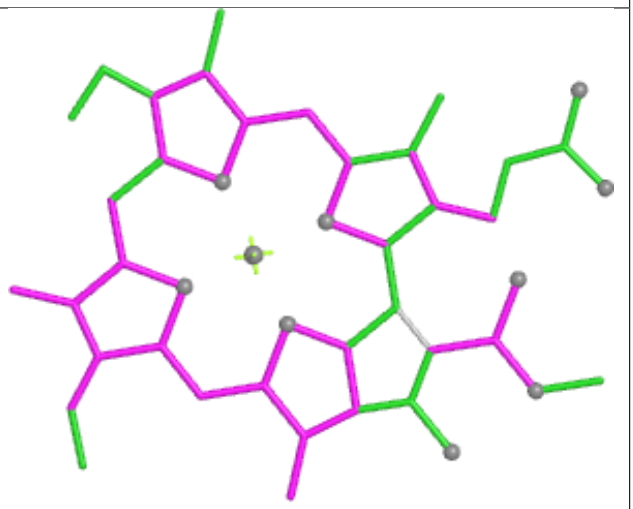
Ligand PQN aB 841	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR aB 844	
	
Bond lengths	Bond angles
	
Torsions	Rings

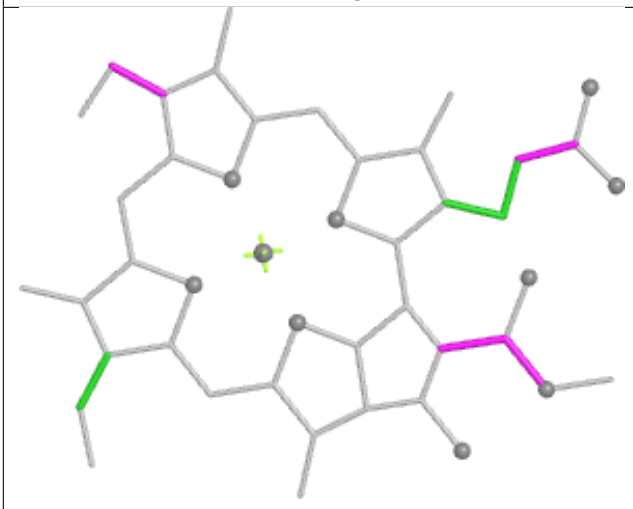
Ligand CLA aA 805



Bond lengths



Bond angles

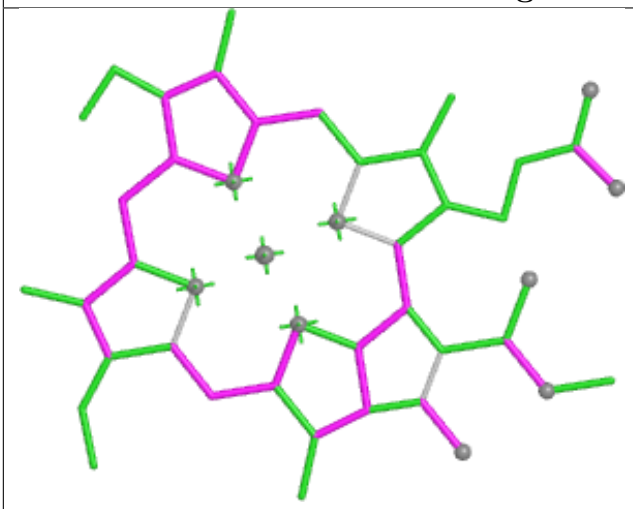


Torsions



Rings

Ligand CLA cB 820



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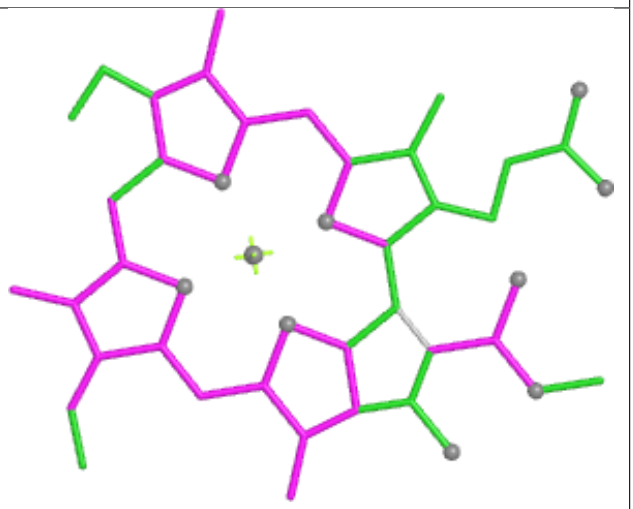
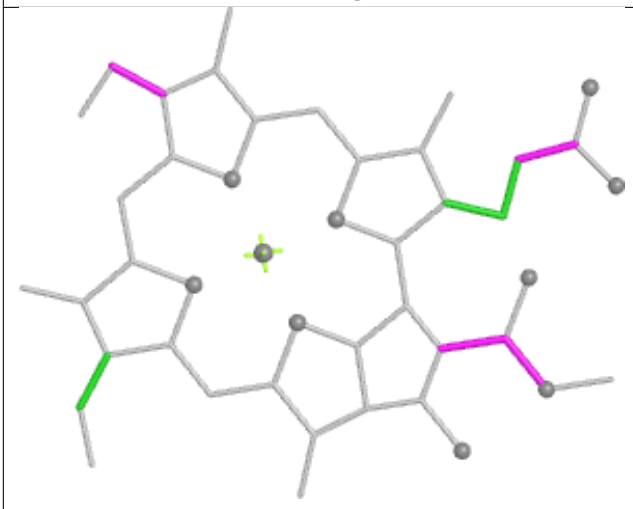


Bond angles

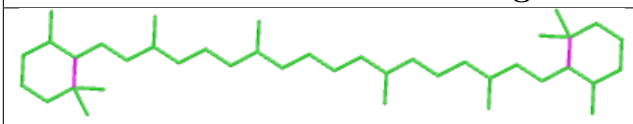


Torsions



Rings

Ligand BCR aA 847



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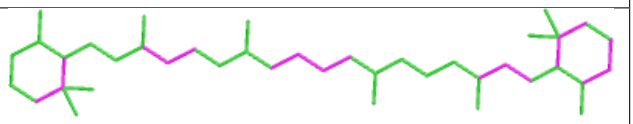
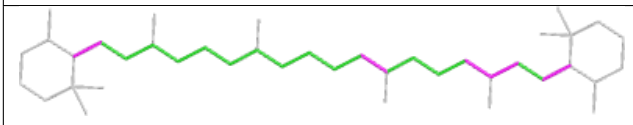


Bond angles



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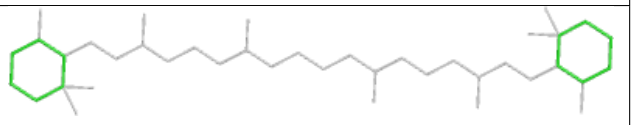
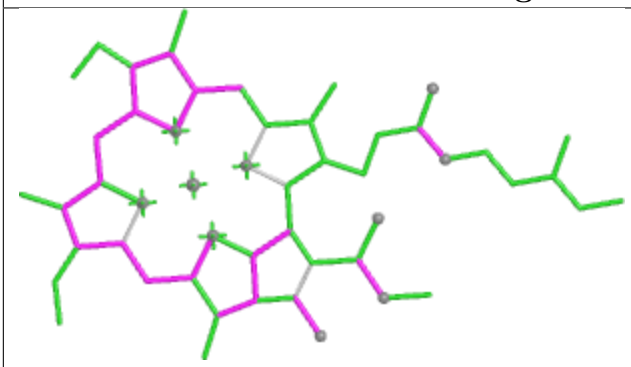
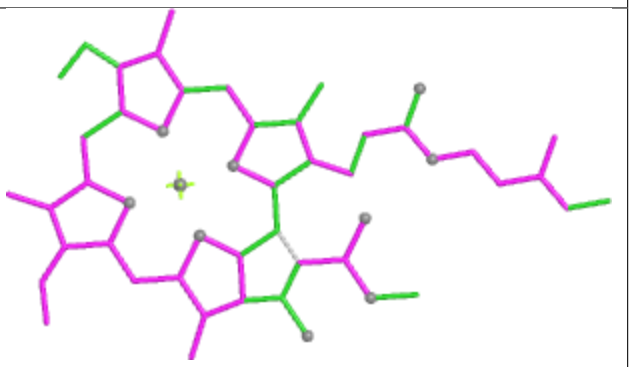
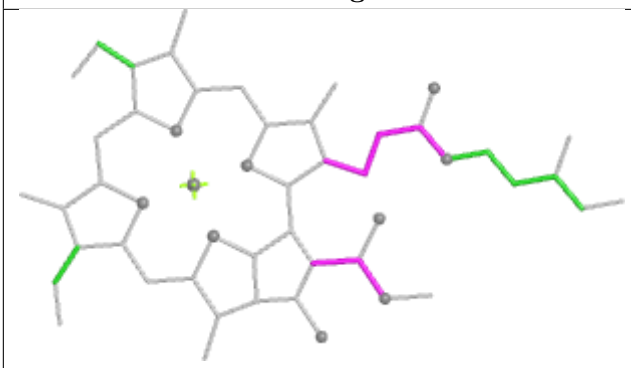
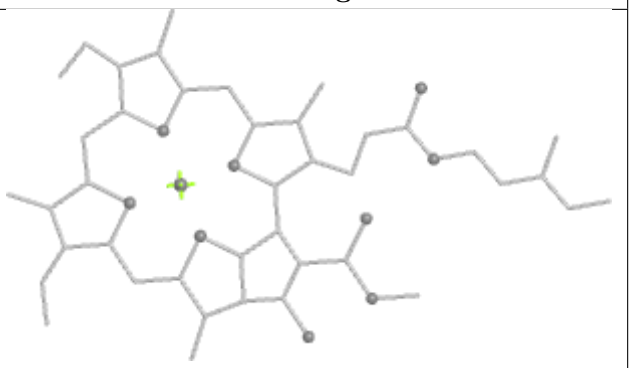


Rings

Ligand CLA aA 838	
 Bond lengths	 Bond angles
 Torsions	 Rings

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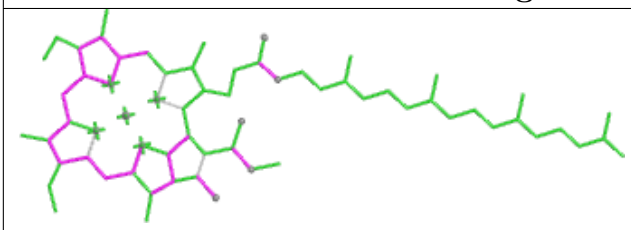
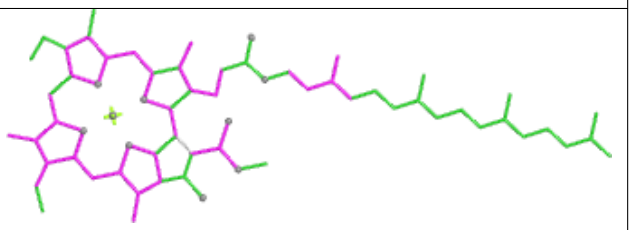
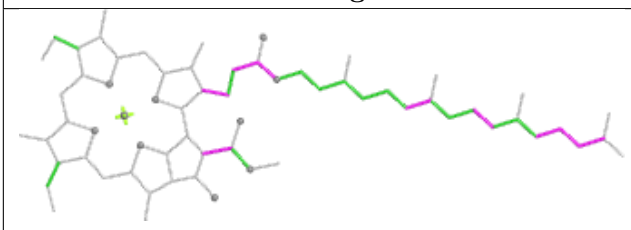
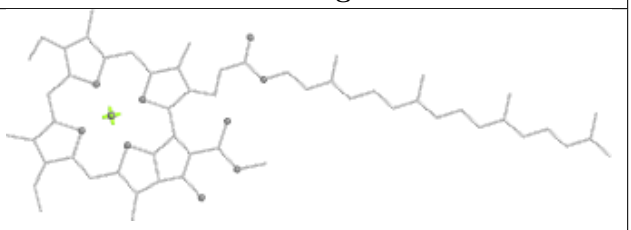
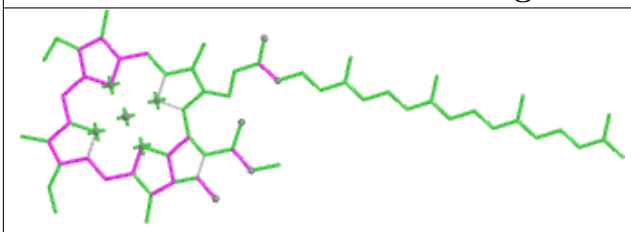
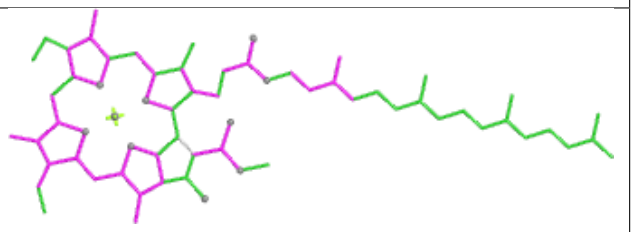
 Bond lengths	 Bond angles
 Torsions	 Rings

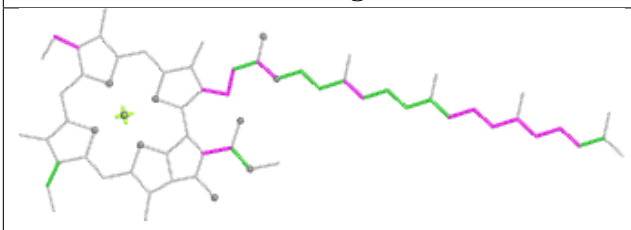
Ligand CLA bB 812



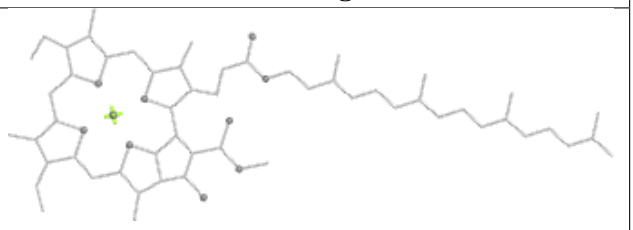
Bond lengths



Bond angles

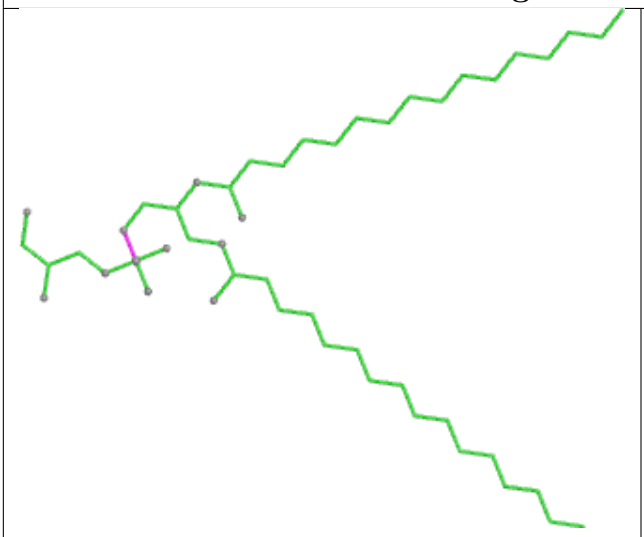


Torsions

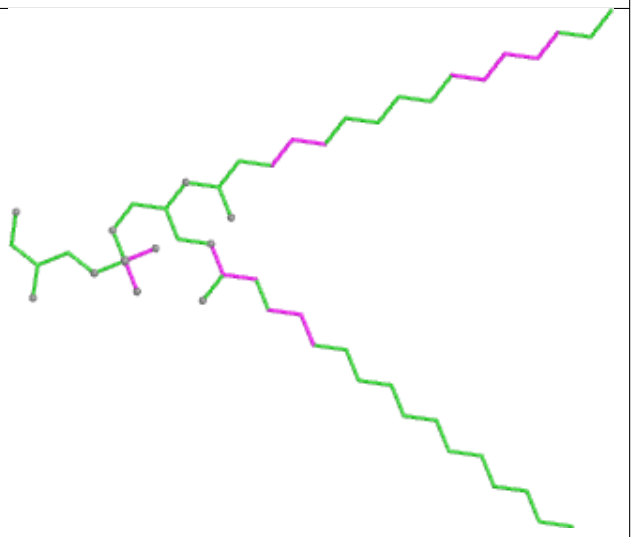


Rings

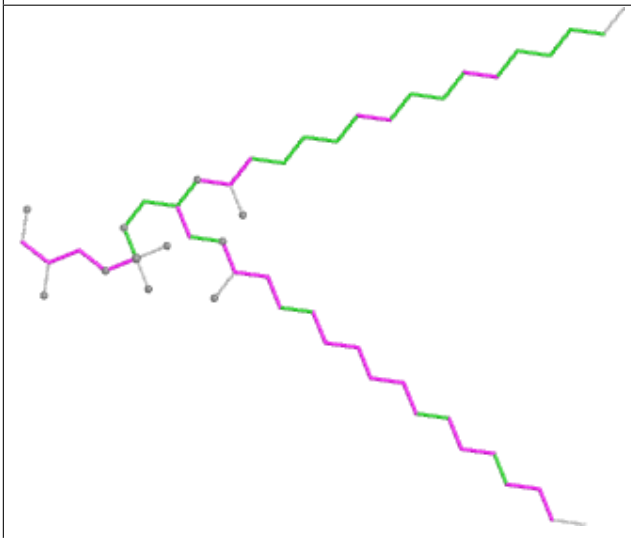
Ligand LHG bA 852



Bond lengths



Bond angles



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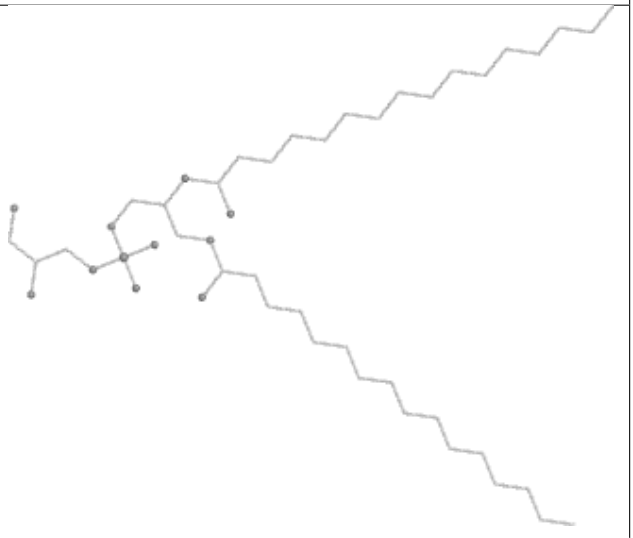
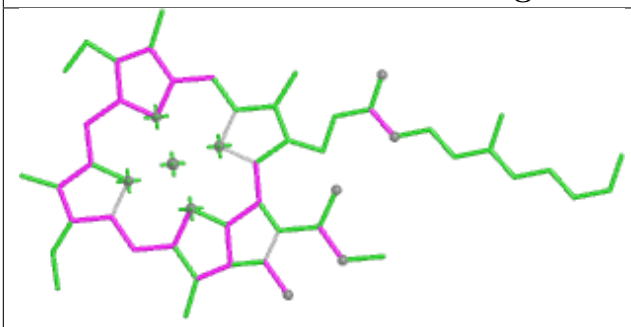


Rings

Ligand CLA bB 823



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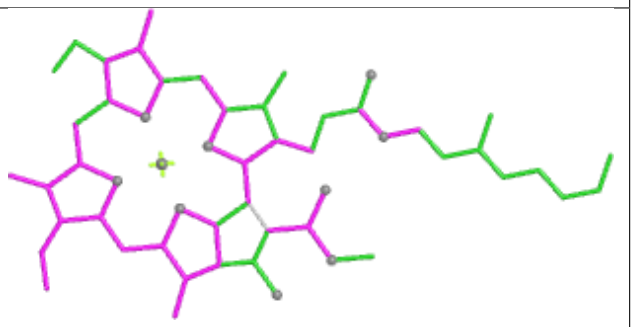
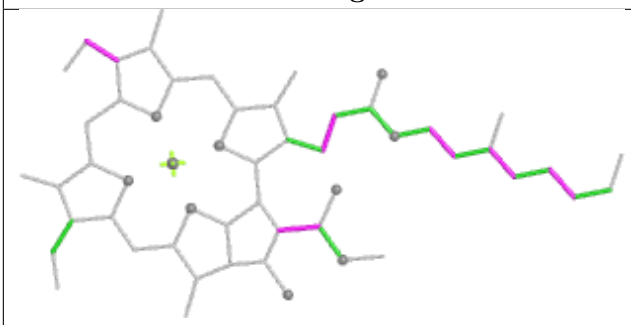


Bond angles



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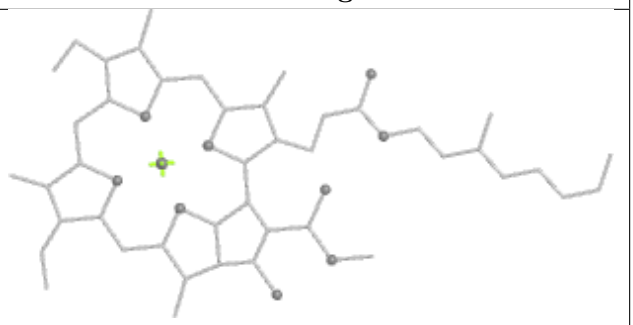
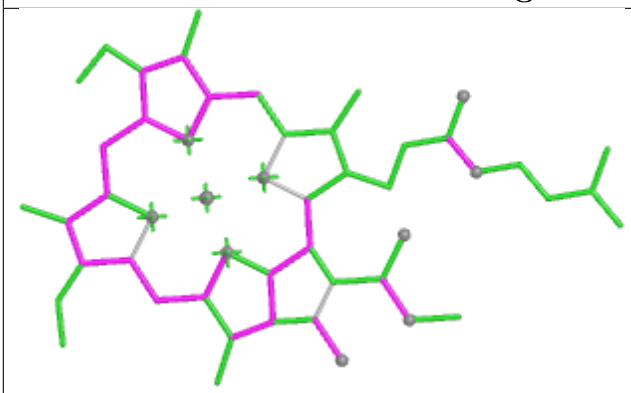
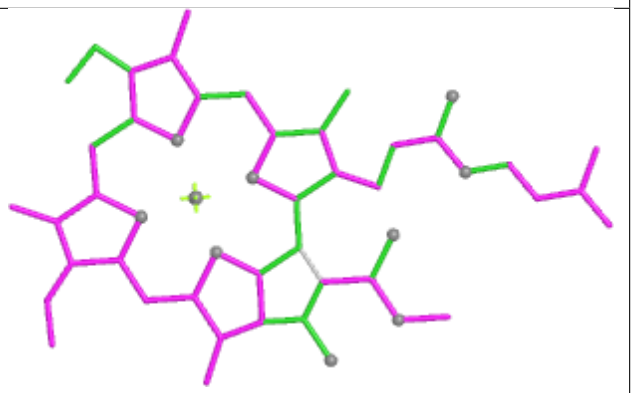


Rings

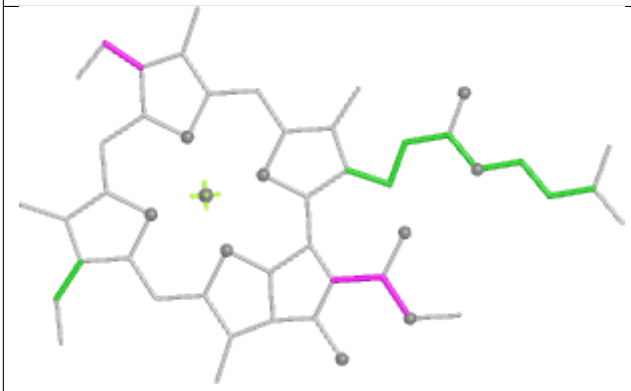
Ligand CLA cA 841



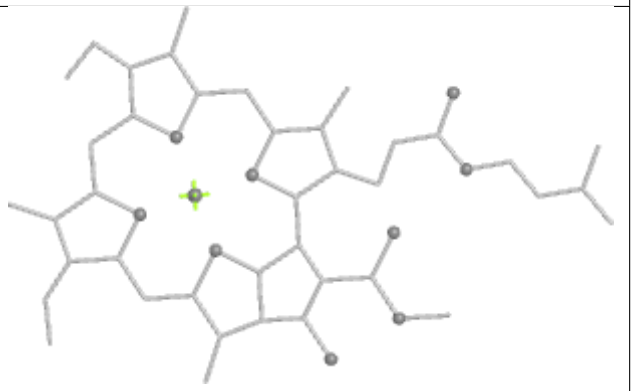
Bond lengths



Bond angles

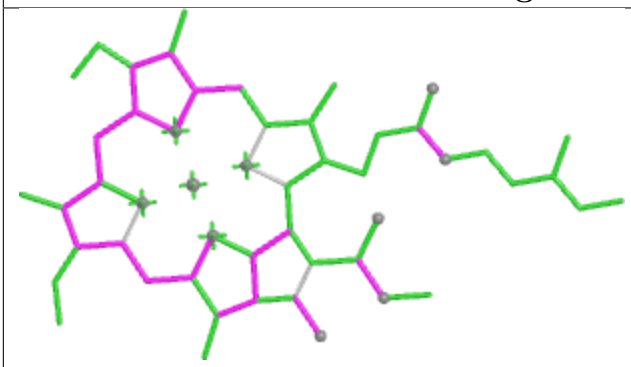


Torsions

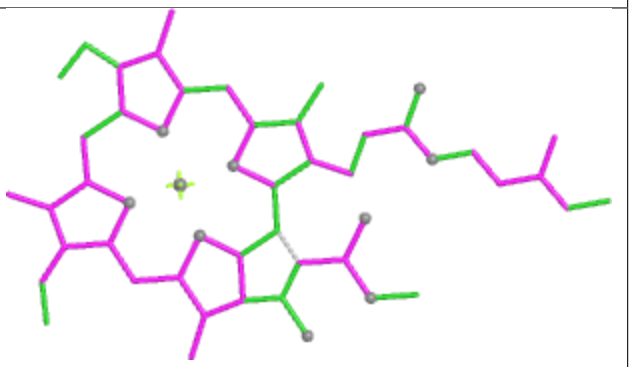


Rings

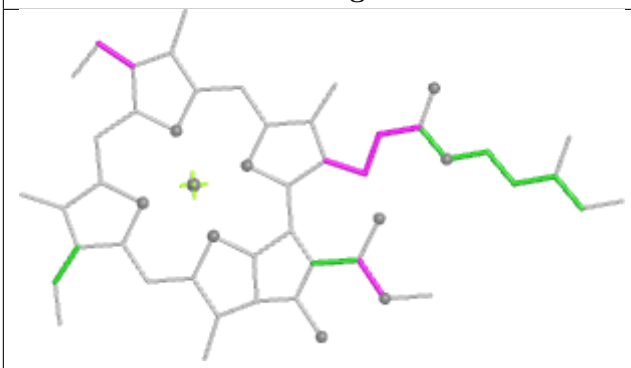
Ligand CLA cA 843



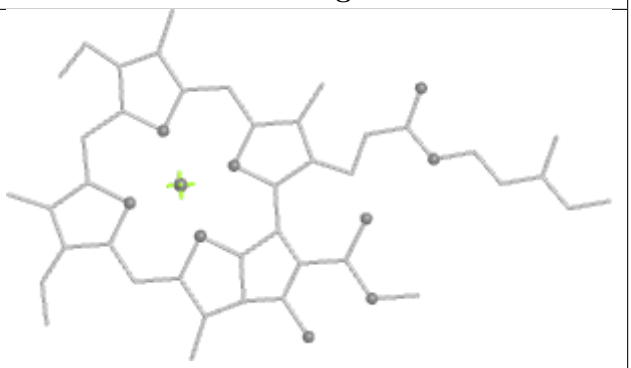
Bond lengths



Bond angles

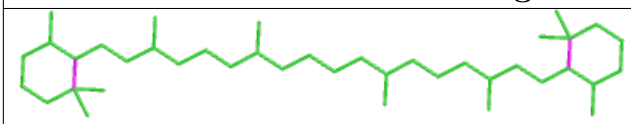


Torsions

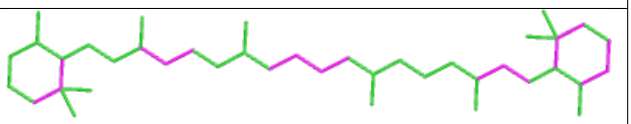


Rings

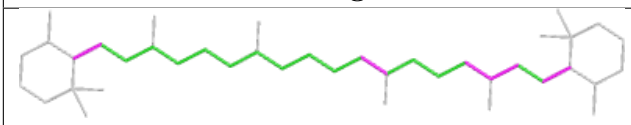
Ligand BCR cA 847



Bond lengths



Bond angles



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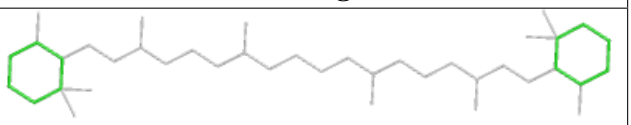
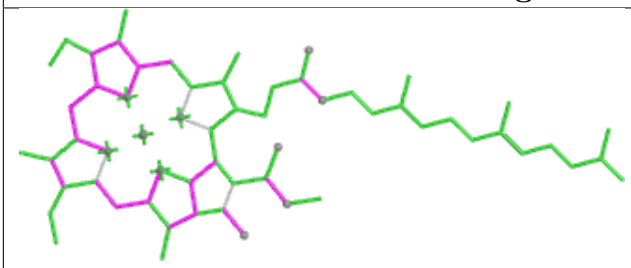


Rings

Ligand CLA aA 828



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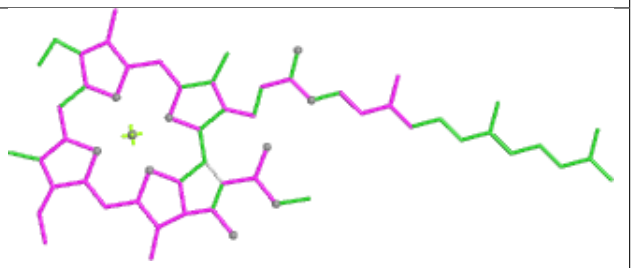
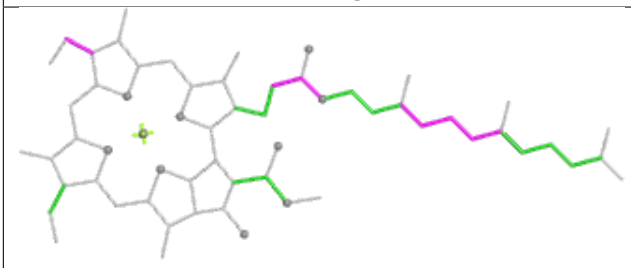


Bond angles



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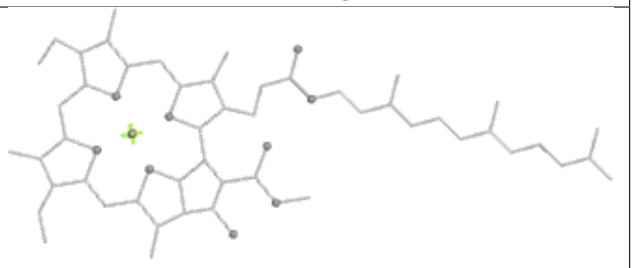
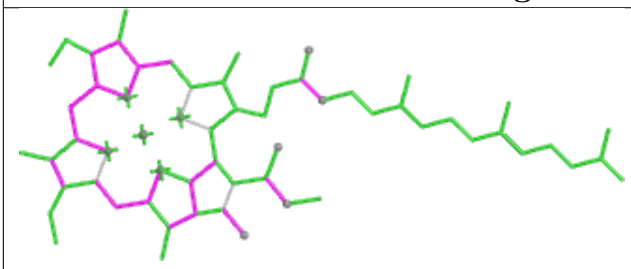
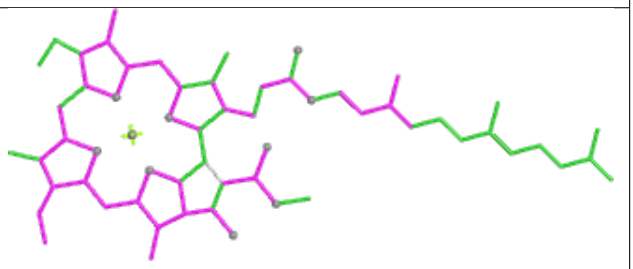


Rings

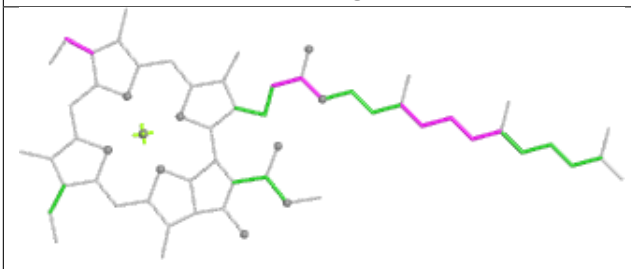
Ligand CLA bA 828



Bond lengths



Bond angles



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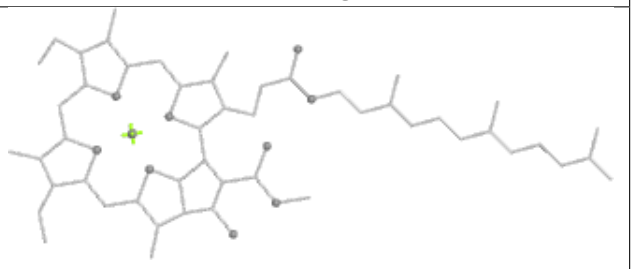
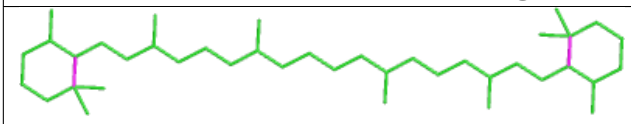


Rings

Ligand BCR cA 848



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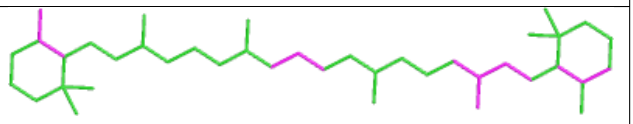
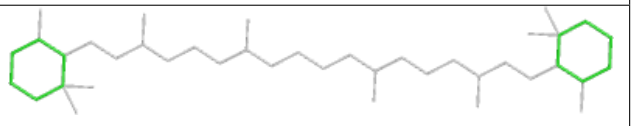


Bond angles

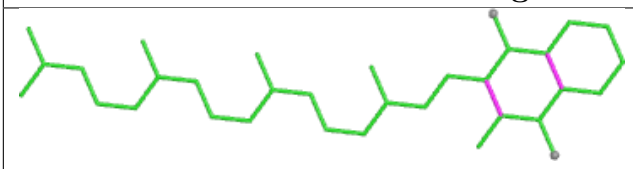


Torsions



Rings

Ligand PQN bA 845



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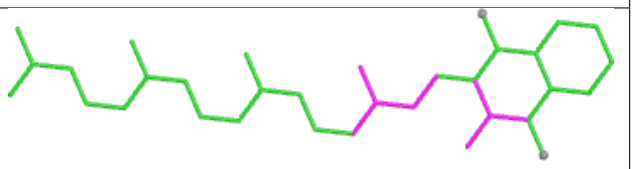
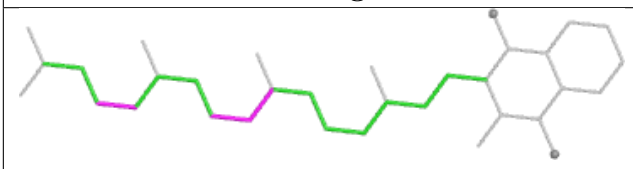


Bond angles



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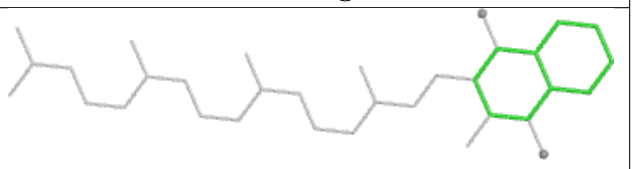
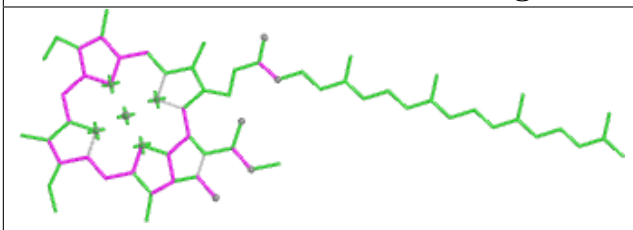


Rings

Ligand CLA bA 825



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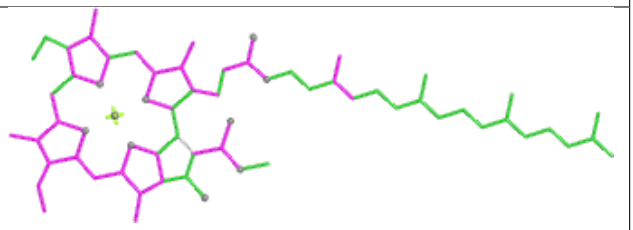
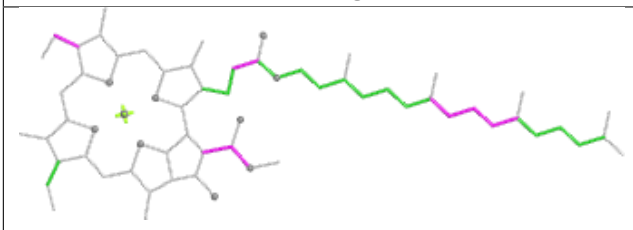


Bond angles



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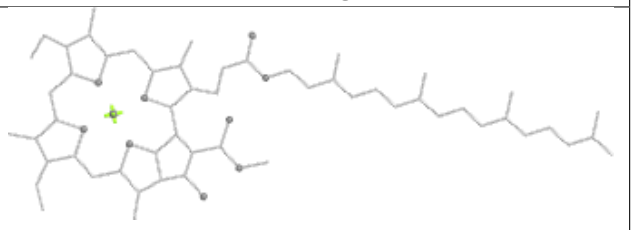
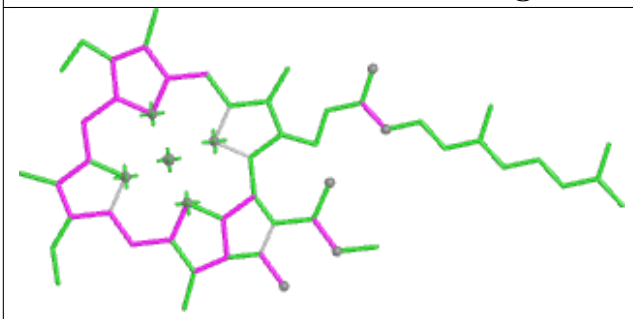


Rings

Ligand CLA bB 837



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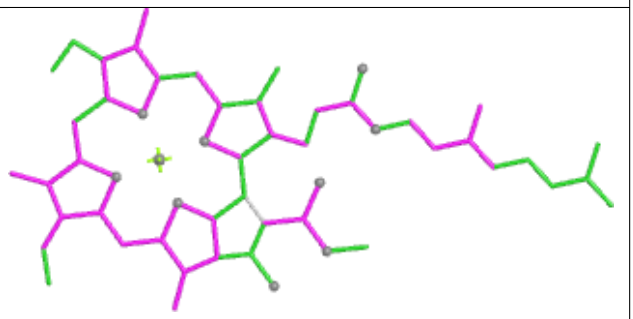
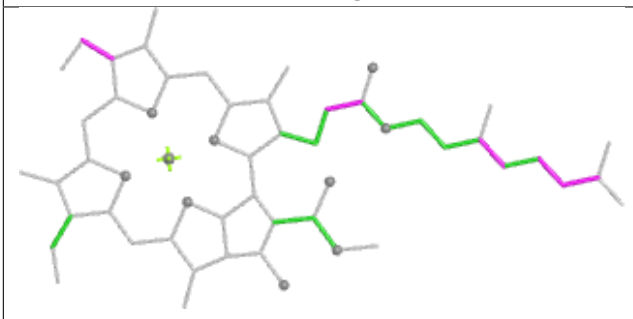


Bond angles



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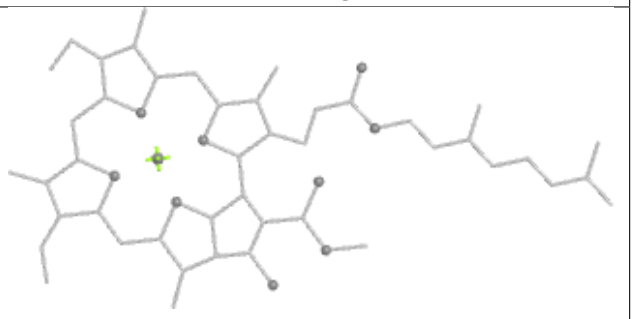
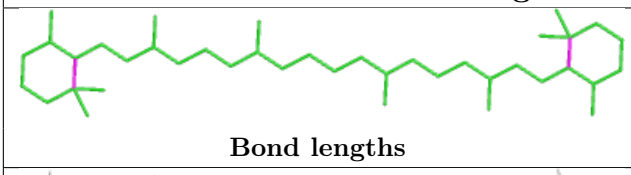


Rings

Ligand BCR aK 102



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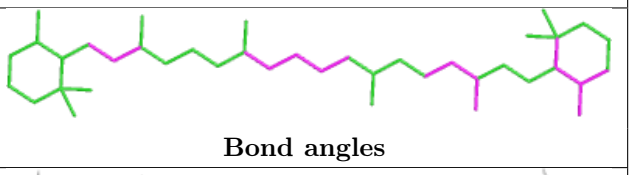
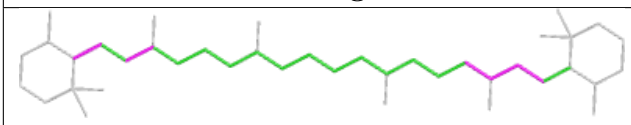
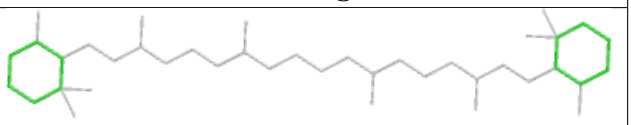


Bond angles

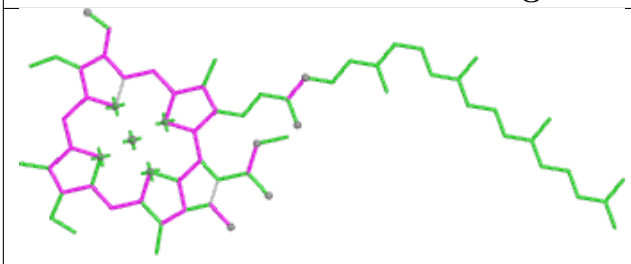


Torsions



Rings

Ligand F6C cL 202



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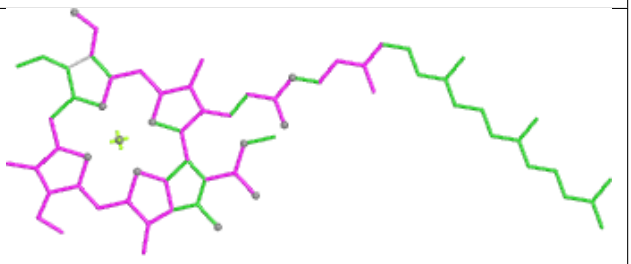
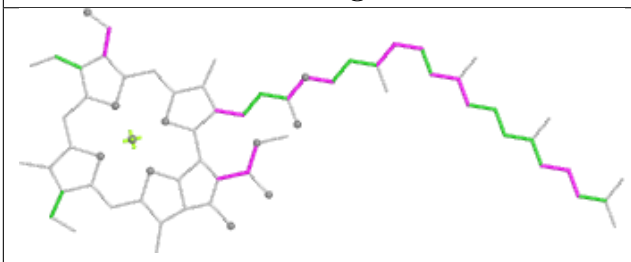


Bond angles



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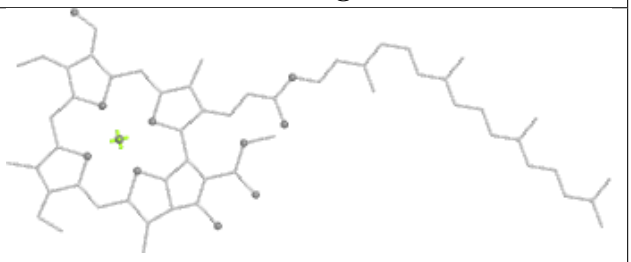
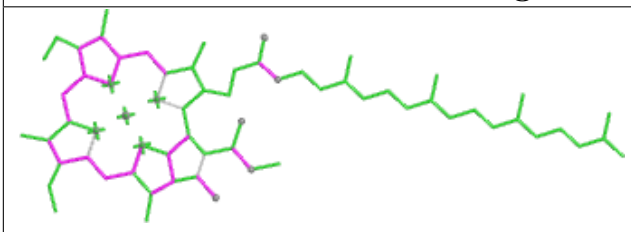
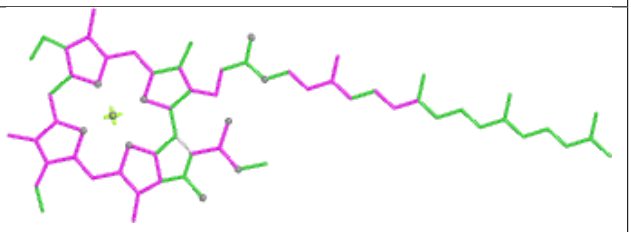


Rings

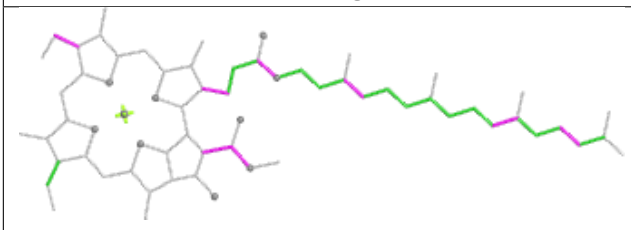
Ligand CLA bA 806



Bond lengths



Bond angles



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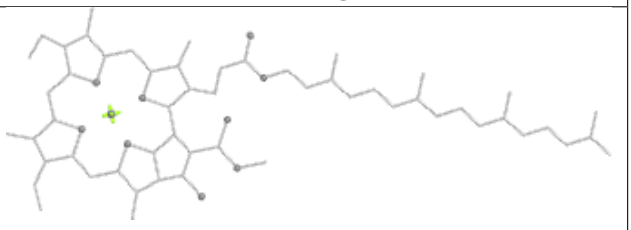
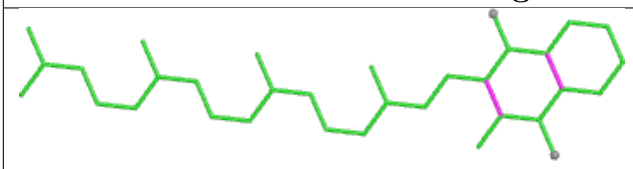


Rings

Ligand PQN aA 845



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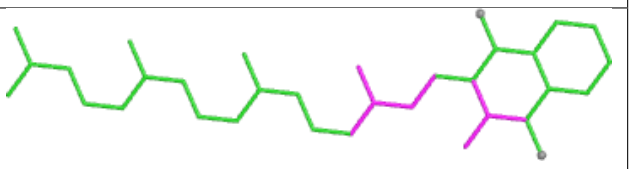
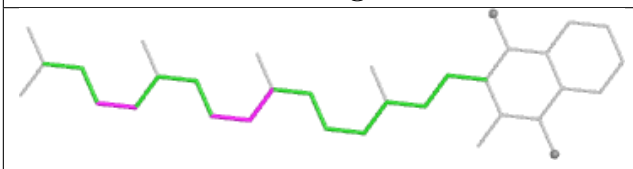


Bond angles



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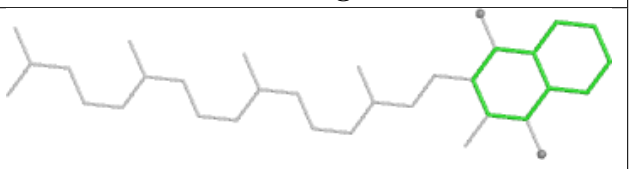
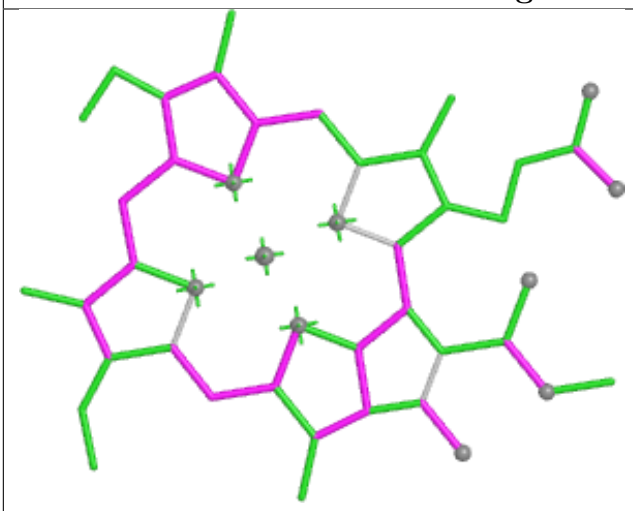
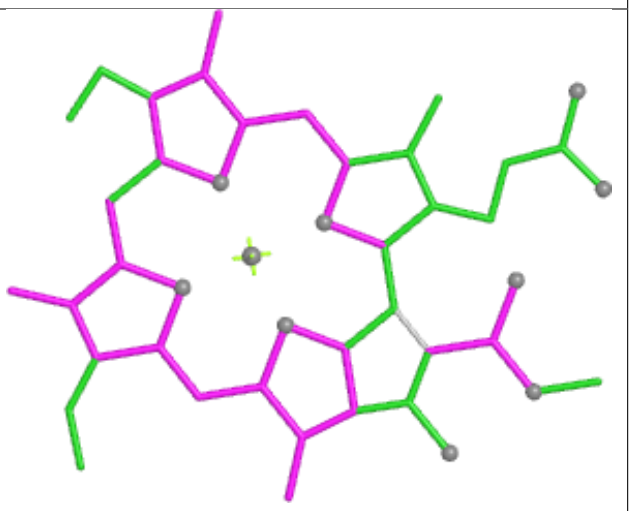


Rings

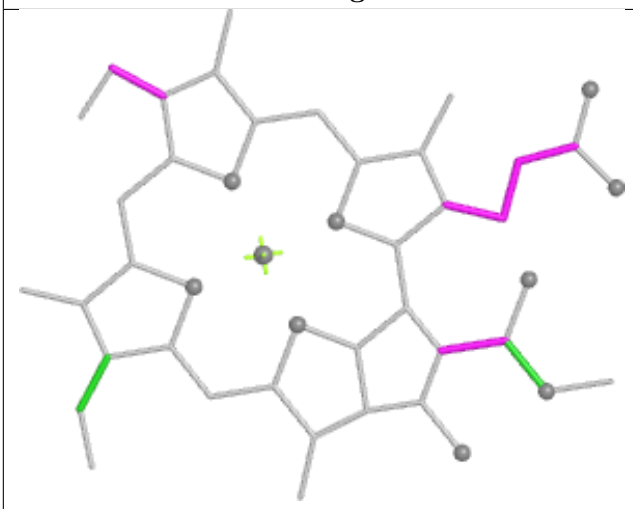
Ligand CLA cA 823



Bond lengths



Bond angles

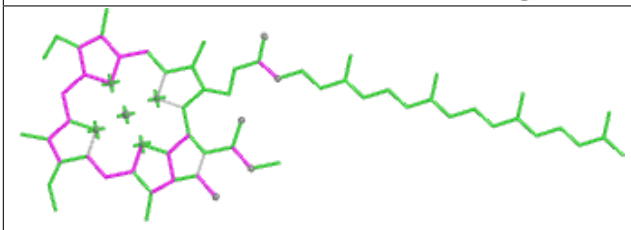


Torsions



Rings

Ligand CLA aB 806



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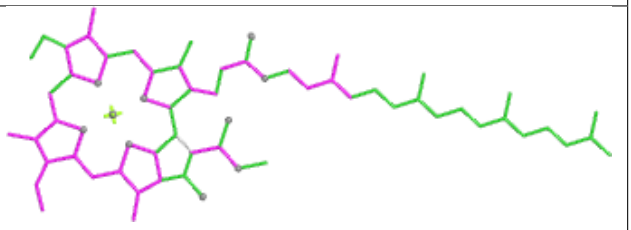
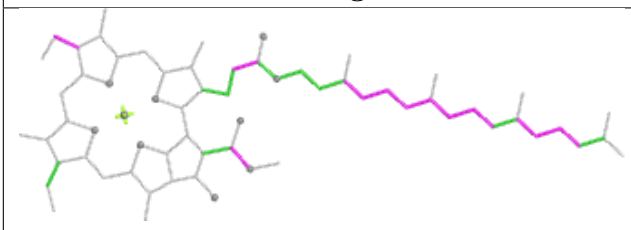
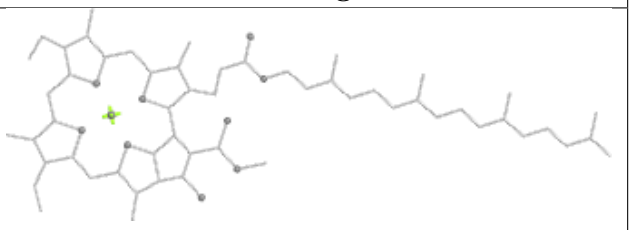


Bond angles

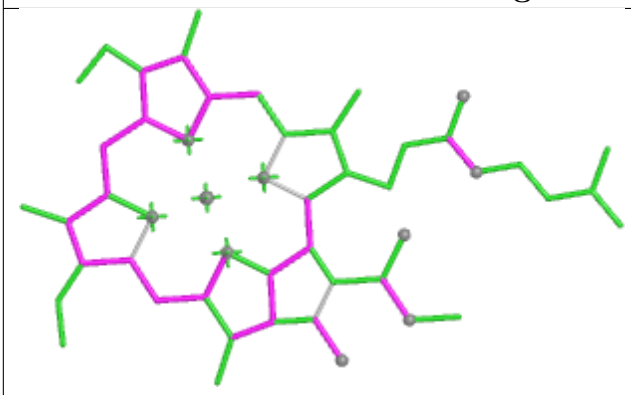


Torsions



Rings

Ligand CLA bA 841



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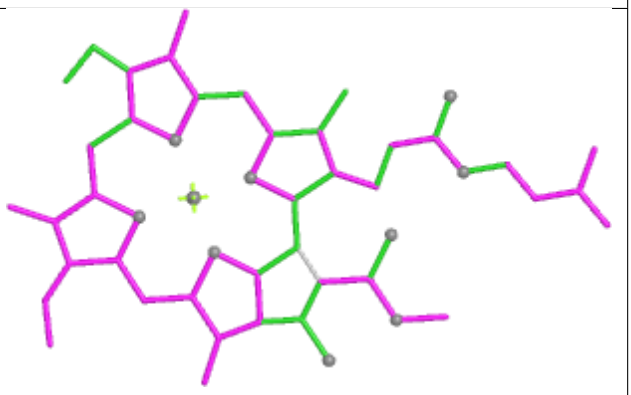
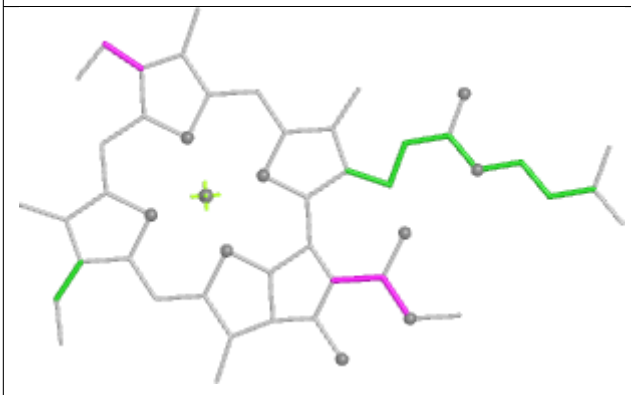
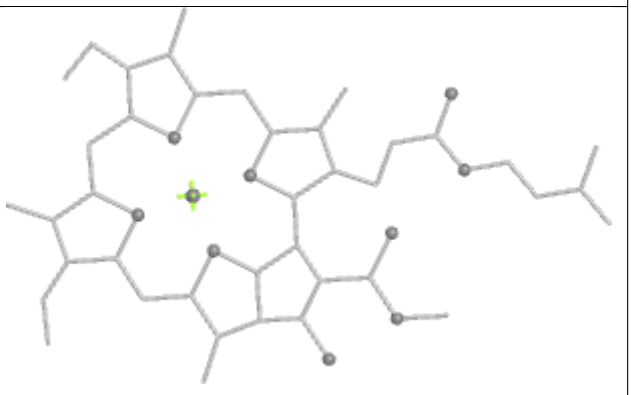


Bond angles

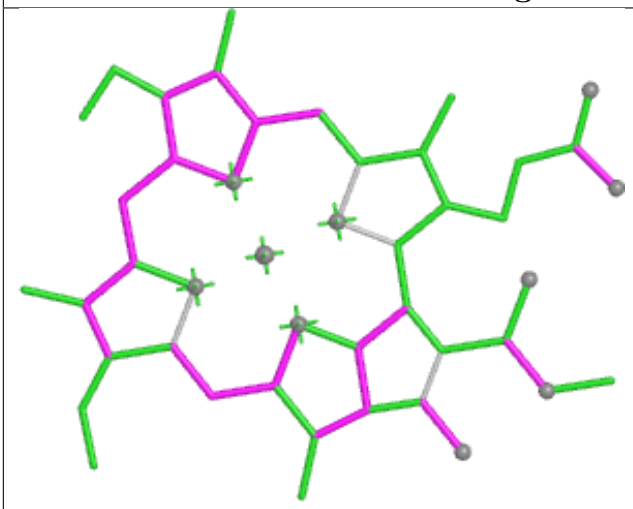


Torsions

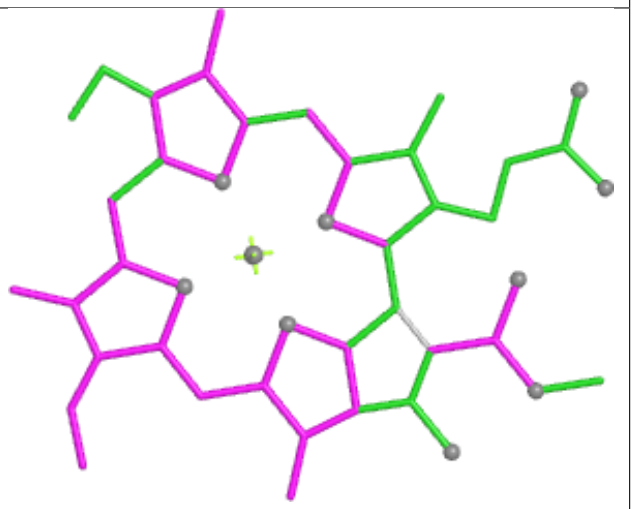


Rings

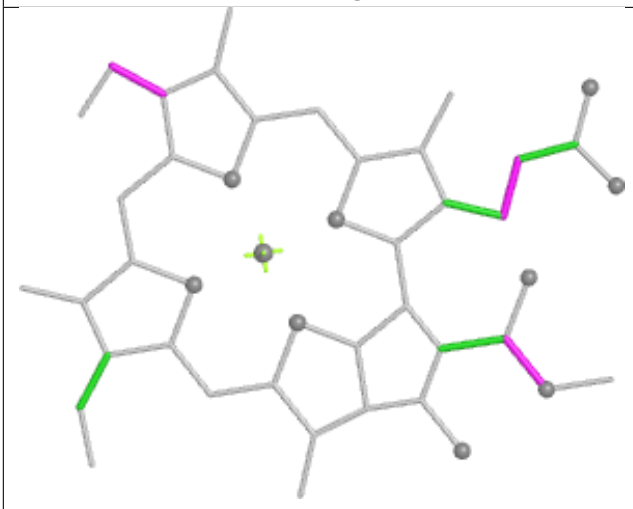
Ligand CLA bB 840



Bond lengths



Bond angles

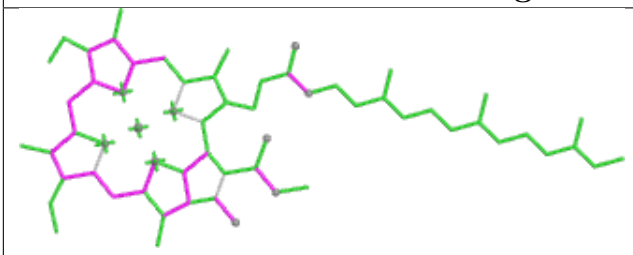


Torsions



Rings

Ligand CLA bB 807



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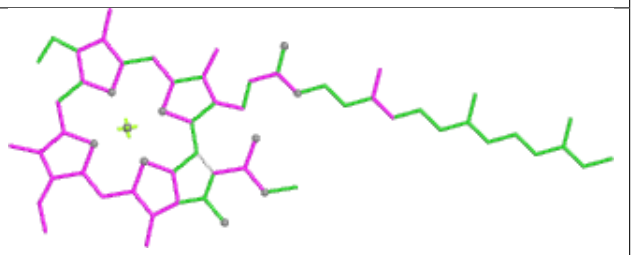
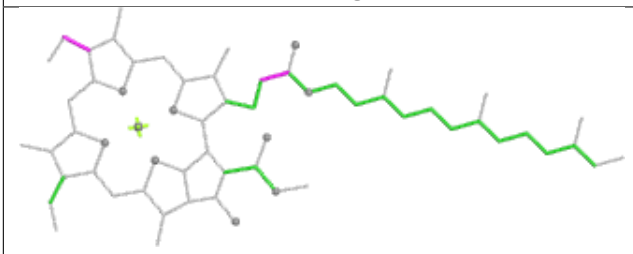


Bond angles



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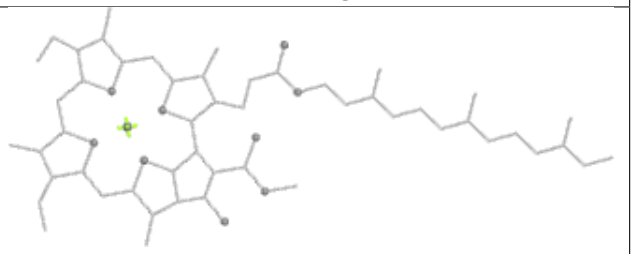
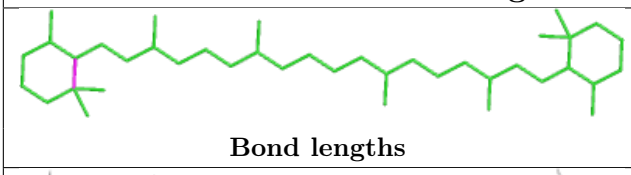


Rings

Ligand BCR bM 101



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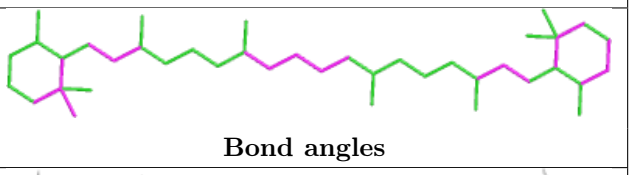
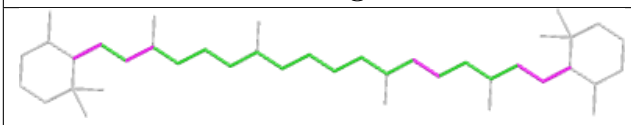


Bond angles



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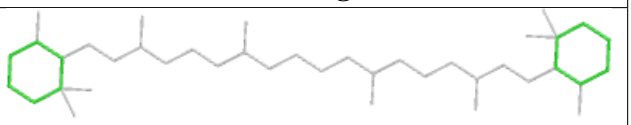
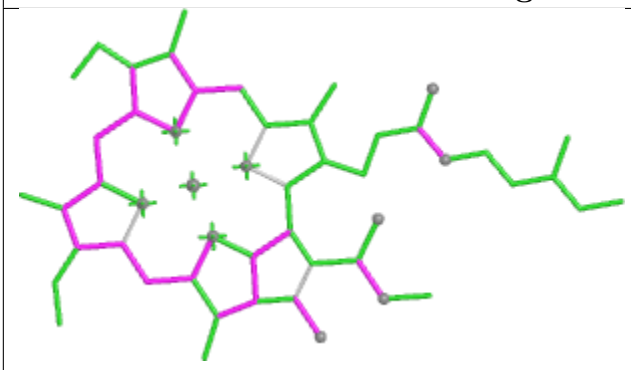


Rings

Ligand CLA aB 836



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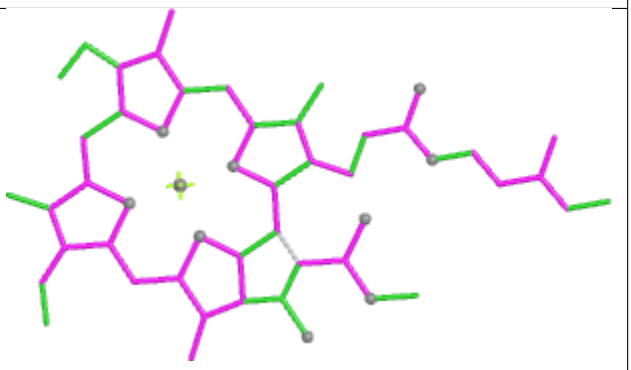
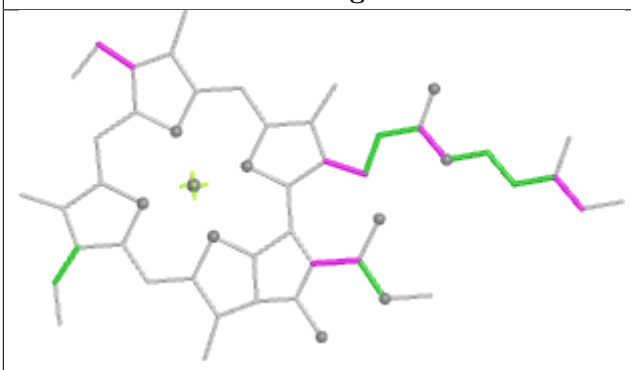


Bond angles



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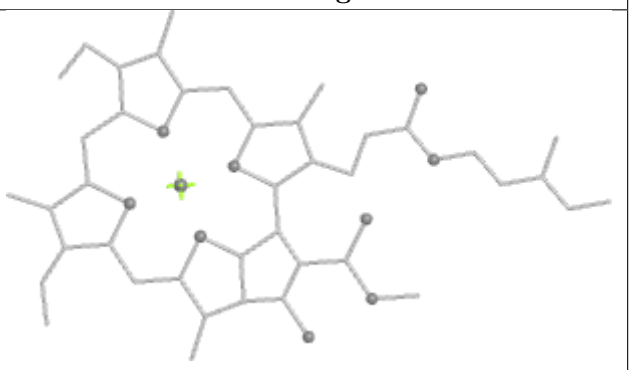
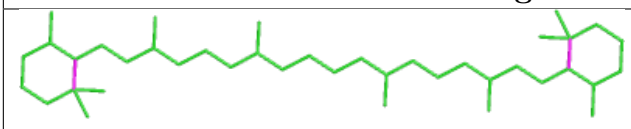


Rings

Ligand BCR cB 844



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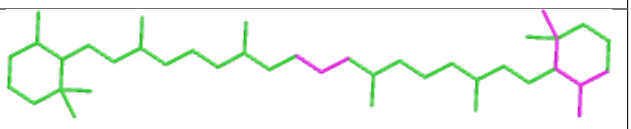
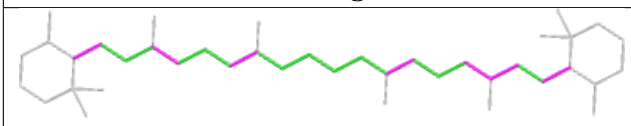


Bond angles



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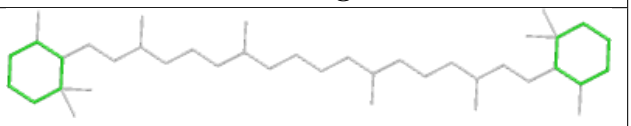
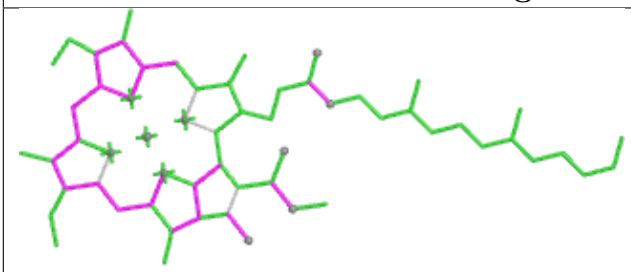
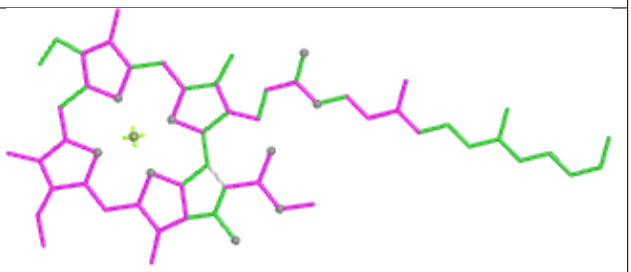
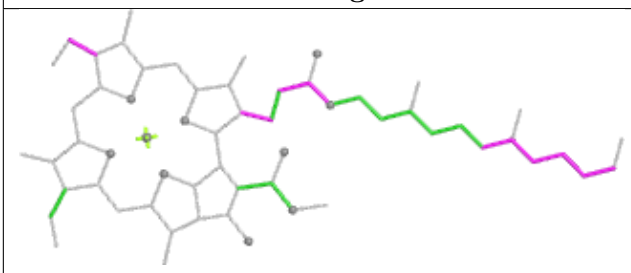
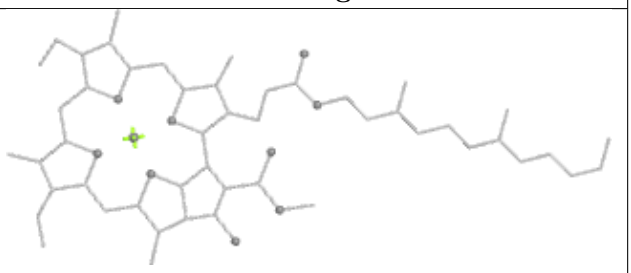
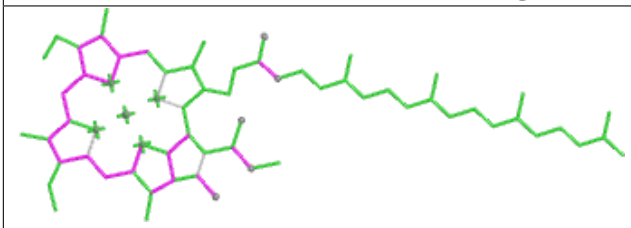
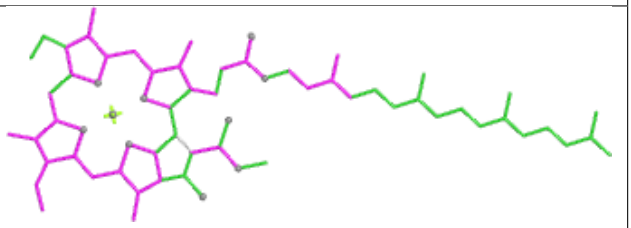
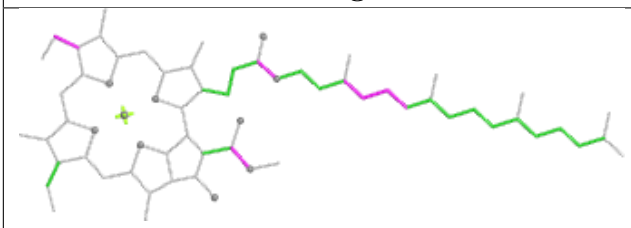
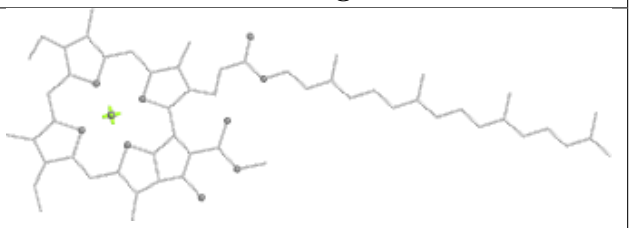
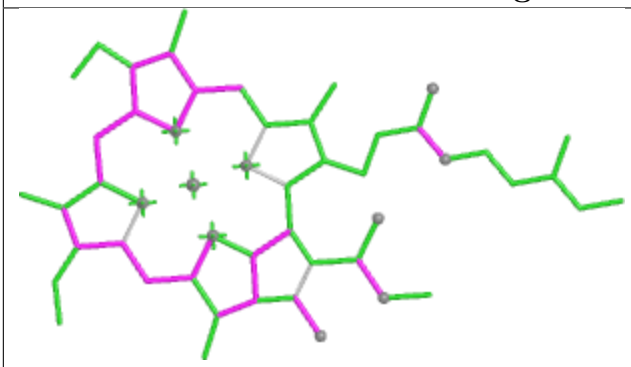


Rings

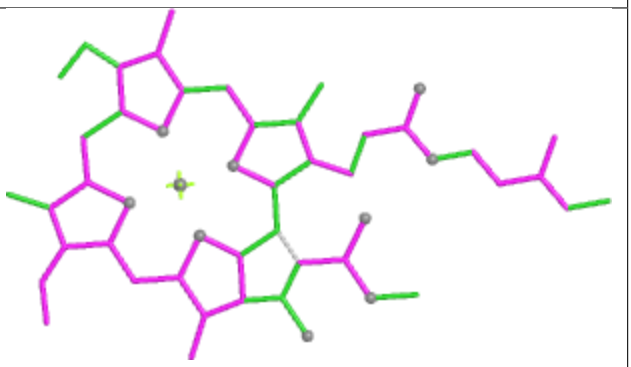
Ligand CLA bB 816	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA bA 834	
	
Bond lengths	Bond angles
	
Torsions	Rings

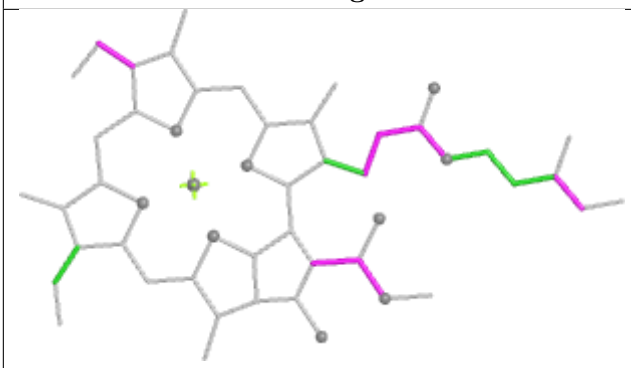
Ligand CLA bA 824



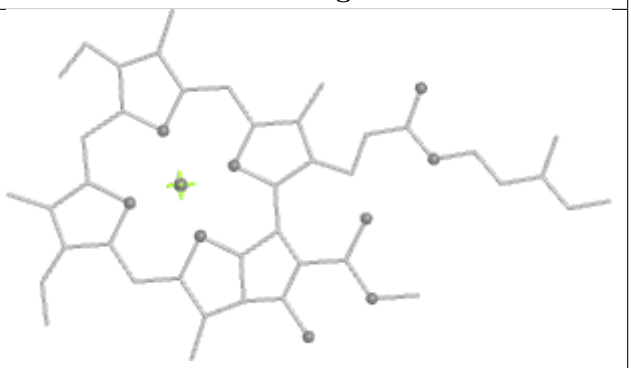
Bond lengths



Bond angles

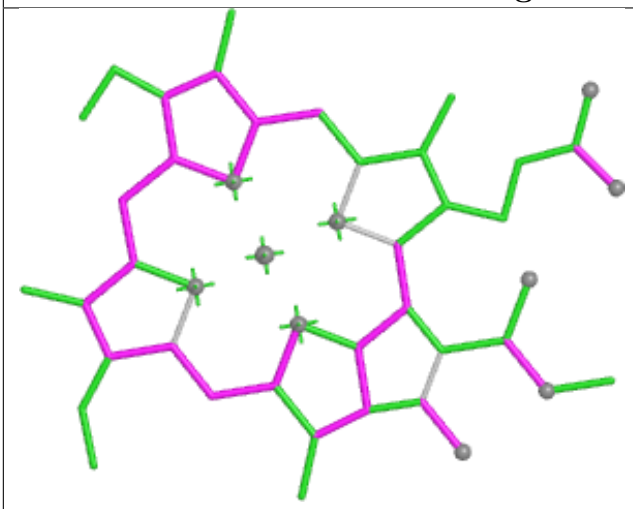


Torsions



Rings

Ligand CLA aA 809



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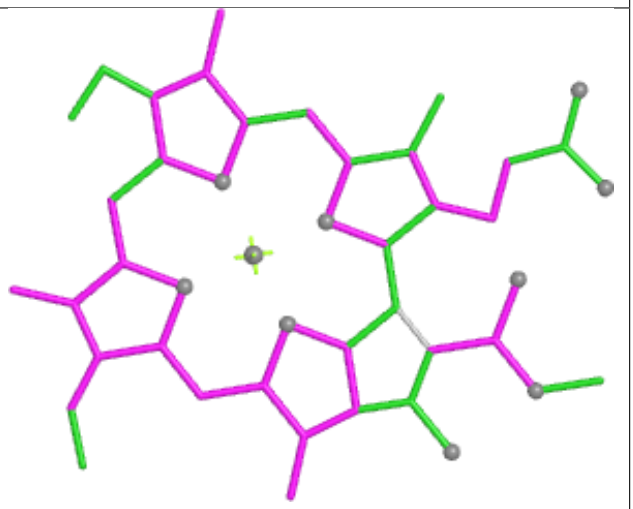
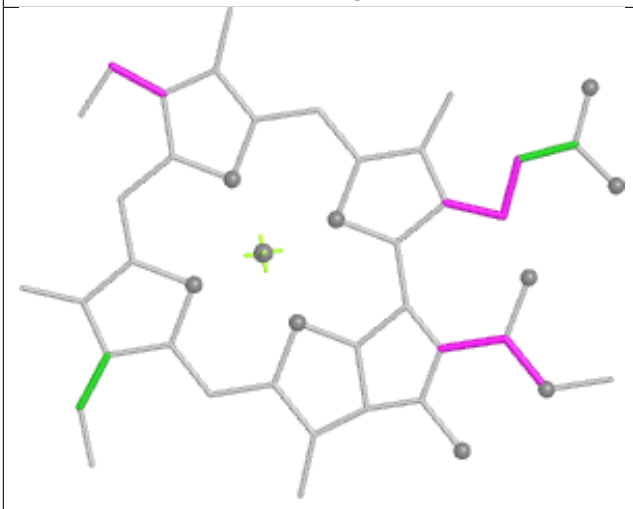


Bond angles

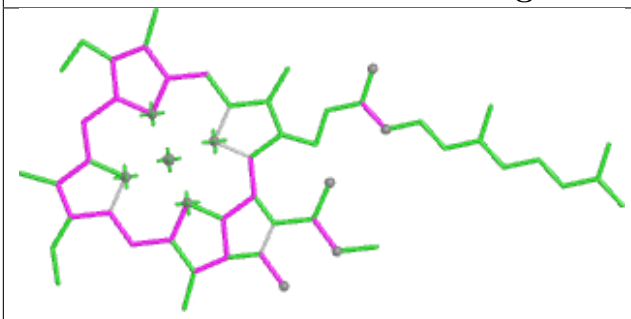


Torsions



Rings

Ligand CLA aB 821



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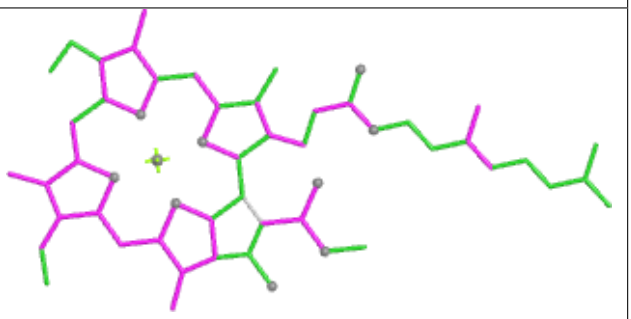
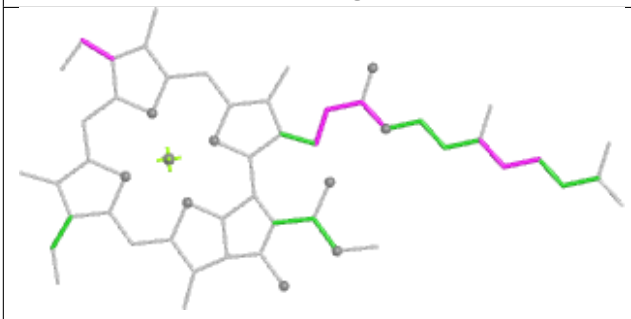


Bond angles



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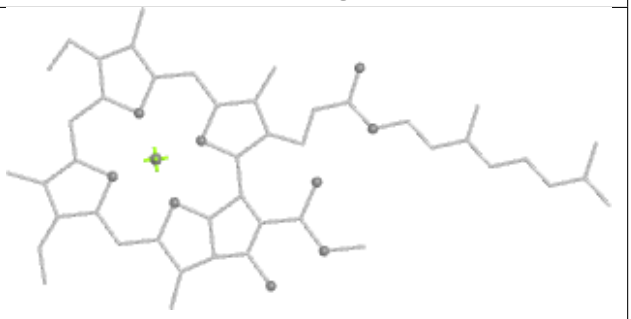
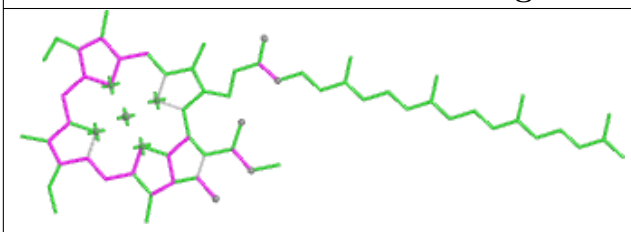


Rings

Ligand CLA aA 834



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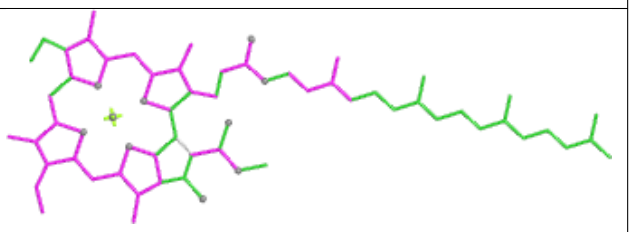
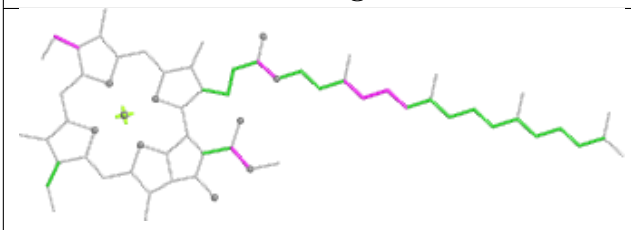


Bond angles



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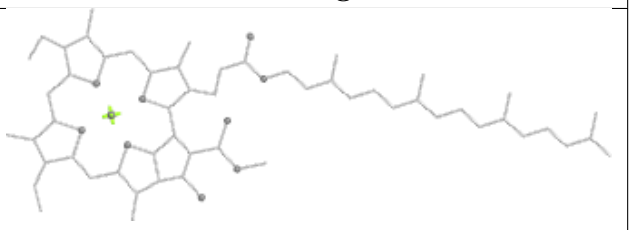
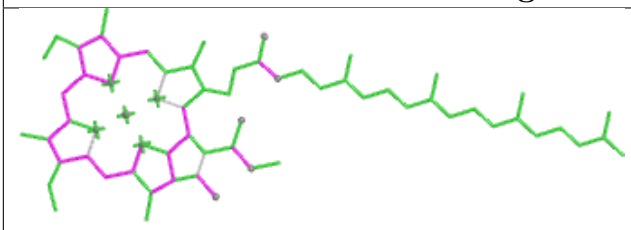
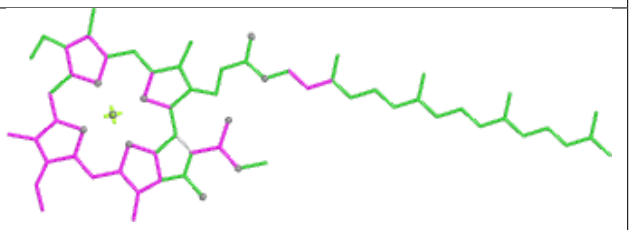
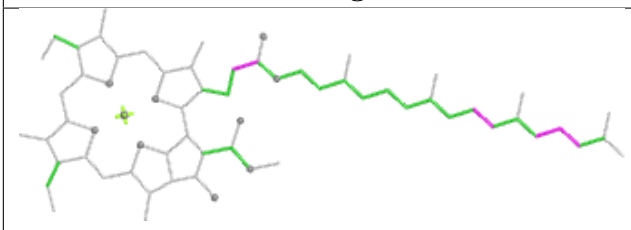
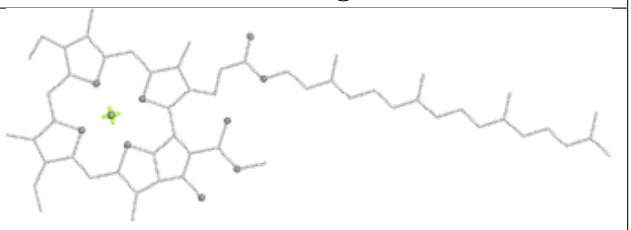
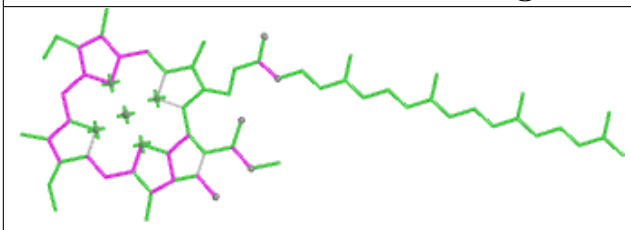
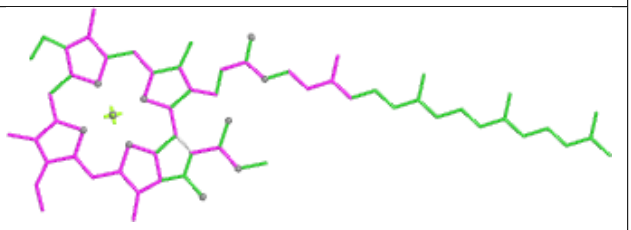
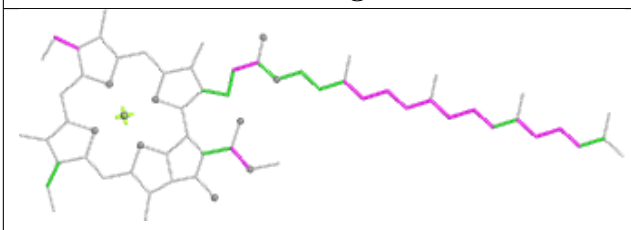
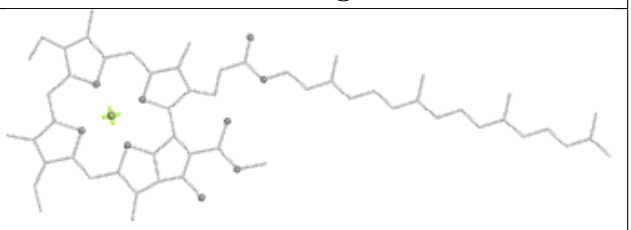
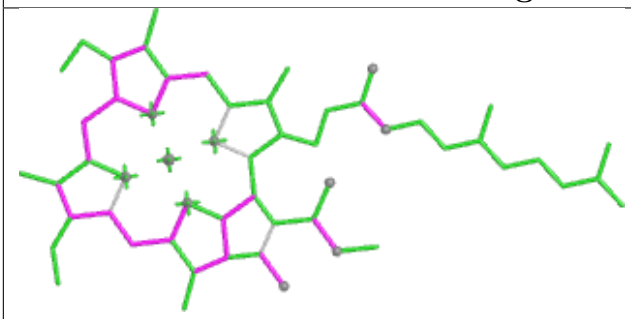


Rings

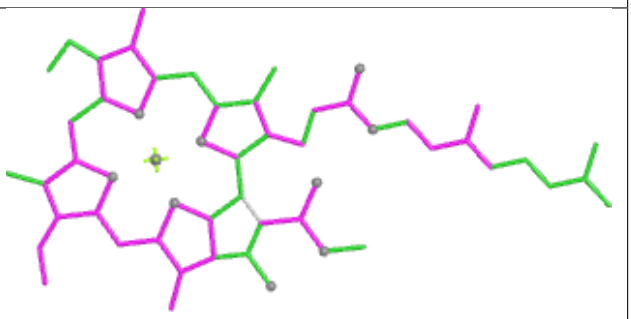
Ligand CLA aL 204	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA cB 806	
	
Bond lengths	Bond angles
	
Torsions	Rings

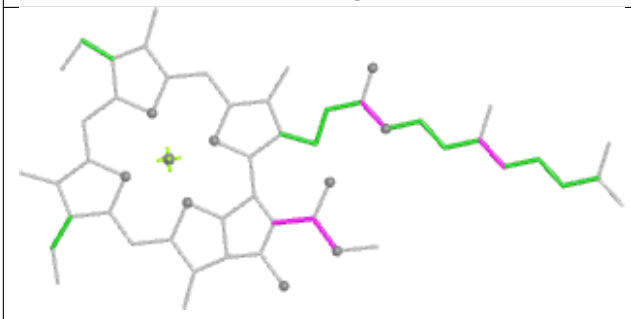
Ligand CLA aB 828



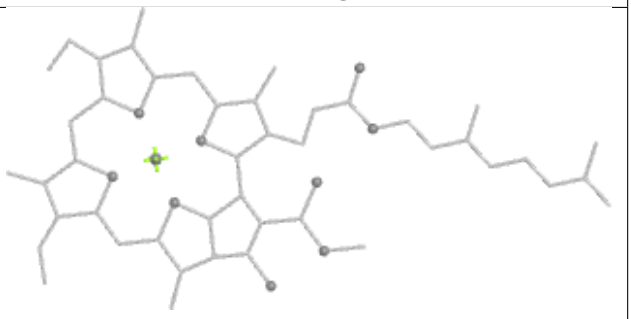
Bond lengths



Bond angles

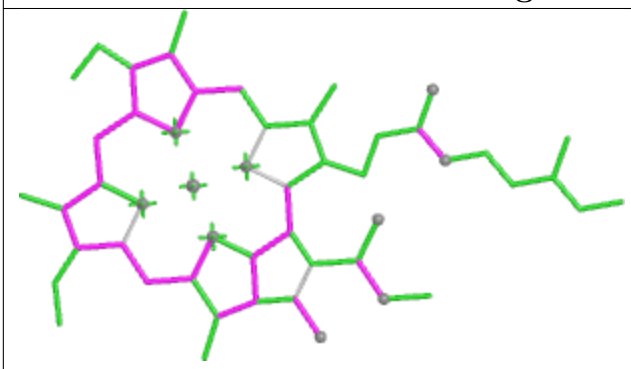


Torsions

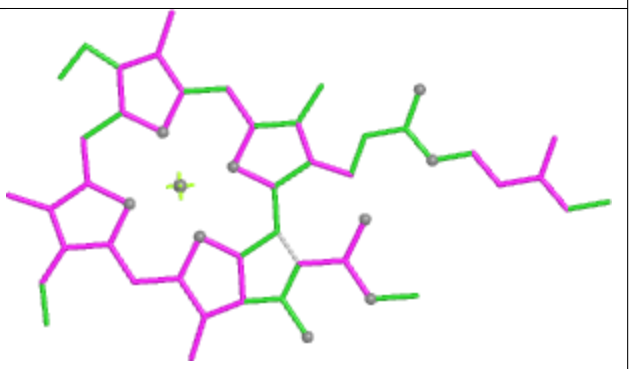


Rings

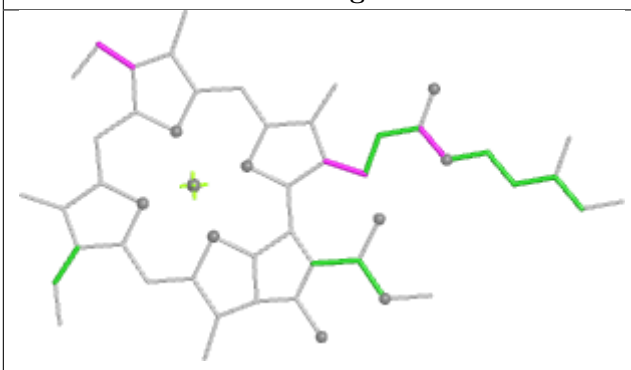
Ligand CLA cA 808



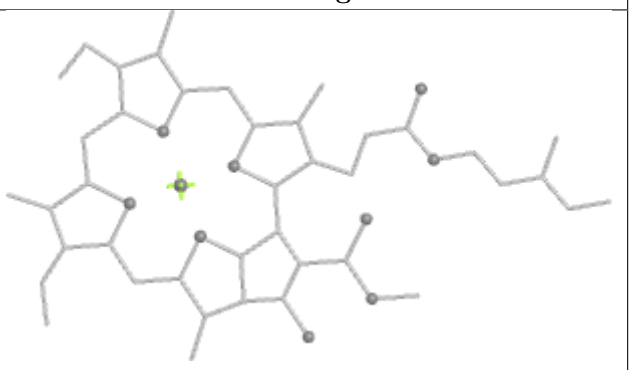
Bond lengths



Bond angles

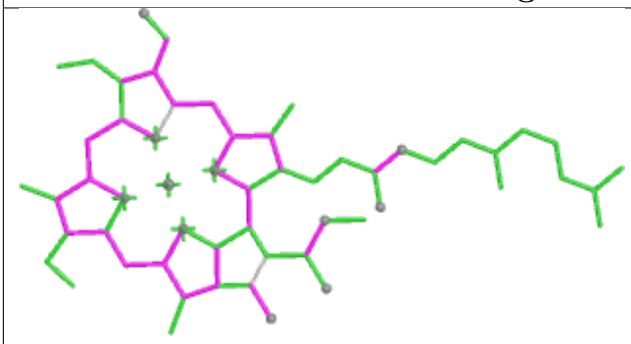


Torsions

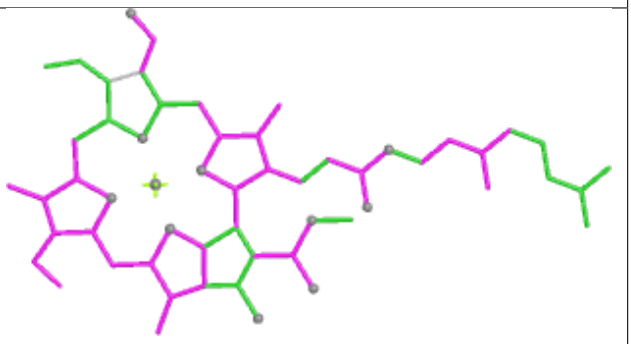


Rings

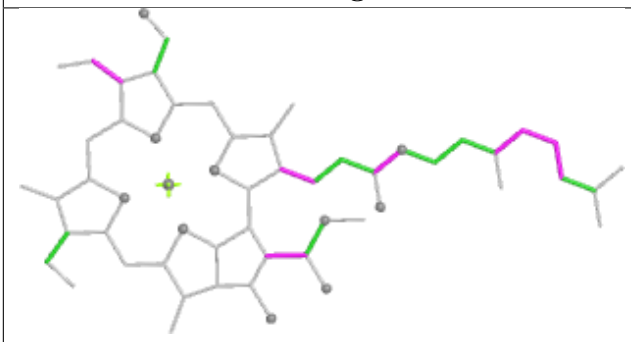
Ligand F6C bA 827



Bond lengths



Bond angles



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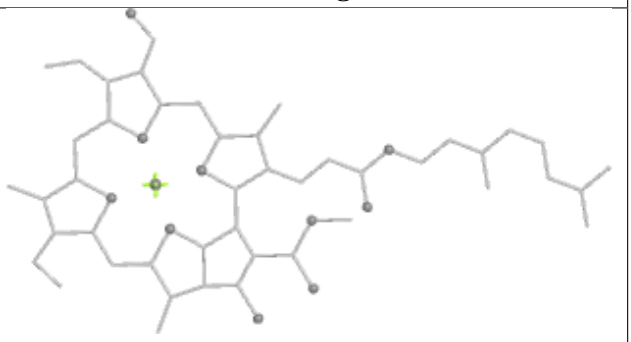
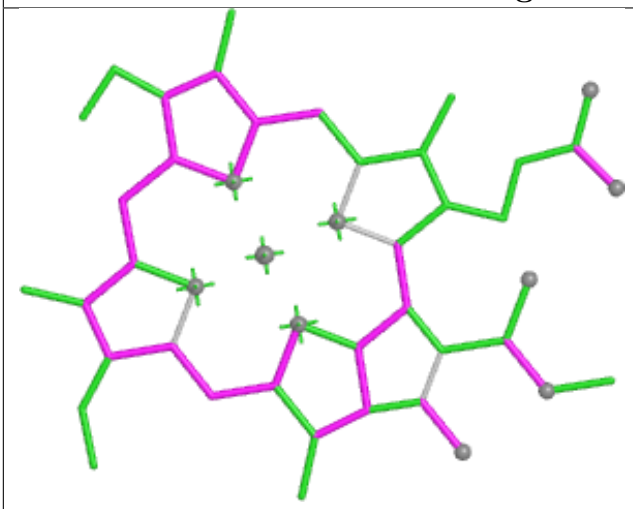


Rings

Ligand CLA cA 837



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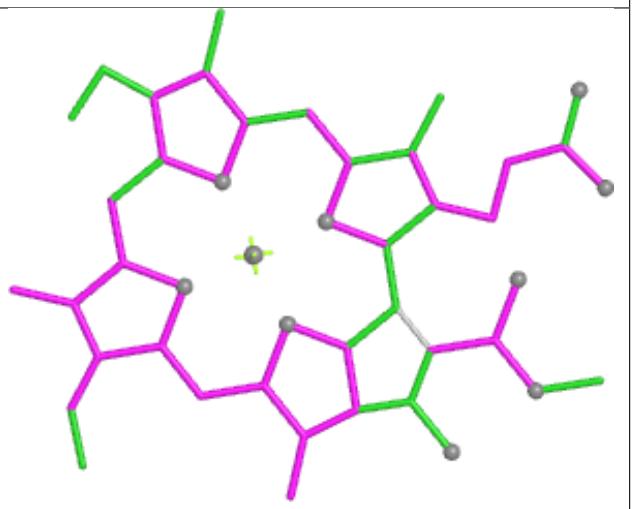
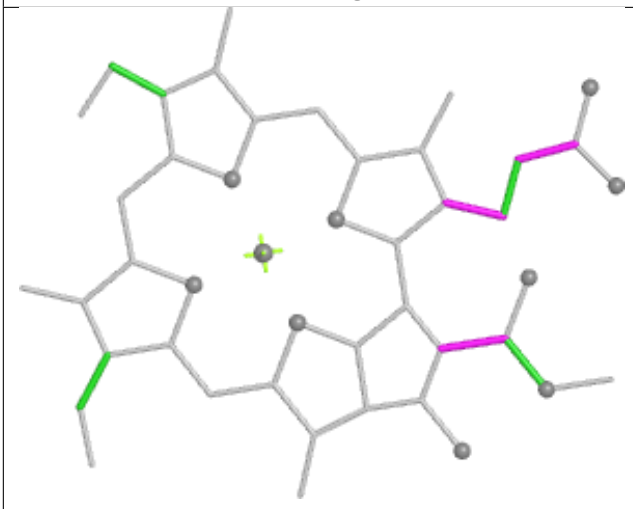


Bond angles

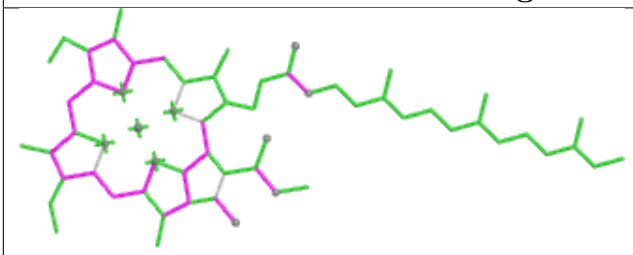


Torsions



Rings

Ligand CLA cB 826



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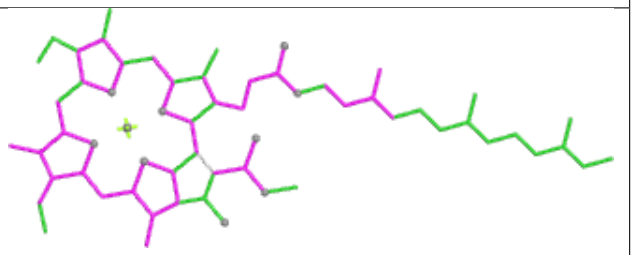
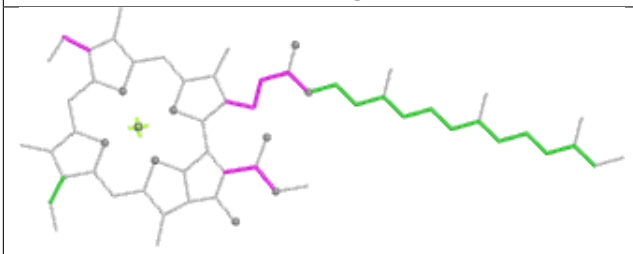


Bond angles



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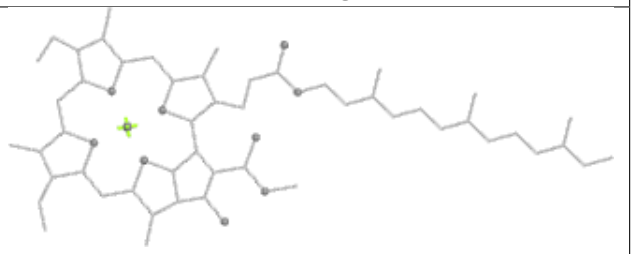
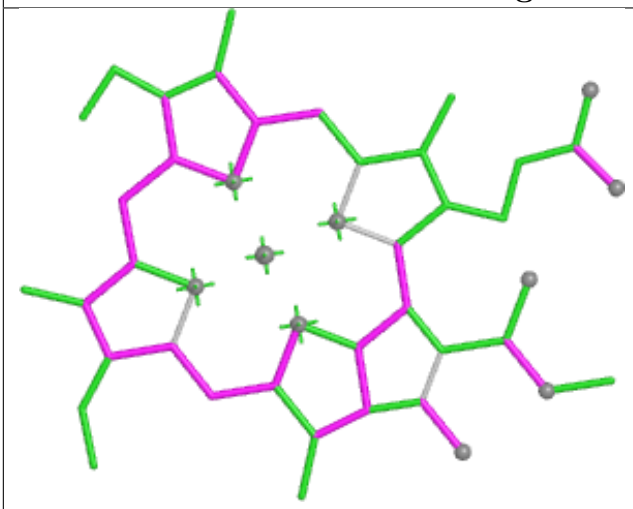


Rings

Ligand CLA aB 834



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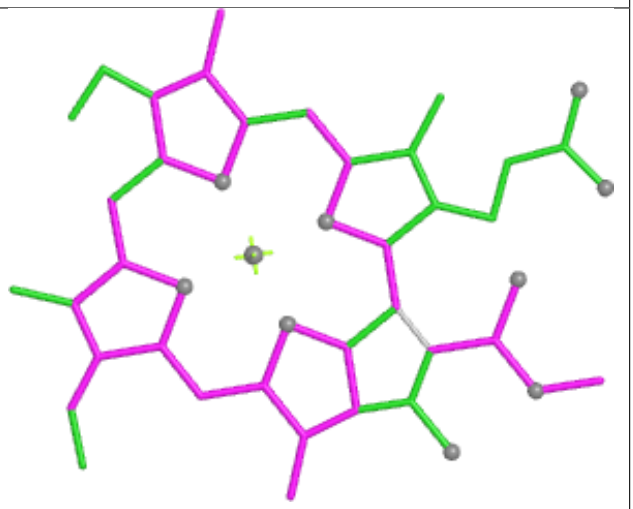
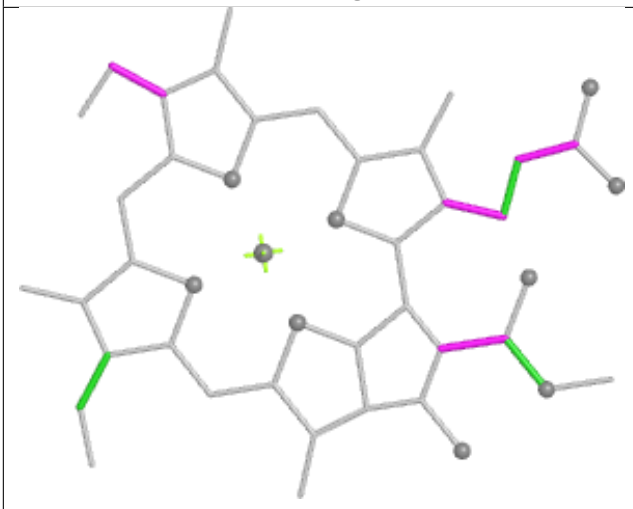


Bond angles

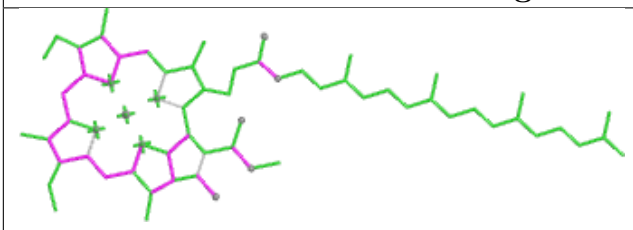


Torsions



Rings

Ligand CLA bB 818



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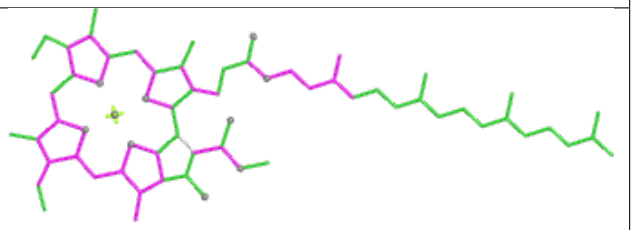
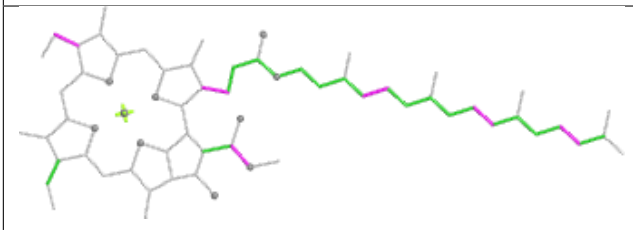


Bond angles



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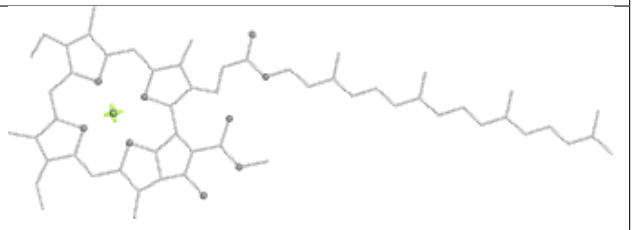
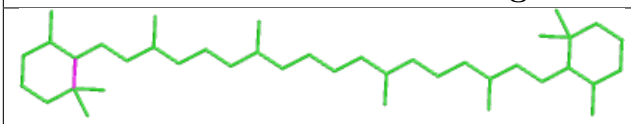


Rings

Ligand BCR aM 101



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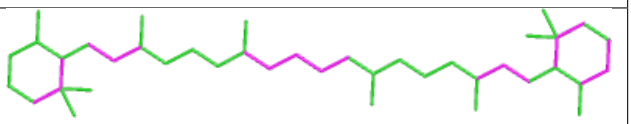

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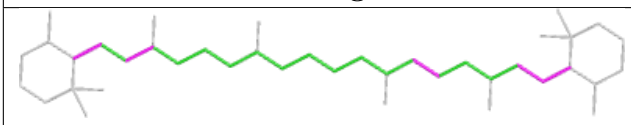

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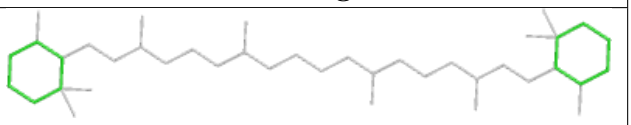
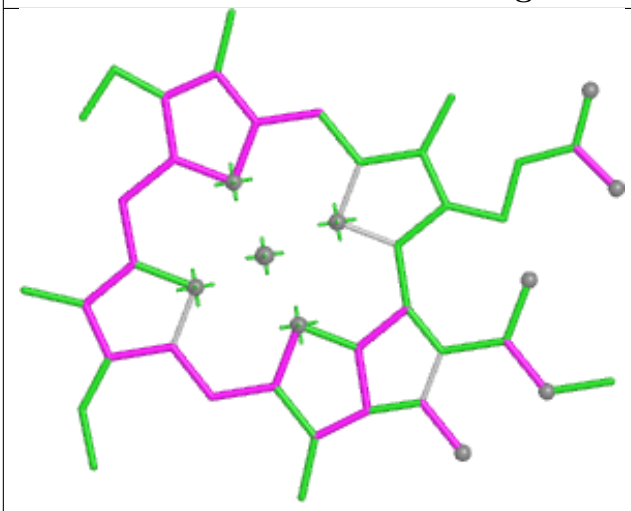


Rings

Ligand CLA aA 804



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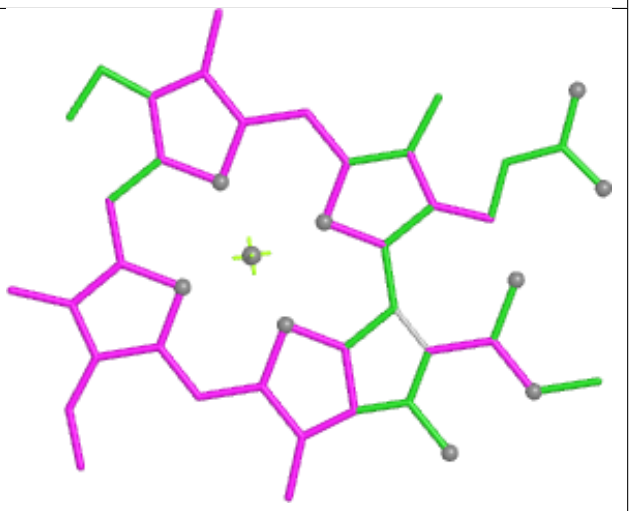

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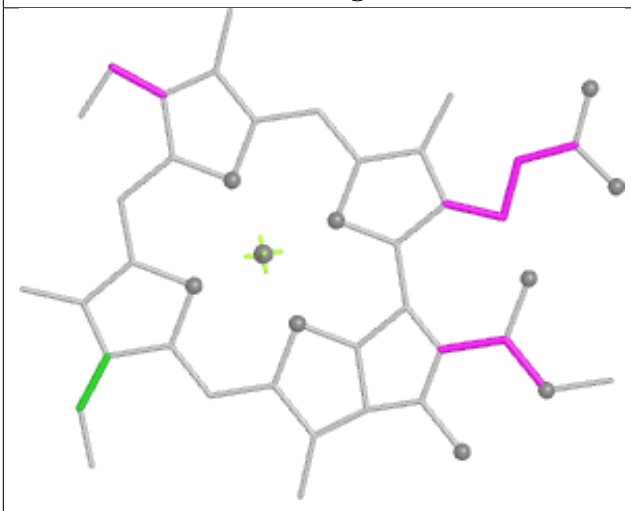

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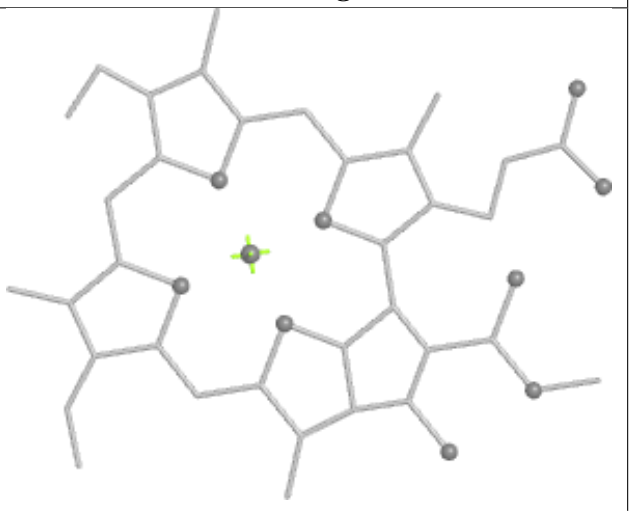
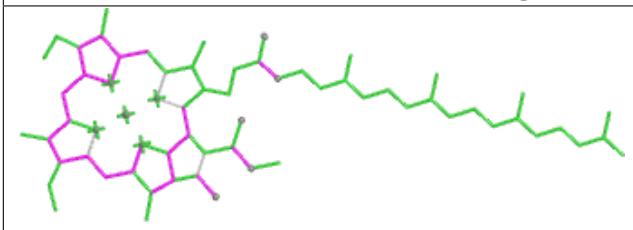


Rings

Ligand CLA aA 812



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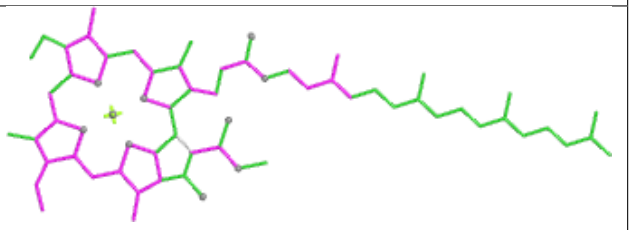

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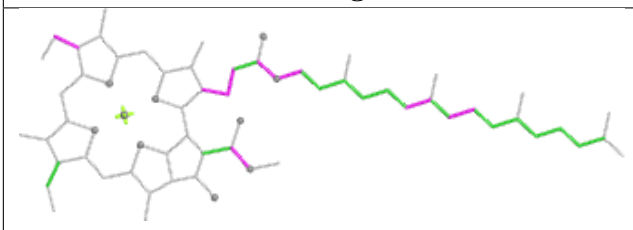

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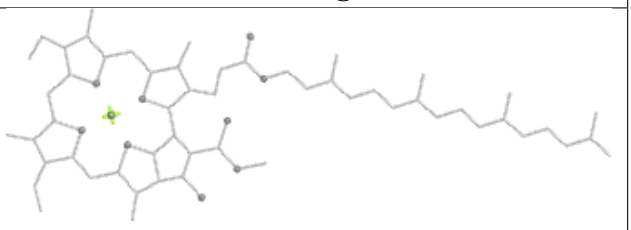
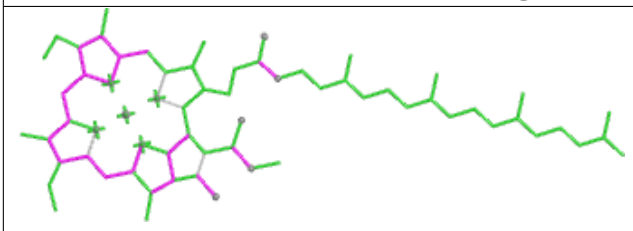


Rings

Ligand CLA aA 814



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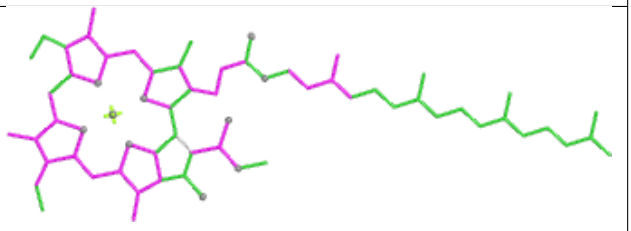
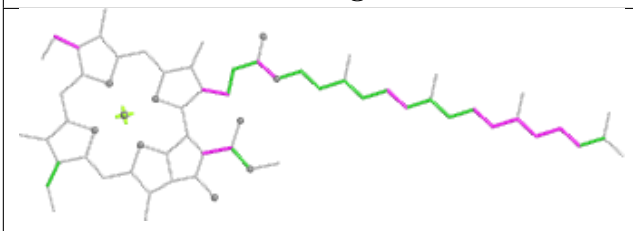


Bond angles



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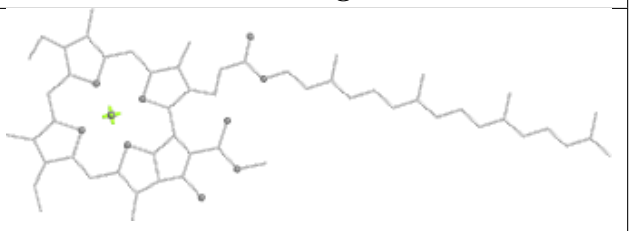
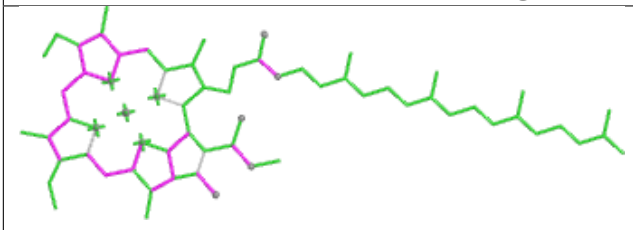


Rings

Ligand CLA bB 839



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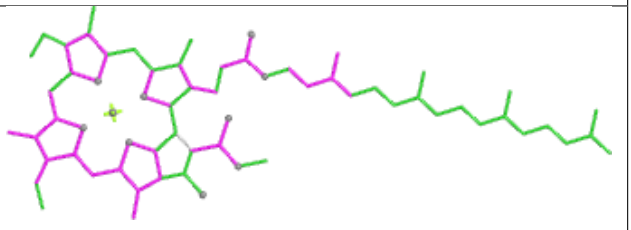
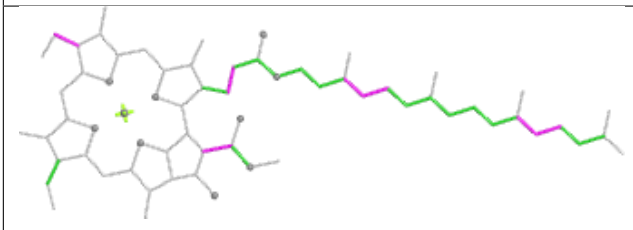


Bond angles



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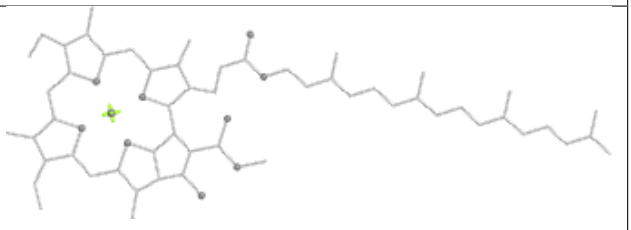
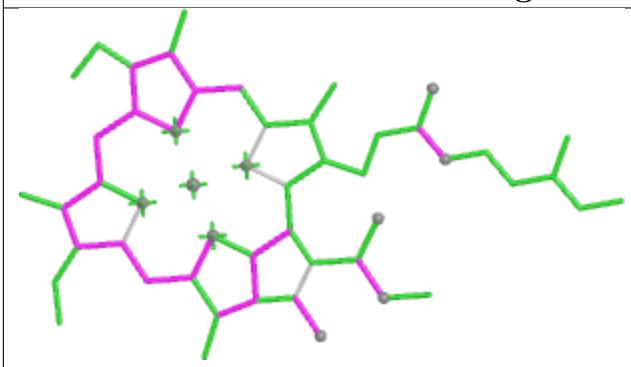
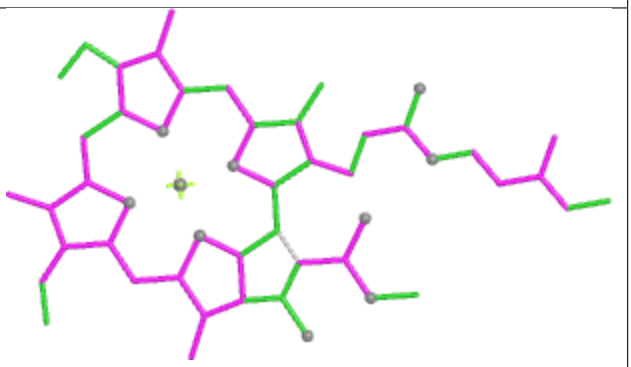
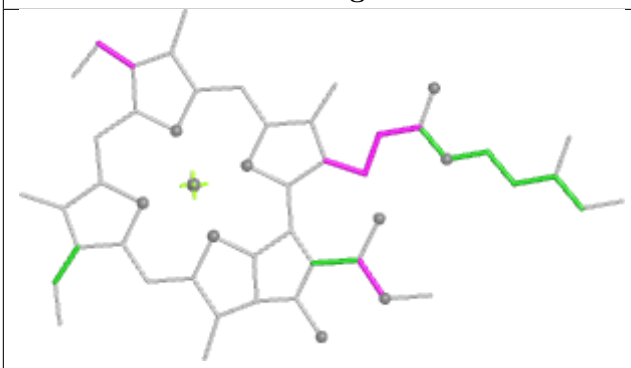
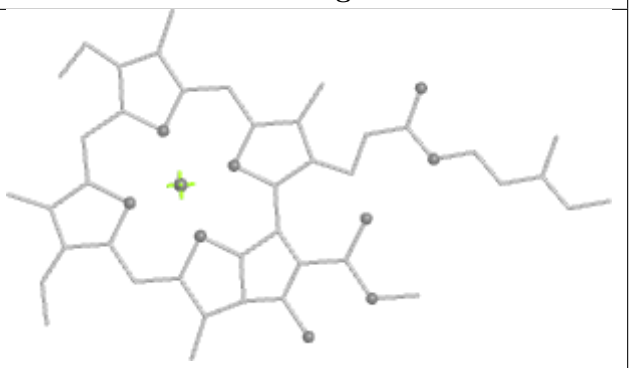
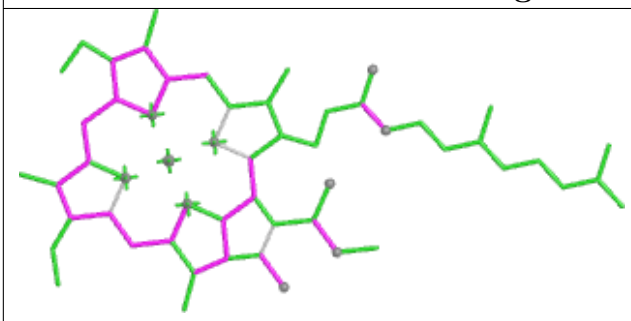
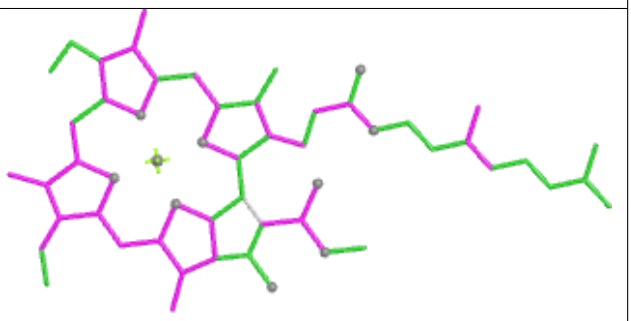
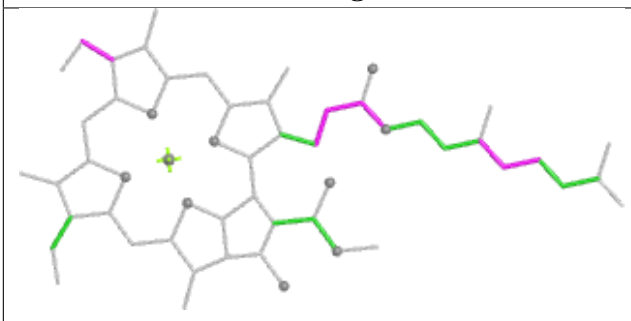
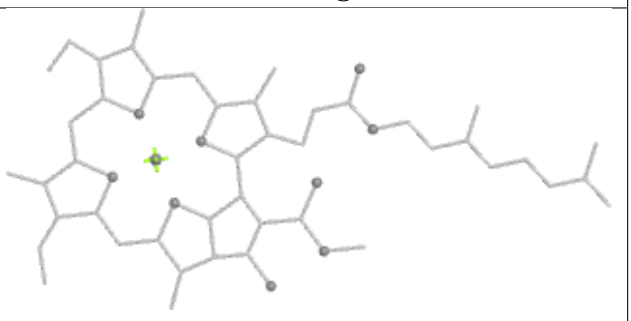
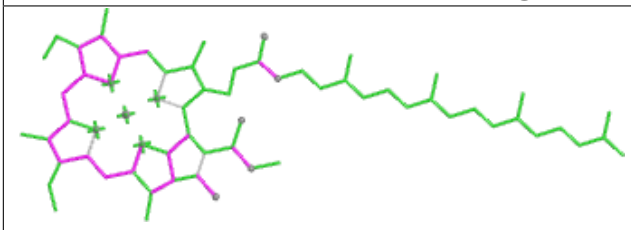


Rings

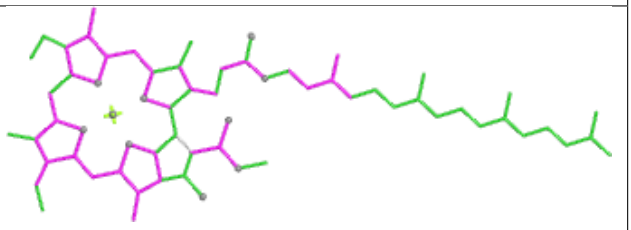
Ligand CLA aA 843	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA bB 821	
 Bond lengths	 Bond angles
 Torsions	 Rings

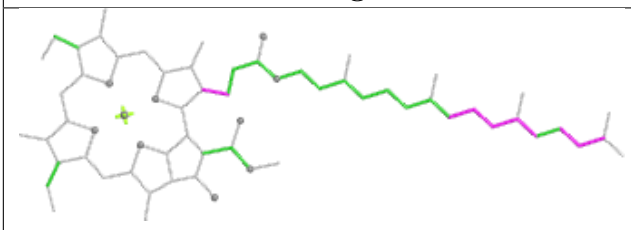
Ligand CLA aB 825



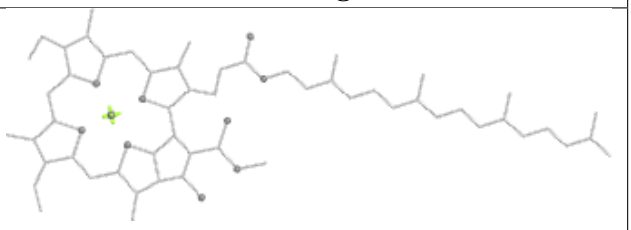
Bond lengths



Bond angles



Torsions

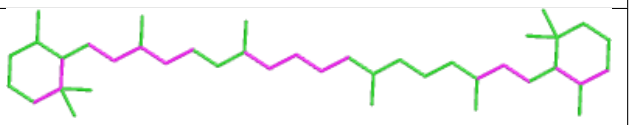


Rings

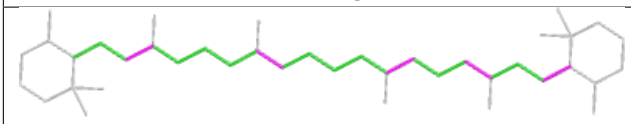
Ligand BCR bL 208



Bond lengths



Bond angles



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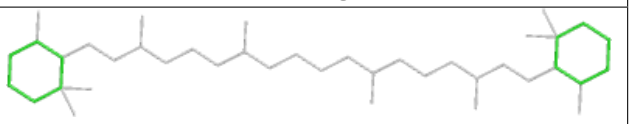
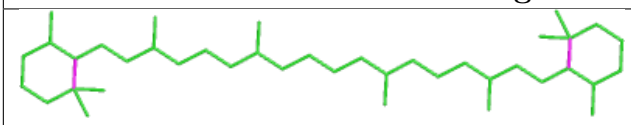
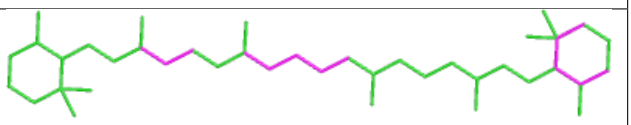


Rings

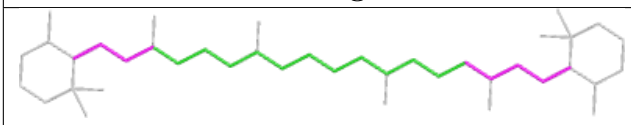
Ligand BCR cA 849



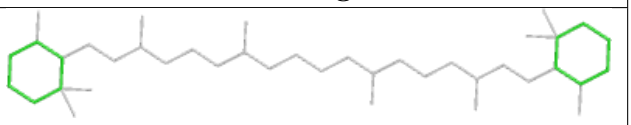
Bond lengths



Bond angles

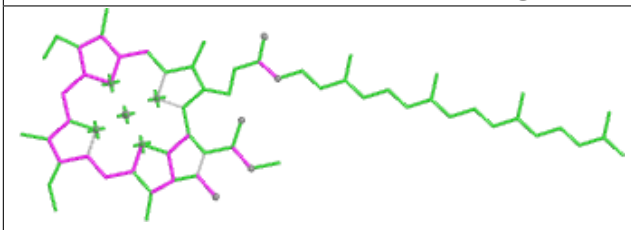


Torsions

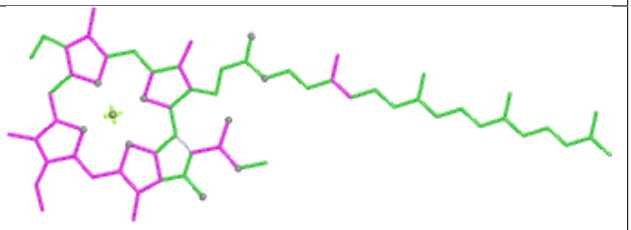


Rings

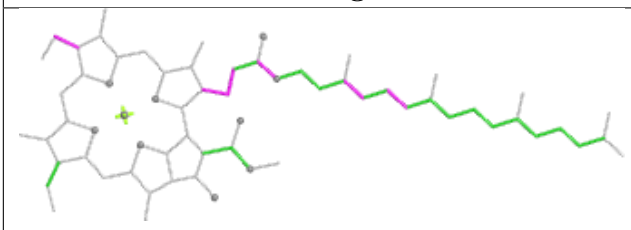
Ligand CLA bB 827



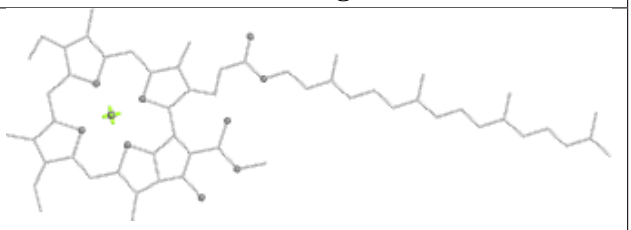
Bond lengths



Bond angles

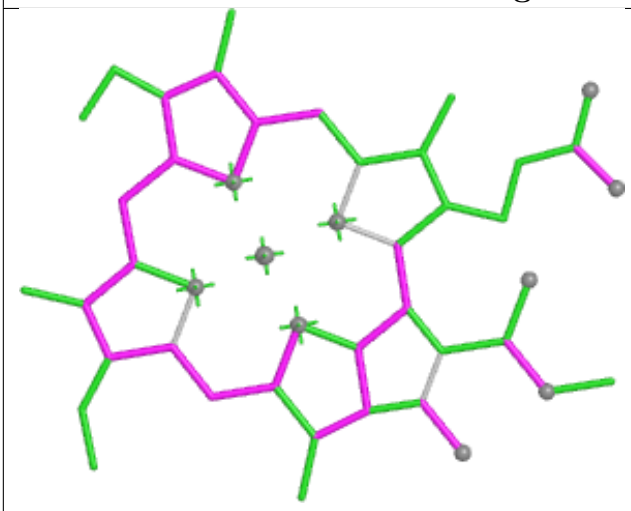


Torsions



Rings

Ligand CLA bA 842



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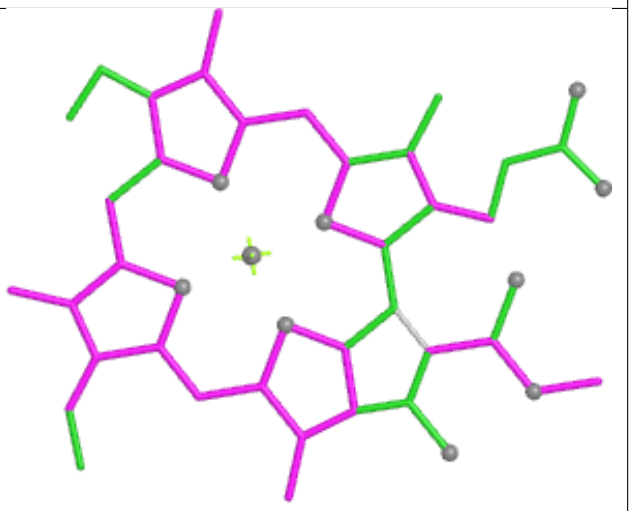
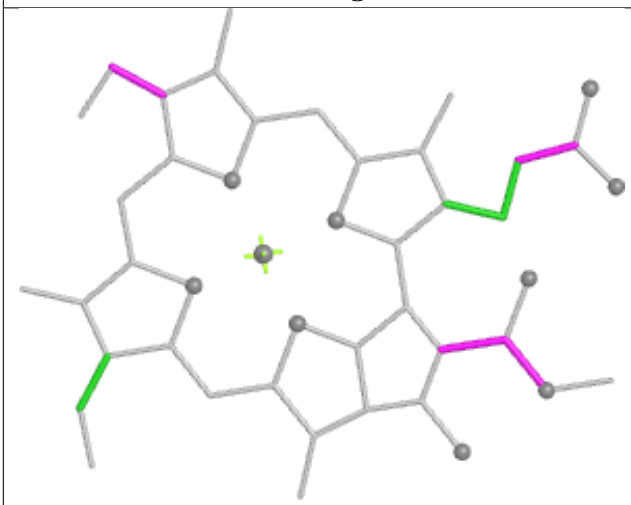


Bond angles



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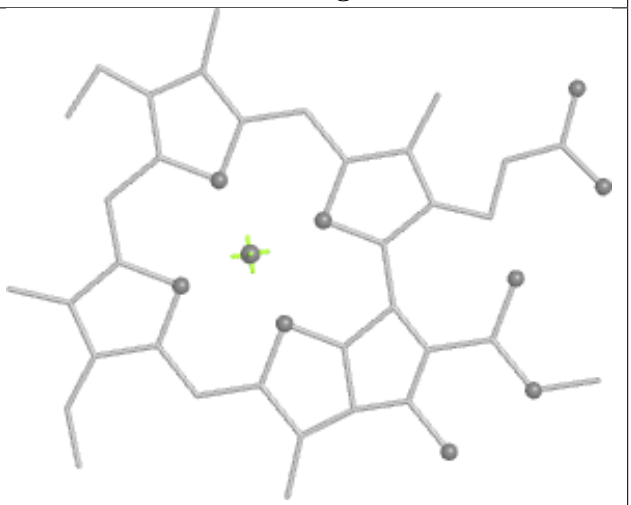
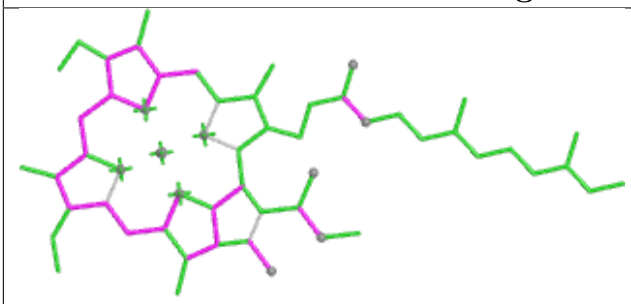
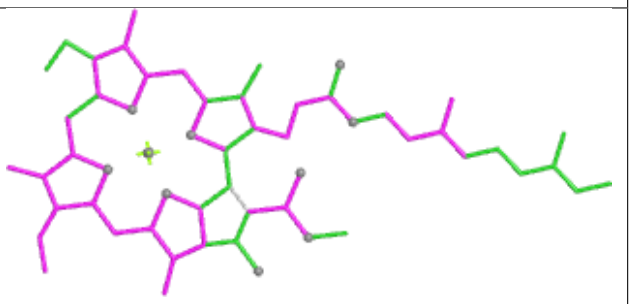
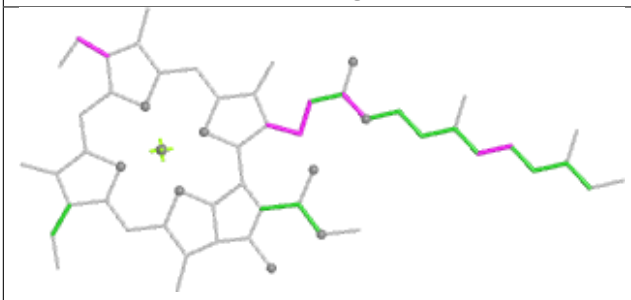
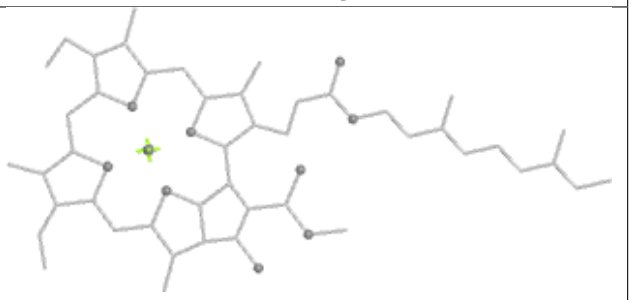
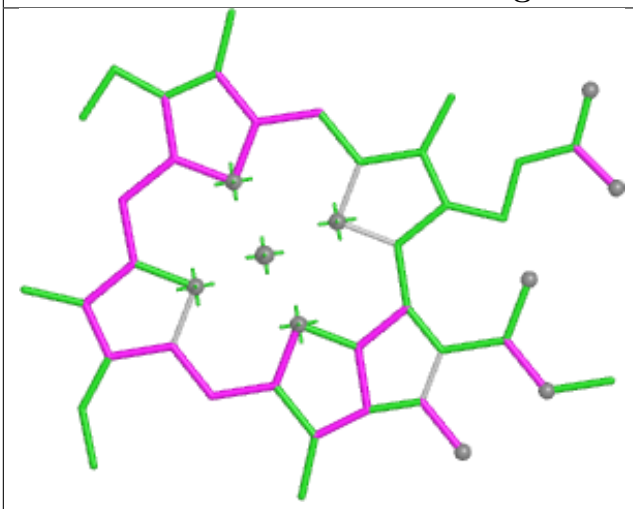


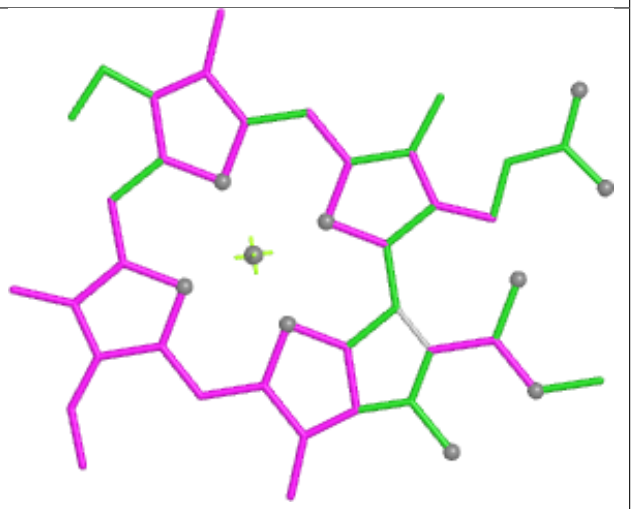
Rings

Ligand CLA aB 831	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

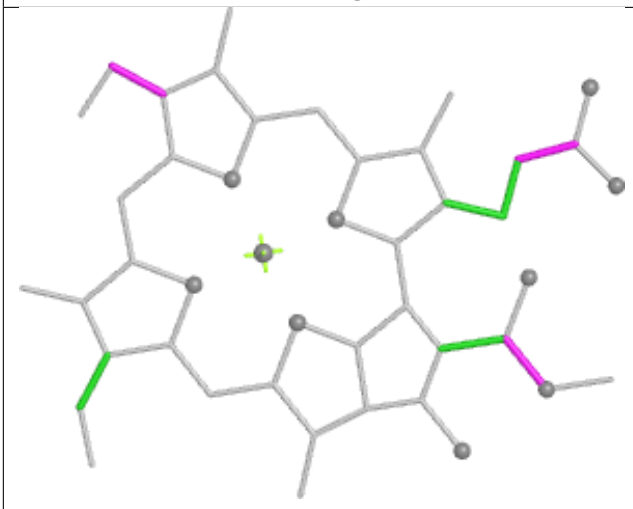
Ligand CLA bA 836



Bond lengths



Bond angles

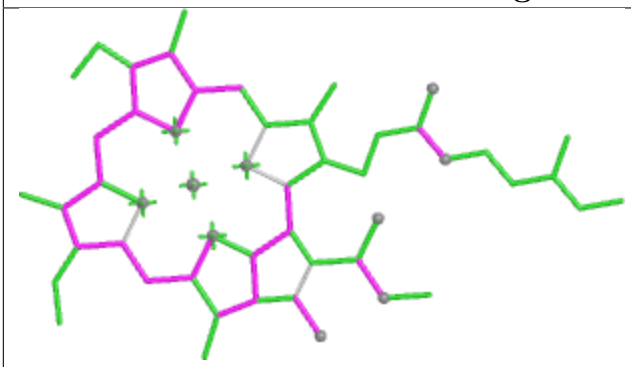


Torsions

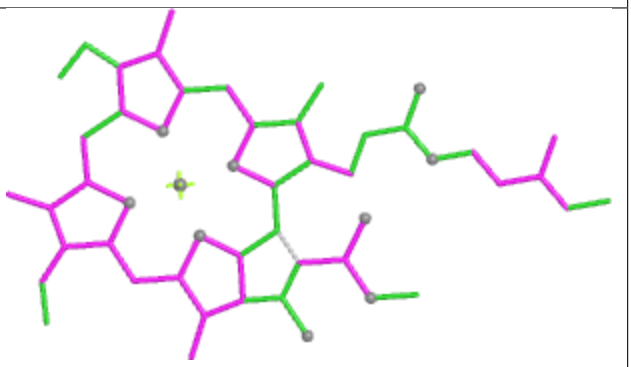


Rings

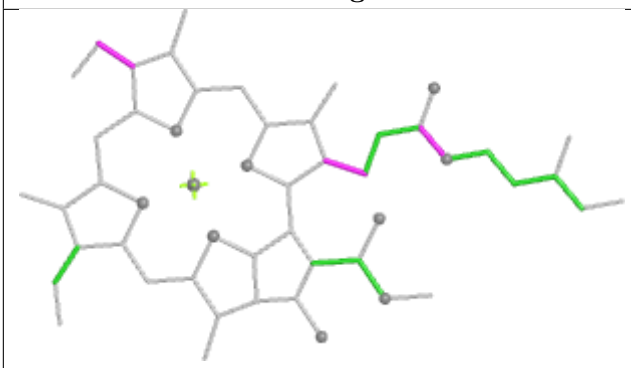
Ligand CLA bA 808



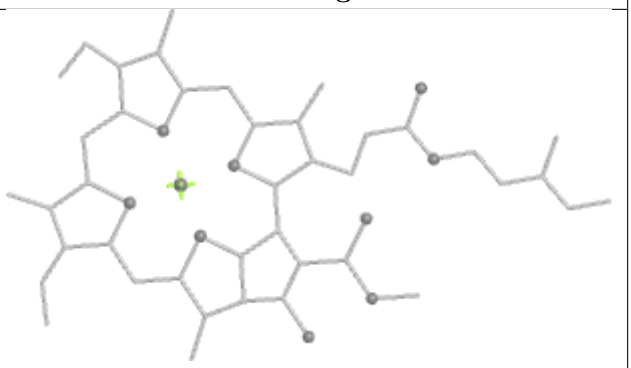
Bond lengths



Bond angles

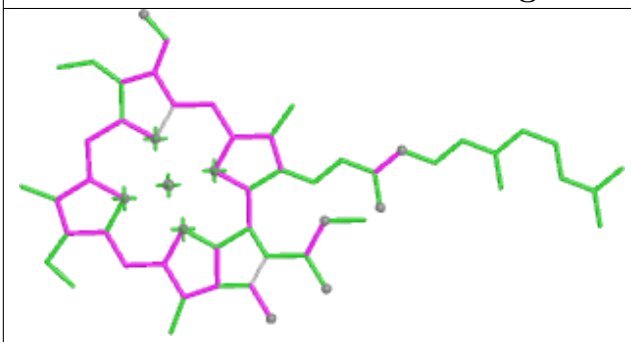


Torsions



Rings

Ligand F6C aA 827



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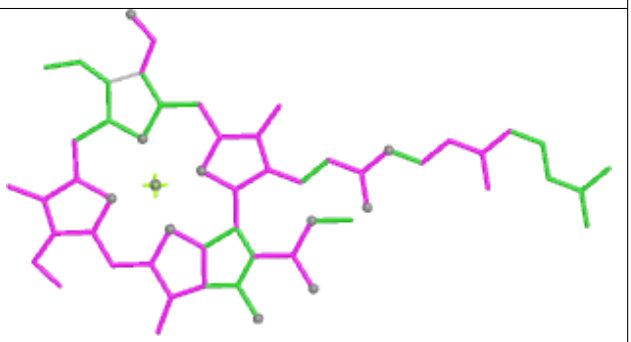
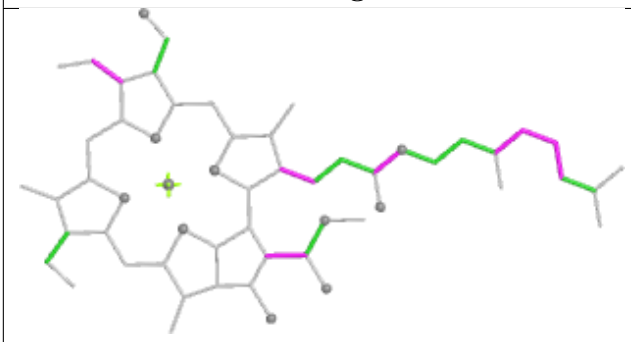


Bond angles



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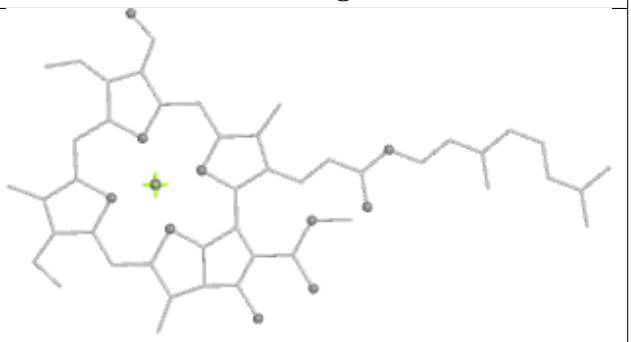
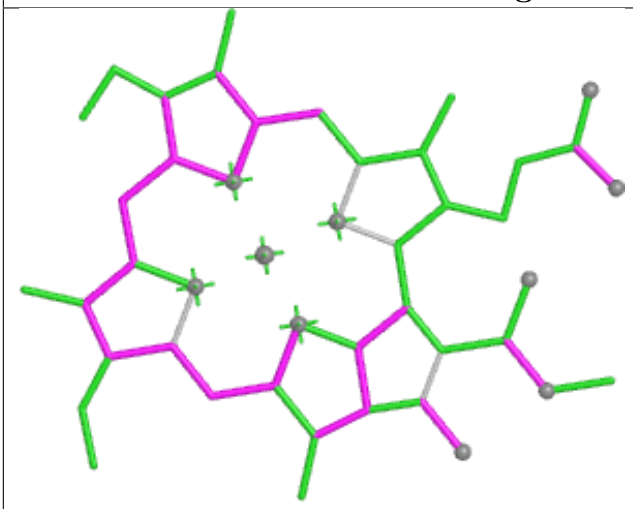


Rings

Ligand CLA aA 836



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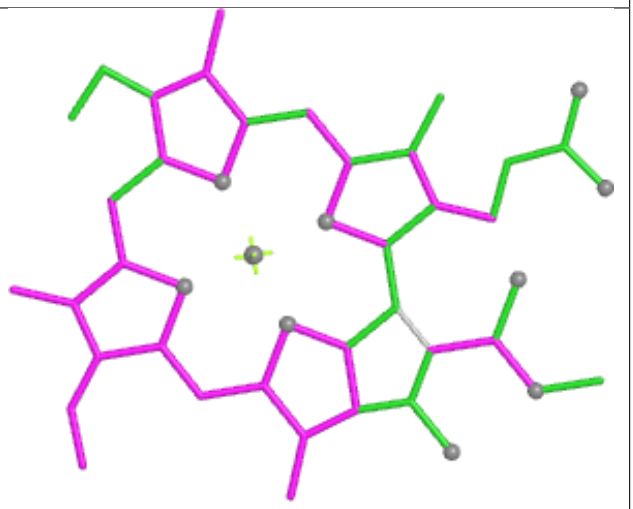
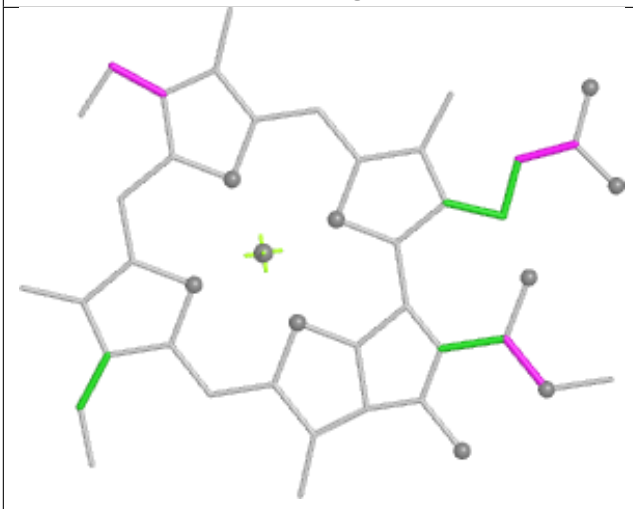


Bond angles

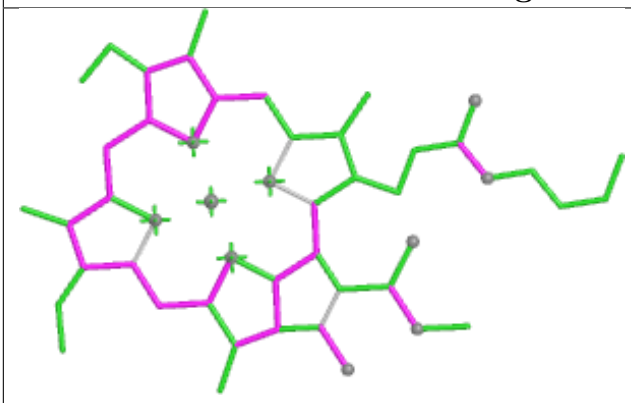


Torsions

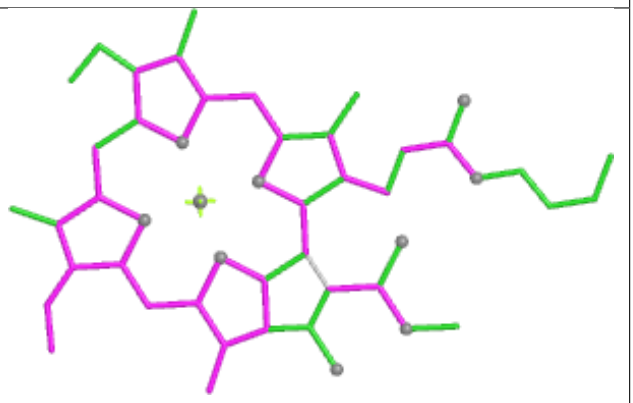


Rings

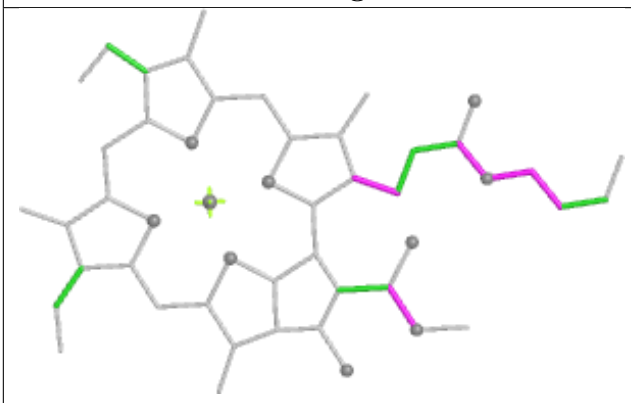
Ligand CLA aA 817



Bond lengths



Bond angles



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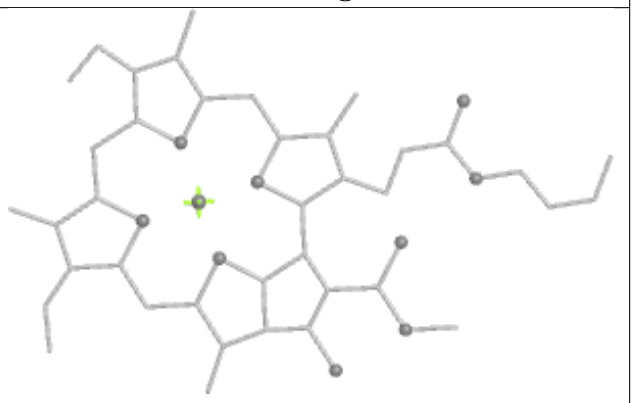
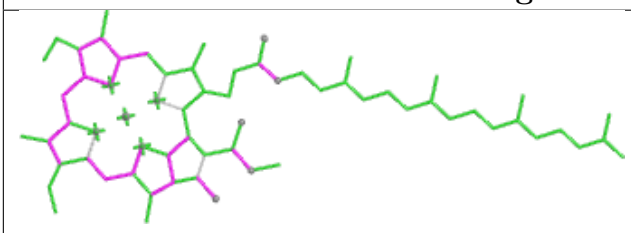


Rings

Ligand CLA aB 839



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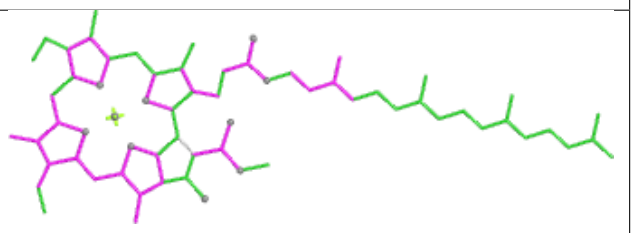
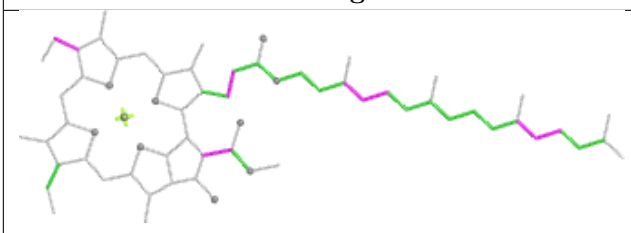
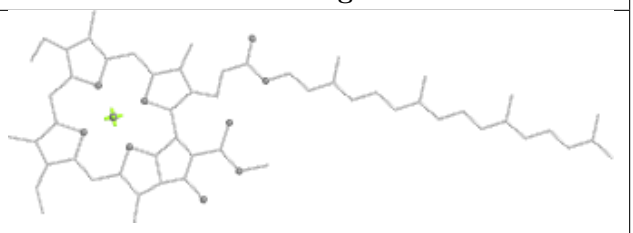


Bond angles

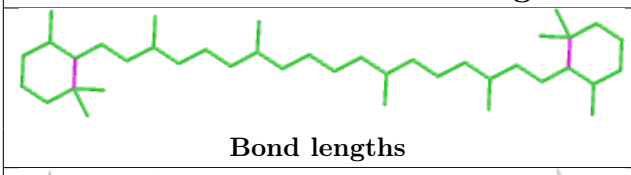


Torsions



Rings

Ligand BCR cK 102



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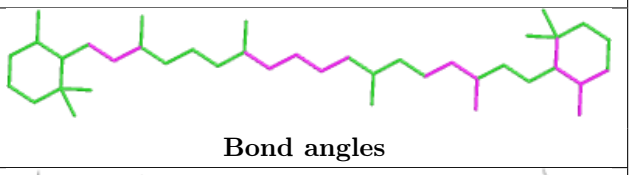
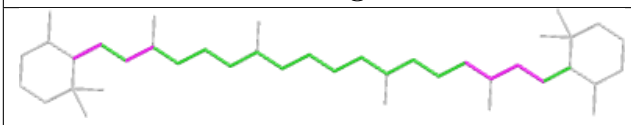


Bond angles



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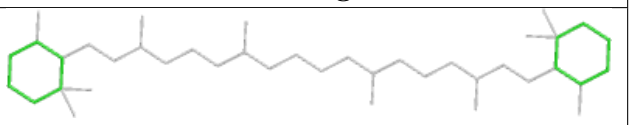
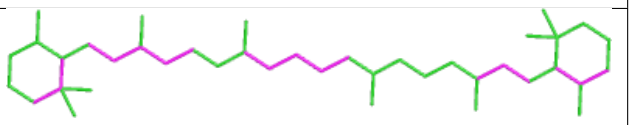


Rings

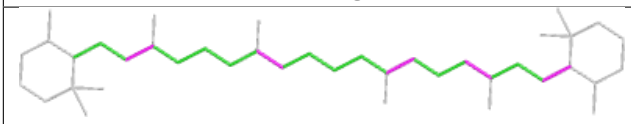
Ligand BCR cL 208



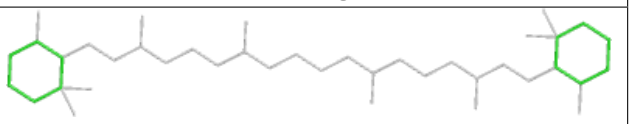
Bond lengths



Bond angles

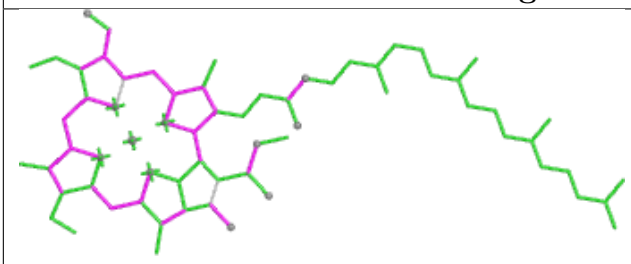


Torsions



Rings

Ligand F6C aA 826



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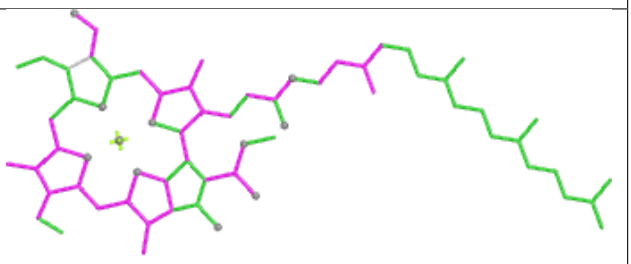
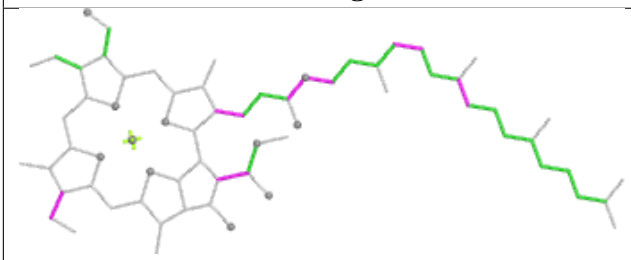


Bond angles



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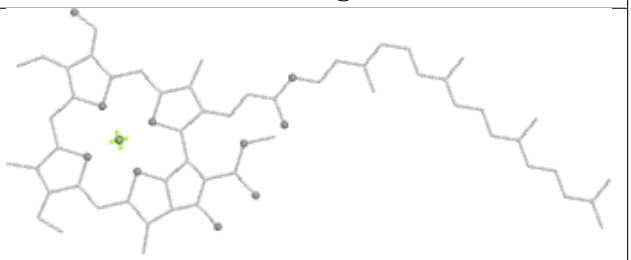
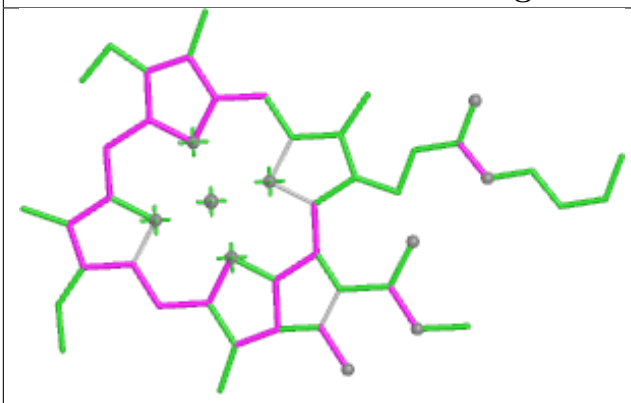
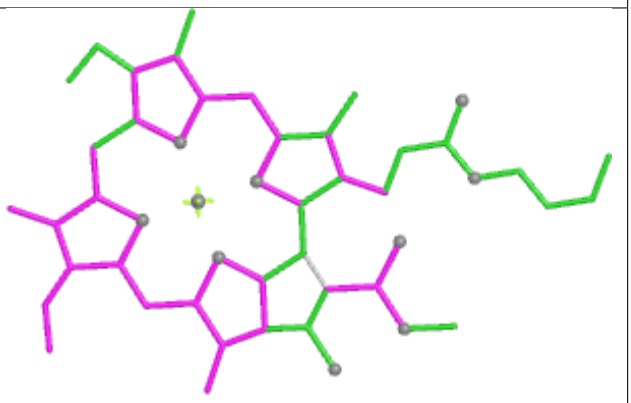


Rings

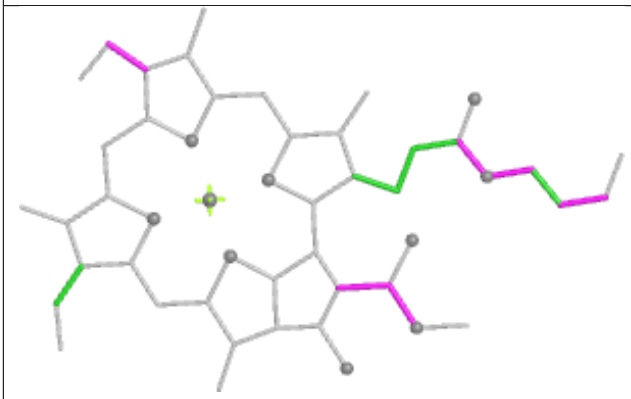
Ligand CLA bB 830



Bond lengths



Bond angles



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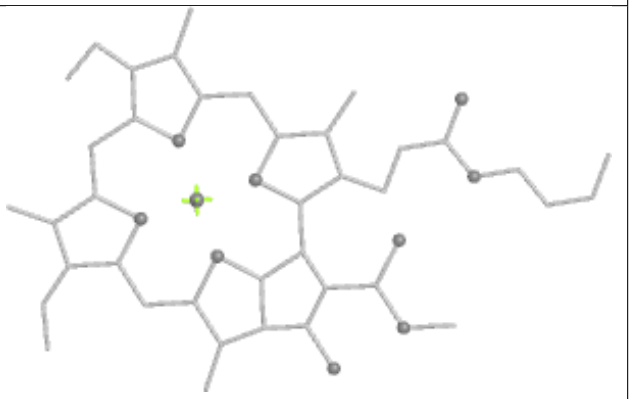
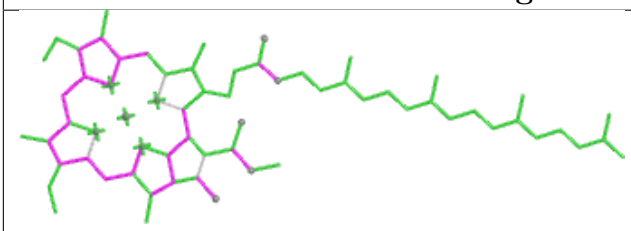
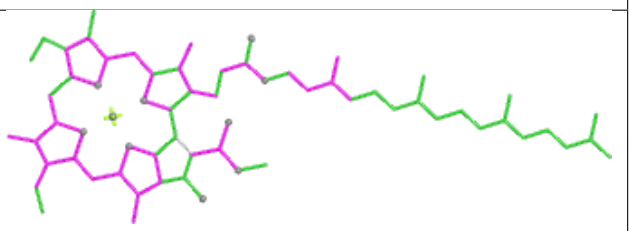


Rings

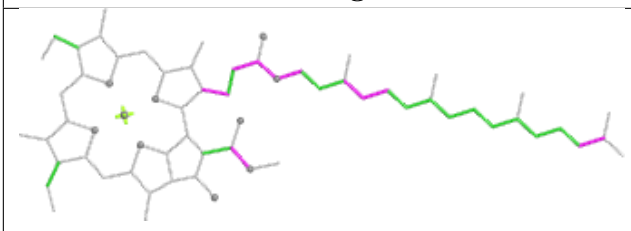
Ligand CLA cA 829



Bond lengths



Bond angles



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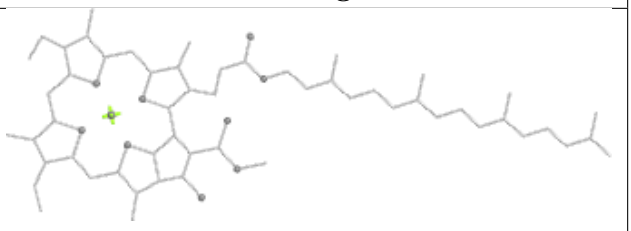
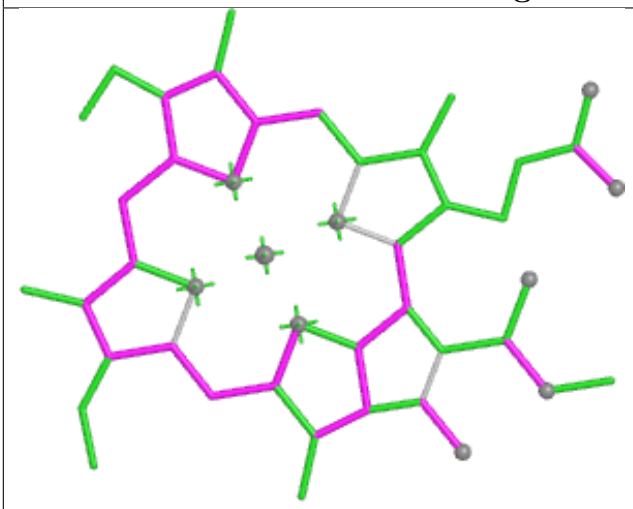
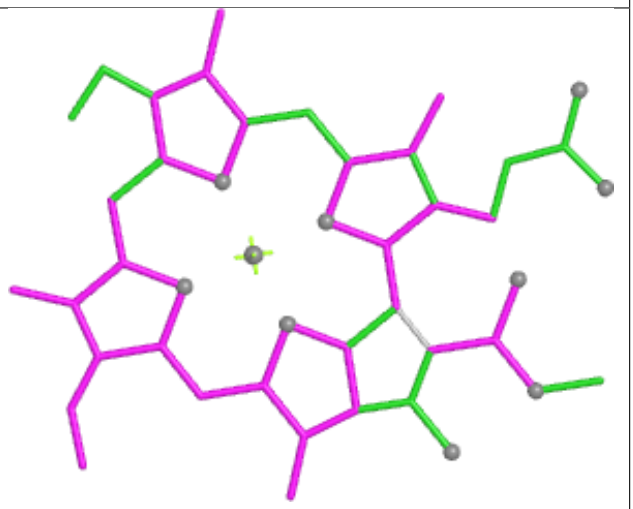


Rings

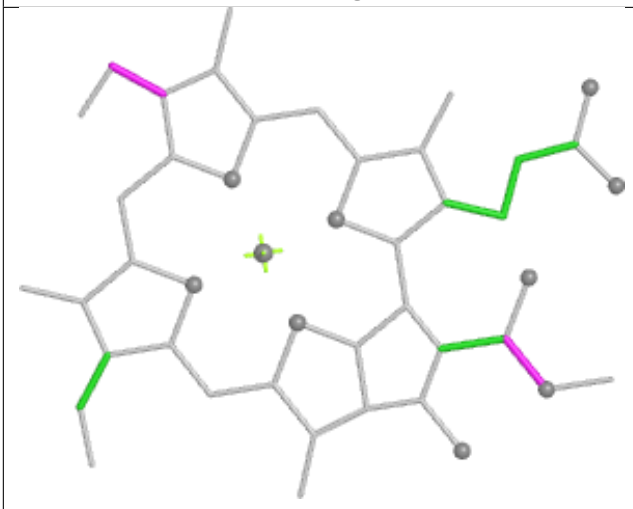
Ligand CLA bA 810



Bond lengths



Bond angles

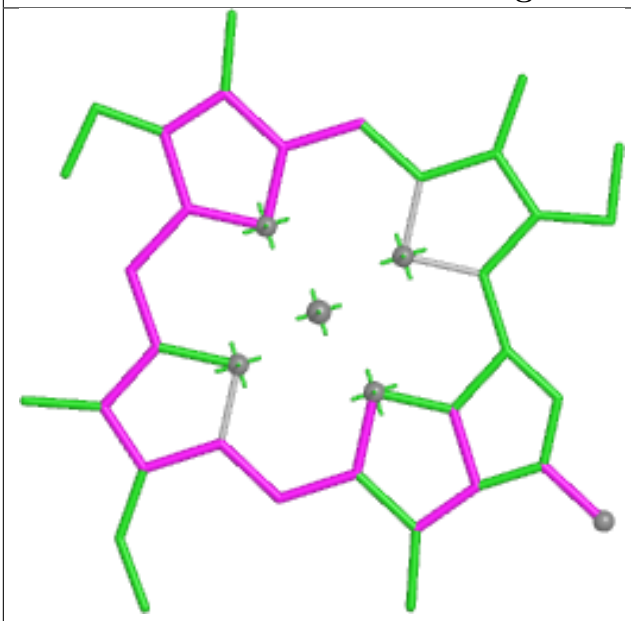


Torsions



Rings

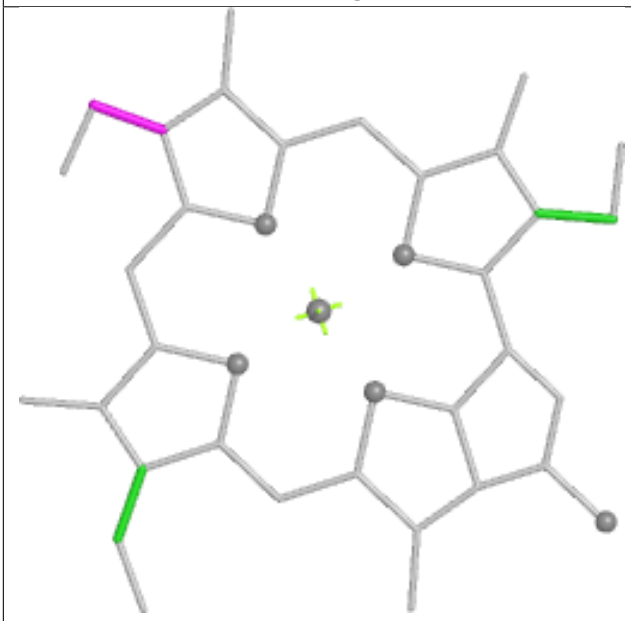
Ligand CLA cK 101



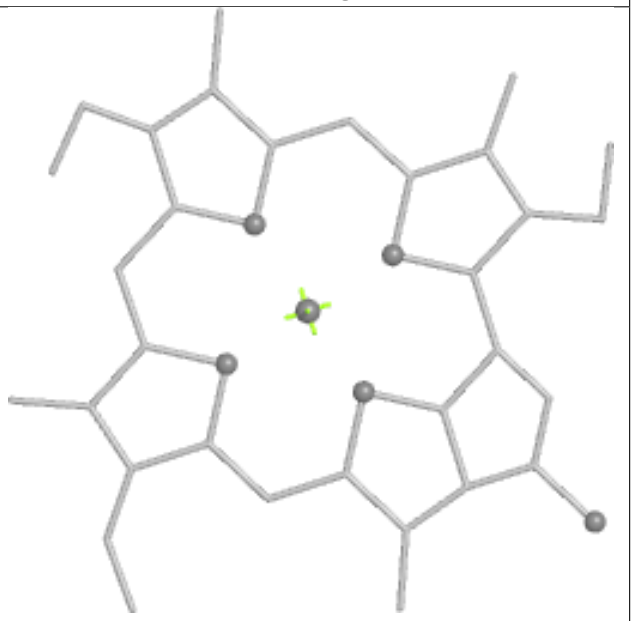
Bond lengths



Bond angles

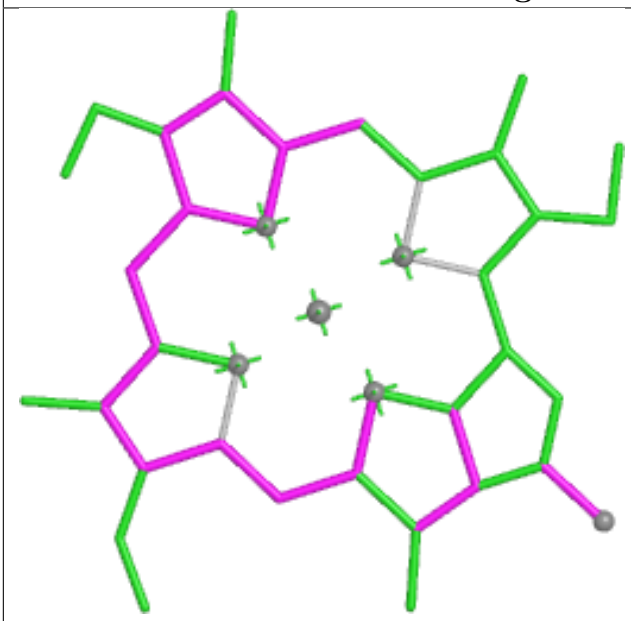


Torsions



Rings

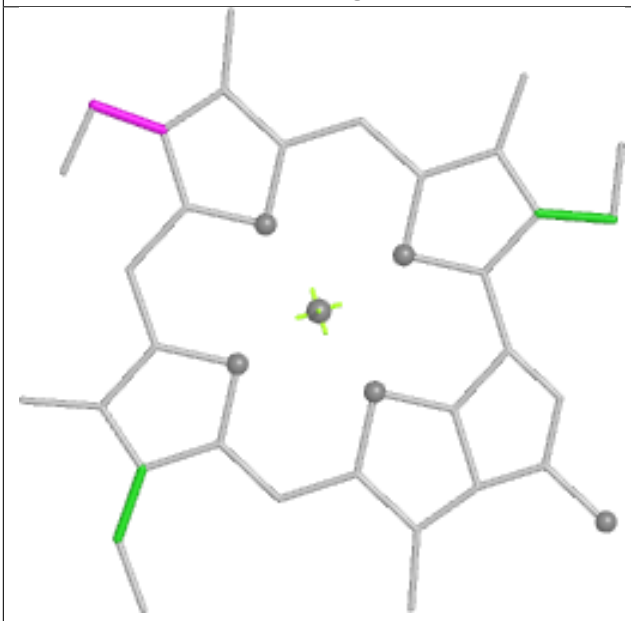
Ligand CLA aK 101



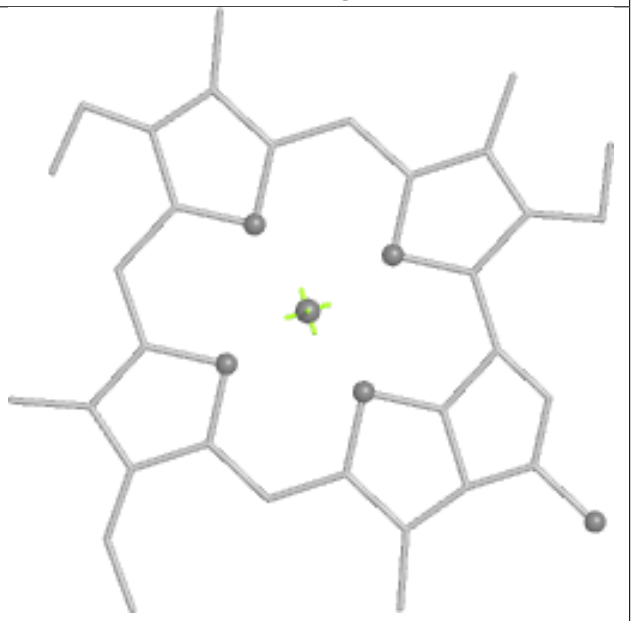
Bond lengths



Bond angles

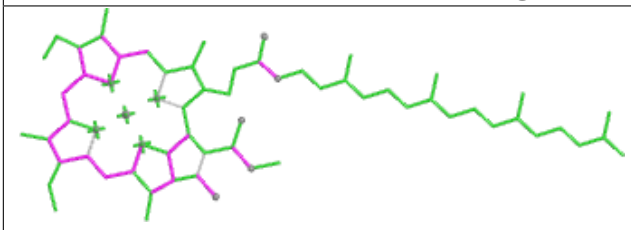


Torsions

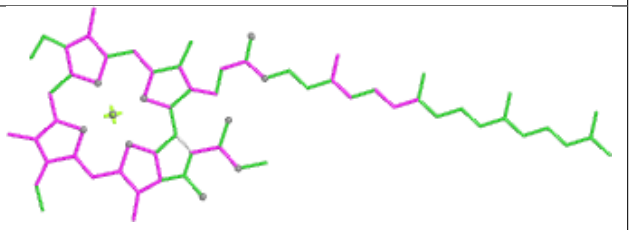


Rings

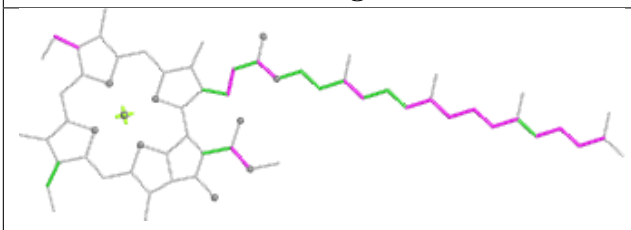
Ligand CLA bA 822



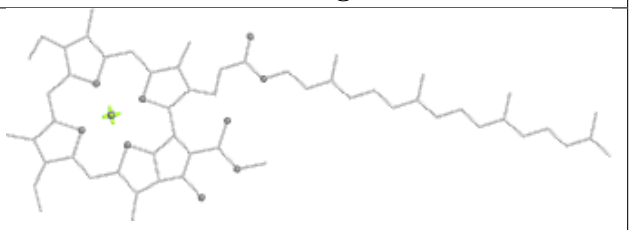
Bond lengths



Bond angles

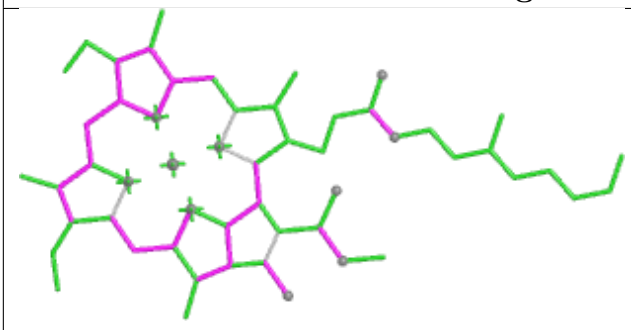


Torsions

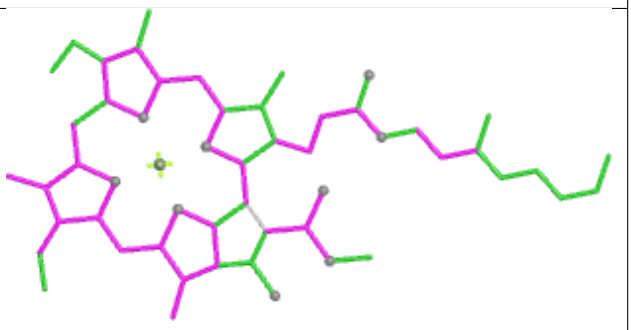


Rings

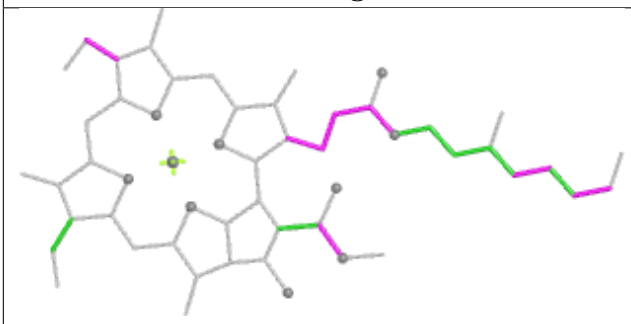
Ligand CLA cA 819



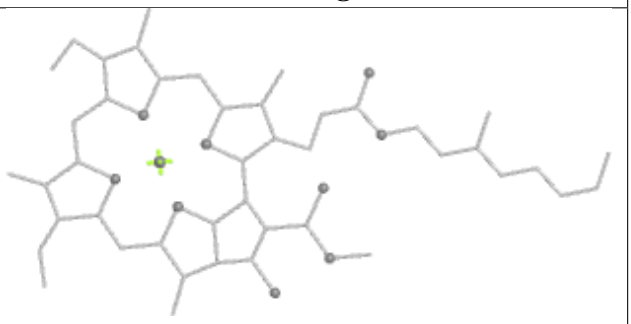
Bond lengths



Bond angles

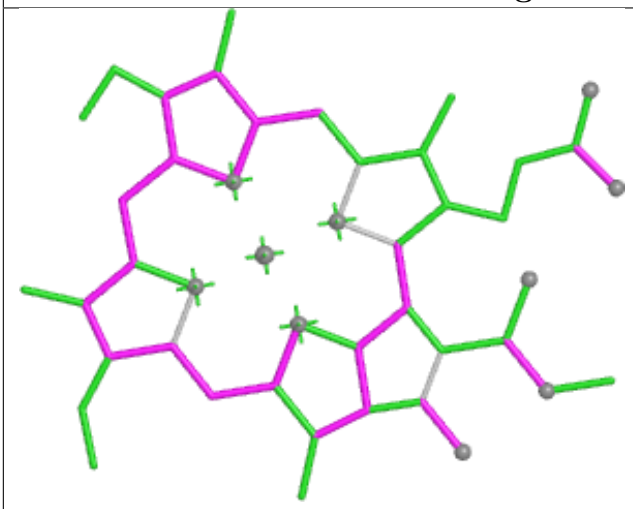


Torsions

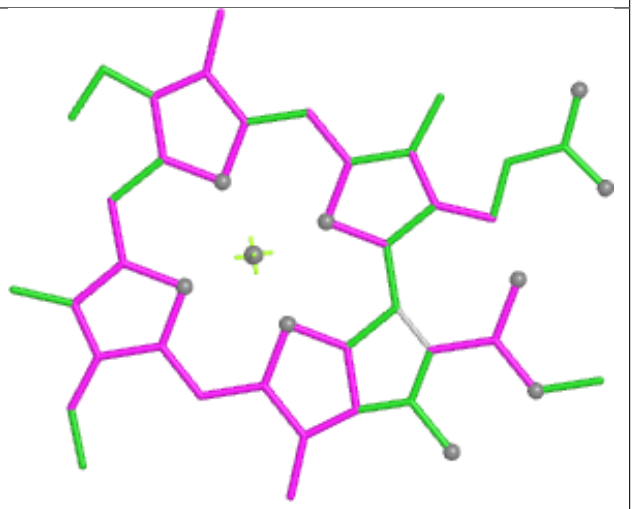


Rings

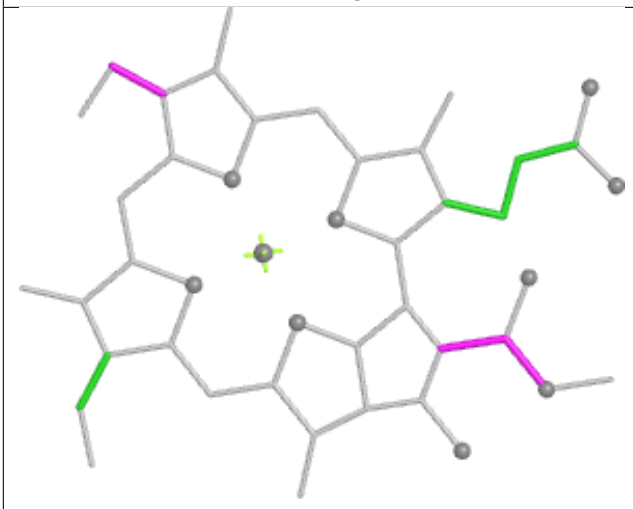
Ligand CLA aA 816



Bond lengths



Bond angles

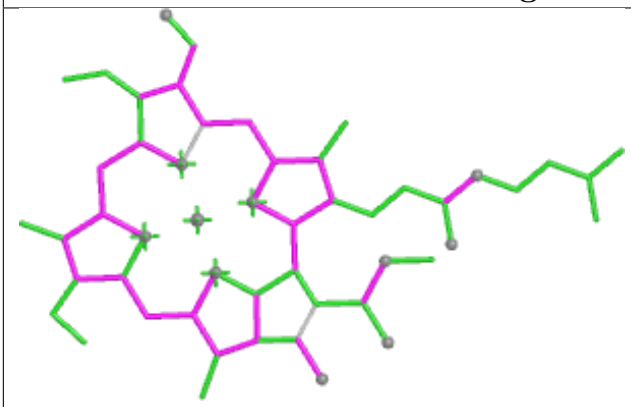


Torsions

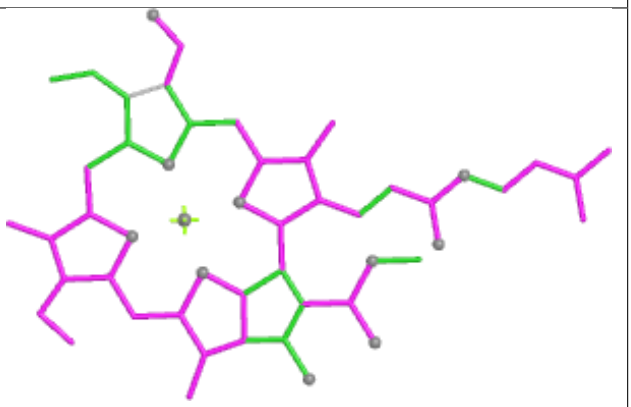


Rings

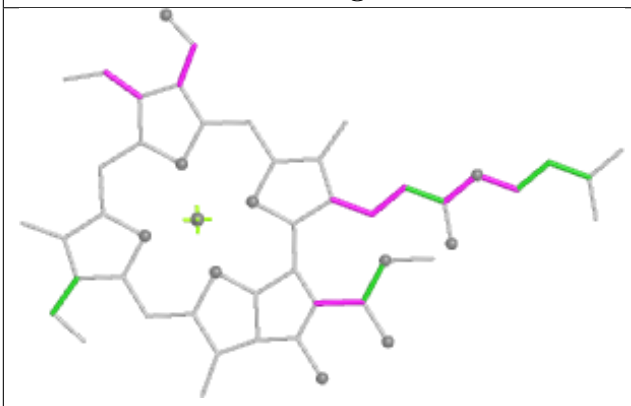
Ligand F6C cA 832



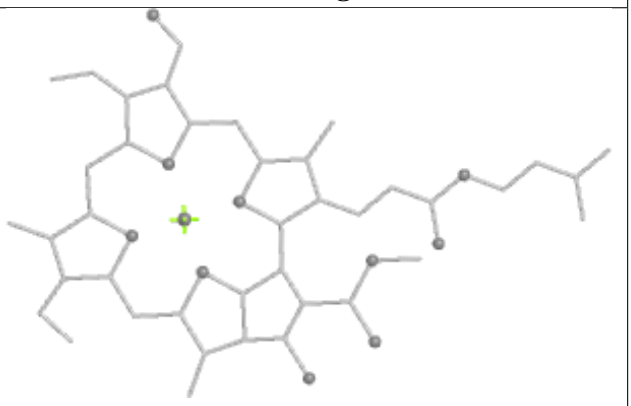
Bond lengths



Bond angles

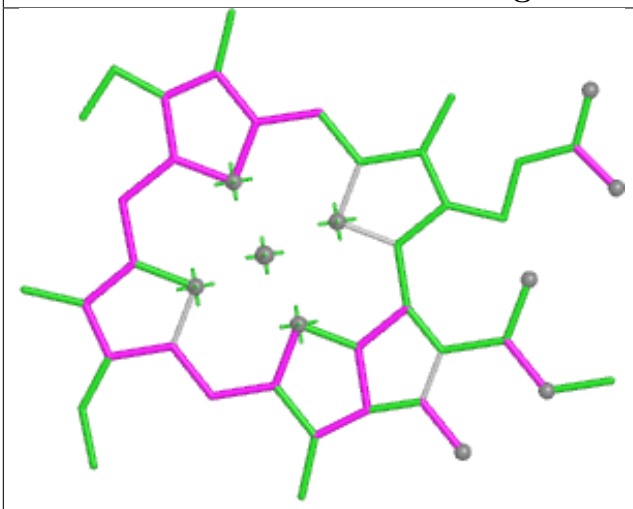


Torsions

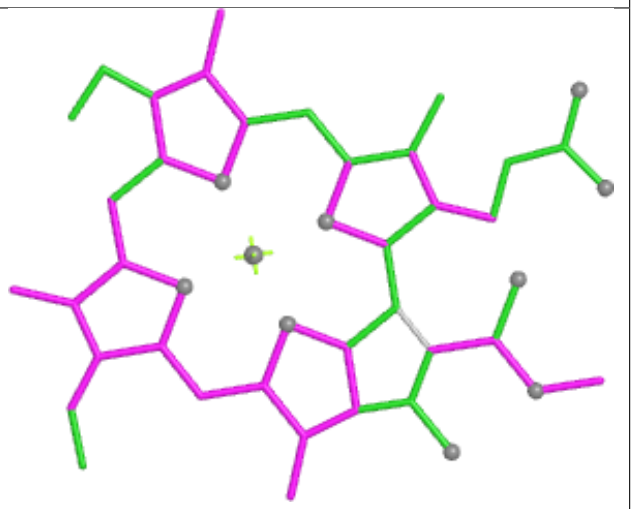


Rings

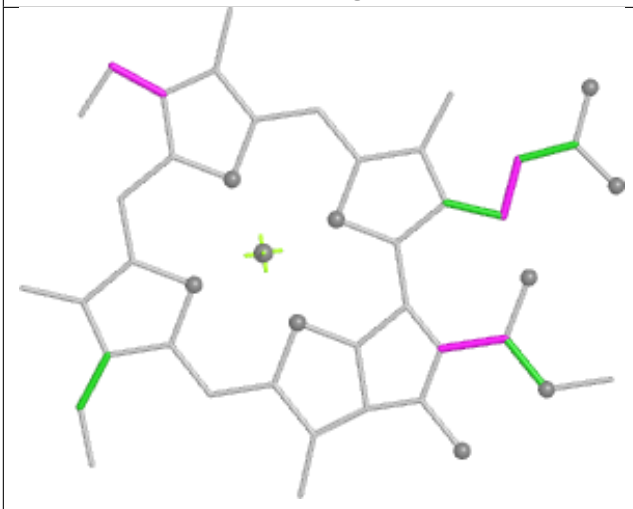
Ligand CLA bA 811



Bond lengths



Bond angles

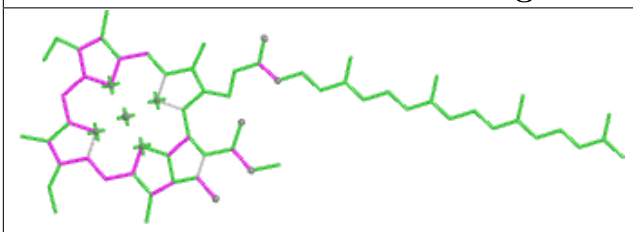


Torsions

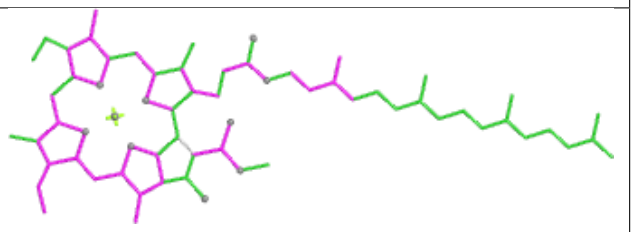


Rings

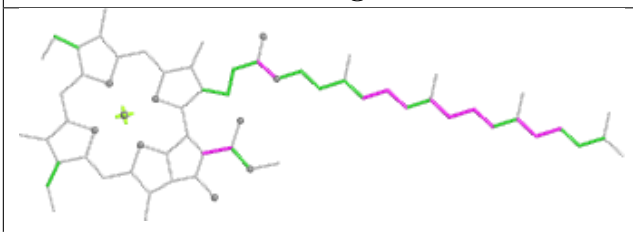
Ligand CLA cA 831



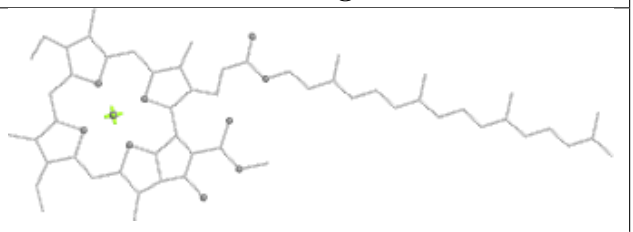
Bond lengths



Bond angles

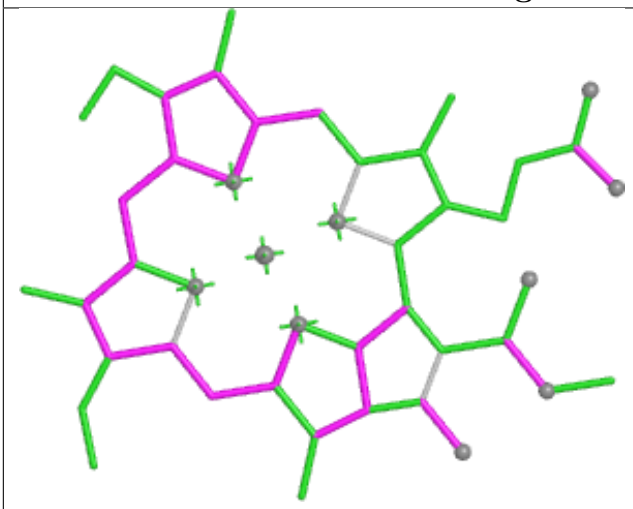


Torsions

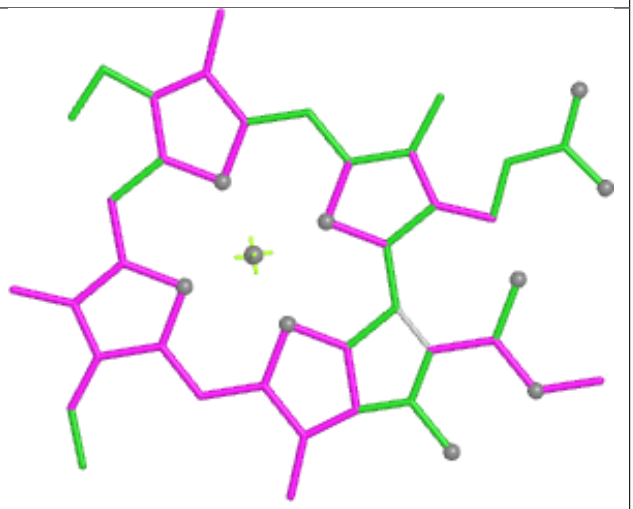


Rings

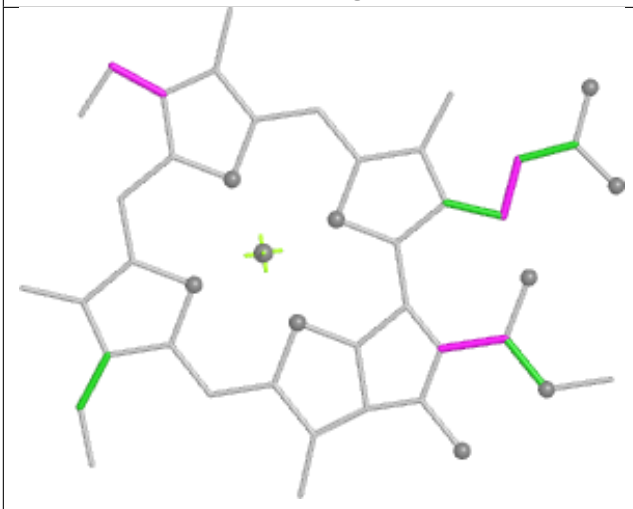
Ligand CLA aA 811



Bond lengths



Bond angles

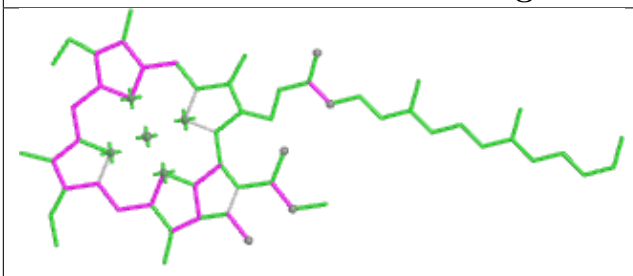


Torsions

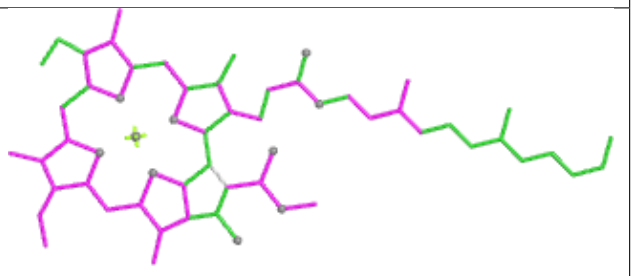


Rings

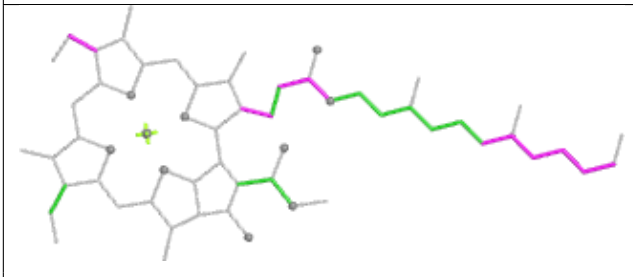
Ligand CLA aB 816



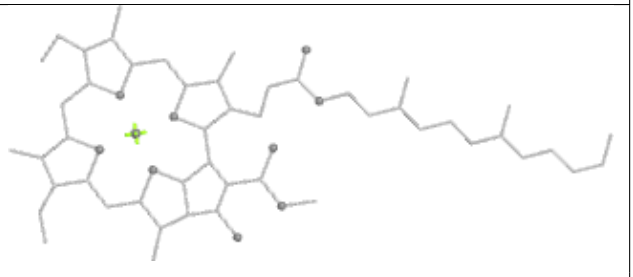
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

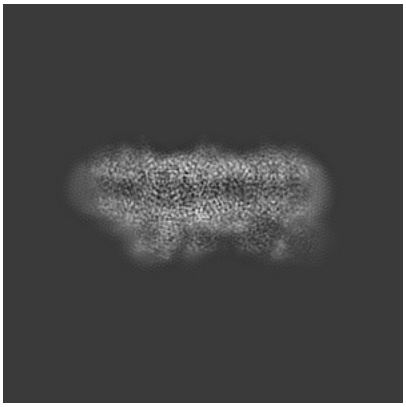
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0727. These allow visual inspection of the internal detail of the map and identification of artifacts.

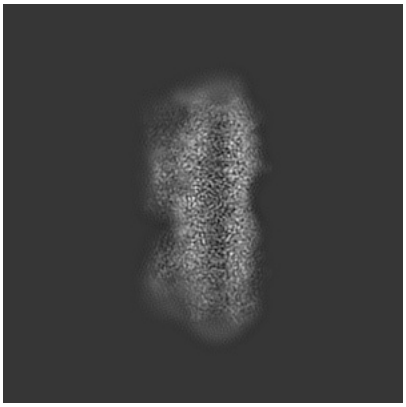
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

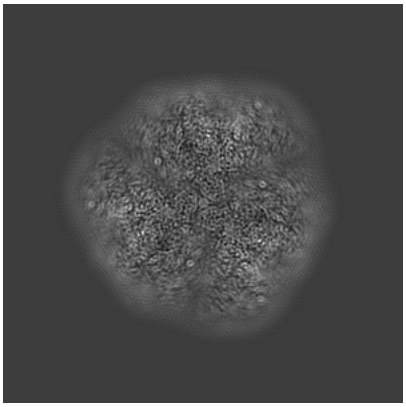
6.1.1 Primary map



X



Y



Z

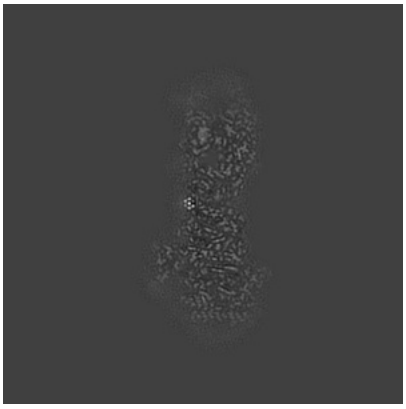
The images above show the map projected in three orthogonal directions.

6.2 Central slices

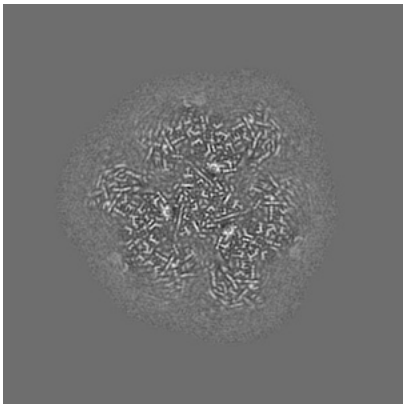
6.2.1 Primary map



X Index: 180



Y Index: 180

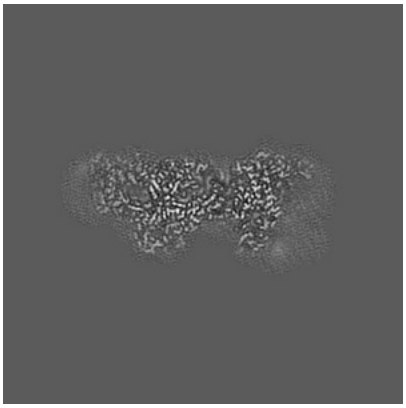


Z Index: 180

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

6.3 Largest variance slices (i)

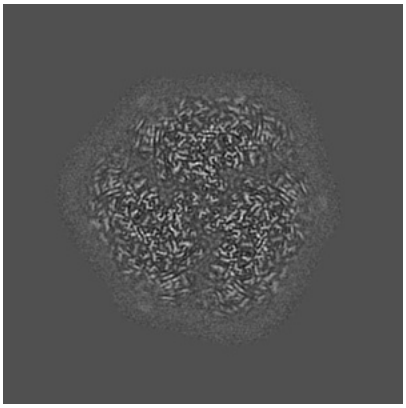
6.3.1 Primary map



X Index: 200



Y Index: 176

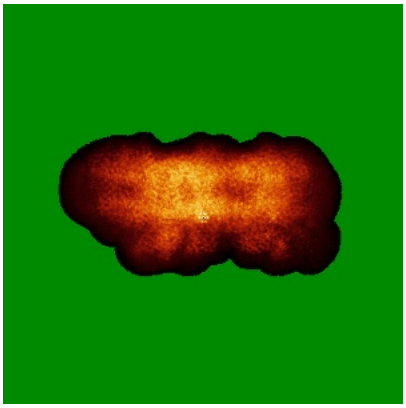


Z Index: 204

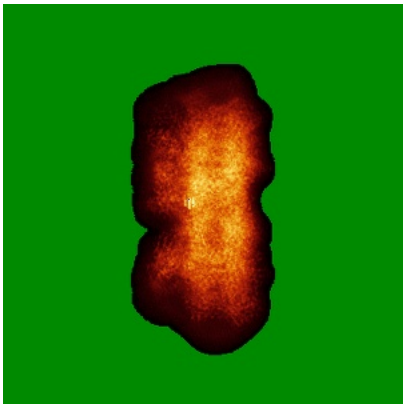
The images above show the largest variance slices of the map in three orthogonal directions.

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

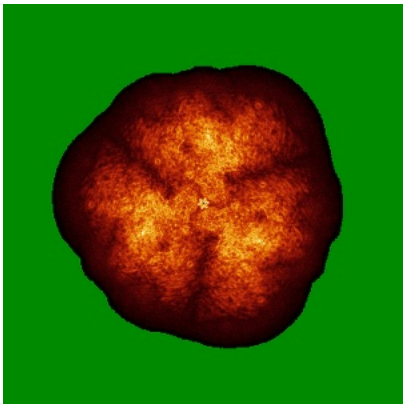
6.4.1 Primary map



X



Y

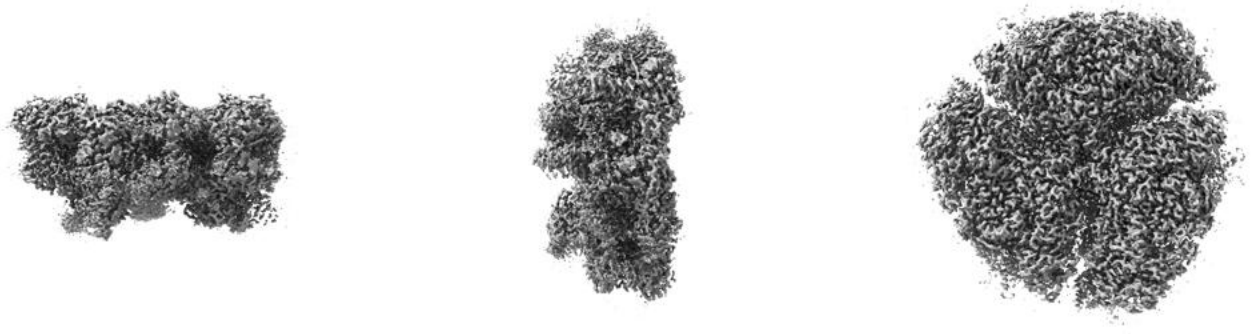


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

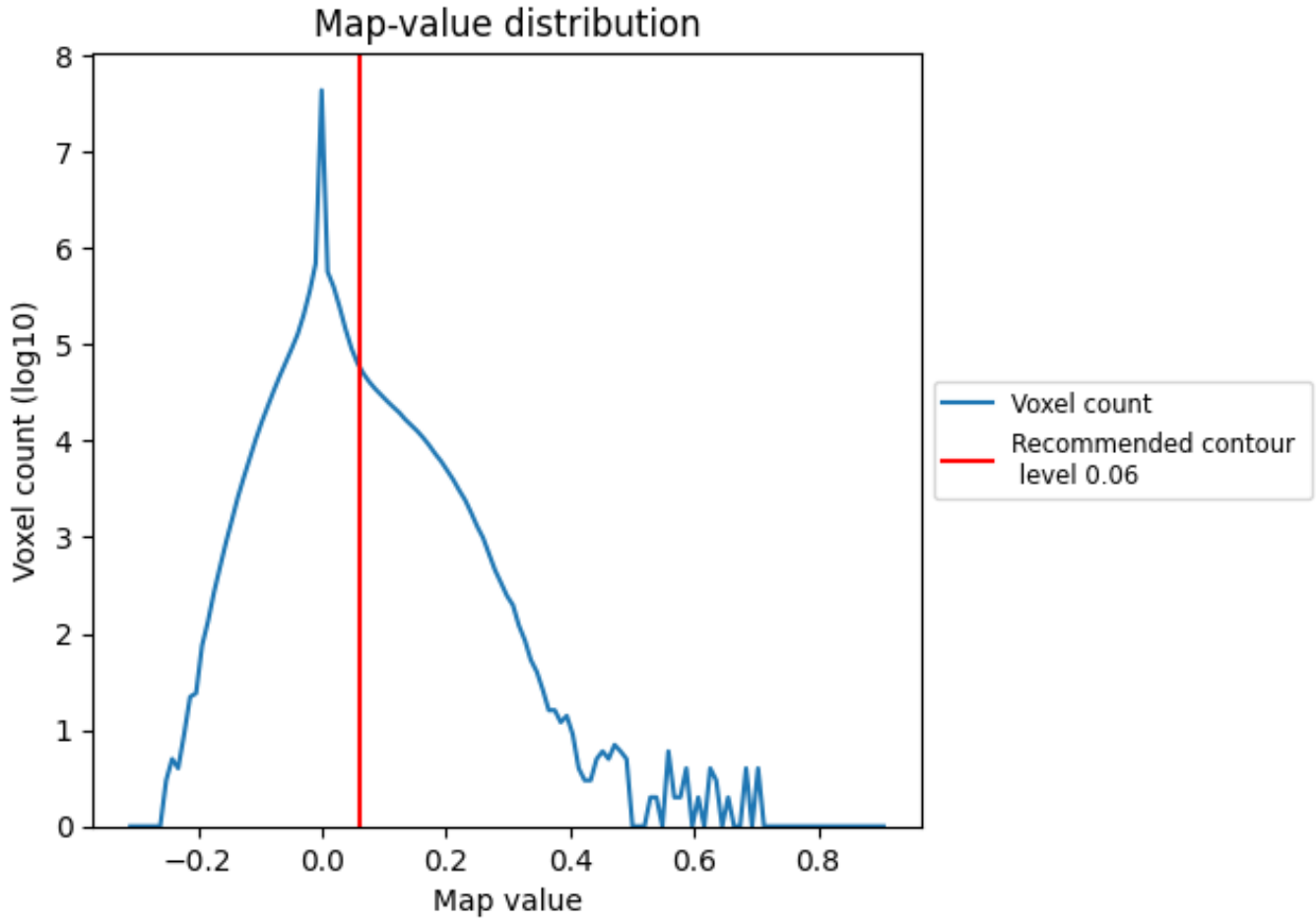
6.6 Mask visualisation (i)

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

7 Map analysis

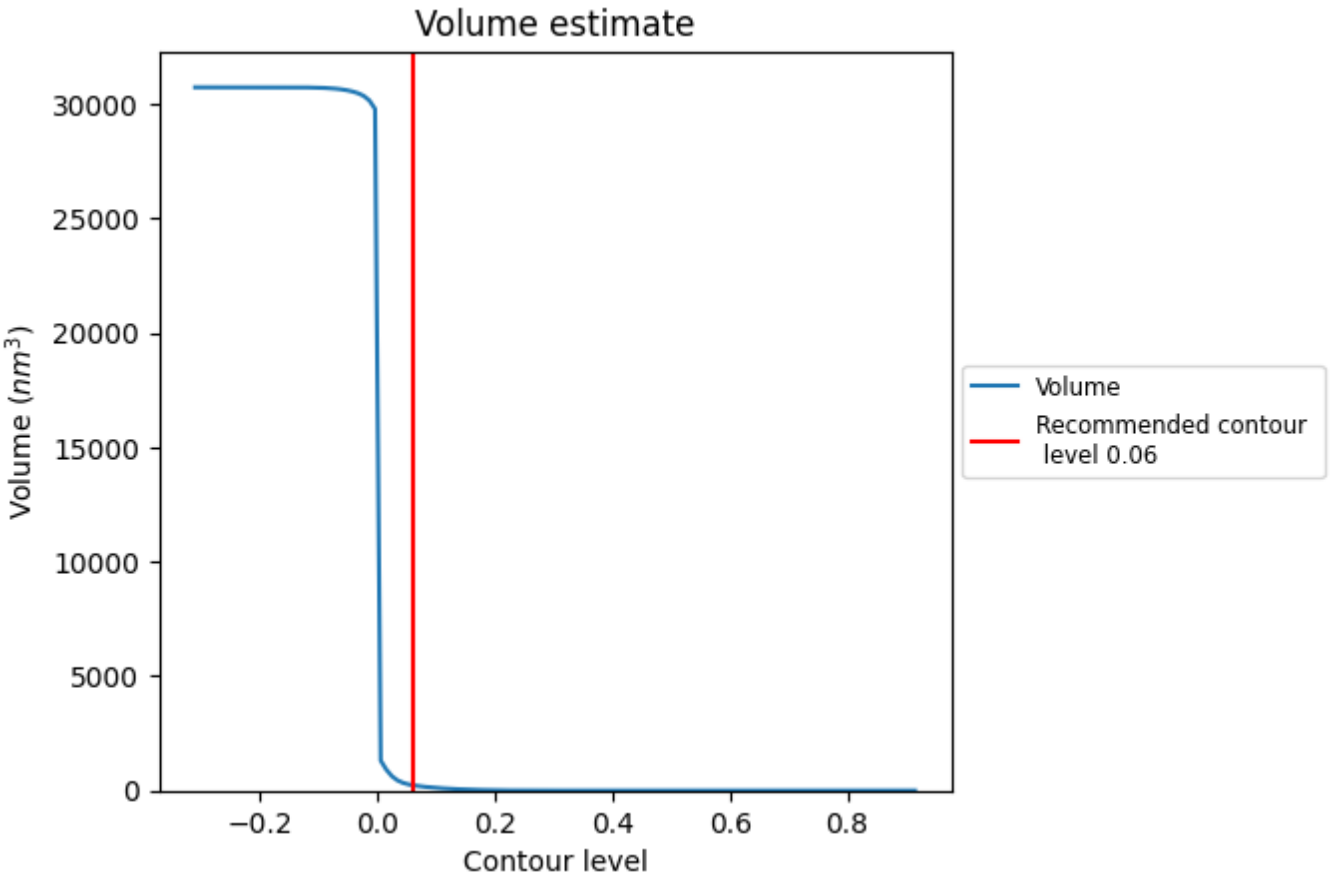
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

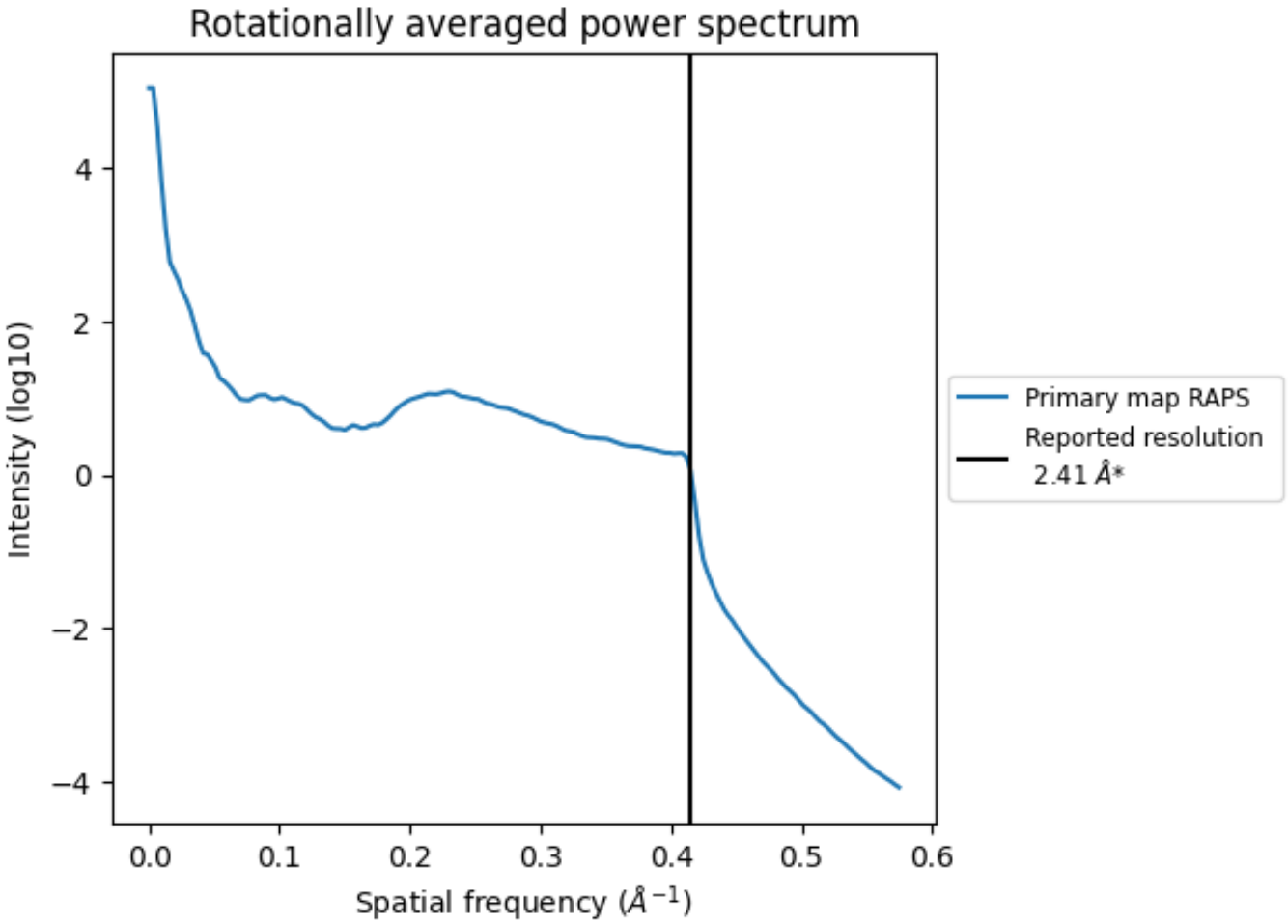
7.2 Volume estimate



The volume at the recommended contour level is 239 nm^3; this corresponds to an approximate mass of 215 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 (i)

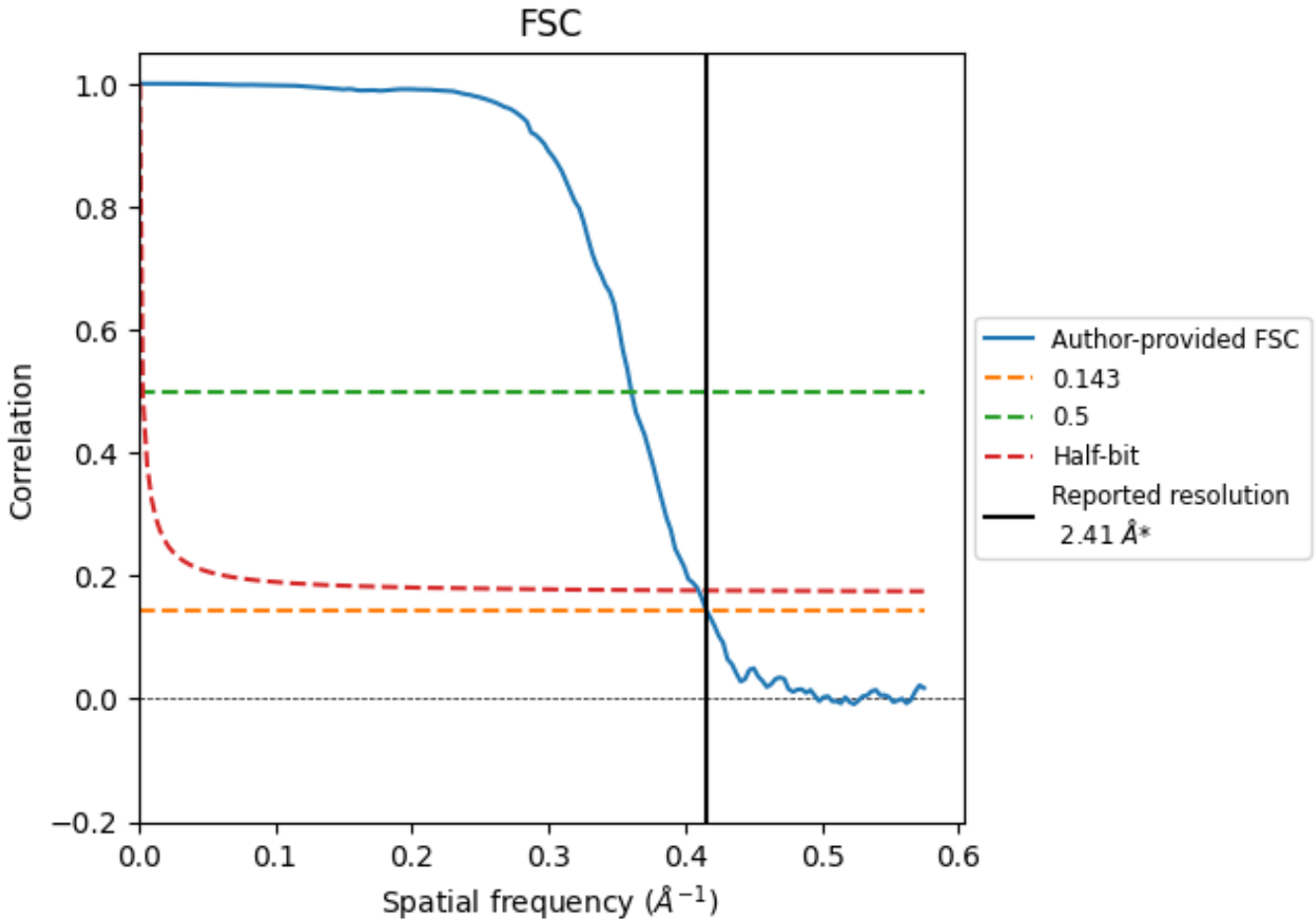


*Reported resolution corresponds to spatial frequency of 0.415 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.415 $Å^{-1}$

8.2 Resolution estimates (i)

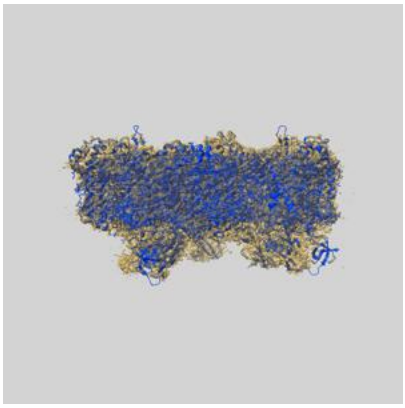
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.41	-	-
Author-provided FSC curve	2.41	2.77	2.44
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

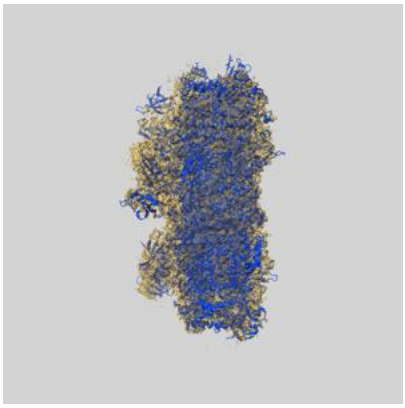
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0727 and PDB model 6KMX. Per-residue inclusion information can be found in section 3 on page 30.

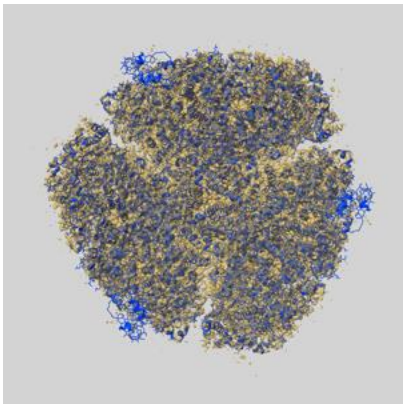
9.1 Map-model overlay



X



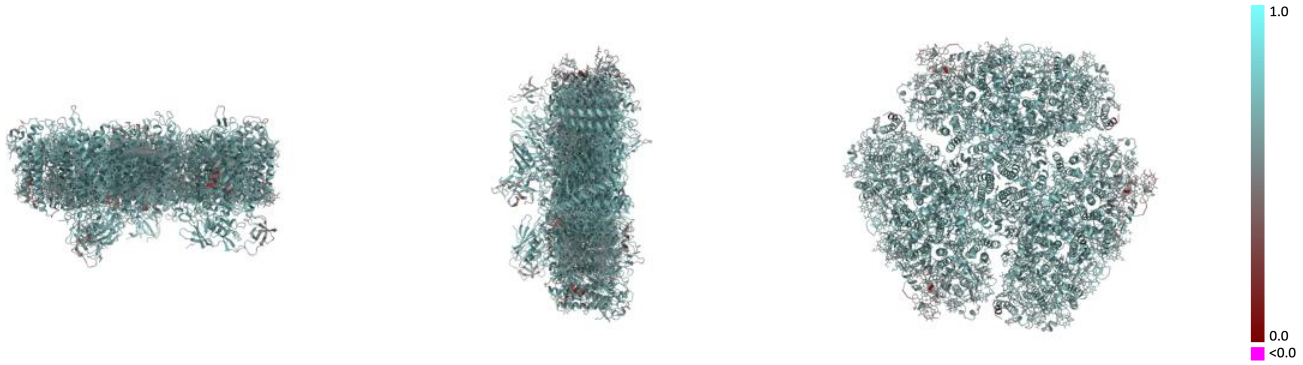
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 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.

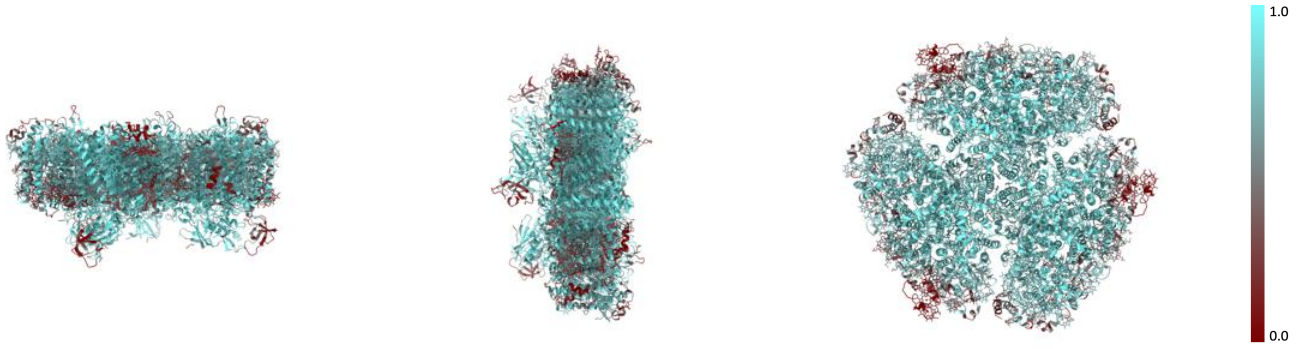
9.2 Q-score mapped to coordinate model



X Y Z

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.

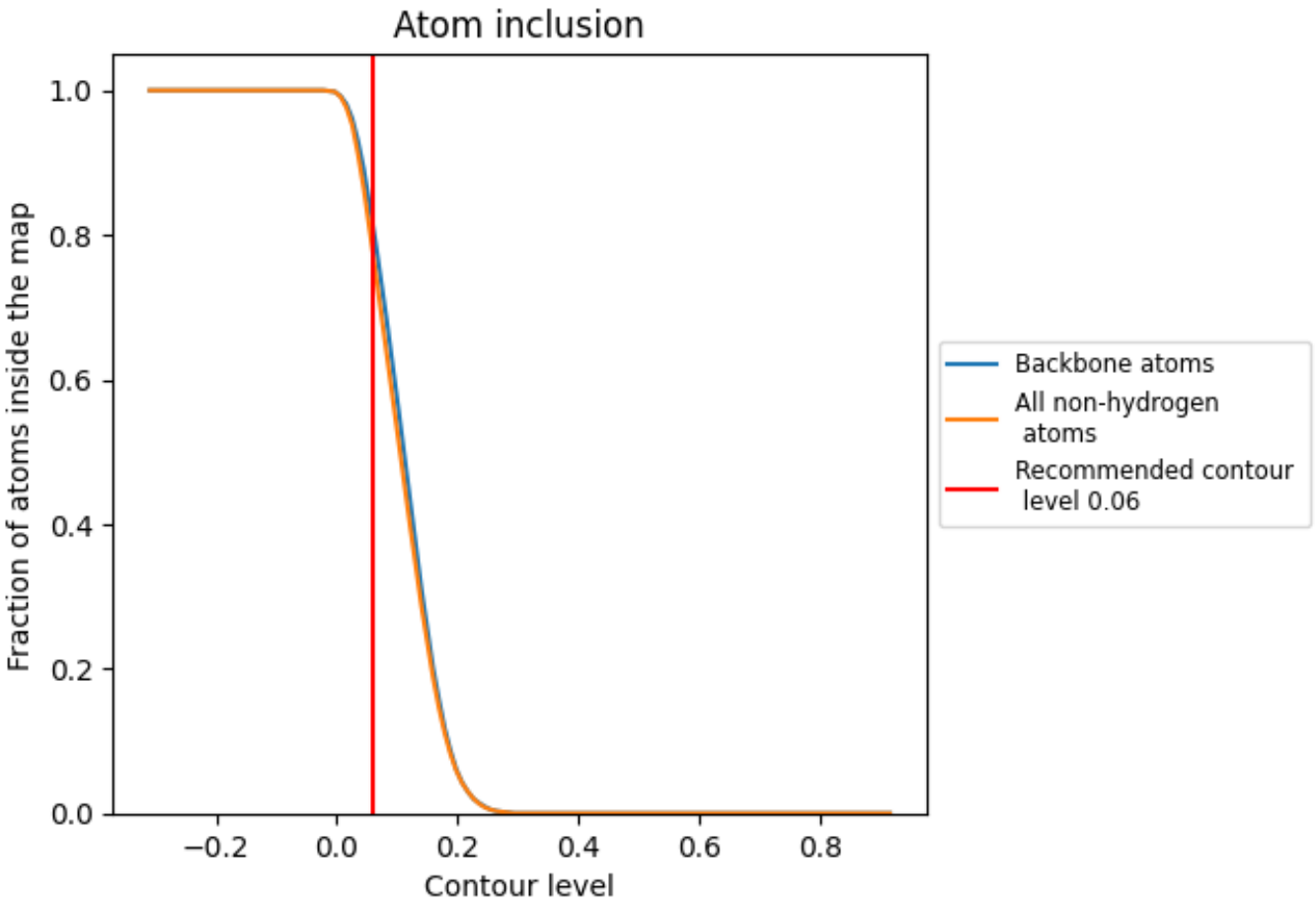
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 77% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7730	0.6490
aA	0.7920	0.6560
aB	0.7450	0.6400
aC	0.9000	0.6780
aD	0.8630	0.6760
aE	0.3350	0.5280
aI	0.8930	0.6970
aK	0.3490	0.5080
aL	0.9090	0.6980
aM	0.7880	0.6400
bA	0.7920	0.6570
bB	0.7500	0.6400
bC	0.9010	0.6780
bD	0.8730	0.6760
bE	0.3310	0.5280
bI	0.8930	0.6980
bK	0.3430	0.5070
bL	0.9130	0.6970
bM	0.7840	0.6440
cA	0.7920	0.6560
cB	0.7490	0.6410
cC	0.8960	0.6800
cD	0.8700	0.6740
cE	0.3240	0.5240
cI	0.8800	0.6940
cK	0.3330	0.5040
cL	0.9140	0.6970
cM	0.7880	0.6400

