Full wwPDB EM Validation Report ⓘ

Sep 15, 2026 – 02:45 PM JST

PDB ID	:	9L0A / pdb_00009l0a
EMDB ID	:	EMD-62693
Title	:	PSI trimer of Arthrospira platensis NIES-39
Authors	:	Kato, K.; Nakajima, Y.; Shen, J.R.; Nagao, R.
Deposited on	:	2024-12-12
Resolution	:	2.17 Å(reported)
Based on initial model	:	.

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:

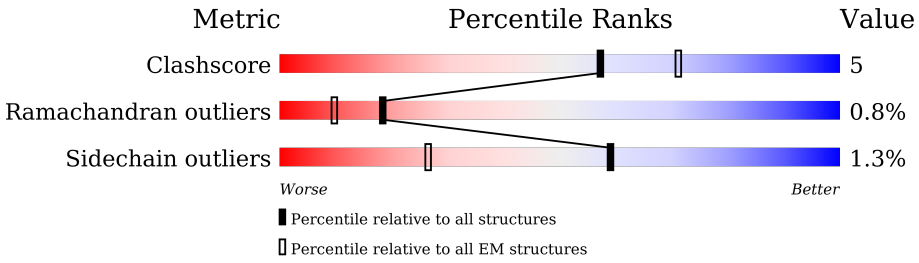
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

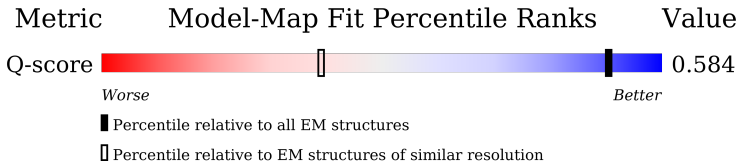
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.17 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	2651 (1.67 - 2.67)

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	A	751	23% 93%
1	bA	751	23% 93%
1	cA	751	22% 93%
2	B	741	17% 91% 8%

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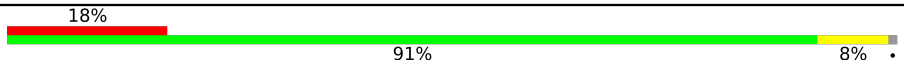
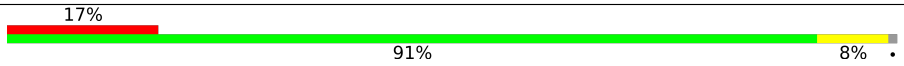
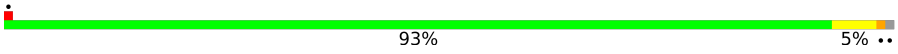
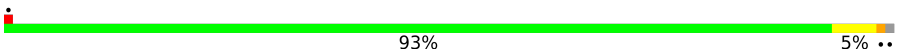
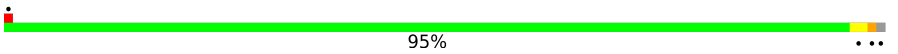
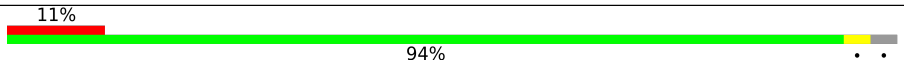
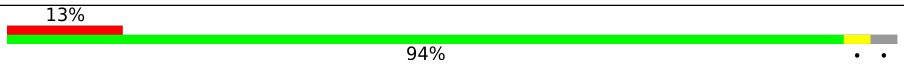
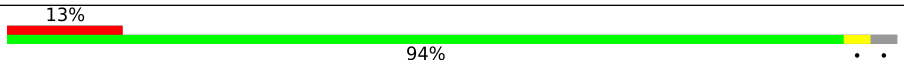
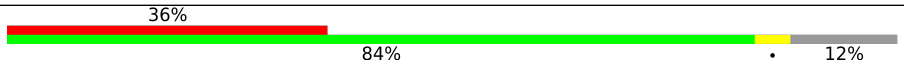
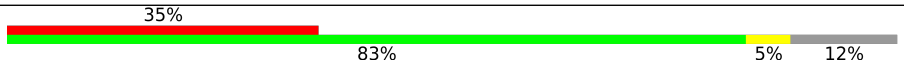
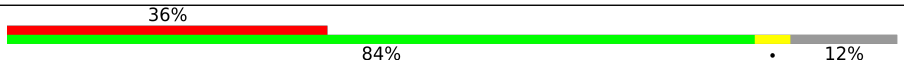
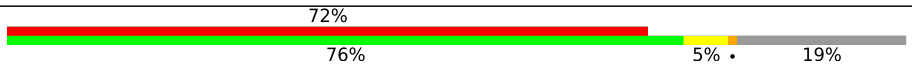
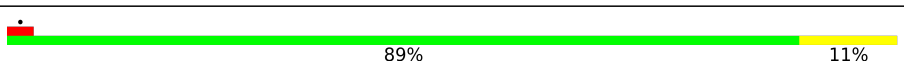
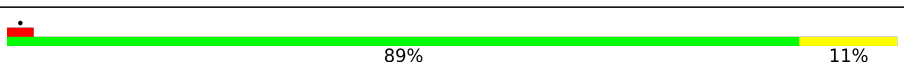
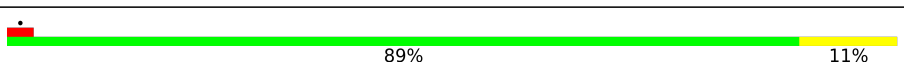
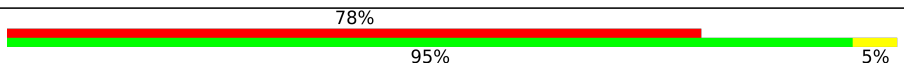
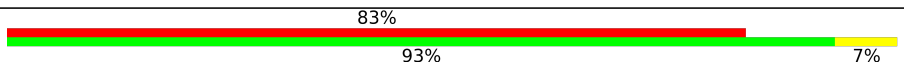
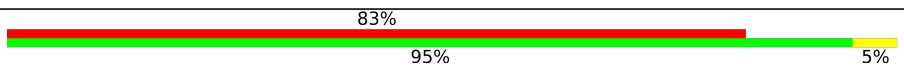
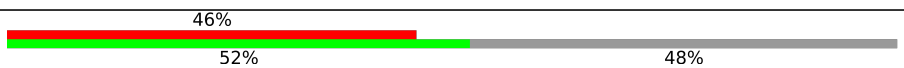
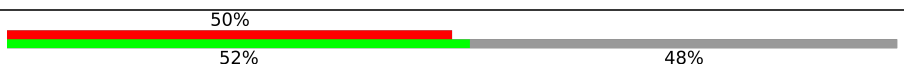
Mol	Chain	Length	Quality of chain
2	bB	741	
2	cB	741	
3	C	81	
3	bC	81	
3	cC	81	
4	D	142	
4	bD	142	
4	cD	142	
5	E	77	
5	bE	77	
5	cE	77	
6	F	162	
6	bF	162	
6	cF	162	
7	I	38	
7	bI	38	
7	cI	38	
8	J	41	
8	bJ	41	
8	cJ	41	
9	K	82	
9	bK	82	
9	cK	82	
10	L	161	
10	bL	161	

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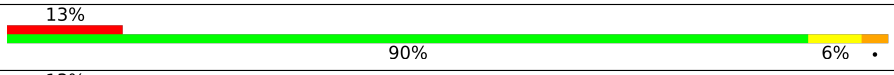
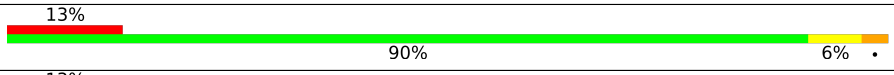
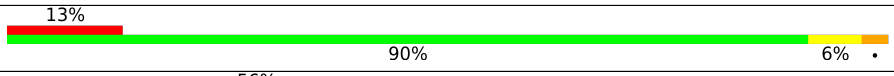
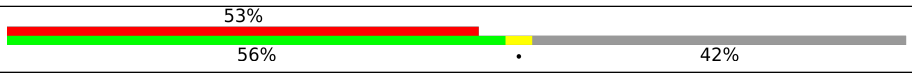
Mol	Chain	Length	Quality of chain
10	cL	161	
11	M	31	
11	bM	31	
11	cM	31	
12	X	36	
12	bX	36	
12	cX	36	

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 70131 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	731	Total	C	N	O	S	0	0
			5742	3755	981	979	27		
1	bA	731	Total	C	N	O	S	0	0
			5742	3755	981	979	27		
1	cA	731	Total	C	N	O	S	0	0
			5742	3755	981	979	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	736	Total	C	N	O	S	0	0
			5886	3873	989	1004	20		
2	bB	736	Total	C	N	O	S	0	0
			5886	3873	989	1004	20		
2	cB	736	Total	C	N	O	S	0	0
			5886	3873	989	1004	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			599	368	103	117	11		
3	bC	80	Total	C	N	O	S	0	0
			599	368	103	117	11		
3	cC	80	Total	C	N	O	S	0	0
			599	368	103	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	138	Total	C	N	O	S	0	0
			1084	692	183	205	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	bD	138	Total	C	N	O	S	0	0
			1084	692	183	205	4		
4	cD	138	Total	C	N	O	S	0	0
			1084	692	183	205	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	68	Total	C	N	O	S	0	0
			544	344	95	104	1		
5	bE	68	Total	C	N	O	S	0	0
			544	344	95	104	1		
5	cE	68	Total	C	N	O	S	0	0
			544	344	95	104	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	132	Total	C	N	O	S	0	0
			1023	656	169	193	5		
6	bF	132	Total	C	N	O	S	0	0
			1023	656	169	193	5		
6	cF	132	Total	C	N	O	S	0	0
			1023	656	169	193	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	38	Total	C	N	O	S	0	0
			297	202	42	49	4		
7	bI	38	Total	C	N	O	S	0	0
			297	202	42	49	4		
7	cI	38	Total	C	N	O	S	0	0
			297	202	42	49	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	41	Total	C	N	O	S	0	0
			339	234	51	53	1		
8	bJ	41	Total	C	N	O	S	0	0
			339	234	51	53	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	cJ	41	Total	C	N	O	S	0	0
			339	234	51	53	1		

- Molecule 9 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	K	43	Total	C	N	O	0	0
			208	122	43	43		
9	bK	43	Total	C	N	O	0	0
			208	122	43	43		
9	cK	43	Total	C	N	O	0	0
			208	122	43	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	158	Total	C	N	O	S	0	0
			1178	765	194	214	5		
10	bL	158	Total	C	N	O	S	0	0
			1178	765	194	214	5		
10	cL	158	Total	C	N	O	S	0	0
			1178	765	194	214	5		

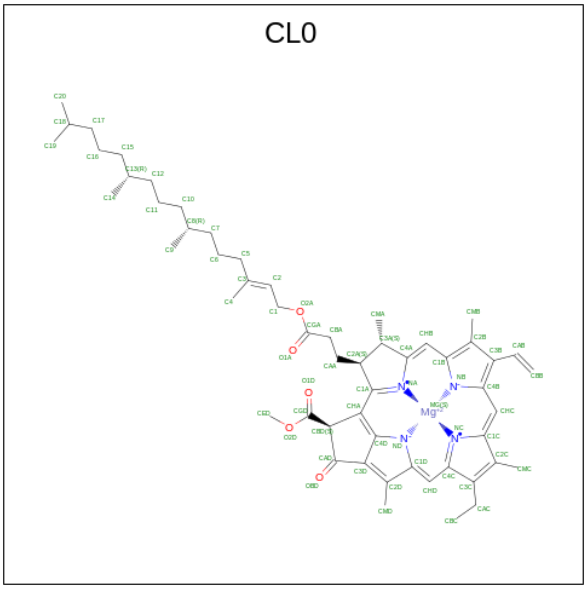
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total	C	N	O	S	0	0
			241	161	36	43	1		
11	bM	31	Total	C	N	O	S	0	0
			241	161	36	43	1		
11	cM	31	Total	C	N	O	S	0	0
			241	161	36	43	1		

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

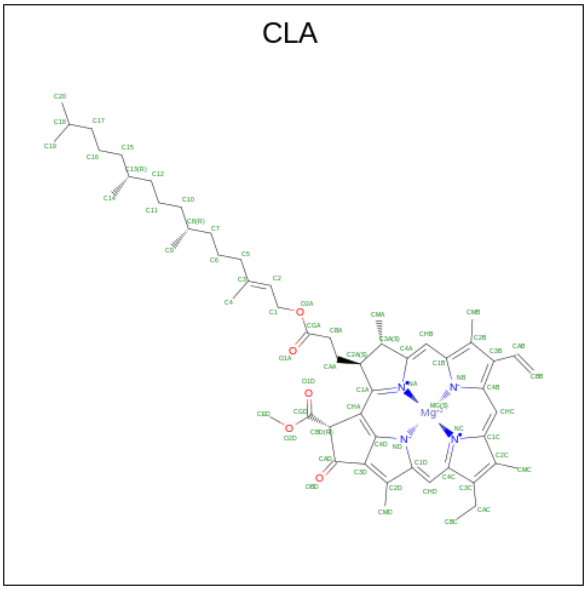
Mol	Chain	Residues	Atoms				AltConf	Trace
12	X	21	Total	C	N	O	0	0
			171	120	26	25		
12	bX	21	Total	C	N	O	0	0
			171	120	26	25		
12	cX	21	Total	C	N	O	0	0
			171	120	26	25		

- Molecule 13 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 14 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	F	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	bA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
14	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	bB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bF	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	bJ	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bJ	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bL	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bX	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	cA	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	cB	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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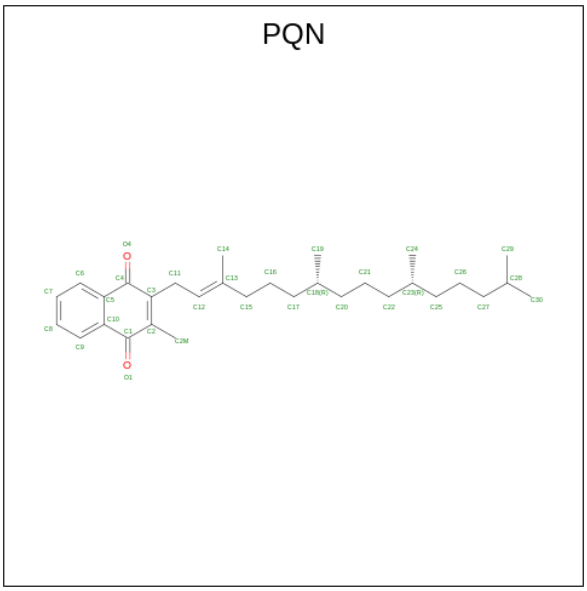
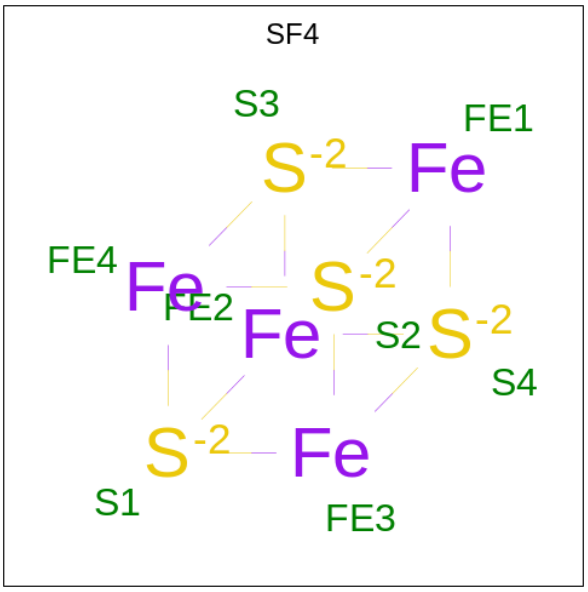
Mol	Chain	Residues	Atoms					AltConf
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
14	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cF	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	cJ	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cJ	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cL	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cX	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 15 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



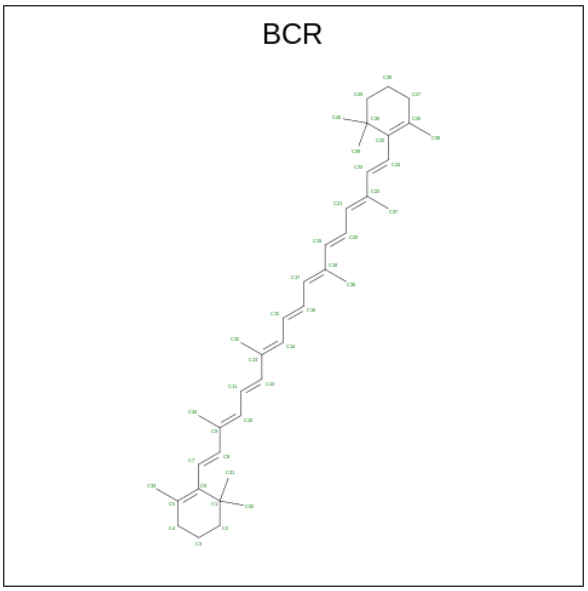
Mol	Chain	Residues	Atoms	AltConf
15	A	1	Total C O 33 31 2	0
15	B	1	Total C O 33 31 2	0
15	bA	1	Total C O 33 31 2	0
15	bB	1	Total C O 33 31 2	0
15	cA	1	Total C O 33 31 2	0
15	cB	1	Total C O 33 31 2	0

- Molecule 16 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
16	A	1	Total Fe S 8 4 4	0
16	C	1	Total Fe S 8 4 4	0
16	C	1	Total Fe S 8 4 4	0
16	bA	1	Total Fe S 8 4 4	0
16	bC	1	Total Fe S 8 4 4	0
16	bC	1	Total Fe S 8 4 4	0
16	cA	1	Total Fe S 8 4 4	0
16	cC	1	Total Fe S 8 4 4	0
16	cC	1	Total Fe S 8 4 4	0

- Molecule 17 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms	AltConf
17	I	1	Total C 40 40	0
17	I	1	Total C 40 40	0
17	J	1	Total C 40 40	0
17	L	1	Total C 40 40	0
17	L	1	Total C 40 40	0
17	M	1	Total C 40 40	0
17	bA	1	Total C 40 40	0
17	bA	1	Total C 40 40	0
17	bA	1	Total C 40 40	0
17	bA	1	Total C 40 40	0
17	bA	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bF	1	Total C 40 40	0
17	bI	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
17	bI	1	Total C 40 40	0
17	bJ	1	Total C 40 40	0
17	bL	1	Total C 40 40	0
17	bL	1	Total C 40 40	0
17	bM	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cF	1	Total C 40 40	0
17	cI	1	Total C 40 40	0
17	cI	1	Total C 40 40	0

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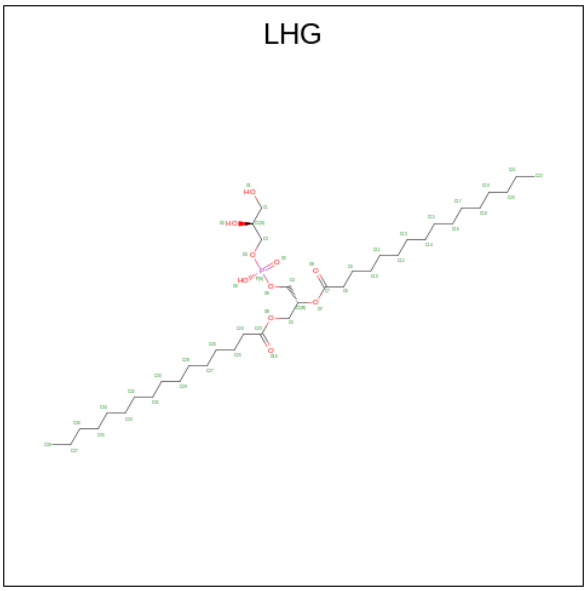
Mol	Chain	Residues	Atoms	AltConf
17	cJ	1	Total C 40 40	0
17	cL	1	Total C 40 40	0
17	cL	1	Total C 40 40	0
17	cM	1	Total C 40 40	0

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).

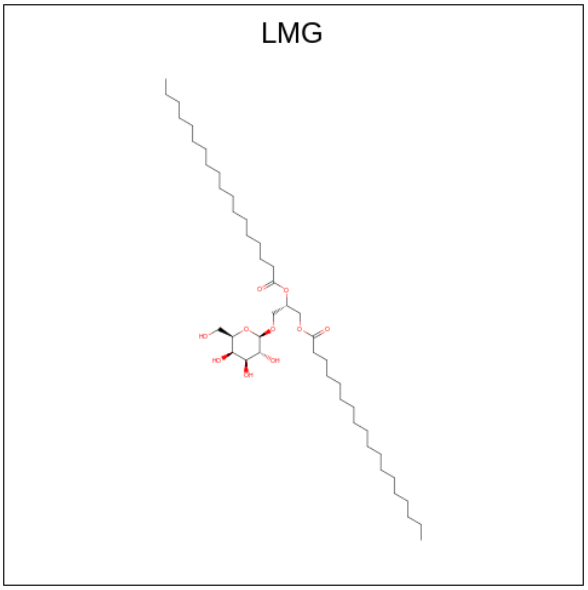


Mol	Chain	Residues	Atoms	AltConf
18	A	1	Total C O P 49 38 10 1	0
18	A	1	Total C O P 27 16 10 1	0
18	bA	1	Total C O P 49 38 10 1	0
18	bA	1	Total C O P 27 16 10 1	0
18	cA	1	Total C O P 49 38 10 1	0
18	cA	1	Total C O P 27 16 10 1	0

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

Mol	Chain	Residues	Atoms	AltConf
19	A	1	Total C 12 12	0
19	I	2	Total C 22 22	0
19	L	2	Total C 29 29	0
19	bA	1	Total C 12 12	0
19	bI	2	Total C 22 22	0
19	bL	2	Total C 29 29	0
19	cA	1	Total C 12 12	0
19	cI	2	Total C 22 22	0
19	cL	2	Total C 29 29	0

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
20	B	1	Total C O 43 33 10	0
20	bB	1	Total C O 43 33 10	0

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Mol	Chain	Residues	Atoms			AltConf
20	cB	1	Total 43	C 33	O 10	0

- Molecule 21 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
21	L	1	Total 1	Ca 1	0
21	bL	1	Total 1	Ca 1	0
21	cL	1	Total 1	Ca 1	0

- Molecule 22 is water.

Mol	Chain	Residues	Atoms		AltConf
22	A	39	Total 39	O 39	0
22	B	30	Total 30	O 30	0
22	C	14	Total 14	O 14	0
22	D	10	Total 10	O 10	0
22	E	3	Total 3	O 3	0
22	I	2	Total 2	O 2	0
22	L	19	Total 19	O 19	0
22	bA	39	Total 39	O 39	0
22	bB	30	Total 30	O 30	0
22	bC	14	Total 14	O 14	0
22	bD	10	Total 10	O 10	0
22	bE	3	Total 3	O 3	0
22	bI	2	Total 2	O 2	0

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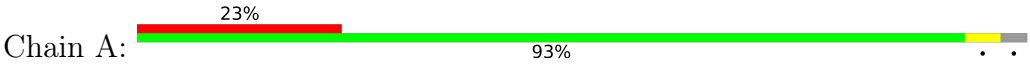
Mol	Chain	Residues	Atoms	AltConf
22	bL	19	Total O 19 19	0
22	cA	39	Total O 39 39	0
22	cB	30	Total O 30 30	0
22	cC	14	Total O 14 14	0
22	cD	10	Total O 10 10	0
22	cE	3	Total O 3 3	0
22	cI	2	Total O 2 2	0
22	cL	19	Total O 19 19	0

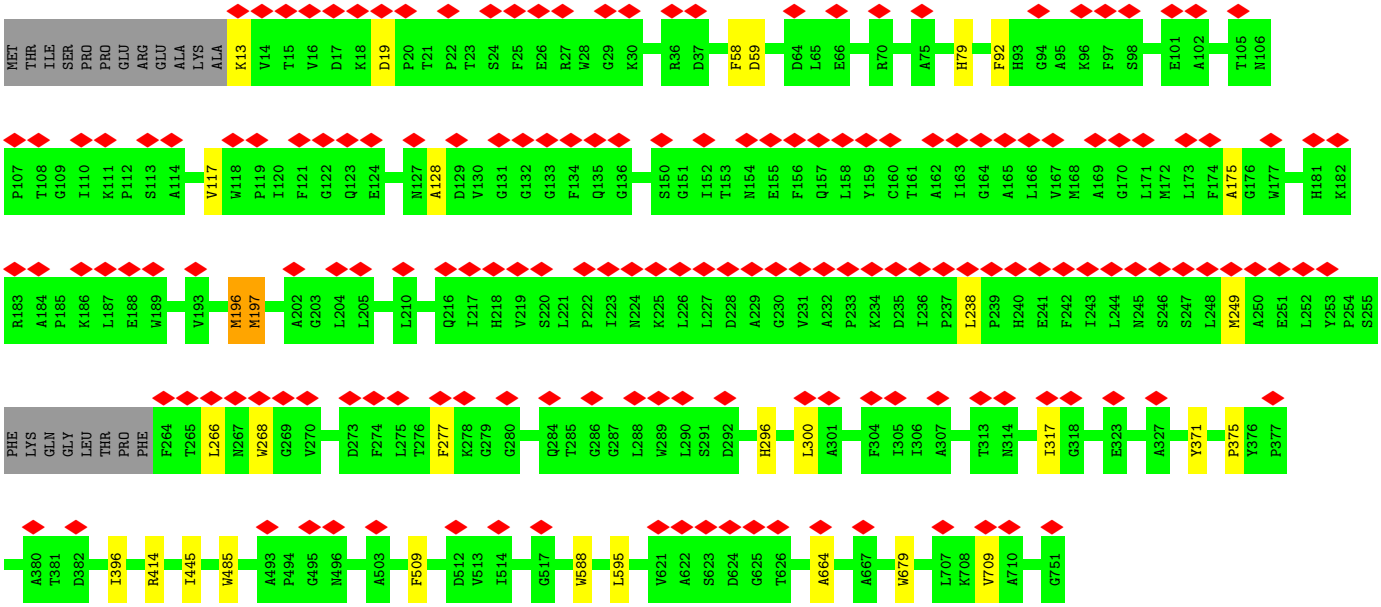
3 Residue-property plots (i)

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

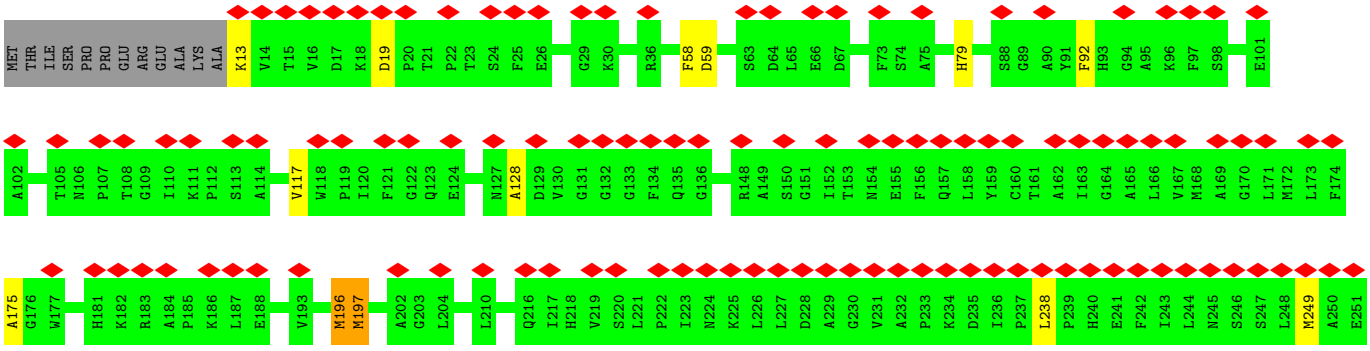
Chain A:

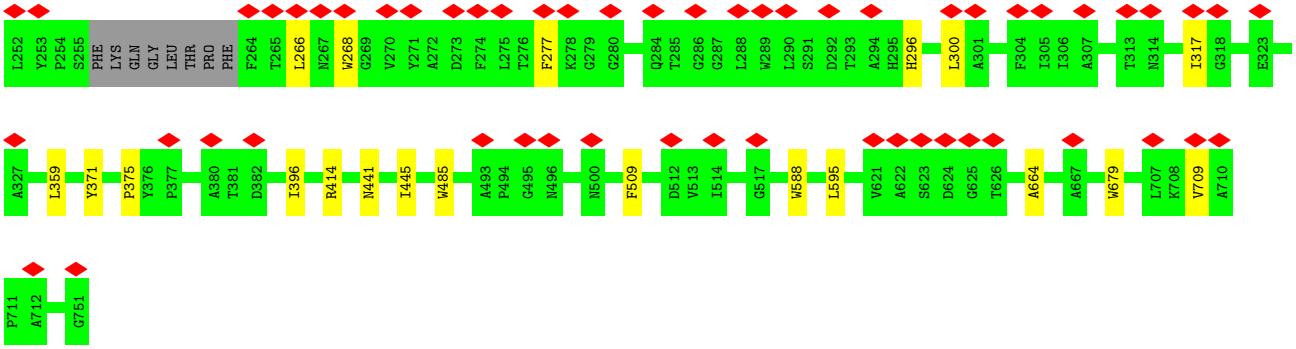




• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

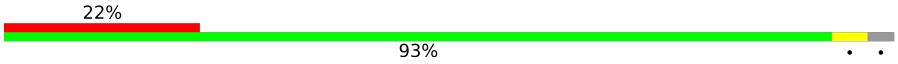
Chain bA:

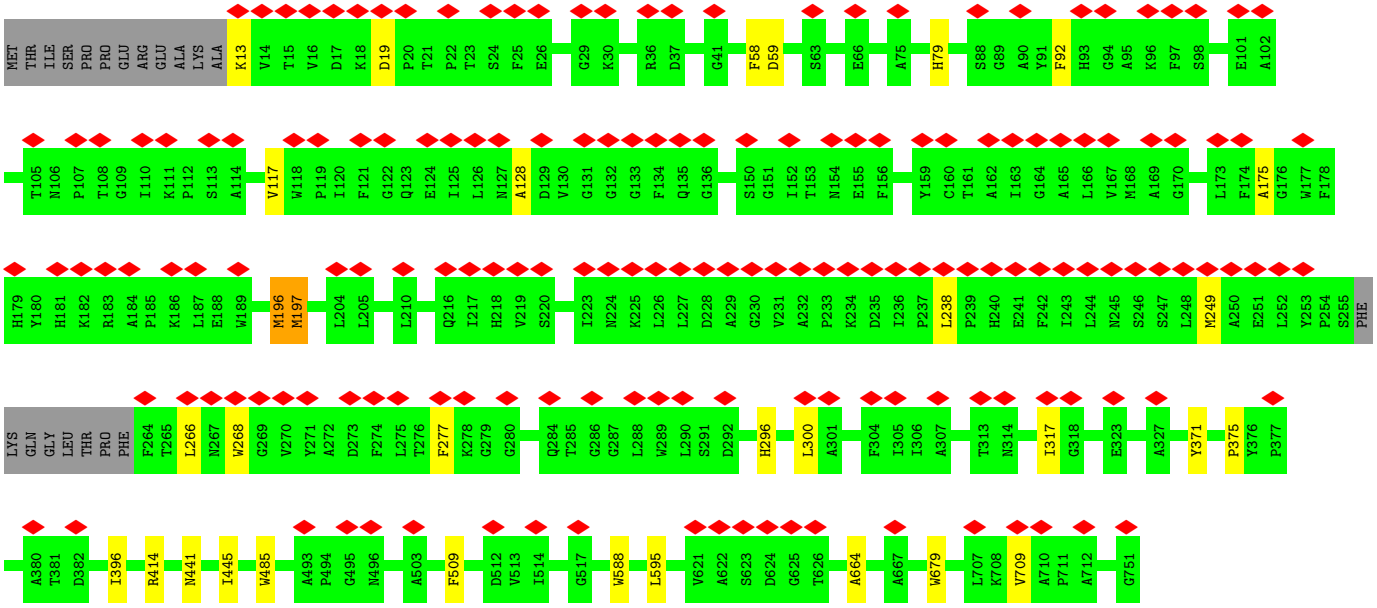




• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

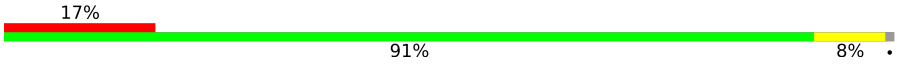
Chain cA:

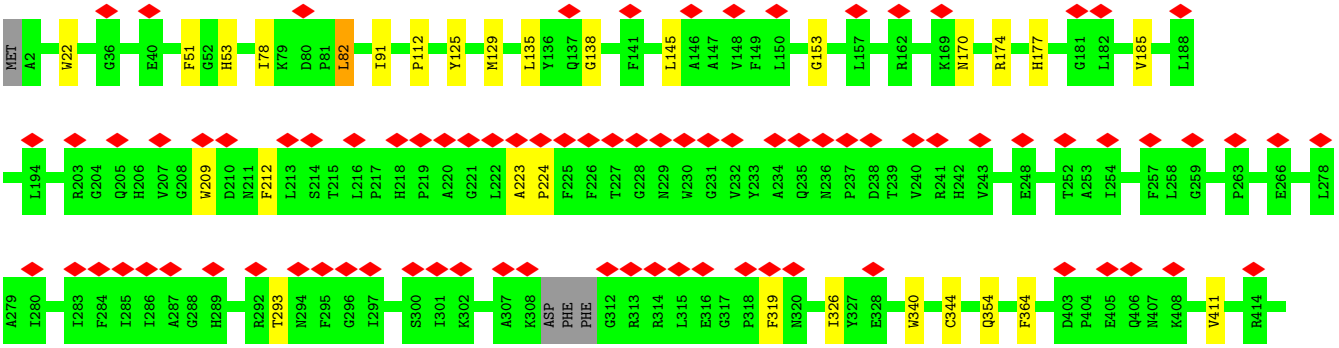


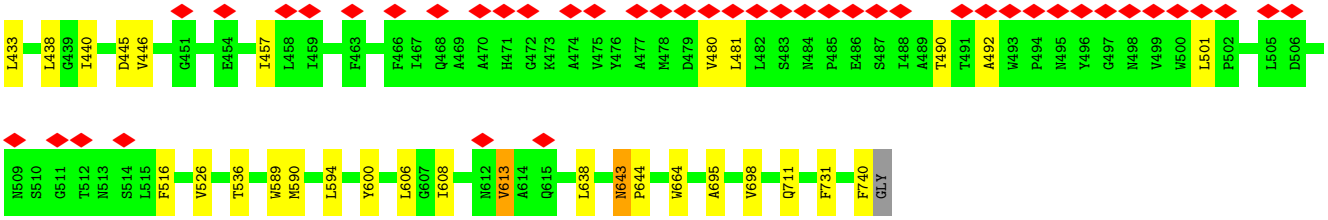


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

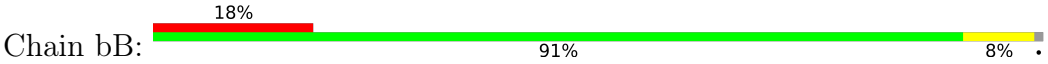
Chain B:

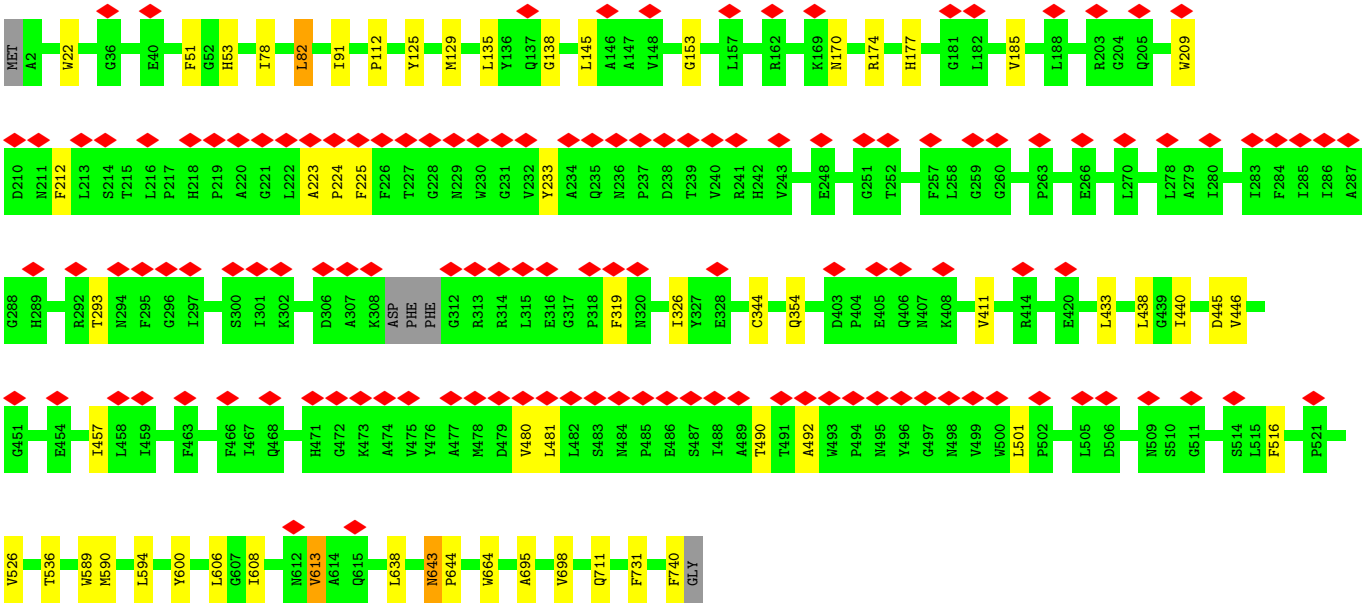




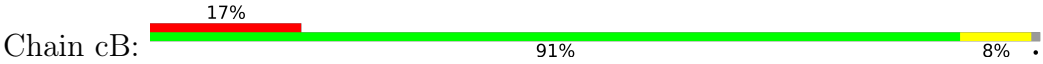


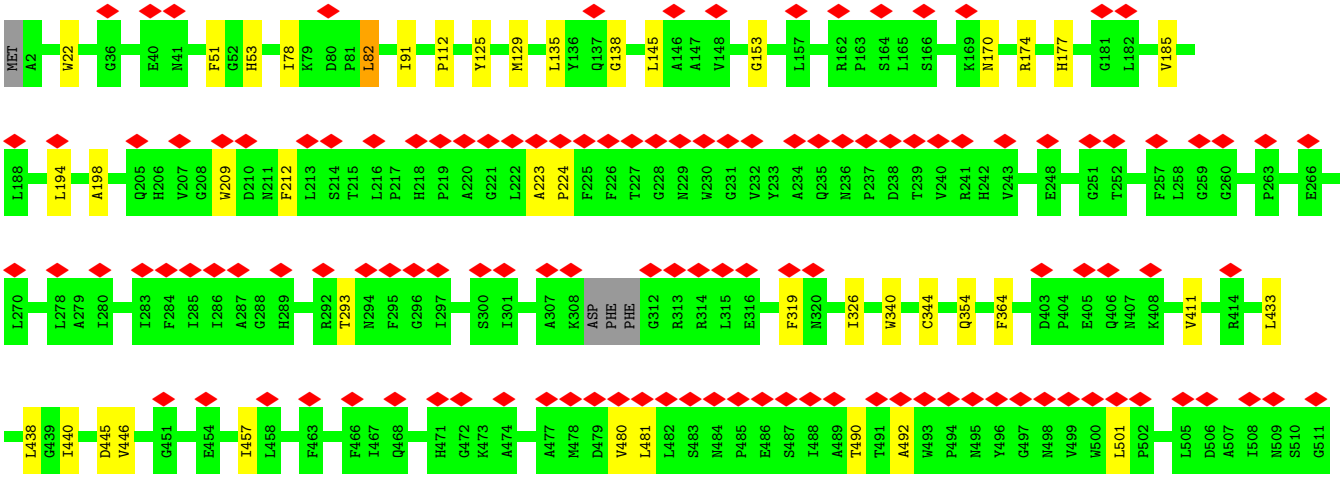
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

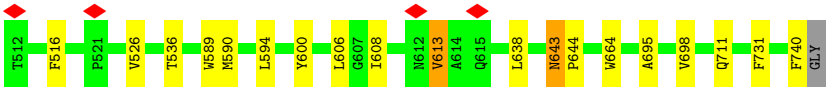




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

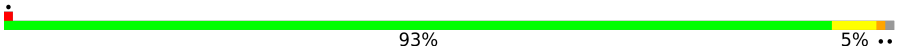


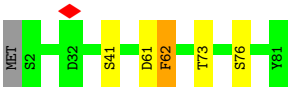




• Molecule 3: Photosystem I iron-sulfur center

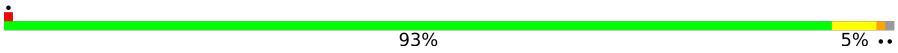
Chain C:

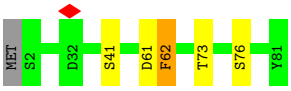




• Molecule 3: Photosystem I iron-sulfur center

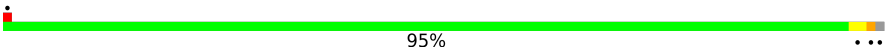
Chain bC:

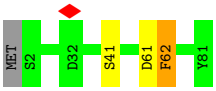




• Molecule 3: Photosystem I iron-sulfur center

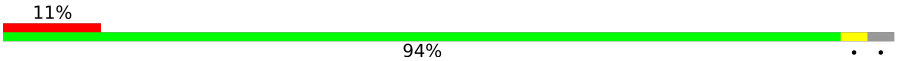
Chain cC:

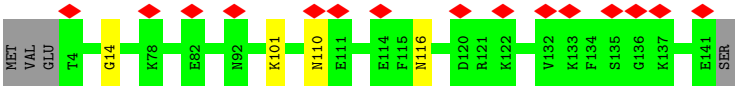




• Molecule 4: Photosystem I reaction center subunit II

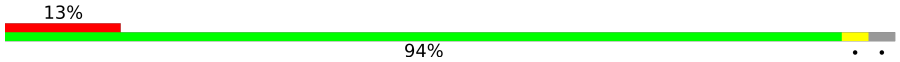
Chain D:

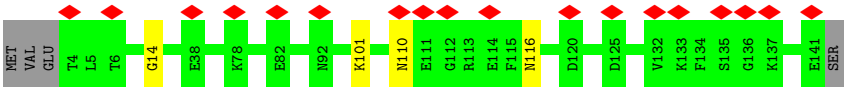




• Molecule 4: Photosystem I reaction center subunit II

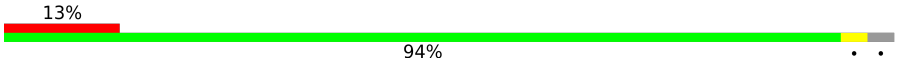
Chain bD:

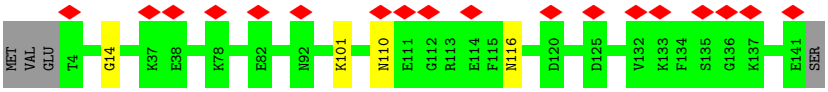




• Molecule 4: Photosystem I reaction center subunit II

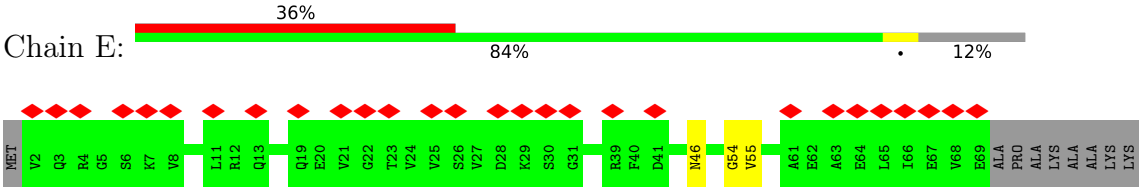
Chain cD:





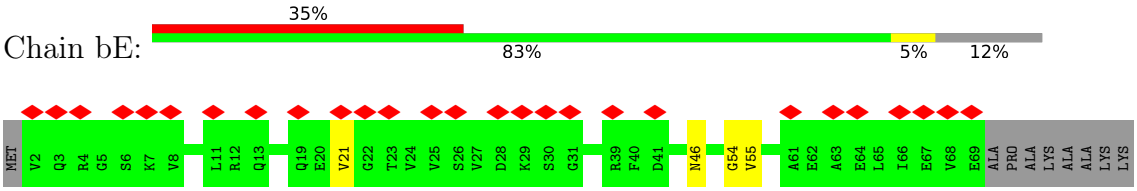
• Molecule 5: Photosystem I reaction center subunit IV

Chain E:



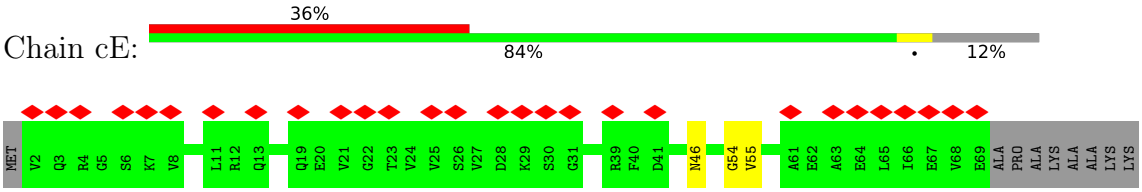
• Molecule 5: Photosystem I reaction center subunit IV

Chain bE:



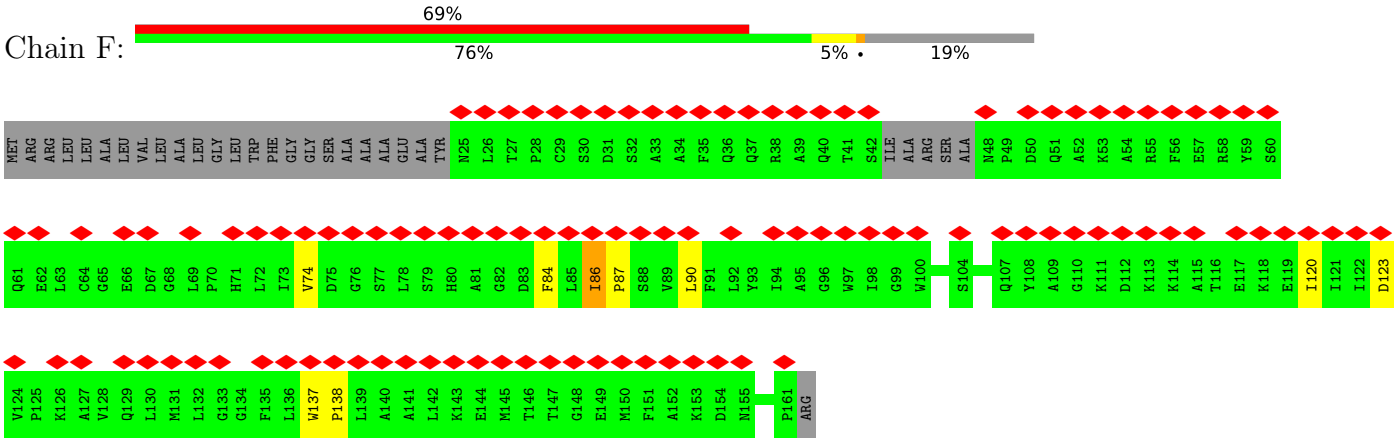
• Molecule 5: Photosystem I reaction center subunit IV

Chain cE:



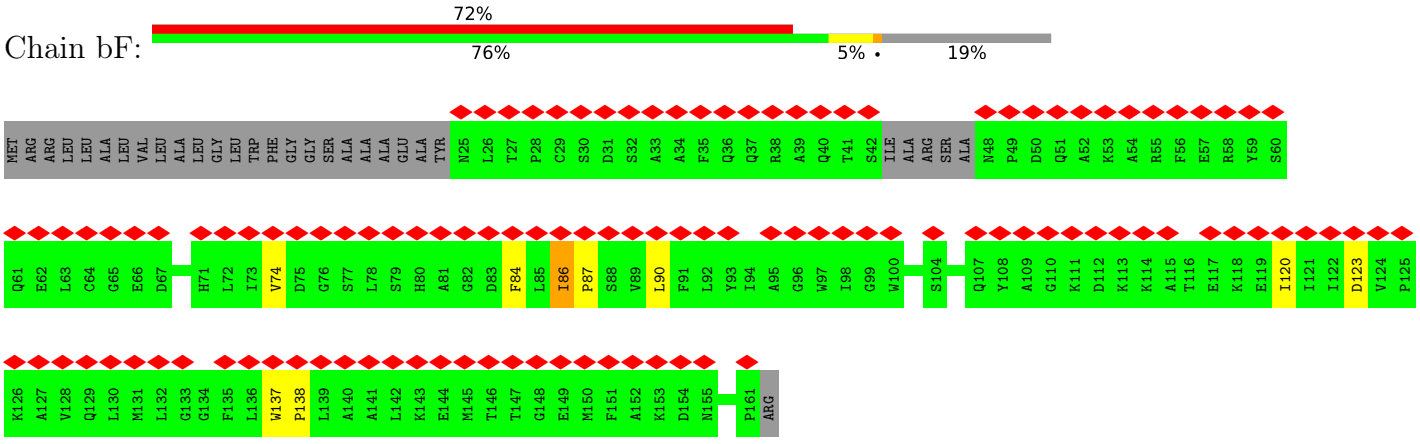
• Molecule 6: Photosystem I reaction center subunit III

Chain F:



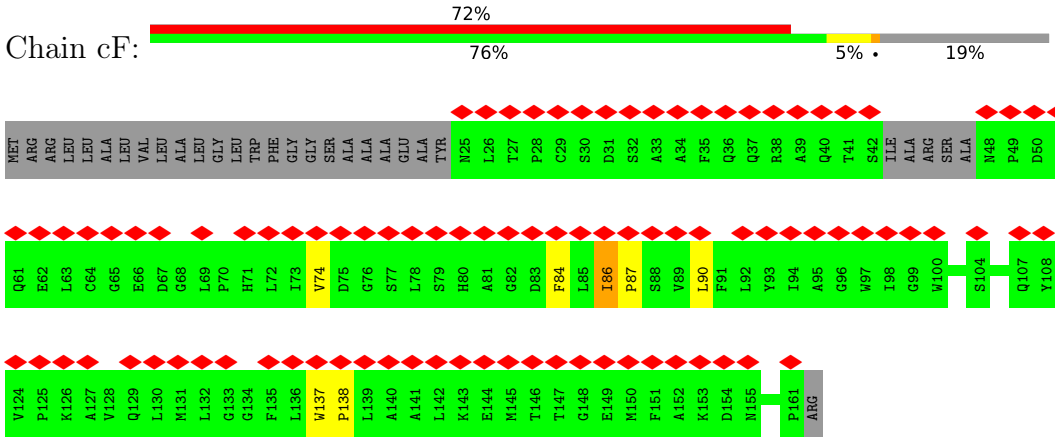
• Molecule 6: Photosystem I reaction center subunit III

Chain bF:



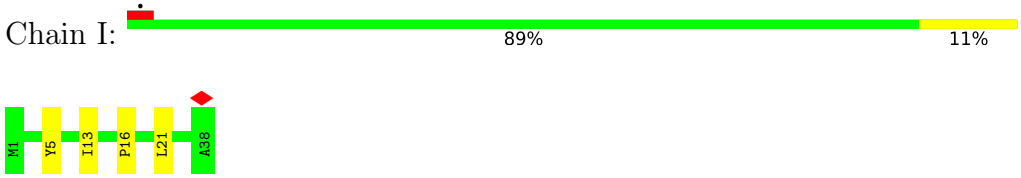
• Molecule 6: Photosystem I reaction center subunit III

Chain cF:



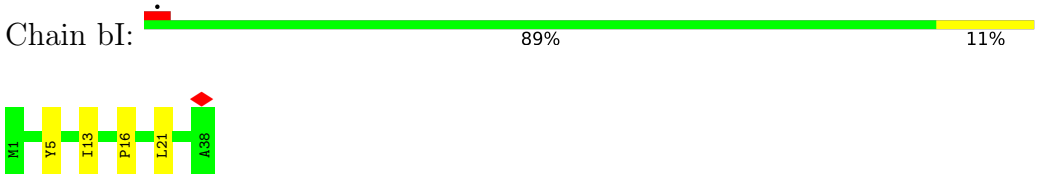
• Molecule 7: Photosystem I reaction center subunit VIII

Chain I:



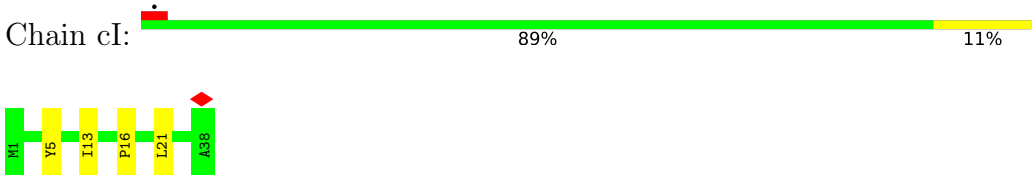
• Molecule 7: Photosystem I reaction center subunit VIII

Chain bI:



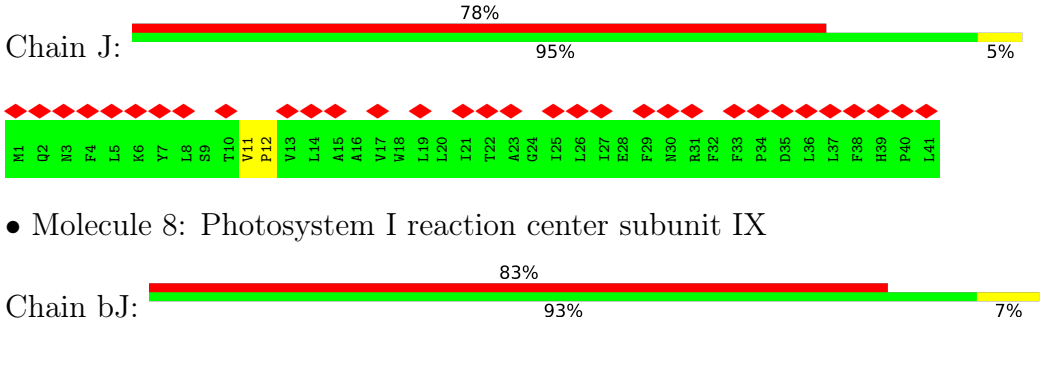
• Molecule 7: Photosystem I reaction center subunit VIII

Chain cI:



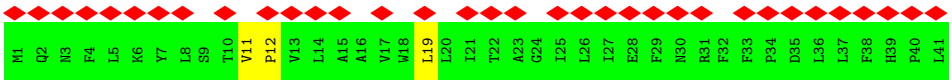
• Molecule 8: Photosystem I reaction center subunit IX

Chain J:

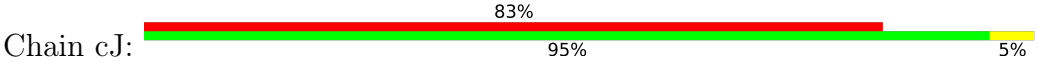


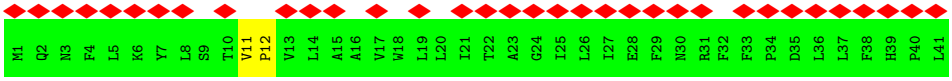
• Molecule 8: Photosystem I reaction center subunit IX

Chain bJ:

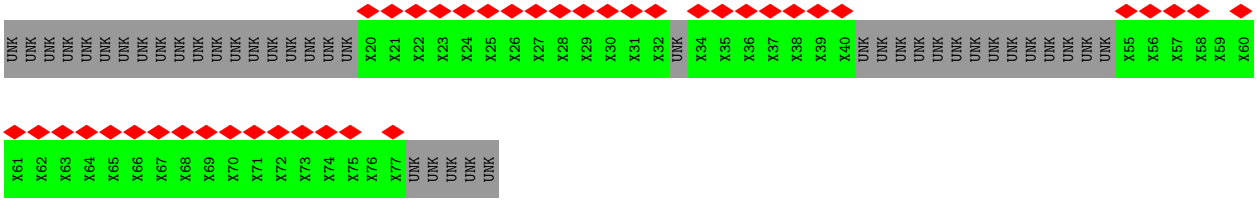


• Molecule 8: Photosystem I reaction center subunit IX

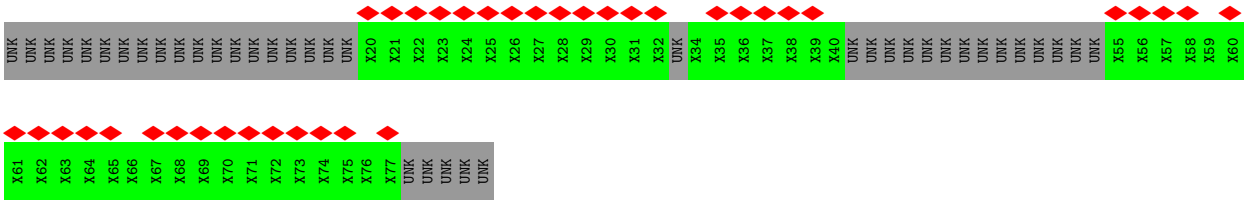




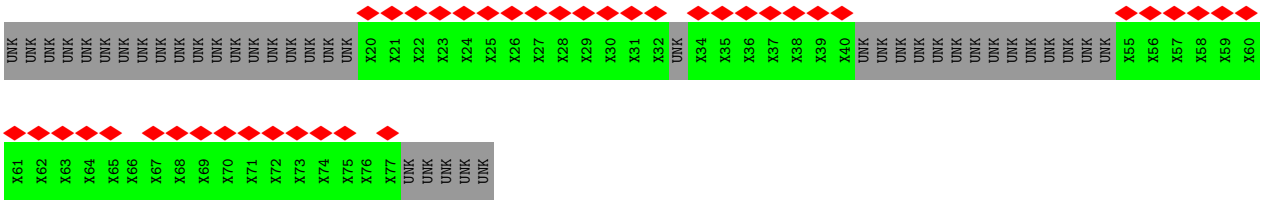
• Molecule 9: Unknown



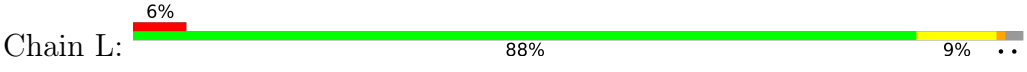
• Molecule 9: Unknown

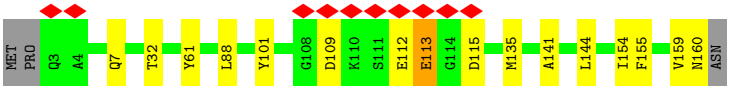


• Molecule 9: Unknown



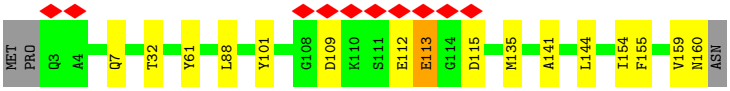
• Molecule 10: Photosystem I reaction center subunit XI





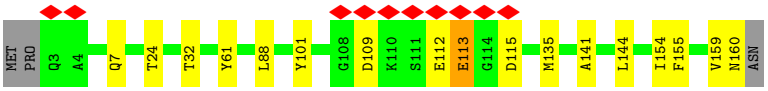
• Molecule 10: Photosystem I reaction center subunit XI

Chain bL:



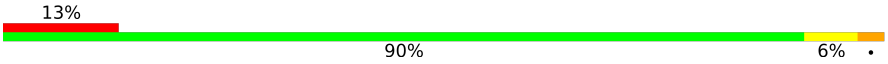
• Molecule 10: Photosystem I reaction center subunit XI

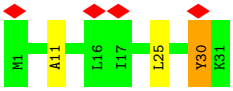
Chain cL:



• Molecule 11: Photosystem I reaction center subunit XII

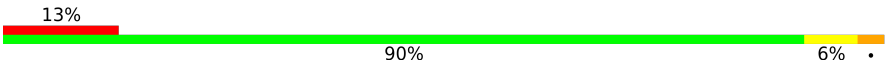
Chain M:

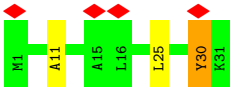




• Molecule 11: Photosystem I reaction center subunit XII

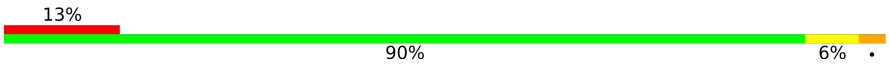
Chain bM:

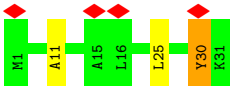




• Molecule 11: Photosystem I reaction center subunit XII

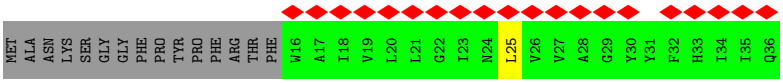
Chain cM:





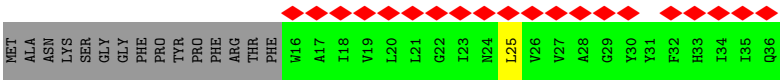
• Molecule 12: Photosystem I reaction center subunit psaX

Chain X:

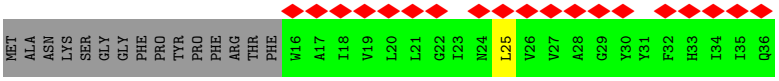


• Molecule 12: Photosystem I reaction center subunit psaX

Chain bX:



• Molecule 12: Photosystem I reaction center subunit psaX



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	121244	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	49	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.207	Depositor
Minimum map value	-0.090	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.019	Depositor
Map size (Å)	222.592, 222.592, 222.592	wwPDB
Map dimensions	296, 296, 296	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.752, 0.752, 0.752	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.03	0/5935	1.58	0/8086
1	bA	1.03	0/5935	1.58	0/8086
1	cA	1.03	0/5935	1.58	0/8086
2	B	1.02	0/6103	1.58	5/8339 (0.1%)
2	bB	1.02	0/6103	1.58	5/8339 (0.1%)
2	cB	1.02	0/6103	1.58	5/8339 (0.1%)
3	C	1.05	0/609	1.43	0/824
3	bC	1.05	0/609	1.43	0/824
3	cC	1.05	0/609	1.43	0/824
4	D	1.05	0/1107	1.39	1/1487 (0.1%)
4	bD	1.05	0/1107	1.39	1/1487 (0.1%)
4	cD	1.05	0/1107	1.39	1/1487 (0.1%)
5	E	1.08	0/553	1.37	0/748
5	bE	1.08	0/553	1.37	2/748 (0.3%)
5	cE	1.08	0/553	1.37	0/748
6	F	1.06	0/1046	1.64	2/1416 (0.1%)
6	bF	1.06	0/1046	1.64	2/1416 (0.1%)
6	cF	1.06	0/1046	1.64	2/1416 (0.1%)
7	I	1.07	0/307	1.52	0/420
7	bI	1.07	0/307	1.52	0/420
7	cI	1.07	0/307	1.52	0/420
8	J	0.99	0/350	1.54	0/477
8	bJ	0.99	0/350	1.54	0/477
8	cJ	0.99	0/350	1.54	0/477
10	L	1.23	2/1208 (0.2%)	1.65	2/1637 (0.1%)
10	bL	1.23	2/1208 (0.2%)	1.65	2/1637 (0.1%)
10	cL	1.23	3/1208 (0.2%)	1.65	2/1637 (0.1%)
11	M	1.06	0/244	1.62	0/330
11	bM	1.05	0/244	1.61	0/330
11	cM	1.05	0/244	1.61	0/330
12	X	1.04	0/176	1.71	0/241
12	bX	1.03	0/176	1.71	0/241

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
12	cX	1.03	0/176	1.71	0/241
All	All	1.05	7/52914 (0.0%)	1.57	32/72015 (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
3	C	0	1
3	bC	0	1
3	cC	0	1
All	All	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cL	113	GLU	CD-OE2	20.57	1.64	1.25
10	bL	113	GLU	CD-OE2	20.57	1.64	1.25
10	L	113	GLU	CD-OE2	20.56	1.64	1.25
10	bL	113	GLU	CD-OE1	12.51	1.49	1.25
10	cL	113	GLU	CD-OE1	12.50	1.49	1.25
10	L	113	GLU	CD-OE1	12.49	1.49	1.25
10	cL	24	THR	N-CA	5.01	1.49	1.46

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	14	GLY	CA-C-O	-6.59	117.94	122.22
4	bD	14	GLY	CA-C-O	-6.57	117.95	122.22
4	cD	14	GLY	CA-C-O	-6.56	117.95	122.22
6	F	123	ASP	CA-C-N	6.28	125.35	120.33
6	F	123	ASP	C-N-CA	6.28	125.35	120.33
6	bF	123	ASP	CA-C-N	6.27	125.34	120.33
6	bF	123	ASP	C-N-CA	6.27	125.34	120.33
6	cF	123	ASP	CA-C-N	6.26	125.34	120.33
6	cF	123	ASP	C-N-CA	6.26	125.34	120.33
10	L	113	GLU	CG-CD-OE1	-6.20	104.15	118.40
10	cL	113	GLU	CG-CD-OE1	-6.19	104.16	118.40
10	bL	113	GLU	CG-CD-OE1	-6.19	104.17	118.40
10	L	113	GLU	OE1-CD-OE2	5.46	136.01	122.90
10	cL	113	GLU	OE1-CD-OE2	5.45	135.99	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	bL	113	GLU	OE1-CD-OE2	5.45	135.97	122.90
2	cB	51	PHE	CA-C-N	5.37	125.94	119.98
2	cB	51	PHE	C-N-CA	5.37	125.94	119.98
2	B	51	PHE	CA-C-N	5.37	125.94	119.98
2	B	51	PHE	C-N-CA	5.37	125.94	119.98
2	bB	51	PHE	CA-C-N	5.37	125.94	119.98
2	bB	51	PHE	C-N-CA	5.37	125.94	119.98
2	bB	433	LEU	CA-C-N	5.09	125.59	119.94
2	bB	433	LEU	C-N-CA	5.09	125.59	119.94
2	cB	433	LEU	CA-C-N	5.09	125.59	119.94
2	cB	433	LEU	C-N-CA	5.09	125.59	119.94
2	B	433	LEU	CA-C-N	5.08	125.58	119.94
2	B	433	LEU	C-N-CA	5.08	125.58	119.94
2	B	643	ASN	CB-CA-C	5.03	116.89	110.76
2	bB	643	ASN	CB-CA-C	5.02	116.89	110.76
2	cB	643	ASN	CB-CA-C	5.02	116.88	110.76
5	bE	21	VAL	CA-C-N	5.00	125.88	121.58
5	bE	21	VAL	C-N-CA	5.00	125.88	121.58

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	62	PHE	Peptide
3	bC	62	PHE	Peptide
3	cC	62	PHE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5742	0	5606	20	0
1	bA	5742	0	5606	22	0
1	cA	5742	0	5606	21	0
2	B	5886	0	5653	37	0
2	bB	5886	0	5653	37	0
2	cB	5886	0	5653	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	599	0	579	2	0
3	bC	599	0	579	2	0
3	cC	599	0	579	1	0
4	D	1084	0	1087	1	0
4	bD	1084	0	1087	1	0
4	cD	1084	0	1087	1	0
5	E	544	0	531	0	0
5	bE	544	0	531	0	0
5	cE	544	0	531	0	0
6	F	1023	0	1007	3	0
6	bF	1023	0	1007	3	0
6	cF	1023	0	1007	3	0
7	I	297	0	303	9	0
7	bI	297	0	303	9	0
7	cI	297	0	303	9	0
8	J	339	0	355	1	0
8	bJ	339	0	355	2	0
8	cJ	339	0	355	1	0
9	K	208	0	45	0	0
9	bK	208	0	45	0	0
9	cK	208	0	45	0	0
10	L	1178	0	1145	18	0
10	bL	1178	0	1145	18	0
10	cL	1178	0	1145	18	0
11	M	241	0	264	2	0
11	bM	241	0	264	2	0
11	cM	241	0	264	2	0
12	X	171	0	177	2	0
12	bX	171	0	177	2	0
12	cX	171	0	177	2	0
13	A	65	0	72	5	0
13	bA	65	0	72	5	0
13	cA	65	0	72	5	0
14	A	2204	0	1960	68	0
14	B	2166	0	1946	62	0
14	F	51	0	41	1	0
14	J	90	0	66	3	0
14	L	254	0	274	14	0
14	X	45	0	33	3	0
14	bA	2204	0	1960	71	0
14	bB	2166	0	1946	62	0
14	bF	51	0	41	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	bJ	90	0	66	3	0
14	bL	254	0	274	15	0
14	bX	45	0	33	3	0
14	cA	2204	0	1960	69	0
14	cB	2166	0	1946	65	0
14	cF	51	0	41	1	0
14	cJ	90	0	66	3	0
14	cL	254	0	274	13	0
14	cX	45	0	33	3	0
15	A	33	0	46	0	0
15	B	33	0	46	1	0
15	bA	33	0	46	0	0
15	bB	33	0	46	1	0
15	cA	33	0	46	0	0
15	cB	33	0	46	1	0
16	A	8	0	0	0	0
16	C	16	0	0	0	0
16	bA	8	0	0	0	0
16	bC	16	0	0	0	0
16	cA	8	0	0	0	0
16	cC	16	0	0	0	0
17	A	200	0	280	5	0
17	B	320	0	448	12	0
17	F	40	0	56	0	0
17	I	80	0	112	2	0
17	J	40	0	56	6	0
17	L	80	0	112	6	0
17	M	40	0	56	2	0
17	bA	200	0	280	5	0
17	bB	320	0	448	13	0
17	bF	40	0	56	0	0
17	bI	80	0	112	2	0
17	bJ	40	0	56	6	0
17	bL	80	0	112	6	0
17	bM	40	0	56	2	0
17	cA	200	0	280	5	0
17	cB	320	0	448	13	0
17	cF	40	0	56	0	0
17	cI	80	0	112	2	0
17	cJ	40	0	56	6	0
17	cL	80	0	112	7	0
17	cM	40	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	A	76	0	98	0	0
18	bA	76	0	98	0	0
18	cA	76	0	98	0	0
19	A	12	0	0	0	0
19	I	22	0	0	0	0
19	L	29	0	0	0	0
19	bA	12	0	0	0	0
19	bI	22	0	0	0	0
19	bL	29	0	0	0	0
19	cA	12	0	0	0	0
19	cI	22	0	0	0	0
19	cL	29	0	0	0	0
20	B	43	0	56	0	0
20	bB	43	0	56	0	0
20	cB	43	0	56	0	0
21	L	1	0	0	0	0
21	bL	1	0	0	0	0
21	cL	1	0	0	0	0
22	A	39	0	0	0	0
22	B	30	0	0	0	0
22	C	14	0	0	0	0
22	D	10	0	0	0	0
22	E	3	0	0	0	0
22	I	2	0	0	0	0
22	L	19	0	0	1	0
22	bA	39	0	0	0	0
22	bB	30	0	0	0	0
22	bC	14	0	0	0	0
22	bD	10	0	0	0	0
22	bE	3	0	0	0	0
22	bI	2	0	0	0	0
22	bL	19	0	0	0	0
22	cA	39	0	0	0	0
22	cB	30	0	0	0	0
22	cC	14	0	0	0	0
22	cD	10	0	0	0	0
22	cE	3	0	0	0	0
22	cI	2	0	0	0	0
22	cL	19	0	0	0	0
All	All	70131	0	67530	652	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 (652) 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)
10:cL:113:GLU:CD	10:cL:113:GLU:OE2	1.64	1.41
10:bL:113:GLU:CD	10:bL:113:GLU:OE2	1.64	1.39
10:L:113:GLU:CD	10:L:113:GLU:OE2	1.64	1.38
14:bA:829:CLA:H191	14:bB:801:CLA:H191	1.70	0.73
14:cA:829:CLA:H191	14:cB:802:CLA:H191	1.70	0.73
14:A:829:CLA:H191	14:B:801:CLA:H191	1.70	0.72
17:cM:101:BCR:H403	17:cM:101:BCR:H23C	1.74	0.69
17:M:101:BCR:H403	17:M:101:BCR:H23C	1.74	0.69
17:bM:101:BCR:H321	17:bM:101:BCR:HC8	1.75	0.68
14:bA:827:CLA:H93	17:bJ:103:BCR:H361	1.76	0.68
17:M:101:BCR:H321	17:M:101:BCR:HC8	1.75	0.68
17:cM:101:BCR:H321	17:cM:101:BCR:HC8	1.75	0.68
17:bM:101:BCR:H403	17:bM:101:BCR:H23C	1.74	0.68
14:cA:827:CLA:H93	17:cJ:103:BCR:H361	1.76	0.68
14:A:827:CLA:H93	17:J:103:BCR:H361	1.76	0.67
7:I:16:PRO:CG	10:bL:155:PHE:HE2	2.09	0.65
10:L:155:PHE:HE2	7:cI:16:PRO:CG	2.09	0.65
7:bI:16:PRO:CG	10:cL:155:PHE:HE2	2.09	0.65
7:bI:13:ILE:CD1	14:cL:205:CLA:C9	2.75	0.64
7:I:13:ILE:CD1	14:bL:204:CLA:C9	2.75	0.64
14:L:204:CLA:C9	7:cI:13:ILE:CD1	2.75	0.64
14:B:804:CLA:HBC3	14:B:828:CLA:H41	1.82	0.62
14:cB:805:CLA:HBC3	14:cB:829:CLA:H41	1.82	0.60
14:bB:804:CLA:HBC3	14:bB:828:CLA:H41	1.82	0.59
10:cL:141:ALA:HB1	14:cL:205:CLA:HED1	1.84	0.59
10:L:141:ALA:HB1	14:L:204:CLA:HED1	1.84	0.58
17:bB:842:BCR:H11C	17:bB:842:BCR:H331	1.86	0.58
10:bL:141:ALA:HB1	14:bL:204:CLA:HED1	1.84	0.58
14:A:802:CLA:OBD	14:B:802:CLA:HMB2	2.04	0.58
1:A:396:ILE:HD13	14:A:827:CLA:HBC3	1.86	0.57
1:bA:396:ILE:HD13	14:bA:827:CLA:HBC3	1.86	0.57
17:B:842:BCR:H11C	17:B:842:BCR:H331	1.86	0.57
14:cA:841:CLA:HMB2	2:cB:698:VAL:HG11	1.87	0.57
6:F:86:ILE:HG13	6:F:87:PRO:HD3	1.86	0.57
14:bA:802:CLA:OBD	14:bB:802:CLA:HMB2	2.04	0.57
14:A:841:CLA:HMB2	2:B:698:VAL:HG11	1.87	0.57
14:bA:841:CLA:HMB2	2:bB:698:VAL:HG11	1.87	0.57
17:bB:844:BCR:H321	17:bB:844:BCR:HC8	1.87	0.56
6:bF:86:ILE:HG13	6:bF:87:PRO:HD3	1.86	0.56
17:cB:845:BCR:H321	17:cB:845:BCR:HC8	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:cA:277:PHE:CE2	14:cA:835:CLA:HED2	2.40	0.56
17:cB:843:BCR:H11C	17:cB:843:BCR:H331	1.86	0.56
14:cA:802:CLA:OBD	14:cB:803:CLA:HMB2	2.04	0.56
1:cA:396:ILE:HD13	14:cA:827:CLA:HBC3	1.86	0.56
17:cJ:103:BCR:H372	17:cJ:103:BCR:H19C	1.88	0.56
1:A:277:PHE:CE2	14:A:835:CLA:HED2	2.40	0.56
17:B:844:BCR:H321	17:B:844:BCR:HC8	1.87	0.56
2:B:344:CYS:HB3	14:B:823:CLA:H42	1.88	0.56
14:B:831:CLA:CBB	17:B:846:BCR:H323	2.37	0.55
17:J:103:BCR:H19C	17:J:103:BCR:H372	1.88	0.55
7:I:13:ILE:HD13	14:bL:204:CLA:C9	2.36	0.55
6:cF:86:ILE:HG13	6:cF:87:PRO:HD3	1.86	0.55
7:I:13:ILE:CD1	14:bL:204:CLA:H91	2.37	0.55
14:bB:801:CLA:HMB3	14:bB:801:CLA:HBB1	1.88	0.55
14:cB:832:CLA:CBB	17:cB:847:BCR:H323	2.37	0.55
14:bA:802:CLA:H91	14:bA:852:CLA:H102	1.88	0.55
2:bB:698:VAL:HG23	10:bL:101:TYR:CE2	2.41	0.55
7:bI:13:ILE:CD1	14:cL:205:CLA:H91	2.37	0.55
7:bI:13:ILE:HD13	14:cL:205:CLA:C9	2.36	0.55
2:cB:698:VAL:HG23	10:cL:101:TYR:CE2	2.41	0.55
14:B:801:CLA:HBB1	14:B:801:CLA:HMB3	1.88	0.55
1:A:197:MET:HE3	14:A:820:CLA:HMA2	1.89	0.55
1:bA:277:PHE:CE2	14:bA:835:CLA:HED2	2.40	0.55
17:cI:102:BCR:H383	14:cL:204:CLA:H43	1.89	0.55
17:cJ:103:BCR:H321	17:cJ:103:BCR:HC8	1.89	0.55
14:B:826:CLA:HBC3	14:B:826:CLA:HHD	1.89	0.55
14:cA:802:CLA:H91	14:cA:852:CLA:H102	1.88	0.55
14:cB:827:CLA:HBC3	14:cB:827:CLA:HHD	1.89	0.55
14:bB:826:CLA:HBC3	14:bB:826:CLA:HHD	1.89	0.54
17:bJ:103:BCR:H19C	17:bJ:103:BCR:H372	1.88	0.54
17:bJ:103:BCR:H321	17:bJ:103:BCR:HC8	1.89	0.54
1:cA:197:MET:HE3	14:cA:820:CLA:HMA2	1.89	0.54
2:B:698:VAL:HG23	10:L:101:TYR:CE2	2.41	0.54
14:bB:831:CLA:CBB	17:bB:846:BCR:H323	2.37	0.54
2:cB:344:CYS:HB3	14:cB:824:CLA:H42	1.88	0.54
14:A:802:CLA:H91	14:A:852:CLA:H102	1.88	0.54
2:bB:22:TRP:CG	2:bB:711:GLN:HE22	2.26	0.54
14:A:802:CLA:HBB1	14:A:802:CLA:HMB3	1.89	0.54
2:bB:344:CYS:HB3	14:bB:823:CLA:H42	1.88	0.54
2:cB:22:TRP:CG	2:cB:711:GLN:HE22	2.26	0.54
2:B:53:HIS:CE1	14:B:805:CLA:HMA2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:cB:53:HIS:CE1	14:cB:806:CLA:HMA2	2.43	0.54
2:bB:53:HIS:CE1	14:bB:805:CLA:HMA2	2.43	0.54
14:L:204:CLA:H91	7:cI:13:ILE:CD1	2.37	0.54
2:B:22:TRP:CG	2:B:711:GLN:HE22	2.26	0.54
17:I:102:BCR:H383	14:L:203:CLA:H43	1.89	0.54
14:L:204:CLA:C9	7:cI:13:ILE:HD13	2.36	0.54
14:cA:825:CLA:HBB1	14:cA:825:CLA:HMB3	1.90	0.54
14:cB:802:CLA:HMB3	14:cB:802:CLA:HBB1	1.88	0.53
17:J:103:BCR:H321	17:J:103:BCR:HC8	1.89	0.53
1:bA:197:MET:HE3	14:bA:820:CLA:HMA2	1.89	0.53
14:bB:831:CLA:HHD	14:bB:831:CLA:HBC2	1.91	0.53
17:bI:102:BCR:H383	14:bL:203:CLA:H43	1.89	0.53
2:cB:643:ASN:HB2	2:cB:644:PRO:HD2	1.91	0.53
12:cX:25:LEU:CD2	14:cX:201:CLA:HED1	2.39	0.53
2:B:138:GLY:HA2	17:B:843:BCR:H381	1.91	0.53
2:cB:138:GLY:HA2	17:cB:844:BCR:H381	1.91	0.53
14:A:825:CLA:HBB1	14:A:825:CLA:HMB3	1.90	0.52
17:cA:847:BCR:H331	17:cA:847:BCR:C8	2.39	0.52
14:bA:802:CLA:HBB1	14:bA:802:CLA:HMB3	1.89	0.52
14:bA:826:CLA:HBB1	14:bA:826:CLA:HMB1	1.92	0.52
14:L:204:CLA:H92	7:cI:13:ILE:HD13	1.92	0.52
12:bX:25:LEU:CD2	14:bX:201:CLA:HED1	2.39	0.52
14:cA:802:CLA:HBB1	14:cA:802:CLA:HMB3	1.90	0.52
14:bA:837:CLA:HHC	14:bA:837:CLA:HBB1	1.92	0.52
14:cA:837:CLA:HHC	14:cA:837:CLA:HBB1	1.92	0.52
14:bA:825:CLA:HBB1	14:bA:825:CLA:HMB3	1.90	0.52
2:bB:138:GLY:HA2	17:bB:843:BCR:H381	1.91	0.52
14:A:826:CLA:HBB1	14:A:826:CLA:HMB1	1.92	0.52
10:L:113:GLU:HB3	10:bL:115:ASP:HB2	1.92	0.52
17:A:847:BCR:H331	17:A:847:BCR:C8	2.39	0.52
14:B:831:CLA:HBC2	14:B:831:CLA:HHD	1.90	0.52
14:A:837:CLA:HHC	14:A:837:CLA:HBB1	1.92	0.52
12:X:25:LEU:CD2	14:X:201:CLA:HED1	2.39	0.52
14:cA:826:CLA:HBB1	14:cA:826:CLA:HMB1	1.92	0.52
2:bB:643:ASN:HB2	2:bB:644:PRO:HD2	1.91	0.52
14:bB:813:CLA:HMB1	14:bB:813:CLA:HBB1	1.92	0.52
14:cB:832:CLA:HBC2	14:cB:832:CLA:HHD	1.90	0.51
10:bL:113:GLU:HB3	10:cL:115:ASP:HB2	1.92	0.51
2:bB:326:ILE:HD11	2:bB:411:VAL:HG12	1.92	0.51
14:cB:814:CLA:HBB1	14:cB:814:CLA:HMB1	1.92	0.51
2:B:643:ASN:HB2	2:B:644:PRO:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:GLY:HA3	11:M:25:LEU:HD13	1.93	0.51
14:B:803:CLA:HBB1	14:B:803:CLA:HMB3	1.92	0.51
7:I:13:ILE:HD13	14:bL:204:CLA:H92	1.91	0.51
2:bB:153:GLY:HA3	11:bM:25:LEU:HD13	1.93	0.51
7:bI:13:ILE:HD13	14:cL:205:CLA:H92	1.92	0.51
14:A:838:CLA:HHC	14:A:838:CLA:HBB1	1.92	0.51
14:cA:834:CLA:HHC	14:cA:834:CLA:HBB1	1.93	0.51
2:B:129:MET:HE3	2:B:135:LEU:HD23	1.93	0.51
14:A:828:CLA:HMB3	14:A:828:CLA:HBB1	1.93	0.51
14:B:813:CLA:HMB1	14:B:813:CLA:HBB1	1.92	0.51
14:B:827:CLA:H143	17:B:842:BCR:C17	2.41	0.51
14:L:201:CLA:HHC	14:L:201:CLA:HBB1	1.93	0.51
10:L:115:ASP:HB2	10:cL:113:GLU:HB3	1.92	0.51
2:cB:326:ILE:HD11	2:cB:411:VAL:HG12	1.92	0.51
14:cL:202:CLA:HHC	14:cL:202:CLA:HBB1	1.93	0.50
14:bB:803:CLA:HMB3	14:bB:803:CLA:HBB1	1.92	0.50
14:bL:201:CLA:HHC	14:bL:201:CLA:HBB1	1.93	0.50
14:cB:828:CLA:H143	17:cB:843:BCR:C17	2.41	0.50
2:B:326:ILE:HD11	2:B:411:VAL:HG12	1.92	0.50
14:cA:828:CLA:HMB3	14:cA:828:CLA:HBB1	1.93	0.50
14:cA:841:CLA:HHC	14:cA:841:CLA:HBB1	1.94	0.50
14:cA:852:CLA:H112	17:cB:848:BCR:H362	1.94	0.50
14:bA:806:CLA:HHC	14:bA:806:CLA:HBB1	1.94	0.50
14:bA:841:CLA:HHC	14:bA:841:CLA:HBB1	1.94	0.50
14:bA:834:CLA:HHC	14:bA:834:CLA:HBB1	1.93	0.50
17:bA:847:BCR:H331	17:bA:847:BCR:C8	2.39	0.50
14:cB:807:CLA:HHC	14:cB:807:CLA:HBB1	1.94	0.50
17:cL:206:BCR:H403	17:cL:206:BCR:H23C	1.94	0.50
14:A:834:CLA:HHC	14:A:834:CLA:HBB1	1.93	0.50
14:J:102:CLA:HHC	14:J:102:CLA:HBB1	1.94	0.50
14:bA:828:CLA:HBB1	14:bA:828:CLA:HMB3	1.93	0.50
14:bB:827:CLA:H143	17:bB:842:BCR:C17	2.41	0.50
14:cB:804:CLA:HBB1	14:cB:804:CLA:HMB3	1.92	0.50
17:bA:849:BCR:H331	17:bA:849:BCR:C8	2.42	0.50
14:bL:202:CLA:HBB1	14:bL:202:CLA:HMB3	1.94	0.50
14:cA:838:CLA:HHC	14:cA:838:CLA:HBB1	1.92	0.50
2:cB:129:MET:HE3	2:cB:135:LEU:HD23	1.93	0.50
2:cB:153:GLY:HA3	11:cM:25:LEU:HD13	1.93	0.50
2:B:177:HIS:ND1	14:B:812:CLA:HMC2	2.27	0.49
14:bJ:102:CLA:HHC	14:bJ:102:CLA:HBB1	1.94	0.49
17:cB:845:BCR:C31	17:cB:846:BCR:H402	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:202:CLA:HBB1	14:L:202:CLA:HMB3	1.94	0.49
14:bA:838:CLA:HHC	14:bA:838:CLA:HBB1	1.92	0.49
2:cB:177:HIS:ND1	14:cB:813:CLA:HMC2	2.27	0.49
14:A:806:CLA:HHC	14:A:806:CLA:HBB1	1.94	0.49
14:B:806:CLA:HHC	14:B:806:CLA:HBB1	1.94	0.49
17:B:850:BCR:C8	17:B:850:BCR:H311	2.42	0.49
14:bA:809:CLA:HMB1	14:bA:809:CLA:HBB1	1.95	0.49
14:bA:832:CLA:HBB1	14:bA:832:CLA:HHC	1.94	0.49
17:bB:850:BCR:C8	17:bB:850:BCR:H311	2.42	0.49
14:cJ:102:CLA:HBB1	14:cJ:102:CLA:HHC	1.94	0.49
1:A:79:HIS:CE1	14:A:805:CLA:HMA2	2.48	0.49
14:A:841:CLA:HHC	14:A:841:CLA:HBB1	1.94	0.49
14:bA:852:CLA:H112	17:bB:847:BCR:H362	1.94	0.49
2:bB:177:HIS:ND1	14:bB:812:CLA:HMC2	2.27	0.49
13:A:801:CL0:H12	14:B:803:CLA:OBD	2.13	0.49
17:A:849:BCR:H331	17:A:849:BCR:C8	2.42	0.49
1:cA:79:HIS:CE1	14:cA:805:CLA:HMA2	2.48	0.49
14:cA:809:CLA:HBB1	14:cA:809:CLA:HMB1	1.95	0.49
14:A:832:CLA:HHC	14:A:832:CLA:HBB1	1.94	0.49
14:A:852:CLA:H112	17:B:847:BCR:H362	1.94	0.49
14:bB:839:CLA:HHC	14:bB:839:CLA:HBB1	1.95	0.49
17:bL:205:BCR:H403	17:bL:205:BCR:H23C	1.94	0.49
2:bB:129:MET:HE3	2:bB:135:LEU:HD23	1.93	0.49
17:cB:851:BCR:H311	17:cB:851:BCR:C8	2.42	0.49
17:bB:844:BCR:C31	17:bB:845:BCR:H402	2.42	0.49
14:cA:832:CLA:HHC	14:cA:832:CLA:HBB1	1.94	0.49
1:A:396:ILE:CD1	14:A:827:CLA:HBC3	2.43	0.49
17:A:849:BCR:H272	17:J:103:BCR:H313	1.95	0.49
14:B:827:CLA:HMB3	14:B:827:CLA:HBB1	1.94	0.49
17:B:844:BCR:C31	17:B:845:BCR:H402	2.42	0.48
14:bA:822:CLA:HHC	14:bA:822:CLA:HBB1	1.95	0.48
14:A:822:CLA:HHC	14:A:822:CLA:HBB1	1.95	0.48
1:bA:396:ILE:CD1	14:bA:827:CLA:HBC3	2.43	0.48
2:bB:695:ALA:O	2:bB:698:VAL:HG12	2.13	0.48
13:cA:801:CL0:H12	14:cB:804:CLA:OBD	2.13	0.48
17:cA:849:BCR:H272	17:cJ:103:BCR:H313	1.95	0.48
17:cA:849:BCR:H331	17:cA:849:BCR:C8	2.42	0.48
17:L:205:BCR:H403	17:L:205:BCR:H23C	1.94	0.48
2:B:695:ALA:O	2:B:698:VAL:HG12	2.13	0.48
14:B:813:CLA:HAB	14:B:827:CLA:H193	1.96	0.48
14:B:836:CLA:HBB1	14:B:836:CLA:HMB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:bB:827:CLA:HBB1	14:bB:827:CLA:HMB3	1.94	0.48
17:bJ:103:BCR:C8	17:bJ:103:BCR:H311	2.43	0.48
10:L:155:PHE:CE2	7:cI:16:PRO:CG	2.94	0.48
14:bB:806:CLA:HHC	14:bB:806:CLA:HBB1	1.94	0.48
1:cA:396:ILE:CD1	14:cA:827:CLA:HBC3	2.43	0.48
14:cA:806:CLA:HHC	14:cA:806:CLA:HBB1	1.94	0.48
14:cB:837:CLA:HBB1	14:cB:837:CLA:HMB3	1.95	0.48
14:A:809:CLA:HBB1	14:A:809:CLA:HMB1	1.95	0.48
14:B:828:CLA:H93	14:B:839:CLA:HED1	1.96	0.48
14:bB:813:CLA:HAB	14:bB:827:CLA:H193	1.96	0.48
14:cB:817:CLA:HHC	14:cB:817:CLA:HBB1	1.96	0.48
14:B:838:CLA:HBB2	15:B:840:PQN:H141	1.95	0.48
14:B:839:CLA:HBB1	14:B:839:CLA:HHC	1.95	0.48
17:J:103:BCR:C8	17:J:103:BCR:H311	2.43	0.48
1:bA:79:HIS:CE1	14:bA:805:CLA:HMA2	2.48	0.48
13:bA:801:CL0:H12	14:bB:803:CLA:OBD	2.13	0.48
14:bA:823:CLA:HHC	14:bA:823:CLA:HBB1	1.96	0.48
14:bB:838:CLA:HBB1	14:bB:838:CLA:HHC	1.96	0.48
14:cA:822:CLA:HHC	14:cA:822:CLA:HBB1	1.95	0.48
14:cA:823:CLA:HHC	14:cA:823:CLA:HBB1	1.96	0.48
2:cB:664:TRP:CD2	14:cB:803:CLA:HMA2	2.49	0.48
13:bA:801:CL0:H15	13:bA:801:CL0:H2	1.95	0.48
14:bB:828:CLA:H93	14:bB:839:CLA:HED1	1.96	0.48
14:cB:828:CLA:HBB1	14:cB:828:CLA:HMB3	1.94	0.48
14:A:802:CLA:H91	14:A:852:CLA:C10	2.44	0.48
14:A:839:CLA:HBB1	14:A:839:CLA:HMB1	1.96	0.48
14:bA:839:CLA:HMB1	14:bA:839:CLA:HBB1	1.96	0.48
2:cB:695:ALA:O	2:cB:698:VAL:HG12	2.13	0.48
17:cJ:103:BCR:H311	17:cJ:103:BCR:C8	2.43	0.48
2:B:664:TRP:CD2	14:B:802:CLA:HMA2	2.49	0.47
14:bA:802:CLA:H91	14:bA:852:CLA:C10	2.44	0.47
14:cA:813:CLA:HHC	14:cA:813:CLA:HBB1	1.96	0.47
1:A:445:ILE:HG22	14:A:832:CLA:HED3	1.96	0.47
14:bB:811:CLA:HHC	14:bB:811:CLA:HBB1	1.96	0.47
14:bB:838:CLA:HBB2	15:bB:840:PQN:H141	1.95	0.47
14:bB:851:CLA:HHC	14:bB:851:CLA:HBB1	1.96	0.47
13:cA:801:CL0:CGD	13:cA:801:CL0:H8	2.44	0.47
14:cB:839:CLA:HBB2	15:cB:841:PQN:H141	1.95	0.47
1:A:509:PHE:CE1	14:A:826:CLA:HBC2	2.49	0.47
14:A:823:CLA:HHC	14:A:823:CLA:HBB1	1.96	0.47
3:C:73:THR:H	3:C:76:SER:HG	1.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:88:LEU:CD2	17:bL:206:BCR:H311	2.44	0.47
1:cA:445:ILE:HG22	14:cA:832:CLA:HED3	1.97	0.47
14:B:838:CLA:HHC	14:B:838:CLA:HBB1	1.96	0.47
14:bA:813:CLA:HHC	14:bA:813:CLA:HBB1	1.96	0.47
13:cA:801:CL0:H15	13:cA:801:CL0:H2	1.95	0.47
14:cB:829:CLA:H93	14:cB:840:CLA:HED1	1.96	0.47
13:A:801:CL0:CGD	13:A:801:CL0:H8	2.44	0.47
13:A:801:CL0:H15	13:A:801:CL0:H2	1.95	0.47
14:B:810:CLA:HMB1	14:B:810:CLA:HBB1	1.96	0.47
14:bA:811:CLA:HBB1	14:bA:811:CLA:HHC	1.97	0.47
7:bI:16:PRO:CG	10:cL:155:PHE:CE2	2.94	0.47
10:bL:88:LEU:CD2	17:cL:207:BCR:H311	2.44	0.47
14:cA:839:CLA:HMB1	14:cA:839:CLA:HBB1	1.96	0.47
14:A:811:CLA:HHC	14:A:811:CLA:HBB1	1.96	0.47
1:cA:509:PHE:CE1	14:cA:826:CLA:HBC2	2.49	0.47
14:cA:802:CLA:H91	14:cA:852:CLA:C10	2.44	0.47
14:cB:811:CLA:HMB1	14:cB:811:CLA:HBB1	1.96	0.47
14:cF:201:CLA:HHC	14:cF:201:CLA:HBB1	1.96	0.47
14:cL:203:CLA:HMB1	14:cL:203:CLA:HBB1	1.96	0.47
14:B:811:CLA:HHC	14:B:811:CLA:HBB1	1.97	0.47
14:B:825:CLA:HHC	14:B:825:CLA:HBB1	1.97	0.47
1:bA:445:ILE:HG22	14:bA:832:CLA:HED3	1.96	0.47
1:bA:509:PHE:CE1	14:bA:826:CLA:HBC2	2.49	0.47
13:bA:801:CL0:CGD	13:bA:801:CL0:H8	2.44	0.47
14:bB:836:CLA:HBB1	14:bB:836:CLA:HMB3	1.95	0.47
14:bF:201:CLA:HHC	14:bF:201:CLA:HBB1	1.96	0.47
14:cA:819:CLA:HHC	14:cA:819:CLA:HBB1	1.97	0.47
14:cA:842:CLA:HBB1	14:cA:842:CLA:HMB1	1.97	0.47
14:cB:839:CLA:HHC	14:cB:839:CLA:HBB1	1.96	0.47
14:cB:840:CLA:HHC	14:cB:840:CLA:HBB1	1.95	0.47
2:bB:490:THR:HG23	2:bB:501:LEU:HD21	1.97	0.47
14:bB:816:CLA:HHC	14:bB:816:CLA:HBB1	1.96	0.47
14:bB:849:CLA:HHC	14:bB:849:CLA:HBB1	1.97	0.47
17:L:206:BCR:H311	10:cL:88:LEU:CD2	2.44	0.47
14:bA:810:CLA:HHC	14:bA:810:CLA:HBB1	1.97	0.47
14:bA:842:CLA:HBB1	14:bA:842:CLA:HMB1	1.97	0.47
17:bA:849:BCR:H272	17:bJ:103:BCR:H313	1.95	0.47
2:bB:664:TRP:CD2	14:bB:802:CLA:HMA2	2.49	0.47
14:cA:811:CLA:HHC	14:cA:811:CLA:HBB1	1.96	0.47
14:cB:801:CLA:HHC	14:cB:801:CLA:HBB1	1.96	0.47
14:A:813:CLA:HHC	14:A:813:CLA:HBB1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:816:CLA:HBB1	14:B:816:CLA:HHC	1.96	0.47
14:F:201:CLA:HHC	14:F:201:CLA:HBB1	1.96	0.47
14:bB:810:CLA:HMB1	14:bB:810:CLA:HBB1	1.96	0.47
14:bJ:101:CLA:HHC	14:bJ:101:CLA:HBB1	1.97	0.47
14:cJ:101:CLA:HHC	14:cJ:101:CLA:HBB1	1.97	0.47
14:A:821:CLA:HMB1	14:A:821:CLA:HBB1	1.96	0.46
14:A:835:CLA:HHC	14:A:835:CLA:HBB1	1.98	0.46
14:A:842:CLA:HMB1	14:A:842:CLA:HBB1	1.97	0.46
14:B:833:CLA:HHC	14:B:833:CLA:HBB1	1.97	0.46
12:X:25:LEU:HD21	14:X:201:CLA:HED1	1.96	0.46
14:X:201:CLA:HHC	14:X:201:CLA:HBB1	1.97	0.46
12:bX:25:LEU:HD21	14:bX:201:CLA:HED1	1.96	0.46
14:cB:814:CLA:HAB	14:cB:828:CLA:H193	1.96	0.46
14:cX:201:CLA:HHC	14:cX:201:CLA:HBB1	1.97	0.46
14:bA:807:CLA:HHC	14:bA:807:CLA:HBB1	1.97	0.46
14:bB:825:CLA:HHC	14:bB:825:CLA:HBB1	1.97	0.46
14:bB:833:CLA:HHC	14:bB:833:CLA:HBB1	1.97	0.46
14:bX:201:CLA:HHC	14:bX:201:CLA:HBB1	1.97	0.46
2:B:145:LEU:CD2	17:B:843:BCR:H373	2.46	0.46
14:B:815:CLA:HHC	14:B:815:CLA:HBB1	1.97	0.46
14:J:101:CLA:HBB1	14:J:101:CLA:HHC	1.97	0.46
1:cA:58:PHE:CD2	14:cA:805:CLA:HMC2	2.51	0.46
14:cA:803:CLA:HMB1	14:cA:803:CLA:HBB1	1.97	0.46
2:cB:490:THR:HG23	2:cB:501:LEU:HD21	1.97	0.46
14:cB:820:CLA:HBB1	14:cB:820:CLA:HHC	1.97	0.46
14:cB:850:CLA:HHC	14:cB:850:CLA:HBB1	1.97	0.46
14:A:803:CLA:HMB1	14:A:803:CLA:HBB1	1.97	0.46
7:I:16:PRO:CG	10:bL:155:PHE:CE2	2.94	0.46
1:bA:58:PHE:CD2	14:bA:805:CLA:HMC2	2.51	0.46
14:bA:835:CLA:HHC	14:bA:835:CLA:HBB1	1.98	0.46
2:bB:145:LEU:CD2	17:bB:843:BCR:H373	2.46	0.46
14:bB:807:CLA:HBC1	11:bM:11:ALA:HB1	1.97	0.46
14:cA:840:CLA:HHC	14:cA:840:CLA:HBB1	1.98	0.46
2:cB:174:ARG:HB2	14:cB:813:CLA:HBC2	1.98	0.46
14:B:849:CLA:HHC	14:B:849:CLA:HBB1	1.96	0.46
14:B:851:CLA:HHC	14:B:851:CLA:HBB1	1.96	0.46
14:bA:818:CLA:HHC	14:bA:818:CLA:HBB1	1.97	0.46
2:bB:225:PHE:H	2:bB:233:TYR:HH	1.64	0.46
14:cB:808:CLA:HBC1	11:cM:11:ALA:HB1	1.98	0.46
14:cB:822:CLA:HBB1	14:cB:822:CLA:HMB3	1.97	0.46
1:A:679:TRP:CG	13:A:801:CL0:H5	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:807:CLA:HHC	14:A:807:CLA:HBB1	1.97	0.46
2:B:490:THR:HG23	2:B:501:LEU:HD21	1.97	0.46
2:B:438:LEU:HA	14:B:802:CLA:H201	1.98	0.46
1:bA:679:TRP:CG	13:bA:801:CL0:H5	2.51	0.46
14:bB:815:CLA:HHC	14:bB:815:CLA:HBB1	1.98	0.46
14:cA:806:CLA:H112	14:cA:827:CLA:HBC1	1.97	0.46
14:cB:833:CLA:HHC	14:cB:833:CLA:HBB1	1.98	0.46
14:cB:834:CLA:HHC	14:cB:834:CLA:HBB1	1.97	0.46
14:B:819:CLA:HHC	14:B:819:CLA:HBB1	1.97	0.46
14:B:822:CLA:HBB1	14:B:822:CLA:HMB3	1.98	0.46
14:B:834:CLA:HHC	14:B:834:CLA:HBB1	1.98	0.46
14:bB:834:CLA:HHC	14:bB:834:CLA:HBB1	1.98	0.46
14:cA:810:CLA:HHC	14:cA:810:CLA:HBB1	1.97	0.46
14:cA:831:CLA:HBB1	14:cA:831:CLA:HMB3	1.98	0.46
14:A:840:CLA:HHC	14:A:840:CLA:HBB1	1.98	0.46
14:cB:835:CLA:HBB1	14:cB:835:CLA:HHC	1.98	0.46
14:A:816:CLA:HBB1	14:A:816:CLA:HMB3	1.98	0.46
14:bA:819:CLA:HHC	14:bA:819:CLA:HBB1	1.97	0.46
14:bB:822:CLA:HMB3	14:bB:822:CLA:HBB1	1.98	0.46
12:cX:25:LEU:HD21	14:cX:201:CLA:HED1	1.96	0.46
14:A:819:CLA:HBB1	14:A:819:CLA:HHC	1.97	0.45
7:I:16:PRO:HG3	10:bL:155:PHE:HE2	1.81	0.45
2:cB:145:LEU:CD2	17:cB:844:BCR:H373	2.46	0.45
14:cB:821:CLA:HMB3	14:cB:821:CLA:HBB1	1.99	0.45
14:cB:836:CLA:HMB2	14:cB:838:CLA:HED1	1.98	0.45
14:A:802:CLA:H143	14:L:201:CLA:HBC3	1.98	0.45
1:bA:679:TRP:CD2	13:bA:801:CL0:H5	2.52	0.45
14:bA:815:CLA:HBB1	14:bA:815:CLA:HMB3	1.98	0.45
14:bA:840:CLA:HBB1	14:bA:840:CLA:HHC	1.98	0.45
14:cA:807:CLA:HHC	14:cA:807:CLA:HBB1	1.97	0.45
14:cA:835:CLA:HHC	14:cA:835:CLA:HBB1	1.98	0.45
17:cB:847:BCR:C8	17:cB:847:BCR:H331	2.46	0.45
1:A:58:PHE:CD2	14:A:805:CLA:HMC2	2.51	0.45
14:A:806:CLA:H112	14:A:827:CLA:HBC1	1.97	0.45
14:A:810:CLA:HHC	14:A:810:CLA:HBB1	1.97	0.45
14:B:835:CLA:HMB2	14:B:837:CLA:HED1	1.99	0.45
14:bA:806:CLA:H112	14:bA:827:CLA:HBC1	1.97	0.45
17:bA:845:BCR:H372	17:bA:845:BCR:H19C	1.98	0.45
14:cA:818:CLA:HHC	14:cA:818:CLA:HBB1	1.97	0.45
14:cB:812:CLA:HHC	14:cB:812:CLA:HBB1	1.97	0.45
14:cB:826:CLA:HHC	14:cB:826:CLA:HBB1	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:818:CLA:HHC	14:A:818:CLA:HBB1	1.97	0.45
2:B:174:ARG:HB2	14:B:812:CLA:HBC2	1.98	0.45
14:B:821:CLA:HBB1	14:B:821:CLA:HMB3	1.97	0.45
14:bA:802:CLA:H143	14:bL:201:CLA:HBC3	1.98	0.45
2:B:516:PHE:CD1	14:B:825:CLA:HBC2	2.52	0.45
2:B:608:ILE:HD13	2:B:613:VAL:HG12	1.99	0.45
1:cA:679:TRP:CG	13:cA:801:CL0:H5	2.51	0.45
2:cB:516:PHE:CD1	14:cB:826:CLA:HBC2	2.52	0.45
1:A:679:TRP:CD2	13:A:801:CL0:H5	2.52	0.45
14:A:808:CLA:HHC	14:A:808:CLA:HBB1	1.99	0.45
14:A:824:CLA:HHC	14:A:824:CLA:HBB1	1.99	0.45
17:A:845:BCR:H19C	17:A:845:BCR:H372	1.98	0.45
14:cA:808:CLA:HHC	14:cA:808:CLA:HBB1	1.99	0.45
14:A:831:CLA:HBB1	14:A:831:CLA:HMB3	1.98	0.45
17:B:846:BCR:H331	17:B:846:BCR:C8	2.46	0.45
14:bA:803:CLA:HBB1	14:bA:803:CLA:HMB3	1.99	0.45
14:bA:816:CLA:HMB3	14:bA:816:CLA:HBB1	1.98	0.45
14:bB:821:CLA:HBB1	14:bB:821:CLA:HMB3	1.97	0.45
14:bB:832:CLA:HHC	14:bB:832:CLA:HBB1	1.98	0.45
14:cB:823:CLA:HMB3	14:cB:823:CLA:HBB1	1.98	0.45
2:cB:438:LEU:HA	14:cB:803:CLA:H201	1.98	0.45
14:cB:816:CLA:HBB1	14:cB:816:CLA:HHC	1.97	0.45
14:B:807:CLA:HBC1	11:M:11:ALA:HB1	1.98	0.45
2:bB:438:LEU:HA	14:bB:802:CLA:H201	1.98	0.45
7:bI:21:LEU:HB2	14:cL:205:CLA:H141	1.99	0.45
14:A:815:CLA:HBB1	14:A:815:CLA:HMB3	1.98	0.45
2:bB:608:ILE:HD13	2:bB:613:VAL:HG12	1.99	0.45
14:bB:835:CLA:HMB2	14:bB:837:CLA:HED1	1.98	0.45
1:cA:679:TRP:CD2	13:cA:801:CL0:H5	2.52	0.45
14:cA:816:CLA:HBB1	14:cA:816:CLA:HMB3	1.98	0.45
14:B:820:CLA:HBB1	14:B:820:CLA:HMB3	1.98	0.44
14:B:835:CLA:HMB1	14:B:835:CLA:HBB1	1.99	0.44
14:bB:819:CLA:HHC	14:bB:819:CLA:HBB1	1.97	0.44
14:bB:820:CLA:HMB1	14:bB:820:CLA:HBB1	1.98	0.44
17:bB:846:BCR:H331	17:bB:846:BCR:C8	2.46	0.44
14:cA:821:CLA:HBB1	14:cA:821:CLA:HMB3	2.00	0.44
14:A:836:CLA:HBB1	14:A:836:CLA:HMB3	1.99	0.44
14:B:814:CLA:HMB1	14:B:814:CLA:HBB1	1.99	0.44
2:bB:174:ARG:HB2	14:bB:812:CLA:HBC2	1.98	0.44
14:bB:814:CLA:HBB1	14:bB:814:CLA:HMB1	1.99	0.44
14:cA:836:CLA:HBB1	14:cA:836:CLA:HMB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:818:CLA:HBB1	14:B:818:CLA:HHC	2.00	0.44
14:B:832:CLA:HHC	14:B:832:CLA:HBB1	1.98	0.44
14:bA:808:CLA:HHC	14:bA:808:CLA:HBB1	1.99	0.44
14:cA:815:CLA:HBB1	14:cA:815:CLA:HMB3	1.98	0.44
14:cB:815:CLA:HMB1	14:cB:815:CLA:HBB1	1.99	0.44
14:B:812:CLA:HHC	14:B:812:CLA:HBB1	2.00	0.44
14:bA:831:CLA:HBB1	14:bA:831:CLA:HMB3	1.98	0.44
2:bB:223:ALA:N	2:bB:224:PRO:CD	2.81	0.44
14:bB:835:CLA:HBB1	14:bB:835:CLA:HMB1	1.99	0.44
14:L:204:CLA:H141	7:cI:21:LEU:HB2	1.99	0.44
14:bB:818:CLA:HHC	14:bB:818:CLA:HBB1	2.00	0.44
10:bL:159:VAL:C	10:bL:160:ASN:HD22	2.26	0.44
14:cA:817:CLA:HBB1	14:cA:817:CLA:HMB3	2.00	0.44
17:cB:851:BCR:H24C	14:cJ:101:CLA:HBC3	2.00	0.44
17:B:850:BCR:H24C	14:J:101:CLA:HBC3	2.00	0.44
10:L:159:VAL:C	10:L:160:ASN:HD22	2.26	0.44
2:bB:516:PHE:CD1	14:bB:825:CLA:HBC2	2.52	0.44
14:cA:824:CLA:HHC	14:cA:824:CLA:HBB1	1.99	0.44
14:cB:836:CLA:HBB1	14:cB:836:CLA:HMB1	1.99	0.44
14:A:830:CLA:HAB	14:A:838:CLA:CBB	2.48	0.44
6:F:137:TRP:N	6:F:138:PRO:CD	2.81	0.44
14:cA:830:CLA:HAB	14:cA:838:CLA:CBB	2.48	0.44
17:cA:845:BCR:H19C	17:cA:845:BCR:H372	1.98	0.44
17:A:845:BCR:H331	17:A:845:BCR:HC8	2.00	0.44
14:cB:819:CLA:HHC	14:cB:819:CLA:HBB1	2.00	0.44
7:I:21:LEU:HB2	14:bL:204:CLA:H141	1.99	0.44
14:bA:824:CLA:HHC	14:bA:824:CLA:HBB1	1.99	0.44
10:cL:159:VAL:C	10:cL:160:ASN:HD22	2.26	0.44
14:bA:814:CLA:HMB3	14:bA:814:CLA:HBB1	2.00	0.43
14:bA:817:CLA:HBB1	14:bA:817:CLA:HMB3	2.00	0.43
14:bA:821:CLA:HBB1	14:bA:821:CLA:HMB3	1.99	0.43
17:cA:845:BCR:H331	17:cA:845:BCR:HC8	2.00	0.43
2:cB:608:ILE:HD13	2:cB:613:VAL:HG12	1.99	0.43
14:L:201:CLA:C1	10:bL:154:ILE:HG21	2.48	0.43
14:bB:812:CLA:HHC	14:bB:812:CLA:HBB1	2.00	0.43
2:cB:78:ILE:HD12	2:cB:125:TYR:CD1	2.53	0.43
2:cB:536:THR:HG21	2:cB:589:TRP:CZ2	2.53	0.43
6:cF:137:TRP:N	6:cF:138:PRO:CD	2.81	0.43
14:A:820:CLA:HHC	14:A:820:CLA:HBB1	2.00	0.43
14:A:831:CLA:H62	14:A:831:CLA:H41	1.88	0.43
14:bA:831:CLA:H62	14:bA:831:CLA:H41	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:bB:536:THR:HG21	2:bB:589:TRP:CZ2	2.53	0.43
14:cA:802:CLA:H143	14:cL:202:CLA:HBC3	1.98	0.43
2:cB:209:TRP:HA	14:cB:814:CLA:HMD3	2.00	0.43
2:B:536:THR:HG21	2:B:589:TRP:CZ2	2.53	0.43
10:L:154:ILE:HG21	14:cL:202:CLA:C1	2.48	0.43
14:bA:836:CLA:HBB1	14:bA:836:CLA:HMB3	1.99	0.43
2:bB:212:PHE:O	14:bB:814:CLA:HED1	2.18	0.43
2:cB:223:ALA:N	2:cB:224:PRO:CD	2.81	0.43
1:bA:296:HIS:CE1	1:bA:300:LEU:HD11	2.54	0.43
3:bC:73:THR:H	3:bC:76:SER:HG	1.65	0.43
6:bF:137:TRP:N	6:bF:138:PRO:CD	2.81	0.43
14:cB:809:CLA:HAA1	14:cB:809:CLA:HBD	2.01	0.43
2:B:78:ILE:HD12	2:B:125:TYR:CD1	2.53	0.43
2:B:209:TRP:HA	14:B:813:CLA:HMD3	2.00	0.43
7:I:16:PRO:HG3	10:bL:155:PHE:CE2	2.54	0.43
14:bA:831:CLA:HBC2	14:bA:838:CLA:HMC2	2.01	0.43
2:bB:78:ILE:HD12	2:bB:125:TYR:CD1	2.53	0.43
17:bB:850:BCR:H24C	14:bJ:101:CLA:HBC3	2.00	0.43
7:bI:16:PRO:HG3	10:cL:155:PHE:HE2	1.81	0.43
1:cA:296:HIS:CE1	1:cA:300:LEU:HD11	2.54	0.43
14:cA:804:CLA:HBB1	14:cA:804:CLA:HMB1	2.01	0.43
14:cA:814:CLA:HBB1	14:cA:814:CLA:HMB3	2.00	0.43
14:B:808:CLA:HBD	14:B:808:CLA:HAA1	2.01	0.43
10:L:155:PHE:HE2	7:cI:16:PRO:HG3	1.81	0.43
1:bA:238:LEU:HD13	14:bA:815:CLA:HED1	2.01	0.43
14:bA:829:CLA:HMB3	14:bA:829:CLA:HBB1	2.01	0.43
14:bB:808:CLA:HAA1	14:bB:808:CLA:HBD	2.01	0.43
14:bL:201:CLA:C1	10:cL:154:ILE:HG21	2.48	0.43
2:cB:212:PHE:O	14:cB:815:CLA:HED1	2.19	0.43
14:cB:831:CLA:HBB1	14:cB:831:CLA:HMB3	2.00	0.43
14:A:831:CLA:HBC2	14:A:838:CLA:HMC2	2.01	0.43
2:B:223:ALA:N	2:B:224:PRO:CD	2.81	0.43
14:bA:820:CLA:HHC	14:bA:820:CLA:HBB1	2.00	0.43
14:bB:828:CLA:HBB1	14:bB:828:CLA:HMB3	2.01	0.43
14:bB:830:CLA:HMB3	14:bB:830:CLA:HBB1	2.00	0.43
7:bI:16:PRO:HG3	10:cL:155:PHE:CE2	2.54	0.43
1:cA:266:LEU:HD23	1:cA:266:LEU:N	2.34	0.43
14:cA:820:CLA:HHC	14:cA:820:CLA:HBB1	2.00	0.43
2:cB:319:PHE:HB2	14:cB:823:CLA:CMA	2.49	0.43
1:A:296:HIS:CE1	1:A:300:LEU:HD11	2.54	0.43
2:B:319:PHE:HB2	14:B:822:CLA:CMA	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:bA:845:BCR:HC8	17:bA:845:BCR:H331	2.00	0.43
14:cA:809:CLA:HMC2	2:cB:446:VAL:HG13	2.01	0.43
14:cA:841:CLA:HMB2	2:cB:698:VAL:CG1	2.48	0.43
14:cB:813:CLA:HHC	14:cB:813:CLA:HBB1	2.00	0.43
14:cB:818:CLA:HBB1	14:cB:818:CLA:HMB3	2.00	0.43
2:B:526:VAL:HG11	2:B:600:TYR:HB2	2.01	0.43
1:A:92:PHE:CG	14:A:807:CLA:HBC3	2.54	0.42
2:B:212:PHE:O	14:B:814:CLA:HED1	2.19	0.42
14:B:817:CLA:HMB3	14:B:817:CLA:HBB1	2.00	0.42
1:bA:196:MET:HG3	14:bA:813:CLA:HBC2	2.01	0.42
2:bB:177:HIS:CD2	14:bB:819:CLA:HMD1	2.54	0.42
10:bL:88:LEU:HD22	17:cL:207:BCR:H311	2.01	0.42
17:bL:206:BCR:H23C	17:bL:206:BCR:H403	2.01	0.42
1:cA:92:PHE:CG	14:cA:807:CLA:HBC3	2.54	0.42
14:cA:831:CLA:HBC2	14:cA:838:CLA:HMC2	2.01	0.42
2:cB:526:VAL:HG11	2:cB:600:TYR:HB2	2.01	0.42
14:cB:832:CLA:HHC	14:cB:832:CLA:HBB1	2.01	0.42
1:A:175:ALA:HB2	14:A:810:CLA:HBC2	2.01	0.42
14:A:817:CLA:HBB1	14:A:817:CLA:HMB3	2.00	0.42
14:bA:809:CLA:HMC2	2:bB:446:VAL:HG13	2.01	0.42
14:bA:830:CLA:HAB	14:bA:838:CLA:CBB	2.48	0.42
14:bB:817:CLA:HBB1	14:bB:817:CLA:HMB3	2.00	0.42
14:cB:827:CLA:CGA	14:cB:827:CLA:H3A	2.49	0.42
1:A:196:MET:HG3	14:A:813:CLA:HBC2	2.01	0.42
14:B:828:CLA:HBB1	14:B:828:CLA:HMB3	2.01	0.42
2:bB:209:TRP:HA	14:bB:813:CLA:HMD3	2.00	0.42
14:bB:806:CLA:H152	14:bB:826:CLA:HBC1	2.01	0.42
10:cL:61:TYR:CZ	14:cL:205:CLA:HED3	2.54	0.42
2:B:82:LEU:HD12	2:B:82:LEU:HA	1.92	0.42
2:B:177:HIS:CD2	14:B:819:CLA:HMD1	2.54	0.42
14:B:837:CLA:HBB1	14:B:837:CLA:HMB1	2.02	0.42
10:L:155:PHE:CE2	7:cI:16:PRO:HG3	2.54	0.42
2:bB:319:PHE:HB2	14:bB:822:CLA:CMA	2.49	0.42
6:bF:74:VAL:HG12	6:bF:84:PHE:HB2	2.01	0.42
10:bL:61:TYR:CZ	14:bL:204:CLA:HED3	2.54	0.42
1:A:595:LEU:HD21	14:A:829:CLA:HBC1	2.02	0.42
14:B:806:CLA:H152	14:B:826:CLA:HBC1	2.01	0.42
6:F:74:VAL:HG12	6:F:84:PHE:HB2	2.01	0.42
1:cA:238:LEU:HD13	14:cA:815:CLA:HED1	2.01	0.42
14:cB:807:CLA:H152	14:cB:827:CLA:HBC1	2.01	0.42
14:A:814:CLA:HBB1	14:A:814:CLA:HMB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:852:CLA:CGA	14:A:852:CLA:H3A	2.50	0.42
2:B:91:ILE:HB	2:B:112:PRO:HB2	2.02	0.42
14:cA:852:CLA:CGA	14:cA:852:CLA:H3A	2.50	0.42
17:cB:846:BCR:C8	17:cB:846:BCR:H331	2.50	0.42
1:A:238:LEU:HD13	14:A:815:CLA:HED1	2.01	0.42
1:bA:92:PHE:CG	14:bA:807:CLA:HBC3	2.54	0.42
14:bA:804:CLA:HBB1	14:bA:804:CLA:HMB1	2.01	0.42
14:bA:831:CLA:H42	10:bL:32:THR:HG23	2.01	0.42
14:cA:830:CLA:HMB2	14:cA:831:CLA:C1D	2.50	0.42
2:cB:91:ILE:HB	2:cB:112:PRO:HB2	2.02	0.42
1:A:266:LEU:HD23	1:A:266:LEU:N	2.34	0.42
1:bA:588:TRP:CD1	14:bA:829:CLA:HMD1	2.55	0.42
14:bB:831:CLA:HHC	14:bB:831:CLA:HBB1	2.01	0.42
17:bB:845:BCR:C8	17:bB:845:BCR:H331	2.50	0.42
1:cA:128:ALA:HB2	1:cA:664:ALA:HB1	2.02	0.42
17:L:206:BCR:H311	10:cL:88:LEU:HD22	2.01	0.42
6:cF:74:VAL:HG12	6:cF:84:PHE:HB2	2.01	0.42
17:cJ:103:BCR:C23	17:cJ:103:BCR:H382	2.50	0.42
10:L:88:LEU:HD22	17:bL:206:BCR:H311	2.01	0.42
14:bA:830:CLA:HMB2	14:bA:831:CLA:C1D	2.50	0.42
14:bA:841:CLA:HMB2	2:bB:698:VAL:CG1	2.48	0.42
14:bA:852:CLA:CGA	14:bA:852:CLA:H3A	2.50	0.42
14:A:829:CLA:HBB1	14:A:829:CLA:HMB3	2.01	0.41
17:L:206:BCR:C23	17:L:206:BCR:H403	2.50	0.41
2:bB:590:MET:SD	2:bB:594:LEU:HD22	2.60	0.41
14:bB:826:CLA:CGA	14:bB:826:CLA:H3A	2.49	0.41
17:bJ:103:BCR:C23	17:bJ:103:BCR:H382	2.50	0.41
17:bL:206:BCR:H403	17:bL:206:BCR:C23	2.50	0.41
1:cA:588:TRP:CD1	14:cA:829:CLA:HMD1	2.55	0.41
2:cB:590:MET:SD	2:cB:594:LEU:HD22	2.60	0.41
14:cB:829:CLA:HBB1	14:cB:829:CLA:HMB3	2.01	0.41
14:A:809:CLA:HMC2	2:B:446:VAL:HG13	2.01	0.41
14:B:824:CLA:HMB1	14:B:824:CLA:HBB1	2.02	0.41
14:B:830:CLA:HBB1	14:B:830:CLA:HMB3	2.00	0.41
1:bA:175:ALA:HB2	14:bA:810:CLA:HBC2	2.01	0.41
1:bA:595:LEU:HD21	14:bA:829:CLA:HBC1	2.02	0.41
14:bB:837:CLA:HBB1	14:bB:837:CLA:HMB1	2.02	0.41
1:cA:59:ASP:OD1	1:cA:414:ARG:NH1	2.53	0.41
1:cA:196:MET:HG3	14:cA:813:CLA:HBC2	2.01	0.41
14:cA:829:CLA:HBB1	14:cA:829:CLA:HMB3	2.01	0.41
14:cA:831:CLA:H42	10:cL:32:THR:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:cB:177:HIS:CD2	14:cB:820:CLA:HMD1	2.54	0.41
17:cI:102:BCR:C8	17:cI:102:BCR:H331	2.50	0.41
14:A:831:CLA:H42	10:L:32:THR:HG23	2.01	0.41
2:B:526:VAL:HG11	2:B:600:TYR:CG	2.56	0.41
17:I:102:BCR:H331	17:I:102:BCR:C8	2.50	0.41
2:bB:91:ILE:HB	2:bB:112:PRO:HB2	2.02	0.41
17:cL:207:BCR:C23	17:cL:207:BCR:H403	2.50	0.41
14:B:831:CLA:HHC	14:B:831:CLA:HBB1	2.01	0.41
8:J:11:VAL:N	8:J:12:PRO:HD2	2.35	0.41
1:bA:128:ALA:HB2	1:bA:664:ALA:HB1	2.02	0.41
17:bI:102:BCR:H331	17:bI:102:BCR:C8	2.50	0.41
1:A:59:ASP:OD1	1:A:414:ARG:NH1	2.53	0.41
14:B:826:CLA:CGA	14:B:826:CLA:H3A	2.50	0.41
14:B:835:CLA:HBC2	14:B:835:CLA:HHD	2.03	0.41
17:J:103:BCR:C23	17:J:103:BCR:H382	2.50	0.41
2:cB:638:LEU:HD22	2:cB:731:PHE:HA	2.03	0.41
14:cB:838:CLA:HBB1	14:cB:838:CLA:HMB1	2.02	0.41
14:A:804:CLA:HMB1	14:A:804:CLA:HBB1	2.01	0.41
14:A:830:CLA:HMB2	14:A:831:CLA:C1D	2.50	0.41
17:B:845:BCR:H331	17:B:845:BCR:C8	2.50	0.41
2:bB:82:LEU:HD12	2:bB:82:LEU:HA	1.92	0.41
1:cA:175:ALA:HB2	14:cA:810:CLA:HBC2	2.02	0.41
1:cA:595:LEU:HD21	14:cA:829:CLA:HBC1	2.02	0.41
10:L:154:ILE:O	22:L:301:HOH:O	2.22	0.41
17:L:206:BCR:H403	17:L:206:BCR:H23C	2.01	0.41
1:bA:59:ASP:OD1	1:bA:414:ARG:NH1	2.53	0.41
1:bA:266:LEU:N	1:bA:266:LEU:HD23	2.34	0.41
14:cA:812:CLA:HBC3	14:cA:813:CLA:CBB	2.51	0.41
14:cA:831:CLA:H62	14:cA:831:CLA:H41	1.88	0.41
17:cL:207:BCR:H403	17:cL:207:BCR:H23C	2.01	0.41
1:A:588:TRP:CD1	14:A:829:CLA:HMD1	2.55	0.41
2:B:638:LEU:HD22	2:B:731:PHE:HA	2.03	0.41
3:C:41:SER:HG	4:D:116:ASN:H	1.69	0.41
10:L:61:TYR:CZ	14:L:204:CLA:HED3	2.54	0.41
1:bA:359:LEU:HD22	14:bA:805:CLA:HED2	2.03	0.41
14:bA:812:CLA:HBC3	14:bA:813:CLA:CBB	2.51	0.41
2:bB:440:ILE:HD12	2:bB:457:ILE:HG21	2.03	0.41
2:bB:526:VAL:HG11	2:bB:600:TYR:HB2	2.01	0.41
3:bC:41:SER:HG	4:bD:116:ASN:H	1.69	0.41
10:bL:135:MET:HE3	17:cL:207:BCR:H342	2.03	0.41
1:A:128:ALA:HB2	1:A:664:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:812:CLA:HBC3	14:A:813:CLA:CBB	2.51	0.41
2:B:440:ILE:HD12	2:B:457:ILE:HG21	2.03	0.41
1:bA:441:ASN:OD1	14:bA:852:CLA:HED2	2.21	0.41
8:bJ:11:VAL:N	8:bJ:12:PRO:HD2	2.35	0.41
14:bL:203:CLA:HBC2	14:bL:203:CLA:HHD	2.03	0.41
8:cJ:11:VAL:N	8:cJ:12:PRO:HD2	2.35	0.41
2:B:340:TRP:CZ3	14:B:825:CLA:H91	2.56	0.41
2:B:590:MET:SD	2:B:594:LEU:HD22	2.60	0.41
17:L:206:BCR:H342	10:cL:135:MET:HE3	2.03	0.41
10:bL:144:LEU:HB3	14:bL:204:CLA:H41	2.03	0.41
14:bL:201:CLA:H12	10:cL:154:ILE:HG21	2.03	0.41
1:cA:441:ASN:OD1	14:cA:852:CLA:HED2	2.21	0.41
2:cB:340:TRP:CZ3	14:cB:826:CLA:H91	2.56	0.41
14:A:841:CLA:HMB2	2:B:698:VAL:CG1	2.48	0.40
2:B:82:LEU:HD13	2:B:364:PHE:HB3	2.03	0.40
14:bB:824:CLA:HBB1	14:bB:824:CLA:HMB1	2.02	0.40
2:cB:731:PHE:CD1	14:cB:803:CLA:HMD2	2.56	0.40
14:cB:803:CLA:H193	14:cB:804:CLA:HMB2	2.03	0.40
14:B:802:CLA:H193	14:B:803:CLA:HMB2	2.03	0.40
10:L:135:MET:HE3	17:bL:206:BCR:H342	2.03	0.40
2:bB:638:LEU:HD22	2:bB:731:PHE:HA	2.03	0.40
14:bB:831:CLA:HBB1	17:bB:846:BCR:H323	2.02	0.40
14:bB:835:CLA:HBC2	14:bB:835:CLA:HHD	2.03	0.40
2:cB:194:LEU:HA	2:cB:198:ALA:HB3	2.03	0.40
14:cB:825:CLA:HBB1	14:cB:825:CLA:HMB1	2.02	0.40
10:cL:144:LEU:HB3	14:cL:205:CLA:H41	2.04	0.40
14:L:201:CLA:H12	10:bL:154:ILE:HG21	2.03	0.40
2:bB:526:VAL:HG11	2:bB:600:TYR:CG	2.56	0.40
3:cC:41:SER:HG	4:cD:116:ASN:H	1.69	0.40
17:cL:206:BCR:C8	17:cL:206:BCR:H331	2.52	0.40
14:bA:840:CLA:H161	8:bJ:19:LEU:HD22	2.04	0.40
2:bB:731:PHE:CD1	14:bB:802:CLA:HMD2	2.56	0.40
2:cB:82:LEU:HD13	2:cB:364:PHE:HB3	2.03	0.40
14:cB:830:CLA:HMB1	14:cB:830:CLA:HBB1	2.04	0.40
10:L:144:LEU:HB3	14:L:204:CLA:H41	2.04	0.40
2:cB:440:ILE:HD12	2:cB:457:ILE:HG21	2.03	0.40
14:cB:832:CLA:HBB1	17:cB:847:BCR:H323	2.03	0.40
14:cB:836:CLA:HBC2	14:cB:836:CLA:HHD	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	727/751 (97%)	676 (93%)	47 (6%)	4 (1%)	21	20
1	bA	727/751 (97%)	677 (93%)	46 (6%)	4 (1%)	21	20
1	cA	727/751 (97%)	676 (93%)	47 (6%)	4 (1%)	21	20
2	B	732/741 (99%)	681 (93%)	47 (6%)	4 (0%)	24	25
2	bB	732/741 (99%)	681 (93%)	47 (6%)	4 (0%)	24	25
2	cB	732/741 (99%)	681 (93%)	47 (6%)	4 (0%)	24	25
3	C	78/81 (96%)	74 (95%)	2 (3%)	2 (3%)	4	2
3	bC	78/81 (96%)	74 (95%)	2 (3%)	2 (3%)	4	2
3	cC	78/81 (96%)	74 (95%)	2 (3%)	2 (3%)	4	2
4	D	136/142 (96%)	131 (96%)	5 (4%)	0	100	100
4	bD	136/142 (96%)	131 (96%)	5 (4%)	0	100	100
4	cD	136/142 (96%)	131 (96%)	5 (4%)	0	100	100
5	E	66/77 (86%)	60 (91%)	3 (4%)	3 (4%)	2	0
5	bE	66/77 (86%)	60 (91%)	3 (4%)	3 (4%)	2	0
5	cE	66/77 (86%)	60 (91%)	3 (4%)	3 (4%)	2	0
6	F	128/162 (79%)	116 (91%)	12 (9%)	0	100	100
6	bF	128/162 (79%)	116 (91%)	12 (9%)	0	100	100
6	cF	128/162 (79%)	116 (91%)	12 (9%)	0	100	100
7	I	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	4	1
7	bI	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	4	1
7	cI	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	4	1
8	J	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
8	bJ	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
8	cJ	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
10	L	156/161 (97%)	149 (96%)	5 (3%)	2 (1%)	9	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
10	bL	156/161 (97%)	149 (96%)	5 (3%)	2 (1%)	9 7
10	cL	156/161 (97%)	149 (96%)	5 (3%)	2 (1%)	9 7
11	M	29/31 (94%)	28 (97%)	0	1 (3%)	3 1
11	bM	29/31 (94%)	28 (97%)	0	1 (3%)	3 1
11	cM	29/31 (94%)	28 (97%)	0	1 (3%)	3 1
12	X	19/36 (53%)	18 (95%)	1 (5%)	0	100 100
12	bX	19/36 (53%)	18 (95%)	1 (5%)	0	100 100
12	cX	19/36 (53%)	18 (95%)	1 (5%)	0	100 100
All	All	6438/6783 (95%)	6013 (93%)	374 (6%)	51 (1%)	18 14

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	ILE
1	bA	317	ILE
1	cA	317	ILE
1	A	268	TRP
2	B	492	ALA
3	C	62	PHE
5	E	46	ASN
10	L	112	GLU
1	bA	268	TRP
2	bB	492	ALA
3	bC	62	PHE
5	bE	46	ASN
10	bL	112	GLU
1	cA	268	TRP
2	cB	492	ALA
3	cC	62	PHE
5	cE	46	ASN
10	cL	112	GLU
3	C	61	ASP
10	L	109	ASP
11	M	30	TYR
3	bC	61	ASP
10	bL	109	ASP
11	bM	30	TYR
3	cC	61	ASP
10	cL	109	ASP

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Mol	Chain	Res	Type
11	cM	30	TYR
1	A	19	ASP
5	E	55	VAL
7	I	5	TYR
1	bA	19	ASP
5	bE	55	VAL
7	bI	5	TYR
1	cA	19	ASP
5	cE	55	VAL
7	cI	5	TYR
2	B	170	ASN
2	B	481	LEU
5	E	54	GLY
2	bB	170	ASN
2	bB	481	LEU
5	bE	54	GLY
2	cB	170	ASN
2	cB	481	LEU
5	cE	54	GLY
2	B	480	VAL
2	bB	480	VAL
2	cB	480	VAL
1	A	375	PRO
1	bA	375	PRO
1	cA	375	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	A	592/609 (97%)	584 (99%)	8 (1%)	59	72
1	bA	592/609 (97%)	584 (99%)	8 (1%)	59	72
1	cA	592/609 (97%)	584 (99%)	8 (1%)	59	72
2	B	600/604 (99%)	592 (99%)	8 (1%)	61	74
2	bB	600/604 (99%)	592 (99%)	8 (1%)	61	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	cB	600/604 (99%)	592 (99%)	8 (1%)	61	74
3	C	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	D	114/118 (97%)	112 (98%)	2 (2%)	51	65
4	bD	114/118 (97%)	112 (98%)	2 (2%)	51	65
4	cD	114/118 (97%)	112 (98%)	2 (2%)	51	65
5	E	59/64 (92%)	59 (100%)	0	100	100
5	bE	59/64 (92%)	59 (100%)	0	100	100
5	cE	59/64 (92%)	59 (100%)	0	100	100
6	F	108/127 (85%)	105 (97%)	3 (3%)	38	49
6	bF	108/127 (85%)	105 (97%)	3 (3%)	38	49
6	cF	108/127 (85%)	105 (97%)	3 (3%)	38	49
7	I	32/32 (100%)	32 (100%)	0	100	100
7	bI	32/32 (100%)	32 (100%)	0	100	100
7	cI	32/32 (100%)	32 (100%)	0	100	100
8	J	37/37 (100%)	37 (100%)	0	100	100
8	bJ	37/37 (100%)	37 (100%)	0	100	100
8	cJ	37/37 (100%)	37 (100%)	0	100	100
10	L	116/119 (98%)	115 (99%)	1 (1%)	70	81
10	bL	116/119 (98%)	115 (99%)	1 (1%)	70	81
10	cL	116/119 (98%)	115 (99%)	1 (1%)	70	81
11	M	27/27 (100%)	26 (96%)	1 (4%)	30	38
11	bM	27/27 (100%)	26 (96%)	1 (4%)	30	38
11	cM	27/27 (100%)	26 (96%)	1 (4%)	30	38
12	X	17/29 (59%)	17 (100%)	0	100	100
12	bX	17/29 (59%)	17 (100%)	0	100	100
12	cX	17/29 (59%)	17 (100%)	0	100	100
All	All	5310/5505 (96%)	5241 (99%)	69 (1%)	59	74

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	117	VAL
1	A	196	MET
1	A	197	MET
1	A	249	MET
1	A	371	TYR
1	A	485	TRP
1	A	709	VAL
2	B	82	LEU
2	B	185	VAL
2	B	293	THR
2	B	354	GLN
2	B	445	ASP
2	B	606	LEU
2	B	613	VAL
2	B	740	PHE
4	D	101	LYS
4	D	110	ASN
6	F	86	ILE
6	F	90	LEU
6	F	120	ILE
10	L	7	GLN
11	M	30	TYR
1	bA	13	LYS
1	bA	117	VAL
1	bA	196	MET
1	bA	197	MET
1	bA	249	MET
1	bA	371	TYR
1	bA	485	TRP
1	bA	709	VAL
2	bB	82	LEU
2	bB	185	VAL
2	bB	293	THR
2	bB	354	GLN
2	bB	445	ASP
2	bB	606	LEU
2	bB	613	VAL
2	bB	740	PHE
4	bD	101	LYS
4	bD	110	ASN
6	bF	86	ILE
6	bF	90	LEU

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Mol	Chain	Res	Type
6	bF	120	ILE
10	bL	7	GLN
11	bM	30	TYR
1	cA	13	LYS
1	cA	117	VAL
1	cA	196	MET
1	cA	197	MET
1	cA	249	MET
1	cA	371	TYR
1	cA	485	TRP
1	cA	709	VAL
2	cB	82	LEU
2	cB	185	VAL
2	cB	293	THR
2	cB	354	GLN
2	cB	445	ASP
2	cB	606	LEU
2	cB	613	VAL
2	cB	740	PHE
4	cD	101	LYS
4	cD	110	ASN
6	cF	86	ILE
6	cF	90	LEU
6	cF	120	ILE
10	cL	7	GLN
11	cM	30	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	HIS
1	A	157	GLN
1	A	181	HIS
1	A	216	GLN
2	B	178	HIS
2	B	407	ASN
2	B	468	GLN
2	B	617	ASN
6	F	107	GLN
7	I	33	HIS
8	J	39	HIS
10	L	3	GLN

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Mol	Chain	Res	Type
10	L	38	ASN
10	L	73	GLN
10	L	82	ASN
10	L	125	GLN
10	L	160	ASN
11	M	7	GLN
1	bA	79	HIS
1	bA	157	GLN
1	bA	181	HIS
1	bA	216	GLN
2	bB	50	HIS
2	bB	178	HIS
2	bB	289	HIS
2	bB	407	ASN
2	bB	468	GLN
2	bB	617	ASN
4	bD	116	ASN
6	bF	107	GLN
7	bI	33	HIS
8	bJ	39	HIS
10	bL	3	GLN
10	bL	7	GLN
10	bL	38	ASN
10	bL	73	GLN
10	bL	82	ASN
10	bL	125	GLN
10	bL	160	ASN
1	cA	79	HIS
1	cA	157	GLN
1	cA	181	HIS
1	cA	216	GLN
2	cB	50	HIS
2	cB	178	HIS
2	cB	205	GLN
2	cB	289	HIS
2	cB	407	ASN
2	cB	468	GLN
2	cB	617	ASN
5	cE	56	ASN
6	cF	107	GLN
7	cI	33	HIS
8	cJ	39	HIS

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Mol	Chain	Res	Type
10	cL	3	GLN
10	cL	38	ASN
10	cL	125	GLN
10	cL	160	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 378 ligands modelled in this entry, 15 are unknown and 3 are monoatomic - leaving 360 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	CLA	A	852	-	69,73,73	1.86	18 (26%)	83,113,113	2.50	28 (33%)
17	BCR	cL	206	-	41,41,41	1.70	8 (19%)	56,56,56	1.40	9 (16%)
14	CLA	bA	830	1	54,58,73	2.25	19 (35%)	65,95,113	3.07	29 (44%)
17	BCR	bB	850	-	41,41,41	1.76	8 (19%)	56,56,56	1.38	8 (14%)
14	CLA	cB	815	-	49,53,73	2.50	21 (42%)	59,89,113	3.24	27 (45%)
14	CLA	cA	806	1	69,73,73	2.06	20 (28%)	83,113,113	2.74	28 (33%)
14	CLA	X	201	-	49,53,73	2.50	21 (42%)	59,89,113	3.23	28 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	cB	828	2	69,73,73	2.10	20 (28%)	83,113,113	2.71	28 (33%)
15	PQN	bA	843	-	34,34,34	0.47	1 (2%)	42,45,45	0.34	0
14	CLA	cA	811	1	49,53,73	2.47	20 (40%)	59,89,113	3.21	28 (47%)
14	CLA	B	821	-	49,53,73	2.49	21 (42%)	59,89,113	3.23	26 (44%)
14	CLA	J	102	8	49,53,73	2.50	21 (42%)	59,89,113	3.20	26 (44%)
17	BCR	A	848	-	41,41,41	1.68	8 (19%)	56,56,56	1.51	13 (23%)
14	CLA	A	826	1	50,54,73	2.43	20 (40%)	60,90,113	3.24	27 (45%)
14	CLA	bB	824	22	50,54,73	2.48	20 (40%)	60,90,113	3.20	26 (43%)
14	CLA	bA	838	1	49,53,73	2.32	19 (38%)	59,89,113	3.30	27 (45%)
16	SF4	bC	101	3	0,12,12	-	-	-		
13	CL0	bA	801	1	69,73,73	2.01	20 (28%)	83,113,113	2.74	32 (38%)
14	CLA	A	837	1	69,73,73	1.99	20 (28%)	83,113,113	2.72	28 (33%)
14	CLA	bA	818	1	64,68,73	2.18	21 (32%)	77,107,113	2.94	31 (40%)
14	CLA	B	813	-	52,56,73	2.42	20 (38%)	62,92,113	3.13	30 (48%)
17	BCR	cB	843	-	41,41,41	1.80	7 (17%)	56,56,56	1.60	12 (21%)
14	CLA	A	820	22	49,53,73	2.51	21 (42%)	59,89,113	3.17	28 (47%)
14	CLA	bA	816	1	49,53,73	2.48	20 (40%)	59,89,113	3.18	26 (44%)
14	CLA	cB	804	22	59,63,73	2.17	20 (33%)	71,101,113	2.96	30 (42%)
14	CLA	bA	828	1	64,68,73	2.13	20 (31%)	77,107,113	2.80	25 (32%)
14	CLA	cB	832	2	69,73,73	2.10	20 (28%)	83,113,113	2.84	27 (32%)
14	CLA	bA	839	1	69,73,73	2.07	20 (28%)	83,113,113	2.72	28 (33%)
14	CLA	bA	825	22	54,58,73	2.31	20 (37%)	65,95,113	3.19	30 (46%)
16	SF4	bA	844	1,2	0,12,12	-	-	-		
18	LHG	A	850	-	48,48,48	0.27	0	51,54,54	0.31	0
14	CLA	cA	829	1	69,73,73	2.05	20 (28%)	83,113,113	2.69	29 (34%)
14	CLA	bA	819	1	49,53,73	2.51	20 (40%)	59,89,113	3.19	29 (49%)
14	CLA	A	809	1	49,53,73	2.47	20 (40%)	59,89,113	3.18	26 (44%)
14	CLA	F	201	22	55,59,73	2.29	19 (34%)	66,96,113	3.05	31 (46%)
14	CLA	cB	827	2	69,73,73	2.02	21 (30%)	83,113,113	2.82	32 (38%)
17	BCR	B	847	-	41,41,41	1.73	8 (19%)	56,56,56	1.47	13 (23%)
14	CLA	A	827	1	65,69,73	2.16	20 (30%)	78,108,113	2.87	29 (37%)
14	CLA	cA	837	1	69,73,73	2.00	20 (28%)	83,113,113	2.73	28 (33%)
14	CLA	B	805	2	69,73,73	2.08	21 (30%)	83,113,113	2.83	30 (36%)
17	BCR	B	850	-	41,41,41	1.76	8 (19%)	56,56,56	1.38	8 (14%)
14	CLA	cA	839	1	69,73,73	2.07	20 (28%)	83,113,113	2.72	28 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	A	822	1	49,53,73	2.49	21 (42%)	59,89,113	3.23	26 (44%)
14	CLA	bA	804	1	57,61,73	2.32	21 (36%)	68,98,113	3.11	29 (42%)
14	CLA	cA	810	-	49,53,73	2.49	21 (42%)	59,89,113	3.16	25 (42%)
17	BCR	bB	847	-	41,41,41	1.73	8 (19%)	56,56,56	1.48	13 (23%)
14	CLA	B	809	2	69,73,73	1.94	19 (27%)	83,113,113	2.70	30 (36%)
14	CLA	A	841	22	69,73,73	1.97	19 (27%)	83,113,113	2.66	31 (37%)
14	CLA	bB	837	2	51,55,73	2.41	20 (39%)	61,91,113	3.20	25 (40%)
14	CLA	bB	808	2	56,60,73	2.24	20 (35%)	67,97,113	3.08	30 (44%)
17	BCR	cI	101	-	41,41,41	1.68	8 (19%)	56,56,56	1.39	10 (17%)
14	CLA	bA	807	1	49,53,73	2.50	20 (40%)	59,89,113	3.19	26 (44%)
17	BCR	bA	845	-	41,41,41	1.80	7 (17%)	56,56,56	1.49	11 (19%)
14	CLA	B	836	2	49,53,73	2.47	20 (40%)	59,89,113	3.21	26 (44%)
14	CLA	cB	826	2	59,63,73	2.26	20 (33%)	71,101,113	2.99	32 (45%)
14	CLA	bA	833	1	69,73,73	2.00	21 (30%)	83,113,113	2.71	30 (36%)
14	CLA	bA	821	-	49,53,73	2.52	20 (40%)	59,89,113	3.23	26 (44%)
14	CLA	cA	826	1	50,54,73	2.43	20 (40%)	60,90,113	3.24	27 (45%)
14	CLA	B	804	2	55,59,73	2.33	20 (36%)	66,96,113	3.12	30 (45%)
14	CLA	bB	823	2	54,58,73	2.38	20 (37%)	65,95,113	3.13	28 (43%)
14	CLA	A	838	1	49,53,73	2.32	19 (38%)	59,89,113	3.30	27 (45%)
14	CLA	bA	831	1	59,63,73	2.23	20 (33%)	71,101,113	2.99	32 (45%)
14	CLA	cB	817	2	49,53,73	2.52	21 (42%)	59,89,113	3.24	29 (49%)
14	CLA	cX	201	-	49,53,73	2.50	21 (42%)	59,89,113	3.23	28 (47%)
14	CLA	B	851	-	49,53,73	2.50	20 (40%)	59,89,113	3.23	26 (44%)
14	CLA	bJ	102	8	49,53,73	2.50	21 (42%)	59,89,113	3.20	26 (44%)
14	CLA	cB	839	22	69,73,73	1.95	20 (28%)	83,113,113	2.63	27 (32%)
17	BCR	cA	849	-	41,41,41	1.72	7 (17%)	56,56,56	1.48	10 (17%)
14	CLA	B	837	2	51,55,73	2.41	20 (39%)	61,91,113	3.21	25 (40%)
14	CLA	cB	836	2	49,53,73	2.49	20 (40%)	59,89,113	3.22	26 (44%)
17	BCR	bF	202	-	41,41,41	1.80	6 (14%)	56,56,56	1.49	8 (14%)
14	CLA	bB	834	-	49,53,73	2.48	21 (42%)	59,89,113	3.14	27 (45%)
14	CLA	cA	841	22	69,73,73	1.97	19 (27%)	83,113,113	2.65	31 (37%)
17	BCR	A	846	-	41,41,41	1.76	6 (14%)	56,56,56	1.76	14 (25%)
17	BCR	bB	841	-	41,41,41	1.75	6 (14%)	56,56,56	1.37	9 (16%)
14	CLA	B	808	2	56,60,73	2.23	20 (35%)	67,97,113	3.08	30 (44%)
14	CLA	A	803	1	49,53,73	2.49	20 (40%)	59,89,113	3.21	28 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	bB	806	2	69,73,73	2.07	20 (28%)	83,113,113	2.75	31 (37%)
14	CLA	cA	818	1	64,68,73	2.18	21 (32%)	77,107,113	2.94	31 (40%)
14	CLA	cB	812	2	49,53,73	2.49	20 (40%)	59,89,113	3.15	26 (44%)
14	CLA	B	802	2	69,73,73	2.02	20 (28%)	83,113,113	2.75	32 (38%)
18	LHG	bA	851	14	26,26,48	0.33	0	29,32,54	0.39	0
14	CLA	A	836	1	55,59,73	2.26	19 (34%)	66,96,113	3.10	31 (46%)
14	CLA	A	832	1	69,73,73	1.98	20 (28%)	83,113,113	2.74	31 (37%)
14	CLA	cB	810	2	69,73,73	1.94	19 (27%)	83,113,113	2.71	30 (36%)
14	CLA	A	810	-	49,53,73	2.49	21 (42%)	59,89,113	3.16	25 (42%)
14	CLA	L	201	2	69,73,73	1.95	21 (30%)	83,113,113	2.87	31 (37%)
14	CLA	cB	813	2	69,73,73	2.10	21 (30%)	83,113,113	2.88	29 (34%)
14	CLA	B	806	2	69,73,73	2.07	20 (28%)	83,113,113	2.75	31 (37%)
14	CLA	B	834	-	49,53,73	2.47	21 (42%)	59,89,113	3.14	27 (45%)
14	CLA	cB	835	-	49,53,73	2.47	21 (42%)	59,89,113	3.13	27 (45%)
14	CLA	bL	201	2	69,73,73	1.95	21 (30%)	83,113,113	2.88	31 (37%)
17	BCR	cB	846	-	41,41,41	1.79	7 (17%)	56,56,56	1.46	12 (21%)
17	BCR	cB	851	-	41,41,41	1.76	8 (19%)	56,56,56	1.38	8 (14%)
14	CLA	cB	808	2	69,73,73	2.06	20 (28%)	83,113,113	2.75	27 (32%)
14	CLA	bB	838	22	69,73,73	1.95	20 (28%)	83,113,113	2.64	27 (32%)
14	CLA	bL	204	22	69,73,73	2.09	20 (28%)	83,113,113	2.72	27 (32%)
17	BCR	cA	846	-	41,41,41	1.76	6 (14%)	56,56,56	1.76	14 (25%)
14	CLA	bA	829	1	69,73,73	2.05	20 (28%)	83,113,113	2.69	29 (34%)
17	BCR	bJ	103	-	41,41,41	1.84	7 (17%)	56,56,56	1.61	11 (19%)
14	CLA	B	820	2	49,53,73	2.51	20 (40%)	59,89,113	3.23	27 (45%)
16	SF4	cA	844	1,2	0,12,12	-	-	-		
14	CLA	cB	824	2	54,58,73	2.38	20 (37%)	65,95,113	3.13	28 (43%)
17	BCR	F	202	-	41,41,41	1.80	6 (14%)	56,56,56	1.49	8 (14%)
14	CLA	cB	801	-	49,53,73	2.51	20 (40%)	59,89,113	3.23	26 (44%)
14	CLA	cB	806	2	69,73,73	2.08	21 (30%)	83,113,113	2.83	30 (36%)
18	LHG	cA	851	14	26,26,48	0.33	0	29,32,54	0.39	0
13	CL0	cA	801	1	69,73,73	2.01	20 (28%)	83,113,113	2.74	32 (38%)
14	CLA	bB	816	2	49,53,73	2.52	21 (42%)	59,89,113	3.25	30 (50%)
14	CLA	bX	201	-	49,53,73	2.50	21 (42%)	59,89,113	3.22	28 (47%)
14	CLA	cA	836	1	55,59,73	2.27	19 (34%)	66,96,113	3.10	31 (46%)
14	CLA	B	824	22	50,54,73	2.48	20 (40%)	60,90,113	3.20	26 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	bA	840	1	69,73,73	2.11	20 (28%)	83,113,113	2.69	26 (31%)
14	CLA	bA	813	1	49,53,73	2.47	20 (40%)	59,89,113	3.23	26 (44%)
14	CLA	A	815	-	49,53,73	2.51	21 (42%)	59,89,113	3.22	27 (45%)
14	CLA	cB	814	-	52,56,73	2.42	20 (38%)	62,92,113	3.13	30 (48%)
17	BCR	cB	847	-	41,41,41	1.71	7 (17%)	56,56,56	1.41	10 (17%)
17	BCR	A	847	-	41,41,41	1.77	7 (17%)	56,56,56	1.37	8 (14%)
14	CLA	cA	828	1	64,68,73	2.13	20 (31%)	77,107,113	2.80	25 (32%)
14	CLA	cA	834	1	49,53,73	2.50	20 (40%)	59,89,113	3.18	27 (45%)
14	CLA	cB	805	2	55,59,73	2.33	20 (36%)	66,96,113	3.12	30 (45%)
14	CLA	bB	821	-	49,53,73	2.49	21 (42%)	59,89,113	3.23	26 (44%)
14	CLA	B	829	2	49,53,73	2.49	20 (40%)	59,89,113	3.17	26 (44%)
14	CLA	cA	805	1	59,63,73	2.24	21 (35%)	71,101,113	3.03	29 (40%)
14	CLA	cB	820	-	51,55,73	2.45	20 (39%)	61,91,113	3.22	32 (52%)
14	CLA	cJ	102	8	49,53,73	2.50	21 (42%)	59,89,113	3.20	26 (44%)
14	CLA	bA	815	-	49,53,73	2.51	21 (42%)	59,89,113	3.22	27 (45%)
17	BCR	bB	843	-	41,41,41	1.86	7 (17%)	56,56,56	1.57	11 (19%)
17	BCR	B	844	-	41,41,41	1.72	8 (19%)	56,56,56	1.43	10 (17%)
14	CLA	cB	809	2	56,60,73	2.24	20 (35%)	67,97,113	3.07	30 (44%)
20	LMG	bB	848	-	43,43,55	0.21	0	51,51,63	0.30	0
14	CLA	bA	817	1	58,62,73	2.30	20 (34%)	69,99,113	2.95	26 (37%)
14	CLA	bB	829	2	49,53,73	2.49	20 (40%)	59,89,113	3.17	26 (44%)
14	CLA	bB	803	22	59,63,73	2.17	20 (33%)	71,101,113	2.96	30 (42%)
14	CLA	A	817	1	58,62,73	2.30	20 (34%)	69,99,113	2.95	26 (37%)
14	CLA	A	835	1	49,53,73	2.49	20 (40%)	59,89,113	3.15	28 (47%)
14	CLA	cA	823	1	49,53,73	2.48	20 (40%)	59,89,113	3.21	28 (47%)
17	BCR	bL	205	-	41,41,41	1.69	8 (19%)	56,56,56	1.40	9 (16%)
14	CLA	cA	803	1	49,53,73	2.49	20 (40%)	59,89,113	3.21	28 (47%)
14	CLA	cB	831	2	46,50,73	2.51	20 (43%)	55,85,113	3.30	25 (45%)
14	CLA	bA	814	-	49,53,73	2.52	20 (40%)	59,89,113	3.19	26 (44%)
17	BCR	B	843	-	41,41,41	1.85	8 (19%)	56,56,56	1.57	11 (19%)
14	CLA	bA	835	1	49,53,73	2.49	20 (40%)	59,89,113	3.16	28 (47%)
13	CL0	A	801	1	69,73,73	2.01	20 (28%)	83,113,113	2.74	32 (38%)
14	CLA	L	203	10	63,67,73	2.11	21 (33%)	75,105,113	2.96	30 (40%)
14	CLA	cL	204	10	63,67,73	2.11	21 (33%)	75,105,113	2.96	30 (40%)
14	CLA	bB	833	-	49,53,73	2.51	21 (42%)	59,89,113	3.17	28 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	cA	802	22	69,73,73	1.94	21 (30%)	83,113,113	2.85	31 (37%)
14	CLA	cA	824	22	63,67,73	2.17	20 (31%)	75,105,113	2.83	30 (40%)
14	CLA	A	821	-	49,53,73	2.52	20 (40%)	59,89,113	3.23	26 (44%)
17	BCR	bA	849	-	41,41,41	1.72	7 (17%)	56,56,56	1.48	10 (17%)
14	CLA	bB	839	2	69,73,73	2.04	21 (30%)	83,113,113	2.78	28 (33%)
14	CLA	B	832	2	49,53,73	2.44	19 (38%)	59,89,113	3.22	27 (45%)
14	CLA	bB	825	2	59,63,73	2.26	20 (33%)	71,101,113	2.99	32 (45%)
14	CLA	bL	202	10	69,73,73	2.10	21 (30%)	83,113,113	3.98	30 (36%)
15	PQN	B	840	-	34,34,34	0.45	1 (2%)	42,45,45	0.35	0
14	CLA	A	808	1	49,53,73	2.45	20 (40%)	59,89,113	3.24	30 (50%)
14	CLA	B	816	2	49,53,73	2.52	21 (42%)	59,89,113	3.24	29 (49%)
14	CLA	bA	852	-	69,73,73	1.86	18 (26%)	83,113,113	2.50	28 (33%)
14	CLA	A	807	1	49,53,73	2.50	21 (42%)	59,89,113	3.19	27 (45%)
17	BCR	A	845	-	41,41,41	1.79	7 (17%)	56,56,56	1.48	11 (19%)
14	CLA	bB	812	2	69,73,73	2.10	20 (28%)	83,113,113	2.88	29 (34%)
14	CLA	B	839	2	69,73,73	2.04	21 (30%)	83,113,113	2.78	28 (33%)
14	CLA	B	825	2	59,63,73	2.26	20 (33%)	71,101,113	2.99	32 (45%)
14	CLA	bB	818	-	50,54,73	2.45	20 (40%)	60,90,113	3.13	26 (43%)
14	CLA	B	833	-	49,53,73	2.51	21 (42%)	59,89,113	3.17	28 (47%)
14	CLA	bA	837	1	69,73,73	2.00	20 (28%)	83,113,113	2.73	28 (33%)
17	BCR	cB	848	-	41,41,41	1.73	8 (19%)	56,56,56	1.48	13 (23%)
20	LMG	B	848	-	43,43,55	0.21	0	51,51,63	0.30	0
14	CLA	cB	807	2	69,73,73	2.07	20 (28%)	83,113,113	2.74	31 (37%)
14	CLA	bA	812	1	49,53,73	2.51	20 (40%)	59,89,113	3.23	26 (44%)
17	BCR	cF	202	-	41,41,41	1.79	6 (14%)	56,56,56	1.49	8 (14%)
14	CLA	bB	830	2	46,50,73	2.51	20 (43%)	55,85,113	3.30	25 (45%)
17	BCR	L	206	-	41,41,41	1.74	8 (19%)	56,56,56	1.39	8 (14%)
14	CLA	B	812	2	69,73,73	2.10	21 (30%)	83,113,113	2.88	29 (34%)
14	CLA	bA	832	1	69,73,73	1.98	20 (28%)	83,113,113	2.75	31 (37%)
14	CLA	cA	813	1	49,53,73	2.47	20 (40%)	59,89,113	3.23	26 (44%)
14	CLA	A	834	1	49,53,73	2.50	20 (40%)	59,89,113	3.17	27 (45%)
14	CLA	bA	805	1	59,63,73	2.24	21 (35%)	71,101,113	3.04	29 (40%)
14	CLA	bB	828	2	69,73,73	2.01	19 (27%)	83,113,113	2.82	29 (34%)
14	CLA	bA	820	22	49,53,73	2.51	21 (42%)	59,89,113	3.17	28 (47%)
14	CLA	B	817	2	59,63,73	2.26	22 (37%)	71,101,113	3.04	30 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	B	835	2	49,53,73	2.48	20 (40%)	59,89,113	3.22	26 (44%)
14	CLA	cL	202	2	69,73,73	1.95	21 (30%)	83,113,113	2.87	31 (37%)
14	CLA	A	824	22	63,67,73	2.17	20 (31%)	75,105,113	2.83	30 (40%)
14	CLA	bA	808	1	49,53,73	2.45	20 (40%)	59,89,113	3.23	30 (50%)
14	CLA	J	101	8	49,53,73	2.51	21 (42%)	59,89,113	3.21	27 (45%)
14	CLA	bB	819	-	51,55,73	2.45	20 (39%)	61,91,113	3.21	32 (52%)
14	CLA	cB	811	2	49,53,73	2.50	21 (42%)	59,89,113	3.18	25 (42%)
17	BCR	B	846	-	41,41,41	1.71	7 (17%)	56,56,56	1.41	10 (17%)
17	BCR	I	102	-	41,41,41	1.67	8 (19%)	56,56,56	1.46	9 (16%)
14	CLA	bA	822	1	49,53,73	2.49	21 (42%)	59,89,113	3.23	26 (44%)
17	BCR	bB	845	-	41,41,41	1.79	7 (17%)	56,56,56	1.46	12 (21%)
14	CLA	bA	806	1	69,73,73	2.06	20 (28%)	83,113,113	2.75	28 (33%)
14	CLA	cA	821	-	49,53,73	2.52	20 (40%)	59,89,113	3.23	26 (44%)
14	CLA	bA	827	1	65,69,73	2.17	20 (30%)	78,108,113	2.88	29 (37%)
15	PQN	A	843	-	34,34,34	0.47	1 (2%)	42,45,45	0.34	0
17	BCR	bI	101	-	41,41,41	1.68	8 (19%)	56,56,56	1.39	10 (17%)
17	BCR	cB	844	-	41,41,41	1.85	7 (17%)	56,56,56	1.57	11 (19%)
17	BCR	bB	846	-	41,41,41	1.71	7 (17%)	56,56,56	1.41	10 (17%)
17	BCR	bB	842	-	41,41,41	1.79	7 (17%)	56,56,56	1.60	12 (21%)
17	BCR	J	103	-	41,41,41	1.84	7 (17%)	56,56,56	1.61	11 (19%)
14	CLA	A	829	1	69,73,73	2.05	20 (28%)	83,113,113	2.69	29 (34%)
18	LHG	bA	850	-	48,48,48	0.27	0	51,54,54	0.31	0
14	CLA	cA	840	1	69,73,73	2.11	20 (28%)	83,113,113	2.69	26 (31%)
17	BCR	bA	847	-	41,41,41	1.77	7 (17%)	56,56,56	1.37	8 (14%)
16	SF4	C	102	3	0,12,12	-	-	-		
17	BCR	B	845	-	41,41,41	1.78	7 (17%)	56,56,56	1.46	12 (21%)
14	CLA	bB	836	2	49,53,73	2.47	20 (40%)	59,89,113	3.20	26 (44%)
14	CLA	bA	826	1	50,54,73	2.43	20 (40%)	60,90,113	3.24	27 (45%)
14	CLA	cA	825	22	54,58,73	2.31	20 (37%)	65,95,113	3.19	30 (46%)
14	CLA	A	839	1	69,73,73	2.07	20 (28%)	83,113,113	2.73	28 (33%)
14	CLA	cA	830	1	54,58,73	2.24	18 (33%)	65,95,113	3.07	29 (44%)
14	CLA	cB	818	2	59,63,73	2.26	22 (37%)	71,101,113	3.03	30 (42%)
17	BCR	B	842	-	41,41,41	1.80	7 (17%)	56,56,56	1.60	12 (21%)
14	CLA	cA	833	1	69,73,73	2.00	21 (30%)	83,113,113	2.71	30 (36%)
14	CLA	cF	201	22	55,59,73	2.29	19 (34%)	66,96,113	3.04	31 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	cA	831	1	59,63,73	2.23	20 (33%)	71,101,113	2.99	32 (45%)
14	CLA	bB	849	-	49,53,73	2.50	20 (40%)	59,89,113	3.18	27 (45%)
15	PQN	cA	843	-	34,34,34	0.47	1 (2%)	42,45,45	0.34	0
14	CLA	B	823	2	54,58,73	2.38	20 (37%)	65,95,113	3.13	28 (43%)
14	CLA	A	812	1	49,53,73	2.50	21 (42%)	59,89,113	3.22	26 (44%)
14	CLA	cA	814	-	49,53,73	2.52	20 (40%)	59,89,113	3.18	26 (44%)
14	CLA	cA	816	1	49,53,73	2.48	20 (40%)	59,89,113	3.18	26 (44%)
14	CLA	bB	826	2	69,73,73	2.02	21 (30%)	83,113,113	2.81	32 (38%)
14	CLA	bL	203	10	63,67,73	2.11	21 (33%)	75,105,113	2.96	30 (40%)
14	CLA	cA	852	-	69,73,73	1.86	18 (26%)	83,113,113	2.50	28 (33%)
14	CLA	bB	815	2	56,60,73	2.33	21 (37%)	67,97,113	3.10	31 (46%)
17	BCR	A	849	-	41,41,41	1.72	7 (17%)	56,56,56	1.48	10 (17%)
14	CLA	cB	803	2	69,73,73	2.01	20 (28%)	83,113,113	2.75	32 (38%)
14	CLA	bA	810	-	49,53,73	2.49	21 (42%)	59,89,113	3.16	25 (42%)
17	BCR	cL	207	-	41,41,41	1.74	8 (19%)	56,56,56	1.39	8 (14%)
14	CLA	cB	802	-	69,73,73	2.02	19 (27%)	83,113,113	2.70	28 (33%)
14	CLA	A	811	1	49,53,73	2.47	20 (40%)	59,89,113	3.21	28 (47%)
17	BCR	bA	846	-	41,41,41	1.77	7 (17%)	56,56,56	1.77	14 (25%)
17	BCR	B	841	-	41,41,41	1.75	7 (17%)	56,56,56	1.37	9 (16%)
14	CLA	A	818	1	64,68,73	2.18	21 (32%)	77,107,113	2.94	31 (40%)
14	CLA	A	802	22	69,73,73	1.94	21 (30%)	83,113,113	2.85	31 (37%)
14	CLA	bA	811	1	49,53,73	2.47	21 (42%)	59,89,113	3.21	28 (47%)
14	CLA	bB	801	-	69,73,73	2.02	19 (27%)	83,113,113	2.70	28 (33%)
17	BCR	cI	102	-	41,41,41	1.66	8 (19%)	56,56,56	1.46	9 (16%)
14	CLA	B	838	22	69,73,73	1.95	20 (28%)	83,113,113	2.63	27 (32%)
14	CLA	B	807	2	69,73,73	2.06	20 (28%)	83,113,113	2.75	27 (32%)
14	CLA	bA	803	1	49,53,73	2.49	20 (40%)	59,89,113	3.21	28 (47%)
14	CLA	cA	820	22	49,53,73	2.51	21 (42%)	59,89,113	3.17	28 (47%)
14	CLA	bB	804	2	55,59,73	2.33	20 (36%)	66,96,113	3.12	30 (45%)
14	CLA	cA	807	1	49,53,73	2.50	21 (42%)	59,89,113	3.18	27 (45%)
17	BCR	I	101	-	41,41,41	1.69	8 (19%)	56,56,56	1.39	10 (17%)
14	CLA	bB	813	-	52,56,73	2.42	20 (38%)	62,92,113	3.12	30 (48%)
16	SF4	A	844	1,2	0,12,12	-	-	-		
14	CLA	bB	835	2	49,53,73	2.48	20 (40%)	59,89,113	3.22	26 (44%)
14	CLA	A	819	1	49,53,73	2.51	20 (40%)	59,89,113	3.19	29 (49%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	LHG	cA	850	-	48,48,48	0.27	0	51,54,54	0.31	0
14	CLA	A	804	1	57,61,73	2.32	21 (36%)	68,98,113	3.10	29 (42%)
14	CLA	cA	809	1	49,53,73	2.47	20 (40%)	59,89,113	3.19	26 (44%)
14	CLA	bB	807	2	69,73,73	2.06	20 (28%)	83,113,113	2.75	27 (32%)
20	LMG	cB	849	-	43,43,55	0.21	0	51,51,63	0.30	0
14	CLA	bB	822	2	49,53,73	2.48	20 (40%)	59,89,113	3.26	26 (44%)
14	CLA	cA	827	1	65,69,73	2.17	20 (30%)	78,108,113	2.88	28 (35%)
17	BCR	cB	842	-	41,41,41	1.75	7 (17%)	56,56,56	1.37	9 (16%)
16	SF4	C	101	3	0,12,12	-	-	-		
14	CLA	B	814	-	49,53,73	2.50	21 (42%)	59,89,113	3.24	28 (47%)
14	CLA	B	828	2	69,73,73	2.01	19 (27%)	83,113,113	2.81	29 (34%)
14	CLA	cB	837	2	49,53,73	2.47	20 (40%)	59,89,113	3.20	26 (44%)
14	CLA	A	828	1	64,68,73	2.13	20 (31%)	77,107,113	2.80	25 (32%)
14	CLA	A	825	22	54,58,73	2.31	20 (37%)	65,95,113	3.19	30 (46%)
14	CLA	bB	814	-	49,53,73	2.50	21 (42%)	59,89,113	3.24	27 (45%)
14	CLA	bB	805	2	69,73,73	2.07	21 (30%)	83,113,113	2.83	30 (36%)
14	CLA	B	830	2	46,50,73	2.51	20 (43%)	55,85,113	3.30	25 (45%)
14	CLA	cA	819	1	49,53,73	2.51	20 (40%)	59,89,113	3.19	29 (49%)
14	CLA	cB	823	2	49,53,73	2.48	20 (40%)	59,89,113	3.25	26 (44%)
14	CLA	cL	203	10	69,73,73	2.10	21 (30%)	83,113,113	3.99	30 (36%)
14	CLA	A	823	1	49,53,73	2.48	20 (40%)	59,89,113	3.21	28 (47%)
14	CLA	cB	821	2	49,53,73	2.52	20 (40%)	59,89,113	3.23	27 (45%)
14	CLA	bB	817	2	59,63,73	2.26	22 (37%)	71,101,113	3.03	30 (42%)
14	CLA	B	815	2	56,60,73	2.33	21 (37%)	67,97,113	3.09	31 (46%)
14	CLA	cA	838	1	49,53,73	2.32	19 (38%)	59,89,113	3.30	27 (45%)
15	PQN	cB	841	-	34,34,34	0.45	1 (2%)	42,45,45	0.35	0
14	CLA	bB	831	2	69,73,73	2.10	20 (28%)	83,113,113	2.85	29 (34%)
14	CLA	bA	836	1	55,59,73	2.26	19 (34%)	66,96,113	3.10	31 (46%)
14	CLA	B	803	22	59,63,73	2.17	20 (33%)	71,101,113	2.96	30 (42%)
17	BCR	bA	848	-	41,41,41	1.68	8 (19%)	56,56,56	1.51	13 (23%)
14	CLA	L	204	22	69,73,73	2.09	20 (28%)	83,113,113	2.72	27 (32%)
17	BCR	cM	101	-	41,41,41	1.75	8 (19%)	56,56,56	1.50	12 (21%)
14	CLA	bB	851	-	49,53,73	2.51	20 (40%)	59,89,113	3.23	26 (44%)
14	CLA	cB	822	-	49,53,73	2.49	21 (42%)	59,89,113	3.23	26 (44%)
14	CLA	A	833	1	69,73,73	2.00	21 (30%)	83,113,113	2.71	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	LHG	A	851	14	26,26,48	0.33	0	29,32,54	0.39	0
14	CLA	B	822	2	49,53,73	2.48	20 (40%)	59,89,113	3.25	26 (44%)
14	CLA	B	831	2	69,73,73	2.10	20 (28%)	83,113,113	2.84	29 (34%)
14	CLA	bB	832	2	49,53,73	2.44	19 (38%)	59,89,113	3.22	27 (45%)
14	CLA	bA	834	1	49,53,73	2.50	20 (40%)	59,89,113	3.17	27 (45%)
14	CLA	bA	841	22	69,73,73	1.97	19 (27%)	83,113,113	2.66	31 (37%)
14	CLA	bB	810	2	49,53,73	2.50	21 (42%)	59,89,113	3.18	25 (42%)
14	CLA	cA	804	1	57,61,73	2.32	21 (36%)	68,98,113	3.10	29 (42%)
14	CLA	cL	205	22	69,73,73	2.09	20 (28%)	83,113,113	2.72	27 (32%)
14	CLA	B	818	-	50,54,73	2.44	20 (40%)	60,90,113	3.12	26 (43%)
17	BCR	M	101	-	41,41,41	1.75	8 (19%)	56,56,56	1.50	12 (21%)
14	CLA	cA	832	1	69,73,73	1.98	20 (28%)	83,113,113	2.74	31 (37%)
14	CLA	cB	838	2	51,55,73	2.41	20 (39%)	61,91,113	3.20	25 (40%)
14	CLA	B	801	-	69,73,73	2.02	19 (27%)	83,113,113	2.71	28 (33%)
14	CLA	bJ	101	8	49,53,73	2.51	21 (42%)	59,89,113	3.21	27 (45%)
14	CLA	cB	850	-	49,53,73	2.50	21 (42%)	59,89,113	3.18	27 (45%)
14	CLA	bA	802	22	69,73,73	1.94	21 (30%)	83,113,113	2.85	31 (37%)
14	CLA	bA	824	22	63,67,73	2.17	20 (31%)	75,105,113	2.83	30 (40%)
14	CLA	cB	834	-	49,53,73	2.51	20 (40%)	59,89,113	3.17	28 (47%)
14	CLA	bF	201	22	55,59,73	2.29	19 (34%)	66,96,113	3.04	31 (46%)
14	CLA	bB	811	2	49,53,73	2.49	20 (40%)	59,89,113	3.15	26 (44%)
14	CLA	bB	802	2	69,73,73	2.02	20 (28%)	83,113,113	2.75	32 (38%)
14	CLA	A	813	1	49,53,73	2.47	20 (40%)	59,89,113	3.23	26 (44%)
14	CLA	cA	822	1	49,53,73	2.49	21 (42%)	59,89,113	3.23	26 (44%)
14	CLA	cB	830	2	49,53,73	2.49	20 (40%)	59,89,113	3.17	26 (44%)
14	CLA	B	819	-	51,55,73	2.45	20 (39%)	61,91,113	3.21	32 (52%)
16	SF4	bC	102	3	0,12,12	-	-	-		
14	CLA	B	810	2	49,53,73	2.50	21 (42%)	59,89,113	3.18	25 (42%)
14	CLA	cB	833	2	49,53,73	2.44	19 (38%)	59,89,113	3.21	27 (45%)
14	CLA	bA	809	1	49,53,73	2.47	20 (40%)	59,89,113	3.20	26 (44%)
17	BCR	bL	206	-	41,41,41	1.74	8 (19%)	56,56,56	1.39	8 (14%)
14	CLA	bB	827	2	69,73,73	2.10	20 (28%)	83,113,113	2.71	28 (33%)
14	CLA	bB	809	2	69,73,73	1.94	19 (27%)	83,113,113	2.71	30 (36%)
14	CLA	cA	815	-	49,53,73	2.51	21 (42%)	59,89,113	3.22	27 (45%)
17	BCR	cA	847	-	41,41,41	1.77	7 (17%)	56,56,56	1.37	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	BCR	cA	848	-	41,41,41	1.68	8 (19%)	56,56,56	1.52	13 (23%)
14	CLA	B	811	2	49,53,73	2.50	20 (40%)	59,89,113	3.15	27 (45%)
14	CLA	cB	829	2	69,73,73	2.01	19 (27%)	83,113,113	2.81	29 (34%)
14	CLA	bB	820	2	49,53,73	2.52	20 (40%)	59,89,113	3.23	27 (45%)
17	BCR	cJ	103	-	41,41,41	1.84	7 (17%)	56,56,56	1.61	11 (19%)
17	BCR	bI	102	-	41,41,41	1.67	8 (19%)	56,56,56	1.46	9 (16%)
14	CLA	A	842	18	49,53,73	2.44	20 (40%)	59,89,113	3.19	26 (44%)
14	CLA	L	202	10	69,73,73	2.10	21 (30%)	83,113,113	3.98	30 (36%)
14	CLA	cJ	101	8	49,53,73	2.51	21 (42%)	59,89,113	3.21	27 (45%)
14	CLA	A	805	1	59,63,73	2.23	21 (35%)	71,101,113	3.03	29 (40%)
14	CLA	cB	816	2	56,60,73	2.33	21 (37%)	67,97,113	3.09	31 (46%)
14	CLA	cB	840	2	69,73,73	2.04	21 (30%)	83,113,113	2.78	28 (33%)
14	CLA	cA	817	1	58,62,73	2.30	20 (34%)	69,99,113	2.95	26 (37%)
14	CLA	A	840	1	69,73,73	2.11	20 (28%)	83,113,113	2.69	26 (31%)
14	CLA	bA	842	18	49,53,73	2.44	20 (40%)	59,89,113	3.19	26 (44%)
17	BCR	cB	845	-	41,41,41	1.72	8 (19%)	56,56,56	1.42	10 (17%)
17	BCR	L	205	-	41,41,41	1.70	8 (19%)	56,56,56	1.40	9 (16%)
14	CLA	B	827	2	69,73,73	2.10	20 (28%)	83,113,113	2.71	28 (33%)
17	BCR	bB	844	-	41,41,41	1.71	8 (19%)	56,56,56	1.43	10 (17%)
14	CLA	A	816	1	49,53,73	2.48	20 (40%)	59,89,113	3.18	26 (44%)
14	CLA	cB	825	22	50,54,73	2.48	20 (40%)	60,90,113	3.20	26 (43%)
14	CLA	A	830	1	54,58,73	2.24	18 (33%)	65,95,113	3.07	29 (44%)
14	CLA	A	831	1	59,63,73	2.23	20 (33%)	71,101,113	2.99	31 (43%)
14	CLA	cA	812	1	49,53,73	2.51	20 (40%)	59,89,113	3.23	26 (44%)
14	CLA	A	806	1	69,73,73	2.06	20 (28%)	83,113,113	2.75	28 (33%)
14	CLA	bA	823	1	49,53,73	2.48	20 (40%)	59,89,113	3.21	28 (47%)
17	BCR	bM	101	-	41,41,41	1.75	8 (19%)	56,56,56	1.50	12 (21%)
14	CLA	cA	842	18	49,53,73	2.44	20 (40%)	59,89,113	3.18	26 (44%)
14	CLA	B	849	-	49,53,73	2.50	21 (42%)	59,89,113	3.18	27 (45%)
14	CLA	B	826	2	69,73,73	2.02	21 (30%)	83,113,113	2.82	32 (38%)
14	CLA	A	814	-	49,53,73	2.52	20 (40%)	59,89,113	3.19	26 (44%)
17	BCR	cA	845	-	41,41,41	1.80	7 (17%)	56,56,56	1.49	11 (19%)
16	SF4	cC	101	3	0,12,12	-	-	-		
15	PQN	bB	840	-	34,34,34	0.45	1 (2%)	42,45,45	0.35	0
16	SF4	cC	102	3	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	cA	835	1	49,53,73	2.49	20 (40%)	59,89,113	3.15	28 (47%)
14	CLA	cB	819	-	50,54,73	2.45	20 (40%)	60,90,113	3.13	26 (43%)
14	CLA	cA	808	1	49,53,73	2.45	20 (40%)	59,89,113	3.23	30 (50%)

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	CLA	A	852	-	-	7/39/115/115	-
17	BCR	cL	206	-	-	4/29/63/63	0/2/2/2
14	CLA	bA	830	1	-	4/21/97/115	-
17	BCR	bB	850	-	-	12/29/63/63	0/2/2/2
14	CLA	cB	815	-	-	7/15/91/115	-
14	CLA	cA	806	1	-	11/39/115/115	-
14	CLA	X	201	-	-	5/15/91/115	-
14	CLA	cB	828	2	-	5/39/115/115	-
15	PQN	bA	843	-	-	4/23/43/43	0/2/2/2
14	CLA	cA	811	1	-	5/15/91/115	-
14	CLA	B	821	-	-	8/15/91/115	-
14	CLA	J	102	8	-	2/15/91/115	-
17	BCR	A	848	-	-	3/29/63/63	0/2/2/2
14	CLA	A	826	1	-	6/17/93/115	-
14	CLA	bB	824	22	-	6/17/93/115	-
14	CLA	bA	838	1	-	5/15/91/115	-
16	SF4	bC	101	3	-	-	0/6/5/5
13	CL0	bA	801	1	-	4/39/115/115	-
14	CLA	A	837	1	-	9/39/115/115	-
14	CLA	bA	818	1	-	10/33/109/115	-
14	CLA	B	813	-	-	5/19/95/115	-
17	BCR	cB	843	-	-	9/29/63/63	0/2/2/2
14	CLA	A	820	22	-	5/15/91/115	-
14	CLA	bA	816	1	-	7/15/91/115	-
14	CLA	cB	804	22	-	8/27/103/115	-
14	CLA	bA	828	1	-	7/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	cB	832	2	-	16/39/115/115	-
14	CLA	bA	839	1	-	9/39/115/115	-
14	CLA	bA	825	22	-	2/21/97/115	-
18	LHG	A	850	-	-	15/53/53/53	-
16	SF4	bA	844	1,2	-	-	0/6/5/5
14	CLA	cA	829	1	-	12/39/115/115	-
14	CLA	bA	819	1	-	6/15/91/115	-
14	CLA	A	809	1	-	6/15/91/115	-
14	CLA	F	201	22	-	5/23/99/115	-
14	CLA	cB	827	2	-	6/39/115/115	-
17	BCR	B	847	-	-	2/29/63/63	0/2/2/2
14	CLA	A	827	1	-	3/35/111/115	-
14	CLA	cA	837	1	-	9/39/115/115	-
14	CLA	B	805	2	-	15/39/115/115	-
17	BCR	B	850	-	-	12/29/63/63	0/2/2/2
14	CLA	cA	839	1	-	9/39/115/115	-
14	CLA	A	822	1	-	3/15/91/115	-
14	CLA	bA	804	1	-	8/25/101/115	-
14	CLA	cA	810	-	-	5/15/91/115	-
17	BCR	bB	847	-	-	2/29/63/63	0/2/2/2
14	CLA	B	809	2	-	11/39/115/115	-
14	CLA	A	841	22	-	11/39/115/115	-
14	CLA	bB	837	2	-	6/18/94/115	-
14	CLA	bB	808	2	-	3/24/100/115	-
17	BCR	cI	101	-	-	1/29/63/63	0/2/2/2
14	CLA	bA	807	1	-	8/15/91/115	-
17	BCR	bA	845	-	-	10/29/63/63	0/2/2/2
14	CLA	B	836	2	-	7/15/91/115	-
14	CLA	cB	826	2	-	4/27/103/115	-
14	CLA	bA	833	1	-	8/39/115/115	-
14	CLA	bA	821	-	-	4/15/91/115	-
14	CLA	cA	826	1	-	6/17/93/115	-
14	CLA	B	804	2	-	7/23/99/115	-
14	CLA	bB	823	2	-	6/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	838	1	-	5/15/91/115	-
14	CLA	bA	831	1	-	13/27/103/115	-
14	CLA	cB	817	2	-	6/15/91/115	-
14	CLA	cX	201	-	-	5/15/91/115	-
14	CLA	B	851	-	-	5/15/91/115	-
14	CLA	bJ	102	8	-	3/15/91/115	-
14	CLA	cB	839	22	-	5/39/115/115	-
17	BCR	cA	849	-	-	8/29/63/63	0/2/2/2
14	CLA	B	837	2	-	6/18/94/115	-
14	CLA	cB	836	2	-	3/15/91/115	-
17	BCR	bF	202	-	-	6/29/63/63	0/2/2/2
14	CLA	bB	834	-	-	3/15/91/115	-
14	CLA	cA	841	22	-	11/39/115/115	-
17	BCR	A	846	-	-	15/29/63/63	0/2/2/2
17	BCR	bB	841	-	-	7/29/63/63	0/2/2/2
14	CLA	B	808	2	-	3/24/100/115	-
14	CLA	A	803	1	-	8/15/91/115	-
14	CLA	bB	806	2	-	10/39/115/115	-
14	CLA	cA	818	1	-	10/33/109/115	-
14	CLA	cB	812	2	-	3/15/91/115	-
14	CLA	B	802	2	-	11/39/115/115	-
18	LHG	bA	851	14	-	13/31/31/53	-
14	CLA	A	836	1	-	6/23/99/115	-
14	CLA	A	832	1	-	8/39/115/115	-
14	CLA	cB	810	2	-	11/39/115/115	-
14	CLA	A	810	-	-	5/15/91/115	-
14	CLA	L	201	2	-	10/39/115/115	-
14	CLA	cB	813	2	-	9/39/115/115	-
14	CLA	B	806	2	-	10/39/115/115	-
14	CLA	B	834	-	-	3/15/91/115	-
14	CLA	cB	835	-	-	3/15/91/115	-
14	CLA	bL	201	2	-	10/39/115/115	-
17	BCR	cB	846	-	-	3/29/63/63	0/2/2/2
17	BCR	cB	851	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	cB	808	2	-	12/39/115/115	-
14	CLA	bB	838	22	-	5/39/115/115	-
14	CLA	bL	204	22	-	17/39/115/115	-
17	BCR	cA	846	-	-	15/29/63/63	0/2/2/2
14	CLA	bA	829	1	-	12/39/115/115	-
17	BCR	bJ	103	-	-	17/29/63/63	0/2/2/2
14	CLA	B	820	2	-	10/15/91/115	-
16	SF4	cA	844	1,2	-	-	0/6/5/5
14	CLA	cB	824	2	-	6/21/97/115	-
17	BCR	F	202	-	-	6/29/63/63	0/2/2/2
14	CLA	cB	801	-	-	6/15/91/115	-
14	CLA	cB	806	2	-	15/39/115/115	-
18	LHG	cA	851	14	-	14/31/31/53	-
13	CL0	cA	801	1	-	4/39/115/115	-
14	CLA	bB	816	2	-	6/15/91/115	-
14	CLA	bX	201	-	-	5/15/91/115	-
14	CLA	cA	836	1	-	6/23/99/115	-
14	CLA	B	824	22	-	6/17/93/115	-
14	CLA	bA	840	1	-	13/39/115/115	-
14	CLA	bA	813	1	-	5/15/91/115	-
14	CLA	A	815	-	-	7/15/91/115	-
14	CLA	cB	814	-	-	5/19/95/115	-
17	BCR	cB	847	-	-	10/29/63/63	0/2/2/2
17	BCR	A	847	-	-	6/29/63/63	0/2/2/2
14	CLA	cA	828	1	-	7/33/109/115	-
14	CLA	cA	834	1	-	3/15/91/115	-
14	CLA	cB	805	2	-	8/23/99/115	-
14	CLA	bB	821	-	-	8/15/91/115	-
14	CLA	B	829	2	-	7/15/91/115	-
14	CLA	cA	805	1	-	6/27/103/115	-
14	CLA	cB	820	-	-	11/18/94/115	-
14	CLA	cJ	102	8	-	3/15/91/115	-
14	CLA	bA	815	-	-	7/15/91/115	-
17	BCR	bB	843	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	B	844	-	-	15/29/63/63	0/2/2/2
14	CLA	cB	809	2	-	3/24/100/115	-
20	LMG	bB	848	-	-	9/38/58/70	0/1/1/1
14	CLA	bA	817	1	-	8/26/102/115	-
14	CLA	bB	829	2	-	7/15/91/115	-
14	CLA	bB	803	22	-	8/27/103/115	-
14	CLA	A	817	1	-	8/26/102/115	-
14	CLA	A	835	1	-	5/15/91/115	-
14	CLA	cA	823	1	-	6/15/91/115	-
17	BCR	bL	205	-	-	4/29/63/63	0/2/2/2
14	CLA	cA	803	1	-	8/15/91/115	-
14	CLA	cB	831	2	-	4/12/88/115	-
14	CLA	bA	814	-	-	1/15/91/115	-
17	BCR	B	843	-	-	10/29/63/63	0/2/2/2
14	CLA	bA	835	1	-	5/15/91/115	-
13	CL0	A	801	1	-	4/39/115/115	-
14	CLA	L	203	10	-	9/32/108/115	-
14	CLA	cL	204	10	-	9/32/108/115	-
14	CLA	bB	833	-	-	2/15/91/115	-
14	CLA	cA	802	22	-	3/39/115/115	-
14	CLA	cA	824	22	-	7/32/108/115	-
14	CLA	A	821	-	-	4/15/91/115	-
17	BCR	bA	849	-	-	8/29/63/63	0/2/2/2
14	CLA	bB	839	2	-	13/39/115/115	-
14	CLA	B	832	2	-	4/15/91/115	-
14	CLA	bB	825	2	-	4/27/103/115	-
14	CLA	bL	202	10	-	15/39/115/115	-
15	PQN	B	840	-	-	4/23/43/43	0/2/2/2
14	CLA	A	808	1	-	7/15/91/115	-
14	CLA	B	816	2	-	5/15/91/115	-
14	CLA	bA	852	-	-	7/39/115/115	-
14	CLA	A	807	1	-	8/15/91/115	-
17	BCR	A	845	-	-	10/29/63/63	0/2/2/2
14	CLA	bB	812	2	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	839	2	-	13/39/115/115	-
14	CLA	B	825	2	-	5/27/103/115	-
14	CLA	bB	818	-	-	5/17/93/115	-
14	CLA	B	833	-	-	2/15/91/115	-
14	CLA	bA	837	1	-	9/39/115/115	-
17	BCR	cB	848	-	-	2/29/63/63	0/2/2/2
20	LMG	B	848	-	-	9/38/58/70	0/1/1/1
14	CLA	cB	807	2	-	10/39/115/115	-
14	CLA	bA	812	1	-	5/15/91/115	-
17	BCR	cF	202	-	-	6/29/63/63	0/2/2/2
14	CLA	bB	830	2	-	4/12/88/115	-
17	BCR	L	206	-	-	3/29/63/63	0/2/2/2
14	CLA	B	812	2	-	9/39/115/115	-
14	CLA	bA	832	1	-	8/39/115/115	-
14	CLA	cA	813	1	-	5/15/91/115	-
14	CLA	A	834	1	-	3/15/91/115	-
14	CLA	bA	805	1	-	6/27/103/115	-
14	CLA	bB	828	2	-	13/39/115/115	-
14	CLA	bA	820	22	-	5/15/91/115	-
14	CLA	B	817	2	-	6/27/103/115	-
14	CLA	B	835	2	-	3/15/91/115	-
14	CLA	cL	202	2	-	10/39/115/115	-
14	CLA	A	824	22	-	7/32/108/115	-
14	CLA	bA	808	1	-	7/15/91/115	-
14	CLA	J	101	8	-	4/15/91/115	-
14	CLA	bB	819	-	-	11/18/94/115	-
14	CLA	cB	811	2	-	5/15/91/115	-
17	BCR	B	846	-	-	10/29/63/63	0/2/2/2
17	BCR	I	102	-	-	3/29/63/63	0/2/2/2
14	CLA	bA	822	1	-	3/15/91/115	-
17	BCR	bB	845	-	-	3/29/63/63	0/2/2/2
14	CLA	bA	806	1	-	11/39/115/115	-
14	CLA	cA	821	-	-	4/15/91/115	-
14	CLA	bA	827	1	-	3/35/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	PQN	A	843	-	-	4/23/43/43	0/2/2/2
17	BCR	bI	101	-	-	1/29/63/63	0/2/2/2
17	BCR	cB	844	-	-	10/29/63/63	0/2/2/2
17	BCR	bB	846	-	-	10/29/63/63	0/2/2/2
17	BCR	bB	842	-	-	9/29/63/63	0/2/2/2
17	BCR	J	103	-	-	17/29/63/63	0/2/2/2
14	CLA	A	829	1	-	12/39/115/115	-
18	LHG	bA	850	-	-	15/53/53/53	-
14	CLA	cA	840	1	-	13/39/115/115	-
17	BCR	bA	847	-	-	6/29/63/63	0/2/2/2
16	SF4	C	102	3	-	-	0/6/5/5
17	BCR	B	845	-	-	3/29/63/63	0/2/2/2
14	CLA	bB	836	2	-	7/15/91/115	-
14	CLA	bA	826	1	-	6/17/93/115	-
14	CLA	cA	825	22	-	2/21/97/115	-
14	CLA	A	839	1	-	9/39/115/115	-
14	CLA	cA	830	1	-	4/21/97/115	-
14	CLA	cB	818	2	-	6/27/103/115	-
17	BCR	B	842	-	-	9/29/63/63	0/2/2/2
14	CLA	cA	833	1	-	8/39/115/115	-
14	CLA	cF	201	22	-	5/23/99/115	-
14	CLA	cA	831	1	-	13/27/103/115	-
14	CLA	bB	849	-	-	4/15/91/115	-
15	PQN	cA	843	-	-	4/23/43/43	0/2/2/2
14	CLA	B	823	2	-	6/21/97/115	-
14	CLA	A	812	1	-	5/15/91/115	-
14	CLA	cA	814	-	-	1/15/91/115	-
14	CLA	cA	816	1	-	7/15/91/115	-
14	CLA	bB	826	2	-	6/39/115/115	-
14	CLA	bL	203	10	-	9/32/108/115	-
14	CLA	cA	852	-	-	7/39/115/115	-
14	CLA	bB	815	2	-	11/24/100/115	-
17	BCR	A	849	-	-	8/29/63/63	0/2/2/2
14	CLA	cB	803	2	-	11/39/115/115	-
14	CLA	bA	810	-	-	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	cL	207	-	-	3/29/63/63	0/2/2/2
14	CLA	cB	802	-	-	9/39/115/115	-
14	CLA	A	811	1	-	5/15/91/115	-
17	BCR	bA	846	-	-	15/29/63/63	0/2/2/2
17	BCR	B	841	-	-	7/29/63/63	0/2/2/2
14	CLA	A	818	1	-	10/33/109/115	-
14	CLA	A	802	22	-	3/39/115/115	-
14	CLA	bA	811	1	-	5/15/91/115	-
14	CLA	bB	801	-	-	9/39/115/115	-
17	BCR	cI	102	-	-	3/29/63/63	0/2/2/2
14	CLA	B	838	22	-	5/39/115/115	-
14	CLA	B	807	2	-	12/39/115/115	-
14	CLA	bA	803	1	-	8/15/91/115	-
14	CLA	cA	820	22	-	5/15/91/115	-
14	CLA	bB	804	2	-	6/23/99/115	-
14	CLA	cA	807	1	-	8/15/91/115	-
17	BCR	I	101	-	-	1/29/63/63	0/2/2/2
14	CLA	bB	813	-	-	5/19/95/115	-
16	SF4	A	844	1,2	-	-	0/6/5/5
14	CLA	bB	835	2	-	3/15/91/115	-
14	CLA	A	819	1	-	6/15/91/115	-
18	LHG	cA	850	-	-	15/53/53/53	-
14	CLA	A	804	1	-	8/25/101/115	-
14	CLA	cA	809	1	-	6/15/91/115	-
14	CLA	bB	807	2	-	12/39/115/115	-
20	LMG	cB	849	-	-	9/38/58/70	0/1/1/1
14	CLA	bB	822	2	-	6/15/91/115	-
14	CLA	cA	827	1	-	3/35/111/115	-
17	BCR	cB	842	-	-	7/29/63/63	0/2/2/2
16	SF4	C	101	3	-	-	0/6/5/5
14	CLA	B	814	-	-	7/15/91/115	-
14	CLA	B	828	2	-	13/39/115/115	-
14	CLA	cB	837	2	-	7/15/91/115	-
14	CLA	A	828	1	-	7/33/109/115	-
14	CLA	A	825	22	-	2/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	bB	814	-	-	7/15/91/115	-
14	CLA	bB	805	2	-	15/39/115/115	-
14	CLA	B	830	2	-	4/12/88/115	-
14	CLA	cA	819	1	-	6/15/91/115	-
14	CLA	cB	823	2	-	6/15/91/115	-
14	CLA	cL	203	10	-	15/39/115/115	-
14	CLA	A	823	1	-	6/15/91/115	-
14	CLA	cB	821	2	-	10/15/91/115	-
14	CLA	bB	817	2	-	6/27/103/115	-
14	CLA	B	815	2	-	11/24/100/115	-
14	CLA	cA	838	1	-	5/15/91/115	-
15	PQN	cB	841	-	-	4/23/43/43	0/2/2/2
14	CLA	bB	831	2	-	16/39/115/115	-
14	CLA	bA	836	1	-	6/23/99/115	-
14	CLA	B	803	22	-	8/27/103/115	-
17	BCR	bA	848	-	-	3/29/63/63	0/2/2/2
14	CLA	L	204	22	-	17/39/115/115	-
17	BCR	cM	101	-	-	6/29/63/63	0/2/2/2
14	CLA	bB	851	-	-	5/15/91/115	-
14	CLA	cB	822	-	-	8/15/91/115	-
14	CLA	A	833	1	-	8/39/115/115	-
18	LHG	A	851	14	-	14/31/31/53	-
14	CLA	B	822	2	-	6/15/91/115	-
14	CLA	B	831	2	-	16/39/115/115	-
14	CLA	bB	832	2	-	4/15/91/115	-
14	CLA	bA	834	1	-	3/15/91/115	-
14	CLA	bA	841	22	-	10/39/115/115	-
14	CLA	bB	810	2	-	5/15/91/115	-
14	CLA	cA	804	1	-	8/25/101/115	-
14	CLA	cL	205	22	-	17/39/115/115	-
14	CLA	B	818	-	-	5/17/93/115	-
17	BCR	M	101	-	-	6/29/63/63	0/2/2/2
14	CLA	cA	832	1	-	8/39/115/115	-
14	CLA	cB	838	2	-	6/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	801	-	-	9/39/115/115	-
14	CLA	bJ	101	8	-	4/15/91/115	-
14	CLA	cB	850	-	-	4/15/91/115	-
14	CLA	bA	802	22	-	3/39/115/115	-
14	CLA	bA	824	22	-	7/32/108/115	-
14	CLA	cB	834	-	-	2/15/91/115	-
14	CLA	bF	201	22	-	5/23/99/115	-
14	CLA	bB	811	2	-	3/15/91/115	-
14	CLA	bB	802	2	-	11/39/115/115	-
14	CLA	A	813	1	-	4/15/91/115	-
14	CLA	cA	822	1	-	3/15/91/115	-
14	CLA	cB	830	2	-	7/15/91/115	-
14	CLA	B	819	-	-	11/18/94/115	-
16	SF4	bC	102	3	-	-	0/6/5/5
14	CLA	B	810	2	-	5/15/91/115	-
14	CLA	cB	833	2	-	4/15/91/115	-
14	CLA	bA	809	1	-	6/15/91/115	-
17	BCR	bL	206	-	-	3/29/63/63	0/2/2/2
14	CLA	bB	827	2	-	5/39/115/115	-
14	CLA	bB	809	2	-	11/39/115/115	-
14	CLA	cA	815	-	-	7/15/91/115	-
17	BCR	cA	847	-	-	6/29/63/63	0/2/2/2
17	BCR	cA	848	-	-	3/29/63/63	0/2/2/2
14	CLA	B	811	2	-	3/15/91/115	-
14	CLA	cB	829	2	-	13/39/115/115	-
14	CLA	bB	820	2	-	10/15/91/115	-
17	BCR	cJ	103	-	-	17/29/63/63	0/2/2/2
17	BCR	bI	102	-	-	3/29/63/63	0/2/2/2
14	CLA	A	842	18	-	8/15/91/115	-
14	CLA	L	202	10	-	15/39/115/115	-
14	CLA	cJ	101	8	-	4/15/91/115	-
14	CLA	A	805	1	-	6/27/103/115	-
14	CLA	cB	816	2	-	11/24/100/115	-
14	CLA	cB	840	2	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	cA	817	1	-	8/26/102/115	-
14	CLA	A	840	1	-	13/39/115/115	-
14	CLA	bA	842	18	-	8/15/91/115	-
17	BCR	cB	845	-	-	15/29/63/63	0/2/2/2
17	BCR	L	205	-	-	4/29/63/63	0/2/2/2
14	CLA	B	827	2	-	5/39/115/115	-
17	BCR	bB	844	-	-	15/29/63/63	0/2/2/2
14	CLA	A	816	1	-	7/15/91/115	-
14	CLA	cB	825	22	-	6/17/93/115	-
14	CLA	A	830	1	-	4/21/97/115	-
14	CLA	A	831	1	-	13/27/103/115	-
14	CLA	cA	812	1	-	5/15/91/115	-
14	CLA	A	806	1	-	11/39/115/115	-
14	CLA	bA	823	1	-	6/15/91/115	-
17	BCR	bM	101	-	-	5/29/63/63	0/2/2/2
14	CLA	cA	842	18	-	8/15/91/115	-
14	CLA	B	849	-	-	4/15/91/115	-
14	CLA	B	826	2	-	6/39/115/115	-
14	CLA	A	814	-	-	1/15/91/115	-
17	BCR	cA	845	-	-	10/29/63/63	0/2/2/2
16	SF4	cC	101	3	-	-	0/6/5/5
15	PQN	bB	840	-	-	4/23/43/43	0/2/2/2
16	SF4	cC	102	3	-	-	0/6/5/5
14	CLA	cA	835	1	-	5/15/91/115	-
14	CLA	cB	819	-	-	5/17/93/115	-
14	CLA	cA	808	1	-	7/15/91/115	-

All (6021) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bB	820	CLA	C3C-C2C	5.55	1.48	1.36
14	cB	821	CLA	C3C-C2C	5.53	1.48	1.36
14	B	820	CLA	C3C-C2C	5.51	1.48	1.36
14	bB	831	CLA	C3C-C2C	5.49	1.48	1.36
14	bA	820	CLA	C3C-C2C	5.48	1.48	1.36
14	cA	820	CLA	C3C-C2C	5.48	1.48	1.36
14	A	820	CLA	C3C-C2C	5.48	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bB	830	CLA	C3C-C2C	5.47	1.48	1.36
14	cB	831	CLA	C3C-C2C	5.46	1.48	1.36
14	B	830	CLA	C3C-C2C	5.46	1.48	1.36
14	B	831	CLA	C3C-C2C	5.45	1.48	1.36
14	B	824	CLA	C3C-C2C	5.45	1.48	1.36
14	cB	832	CLA	C3C-C2C	5.45	1.48	1.36
14	bB	824	CLA	C3C-C2C	5.45	1.48	1.36
14	cB	825	CLA	C3C-C2C	5.45	1.48	1.36
14	bB	825	CLA	C1D-ND	5.44	1.44	1.37
14	B	829	CLA	C3C-C2C	5.44	1.48	1.36
14	bA	821	CLA	O2D-CGD	5.44	1.46	1.33
14	A	840	CLA	C3C-C2C	5.43	1.48	1.36
14	cA	821	CLA	O2D-CGD	5.43	1.46	1.33
14	A	821	CLA	O2D-CGD	5.43	1.46	1.33
14	cA	840	CLA	C3C-C2C	5.43	1.48	1.36
14	cB	827	CLA	C1D-ND	5.43	1.44	1.37
14	bA	840	CLA	C3C-C2C	5.43	1.48	1.36
14	A	821	CLA	C1D-ND	5.43	1.44	1.37
14	bJ	102	CLA	C1D-ND	5.42	1.44	1.37
14	bB	829	CLA	C3C-C2C	5.42	1.48	1.36
14	cB	830	CLA	C3C-C2C	5.42	1.48	1.36
14	bB	851	CLA	C1D-ND	5.42	1.44	1.37
14	B	825	CLA	C1D-ND	5.42	1.44	1.37
14	bB	813	CLA	O2D-CGD	5.42	1.46	1.33
14	cA	834	CLA	O2D-CGD	5.42	1.46	1.33
14	bA	821	CLA	C1D-ND	5.42	1.44	1.37
14	B	813	CLA	O2D-CGD	5.42	1.46	1.33
14	cB	804	CLA	C3C-C2C	5.41	1.48	1.36
14	A	823	CLA	C1D-ND	5.41	1.44	1.37
14	cB	806	CLA	C1D-ND	5.41	1.44	1.37
14	cB	814	CLA	O2D-CGD	5.41	1.46	1.33
14	B	826	CLA	C1D-ND	5.41	1.44	1.37
14	bB	818	CLA	C3C-C2C	5.41	1.48	1.36
14	cB	819	CLA	C3C-C2C	5.41	1.48	1.36
14	cA	825	CLA	O2D-CGD	5.41	1.46	1.33
14	cA	821	CLA	C1D-ND	5.41	1.44	1.37
14	B	818	CLA	C3C-C2C	5.41	1.48	1.36
14	bA	825	CLA	O2D-CGD	5.41	1.46	1.33
14	bA	819	CLA	C1D-ND	5.41	1.44	1.37
14	cB	813	CLA	O2D-CGD	5.41	1.46	1.33
14	bB	805	CLA	C1D-ND	5.41	1.44	1.37
14	B	805	CLA	C1D-ND	5.40	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bA	823	CLA	C1D-ND	5.40	1.44	1.37
14	B	812	CLA	O2D-CGD	5.40	1.46	1.33
14	A	825	CLA	O2D-CGD	5.40	1.46	1.33
14	B	803	CLA	C3C-C2C	5.40	1.48	1.36
14	B	851	CLA	C1D-ND	5.40	1.44	1.37
14	cB	817	CLA	C3C-C2C	5.40	1.48	1.36
14	bB	819	CLA	C3C-C2C	5.40	1.48	1.36
14	B	806	CLA	C1D-ND	5.39	1.44	1.37
14	cB	826	CLA	C1D-ND	5.39	1.44	1.37
14	bX	201	CLA	C1D-ND	5.39	1.44	1.37
14	A	834	CLA	O2D-CGD	5.39	1.46	1.33
14	cB	820	CLA	O2D-CGD	5.39	1.46	1.33
14	X	201	CLA	C1D-ND	5.39	1.44	1.37
14	B	811	CLA	C3C-C2C	5.39	1.48	1.36
14	cJ	102	CLA	C1D-ND	5.39	1.44	1.37
14	cA	823	CLA	C1D-ND	5.39	1.44	1.37
14	B	825	CLA	O2D-CGD	5.39	1.46	1.33
14	bB	803	CLA	C3C-C2C	5.39	1.48	1.36
14	bA	821	CLA	C3C-C2C	5.39	1.48	1.36
14	bB	811	CLA	C3C-C2C	5.39	1.48	1.36
14	bJ	102	CLA	O2D-CGD	5.39	1.46	1.33
14	B	816	CLA	C3C-C2C	5.39	1.48	1.36
14	bA	834	CLA	O2D-CGD	5.39	1.46	1.33
14	B	819	CLA	C3C-C2C	5.39	1.48	1.36
14	B	819	CLA	O2D-CGD	5.39	1.46	1.33
14	cB	820	CLA	C3C-C2C	5.38	1.48	1.36
14	cB	801	CLA	C1D-ND	5.38	1.44	1.37
14	bB	812	CLA	O2D-CGD	5.38	1.46	1.33
14	bB	819	CLA	O2D-CGD	5.38	1.46	1.33
14	cX	201	CLA	C1D-ND	5.38	1.44	1.37
14	bB	816	CLA	C3C-C2C	5.38	1.48	1.36
14	cB	801	CLA	C3C-C2C	5.38	1.48	1.36
14	bB	826	CLA	C1D-ND	5.38	1.44	1.37
14	cJ	102	CLA	O2D-CGD	5.38	1.46	1.33
14	B	833	CLA	C3C-C2C	5.38	1.48	1.36
14	A	824	CLA	O2D-CGD	5.38	1.46	1.33
14	cB	826	CLA	O2D-CGD	5.38	1.46	1.33
14	cA	819	CLA	C1D-ND	5.37	1.44	1.37
14	cA	821	CLA	C3C-C2C	5.37	1.48	1.36
14	cJ	101	CLA	C1D-ND	5.37	1.44	1.37
14	bA	814	CLA	O2D-CGD	5.37	1.46	1.33
14	bA	815	CLA	C3C-C2C	5.37	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bA	824	CLA	O2D-CGD	5.37	1.46	1.33
14	bB	806	CLA	C1D-ND	5.37	1.44	1.37
14	J	102	CLA	C1D-ND	5.37	1.44	1.37
14	B	851	CLA	C3C-C2C	5.37	1.48	1.36
14	cA	824	CLA	O2D-CGD	5.37	1.46	1.33
14	bB	851	CLA	C3C-C2C	5.37	1.48	1.36
14	J	101	CLA	C1D-ND	5.37	1.44	1.37
14	cB	812	CLA	C3C-C2C	5.37	1.48	1.36
14	bA	803	CLA	O2D-CGD	5.37	1.46	1.33
14	bB	833	CLA	C3C-C2C	5.36	1.48	1.36
14	A	821	CLA	C3C-C2C	5.36	1.48	1.36
14	J	102	CLA	O2D-CGD	5.36	1.46	1.33
14	cA	815	CLA	C3C-C2C	5.36	1.48	1.36
14	bB	816	CLA	C1D-ND	5.36	1.44	1.37
14	bB	829	CLA	O2D-CGD	5.36	1.46	1.33
14	bB	828	CLA	C3C-C2C	5.36	1.48	1.36
14	cB	812	CLA	O2D-CGD	5.36	1.46	1.33
14	B	811	CLA	O2D-CGD	5.36	1.46	1.33
14	cA	803	CLA	O2D-CGD	5.36	1.46	1.33
14	bB	825	CLA	O2D-CGD	5.36	1.46	1.33
14	cB	817	CLA	C1D-ND	5.36	1.44	1.37
14	A	803	CLA	O2D-CGD	5.36	1.46	1.33
14	cB	834	CLA	C3C-C2C	5.35	1.48	1.36
14	A	807	CLA	O2D-CGD	5.35	1.46	1.33
14	B	816	CLA	C1D-ND	5.35	1.44	1.37
14	bB	830	CLA	C1D-ND	5.35	1.44	1.37
14	cA	807	CLA	C3C-C2C	5.35	1.48	1.36
14	bA	827	CLA	O2D-CGD	5.35	1.46	1.33
14	A	814	CLA	O2D-CGD	5.35	1.46	1.33
14	cA	839	CLA	O2D-CGD	5.35	1.46	1.33
14	A	819	CLA	C1D-ND	5.35	1.44	1.37
14	cA	828	CLA	C3C-C2C	5.35	1.48	1.36
14	bB	849	CLA	C1D-ND	5.35	1.44	1.37
14	bB	816	CLA	O2D-CGD	5.35	1.46	1.33
14	cB	807	CLA	C1D-ND	5.35	1.44	1.37
14	A	815	CLA	C3C-C2C	5.35	1.48	1.36
14	bB	811	CLA	O2D-CGD	5.35	1.46	1.33
14	cB	817	CLA	O2D-CGD	5.35	1.46	1.33
14	B	828	CLA	C3C-C2C	5.35	1.48	1.36
14	A	828	CLA	C3C-C2C	5.35	1.48	1.36
14	cA	814	CLA	O2D-CGD	5.34	1.46	1.33
14	bA	828	CLA	C3C-C2C	5.34	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cB	821	CLA	O2D-CGD	5.34	1.46	1.33
14	B	823	CLA	C1D-ND	5.34	1.44	1.37
14	B	849	CLA	C1D-ND	5.34	1.44	1.37
14	bB	823	CLA	O2D-CGD	5.34	1.46	1.33
14	B	820	CLA	O2D-CGD	5.34	1.46	1.33
14	bB	813	CLA	C3C-C2C	5.34	1.48	1.36
14	A	835	CLA	C3C-C2C	5.34	1.48	1.36
14	bA	835	CLA	C3C-C2C	5.34	1.48	1.36
14	cA	808	CLA	O2D-CGD	5.34	1.46	1.33
14	A	808	CLA	O2D-CGD	5.34	1.46	1.33
14	cB	823	CLA	C1D-ND	5.34	1.44	1.37
14	bA	808	CLA	O2D-CGD	5.34	1.46	1.33
14	cA	835	CLA	C3C-C2C	5.34	1.48	1.36
14	A	839	CLA	O2D-CGD	5.34	1.46	1.33
14	bA	807	CLA	C3C-C2C	5.34	1.48	1.36
14	A	807	CLA	C3C-C2C	5.33	1.48	1.36
14	cA	807	CLA	O2D-CGD	5.33	1.46	1.33
14	cA	817	CLA	O2D-CGD	5.33	1.46	1.33
14	B	817	CLA	C3C-C2C	5.33	1.48	1.36
14	bA	807	CLA	O2D-CGD	5.33	1.46	1.33
14	cA	827	CLA	O2D-CGD	5.33	1.46	1.33
14	cB	824	CLA	C1D-ND	5.33	1.44	1.37
14	A	827	CLA	O2D-CGD	5.33	1.46	1.33
14	cB	818	CLA	C3C-C2C	5.33	1.48	1.36
14	A	817	CLA	C3C-C2C	5.33	1.48	1.36
14	cB	830	CLA	O2D-CGD	5.33	1.46	1.33
14	B	829	CLA	O2D-CGD	5.33	1.46	1.33
14	B	816	CLA	O2D-CGD	5.33	1.46	1.33
14	cB	831	CLA	C1D-ND	5.33	1.44	1.37
14	bA	810	CLA	C1D-ND	5.33	1.44	1.37
14	bA	812	CLA	C3C-C2C	5.33	1.48	1.36
14	bA	839	CLA	O2D-CGD	5.32	1.46	1.33
14	cB	814	CLA	C3C-C2C	5.32	1.48	1.36
14	cA	807	CLA	C1D-ND	5.32	1.44	1.37
14	bA	817	CLA	O2D-CGD	5.32	1.46	1.33
14	bA	817	CLA	C3C-C2C	5.32	1.48	1.36
14	cB	824	CLA	O2D-CGD	5.32	1.46	1.33
14	A	810	CLA	C1D-ND	5.32	1.44	1.37
14	B	849	CLA	O2D-CGD	5.32	1.46	1.33
14	bB	820	CLA	O2D-CGD	5.32	1.46	1.33
14	bB	817	CLA	C3C-C2C	5.32	1.48	1.36
14	bB	823	CLA	C1D-ND	5.32	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cA	810	CLA	C1D-ND	5.32	1.44	1.37
14	bB	849	CLA	O2D-CGD	5.32	1.46	1.33
14	cA	817	CLA	C3C-C2C	5.32	1.48	1.36
14	A	817	CLA	O2D-CGD	5.32	1.46	1.33
14	B	814	CLA	C1D-ND	5.32	1.44	1.37
14	cB	828	CLA	O2D-CGD	5.32	1.46	1.33
14	B	813	CLA	C3C-C2C	5.32	1.48	1.36
14	cB	850	CLA	C1D-ND	5.31	1.44	1.37
14	X	201	CLA	O2D-CGD	5.31	1.46	1.33
14	bL	202	CLA	C3C-C2C	5.31	1.48	1.36
14	cA	812	CLA	C3C-C2C	5.31	1.48	1.36
14	bB	814	CLA	C1D-ND	5.31	1.44	1.37
14	bB	827	CLA	O2D-CGD	5.31	1.46	1.33
14	bJ	101	CLA	C1D-ND	5.31	1.44	1.37
14	cA	809	CLA	O2D-CGD	5.31	1.46	1.33
14	cB	850	CLA	O2D-CGD	5.31	1.46	1.33
14	cB	829	CLA	C3C-C2C	5.31	1.48	1.36
14	bB	822	CLA	C1D-ND	5.31	1.44	1.37
14	A	812	CLA	C3C-C2C	5.31	1.48	1.36
14	B	823	CLA	O2D-CGD	5.31	1.46	1.33
14	cA	834	CLA	C3C-C2C	5.31	1.48	1.36
14	bB	833	CLA	C1D-ND	5.31	1.44	1.37
14	cB	815	CLA	C3C-C2C	5.31	1.48	1.36
14	B	810	CLA	O2D-CGD	5.31	1.46	1.33
14	cX	201	CLA	O2D-CGD	5.31	1.46	1.33
14	cL	203	CLA	C3C-C2C	5.31	1.48	1.36
14	B	830	CLA	C1D-ND	5.31	1.44	1.37
14	A	834	CLA	C3C-C2C	5.31	1.48	1.36
14	cA	812	CLA	C1D-ND	5.31	1.44	1.37
14	A	831	CLA	C3C-C2C	5.30	1.48	1.36
14	L	202	CLA	C3C-C2C	5.30	1.48	1.36
14	cB	805	CLA	C3C-C2C	5.30	1.48	1.36
14	cB	815	CLA	C1D-ND	5.30	1.44	1.37
14	bA	809	CLA	O2D-CGD	5.30	1.46	1.33
14	bB	810	CLA	C1D-ND	5.30	1.44	1.37
14	A	807	CLA	C1D-ND	5.30	1.44	1.37
14	cB	811	CLA	O2D-CGD	5.30	1.46	1.33
14	B	827	CLA	O2D-CGD	5.30	1.46	1.33
14	bA	831	CLA	C3C-C2C	5.30	1.48	1.36
14	L	202	CLA	C1D-ND	5.30	1.44	1.37
14	bA	815	CLA	C1D-ND	5.30	1.44	1.37
14	B	804	CLA	C3C-C2C	5.30	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cL	203	CLA	C1D-ND	5.30	1.44	1.37
14	bA	822	CLA	O2D-CGD	5.30	1.46	1.33
14	bB	804	CLA	C3C-C2C	5.30	1.48	1.36
14	bB	824	CLA	O2D-CGD	5.30	1.46	1.33
14	bB	822	CLA	O2D-CGD	5.29	1.46	1.33
14	bB	810	CLA	O2D-CGD	5.29	1.46	1.33
14	bX	201	CLA	O2D-CGD	5.29	1.46	1.33
14	B	814	CLA	C3C-C2C	5.29	1.48	1.36
14	A	822	CLA	O2D-CGD	5.29	1.46	1.33
14	B	822	CLA	O2D-CGD	5.29	1.46	1.33
14	bB	836	CLA	O2D-CGD	5.29	1.46	1.33
14	cB	816	CLA	O2D-CGD	5.29	1.46	1.33
14	bA	813	CLA	O2D-CGD	5.29	1.46	1.33
14	bA	812	CLA	C1D-ND	5.29	1.44	1.37
14	cA	819	CLA	C3C-C2C	5.29	1.48	1.36
14	bB	814	CLA	C3C-C2C	5.29	1.48	1.36
14	bA	816	CLA	O2D-CGD	5.29	1.46	1.33
14	X	201	CLA	C3C-C2C	5.29	1.48	1.36
14	cA	810	CLA	C3C-C2C	5.29	1.48	1.36
14	cA	841	CLA	O2D-CGD	5.29	1.46	1.33
14	cB	834	CLA	O2D-CGD	5.28	1.46	1.33
14	L	203	CLA	C3C-C2C	5.28	1.48	1.36
14	bB	836	CLA	C3C-C2C	5.28	1.48	1.36
14	A	809	CLA	O2D-CGD	5.28	1.46	1.33
14	B	817	CLA	O2D-CGD	5.28	1.46	1.33
14	bB	815	CLA	O2D-CGD	5.28	1.46	1.33
14	cB	825	CLA	O2D-CGD	5.28	1.46	1.33
14	bB	817	CLA	O2D-CGD	5.28	1.46	1.33
14	B	824	CLA	O2D-CGD	5.28	1.46	1.33
14	B	836	CLA	C3C-C2C	5.28	1.48	1.36
14	bB	832	CLA	O2D-CGD	5.28	1.46	1.33
14	bA	834	CLA	C3C-C2C	5.28	1.48	1.36
14	cB	818	CLA	O2D-CGD	5.28	1.46	1.33
14	bL	203	CLA	C3C-C2C	5.28	1.48	1.36
14	bX	201	CLA	C3C-C2C	5.28	1.48	1.36
14	A	813	CLA	O2D-CGD	5.28	1.46	1.33
14	B	833	CLA	O2D-CGD	5.28	1.46	1.33
14	B	832	CLA	O2D-CGD	5.28	1.46	1.33
14	cB	823	CLA	O2D-CGD	5.28	1.46	1.33
14	A	816	CLA	O2D-CGD	5.28	1.46	1.33
14	A	841	CLA	O2D-CGD	5.28	1.46	1.33
14	cL	204	CLA	C3C-C2C	5.28	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bA	807	CLA	C1D-ND	5.28	1.44	1.37
14	A	811	CLA	O2D-CGD	5.27	1.46	1.33
14	B	815	CLA	O2D-CGD	5.27	1.46	1.33
14	bA	811	CLA	O2D-CGD	5.27	1.46	1.33
14	cA	811	CLA	O2D-CGD	5.27	1.46	1.33
14	cA	816	CLA	O2D-CGD	5.27	1.46	1.33
14	bB	833	CLA	O2D-CGD	5.27	1.46	1.33
14	cA	822	CLA	O2D-CGD	5.27	1.46	1.33
14	cX	201	CLA	C3C-C2C	5.27	1.47	1.36
14	B	836	CLA	O2D-CGD	5.27	1.46	1.33
14	bB	827	CLA	C3C-C2C	5.27	1.47	1.36
14	cB	833	CLA	O2D-CGD	5.27	1.46	1.33
14	A	822	CLA	C1D-ND	5.27	1.44	1.37
14	cB	831	CLA	O2D-CGD	5.27	1.46	1.33
14	cA	839	CLA	C3C-C2C	5.27	1.47	1.36
14	cB	828	CLA	C3C-C2C	5.27	1.47	1.36
14	cB	836	CLA	C3C-C2C	5.27	1.47	1.36
14	cB	837	CLA	C3C-C2C	5.27	1.47	1.36
14	bA	841	CLA	O2D-CGD	5.27	1.46	1.33
14	bA	819	CLA	C3C-C2C	5.27	1.47	1.36
17	B	843	BCR	C21-C22	5.27	1.42	1.35
14	bB	825	CLA	C3C-C2C	5.27	1.47	1.36
14	bB	830	CLA	O2D-CGD	5.27	1.46	1.33
14	cA	819	CLA	O2D-CGD	5.27	1.46	1.33
14	B	830	CLA	O2D-CGD	5.27	1.46	1.33
14	B	837	CLA	C3C-C2C	5.26	1.47	1.36
14	cA	813	CLA	O2D-CGD	5.26	1.46	1.33
14	bB	837	CLA	C3C-C2C	5.26	1.47	1.36
14	B	815	CLA	C3C-C2C	5.26	1.47	1.36
14	cA	831	CLA	C3C-C2C	5.26	1.47	1.36
14	A	815	CLA	C1D-ND	5.26	1.44	1.37
14	B	822	CLA	C1D-ND	5.26	1.44	1.37
14	B	833	CLA	C1D-ND	5.26	1.44	1.37
14	A	819	CLA	C3C-C2C	5.26	1.47	1.36
14	cB	834	CLA	C1D-ND	5.26	1.44	1.37
14	bB	815	CLA	C3C-C2C	5.26	1.47	1.36
14	B	835	CLA	C3C-C2C	5.26	1.47	1.36
14	bA	805	CLA	O2D-CGD	5.26	1.46	1.33
17	cB	844	BCR	C21-C22	5.26	1.42	1.35
14	bA	819	CLA	O2D-CGD	5.26	1.46	1.33
14	bA	818	CLA	C3C-C2C	5.26	1.47	1.36
14	cA	815	CLA	C1D-ND	5.26	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cB	837	CLA	O2D-CGD	5.26	1.46	1.33
14	bJ	101	CLA	C3C-C2C	5.26	1.47	1.36
14	cB	838	CLA	C3C-C2C	5.26	1.47	1.36
14	A	813	CLA	C1D-ND	5.26	1.44	1.37
14	cA	804	CLA	C1D-ND	5.26	1.44	1.37
14	B	827	CLA	C3C-C2C	5.26	1.47	1.36
14	cB	816	CLA	C3C-C2C	5.26	1.47	1.36
17	bB	843	BCR	C21-C22	5.26	1.42	1.35
14	cB	826	CLA	C3C-C2C	5.26	1.47	1.36
14	bL	202	CLA	C1D-ND	5.26	1.44	1.37
14	A	810	CLA	C3C-C2C	5.26	1.47	1.36
14	bA	813	CLA	C1D-ND	5.26	1.44	1.37
14	cA	813	CLA	C1D-ND	5.26	1.44	1.37
14	L	204	CLA	C3C-C2C	5.26	1.47	1.36
14	bA	822	CLA	C1D-ND	5.26	1.44	1.37
14	cB	811	CLA	C1D-ND	5.26	1.44	1.37
14	cA	805	CLA	O2D-CGD	5.26	1.46	1.33
14	B	825	CLA	C3C-C2C	5.25	1.47	1.36
14	A	814	CLA	C1D-ND	5.25	1.44	1.37
14	bA	810	CLA	O2D-CGD	5.25	1.46	1.33
14	cA	804	CLA	O2D-CGD	5.25	1.46	1.33
14	cA	810	CLA	O2D-CGD	5.25	1.46	1.33
14	cB	822	CLA	C3C-C2C	5.25	1.47	1.36
14	B	849	CLA	C3C-C2C	5.25	1.47	1.36
14	cA	822	CLA	C1D-ND	5.25	1.44	1.37
14	cA	825	CLA	C1D-ND	5.25	1.44	1.37
14	bA	810	CLA	C3C-C2C	5.25	1.47	1.36
14	bB	849	CLA	C3C-C2C	5.25	1.47	1.36
14	cJ	101	CLA	O2D-CGD	5.25	1.46	1.33
14	A	818	CLA	C3C-C2C	5.25	1.47	1.36
14	bB	835	CLA	C3C-C2C	5.25	1.47	1.36
14	A	839	CLA	C3C-C2C	5.25	1.47	1.36
14	bF	201	CLA	O2D-CGD	5.25	1.46	1.33
14	A	819	CLA	O2D-CGD	5.25	1.46	1.33
14	bJ	101	CLA	O2D-CGD	5.25	1.46	1.33
14	A	804	CLA	O2D-CGD	5.25	1.46	1.33
14	bB	821	CLA	C3C-C2C	5.24	1.47	1.36
14	cL	205	CLA	C3C-C2C	5.24	1.47	1.36
14	B	823	CLA	C3C-C2C	5.24	1.47	1.36
14	bA	814	CLA	C3C-C2C	5.24	1.47	1.36
14	A	810	CLA	O2D-CGD	5.24	1.46	1.33
14	cB	835	CLA	C3C-C2C	5.24	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	J	101	CLA	C3C-C2C	5.24	1.47	1.36
14	bB	822	CLA	C3C-C2C	5.24	1.47	1.36
14	A	804	CLA	C1D-ND	5.24	1.44	1.37
14	F	201	CLA	O2D-CGD	5.24	1.46	1.33
14	bA	815	CLA	O2D-CGD	5.24	1.46	1.33
14	cJ	102	CLA	C3C-C2C	5.24	1.47	1.36
14	bB	851	CLA	O2D-CGD	5.24	1.46	1.33
14	B	810	CLA	C1D-ND	5.24	1.44	1.37
14	cA	814	CLA	C1D-ND	5.24	1.44	1.37
14	bL	204	CLA	C3C-C2C	5.24	1.47	1.36
14	B	834	CLA	O2D-CGD	5.24	1.46	1.33
14	bA	804	CLA	O2D-CGD	5.24	1.46	1.33
14	B	807	CLA	C1D-ND	5.24	1.44	1.37
14	cB	823	CLA	C3C-C2C	5.24	1.47	1.36
14	A	812	CLA	C1D-ND	5.23	1.44	1.37
14	cB	835	CLA	O2D-CGD	5.23	1.46	1.33
14	B	822	CLA	C3C-C2C	5.23	1.47	1.36
14	B	818	CLA	O2D-CGD	5.23	1.46	1.33
14	bB	834	CLA	O2D-CGD	5.23	1.46	1.33
14	bA	827	CLA	C1D-ND	5.23	1.44	1.37
14	bB	823	CLA	C3C-C2C	5.23	1.47	1.36
14	bB	818	CLA	O2D-CGD	5.23	1.46	1.33
14	bJ	102	CLA	C3C-C2C	5.23	1.47	1.36
14	cB	829	CLA	O2D-CGD	5.23	1.46	1.33
14	bA	839	CLA	C3C-C2C	5.23	1.47	1.36
14	bA	804	CLA	C1D-ND	5.23	1.44	1.37
14	A	815	CLA	O2D-CGD	5.23	1.46	1.33
14	cB	819	CLA	O2D-CGD	5.23	1.46	1.33
14	A	805	CLA	O2D-CGD	5.23	1.46	1.33
14	B	819	CLA	C1D-ND	5.23	1.44	1.37
14	cA	818	CLA	C3C-C2C	5.23	1.47	1.36
17	cJ	103	BCR	C21-C22	5.23	1.42	1.35
14	bA	829	CLA	C3C-C2C	5.23	1.47	1.36
14	B	828	CLA	O2D-CGD	5.23	1.46	1.33
14	cF	201	CLA	O2D-CGD	5.23	1.46	1.33
14	bA	814	CLA	C1D-ND	5.23	1.44	1.37
14	cA	827	CLA	C1D-ND	5.23	1.44	1.37
14	cA	814	CLA	C3C-C2C	5.23	1.47	1.36
14	cA	829	CLA	C3C-C2C	5.23	1.47	1.36
14	bA	805	CLA	C1D-ND	5.23	1.44	1.37
14	cB	824	CLA	C3C-C2C	5.23	1.47	1.36
14	J	101	CLA	O2D-CGD	5.22	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	814	CLA	C3C-C2C	5.22	1.47	1.36
14	bA	811	CLA	C3C-C2C	5.22	1.47	1.36
14	cB	801	CLA	O2D-CGD	5.22	1.45	1.33
14	bB	828	CLA	O2D-CGD	5.22	1.45	1.33
14	J	102	CLA	C3C-C2C	5.22	1.47	1.36
14	cB	850	CLA	C3C-C2C	5.22	1.47	1.36
14	bB	819	CLA	C1D-ND	5.22	1.44	1.37
14	bB	826	CLA	O2D-CGD	5.22	1.45	1.33
14	B	851	CLA	O2D-CGD	5.22	1.45	1.33
14	cB	820	CLA	C1D-ND	5.22	1.44	1.37
14	B	826	CLA	O2D-CGD	5.22	1.45	1.33
14	cA	816	CLA	C3C-C2C	5.22	1.47	1.36
14	cA	835	CLA	C1D-ND	5.22	1.44	1.37
14	bA	809	CLA	C3C-C2C	5.22	1.47	1.36
14	cB	808	CLA	C1D-ND	5.22	1.44	1.37
14	cA	820	CLA	O2D-CGD	5.22	1.45	1.33
14	A	826	CLA	C3C-C2C	5.22	1.47	1.36
14	cB	827	CLA	O2D-CGD	5.22	1.45	1.33
14	B	835	CLA	O2D-CGD	5.21	1.45	1.33
14	A	805	CLA	C1D-ND	5.21	1.44	1.37
14	bA	820	CLA	O2D-CGD	5.21	1.45	1.33
14	B	821	CLA	C3C-C2C	5.21	1.47	1.36
14	cA	804	CLA	C3C-C2C	5.21	1.47	1.36
14	A	811	CLA	C3C-C2C	5.21	1.47	1.36
14	cA	815	CLA	O2D-CGD	5.21	1.45	1.33
14	A	816	CLA	C3C-C2C	5.21	1.47	1.36
14	A	829	CLA	C3C-C2C	5.21	1.47	1.36
14	B	834	CLA	C3C-C2C	5.21	1.47	1.36
14	bB	834	CLA	C3C-C2C	5.21	1.47	1.36
14	A	827	CLA	C1D-ND	5.21	1.44	1.37
14	cJ	101	CLA	C3C-C2C	5.21	1.47	1.36
14	bA	828	CLA	O2D-CGD	5.21	1.45	1.33
14	cA	809	CLA	C3C-C2C	5.21	1.47	1.36
14	bA	804	CLA	C3C-C2C	5.21	1.47	1.36
13	cA	801	CL0	C3C-C2C	5.21	1.47	1.36
14	B	832	CLA	C3C-C2C	5.21	1.47	1.36
14	cA	805	CLA	C1D-ND	5.20	1.44	1.37
14	A	820	CLA	O2D-CGD	5.20	1.45	1.33
14	cB	819	CLA	C1D-ND	5.20	1.44	1.37
14	bA	834	CLA	C1D-ND	5.20	1.44	1.37
14	cA	828	CLA	O2D-CGD	5.20	1.45	1.33
14	bA	825	CLA	C1D-ND	5.20	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	813	CLA	C3C-C2C	5.20	1.47	1.36
14	A	804	CLA	C3C-C2C	5.20	1.47	1.36
14	bA	813	CLA	C3C-C2C	5.20	1.47	1.36
14	bB	812	CLA	C3C-C2C	5.20	1.47	1.36
14	B	834	CLA	C1D-ND	5.20	1.44	1.37
13	A	801	CL0	C3C-C2C	5.20	1.47	1.36
14	cA	813	CLA	C3C-C2C	5.20	1.47	1.36
14	cA	826	CLA	C3C-C2C	5.20	1.47	1.36
14	A	809	CLA	C3C-C2C	5.20	1.47	1.36
14	bB	835	CLA	O2D-CGD	5.20	1.45	1.33
14	A	828	CLA	O2D-CGD	5.20	1.45	1.33
14	cB	839	CLA	O2D-CGD	5.19	1.45	1.33
14	cA	811	CLA	C3C-C2C	5.19	1.47	1.36
14	cB	836	CLA	O2D-CGD	5.19	1.45	1.33
14	bA	826	CLA	C3C-C2C	5.19	1.47	1.36
14	A	830	CLA	O2D-CGD	5.19	1.45	1.33
14	bB	832	CLA	C3C-C2C	5.19	1.47	1.36
14	B	838	CLA	O2D-CGD	5.19	1.45	1.33
14	B	821	CLA	O2D-CGD	5.19	1.45	1.33
17	bJ	103	BCR	C21-C22	5.19	1.42	1.35
14	bB	818	CLA	C1D-ND	5.19	1.44	1.37
14	cB	812	CLA	C1D-ND	5.19	1.44	1.37
14	B	812	CLA	C3C-C2C	5.19	1.47	1.36
14	bB	810	CLA	C3C-C2C	5.19	1.47	1.36
14	cB	813	CLA	C3C-C2C	5.19	1.47	1.36
14	bB	838	CLA	O2D-CGD	5.19	1.45	1.33
14	bB	811	CLA	C1D-ND	5.18	1.44	1.37
14	A	823	CLA	O2D-CGD	5.18	1.45	1.33
14	cB	811	CLA	C3C-C2C	5.18	1.47	1.36
14	cB	822	CLA	O2D-CGD	5.18	1.45	1.33
14	bA	816	CLA	C3C-C2C	5.18	1.47	1.36
14	bA	836	CLA	O2D-CGD	5.18	1.45	1.33
14	B	821	CLA	C1D-ND	5.18	1.44	1.37
17	J	103	BCR	C21-C22	5.18	1.42	1.35
14	bB	821	CLA	C1D-ND	5.18	1.44	1.37
14	B	810	CLA	C3C-C2C	5.18	1.47	1.36
14	cA	806	CLA	O2D-CGD	5.18	1.45	1.33
14	cA	836	CLA	O2D-CGD	5.18	1.45	1.33
14	cB	833	CLA	C3C-C2C	5.18	1.47	1.36
14	bA	826	CLA	C1D-ND	5.18	1.44	1.37
14	bA	827	CLA	C3C-C2C	5.18	1.47	1.36
14	A	806	CLA	C1D-ND	5.18	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	bA	801	CL0	C3C-C2C	5.18	1.47	1.36
14	cA	823	CLA	C3C-C2C	5.18	1.47	1.36
14	A	826	CLA	O2D-CGD	5.17	1.45	1.33
14	bA	823	CLA	O2D-CGD	5.17	1.45	1.33
14	bB	821	CLA	O2D-CGD	5.17	1.45	1.33
14	bA	823	CLA	C3C-C2C	5.17	1.47	1.36
14	B	811	CLA	C1D-ND	5.17	1.44	1.37
14	A	836	CLA	O2D-CGD	5.17	1.45	1.33
14	A	835	CLA	C1D-ND	5.17	1.44	1.37
14	cA	823	CLA	O2D-CGD	5.17	1.45	1.33
14	cA	826	CLA	O2D-CGD	5.17	1.45	1.33
14	bA	830	CLA	O2D-CGD	5.17	1.45	1.33
14	cA	812	CLA	O2D-CGD	5.17	1.45	1.33
14	A	825	CLA	C1D-ND	5.17	1.44	1.37
14	bA	812	CLA	O2D-CGD	5.17	1.45	1.33
14	A	812	CLA	O2D-CGD	5.17	1.45	1.33
14	A	806	CLA	O2D-CGD	5.17	1.45	1.33
14	bA	826	CLA	O2D-CGD	5.17	1.45	1.33
14	A	826	CLA	C1D-ND	5.17	1.44	1.37
14	bA	806	CLA	O2D-CGD	5.16	1.45	1.33
14	B	831	CLA	O2D-CGD	5.16	1.45	1.33
14	bB	831	CLA	O2D-CGD	5.16	1.45	1.33
14	bA	836	CLA	C3C-C2C	5.16	1.47	1.36
14	cA	836	CLA	C3C-C2C	5.16	1.47	1.36
14	cB	822	CLA	C1D-ND	5.16	1.44	1.37
14	cA	827	CLA	C3C-C2C	5.16	1.47	1.36
14	cB	840	CLA	C3C-C2C	5.16	1.47	1.36
14	bB	814	CLA	O2D-CGD	5.16	1.45	1.33
14	B	839	CLA	C3C-C2C	5.16	1.47	1.36
14	bB	807	CLA	C1D-ND	5.16	1.44	1.37
14	cA	830	CLA	O2D-CGD	5.16	1.45	1.33
14	bB	839	CLA	C3C-C2C	5.16	1.47	1.36
14	cB	832	CLA	O2D-CGD	5.16	1.45	1.33
14	cL	202	CLA	C3C-C2C	5.15	1.47	1.36
14	cB	832	CLA	CHC-C1C	5.15	1.49	1.38
14	cA	818	CLA	O2D-CGD	5.15	1.45	1.33
14	B	809	CLA	O2D-CGD	5.15	1.45	1.33
14	bB	809	CLA	O2D-CGD	5.15	1.45	1.33
14	A	836	CLA	C3C-C2C	5.15	1.47	1.36
14	cB	810	CLA	O2D-CGD	5.15	1.45	1.33
14	cA	806	CLA	C1D-ND	5.15	1.44	1.37
14	cA	834	CLA	C1D-ND	5.15	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	L	201	CLA	C3C-C2C	5.15	1.47	1.36
14	bL	201	CLA	C3C-C2C	5.15	1.47	1.36
14	bA	818	CLA	O2D-CGD	5.15	1.45	1.33
14	B	818	CLA	C1D-ND	5.15	1.44	1.37
14	A	823	CLA	C3C-C2C	5.15	1.47	1.36
14	B	803	CLA	O2D-CGD	5.15	1.45	1.33
14	bB	834	CLA	C1D-ND	5.14	1.44	1.37
14	bA	806	CLA	C1D-ND	5.14	1.44	1.37
14	cB	835	CLA	C1D-ND	5.14	1.44	1.37
14	cA	803	CLA	C3C-C2C	5.14	1.47	1.36
14	A	827	CLA	C3C-C2C	5.14	1.47	1.36
14	cA	826	CLA	C1D-ND	5.14	1.44	1.37
14	bB	831	CLA	CHC-C1C	5.14	1.49	1.38
14	cA	817	CLA	C1D-ND	5.14	1.44	1.37
14	bA	817	CLA	C1D-ND	5.14	1.44	1.37
14	bA	816	CLA	C1D-ND	5.14	1.44	1.37
14	bB	824	CLA	C1D-ND	5.14	1.44	1.37
14	cA	842	CLA	C3C-C2C	5.14	1.47	1.36
14	bB	803	CLA	O2D-CGD	5.14	1.45	1.33
14	A	803	CLA	C3C-C2C	5.14	1.47	1.36
14	cB	804	CLA	O2D-CGD	5.14	1.45	1.33
14	A	817	CLA	C1D-ND	5.14	1.44	1.37
14	A	820	CLA	C1D-ND	5.14	1.44	1.37
14	cB	838	CLA	C1D-ND	5.13	1.44	1.37
14	A	818	CLA	O2D-CGD	5.13	1.45	1.33
14	bA	803	CLA	C3C-C2C	5.13	1.47	1.36
14	bB	812	CLA	CHC-C1C	5.13	1.48	1.38
14	B	814	CLA	O2D-CGD	5.13	1.45	1.33
14	cB	813	CLA	CHC-C1C	5.13	1.48	1.38
14	A	834	CLA	C1D-ND	5.13	1.44	1.37
14	B	815	CLA	C1D-ND	5.13	1.44	1.37
14	bB	837	CLA	C1D-ND	5.13	1.44	1.37
14	B	812	CLA	CHC-C1C	5.13	1.48	1.38
14	cB	815	CLA	O2D-CGD	5.13	1.45	1.33
14	cA	808	CLA	C1D-ND	5.13	1.44	1.37
14	A	842	CLA	C3C-C2C	5.13	1.47	1.36
14	bA	835	CLA	C1D-ND	5.13	1.44	1.37
14	bB	815	CLA	C1D-ND	5.13	1.44	1.37
14	cA	830	CLA	C3C-C2C	5.12	1.47	1.36
14	B	824	CLA	C1D-ND	5.12	1.44	1.37
14	A	829	CLA	O2D-CGD	5.12	1.45	1.33
14	cB	825	CLA	C1D-ND	5.12	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bA	840	CLA	O2D-CGD	5.12	1.45	1.33
14	bA	842	CLA	C3C-C2C	5.12	1.47	1.36
14	bA	830	CLA	C3C-C2C	5.12	1.47	1.36
14	bF	201	CLA	C3C-C2C	5.12	1.47	1.36
14	B	831	CLA	CHC-C1C	5.11	1.48	1.38
14	cB	813	CLA	C1D-ND	5.11	1.44	1.37
14	bB	812	CLA	C1D-ND	5.11	1.44	1.37
14	cA	806	CLA	C3C-C2C	5.11	1.47	1.36
14	A	824	CLA	C3C-C2C	5.11	1.47	1.36
14	B	812	CLA	C1D-ND	5.11	1.44	1.37
14	cA	840	CLA	O2D-CGD	5.11	1.45	1.33
14	F	201	CLA	C3C-C2C	5.11	1.47	1.36
14	A	816	CLA	C1D-ND	5.11	1.44	1.37
14	cA	824	CLA	C1D-ND	5.11	1.44	1.37
14	A	831	CLA	O2D-CGD	5.11	1.45	1.33
14	bA	824	CLA	C3C-C2C	5.11	1.47	1.36
14	bA	820	CLA	C1D-ND	5.11	1.44	1.37
14	B	801	CLA	C3C-C2C	5.11	1.47	1.36
14	cA	831	CLA	O2D-CGD	5.11	1.45	1.33
14	B	837	CLA	C1D-ND	5.10	1.44	1.37
14	bB	808	CLA	O2D-CGD	5.10	1.45	1.33
14	bA	806	CLA	C3C-C2C	5.10	1.47	1.36
14	cA	829	CLA	O2D-CGD	5.10	1.45	1.33
14	cB	816	CLA	C1D-ND	5.10	1.44	1.37
14	bA	831	CLA	O2D-CGD	5.10	1.45	1.33
14	bB	801	CLA	C3C-C2C	5.10	1.47	1.36
14	cA	824	CLA	C3C-C2C	5.10	1.47	1.36
14	cB	802	CLA	C3C-C2C	5.10	1.47	1.36
14	B	835	CLA	C1D-ND	5.10	1.44	1.37
14	A	840	CLA	O2D-CGD	5.10	1.45	1.33
14	bA	842	CLA	O2D-CGD	5.10	1.45	1.33
14	B	802	CLA	C3C-C2C	5.10	1.47	1.36
14	cB	806	CLA	O2D-CGD	5.09	1.45	1.33
14	bA	808	CLA	C1D-ND	5.09	1.44	1.37
14	bA	824	CLA	C1D-ND	5.09	1.44	1.37
14	cB	836	CLA	C1D-ND	5.09	1.44	1.37
14	cF	201	CLA	C3C-C2C	5.09	1.47	1.36
14	cB	803	CLA	C3C-C2C	5.09	1.47	1.36
14	cA	842	CLA	O2D-CGD	5.09	1.45	1.33
14	A	808	CLA	C1D-ND	5.09	1.44	1.37
14	A	824	CLA	C1D-ND	5.09	1.44	1.37
14	A	830	CLA	C3C-C2C	5.09	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cA	820	CLA	C1D-ND	5.09	1.44	1.37
14	A	806	CLA	C3C-C2C	5.09	1.47	1.36
14	B	805	CLA	O2D-CGD	5.09	1.45	1.33
14	bB	835	CLA	C1D-ND	5.09	1.44	1.37
14	cB	809	CLA	O2D-CGD	5.09	1.45	1.33
14	A	842	CLA	O2D-CGD	5.08	1.45	1.33
14	cA	816	CLA	C1D-ND	5.08	1.44	1.37
14	bA	829	CLA	O2D-CGD	5.08	1.45	1.33
14	cB	818	CLA	C1D-ND	5.08	1.44	1.37
14	A	803	CLA	C1D-ND	5.08	1.44	1.37
14	bB	802	CLA	C3C-C2C	5.08	1.47	1.36
14	cA	822	CLA	C3C-C2C	5.08	1.47	1.36
14	bA	835	CLA	O2D-CGD	5.08	1.45	1.33
14	A	835	CLA	O2D-CGD	5.08	1.45	1.33
14	bA	822	CLA	C3C-C2C	5.08	1.47	1.36
14	cA	835	CLA	O2D-CGD	5.08	1.45	1.33
14	A	838	CLA	C3C-C2C	5.08	1.47	1.36
14	cA	838	CLA	C3C-C2C	5.07	1.47	1.36
14	B	808	CLA	O2D-CGD	5.07	1.45	1.33
14	bA	818	CLA	C1D-ND	5.07	1.44	1.37
14	cA	803	CLA	C1D-ND	5.07	1.44	1.37
14	cB	837	CLA	C1D-ND	5.07	1.44	1.37
14	A	809	CLA	C1D-ND	5.07	1.44	1.37
14	bA	838	CLA	C3C-C2C	5.07	1.47	1.36
14	bA	803	CLA	C1D-ND	5.07	1.44	1.37
14	B	817	CLA	C1D-ND	5.07	1.44	1.37
14	cL	204	CLA	O2D-CGD	5.06	1.45	1.33
14	A	822	CLA	C3C-C2C	5.06	1.47	1.36
14	A	825	CLA	C3C-C2C	5.06	1.47	1.36
14	bB	805	CLA	O2D-CGD	5.06	1.45	1.33
14	B	820	CLA	C1D-ND	5.06	1.44	1.37
14	bB	820	CLA	C1D-ND	5.05	1.44	1.37
14	cA	837	CLA	C3C-C2C	5.05	1.47	1.36
14	L	203	CLA	O2D-CGD	5.05	1.45	1.33
14	A	840	CLA	C1D-ND	5.05	1.44	1.37
14	cA	825	CLA	C3C-C2C	5.05	1.47	1.36
14	A	837	CLA	C3C-C2C	5.05	1.47	1.36
14	bA	809	CLA	C1D-ND	5.05	1.44	1.37
14	bA	825	CLA	C3C-C2C	5.05	1.47	1.36
14	bA	837	CLA	C3C-C2C	5.05	1.47	1.36
14	bA	832	CLA	C3C-C2C	5.05	1.47	1.36
14	cA	832	CLA	C3C-C2C	5.05	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bB	831	CLA	C1D-ND	5.04	1.44	1.37
14	bB	836	CLA	C1D-ND	5.04	1.44	1.37
14	cA	840	CLA	C1D-ND	5.04	1.44	1.37
14	A	832	CLA	C3C-C2C	5.04	1.47	1.36
14	bL	203	CLA	O2D-CGD	5.04	1.45	1.33
14	cB	805	CLA	C1D-ND	5.04	1.44	1.37
14	A	818	CLA	C1D-ND	5.03	1.44	1.37
14	bB	804	CLA	C1D-ND	5.03	1.44	1.37
14	B	839	CLA	C1D-ND	5.03	1.44	1.37
17	bB	842	BCR	C14-C13	5.03	1.42	1.35
14	cB	807	CLA	O2D-CGD	5.03	1.45	1.33
14	B	836	CLA	C1D-ND	5.03	1.44	1.37
14	B	806	CLA	O2D-CGD	5.03	1.45	1.33
14	bB	806	CLA	O2D-CGD	5.02	1.45	1.33
17	cB	843	BCR	C14-C13	5.02	1.42	1.35
14	bA	840	CLA	C1D-ND	5.02	1.44	1.37
14	bB	817	CLA	C1D-ND	5.02	1.44	1.37
14	cB	840	CLA	C1D-ND	5.02	1.44	1.37
14	B	804	CLA	C1D-ND	5.02	1.44	1.37
14	cA	809	CLA	C1D-ND	5.02	1.44	1.37
14	cB	821	CLA	C1D-ND	5.01	1.43	1.37
14	cB	832	CLA	C1D-ND	5.01	1.43	1.37
14	bA	837	CLA	O2D-CGD	5.01	1.45	1.33
14	B	806	CLA	C3C-C2C	5.01	1.47	1.36
14	bB	839	CLA	C1D-ND	5.00	1.43	1.37
14	cB	810	CLA	C3C-C2C	5.00	1.47	1.36
14	cA	837	CLA	O2D-CGD	5.00	1.45	1.33
14	A	811	CLA	C1D-ND	5.00	1.43	1.37
14	cA	818	CLA	C1D-ND	5.00	1.43	1.37
14	bB	807	CLA	O2D-CGD	5.00	1.45	1.33
14	L	204	CLA	C1D-ND	5.00	1.43	1.37
14	bL	204	CLA	C1D-ND	5.00	1.43	1.37
14	cB	805	CLA	O2D-CGD	5.00	1.45	1.33
14	cL	205	CLA	C1D-ND	5.00	1.43	1.37
14	bA	839	CLA	C1D-ND	4.99	1.43	1.37
14	B	805	CLA	C3C-C2C	4.99	1.47	1.36
14	cA	826	CLA	CHC-C1C	4.99	1.48	1.38
14	bB	805	CLA	C3C-C2C	4.99	1.47	1.36
14	cA	808	CLA	C3C-C2C	4.99	1.47	1.36
14	B	832	CLA	C1D-ND	4.99	1.43	1.37
17	B	843	BCR	C14-C13	4.99	1.42	1.35
14	A	837	CLA	O2D-CGD	4.99	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bB	806	CLA	C3C-C2C	4.99	1.47	1.36
14	cL	203	CLA	O2D-CGD	4.99	1.45	1.33
17	B	842	BCR	C14-C13	4.99	1.42	1.35
14	L	202	CLA	O2D-CGD	4.99	1.45	1.33
17	cB	844	BCR	C14-C13	4.99	1.42	1.35
14	A	808	CLA	C3C-C2C	4.98	1.47	1.36
14	cB	806	CLA	C3C-C2C	4.98	1.47	1.36
14	cA	811	CLA	C1D-ND	4.98	1.43	1.37
14	bB	809	CLA	C3C-C2C	4.98	1.47	1.36
14	B	831	CLA	C1D-ND	4.98	1.43	1.37
14	bA	808	CLA	C3C-C2C	4.98	1.47	1.36
14	bA	820	CLA	CHC-C1C	4.98	1.48	1.38
14	bL	202	CLA	O2D-CGD	4.98	1.45	1.33
14	bA	826	CLA	CHC-C1C	4.98	1.48	1.38
14	B	804	CLA	O2D-CGD	4.98	1.45	1.33
14	B	807	CLA	O2D-CGD	4.98	1.45	1.33
14	A	826	CLA	CHC-C1C	4.98	1.48	1.38
14	cA	808	CLA	CHC-C1C	4.98	1.48	1.38
14	cB	808	CLA	O2D-CGD	4.98	1.45	1.33
14	A	820	CLA	CHC-C1C	4.97	1.48	1.38
17	bB	843	BCR	C14-C13	4.97	1.42	1.35
14	B	809	CLA	C3C-C2C	4.97	1.47	1.36
14	cL	202	CLA	O2D-CGD	4.97	1.45	1.33
14	bB	837	CLA	O2D-CGD	4.97	1.45	1.33
14	cB	807	CLA	C3C-C2C	4.97	1.47	1.36
14	A	827	CLA	CHC-C1C	4.97	1.48	1.38
14	L	201	CLA	O2D-CGD	4.97	1.45	1.33
14	bA	808	CLA	CHC-C1C	4.96	1.48	1.38
14	cA	840	CLA	CHC-C1C	4.96	1.48	1.38
14	bB	804	CLA	O2D-CGD	4.96	1.45	1.33
14	cB	838	CLA	O2D-CGD	4.96	1.45	1.33
14	bA	811	CLA	C1D-ND	4.96	1.43	1.37
14	bL	201	CLA	O2D-CGD	4.96	1.45	1.33
14	bA	840	CLA	CHC-C1C	4.96	1.48	1.38
14	A	840	CLA	CHC-C1C	4.96	1.48	1.38
14	B	837	CLA	O2D-CGD	4.96	1.45	1.33
14	bA	827	CLA	CHC-C1C	4.96	1.48	1.38
14	bB	832	CLA	C1D-ND	4.95	1.43	1.37
14	cA	820	CLA	CHC-C1C	4.95	1.48	1.38
14	cB	833	CLA	C1D-ND	4.95	1.43	1.37
17	cA	847	BCR	C10-C9	4.95	1.42	1.35
14	B	827	CLA	C1D-ND	4.95	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	808	CLA	CHC-C1C	4.95	1.48	1.38
14	bA	818	CLA	CHC-C1C	4.95	1.48	1.38
14	cB	808	CLA	C3C-C2C	4.95	1.47	1.36
14	bB	807	CLA	C3C-C2C	4.94	1.47	1.36
14	A	804	CLA	CHC-C1C	4.94	1.48	1.38
14	cA	827	CLA	CHC-C1C	4.94	1.48	1.38
14	B	802	CLA	O2D-CGD	4.94	1.45	1.33
14	cA	818	CLA	CHC-C1C	4.94	1.48	1.38
14	bB	819	CLA	CHC-C1C	4.94	1.48	1.38
14	A	818	CLA	CHC-C1C	4.94	1.48	1.38
14	A	839	CLA	C1D-ND	4.94	1.43	1.37
17	bA	847	BCR	C10-C9	4.94	1.42	1.35
14	A	833	CLA	C3C-C2C	4.94	1.47	1.36
17	A	847	BCR	C10-C9	4.94	1.42	1.35
13	cA	801	CL0	O2D-CGD	4.93	1.45	1.33
14	bB	802	CLA	O2D-CGD	4.93	1.45	1.33
14	bB	801	CLA	CHC-C1C	4.93	1.48	1.38
14	cB	803	CLA	O2D-CGD	4.93	1.45	1.33
14	B	807	CLA	C3C-C2C	4.93	1.47	1.36
14	bA	833	CLA	C3C-C2C	4.93	1.47	1.36
14	B	824	CLA	CHC-C1C	4.93	1.48	1.38
14	cB	828	CLA	C1D-ND	4.93	1.43	1.37
14	cA	833	CLA	C3C-C2C	4.93	1.47	1.36
14	cB	825	CLA	CHC-C1C	4.93	1.48	1.38
14	cB	820	CLA	CHC-C1C	4.93	1.48	1.38
14	cA	804	CLA	CHC-C1C	4.93	1.48	1.38
14	B	819	CLA	CHC-C1C	4.93	1.48	1.38
14	cA	832	CLA	O2D-CGD	4.93	1.45	1.33
14	cA	802	CLA	C1D-ND	4.93	1.43	1.37
14	cB	809	CLA	C1D-ND	4.93	1.43	1.37
14	cB	802	CLA	O2D-CGD	4.93	1.45	1.33
14	bA	832	CLA	O2D-CGD	4.93	1.45	1.33
14	bB	808	CLA	C3C-C2C	4.92	1.47	1.36
14	B	801	CLA	CHC-C1C	4.92	1.48	1.38
14	bB	801	CLA	O2D-CGD	4.92	1.45	1.33
13	bA	801	CL0	O2D-CGD	4.92	1.45	1.33
14	cA	839	CLA	C1D-ND	4.92	1.43	1.37
14	cB	802	CLA	CHC-C1C	4.92	1.48	1.38
14	A	832	CLA	O2D-CGD	4.92	1.45	1.33
14	bB	824	CLA	CHC-C1C	4.92	1.48	1.38
14	bB	813	CLA	C1D-ND	4.92	1.43	1.37
14	cB	809	CLA	C3C-C2C	4.92	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bB	816	CLA	CHC-C1C	4.92	1.48	1.38
14	cB	801	CLA	CHC-C1C	4.92	1.48	1.38
14	B	808	CLA	C3C-C2C	4.92	1.47	1.36
14	bA	804	CLA	CHC-C1C	4.92	1.48	1.38
14	bB	851	CLA	CHC-C1C	4.92	1.48	1.38
14	bA	842	CLA	C1D-ND	4.92	1.43	1.37
14	cB	828	CLA	CHC-C1C	4.91	1.48	1.38
13	A	801	CL0	O2D-CGD	4.91	1.45	1.33
14	A	802	CLA	C1D-ND	4.91	1.43	1.37
14	cB	814	CLA	C1D-ND	4.91	1.43	1.37
14	B	801	CLA	O2D-CGD	4.91	1.45	1.33
14	cB	834	CLA	CHC-C1C	4.91	1.48	1.38
14	cA	842	CLA	C1D-ND	4.91	1.43	1.37
14	cB	817	CLA	CHC-C1C	4.91	1.48	1.38
14	A	842	CLA	C1D-ND	4.91	1.43	1.37
14	bA	802	CLA	C1D-ND	4.90	1.43	1.37
14	B	826	CLA	C3C-C2C	4.90	1.47	1.36
14	B	851	CLA	CHC-C1C	4.90	1.48	1.38
14	B	808	CLA	C1D-ND	4.90	1.43	1.37
14	bB	827	CLA	CHC-C1C	4.90	1.48	1.38
14	bA	841	CLA	C3C-C2C	4.90	1.47	1.36
14	B	816	CLA	CHC-C1C	4.89	1.48	1.38
14	bB	808	CLA	C1D-ND	4.89	1.43	1.37
14	bB	839	CLA	O2D-CGD	4.89	1.45	1.33
14	J	101	CLA	CHC-C1C	4.89	1.48	1.38
14	B	839	CLA	O2D-CGD	4.89	1.45	1.33
14	B	827	CLA	CHC-C1C	4.89	1.48	1.38
14	bB	820	CLA	CHC-C1C	4.89	1.48	1.38
17	cA	845	BCR	C21-C22	4.88	1.42	1.35
14	bJ	101	CLA	CHC-C1C	4.88	1.48	1.38
14	bB	825	CLA	CHC-C1C	4.88	1.48	1.38
17	A	845	BCR	C21-C22	4.88	1.42	1.35
14	bB	826	CLA	C3C-C2C	4.88	1.47	1.36
14	cA	841	CLA	C3C-C2C	4.88	1.47	1.36
14	B	813	CLA	C1D-ND	4.88	1.43	1.37
14	B	825	CLA	CHC-C1C	4.88	1.48	1.38
14	bA	812	CLA	CHC-C1C	4.88	1.48	1.38
14	cB	840	CLA	O2D-CGD	4.88	1.45	1.33
14	cA	812	CLA	CHC-C1C	4.88	1.48	1.38
14	cA	831	CLA	C1D-ND	4.88	1.43	1.37
14	B	833	CLA	CHC-C1C	4.88	1.48	1.38
14	bB	827	CLA	C1D-ND	4.88	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cB	827	CLA	C3C-C2C	4.87	1.47	1.36
14	X	201	CLA	CHC-C1C	4.87	1.48	1.38
14	bB	833	CLA	CHC-C1C	4.87	1.48	1.38
14	cB	821	CLA	CHC-C1C	4.87	1.48	1.38
14	cX	201	CLA	CHC-C1C	4.87	1.48	1.38
14	A	841	CLA	C3C-C2C	4.87	1.47	1.36
14	cJ	101	CLA	CHC-C1C	4.87	1.48	1.38
14	A	812	CLA	CHC-C1C	4.87	1.48	1.38
14	bX	201	CLA	CHC-C1C	4.87	1.48	1.38
17	bA	845	BCR	C21-C22	4.86	1.42	1.35
14	cB	826	CLA	CHC-C1C	4.86	1.48	1.38
14	B	820	CLA	CHC-C1C	4.86	1.48	1.38
14	bA	831	CLA	C1D-ND	4.86	1.43	1.37
17	bA	846	BCR	C21-C22	4.86	1.42	1.35
14	A	831	CLA	C1D-ND	4.86	1.43	1.37
14	B	836	CLA	CHC-C1C	4.85	1.48	1.38
14	A	814	CLA	CHC-C1C	4.85	1.48	1.38
17	cA	846	BCR	C21-C22	4.85	1.42	1.35
14	bB	836	CLA	CHC-C1C	4.85	1.48	1.38
14	bB	804	CLA	CHC-C1C	4.85	1.48	1.38
14	B	802	CLA	C1D-ND	4.85	1.43	1.37
14	cA	813	CLA	CHC-C1C	4.85	1.48	1.38
14	A	813	CLA	CHC-C1C	4.85	1.48	1.38
14	bA	838	CLA	O2D-CGD	4.85	1.45	1.33
14	bA	814	CLA	CHC-C1C	4.84	1.48	1.38
14	B	804	CLA	CHC-C1C	4.84	1.48	1.38
14	A	816	CLA	CHC-C1C	4.84	1.48	1.38
14	cA	838	CLA	O2D-CGD	4.84	1.45	1.33
14	bA	813	CLA	CHC-C1C	4.84	1.48	1.38
14	bB	802	CLA	C1D-ND	4.84	1.43	1.37
14	cB	819	CLA	CHC-C1C	4.84	1.48	1.38
14	cB	837	CLA	CHC-C1C	4.84	1.48	1.38
14	cA	814	CLA	CHC-C1C	4.84	1.48	1.38
14	cB	803	CLA	C1D-ND	4.84	1.43	1.37
14	B	815	CLA	CHC-C1C	4.84	1.48	1.38
14	bA	805	CLA	C3C-C2C	4.84	1.47	1.36
14	cA	816	CLA	CHC-C1C	4.84	1.48	1.38
14	B	829	CLA	C1D-ND	4.84	1.43	1.37
14	cB	805	CLA	CHC-C1C	4.83	1.48	1.38
14	A	838	CLA	O2D-CGD	4.83	1.45	1.33
17	bF	202	BCR	C14-C13	4.83	1.42	1.35
14	F	201	CLA	C1D-ND	4.83	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cA	815	CLA	CHC-C1C	4.83	1.48	1.38
17	A	846	BCR	C21-C22	4.83	1.42	1.35
14	bB	815	CLA	CHC-C1C	4.83	1.48	1.38
14	cB	816	CLA	CHC-C1C	4.83	1.48	1.38
14	bA	816	CLA	CHC-C1C	4.83	1.48	1.38
14	bA	835	CLA	CHC-C1C	4.83	1.48	1.38
14	B	835	CLA	CHC-C1C	4.82	1.48	1.38
14	cB	836	CLA	CHC-C1C	4.82	1.48	1.38
14	A	835	CLA	CHC-C1C	4.82	1.48	1.38
14	bB	835	CLA	CHC-C1C	4.82	1.48	1.38
14	cL	203	CLA	CHC-C1C	4.82	1.48	1.38
14	cA	805	CLA	C3C-C2C	4.81	1.47	1.36
14	L	202	CLA	CHC-C1C	4.81	1.48	1.38
14	cB	812	CLA	CHC-C1C	4.81	1.48	1.38
14	B	811	CLA	CHC-C1C	4.81	1.48	1.38
14	B	818	CLA	CHC-C1C	4.81	1.48	1.38
14	cA	835	CLA	CHC-C1C	4.81	1.48	1.38
14	A	805	CLA	C3C-C2C	4.80	1.46	1.36
14	bL	202	CLA	CHC-C1C	4.80	1.48	1.38
17	F	202	BCR	C14-C13	4.80	1.42	1.35
14	bA	815	CLA	CHC-C1C	4.80	1.48	1.38
17	cF	202	BCR	C14-C13	4.80	1.42	1.35
14	bB	818	CLA	CHC-C1C	4.80	1.48	1.38
14	A	815	CLA	CHC-C1C	4.79	1.48	1.38
14	B	830	CLA	CHC-C1C	4.79	1.48	1.38
14	bF	201	CLA	C1D-ND	4.79	1.43	1.37
14	bB	811	CLA	CHC-C1C	4.79	1.48	1.38
14	cB	830	CLA	C1D-ND	4.79	1.43	1.37
14	cA	811	CLA	CHC-C1C	4.79	1.48	1.38
14	bB	806	CLA	CHC-C1C	4.79	1.48	1.38
14	cB	807	CLA	CHC-C1C	4.79	1.48	1.38
14	A	811	CLA	CHC-C1C	4.78	1.48	1.38
14	bF	201	CLA	CHC-C1C	4.78	1.48	1.38
14	cF	201	CLA	C1D-ND	4.78	1.43	1.37
14	A	819	CLA	CHC-C1C	4.78	1.48	1.38
14	B	806	CLA	CHC-C1C	4.78	1.48	1.38
14	cA	819	CLA	CHC-C1C	4.78	1.48	1.38
14	cF	201	CLA	CHC-C1C	4.78	1.48	1.38
17	B	842	BCR	C21-C22	4.78	1.42	1.35
13	cA	801	CL0	C1D-ND	4.78	1.43	1.37
14	F	201	CLA	CHC-C1C	4.77	1.48	1.38
14	bJ	102	CLA	CHC-C1C	4.77	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	bB	843	BCR	C17-C18	4.77	1.42	1.35
17	cB	843	BCR	C21-C22	4.77	1.42	1.35
14	bB	829	CLA	C1D-ND	4.77	1.43	1.37
14	bA	811	CLA	CHC-C1C	4.77	1.48	1.38
14	cB	831	CLA	CHC-C1C	4.77	1.48	1.38
14	A	809	CLA	CHC-C1C	4.77	1.48	1.38
17	J	103	BCR	C14-C13	4.76	1.42	1.35
14	bB	830	CLA	CHC-C1C	4.76	1.48	1.38
14	bA	809	CLA	CHC-C1C	4.76	1.48	1.38
14	bA	819	CLA	CHC-C1C	4.76	1.48	1.38
13	bA	801	CL0	C1D-ND	4.76	1.43	1.37
13	A	801	CL0	C1D-ND	4.76	1.43	1.37
14	J	102	CLA	CHC-C1C	4.76	1.48	1.38
17	bJ	103	BCR	C14-C13	4.76	1.42	1.35
14	bA	803	CLA	CHC-C1C	4.76	1.48	1.38
14	cB	850	CLA	CHC-C1C	4.76	1.48	1.38
14	cJ	102	CLA	CHC-C1C	4.76	1.48	1.38
14	bB	822	CLA	CHC-C1C	4.75	1.48	1.38
17	cB	844	BCR	C17-C18	4.75	1.42	1.35
17	B	843	BCR	C17-C18	4.75	1.42	1.35
14	A	803	CLA	CHC-C1C	4.75	1.48	1.38
14	cB	811	CLA	CHC-C1C	4.74	1.48	1.38
14	cL	205	CLA	O2D-CGD	4.74	1.44	1.33
14	cA	803	CLA	CHC-C1C	4.74	1.48	1.38
14	B	822	CLA	CHC-C1C	4.74	1.48	1.38
14	B	814	CLA	CHC-C1C	4.74	1.48	1.38
14	B	849	CLA	CHC-C1C	4.74	1.48	1.38
14	bB	849	CLA	CHC-C1C	4.73	1.48	1.38
14	L	204	CLA	O2D-CGD	4.73	1.44	1.33
14	bA	829	CLA	CHC-C1C	4.73	1.48	1.38
14	cB	815	CLA	CHC-C1C	4.73	1.48	1.38
14	cA	809	CLA	CHC-C1C	4.73	1.48	1.38
17	cJ	103	BCR	C14-C13	4.73	1.42	1.35
14	cA	836	CLA	CHC-C1C	4.73	1.48	1.38
14	bA	836	CLA	CHC-C1C	4.73	1.48	1.38
14	bA	828	CLA	C1D-ND	4.73	1.43	1.37
14	cB	823	CLA	CHC-C1C	4.73	1.48	1.38
14	A	829	CLA	CHC-C1C	4.73	1.48	1.38
14	bA	817	CLA	CHC-C1C	4.73	1.48	1.38
14	bL	204	CLA	O2D-CGD	4.73	1.44	1.33
17	bB	842	BCR	C21-C22	4.72	1.42	1.35
14	A	836	CLA	CHC-C1C	4.72	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bB	810	CLA	CHC-C1C	4.72	1.48	1.38
14	B	810	CLA	CHC-C1C	4.72	1.48	1.38
14	bA	821	CLA	CHC-C1C	4.72	1.48	1.38
14	bB	814	CLA	CHC-C1C	4.72	1.48	1.38
14	A	833	CLA	O2D-CGD	4.72	1.44	1.33
14	A	828	CLA	C1D-ND	4.71	1.43	1.37
14	bA	833	CLA	O2D-CGD	4.71	1.44	1.33
14	cA	829	CLA	CHC-C1C	4.71	1.48	1.38
14	cA	828	CLA	C1D-ND	4.71	1.43	1.37
14	A	817	CLA	CHC-C1C	4.71	1.48	1.38
14	bB	832	CLA	CHC-C1C	4.71	1.48	1.38
14	bA	810	CLA	CHC-C1C	4.70	1.48	1.38
14	cA	817	CLA	CHC-C1C	4.70	1.48	1.38
14	cB	833	CLA	CHC-C1C	4.70	1.48	1.38
17	bA	845	BCR	C10-C9	4.70	1.42	1.35
14	A	821	CLA	CHC-C1C	4.70	1.48	1.38
14	cA	833	CLA	O2D-CGD	4.70	1.44	1.33
14	L	201	CLA	O2A-CGA	4.70	1.47	1.33
14	A	852	CLA	C3C-C2C	4.69	1.46	1.36
14	cA	807	CLA	CHC-C1C	4.69	1.48	1.38
14	bA	822	CLA	CHD-C1D	4.69	1.47	1.38
17	cB	848	BCR	C10-C9	4.69	1.42	1.35
17	bF	202	BCR	C10-C9	4.69	1.42	1.35
14	cL	202	CLA	O2A-CGA	4.69	1.47	1.33
14	bL	201	CLA	O2A-CGA	4.69	1.47	1.33
14	B	832	CLA	CHC-C1C	4.69	1.48	1.38
14	bA	824	CLA	CHC-C1C	4.69	1.48	1.38
14	bA	852	CLA	C3C-C2C	4.69	1.46	1.36
14	A	822	CLA	CHD-C1D	4.69	1.47	1.38
14	A	810	CLA	CHC-C1C	4.69	1.48	1.38
14	cA	824	CLA	CHC-C1C	4.69	1.48	1.38
14	cB	814	CLA	CHC-C1C	4.69	1.48	1.38
14	cA	822	CLA	CHD-C1D	4.69	1.47	1.38
14	cA	821	CLA	CHC-C1C	4.68	1.48	1.38
14	bA	829	CLA	C1D-ND	4.68	1.43	1.37
17	cF	202	BCR	C21-C22	4.68	1.42	1.35
14	A	807	CLA	CHC-C1C	4.68	1.48	1.38
14	B	813	CLA	CHC-C1C	4.68	1.48	1.38
17	B	847	BCR	C10-C9	4.68	1.42	1.35
14	B	821	CLA	CHC-C1C	4.68	1.48	1.38
14	bA	807	CLA	CHC-C1C	4.68	1.48	1.38
14	cA	810	CLA	CHC-C1C	4.68	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bB	821	CLA	CHC-C1C	4.68	1.48	1.38
14	cA	829	CLA	C1D-ND	4.68	1.43	1.37
14	cB	822	CLA	CHC-C1C	4.68	1.48	1.38
17	F	202	BCR	C10-C9	4.68	1.42	1.35
14	bB	813	CLA	CHC-C1C	4.68	1.48	1.38
14	cA	852	CLA	C3C-C2C	4.68	1.46	1.36
14	cB	806	CLA	CHC-C1C	4.68	1.48	1.38
14	A	824	CLA	CHC-C1C	4.68	1.48	1.38
17	A	845	BCR	C10-C9	4.67	1.42	1.35
14	B	805	CLA	CHC-C1C	4.67	1.48	1.38
17	cA	845	BCR	C10-C9	4.67	1.42	1.35
14	bA	837	CLA	CHC-C1C	4.67	1.48	1.38
17	F	202	BCR	C21-C22	4.66	1.42	1.35
14	bB	805	CLA	CHC-C1C	4.66	1.48	1.38
14	cA	852	CLA	O2D-CGD	4.66	1.44	1.33
14	cA	837	CLA	CHC-C1C	4.66	1.48	1.38
17	bB	847	BCR	C10-C9	4.66	1.42	1.35
17	cB	846	BCR	C10-C9	4.66	1.42	1.35
14	A	837	CLA	CHC-C1C	4.65	1.48	1.38
14	A	823	CLA	CHC-C1C	4.65	1.48	1.38
14	bA	823	CLA	CHC-C1C	4.65	1.48	1.38
14	cA	823	CLA	O2A-CGA	4.65	1.46	1.30
17	bF	202	BCR	C21-C22	4.65	1.41	1.35
14	bA	823	CLA	O2A-CGA	4.65	1.46	1.30
17	cF	202	BCR	C10-C9	4.65	1.41	1.35
14	A	829	CLA	C1D-ND	4.65	1.43	1.37
14	A	823	CLA	O2A-CGA	4.65	1.46	1.30
14	cA	823	CLA	CHC-C1C	4.65	1.48	1.38
14	A	802	CLA	O2D-CGD	4.65	1.44	1.33
17	cB	842	BCR	C10-C9	4.64	1.41	1.35
17	B	841	BCR	C10-C9	4.64	1.41	1.35
17	B	845	BCR	C10-C9	4.64	1.41	1.35
14	bA	839	CLA	CHC-C1C	4.64	1.47	1.38
14	bA	852	CLA	O2D-CGD	4.64	1.44	1.33
14	A	852	CLA	O2D-CGD	4.64	1.44	1.33
17	bB	841	BCR	C10-C9	4.64	1.41	1.35
14	cA	802	CLA	O2D-CGD	4.63	1.44	1.33
14	A	822	CLA	CHC-C1C	4.63	1.47	1.38
14	cA	822	CLA	CHC-C1C	4.63	1.47	1.38
14	cB	824	CLA	CHC-C1C	4.63	1.47	1.38
14	bA	842	CLA	CHC-C1C	4.63	1.47	1.38
14	cB	838	CLA	CHC-C1C	4.62	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	bB	845	BCR	C10-C9	4.62	1.41	1.35
14	A	842	CLA	CHC-C1C	4.62	1.47	1.38
14	bA	802	CLA	O2D-CGD	4.62	1.44	1.33
14	bA	805	CLA	CHC-C1C	4.62	1.47	1.38
14	bB	828	CLA	CHC-C1C	4.62	1.47	1.38
14	B	823	CLA	CHC-C1C	4.62	1.47	1.38
14	bA	838	CLA	O2A-CGA	4.62	1.46	1.30
14	A	838	CLA	O2A-CGA	4.61	1.46	1.30
14	B	837	CLA	CHC-C1C	4.61	1.47	1.38
14	cA	838	CLA	O2A-CGA	4.61	1.46	1.30
14	A	805	CLA	CHC-C1C	4.61	1.47	1.38
14	bB	837	CLA	CHC-C1C	4.61	1.47	1.38
14	B	828	CLA	CHC-C1C	4.61	1.47	1.38
14	cA	842	CLA	CHC-C1C	4.60	1.47	1.38
14	bB	823	CLA	CHC-C1C	4.60	1.47	1.38
14	A	839	CLA	CHC-C1C	4.60	1.47	1.38
14	cB	835	CLA	CHC-C1C	4.60	1.47	1.38
14	cB	824	CLA	O2A-CGA	4.60	1.46	1.33
14	bB	834	CLA	CHC-C1C	4.60	1.47	1.38
14	cB	829	CLA	CHC-C1C	4.60	1.47	1.38
14	B	823	CLA	O2A-CGA	4.60	1.46	1.33
14	B	834	CLA	CHC-C1C	4.60	1.47	1.38
17	F	202	BCR	C17-C18	4.60	1.41	1.35
14	cA	805	CLA	CHC-C1C	4.59	1.47	1.38
14	cA	839	CLA	CHC-C1C	4.59	1.47	1.38
17	bF	202	BCR	C17-C18	4.59	1.41	1.35
14	bA	822	CLA	CHC-C1C	4.59	1.47	1.38
14	bB	823	CLA	O2A-CGA	4.59	1.46	1.33
14	B	829	CLA	CHC-C1C	4.59	1.47	1.38
14	bB	816	CLA	O2A-CGA	4.59	1.46	1.30
14	bB	829	CLA	CHC-C1C	4.58	1.47	1.38
14	cB	805	CLA	O2A-CGA	4.58	1.46	1.33
17	cF	202	BCR	C17-C18	4.58	1.41	1.35
14	bA	834	CLA	CHC-C1C	4.58	1.47	1.38
17	bA	847	BCR	C21-C22	4.58	1.41	1.35
17	bB	846	BCR	C21-C22	4.58	1.41	1.35
14	cB	817	CLA	O2A-CGA	4.58	1.46	1.30
14	bA	821	CLA	O2A-CGA	4.57	1.46	1.30
14	cA	821	CLA	O2A-CGA	4.57	1.46	1.30
14	cB	830	CLA	CHC-C1C	4.57	1.47	1.38
14	B	816	CLA	O2A-CGA	4.57	1.46	1.30
17	bB	845	BCR	C17-C18	4.57	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	cA	847	BCR	C21-C22	4.57	1.41	1.35
14	A	834	CLA	CHC-C1C	4.57	1.47	1.38
14	B	804	CLA	O2A-CGA	4.57	1.46	1.33
14	cB	835	CLA	O2A-CGA	4.57	1.46	1.30
14	B	832	CLA	O2A-CGA	4.57	1.46	1.30
17	B	846	BCR	C21-C22	4.57	1.41	1.35
14	bA	809	CLA	O2A-CGA	4.57	1.46	1.30
17	cB	846	BCR	C17-C18	4.57	1.41	1.35
14	B	834	CLA	O2A-CGA	4.57	1.46	1.30
14	cA	809	CLA	O2A-CGA	4.57	1.46	1.30
14	A	821	CLA	O2A-CGA	4.57	1.46	1.30
14	bB	834	CLA	O2A-CGA	4.57	1.46	1.30
14	cB	833	CLA	O2A-CGA	4.56	1.46	1.30
14	bB	804	CLA	O2A-CGA	4.56	1.46	1.33
14	bB	832	CLA	O2A-CGA	4.56	1.46	1.30
17	cM	101	BCR	C10-C9	4.56	1.41	1.35
14	A	809	CLA	O2A-CGA	4.56	1.46	1.30
14	cA	834	CLA	CHC-C1C	4.56	1.47	1.38
14	B	829	CLA	O2A-CGA	4.55	1.46	1.30
14	A	842	CLA	O2A-CGA	4.55	1.46	1.30
14	B	838	CLA	O2A-CGA	4.55	1.46	1.33
14	cB	839	CLA	O2A-CGA	4.55	1.46	1.33
14	cA	820	CLA	CHD-C1D	4.55	1.47	1.38
17	bM	101	BCR	C10-C9	4.55	1.41	1.35
14	A	820	CLA	CHD-C1D	4.55	1.47	1.38
14	bB	838	CLA	O2A-CGA	4.54	1.46	1.33
14	bB	829	CLA	O2A-CGA	4.54	1.46	1.30
14	bB	838	CLA	C3C-C2C	4.54	1.46	1.36
14	cA	842	CLA	O2A-CGA	4.54	1.46	1.30
14	bB	834	CLA	CHD-C1D	4.54	1.47	1.38
14	cB	822	CLA	O2A-CGA	4.54	1.46	1.30
14	A	831	CLA	CHC-C1C	4.54	1.47	1.38
17	A	846	BCR	C14-C13	4.54	1.41	1.35
14	bA	831	CLA	CHC-C1C	4.54	1.47	1.38
14	cB	815	CLA	O2A-CGA	4.54	1.46	1.30
14	bA	842	CLA	O2A-CGA	4.54	1.46	1.30
14	B	839	CLA	O2A-CGA	4.54	1.46	1.33
14	bA	812	CLA	O2A-CGA	4.54	1.46	1.30
14	B	814	CLA	O2A-CGA	4.54	1.46	1.30
14	bA	822	CLA	O2A-CGA	4.54	1.46	1.30
14	cA	835	CLA	O2A-CGA	4.54	1.46	1.30
14	A	835	CLA	O2A-CGA	4.54	1.46	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	845	BCR	C17-C18	4.54	1.41	1.35
14	A	812	CLA	O2A-CGA	4.54	1.46	1.30
14	cB	840	CLA	O2A-CGA	4.54	1.46	1.33
14	B	838	CLA	C3C-C2C	4.54	1.46	1.36
14	A	822	CLA	O2A-CGA	4.54	1.46	1.30
14	cB	830	CLA	O2A-CGA	4.54	1.46	1.30
17	cB	847	BCR	C21-C22	4.54	1.41	1.35
14	bA	820	CLA	CHD-C1D	4.54	1.47	1.38
14	cX	201	CLA	O2A-CGA	4.53	1.46	1.30
14	bB	814	CLA	O2A-CGA	4.53	1.46	1.30
14	cA	812	CLA	O2A-CGA	4.53	1.46	1.30
17	bB	845	BCR	C14-C13	4.53	1.41	1.35
14	B	821	CLA	O2A-CGA	4.53	1.46	1.30
14	bB	820	CLA	O2A-CGA	4.53	1.46	1.30
14	A	820	CLA	O2A-CGA	4.53	1.46	1.30
14	cB	808	CLA	O2A-CGA	4.53	1.46	1.33
14	bA	802	CLA	C3C-C2C	4.53	1.46	1.36
14	A	810	CLA	O2A-CGA	4.53	1.46	1.30
14	bA	820	CLA	O2A-CGA	4.53	1.46	1.30
14	B	817	CLA	CHC-C1C	4.53	1.47	1.38
14	cA	820	CLA	O2A-CGA	4.53	1.46	1.30
14	bB	821	CLA	O2A-CGA	4.53	1.46	1.30
14	B	820	CLA	O2A-CGA	4.53	1.46	1.30
14	bJ	101	CLA	O2A-CGA	4.53	1.46	1.30
14	cB	839	CLA	C3C-C2C	4.53	1.46	1.36
14	bA	835	CLA	O2A-CGA	4.53	1.46	1.30
14	J	101	CLA	O2A-CGA	4.53	1.46	1.30
14	bX	201	CLA	O2A-CGA	4.53	1.46	1.30
14	A	807	CLA	O2A-CGA	4.53	1.46	1.30
14	A	814	CLA	O2A-CGA	4.53	1.46	1.30
14	cA	819	CLA	CHD-C1D	4.53	1.47	1.38
14	cB	835	CLA	CHD-C1D	4.53	1.47	1.38
17	A	847	BCR	C21-C22	4.53	1.41	1.35
14	B	836	CLA	O2A-CGA	4.53	1.46	1.30
14	cJ	101	CLA	O2A-CGA	4.52	1.46	1.30
14	A	806	CLA	CHC-C1C	4.52	1.47	1.38
14	cA	822	CLA	O2A-CGA	4.52	1.46	1.30
14	cB	837	CLA	O2A-CGA	4.52	1.46	1.30
14	bB	822	CLA	O2A-CGA	4.52	1.46	1.30
14	cB	823	CLA	O2A-CGA	4.52	1.46	1.30
14	bA	807	CLA	O2A-CGA	4.52	1.45	1.30
14	B	822	CLA	O2A-CGA	4.52	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cA	810	CLA	O2A-CGA	4.52	1.45	1.30
14	A	802	CLA	C3C-C2C	4.52	1.46	1.36
14	cA	814	CLA	O2A-CGA	4.52	1.45	1.30
17	I	102	BCR	C14-C13	4.52	1.41	1.35
14	B	810	CLA	O2A-CGA	4.52	1.45	1.30
17	bA	846	BCR	C14-C13	4.52	1.41	1.35
17	bI	102	BCR	C14-C13	4.52	1.41	1.35
14	cL	205	CLA	CHC-C1C	4.52	1.47	1.38
14	B	811	CLA	O2A-CGA	4.52	1.45	1.30
14	cB	821	CLA	O2A-CGA	4.52	1.45	1.30
14	bA	810	CLA	O2A-CGA	4.52	1.45	1.30
14	cA	802	CLA	C3C-C2C	4.52	1.46	1.36
14	X	201	CLA	O2A-CGA	4.52	1.45	1.30
14	B	807	CLA	O2A-CGA	4.52	1.46	1.33
17	cI	102	BCR	C14-C13	4.52	1.41	1.35
14	bA	814	CLA	O2A-CGA	4.52	1.45	1.30
14	bA	806	CLA	CHC-C1C	4.52	1.47	1.38
14	cA	834	CLA	CHD-C1D	4.52	1.47	1.38
17	M	101	BCR	C10-C9	4.52	1.41	1.35
14	cA	811	CLA	O2A-CGA	4.52	1.45	1.30
14	bA	811	CLA	O2A-CGA	4.52	1.45	1.30
14	bB	807	CLA	O2A-CGA	4.52	1.46	1.33
14	bB	811	CLA	O2A-CGA	4.51	1.45	1.30
17	B	845	BCR	C14-C13	4.51	1.41	1.35
14	bB	836	CLA	O2A-CGA	4.51	1.45	1.30
14	cA	807	CLA	O2A-CGA	4.51	1.45	1.30
14	B	834	CLA	CHD-C1D	4.51	1.47	1.38
14	cB	812	CLA	O2A-CGA	4.51	1.45	1.30
14	bB	839	CLA	O2A-CGA	4.51	1.46	1.33
14	L	204	CLA	CHC-C1C	4.51	1.47	1.38
14	bL	204	CLA	CHC-C1C	4.51	1.47	1.38
14	bA	815	CLA	O2A-CGA	4.51	1.45	1.30
14	bB	810	CLA	O2A-CGA	4.51	1.45	1.30
14	cB	811	CLA	O2A-CGA	4.51	1.45	1.30
14	A	811	CLA	O2A-CGA	4.51	1.45	1.30
17	cA	845	BCR	C14-C13	4.51	1.41	1.35
14	bA	834	CLA	O2A-CGA	4.51	1.45	1.30
14	A	815	CLA	O2A-CGA	4.51	1.45	1.30
14	bA	834	CLA	CHD-C1D	4.51	1.47	1.38
14	bA	819	CLA	CHD-C1D	4.51	1.47	1.38
14	A	834	CLA	CHD-C1D	4.51	1.47	1.38
14	B	833	CLA	O2A-CGA	4.51	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cA	831	CLA	CHC-C1C	4.51	1.47	1.38
17	bA	845	BCR	C14-C13	4.51	1.41	1.35
14	B	849	CLA	O2A-CGA	4.50	1.45	1.30
14	bB	849	CLA	O2A-CGA	4.50	1.45	1.30
14	A	819	CLA	CHD-C1D	4.50	1.47	1.38
14	cB	818	CLA	CHC-C1C	4.50	1.47	1.38
14	cB	834	CLA	O2A-CGA	4.50	1.45	1.30
17	A	845	BCR	C14-C13	4.50	1.41	1.35
17	cB	846	BCR	C14-C13	4.50	1.41	1.35
14	cB	801	CLA	O2A-CGA	4.50	1.45	1.30
14	B	851	CLA	O2A-CGA	4.50	1.45	1.30
17	B	850	BCR	C21-C22	4.50	1.41	1.35
14	cA	819	CLA	O2A-CGA	4.50	1.45	1.30
14	cB	815	CLA	CHD-C1D	4.50	1.47	1.38
17	B	842	BCR	C10-C9	4.50	1.41	1.35
14	bA	819	CLA	O2A-CGA	4.50	1.45	1.30
14	bB	810	CLA	CHD-C1D	4.50	1.47	1.38
14	bB	833	CLA	O2A-CGA	4.50	1.45	1.30
14	J	102	CLA	O2A-CGA	4.50	1.45	1.30
14	cA	806	CLA	CHC-C1C	4.50	1.47	1.38
14	bL	202	CLA	O2A-CGA	4.49	1.46	1.33
14	cB	850	CLA	O2A-CGA	4.49	1.45	1.30
14	B	810	CLA	CHD-C1D	4.49	1.47	1.38
14	cA	834	CLA	O2A-CGA	4.49	1.45	1.30
14	B	814	CLA	CHD-C1D	4.49	1.47	1.38
17	cA	846	BCR	C14-C13	4.49	1.41	1.35
14	cA	815	CLA	O2A-CGA	4.49	1.45	1.30
14	B	835	CLA	O2A-CGA	4.49	1.45	1.30
14	cJ	102	CLA	O2A-CGA	4.49	1.45	1.30
14	bB	851	CLA	O2A-CGA	4.49	1.45	1.30
14	A	834	CLA	O2A-CGA	4.49	1.45	1.30
17	B	850	BCR	C14-C13	4.49	1.41	1.35
14	bA	803	CLA	O2A-CGA	4.49	1.45	1.30
14	B	803	CLA	C1D-ND	4.49	1.43	1.37
14	cA	816	CLA	O2A-CGA	4.49	1.45	1.30
14	A	816	CLA	O2A-CGA	4.49	1.45	1.30
14	bB	817	CLA	CHC-C1C	4.49	1.47	1.38
14	cB	811	CLA	CHD-C1D	4.49	1.47	1.38
14	cB	850	CLA	CHD-C1D	4.49	1.47	1.38
14	bA	816	CLA	O2A-CGA	4.49	1.45	1.30
17	cB	851	BCR	C21-C22	4.49	1.41	1.35
14	cB	836	CLA	O2A-CGA	4.49	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	819	CLA	O2A-CGA	4.48	1.45	1.30
14	bB	835	CLA	O2A-CGA	4.48	1.45	1.30
17	cB	843	BCR	C10-C9	4.48	1.41	1.35
14	A	803	CLA	O2A-CGA	4.48	1.45	1.30
14	bJ	102	CLA	O2A-CGA	4.48	1.45	1.30
14	cL	203	CLA	O2A-CGA	4.48	1.46	1.33
17	bB	842	BCR	C10-C9	4.48	1.41	1.35
14	cA	803	CLA	O2A-CGA	4.48	1.45	1.30
14	A	802	CLA	CHD-C1D	4.48	1.47	1.38
14	cB	838	CLA	CHD-C1D	4.48	1.47	1.38
14	A	813	CLA	O2A-CGA	4.48	1.45	1.30
14	bB	813	CLA	O2A-CGA	4.48	1.46	1.33
14	B	849	CLA	CHD-C1D	4.48	1.47	1.38
14	cA	802	CLA	CHD-C1D	4.48	1.47	1.38
14	bB	814	CLA	CHD-C1D	4.48	1.47	1.38
17	cB	846	BCR	C21-C22	4.48	1.41	1.35
14	L	202	CLA	O2A-CGA	4.48	1.46	1.33
14	bA	835	CLA	CHD-C1D	4.47	1.47	1.38
17	B	845	BCR	C21-C22	4.47	1.41	1.35
14	bA	813	CLA	O2A-CGA	4.47	1.45	1.30
14	bB	849	CLA	CHD-C1D	4.47	1.47	1.38
14	A	835	CLA	CHD-C1D	4.47	1.47	1.38
17	bB	850	BCR	C14-C13	4.47	1.41	1.35
14	B	837	CLA	CHD-C1D	4.47	1.47	1.38
14	bA	802	CLA	CHD-C1D	4.47	1.47	1.38
17	bB	845	BCR	C21-C22	4.47	1.41	1.35
14	cB	804	CLA	C1D-ND	4.47	1.43	1.37
14	F	201	CLA	O2A-CGA	4.47	1.46	1.33
14	B	813	CLA	O2A-CGA	4.47	1.46	1.33
14	A	815	CLA	CHD-C1D	4.47	1.47	1.38
14	cA	813	CLA	O2A-CGA	4.46	1.45	1.30
14	cL	205	CLA	CHD-C1D	4.46	1.47	1.38
14	cB	838	CLA	O2A-CGA	4.46	1.46	1.33
14	bA	815	CLA	CHD-C1D	4.46	1.47	1.38
17	B	842	BCR	C17-C18	4.46	1.41	1.35
17	bJ	103	BCR	C10-C9	4.46	1.41	1.35
14	B	805	CLA	CHD-C1D	4.46	1.47	1.38
14	cA	815	CLA	CHD-C1D	4.46	1.47	1.38
17	J	103	BCR	C10-C9	4.46	1.41	1.35
14	bF	201	CLA	O2A-CGA	4.46	1.46	1.33
14	bB	818	CLA	CHD-C1D	4.46	1.47	1.38
14	cB	806	CLA	CHD-C1D	4.46	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bB	837	CLA	O2A-CGA	4.46	1.46	1.33
14	B	837	CLA	O2A-CGA	4.46	1.46	1.33
17	cA	849	BCR	C10-C9	4.45	1.41	1.35
17	cB	843	BCR	C17-C18	4.45	1.41	1.35
14	A	821	CLA	CHD-C1D	4.45	1.47	1.38
14	bB	815	CLA	O2A-CGA	4.45	1.46	1.33
17	M	101	BCR	C21-C22	4.45	1.41	1.35
17	cJ	103	BCR	C10-C9	4.45	1.41	1.35
14	A	810	CLA	CHD-C1D	4.45	1.47	1.38
14	B	815	CLA	O2A-CGA	4.45	1.46	1.33
17	cB	842	BCR	C14-C13	4.45	1.41	1.35
14	cB	814	CLA	O2A-CGA	4.45	1.46	1.33
14	bA	840	CLA	CHD-C1D	4.45	1.47	1.38
17	bB	850	BCR	C21-C22	4.45	1.41	1.35
14	bB	837	CLA	CHD-C1D	4.45	1.47	1.38
14	B	818	CLA	CHD-C1D	4.45	1.47	1.38
17	J	103	BCR	C17-C18	4.45	1.41	1.35
14	cF	201	CLA	O2A-CGA	4.45	1.46	1.33
17	bB	841	BCR	C14-C13	4.45	1.41	1.35
14	bA	821	CLA	CHD-C1D	4.45	1.47	1.38
14	cB	828	CLA	O2A-CGA	4.45	1.46	1.33
14	bB	805	CLA	CHD-C1D	4.44	1.47	1.38
14	cB	816	CLA	O2A-CGA	4.44	1.46	1.33
14	bA	810	CLA	CHD-C1D	4.44	1.47	1.38
14	cB	819	CLA	CHD-C1D	4.44	1.47	1.38
17	B	841	BCR	C14-C13	4.44	1.41	1.35
14	bA	825	CLA	CHC-C1C	4.44	1.47	1.38
14	L	204	CLA	CHD-C1D	4.44	1.47	1.38
14	cB	817	CLA	CHD-C1D	4.44	1.47	1.38
17	cJ	103	BCR	C17-C18	4.44	1.41	1.35
14	B	812	CLA	O2A-CGA	4.44	1.46	1.33
14	cB	813	CLA	O2A-CGA	4.44	1.46	1.33
14	cA	835	CLA	CHD-C1D	4.44	1.47	1.38
14	A	808	CLA	O2A-CGA	4.44	1.45	1.30
14	A	825	CLA	CHC-C1C	4.44	1.47	1.38
14	cA	808	CLA	O2A-CGA	4.43	1.45	1.30
14	cA	810	CLA	CHD-C1D	4.43	1.47	1.38
14	bA	808	CLA	O2A-CGA	4.43	1.45	1.30
14	bL	204	CLA	CHD-C1D	4.43	1.47	1.38
17	B	841	BCR	C17-C18	4.43	1.41	1.35
14	A	805	CLA	O2A-CGA	4.43	1.46	1.33
14	cA	805	CLA	O2A-CGA	4.43	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	840	CLA	CHD-C1D	4.43	1.47	1.38
17	cB	842	BCR	C17-C18	4.43	1.41	1.35
14	cB	825	CLA	CHD-C1D	4.43	1.47	1.38
14	cA	821	CLA	CHD-C1D	4.43	1.47	1.38
14	bB	816	CLA	CHD-C1D	4.43	1.47	1.38
14	bJ	101	CLA	CHD-C1D	4.43	1.47	1.38
14	bB	812	CLA	O2A-CGA	4.43	1.46	1.33
14	bB	827	CLA	O2A-CGA	4.43	1.46	1.33
14	B	824	CLA	CHD-C1D	4.42	1.47	1.38
14	bB	803	CLA	C1D-ND	4.42	1.43	1.37
14	J	101	CLA	CHD-C1D	4.42	1.47	1.38
14	cA	839	CLA	O2A-CGA	4.42	1.46	1.33
17	cA	845	BCR	C17-C18	4.42	1.41	1.35
14	bB	824	CLA	CHD-C1D	4.42	1.47	1.38
14	cA	825	CLA	CHC-C1C	4.42	1.47	1.38
17	cB	851	BCR	C14-C13	4.42	1.41	1.35
17	cM	101	BCR	C21-C22	4.42	1.41	1.35
14	bA	805	CLA	O2A-CGA	4.42	1.46	1.33
14	cA	840	CLA	CHD-C1D	4.42	1.47	1.38
14	B	827	CLA	O2A-CGA	4.42	1.46	1.33
14	cA	832	CLA	C1D-ND	4.42	1.43	1.37
17	bB	841	BCR	C17-C18	4.42	1.41	1.35
17	bM	101	BCR	C21-C22	4.42	1.41	1.35
14	bA	832	CLA	C1D-ND	4.42	1.43	1.37
14	B	816	CLA	CHD-C1D	4.42	1.47	1.38
14	bA	814	CLA	CHD-C1D	4.42	1.47	1.38
14	bA	839	CLA	O2A-CGA	4.42	1.46	1.33
14	cB	826	CLA	O2A-CGA	4.42	1.46	1.33
14	A	832	CLA	C1D-ND	4.42	1.43	1.37
17	L	206	BCR	C14-C13	4.42	1.41	1.35
14	A	839	CLA	O2A-CGA	4.42	1.46	1.33
17	L	205	BCR	C14-C13	4.41	1.41	1.35
14	A	817	CLA	O2A-CGA	4.41	1.46	1.33
14	B	825	CLA	O2A-CGA	4.41	1.46	1.33
14	bB	825	CLA	O2A-CGA	4.41	1.46	1.33
14	cJ	101	CLA	CHD-C1D	4.41	1.47	1.38
13	bA	801	CL0	CHC-C1C	4.41	1.47	1.38
17	bA	845	BCR	C17-C18	4.41	1.41	1.35
17	cL	207	BCR	C14-C13	4.41	1.41	1.35
14	bB	813	CLA	CHD-C1D	4.41	1.46	1.38
14	cB	814	CLA	CHD-C1D	4.41	1.46	1.38
14	bA	817	CLA	O2A-CGA	4.41	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	bJ	103	BCR	C17-C18	4.41	1.41	1.35
14	B	813	CLA	CHD-C1D	4.41	1.46	1.38
14	cJ	102	CLA	CHD-C1D	4.41	1.46	1.38
13	cA	801	CL0	CHC-C1C	4.41	1.47	1.38
14	cA	816	CLA	CHD-C1D	4.40	1.46	1.38
14	cA	817	CLA	O2A-CGA	4.40	1.46	1.33
14	bA	804	CLA	CHD-C1D	4.40	1.46	1.38
14	cA	824	CLA	O2A-CGA	4.40	1.46	1.33
14	bA	816	CLA	CHD-C1D	4.40	1.46	1.38
14	A	814	CLA	CHD-C1D	4.40	1.46	1.38
17	A	845	BCR	C17-C18	4.40	1.41	1.35
14	A	816	CLA	CHD-C1D	4.40	1.46	1.38
14	bA	812	CLA	CHD-C1D	4.40	1.46	1.38
14	A	812	CLA	CHD-C1D	4.40	1.46	1.38
14	J	102	CLA	CHD-C1D	4.40	1.46	1.38
14	A	817	CLA	CHD-C1D	4.40	1.46	1.38
13	A	801	CL0	CHC-C1C	4.40	1.47	1.38
17	bB	842	BCR	C17-C18	4.40	1.41	1.35
14	B	830	CLA	CHD-C1D	4.40	1.46	1.38
14	bJ	102	CLA	CHD-C1D	4.40	1.46	1.38
17	bA	849	BCR	C10-C9	4.40	1.41	1.35
14	cA	830	CLA	CHC-C1C	4.40	1.47	1.38
14	bA	817	CLA	CHD-C1D	4.40	1.46	1.38
14	bA	830	CLA	CHC-C1C	4.40	1.47	1.38
14	bB	830	CLA	CHD-C1D	4.40	1.46	1.38
14	bB	802	CLA	CHC-C1C	4.39	1.47	1.38
14	A	823	CLA	CHD-C1D	4.39	1.46	1.38
14	cA	828	CLA	CHC-C1C	4.39	1.47	1.38
14	cB	831	CLA	CHD-C1D	4.39	1.46	1.38
14	cA	812	CLA	CHD-C1D	4.39	1.46	1.38
14	cA	814	CLA	CHD-C1D	4.39	1.46	1.38
14	A	837	CLA	C1D-ND	4.39	1.43	1.37
14	bA	807	CLA	CHD-C1D	4.39	1.46	1.38
14	cA	804	CLA	CHD-C1D	4.39	1.46	1.38
14	cB	832	CLA	O2A-CGA	4.38	1.46	1.33
14	B	831	CLA	O2A-CGA	4.38	1.46	1.33
14	bB	831	CLA	O2A-CGA	4.38	1.46	1.33
14	bA	806	CLA	O2A-CGA	4.38	1.46	1.33
17	A	849	BCR	C10-C9	4.38	1.41	1.35
14	cB	801	CLA	CHD-C1D	4.38	1.46	1.38
14	bA	824	CLA	O2A-CGA	4.38	1.46	1.33
13	cA	801	CL0	O2A-CGA	4.38	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	bL	205	BCR	C14-C13	4.38	1.41	1.35
14	A	806	CLA	O2A-CGA	4.38	1.46	1.33
14	A	824	CLA	O2A-CGA	4.38	1.46	1.33
14	A	804	CLA	CHD-C1D	4.38	1.46	1.38
14	cB	834	CLA	CHD-C1D	4.38	1.46	1.38
14	cA	817	CLA	CHD-C1D	4.38	1.46	1.38
14	B	802	CLA	CHC-C1C	4.38	1.47	1.38
17	cL	206	BCR	C14-C13	4.38	1.41	1.35
17	bL	206	BCR	C14-C13	4.38	1.41	1.35
14	bB	833	CLA	CHD-C1D	4.38	1.46	1.38
14	cA	806	CLA	O2A-CGA	4.38	1.46	1.33
14	B	833	CLA	CHD-C1D	4.37	1.46	1.38
17	A	847	BCR	C17-C18	4.37	1.41	1.35
14	bA	837	CLA	C1D-ND	4.37	1.43	1.37
14	bB	851	CLA	CHD-C1D	4.37	1.46	1.38
14	A	830	CLA	CHC-C1C	4.37	1.47	1.38
14	bA	828	CLA	CHC-C1C	4.37	1.47	1.38
14	cA	823	CLA	CHD-C1D	4.37	1.46	1.38
14	bB	819	CLA	O2A-CGA	4.37	1.46	1.33
14	cB	802	CLA	O2A-CGA	4.37	1.46	1.33
17	cB	847	BCR	C17-C18	4.37	1.41	1.35
13	bA	801	CL0	O2A-CGA	4.37	1.46	1.33
14	B	819	CLA	O2A-CGA	4.37	1.46	1.33
14	cB	830	CLA	CHD-C1D	4.37	1.46	1.38
14	bA	840	CLA	O2A-CGA	4.37	1.46	1.33
14	bB	829	CLA	CHD-C1D	4.37	1.46	1.38
14	bB	820	CLA	CHD-C4C	4.37	1.49	1.39
17	L	206	BCR	C10-C9	4.37	1.41	1.35
17	M	101	BCR	C14-C13	4.37	1.41	1.35
14	cB	820	CLA	O2A-CGA	4.37	1.46	1.33
17	cA	846	BCR	C17-C18	4.37	1.41	1.35
14	A	840	CLA	O2A-CGA	4.37	1.46	1.33
14	cA	811	CLA	CHD-C1D	4.37	1.46	1.38
14	bA	823	CLA	CHD-C1D	4.37	1.46	1.38
14	cA	807	CLA	CHD-C1D	4.37	1.46	1.38
14	A	807	CLA	CHD-C1D	4.36	1.46	1.38
17	bA	849	BCR	C14-C13	4.36	1.41	1.35
14	cA	804	CLA	O2A-CGA	4.36	1.46	1.33
14	cB	803	CLA	CHC-C1C	4.36	1.47	1.38
14	B	851	CLA	CHD-C1D	4.36	1.46	1.38
14	B	801	CLA	O2A-CGA	4.36	1.46	1.33
14	bX	201	CLA	CHD-C1D	4.36	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	bL	206	BCR	C10-C9	4.36	1.41	1.35
14	bA	832	CLA	CHC-C1C	4.36	1.47	1.38
14	cA	830	CLA	O2A-CGA	4.36	1.46	1.33
14	A	805	CLA	CHD-C1D	4.36	1.46	1.38
14	A	830	CLA	O2A-CGA	4.36	1.46	1.33
14	bA	830	CLA	O2A-CGA	4.36	1.46	1.33
14	bA	805	CLA	CHD-C1D	4.36	1.46	1.38
14	A	804	CLA	O2A-CGA	4.36	1.46	1.33
14	bA	804	CLA	O2A-CGA	4.36	1.46	1.33
14	A	828	CLA	CHC-C1C	4.36	1.47	1.38
14	cA	840	CLA	O2A-CGA	4.36	1.46	1.33
14	cA	832	CLA	CHC-C1C	4.36	1.47	1.38
14	bB	801	CLA	O2A-CGA	4.36	1.46	1.33
17	A	846	BCR	C17-C18	4.36	1.41	1.35
14	bA	827	CLA	O2A-CGA	4.36	1.46	1.33
17	bA	846	BCR	C17-C18	4.36	1.41	1.35
14	cA	838	CLA	CHC-C1C	4.36	1.47	1.38
14	cA	827	CLA	O2A-CGA	4.36	1.46	1.33
14	A	832	CLA	CHC-C1C	4.36	1.47	1.38
14	B	803	CLA	O2A-CGA	4.35	1.46	1.33
17	cL	207	BCR	C10-C9	4.35	1.41	1.35
14	A	827	CLA	O2A-CGA	4.35	1.46	1.33
14	cA	805	CLA	CHD-C1D	4.35	1.46	1.38
14	cA	837	CLA	C1D-ND	4.35	1.43	1.37
17	bB	843	BCR	C10-C9	4.35	1.41	1.35
13	A	801	CL0	O2A-CGA	4.35	1.46	1.33
14	A	803	CLA	CHD-C1D	4.35	1.46	1.38
14	bL	204	CLA	O2A-CGA	4.35	1.46	1.33
17	A	849	BCR	C14-C13	4.35	1.41	1.35
14	X	201	CLA	CHD-C1D	4.35	1.46	1.38
17	cA	847	BCR	C17-C18	4.35	1.41	1.35
14	bB	803	CLA	O2A-CGA	4.35	1.46	1.33
17	B	846	BCR	C17-C18	4.35	1.41	1.35
14	cA	809	CLA	CHD-C1D	4.35	1.46	1.38
14	bB	829	CLA	CHD-C4C	4.35	1.49	1.39
14	cA	820	CLA	CHD-C4C	4.35	1.49	1.39
14	A	811	CLA	CHD-C1D	4.35	1.46	1.38
14	bA	809	CLA	CHD-C1D	4.34	1.46	1.38
14	B	829	CLA	CHD-C4C	4.34	1.49	1.39
14	B	829	CLA	CHD-C1D	4.34	1.46	1.38
14	B	827	CLA	CHD-C1D	4.34	1.46	1.38
14	bA	833	CLA	CHC-C1C	4.34	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bB	810	CLA	CHD-C4C	4.34	1.49	1.39
14	cB	804	CLA	O2A-CGA	4.34	1.46	1.33
14	cL	205	CLA	O2A-CGA	4.34	1.46	1.33
14	bB	831	CLA	CHD-C4C	4.34	1.49	1.39
14	B	821	CLA	CHD-C1D	4.34	1.46	1.38
14	bA	811	CLA	CHD-C1D	4.34	1.46	1.38
14	bB	827	CLA	CHD-C1D	4.34	1.46	1.38
14	bA	838	CLA	CHC-C1C	4.34	1.47	1.38
14	cA	803	CLA	CHD-C1D	4.34	1.46	1.38
14	B	810	CLA	CHD-C4C	4.34	1.49	1.39
17	bA	847	BCR	C17-C18	4.34	1.41	1.35
17	cA	849	BCR	C14-C13	4.34	1.41	1.35
14	cB	821	CLA	CHD-C4C	4.34	1.49	1.39
14	bB	808	CLA	CHC-C1C	4.34	1.47	1.38
14	B	811	CLA	CHD-C1D	4.34	1.46	1.38
14	cB	832	CLA	CHD-C4C	4.34	1.49	1.39
14	A	838	CLA	CHC-C1C	4.34	1.47	1.38
17	cM	101	BCR	C14-C13	4.33	1.41	1.35
14	B	820	CLA	CHD-C4C	4.33	1.49	1.39
14	cB	828	CLA	CHD-C1D	4.33	1.46	1.38
14	bB	821	CLA	CHD-C1D	4.33	1.46	1.38
14	cL	202	CLA	C1D-ND	4.33	1.43	1.37
14	bA	820	CLA	CHD-C4C	4.33	1.49	1.39
14	A	833	CLA	CHC-C1C	4.33	1.47	1.38
14	bA	803	CLA	CHD-C1D	4.33	1.46	1.38
14	cA	833	CLA	CHC-C1C	4.33	1.47	1.38
14	B	831	CLA	CHD-C4C	4.33	1.49	1.39
14	cB	811	CLA	CHD-C4C	4.33	1.49	1.39
14	cB	812	CLA	CHD-C1D	4.33	1.46	1.38
14	cB	830	CLA	CHD-C4C	4.33	1.49	1.39
14	bB	811	CLA	CHD-C1D	4.33	1.46	1.38
14	L	204	CLA	O2A-CGA	4.33	1.46	1.33
14	bA	823	CLA	CHD-C4C	4.33	1.49	1.39
14	bB	814	CLA	CHD-C4C	4.33	1.49	1.39
17	bM	101	BCR	C14-C13	4.32	1.41	1.35
14	cB	822	CLA	CHD-C4C	4.32	1.49	1.39
14	cB	821	CLA	CHD-C1D	4.32	1.46	1.38
14	A	820	CLA	CHD-C4C	4.32	1.49	1.39
14	bB	816	CLA	CHD-C4C	4.32	1.49	1.39
14	bB	822	CLA	CHD-C1D	4.32	1.46	1.38
14	cB	822	CLA	CHD-C1D	4.32	1.46	1.38
14	cA	825	CLA	O2A-CGA	4.32	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	822	CLA	CHD-C1D	4.32	1.46	1.38
14	B	820	CLA	CHD-C1D	4.32	1.46	1.38
14	A	822	CLA	CHD-C4C	4.32	1.49	1.39
14	cX	201	CLA	CHD-C1D	4.32	1.46	1.38
14	A	809	CLA	CHD-C1D	4.32	1.46	1.38
14	B	814	CLA	CHD-C4C	4.32	1.49	1.39
14	bB	830	CLA	CHD-C4C	4.32	1.49	1.39
14	cA	818	CLA	CHD-C1D	4.32	1.46	1.38
14	B	808	CLA	CHC-C1C	4.32	1.47	1.38
14	cB	815	CLA	CHD-C4C	4.32	1.49	1.39
14	cB	809	CLA	CHC-C1C	4.32	1.47	1.38
14	A	825	CLA	O2A-CGA	4.32	1.46	1.33
14	bB	821	CLA	CHD-C4C	4.32	1.49	1.39
14	cA	829	CLA	O2A-CGA	4.32	1.46	1.33
17	bB	846	BCR	C17-C18	4.32	1.41	1.35
14	cA	823	CLA	CHD-C4C	4.31	1.49	1.39
14	A	818	CLA	CHD-C4C	4.31	1.49	1.39
14	B	830	CLA	CHD-C4C	4.31	1.49	1.39
14	B	821	CLA	CHD-C4C	4.31	1.49	1.39
17	cB	851	BCR	C10-C9	4.31	1.41	1.35
14	B	816	CLA	CHD-C4C	4.31	1.49	1.39
14	B	815	CLA	CHD-C1D	4.31	1.46	1.38
14	bA	818	CLA	CHD-C1D	4.31	1.46	1.38
14	bB	820	CLA	CHD-C1D	4.31	1.46	1.38
14	cB	823	CLA	CHD-C1D	4.31	1.46	1.38
14	cA	836	CLA	C1D-ND	4.31	1.43	1.37
14	A	829	CLA	O2A-CGA	4.31	1.45	1.33
14	A	818	CLA	CHD-C1D	4.31	1.46	1.38
14	bB	815	CLA	CHD-C1D	4.31	1.46	1.38
14	bB	803	CLA	CHC-C1C	4.31	1.47	1.38
14	cB	831	CLA	CHD-C4C	4.31	1.49	1.39
14	bA	836	CLA	C1D-ND	4.31	1.43	1.37
14	cB	816	CLA	CHD-C1D	4.31	1.46	1.38
14	bA	822	CLA	CHD-C4C	4.31	1.49	1.39
14	bA	828	CLA	CHD-C1D	4.31	1.46	1.38
14	A	831	CLA	O2A-CGA	4.31	1.45	1.33
14	bA	829	CLA	O2A-CGA	4.31	1.45	1.33
17	B	843	BCR	C10-C9	4.31	1.41	1.35
14	cA	818	CLA	CHD-C4C	4.30	1.49	1.39
14	A	833	CLA	CHD-C1D	4.30	1.46	1.38
17	I	101	BCR	C10-C9	4.30	1.41	1.35
14	cA	815	CLA	CHD-C4C	4.30	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	847	BCR	C14-C13	4.30	1.41	1.35
14	cA	822	CLA	CHD-C4C	4.30	1.49	1.39
14	bL	201	CLA	C1D-ND	4.30	1.43	1.37
14	cB	829	CLA	C1D-ND	4.30	1.43	1.37
14	bA	825	CLA	O2A-CGA	4.30	1.45	1.33
14	cA	831	CLA	O2A-CGA	4.30	1.45	1.33
14	cA	833	CLA	CHD-C1D	4.30	1.46	1.38
14	bA	833	CLA	CHD-C1D	4.30	1.46	1.38
14	cB	817	CLA	CHD-C4C	4.30	1.49	1.39
14	bB	828	CLA	C1D-ND	4.30	1.43	1.37
14	cA	834	CLA	CHD-C4C	4.30	1.49	1.39
14	bA	815	CLA	CHD-C4C	4.30	1.49	1.39
14	bA	818	CLA	CHD-C4C	4.30	1.49	1.39
14	cB	827	CLA	O2A-CGA	4.30	1.45	1.33
14	B	828	CLA	C1D-ND	4.30	1.43	1.37
14	bA	807	CLA	CHD-C4C	4.30	1.49	1.39
14	bA	818	CLA	O2A-CGA	4.30	1.45	1.33
14	bA	831	CLA	O2A-CGA	4.30	1.45	1.33
17	bB	844	BCR	C17-C18	4.29	1.41	1.35
14	B	836	CLA	CHD-C1D	4.29	1.46	1.38
14	A	836	CLA	C1D-ND	4.29	1.43	1.37
14	cB	804	CLA	CHC-C1C	4.29	1.47	1.38
14	cA	828	CLA	CHD-C1D	4.29	1.46	1.38
14	bB	826	CLA	O2A-CGA	4.29	1.45	1.33
14	B	826	CLA	O2A-CGA	4.29	1.45	1.33
17	cI	101	BCR	C10-C9	4.29	1.41	1.35
14	cL	203	CLA	CHD-C1D	4.29	1.46	1.38
14	bB	817	CLA	O2A-CGA	4.29	1.45	1.33
14	A	841	CLA	C1B-NB	-4.29	1.32	1.37
14	B	813	CLA	CHD-C4C	4.29	1.49	1.39
17	bB	850	BCR	C10-C9	4.29	1.41	1.35
14	A	834	CLA	CHD-C4C	4.29	1.49	1.39
14	A	815	CLA	CHD-C4C	4.29	1.49	1.39
14	bA	834	CLA	CHD-C4C	4.29	1.49	1.39
14	bB	807	CLA	CHD-C1D	4.29	1.46	1.38
17	B	850	BCR	C10-C9	4.29	1.41	1.35
14	cB	814	CLA	CHD-C4C	4.28	1.49	1.39
14	B	803	CLA	CHC-C1C	4.28	1.47	1.38
17	bI	101	BCR	C10-C9	4.28	1.41	1.35
14	A	828	CLA	CHD-C1D	4.28	1.46	1.38
17	bB	847	BCR	C17-C18	4.28	1.41	1.35
17	cB	848	BCR	C14-C13	4.28	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	cB	848	BCR	C17-C18	4.28	1.41	1.35
14	A	823	CLA	CHD-C4C	4.28	1.49	1.39
14	L	202	CLA	CHD-C1D	4.28	1.46	1.38
14	L	201	CLA	C1D-ND	4.28	1.43	1.37
14	cA	818	CLA	O2A-CGA	4.28	1.45	1.33
14	A	818	CLA	O2A-CGA	4.27	1.45	1.33
14	bL	203	CLA	C1D-ND	4.27	1.43	1.37
14	A	807	CLA	CHD-C4C	4.27	1.49	1.39
17	B	844	BCR	C17-C18	4.27	1.41	1.35
14	cA	807	CLA	CHD-C4C	4.27	1.49	1.39
14	cB	820	CLA	CHD-C1D	4.27	1.46	1.38
17	cB	845	BCR	C17-C18	4.27	1.41	1.35
14	cB	818	CLA	O2A-CGA	4.27	1.45	1.33
14	cB	808	CLA	CHD-C1D	4.27	1.46	1.38
14	bB	836	CLA	CHD-C1D	4.27	1.46	1.38
14	bB	813	CLA	CHD-C4C	4.27	1.49	1.39
17	cA	849	BCR	C17-C18	4.27	1.41	1.35
14	B	807	CLA	CHD-C1D	4.27	1.46	1.38
14	B	819	CLA	CHD-C1D	4.27	1.46	1.38
17	cL	206	BCR	C10-C9	4.27	1.41	1.35
14	bA	812	CLA	CHD-C4C	4.27	1.49	1.39
14	cA	841	CLA	C1B-NB	-4.27	1.32	1.37
14	L	203	CLA	C1D-ND	4.27	1.43	1.37
14	A	812	CLA	CHD-C4C	4.27	1.49	1.39
14	A	821	CLA	CHD-C4C	4.27	1.49	1.39
17	bB	847	BCR	C14-C13	4.27	1.41	1.35
14	cA	812	CLA	CHD-C4C	4.27	1.49	1.39
14	bB	819	CLA	CHD-C1D	4.26	1.46	1.38
14	L	203	CLA	CHC-C1C	4.26	1.47	1.38
14	bL	202	CLA	CHD-C1D	4.26	1.46	1.38
17	L	205	BCR	C10-C9	4.26	1.41	1.35
14	bJ	101	CLA	CHD-C4C	4.26	1.49	1.39
14	B	817	CLA	O2A-CGA	4.26	1.45	1.33
14	cA	821	CLA	CHD-C4C	4.26	1.49	1.39
14	cL	204	CLA	CHC-C1C	4.26	1.47	1.38
14	J	101	CLA	CHD-C4C	4.26	1.49	1.39
14	cJ	101	CLA	CHD-C4C	4.26	1.49	1.39
17	A	849	BCR	C17-C18	4.26	1.41	1.35
14	cA	819	CLA	CHD-C4C	4.26	1.49	1.39
17	bL	205	BCR	C10-C9	4.26	1.41	1.35
14	B	834	CLA	CHD-C4C	4.26	1.48	1.39
14	bL	203	CLA	CHC-C1C	4.25	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cB	835	CLA	CHD-C4C	4.25	1.48	1.39
14	bB	812	CLA	CHC-C4B	4.25	1.48	1.39
14	cB	837	CLA	CHD-C1D	4.25	1.46	1.38
14	B	812	CLA	CHC-C4B	4.25	1.48	1.39
14	cL	204	CLA	C1D-ND	4.25	1.43	1.37
14	bB	834	CLA	CHD-C4C	4.25	1.48	1.39
14	B	837	CLA	CHD-C4C	4.25	1.48	1.39
14	cB	813	CLA	CHC-C4B	4.25	1.48	1.39
17	bM	101	BCR	C17-C18	4.25	1.41	1.35
14	bA	819	CLA	CHD-C4C	4.25	1.48	1.39
14	bB	802	CLA	O2A-CGA	4.25	1.45	1.33
17	cM	101	BCR	C17-C18	4.25	1.41	1.35
14	bA	835	CLA	CHD-C4C	4.25	1.48	1.39
14	bB	837	CLA	CHD-C4C	4.24	1.48	1.39
14	cB	838	CLA	CHD-C4C	4.24	1.48	1.39
14	B	802	CLA	O2A-CGA	4.24	1.45	1.33
14	cB	826	CLA	CHD-C1D	4.24	1.46	1.38
14	A	819	CLA	CHD-C4C	4.24	1.48	1.39
17	bA	849	BCR	C17-C18	4.24	1.41	1.35
17	cA	846	BCR	C10-C9	4.24	1.41	1.35
17	bA	846	BCR	C10-C9	4.24	1.41	1.35
14	bB	825	CLA	CHD-C1D	4.24	1.46	1.38
14	bA	841	CLA	C1B-NB	-4.24	1.32	1.37
14	bA	810	CLA	CHD-C4C	4.24	1.48	1.39
14	B	825	CLA	CHD-C1D	4.24	1.46	1.38
14	A	810	CLA	CHD-C4C	4.24	1.48	1.39
17	A	846	BCR	C10-C9	4.24	1.41	1.35
14	cA	835	CLA	CHD-C4C	4.24	1.48	1.39
14	bA	821	CLA	CHD-C4C	4.24	1.48	1.39
14	cA	810	CLA	CHD-C4C	4.23	1.48	1.39
14	B	809	CLA	C1B-NB	-4.23	1.32	1.37
14	cA	852	CLA	CHC-C1C	4.23	1.47	1.38
14	cB	807	CLA	O2A-CGA	4.23	1.45	1.33
17	cB	844	BCR	C10-C9	4.23	1.41	1.35
14	bB	805	CLA	CHD-C4C	4.23	1.48	1.39
14	bB	833	CLA	CHD-C4C	4.23	1.48	1.39
14	cB	803	CLA	O2A-CGA	4.23	1.45	1.33
14	B	805	CLA	CHD-C4C	4.23	1.48	1.39
14	cA	839	CLA	CHD-C1D	4.23	1.46	1.38
14	cB	834	CLA	CHD-C4C	4.23	1.48	1.39
14	bA	828	CLA	O2A-CGA	4.23	1.45	1.33
14	A	839	CLA	CHD-C1D	4.23	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	807	CLA	CHC-C1C	4.23	1.47	1.38
14	A	835	CLA	CHD-C4C	4.23	1.48	1.39
14	A	852	CLA	CHC-C1C	4.23	1.47	1.38
14	A	828	CLA	O2A-CGA	4.22	1.45	1.33
14	bB	809	CLA	C1B-NB	-4.22	1.32	1.37
14	B	835	CLA	CHD-C1D	4.22	1.46	1.38
14	bA	852	CLA	CHC-C1C	4.22	1.47	1.38
14	bB	817	CLA	CHD-C1D	4.22	1.46	1.38
17	B	847	BCR	C17-C18	4.22	1.41	1.35
14	B	817	CLA	CHD-C1D	4.22	1.46	1.38
14	B	806	CLA	O2A-CGA	4.22	1.45	1.33
14	bB	807	CLA	CHC-C1C	4.22	1.47	1.38
14	bB	806	CLA	O2A-CGA	4.22	1.45	1.33
14	B	833	CLA	CHD-C4C	4.22	1.48	1.39
17	A	847	BCR	C14-C13	4.22	1.41	1.35
14	bB	835	CLA	CHD-C1D	4.22	1.46	1.38
14	cB	836	CLA	CHD-C1D	4.22	1.46	1.38
14	cB	808	CLA	CHC-C1C	4.22	1.47	1.38
14	bA	839	CLA	CHD-C1D	4.22	1.46	1.38
14	cB	837	CLA	CHD-C4C	4.21	1.48	1.39
14	bA	841	CLA	C1D-ND	4.21	1.43	1.37
14	bB	836	CLA	CHD-C4C	4.21	1.48	1.39
17	bA	847	BCR	C14-C13	4.21	1.41	1.35
14	cB	806	CLA	CHD-C4C	4.21	1.48	1.39
14	A	838	CLA	C1D-ND	4.21	1.43	1.37
14	B	836	CLA	CHD-C4C	4.21	1.48	1.39
14	cB	818	CLA	CHD-C1D	4.21	1.46	1.38
17	cA	847	BCR	C14-C13	4.21	1.41	1.35
14	cA	838	CLA	C1D-ND	4.21	1.43	1.37
14	bB	832	CLA	CHD-C1D	4.20	1.46	1.38
14	bB	811	CLA	CHD-C4C	4.20	1.48	1.39
17	M	101	BCR	C17-C18	4.20	1.41	1.35
14	cB	829	CLA	O2A-CGA	4.20	1.45	1.33
14	cA	841	CLA	C1D-ND	4.20	1.43	1.37
17	cI	101	BCR	C14-C13	4.20	1.41	1.35
14	bB	828	CLA	O2A-CGA	4.20	1.45	1.33
14	cB	810	CLA	C1B-NB	-4.20	1.32	1.37
14	cA	828	CLA	O2A-CGA	4.20	1.45	1.33
14	bB	806	CLA	CHD-C1D	4.20	1.46	1.38
17	cB	851	BCR	C17-C18	4.20	1.41	1.35
14	cB	833	CLA	CHD-C1D	4.20	1.46	1.38
14	cL	202	CLA	CHC-C1C	4.20	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	L	203	CLA	O2A-CGA	4.20	1.45	1.33
14	bA	829	CLA	CHD-C1D	4.20	1.46	1.38
14	bA	811	CLA	CHD-C4C	4.20	1.48	1.39
14	cA	840	CLA	CHD-C4C	4.20	1.48	1.39
14	B	811	CLA	CHD-C4C	4.20	1.48	1.39
14	cB	807	CLA	CHD-C1D	4.20	1.46	1.38
17	B	844	BCR	C14-C13	4.19	1.41	1.35
14	bL	203	CLA	O2A-CGA	4.19	1.45	1.33
14	A	829	CLA	CHD-C1D	4.19	1.46	1.38
14	bA	827	CLA	CHD-C4C	4.19	1.48	1.39
14	B	828	CLA	O2A-CGA	4.19	1.45	1.33
14	bB	815	CLA	CHD-C4C	4.19	1.48	1.39
14	A	804	CLA	CHD-C4C	4.19	1.48	1.39
14	cA	813	CLA	CHD-C1D	4.19	1.46	1.38
14	cA	829	CLA	CHD-C1D	4.19	1.46	1.38
14	cA	827	CLA	CHD-C1D	4.19	1.46	1.38
14	bA	827	CLA	CHD-C1D	4.19	1.46	1.38
14	cB	812	CLA	CHD-C4C	4.19	1.48	1.39
14	A	840	CLA	CHD-C4C	4.19	1.48	1.39
14	B	806	CLA	CHD-C1D	4.19	1.46	1.38
14	L	201	CLA	CHC-C1C	4.19	1.47	1.38
14	A	811	CLA	CHD-C4C	4.19	1.48	1.39
14	bA	840	CLA	CHD-C4C	4.19	1.48	1.39
14	bB	806	CLA	CHD-C4C	4.19	1.48	1.39
14	bA	831	CLA	CHD-C1D	4.19	1.46	1.38
14	cJ	102	CLA	CHD-C4C	4.19	1.48	1.39
14	bA	813	CLA	CHD-C1D	4.18	1.46	1.38
14	cA	828	CLA	C3D-C2D	4.18	1.50	1.39
14	J	102	CLA	CHD-C4C	4.18	1.48	1.39
14	bA	804	CLA	CHD-C4C	4.18	1.48	1.39
14	cB	816	CLA	CHD-C4C	4.18	1.48	1.39
14	B	801	CLA	C1D-ND	4.18	1.42	1.37
14	cB	802	CLA	C1D-ND	4.18	1.42	1.37
17	bB	850	BCR	C17-C18	4.18	1.41	1.35
14	bB	818	CLA	CHD-C4C	4.18	1.48	1.39
14	B	832	CLA	CHD-C1D	4.18	1.46	1.38
14	cB	807	CLA	CHD-C4C	4.18	1.48	1.39
14	bL	201	CLA	CHC-C1C	4.18	1.47	1.38
14	A	813	CLA	CHD-C1D	4.18	1.46	1.38
14	cA	804	CLA	CHD-C4C	4.18	1.48	1.39
14	bA	838	CLA	C1D-ND	4.18	1.42	1.37
14	cB	825	CLA	CHD-C4C	4.18	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	849	CLA	CHD-C4C	4.18	1.48	1.39
14	A	831	CLA	CHD-C1D	4.18	1.46	1.38
17	B	847	BCR	C21-C22	4.18	1.41	1.35
14	B	806	CLA	CHD-C4C	4.18	1.48	1.39
14	B	818	CLA	CHD-C4C	4.18	1.48	1.39
14	B	851	CLA	CHD-C4C	4.18	1.48	1.39
14	cA	831	CLA	CHD-C1D	4.18	1.46	1.38
17	I	101	BCR	C14-C13	4.18	1.41	1.35
14	bJ	102	CLA	CHD-C4C	4.18	1.48	1.39
14	cB	850	CLA	CHD-C4C	4.18	1.48	1.39
14	bB	801	CLA	C1D-ND	4.18	1.42	1.37
14	cB	805	CLA	CHD-C1D	4.18	1.46	1.38
14	cX	201	CLA	CHD-C4C	4.18	1.48	1.39
14	A	827	CLA	CHD-C1D	4.18	1.46	1.38
14	cL	204	CLA	O2A-CGA	4.18	1.45	1.33
14	A	841	CLA	C1D-ND	4.18	1.42	1.37
14	bB	824	CLA	CHD-C4C	4.18	1.48	1.39
14	B	815	CLA	CHD-C4C	4.17	1.48	1.39
14	cB	801	CLA	CHD-C4C	4.17	1.48	1.39
17	L	206	BCR	C21-C22	4.17	1.41	1.35
14	bB	851	CLA	CHD-C4C	4.17	1.48	1.39
14	X	201	CLA	CHD-C4C	4.17	1.48	1.39
17	bI	101	BCR	C14-C13	4.17	1.41	1.35
14	cA	824	CLA	CHD-C1D	4.17	1.46	1.38
14	B	824	CLA	CHD-C4C	4.17	1.48	1.39
14	bA	828	CLA	C3D-C2D	4.17	1.50	1.39
14	cA	827	CLA	CHD-C4C	4.17	1.48	1.39
17	I	101	BCR	C21-C22	4.17	1.41	1.35
14	A	827	CLA	CHD-C4C	4.17	1.48	1.39
14	bB	804	CLA	CHD-C1D	4.17	1.46	1.38
14	A	828	CLA	C3D-C2D	4.17	1.50	1.39
14	B	804	CLA	CHD-C1D	4.17	1.46	1.38
14	bB	849	CLA	CHD-C4C	4.17	1.48	1.39
17	bB	847	BCR	C21-C22	4.17	1.41	1.35
14	A	824	CLA	CHD-C1D	4.17	1.46	1.38
14	cB	839	CLA	C1D-ND	4.17	1.42	1.37
14	cB	836	CLA	CHD-C4C	4.16	1.48	1.39
17	A	849	BCR	C21-C22	4.16	1.41	1.35
17	cL	207	BCR	C21-C22	4.16	1.41	1.35
14	cA	803	CLA	CHD-C4C	4.16	1.48	1.39
14	cB	809	CLA	O2A-CGA	4.16	1.45	1.33
17	bA	849	BCR	C21-C22	4.16	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cA	811	CLA	CHD-C4C	4.16	1.48	1.39
14	bX	201	CLA	CHD-C4C	4.16	1.48	1.39
14	bA	803	CLA	CHD-C4C	4.16	1.48	1.39
14	bB	835	CLA	CHD-C4C	4.16	1.48	1.39
14	bB	809	CLA	CHC-C1C	4.16	1.47	1.38
17	bL	206	BCR	C21-C22	4.16	1.41	1.35
17	B	850	BCR	C17-C18	4.16	1.41	1.35
14	cB	819	CLA	CHD-C4C	4.15	1.48	1.39
17	cB	848	BCR	C21-C22	4.15	1.41	1.35
14	B	819	CLA	CHD-C4C	4.15	1.48	1.39
17	I	102	BCR	C10-C9	4.15	1.41	1.35
14	cB	810	CLA	CHC-C1C	4.15	1.47	1.38
17	cB	845	BCR	C14-C13	4.15	1.41	1.35
14	bB	809	CLA	O2A-CGA	4.15	1.45	1.33
14	bA	833	CLA	O2A-CGA	4.15	1.45	1.33
17	bI	102	BCR	C10-C9	4.15	1.41	1.35
14	A	833	CLA	O2A-CGA	4.15	1.45	1.33
14	cA	833	CLA	O2A-CGA	4.15	1.45	1.33
14	B	835	CLA	CHD-C4C	4.15	1.48	1.39
14	A	803	CLA	CHD-C4C	4.15	1.48	1.39
14	bB	838	CLA	C1D-ND	4.15	1.42	1.37
14	B	812	CLA	CHD-C4C	4.15	1.48	1.39
14	bB	819	CLA	CHD-C4C	4.15	1.48	1.39
14	cB	813	CLA	CHD-C1D	4.14	1.46	1.38
14	cB	820	CLA	CHD-C4C	4.14	1.48	1.39
14	bB	812	CLA	CHD-C1D	4.14	1.46	1.38
14	B	809	CLA	CHC-C1C	4.14	1.46	1.38
14	B	808	CLA	O2A-CGA	4.14	1.45	1.33
14	cB	813	CLA	CHD-C4C	4.14	1.48	1.39
14	bB	812	CLA	CHD-C4C	4.14	1.48	1.39
14	B	809	CLA	O2A-CGA	4.14	1.45	1.33
14	bB	808	CLA	O2A-CGA	4.14	1.45	1.33
14	cB	810	CLA	O2A-CGA	4.14	1.45	1.33
17	bI	101	BCR	C21-C22	4.14	1.41	1.35
17	cA	849	BCR	C21-C22	4.14	1.41	1.35
17	cI	102	BCR	C10-C9	4.14	1.41	1.35
17	bA	848	BCR	C21-C22	4.14	1.41	1.35
14	bA	842	CLA	CHD-C1D	4.14	1.46	1.38
17	bB	844	BCR	C14-C13	4.14	1.41	1.35
14	bB	827	CLA	CHD-C4C	4.14	1.48	1.39
14	A	842	CLA	CHD-C1D	4.14	1.46	1.38
14	bA	824	CLA	CHD-C1D	4.13	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	827	CLA	CHD-C4C	4.13	1.48	1.39
14	bA	817	CLA	CHD-C4C	4.13	1.48	1.39
14	cA	814	CLA	CHD-C4C	4.13	1.48	1.39
14	A	831	CLA	CHD-C4C	4.13	1.48	1.39
14	A	830	CLA	CHD-C4C	4.13	1.48	1.39
14	B	812	CLA	CHD-C1D	4.13	1.46	1.38
14	cA	817	CLA	CHD-C4C	4.13	1.48	1.39
14	bA	816	CLA	CHD-C4C	4.13	1.48	1.39
14	cB	828	CLA	CHD-C4C	4.13	1.48	1.39
14	cA	842	CLA	CHD-C1D	4.12	1.46	1.38
14	cA	836	CLA	O2A-CGA	4.12	1.45	1.33
14	A	814	CLA	CHD-C4C	4.12	1.48	1.39
14	bB	839	CLA	CHC-C1C	4.12	1.46	1.38
14	B	838	CLA	C1D-ND	4.12	1.42	1.37
14	B	839	CLA	CHC-C1C	4.12	1.46	1.38
14	cB	840	CLA	CHC-C1C	4.12	1.46	1.38
14	cA	816	CLA	CHD-C4C	4.12	1.48	1.39
14	cA	826	CLA	CHD-C4C	4.12	1.48	1.39
14	A	816	CLA	CHD-C4C	4.12	1.48	1.39
14	bA	830	CLA	CHD-C4C	4.12	1.48	1.39
14	A	826	CLA	CHC-C4B	4.12	1.48	1.39
14	cA	826	CLA	CHC-C4B	4.12	1.48	1.39
14	bA	831	CLA	CHD-C4C	4.12	1.48	1.39
14	bA	826	CLA	O2A-CGA	4.12	1.46	1.33
14	bA	826	CLA	CHC-C4B	4.12	1.48	1.39
17	bB	841	BCR	C21-C22	4.12	1.41	1.35
14	bL	204	CLA	CHD-C4C	4.12	1.48	1.39
14	bA	814	CLA	CHD-C4C	4.12	1.48	1.39
14	A	826	CLA	O2A-CGA	4.11	1.46	1.33
14	A	813	CLA	CHD-C4C	4.11	1.48	1.39
17	B	841	BCR	C21-C22	4.11	1.41	1.35
14	cA	826	CLA	O2A-CGA	4.11	1.46	1.33
17	cI	101	BCR	C21-C22	4.11	1.41	1.35
17	cB	847	BCR	C10-C9	4.11	1.41	1.35
14	A	817	CLA	CHD-C4C	4.11	1.48	1.39
14	A	826	CLA	CHD-C4C	4.11	1.48	1.39
17	A	848	BCR	C21-C22	4.11	1.41	1.35
14	cA	837	CLA	CHD-C1D	4.11	1.46	1.38
14	cA	830	CLA	CHD-C4C	4.11	1.48	1.39
17	cB	842	BCR	C21-C22	4.11	1.41	1.35
14	bA	836	CLA	O2A-CGA	4.11	1.45	1.33
17	cA	848	BCR	C21-C22	4.11	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bA	827	CLA	CHC-C4B	4.11	1.48	1.39
14	cA	831	CLA	CHD-C4C	4.11	1.48	1.39
14	A	827	CLA	CHC-C4B	4.11	1.48	1.39
14	A	806	CLA	CHD-C1D	4.10	1.46	1.38
14	B	808	CLA	CHD-C1D	4.10	1.46	1.38
14	bA	806	CLA	CHD-C1D	4.10	1.46	1.38
14	cA	806	CLA	CHD-C1D	4.10	1.46	1.38
14	bA	813	CLA	CHD-C4C	4.10	1.48	1.39
14	cA	827	CLA	CHC-C4B	4.10	1.48	1.39
14	bA	826	CLA	CHD-C4C	4.10	1.48	1.39
14	A	836	CLA	O2A-CGA	4.10	1.45	1.33
17	bB	846	BCR	C10-C9	4.10	1.41	1.35
14	B	851	CLA	CHC-C4B	4.09	1.48	1.39
14	cA	813	CLA	CHD-C4C	4.09	1.48	1.39
14	bA	841	CLA	O2A-CGA	4.09	1.45	1.33
14	bB	839	CLA	CHD-C1D	4.09	1.46	1.38
17	bA	848	BCR	C14-C13	4.09	1.41	1.35
14	bB	822	CLA	CHD-C4C	4.09	1.48	1.39
14	B	822	CLA	CHD-C4C	4.09	1.48	1.39
14	cB	823	CLA	CHD-C4C	4.09	1.48	1.39
14	bA	837	CLA	CHD-C1D	4.09	1.46	1.38
14	L	204	CLA	CHD-C4C	4.09	1.48	1.39
14	cB	840	CLA	CHD-C1D	4.09	1.46	1.38
14	cA	841	CLA	O2A-CGA	4.09	1.45	1.33
14	B	831	CLA	CHD-C1D	4.08	1.46	1.38
17	cA	848	BCR	C14-C13	4.08	1.41	1.35
14	F	201	CLA	CHD-C1D	4.08	1.46	1.38
14	bA	830	CLA	C1D-ND	4.08	1.42	1.37
14	bB	851	CLA	CHC-C4B	4.08	1.48	1.39
14	bB	831	CLA	CHD-C1D	4.08	1.46	1.38
14	A	837	CLA	CHD-C1D	4.08	1.46	1.38
14	bB	808	CLA	CHD-C1D	4.08	1.46	1.38
14	cL	203	CLA	CHD-C4C	4.08	1.48	1.39
17	A	848	BCR	C14-C13	4.08	1.41	1.35
14	bA	806	CLA	CHD-C4C	4.07	1.48	1.39
14	cL	205	CLA	CHD-C4C	4.07	1.48	1.39
14	cB	801	CLA	CHC-C4B	4.07	1.48	1.39
14	cB	809	CLA	CHD-C1D	4.07	1.46	1.38
14	bL	202	CLA	CHD-C4C	4.07	1.48	1.39
17	B	846	BCR	C10-C9	4.07	1.41	1.35
14	A	806	CLA	CHD-C4C	4.07	1.48	1.39
14	A	841	CLA	O2A-CGA	4.07	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bA	842	CLA	CHD-C4C	4.07	1.48	1.39
14	cA	804	CLA	CHC-C4B	4.07	1.48	1.39
14	bB	831	CLA	CHC-C4B	4.07	1.48	1.39
14	cB	832	CLA	CHD-C1D	4.07	1.46	1.38
14	B	839	CLA	CHD-C1D	4.06	1.46	1.38
14	B	831	CLA	CHC-C4B	4.06	1.48	1.39
14	cA	806	CLA	CHD-C4C	4.06	1.48	1.39
14	bA	808	CLA	CHD-C1D	4.06	1.46	1.38
14	bB	804	CLA	CHD-C4C	4.06	1.48	1.39
14	A	804	CLA	CHC-C4B	4.06	1.48	1.39
14	cB	826	CLA	CHD-C4C	4.06	1.48	1.39
14	cF	201	CLA	CHD-C1D	4.06	1.46	1.38
14	cA	833	CLA	CHD-C4C	4.06	1.48	1.39
14	A	842	CLA	CHD-C4C	4.05	1.48	1.39
14	bA	804	CLA	CHC-C4B	4.05	1.48	1.39
14	B	804	CLA	CHD-C4C	4.05	1.48	1.39
14	A	836	CLA	CHD-C1D	4.05	1.46	1.38
14	cB	832	CLA	CHC-C4B	4.05	1.48	1.39
14	A	808	CLA	CHD-C1D	4.05	1.46	1.38
14	A	805	CLA	CHD-C4C	4.05	1.48	1.39
14	bA	829	CLA	CHD-C4C	4.05	1.48	1.39
14	bB	801	CLA	CHD-C4C	4.05	1.48	1.39
14	bB	802	CLA	CHD-C1D	4.05	1.46	1.38
14	cA	805	CLA	CHD-C4C	4.05	1.48	1.39
14	cB	802	CLA	CHD-C4C	4.05	1.48	1.39
14	A	830	CLA	CHD-C1D	4.05	1.46	1.38
14	B	802	CLA	CHD-C1D	4.05	1.46	1.38
14	bF	201	CLA	CHD-C1D	4.05	1.46	1.38
14	cB	805	CLA	CHD-C4C	4.05	1.48	1.39
14	B	825	CLA	CHD-C4C	4.05	1.48	1.39
14	cA	830	CLA	CHD-C1D	4.05	1.46	1.38
14	B	801	CLA	CHD-C4C	4.04	1.48	1.39
14	cA	802	CLA	O2A-CGA	4.04	1.45	1.33
14	bA	809	CLA	CHD-C4C	4.04	1.48	1.39
14	L	202	CLA	CHD-C4C	4.04	1.48	1.39
14	bA	802	CLA	O2A-CGA	4.04	1.45	1.33
14	A	829	CLA	CHD-C4C	4.04	1.48	1.39
14	bA	805	CLA	CHD-C4C	4.04	1.48	1.39
14	cA	808	CLA	CHD-C4C	4.04	1.48	1.39
17	A	848	BCR	C17-C18	4.04	1.41	1.35
14	cA	830	CLA	C1D-ND	4.04	1.42	1.37
14	A	809	CLA	CHD-C4C	4.04	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	839	CLA	CHD-C4C	4.04	1.48	1.39
14	bB	825	CLA	CHD-C4C	4.04	1.48	1.39
14	cA	829	CLA	CHD-C4C	4.04	1.48	1.39
14	bA	830	CLA	CHD-C1D	4.04	1.46	1.38
14	cA	809	CLA	CHD-C4C	4.04	1.48	1.39
14	cA	837	CLA	O2A-CGA	4.04	1.45	1.33
14	A	802	CLA	O2A-CGA	4.04	1.45	1.33
14	bA	833	CLA	CHD-C4C	4.04	1.48	1.39
17	cA	848	BCR	C10-C9	4.04	1.41	1.35
14	bA	839	CLA	CHD-C4C	4.04	1.48	1.39
14	bB	816	CLA	CHC-C4B	4.04	1.48	1.39
14	bA	808	CLA	CHD-C4C	4.04	1.48	1.39
14	bA	836	CLA	CHD-C1D	4.04	1.46	1.38
14	cL	203	CLA	OBD-CAD	4.03	1.29	1.22
14	bA	826	CLA	CHD-C1D	4.03	1.46	1.38
14	A	837	CLA	O2A-CGA	4.03	1.45	1.33
14	bA	837	CLA	O2A-CGA	4.03	1.45	1.33
14	A	830	CLA	C1D-ND	4.03	1.42	1.37
14	cA	808	CLA	CHD-C1D	4.03	1.46	1.38
14	cB	817	CLA	CHC-C4B	4.03	1.48	1.39
14	cA	842	CLA	CHD-C4C	4.03	1.48	1.39
14	A	826	CLA	CHD-C1D	4.03	1.46	1.38
14	cA	826	CLA	CHD-C1D	4.03	1.46	1.38
14	A	833	CLA	CHD-C4C	4.03	1.48	1.39
14	cB	819	CLA	O2A-CGA	4.03	1.45	1.33
17	A	848	BCR	C10-C9	4.03	1.41	1.35
14	B	816	CLA	CHC-C4B	4.03	1.48	1.39
17	L	205	BCR	C17-C18	4.03	1.41	1.35
14	B	824	CLA	CHC-C4B	4.03	1.48	1.39
14	cA	818	CLA	CHC-C4B	4.03	1.48	1.39
14	B	823	CLA	CHD-C1D	4.03	1.46	1.38
14	bB	824	CLA	CHC-C4B	4.02	1.48	1.39
14	bB	823	CLA	CHD-C1D	4.02	1.46	1.38
14	cB	803	CLA	CHD-C1D	4.02	1.46	1.38
14	cA	839	CLA	CHD-C4C	4.02	1.48	1.39
14	cB	824	CLA	CHD-C1D	4.02	1.46	1.38
14	B	805	CLA	O2A-CGA	4.02	1.45	1.33
14	cB	825	CLA	CHC-C4B	4.02	1.48	1.39
17	bA	848	BCR	C10-C9	4.02	1.41	1.35
14	bA	837	CLA	CHB-C1B	4.02	1.48	1.39
14	cA	837	CLA	CHB-C1B	4.02	1.48	1.39
17	cL	206	BCR	C17-C18	4.02	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cB	806	CLA	O2A-CGA	4.02	1.45	1.33
14	B	818	CLA	O2A-CGA	4.02	1.45	1.33
14	A	818	CLA	CHC-C4B	4.02	1.48	1.39
14	B	823	CLA	CHD-C4C	4.02	1.48	1.39
14	L	202	CLA	OBD-CAD	4.02	1.29	1.22
14	bA	818	CLA	CHC-C4B	4.02	1.48	1.39
14	A	825	CLA	CHD-C1D	4.02	1.46	1.38
14	bB	817	CLA	CHD-C4C	4.01	1.48	1.39
14	bB	818	CLA	O2A-CGA	4.01	1.45	1.33
14	bB	807	CLA	CHB-C1B	4.01	1.48	1.39
14	bB	803	CLA	C3D-C2D	4.01	1.50	1.39
14	A	808	CLA	CHD-C4C	4.01	1.48	1.39
14	bB	805	CLA	O2A-CGA	4.01	1.45	1.33
14	cB	808	CLA	CHB-C1B	4.01	1.48	1.39
17	bL	205	BCR	C17-C18	4.01	1.41	1.35
14	A	825	CLA	CHD-C4C	4.01	1.48	1.39
14	bA	825	CLA	CHD-C1D	4.01	1.46	1.38
14	bL	202	CLA	OBD-CAD	4.01	1.29	1.22
14	B	824	CLA	O2A-CGA	4.01	1.45	1.33
14	bA	825	CLA	CHD-C4C	4.01	1.48	1.39
14	bB	828	CLA	CHD-C4C	4.01	1.48	1.39
14	bB	823	CLA	CHD-C4C	4.01	1.48	1.39
14	B	817	CLA	CHD-C4C	4.00	1.48	1.39
14	cA	836	CLA	CHD-C1D	4.00	1.46	1.38
14	cB	824	CLA	CHD-C4C	4.00	1.48	1.39
17	cA	848	BCR	C17-C18	4.00	1.41	1.35
14	cB	805	CLA	CHC-C4B	4.00	1.48	1.39
14	cB	825	CLA	O2A-CGA	4.00	1.45	1.33
17	bA	848	BCR	C17-C18	4.00	1.41	1.35
14	cA	825	CLA	CHD-C4C	4.00	1.48	1.39
14	B	804	CLA	CHC-C4B	4.00	1.48	1.39
14	A	852	CLA	O2A-CGA	4.00	1.45	1.33
14	cB	818	CLA	CHD-C4C	4.00	1.48	1.39
14	A	837	CLA	CHB-C1B	4.00	1.48	1.39
14	bA	852	CLA	O2A-CGA	3.99	1.45	1.33
14	bA	832	CLA	CHD-C1D	3.99	1.46	1.38
14	cA	820	CLA	CHC-C4B	3.99	1.48	1.39
14	bA	838	CLA	CHD-C4C	3.99	1.48	1.39
14	cA	825	CLA	CHD-C1D	3.99	1.46	1.38
14	cA	817	CLA	CHB-C1B	3.99	1.48	1.39
14	cA	838	CLA	CHD-C4C	3.99	1.48	1.39
14	bB	824	CLA	O2A-CGA	3.99	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cA	830	CLA	C4B-NB	-3.99	1.32	1.37
14	B	807	CLA	CHB-C1B	3.99	1.48	1.39
14	bA	817	CLA	CHB-C1B	3.99	1.48	1.39
14	B	803	CLA	C3D-C2D	3.98	1.50	1.39
14	A	838	CLA	CHD-C4C	3.98	1.48	1.39
14	bB	815	CLA	CHC-C4B	3.98	1.48	1.39
14	cA	852	CLA	O2A-CGA	3.98	1.45	1.33
14	A	840	CLA	CHC-C4B	3.98	1.48	1.39
14	bA	806	CLA	CHC-C4B	3.98	1.48	1.39
14	bB	804	CLA	CHC-C4B	3.98	1.48	1.39
14	cB	816	CLA	CHC-C4B	3.98	1.48	1.39
14	A	806	CLA	CHC-C4B	3.98	1.48	1.39
14	cA	840	CLA	CHC-C4B	3.98	1.48	1.39
14	cB	829	CLA	CHD-C4C	3.98	1.48	1.39
14	cB	804	CLA	C3D-C2D	3.98	1.50	1.39
14	A	832	CLA	CHD-C1D	3.98	1.46	1.38
14	cA	832	CLA	CHD-C1D	3.98	1.46	1.38
14	A	820	CLA	CHC-C4B	3.98	1.48	1.39
14	B	838	CLA	CHC-C1C	3.98	1.46	1.38
14	bA	824	CLA	CHD-C4C	3.98	1.48	1.39
14	A	817	CLA	CHB-C1B	3.98	1.48	1.39
14	B	815	CLA	CHC-C4B	3.98	1.48	1.39
14	bA	840	CLA	CHC-C4B	3.98	1.48	1.39
14	cA	806	CLA	CHC-C4B	3.98	1.48	1.39
14	B	828	CLA	CHD-C4C	3.98	1.48	1.39
14	A	830	CLA	C4B-NB	-3.98	1.32	1.37
14	A	836	CLA	CHD-C4C	3.97	1.48	1.39
14	bA	820	CLA	CHC-C4B	3.97	1.48	1.39
14	bA	836	CLA	CHD-C4C	3.97	1.48	1.39
14	cA	836	CLA	CHD-C4C	3.97	1.48	1.39
14	B	819	CLA	CHC-C4B	3.97	1.48	1.39
14	cA	802	CLA	CHB-C1B	3.97	1.48	1.39
17	B	844	BCR	C21-C22	3.97	1.41	1.35
14	bA	802	CLA	CHB-C1B	3.96	1.48	1.39
14	A	802	CLA	CHB-C1B	3.96	1.48	1.39
14	L	204	CLA	C3D-C2D	3.96	1.49	1.39
14	cA	808	CLA	CHC-C4B	3.96	1.48	1.39
14	bA	833	CLA	C1D-ND	3.96	1.42	1.37
14	bL	204	CLA	C3D-C2D	3.96	1.49	1.39
14	bB	825	CLA	CHC-C4B	3.96	1.48	1.39
14	cL	205	CLA	C3D-C2D	3.96	1.49	1.39
14	cB	826	CLA	CHC-C4B	3.96	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	L	206	BCR	C17-C18	3.95	1.41	1.35
14	bB	838	CLA	CHC-C1C	3.95	1.46	1.38
14	B	825	CLA	CHC-C4B	3.95	1.48	1.39
14	B	806	CLA	CHC-C4B	3.95	1.48	1.39
14	bB	819	CLA	CHC-C4B	3.95	1.48	1.39
14	cB	820	CLA	CHC-C4B	3.95	1.48	1.39
14	A	808	CLA	CHC-C4B	3.95	1.48	1.39
17	cB	845	BCR	C21-C22	3.95	1.41	1.35
14	bB	806	CLA	CHC-C4B	3.95	1.48	1.39
14	bA	830	CLA	C4B-NB	-3.95	1.32	1.37
14	bF	201	CLA	CHC-C4B	3.95	1.48	1.39
14	A	833	CLA	C1D-ND	3.95	1.42	1.37
14	cA	824	CLA	CHD-C4C	3.95	1.48	1.39
13	cA	801	CL0	CHD-C1D	3.95	1.46	1.38
14	cB	839	CLA	CHC-C1C	3.95	1.46	1.38
17	bB	844	BCR	C21-C22	3.94	1.41	1.35
14	A	824	CLA	CHD-C4C	3.94	1.48	1.39
14	bA	813	CLA	CHC-C4B	3.94	1.48	1.39
14	A	813	CLA	CHC-C4B	3.94	1.48	1.39
14	bA	808	CLA	CHC-C4B	3.94	1.48	1.39
14	cL	203	CLA	CHC-C4B	3.94	1.48	1.39
14	cA	813	CLA	CHC-C4B	3.94	1.48	1.39
14	bA	841	CLA	CHC-C1C	3.94	1.46	1.38
14	B	807	CLA	CHD-C4C	3.94	1.48	1.39
14	A	841	CLA	CHC-C1C	3.94	1.46	1.38
14	cA	833	CLA	C1D-ND	3.94	1.42	1.37
14	bB	820	CLA	CHB-C1B	3.93	1.48	1.39
14	bB	807	CLA	CHD-C4C	3.93	1.48	1.39
14	cB	807	CLA	CHC-C4B	3.93	1.48	1.39
14	cL	205	CLA	CHC-C4B	3.93	1.48	1.39
14	cA	841	CLA	CHC-C1C	3.93	1.46	1.38
14	cB	808	CLA	CHD-C4C	3.93	1.48	1.39
14	B	849	CLA	CHC-C4B	3.93	1.48	1.39
14	bL	202	CLA	CHC-C4B	3.93	1.48	1.39
14	L	204	CLA	CHC-C4B	3.93	1.48	1.39
14	cB	821	CLA	CHB-C1B	3.93	1.48	1.39
14	cF	201	CLA	CHC-C4B	3.93	1.48	1.39
14	bL	204	CLA	CHC-C4B	3.93	1.48	1.39
13	bA	801	CL0	CHD-C1D	3.93	1.46	1.38
14	L	202	CLA	CHC-C4B	3.92	1.48	1.39
13	A	801	CL0	CHD-C1D	3.92	1.46	1.38
17	cL	207	BCR	C17-C18	3.92	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	F	201	CLA	CHC-C4B	3.92	1.48	1.39
14	bB	811	CLA	CHC-C4B	3.92	1.48	1.39
14	A	832	CLA	O2A-CGA	3.92	1.44	1.33
14	B	833	CLA	CHC-C4B	3.92	1.48	1.39
14	bA	838	CLA	CHD-C1D	3.92	1.46	1.38
14	bB	818	CLA	C3D-C2D	3.92	1.49	1.39
14	bB	849	CLA	CHC-C4B	3.92	1.48	1.39
14	cB	819	CLA	C3D-C2D	3.92	1.49	1.39
14	bB	803	CLA	CHD-C1D	3.92	1.46	1.38
17	bL	206	BCR	C17-C18	3.92	1.41	1.35
14	B	818	CLA	C3D-C2D	3.92	1.49	1.39
14	A	838	CLA	CHD-C1D	3.92	1.46	1.38
14	cJ	101	CLA	CHC-C4B	3.92	1.48	1.39
14	X	201	CLA	CHC-C4B	3.92	1.48	1.39
14	B	820	CLA	CHB-C1B	3.91	1.48	1.39
14	cB	812	CLA	CHC-C4B	3.91	1.48	1.39
14	cB	834	CLA	CHC-C4B	3.91	1.48	1.39
14	bA	828	CLA	CHD-C4C	3.91	1.48	1.39
14	cA	828	CLA	CHD-C4C	3.91	1.48	1.39
14	A	828	CLA	CHD-C4C	3.91	1.48	1.39
14	cA	832	CLA	O2A-CGA	3.91	1.44	1.33
14	bJ	101	CLA	CHC-C4B	3.91	1.48	1.39
14	cB	837	CLA	CHC-C4B	3.91	1.48	1.39
14	B	830	CLA	CHC-C4B	3.91	1.48	1.39
14	bX	201	CLA	CHC-C4B	3.91	1.48	1.39
14	B	832	CLA	CHD-C4C	3.91	1.48	1.39
14	bB	832	CLA	CHD-C4C	3.91	1.48	1.39
14	cB	831	CLA	CHC-C4B	3.91	1.48	1.39
14	cA	814	CLA	CHB-C1B	3.91	1.48	1.39
14	cB	833	CLA	CHD-C4C	3.90	1.48	1.39
14	B	803	CLA	CHD-C1D	3.90	1.46	1.38
14	bB	838	CLA	CHD-C1D	3.90	1.46	1.38
14	B	811	CLA	CHC-C4B	3.90	1.48	1.39
14	bB	830	CLA	CHC-C4B	3.90	1.48	1.39
14	cA	838	CLA	CHD-C1D	3.90	1.46	1.38
14	cX	201	CLA	CHC-C4B	3.90	1.48	1.39
14	bA	814	CLA	CHC-C4B	3.90	1.48	1.39
14	cA	820	CLA	C3D-C2D	3.90	1.49	1.39
14	bA	829	CLA	C3D-C2D	3.90	1.49	1.39
14	cA	829	CLA	C3D-C2D	3.90	1.49	1.39
14	bA	832	CLA	O2A-CGA	3.90	1.44	1.33
14	bA	820	CLA	C3D-C2D	3.90	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	J	101	CLA	CHC-C4B	3.90	1.48	1.39
14	cB	850	CLA	CHC-C4B	3.89	1.48	1.39
14	bA	817	CLA	CHC-C4B	3.89	1.48	1.39
14	cA	817	CLA	CHC-C4B	3.89	1.48	1.39
14	A	820	CLA	C3D-C2D	3.89	1.49	1.39
14	A	817	CLA	CHC-C4B	3.89	1.48	1.39
14	B	810	CLA	C3D-C2D	3.89	1.49	1.39
14	A	829	CLA	C3D-C2D	3.89	1.49	1.39
14	bA	814	CLA	CHB-C1B	3.89	1.48	1.39
14	bB	810	CLA	C3D-C2D	3.89	1.49	1.39
14	B	801	CLA	CHC-C4B	3.89	1.48	1.39
14	bA	841	CLA	CHD-C1D	3.89	1.45	1.38
17	bI	102	BCR	C21-C22	3.89	1.40	1.35
14	cB	804	CLA	CHD-C1D	3.89	1.45	1.38
14	bB	836	CLA	CHC-C4B	3.89	1.48	1.39
14	bB	833	CLA	CHC-C4B	3.89	1.48	1.39
14	bB	801	CLA	CHC-C4B	3.88	1.48	1.39
14	cA	814	CLA	CHC-C4B	3.88	1.48	1.39
14	B	826	CLA	CHC-C1C	3.88	1.46	1.38
17	cI	102	BCR	C21-C22	3.88	1.40	1.35
14	cB	811	CLA	C3D-C2D	3.88	1.49	1.39
14	A	832	CLA	CHB-C1B	3.88	1.48	1.39
14	bB	826	CLA	CHC-C1C	3.88	1.46	1.38
14	cA	832	CLA	CHB-C1B	3.88	1.48	1.39
14	cB	803	CLA	C3D-C2D	3.88	1.49	1.39
14	B	836	CLA	CHC-C4B	3.88	1.48	1.39
14	A	841	CLA	CHD-C1D	3.88	1.45	1.38
14	bB	828	CLA	CHD-C1D	3.88	1.45	1.38
14	A	814	CLA	CHB-C1B	3.88	1.48	1.39
14	B	827	CLA	CHC-C4B	3.88	1.48	1.39
14	bB	815	CLA	OBD-CAD	3.88	1.29	1.22
14	bA	835	CLA	CHC-C4B	3.87	1.48	1.39
14	B	838	CLA	CHD-C1D	3.87	1.45	1.38
14	A	807	CLA	CHC-C4B	3.87	1.48	1.39
14	bA	832	CLA	CHB-C1B	3.87	1.48	1.39
14	cA	816	CLA	CHC-C4B	3.87	1.48	1.39
14	A	816	CLA	CHC-C4B	3.87	1.48	1.39
14	bA	816	CLA	CHC-C4B	3.87	1.48	1.39
14	cA	835	CLA	CHC-C4B	3.87	1.48	1.39
14	cB	839	CLA	CHD-C1D	3.87	1.45	1.38
14	cB	802	CLA	CHC-C4B	3.87	1.48	1.39
14	cB	827	CLA	CHC-C1C	3.87	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	840	CLA	CHB-C1B	3.87	1.48	1.39
14	bB	802	CLA	C3D-C2D	3.87	1.49	1.39
14	B	802	CLA	C3D-C2D	3.87	1.49	1.39
14	bB	832	CLA	CHC-C4B	3.87	1.48	1.39
14	bA	807	CLA	CHC-C4B	3.87	1.48	1.39
17	bB	846	BCR	C14-C13	3.86	1.40	1.35
14	J	102	CLA	CHC-C4B	3.86	1.48	1.39
14	cB	829	CLA	CHD-C1D	3.86	1.45	1.38
14	bA	837	CLA	CHD-C4C	3.86	1.48	1.39
14	A	814	CLA	CHC-C4B	3.86	1.48	1.39
14	A	837	CLA	CHD-C4C	3.86	1.48	1.39
14	cA	837	CLA	CHD-C4C	3.86	1.48	1.39
14	B	832	CLA	CHC-C4B	3.86	1.48	1.39
14	bA	811	CLA	CHC-C4B	3.86	1.48	1.39
14	cA	841	CLA	C3D-C2D	3.86	1.49	1.39
14	bB	827	CLA	CHC-C4B	3.86	1.48	1.39
14	bA	841	CLA	C3D-C2D	3.86	1.49	1.39
14	bB	813	CLA	C3D-C2D	3.86	1.49	1.39
14	cA	811	CLA	CHC-C4B	3.86	1.48	1.39
14	cB	833	CLA	CHC-C4B	3.86	1.48	1.39
14	A	841	CLA	C3D-C2D	3.86	1.49	1.39
14	B	828	CLA	CHD-C1D	3.86	1.45	1.38
14	bJ	102	CLA	CHC-C4B	3.86	1.48	1.39
14	cB	828	CLA	CHC-C4B	3.86	1.48	1.39
17	I	102	BCR	C21-C22	3.86	1.40	1.35
14	A	835	CLA	CHC-C4B	3.86	1.48	1.39
14	bB	817	CLA	OBD-CAD	3.86	1.29	1.22
14	B	801	CLA	CHD-C1D	3.86	1.45	1.38
14	cA	803	CLA	C3D-C2D	3.86	1.49	1.39
14	A	842	CLA	CHC-C4B	3.86	1.48	1.39
14	bB	822	CLA	CHC-C4B	3.86	1.48	1.39
14	A	814	CLA	C3D-C2D	3.85	1.49	1.39
14	bB	807	CLA	C3D-C2D	3.85	1.49	1.39
14	F	201	CLA	CHD-C4C	3.85	1.48	1.39
14	B	815	CLA	OBD-CAD	3.85	1.29	1.22
14	B	813	CLA	C3D-C2D	3.85	1.49	1.39
14	B	807	CLA	C3D-C2D	3.85	1.49	1.39
14	cB	819	CLA	CHC-C4B	3.85	1.48	1.39
14	bA	803	CLA	C3D-C2D	3.85	1.49	1.39
14	cB	814	CLA	C3D-C2D	3.85	1.49	1.39
14	bB	818	CLA	CHC-C4B	3.85	1.48	1.39
14	cJ	102	CLA	CHC-C4B	3.85	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bL	203	CLA	CHD-C4C	3.85	1.48	1.39
14	cA	841	CLA	CHD-C1D	3.85	1.45	1.38
14	B	810	CLA	CHB-C1B	3.85	1.48	1.39
14	cA	810	CLA	CHC-C4B	3.85	1.48	1.39
14	cA	840	CLA	CHB-C1B	3.85	1.48	1.39
14	bB	801	CLA	CHD-C1D	3.85	1.45	1.38
14	bA	810	CLA	CHC-C4B	3.85	1.48	1.39
14	cA	842	CLA	CHC-C4B	3.85	1.48	1.39
14	bA	842	CLA	CHC-C4B	3.85	1.48	1.39
14	bA	814	CLA	C3D-C2D	3.85	1.49	1.39
14	A	810	CLA	CHB-C1B	3.85	1.48	1.39
14	A	803	CLA	C3D-C2D	3.85	1.49	1.39
14	cB	811	CLA	CHB-C1B	3.84	1.48	1.39
14	cA	815	CLA	CHB-C1B	3.84	1.48	1.39
14	cB	833	CLA	OBD-CAD	3.84	1.29	1.22
14	cA	817	CLA	C3D-C2D	3.84	1.49	1.39
14	A	811	CLA	CHC-C4B	3.84	1.48	1.39
14	B	818	CLA	CHC-C4B	3.84	1.48	1.39
17	cB	847	BCR	C14-C13	3.84	1.40	1.35
14	bA	840	CLA	CHB-C1B	3.84	1.48	1.39
14	L	203	CLA	CHD-C4C	3.84	1.48	1.39
14	cB	823	CLA	CHC-C4B	3.84	1.48	1.39
14	bB	832	CLA	OBD-CAD	3.84	1.29	1.22
14	bB	824	CLA	C3D-C2D	3.84	1.49	1.39
14	cF	201	CLA	CHD-C4C	3.84	1.48	1.39
14	cB	802	CLA	CHD-C1D	3.84	1.45	1.38
14	bA	807	CLA	OBD-CAD	3.84	1.29	1.22
14	B	824	CLA	C3D-C2D	3.84	1.49	1.39
14	cL	204	CLA	CHD-C4C	3.84	1.48	1.39
14	A	810	CLA	CHC-C4B	3.84	1.48	1.39
14	bB	810	CLA	CHB-C1B	3.84	1.48	1.39
14	cB	808	CLA	C3D-C2D	3.84	1.49	1.39
14	cA	807	CLA	CHC-C4B	3.84	1.48	1.39
14	bA	817	CLA	C3D-C2D	3.84	1.49	1.39
14	B	817	CLA	OBD-CAD	3.84	1.29	1.22
14	bA	815	CLA	CHB-C1B	3.84	1.48	1.39
14	bB	809	CLA	CHD-C1D	3.84	1.45	1.38
14	A	807	CLA	OBD-CAD	3.84	1.29	1.22
14	cA	814	CLA	C3D-C2D	3.84	1.49	1.39
14	B	822	CLA	CHC-C4B	3.84	1.48	1.39
14	cB	836	CLA	CHC-C4B	3.84	1.48	1.39
14	A	817	CLA	C3D-C2D	3.83	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cA	810	CLA	CHB-C1B	3.83	1.48	1.39
14	bF	201	CLA	CHD-C4C	3.83	1.48	1.39
14	cA	823	CLA	CHC-C4B	3.83	1.48	1.39
14	bA	839	CLA	OBD-CAD	3.83	1.29	1.22
17	cL	206	BCR	C21-C22	3.83	1.40	1.35
14	cB	820	CLA	OBD-CAD	3.83	1.29	1.22
14	cL	204	CLA	CHB-C1B	3.83	1.48	1.39
14	A	818	CLA	C3B-C4B	3.83	1.51	1.42
14	bA	810	CLA	CHB-C1B	3.83	1.48	1.39
14	B	835	CLA	CHC-C4B	3.83	1.48	1.39
14	cA	810	CLA	C3D-C2D	3.83	1.49	1.39
14	A	819	CLA	CHC-C4B	3.83	1.48	1.39
14	bB	835	CLA	CHC-C4B	3.83	1.48	1.39
14	bB	819	CLA	OBD-CAD	3.83	1.29	1.22
14	bA	819	CLA	CHC-C4B	3.83	1.48	1.39
14	bA	803	CLA	CHB-C1B	3.83	1.48	1.39
14	cB	818	CLA	OBD-CAD	3.83	1.29	1.22
14	A	815	CLA	CHB-C1B	3.83	1.48	1.39
14	cB	836	CLA	CHB-C1B	3.83	1.48	1.39
14	B	839	CLA	C3D-C2D	3.82	1.49	1.39
14	bA	810	CLA	C3D-C2D	3.82	1.49	1.39
14	cB	810	CLA	CHD-C1D	3.82	1.45	1.38
14	cA	818	CLA	C3B-C4B	3.82	1.51	1.42
14	A	821	CLA	CHB-C1B	3.82	1.48	1.39
14	cB	840	CLA	C3D-C2D	3.82	1.49	1.39
17	B	846	BCR	C14-C13	3.82	1.40	1.35
14	A	815	CLA	CHC-C4B	3.82	1.48	1.39
14	bB	835	CLA	CHB-C1B	3.82	1.48	1.39
14	cA	827	CLA	CHB-C1B	3.82	1.48	1.39
14	A	839	CLA	OBD-CAD	3.82	1.29	1.22
14	B	832	CLA	OBD-CAD	3.82	1.29	1.22
14	cB	825	CLA	C3D-C2D	3.82	1.49	1.39
14	bA	818	CLA	C3B-C4B	3.82	1.51	1.42
14	bA	823	CLA	CHC-C4B	3.82	1.48	1.39
14	cA	803	CLA	CHC-C4B	3.82	1.48	1.39
14	bA	803	CLA	CHC-C4B	3.82	1.48	1.39
13	bA	801	CL0	CHC-C4B	3.82	1.48	1.39
14	B	813	CLA	CHB-C1B	3.82	1.48	1.39
14	cA	839	CLA	OBD-CAD	3.82	1.29	1.22
14	B	835	CLA	CHB-C1B	3.82	1.48	1.39
14	A	823	CLA	CHC-C4B	3.82	1.48	1.39
14	bA	804	CLA	C3D-C2D	3.82	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bB	839	CLA	C3D-C2D	3.82	1.49	1.39
14	A	831	CLA	CHB-C1B	3.82	1.48	1.39
14	B	819	CLA	OBD-CAD	3.82	1.29	1.22
14	B	837	CLA	CHB-C1B	3.82	1.48	1.39
14	bA	831	CLA	CHB-C1B	3.82	1.48	1.39
14	bB	837	CLA	CHB-C1B	3.82	1.48	1.39
14	bA	827	CLA	CHB-C1B	3.82	1.48	1.39
14	cA	831	CLA	CHB-C1B	3.82	1.48	1.39
14	cA	807	CLA	OBD-CAD	3.81	1.29	1.22
14	A	810	CLA	C3D-C2D	3.81	1.49	1.39
13	A	801	CL0	CHC-C4B	3.81	1.48	1.39
13	cA	801	CL0	CHC-C4B	3.81	1.48	1.39
14	L	203	CLA	CHB-C1B	3.81	1.48	1.39
14	B	814	CLA	CHB-C1B	3.81	1.48	1.39
14	bA	821	CLA	CHB-C1B	3.81	1.48	1.39
14	cB	816	CLA	OBD-CAD	3.81	1.29	1.22
14	cA	803	CLA	CHB-C1B	3.81	1.48	1.39
14	A	803	CLA	CHC-C4B	3.81	1.48	1.39
14	bB	830	CLA	C3D-C2D	3.81	1.49	1.39
14	A	833	CLA	C4B-NB	-3.81	1.33	1.37
14	cB	831	CLA	C3D-C2D	3.81	1.49	1.39
14	B	830	CLA	C3D-C2D	3.81	1.49	1.39
14	bB	834	CLA	C3D-C2D	3.81	1.49	1.39
14	A	833	CLA	C3D-C2D	3.81	1.49	1.39
14	cA	821	CLA	CHB-C1B	3.81	1.47	1.39
14	A	810	CLA	OBD-CAD	3.81	1.29	1.22
14	A	822	CLA	C3D-C2D	3.80	1.49	1.39
14	A	827	CLA	CHB-C1B	3.80	1.47	1.39
14	cB	815	CLA	CHB-C1B	3.80	1.47	1.39
14	B	809	CLA	CHD-C1D	3.80	1.45	1.38
14	cA	834	CLA	CHC-C4B	3.80	1.47	1.39
14	A	804	CLA	C3D-C2D	3.80	1.49	1.39
14	bA	821	CLA	C3D-C2D	3.80	1.49	1.39
14	bA	816	CLA	CHB-C1B	3.80	1.47	1.39
14	A	816	CLA	CHB-C1B	3.80	1.47	1.39
14	bB	821	CLA	OBD-CAD	3.80	1.29	1.22
14	B	809	CLA	CHB-C1B	3.80	1.47	1.39
14	bL	203	CLA	CHB-C1B	3.80	1.47	1.39
14	B	833	CLA	C3D-C2D	3.80	1.49	1.39
14	bA	810	CLA	OBD-CAD	3.80	1.29	1.22
14	cB	814	CLA	CHB-C1B	3.80	1.47	1.39
14	bB	821	CLA	CHB-C1B	3.80	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cB	822	CLA	OBD-CAD	3.80	1.29	1.22
14	bA	822	CLA	C3D-C2D	3.80	1.49	1.39
14	cA	816	CLA	CHB-C1B	3.80	1.47	1.39
14	cA	819	CLA	CHC-C4B	3.80	1.47	1.39
14	bB	813	CLA	CHB-C1B	3.80	1.47	1.39
14	cA	812	CLA	CHC-C4B	3.80	1.47	1.39
14	cA	804	CLA	C3D-C2D	3.80	1.49	1.39
14	B	821	CLA	OBD-CAD	3.80	1.29	1.22
14	cA	833	CLA	C3D-C2D	3.80	1.49	1.39
14	B	804	CLA	C3D-C2D	3.79	1.49	1.39
14	cB	801	CLA	C3B-C4B	3.79	1.51	1.42
14	bB	833	CLA	C3D-C2D	3.79	1.49	1.39
14	A	803	CLA	CHB-C1B	3.79	1.47	1.39
14	bA	833	CLA	C4B-NB	-3.79	1.33	1.37
14	J	101	CLA	C3D-C2D	3.79	1.49	1.39
14	B	820	CLA	CHC-C4B	3.79	1.47	1.39
14	cB	824	CLA	OBD-CAD	3.79	1.29	1.22
14	bA	833	CLA	C3D-C2D	3.79	1.49	1.39
14	cA	821	CLA	C3D-C2D	3.79	1.49	1.39
14	cA	815	CLA	CHC-C4B	3.79	1.47	1.39
14	cA	814	CLA	OBD-CAD	3.79	1.29	1.22
14	B	834	CLA	C3D-C2D	3.79	1.49	1.39
14	cA	833	CLA	C4B-NB	-3.79	1.33	1.37
14	bA	826	CLA	CHB-C1B	3.79	1.47	1.39
14	cB	821	CLA	CHC-C4B	3.79	1.47	1.39
14	cB	832	CLA	C3B-C4B	3.79	1.51	1.42
14	B	830	CLA	CHB-C1B	3.79	1.47	1.39
14	cB	831	CLA	CHB-C1B	3.79	1.47	1.39
14	cA	815	CLA	C3D-C2D	3.79	1.49	1.39
14	bB	830	CLA	CHB-C1B	3.79	1.47	1.39
14	bJ	101	CLA	C3D-C2D	3.79	1.49	1.39
14	cJ	101	CLA	C3D-C2D	3.79	1.49	1.39
14	bA	835	CLA	OBD-CAD	3.79	1.29	1.22
14	bB	820	CLA	CHC-C4B	3.79	1.47	1.39
14	cB	828	CLA	CHB-C1B	3.79	1.47	1.39
14	A	826	CLA	CHB-C1B	3.79	1.47	1.39
14	bB	804	CLA	C3D-C2D	3.79	1.49	1.39
14	cB	805	CLA	C3D-C2D	3.79	1.49	1.39
14	bB	827	CLA	CHB-C1B	3.79	1.47	1.39
14	A	812	CLA	CHC-C4B	3.79	1.47	1.39
14	B	814	CLA	CHC-C4B	3.79	1.47	1.39
14	A	821	CLA	C3D-C2D	3.79	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	823	CLA	C3D-C2D	3.79	1.49	1.39
14	bB	831	CLA	C3B-C4B	3.79	1.51	1.42
14	bA	839	CLA	C3D-C2D	3.79	1.49	1.39
14	bB	814	CLA	CHC-C4B	3.79	1.47	1.39
14	cB	810	CLA	CHB-C1B	3.79	1.47	1.39
17	I	101	BCR	C17-C18	3.79	1.40	1.35
14	bA	823	CLA	C3D-C2D	3.79	1.49	1.39
14	bB	814	CLA	CHB-C1B	3.79	1.47	1.39
14	B	823	CLA	OBD-CAD	3.79	1.29	1.22
14	B	827	CLA	CHB-C1B	3.79	1.47	1.39
14	cA	823	CLA	C3D-C2D	3.78	1.49	1.39
14	A	835	CLA	OBD-CAD	3.78	1.29	1.22
14	cA	835	CLA	OBD-CAD	3.78	1.29	1.22
14	cA	822	CLA	C3D-C2D	3.78	1.49	1.39
14	bA	815	CLA	CHC-C4B	3.78	1.47	1.39
14	cB	838	CLA	CHB-C1B	3.78	1.47	1.39
14	B	851	CLA	C3B-C4B	3.78	1.51	1.42
14	cA	826	CLA	CHB-C1B	3.78	1.47	1.39
14	B	837	CLA	C3D-C2D	3.78	1.49	1.39
14	bB	834	CLA	CHB-C1B	3.78	1.47	1.39
14	A	815	CLA	C3D-C2D	3.78	1.49	1.39
14	cB	836	CLA	C3D-C2D	3.78	1.49	1.39
14	A	814	CLA	OBD-CAD	3.78	1.29	1.22
14	cB	834	CLA	C3D-C2D	3.78	1.49	1.39
14	bB	849	CLA	C3D-C2D	3.78	1.49	1.39
14	bA	815	CLA	C3D-C2D	3.78	1.49	1.39
14	bL	204	CLA	CHB-C1B	3.78	1.47	1.39
17	bL	205	BCR	C21-C22	3.78	1.40	1.35
14	B	831	CLA	C3B-C4B	3.78	1.51	1.42
14	bA	834	CLA	CHC-C4B	3.78	1.47	1.39
14	B	812	CLA	C3D-C2D	3.78	1.49	1.39
14	bB	829	CLA	CHB-C1B	3.78	1.47	1.39
14	cB	830	CLA	CHB-C1B	3.78	1.47	1.39
14	B	821	CLA	CHB-C1B	3.78	1.47	1.39
14	B	829	CLA	CHB-C1B	3.78	1.47	1.39
14	cB	835	CLA	C3D-C2D	3.78	1.49	1.39
14	bB	809	CLA	CHB-C1B	3.78	1.47	1.39
14	cB	821	CLA	OBD-CAD	3.78	1.29	1.22
14	bA	818	CLA	C3D-C2D	3.78	1.49	1.39
14	cB	834	CLA	C3B-C4B	3.78	1.51	1.42
14	cB	815	CLA	CHC-C4B	3.78	1.47	1.39
17	L	205	BCR	C21-C22	3.78	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	816	CLA	C3D-C2D	3.78	1.49	1.39
14	bB	823	CLA	CHC-C4B	3.78	1.47	1.39
17	cI	101	BCR	C17-C18	3.78	1.40	1.35
14	bA	814	CLA	OBD-CAD	3.77	1.29	1.22
14	bJ	102	CLA	OBD-CAD	3.77	1.29	1.22
14	cB	817	CLA	C3D-C2D	3.77	1.49	1.39
14	bA	812	CLA	CHC-C4B	3.77	1.47	1.39
14	cB	850	CLA	C3D-C2D	3.77	1.49	1.39
14	B	837	CLA	CHC-C4B	3.77	1.47	1.39
14	cA	832	CLA	CHD-C4C	3.77	1.47	1.39
14	cA	816	CLA	C3D-C2D	3.77	1.49	1.39
14	B	835	CLA	C3D-C2D	3.77	1.49	1.39
14	bA	816	CLA	C3D-C2D	3.77	1.49	1.39
14	cB	812	CLA	C3D-C2D	3.77	1.49	1.39
14	A	839	CLA	C3D-C2D	3.77	1.49	1.39
14	cA	812	CLA	C3D-C2D	3.77	1.49	1.39
14	A	834	CLA	CHC-C4B	3.77	1.47	1.39
14	cL	205	CLA	CHB-C1B	3.77	1.47	1.39
14	cJ	102	CLA	OBD-CAD	3.77	1.29	1.22
14	cB	824	CLA	CHC-C4B	3.77	1.47	1.39
14	cB	804	CLA	CHD-C4C	3.77	1.47	1.39
14	bB	823	CLA	OBD-CAD	3.77	1.29	1.22
14	cA	815	CLA	OBD-CAD	3.77	1.29	1.22
14	bA	832	CLA	CHD-C4C	3.77	1.47	1.39
14	cB	838	CLA	CHC-C4B	3.77	1.47	1.39
14	B	849	CLA	C3D-C2D	3.77	1.49	1.39
14	bB	812	CLA	C3D-C2D	3.77	1.49	1.39
14	bB	816	CLA	C3D-C2D	3.77	1.49	1.39
14	bB	851	CLA	C3B-C4B	3.77	1.51	1.42
14	bB	837	CLA	CHC-C4B	3.77	1.47	1.39
14	bB	812	CLA	C3B-C4B	3.77	1.51	1.42
14	B	834	CLA	CHB-C1B	3.77	1.47	1.39
14	cB	813	CLA	C3D-C2D	3.77	1.49	1.39
14	cB	814	CLA	CHC-C4B	3.77	1.47	1.39
14	A	815	CLA	OBD-CAD	3.77	1.29	1.22
14	L	204	CLA	CHB-C1B	3.77	1.47	1.39
14	cB	825	CLA	OBD-CAD	3.77	1.29	1.22
14	B	811	CLA	C3D-C2D	3.77	1.49	1.39
14	B	816	CLA	C3D-C2D	3.76	1.49	1.39
14	cB	812	CLA	CHB-C1B	3.76	1.47	1.39
14	B	823	CLA	CHC-C4B	3.76	1.47	1.39
14	A	852	CLA	C3D-C2D	3.76	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cA	839	CLA	C3D-C2D	3.76	1.49	1.39
14	bB	835	CLA	C3D-C2D	3.76	1.49	1.39
14	B	813	CLA	CHC-C4B	3.76	1.47	1.39
14	bB	811	CLA	C3D-C2D	3.76	1.49	1.39
14	cB	822	CLA	CHB-C1B	3.76	1.47	1.39
14	A	819	CLA	OBD-CAD	3.76	1.29	1.22
14	B	811	CLA	CHB-C1B	3.76	1.47	1.39
14	J	102	CLA	OBD-CAD	3.76	1.29	1.22
14	bA	809	CLA	CHC-C4B	3.76	1.47	1.39
14	bB	811	CLA	CHB-C1B	3.76	1.47	1.39
14	B	812	CLA	C3B-C4B	3.76	1.51	1.42
14	bB	813	CLA	CHC-C4B	3.76	1.47	1.39
14	A	812	CLA	C3D-C2D	3.76	1.49	1.39
14	A	818	CLA	C3D-C2D	3.76	1.49	1.39
14	bB	837	CLA	C3D-C2D	3.76	1.49	1.39
14	A	819	CLA	CHB-C1B	3.76	1.47	1.39
14	bA	819	CLA	CHB-C1B	3.76	1.47	1.39
14	bB	822	CLA	C3D-C2D	3.76	1.49	1.39
14	cB	813	CLA	C3B-C4B	3.76	1.51	1.42
14	A	832	CLA	CHD-C4C	3.76	1.47	1.39
14	cA	803	CLA	OBD-CAD	3.76	1.29	1.22
14	cA	824	CLA	OBD-CAD	3.76	1.29	1.22
14	cA	809	CLA	CHC-C4B	3.76	1.47	1.39
14	cA	821	CLA	CHC-C4B	3.76	1.47	1.39
14	B	820	CLA	OBD-CAD	3.76	1.29	1.22
14	bA	835	CLA	C3D-C2D	3.76	1.49	1.39
14	bA	815	CLA	OBD-CAD	3.76	1.29	1.22
14	cA	835	CLA	C3D-C2D	3.76	1.49	1.39
14	A	829	CLA	CHB-C1B	3.76	1.47	1.39
14	L	201	CLA	CHC-C4B	3.76	1.47	1.39
14	B	824	CLA	OBD-CAD	3.76	1.29	1.22
14	cA	819	CLA	OBD-CAD	3.75	1.28	1.22
14	bB	849	CLA	CHB-C1B	3.75	1.47	1.39
14	bA	852	CLA	C3D-C2D	3.75	1.49	1.39
14	J	101	CLA	OBD-CAD	3.75	1.28	1.22
14	cA	810	CLA	OBD-CAD	3.75	1.28	1.22
14	A	835	CLA	C3D-C2D	3.75	1.49	1.39
14	cB	823	CLA	C3D-C2D	3.75	1.49	1.39
14	cB	838	CLA	C3D-C2D	3.75	1.49	1.39
14	cA	818	CLA	C3D-C2D	3.75	1.49	1.39
14	cA	819	CLA	CHB-C1B	3.75	1.47	1.39
14	cA	832	CLA	CHC-C4B	3.75	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	833	CLA	C3B-C4B	3.75	1.51	1.42
14	bL	201	CLA	CHC-C4B	3.75	1.47	1.39
14	J	102	CLA	C3D-C2D	3.75	1.49	1.39
14	bB	805	CLA	CHC-C4B	3.75	1.47	1.39
14	L	202	CLA	CHB-C1B	3.75	1.47	1.39
14	cA	829	CLA	CHC-C4B	3.75	1.47	1.39
14	bB	824	CLA	OBD-CAD	3.75	1.28	1.22
14	A	821	CLA	CHC-C4B	3.75	1.47	1.39
14	A	809	CLA	CHC-C4B	3.75	1.47	1.39
14	B	805	CLA	CHC-C4B	3.75	1.47	1.39
14	bB	834	CLA	CHC-C4B	3.75	1.47	1.39
14	cA	834	CLA	CHB-C1B	3.75	1.47	1.39
14	B	822	CLA	C3D-C2D	3.75	1.49	1.39
14	cB	806	CLA	CHC-C4B	3.75	1.47	1.39
14	X	201	CLA	OBD-CAD	3.75	1.28	1.22
14	bB	833	CLA	C3B-C4B	3.75	1.51	1.42
14	A	832	CLA	CHC-C4B	3.75	1.47	1.39
14	A	842	CLA	OBD-CAD	3.75	1.28	1.22
14	B	849	CLA	OBD-CAD	3.75	1.28	1.22
14	bA	803	CLA	OBD-CAD	3.75	1.28	1.22
14	cA	829	CLA	CHB-C1B	3.75	1.47	1.39
14	cA	852	CLA	C3D-C2D	3.75	1.49	1.39
14	bB	803	CLA	CHD-C4C	3.75	1.47	1.39
14	bB	836	CLA	C3D-C2D	3.75	1.49	1.39
14	cB	835	CLA	CHB-C1B	3.75	1.47	1.39
14	B	803	CLA	CHD-C4C	3.75	1.47	1.39
14	cJ	101	CLA	OBD-CAD	3.74	1.28	1.22
14	J	102	CLA	CHB-C1B	3.74	1.47	1.39
14	cB	850	CLA	CHB-C1B	3.74	1.47	1.39
14	cB	810	CLA	CHD-C4C	3.74	1.47	1.39
14	bJ	101	CLA	OBD-CAD	3.74	1.28	1.22
14	bA	829	CLA	CHB-C1B	3.74	1.47	1.39
14	A	824	CLA	OBD-CAD	3.74	1.28	1.22
14	bA	829	CLA	CHC-C4B	3.74	1.47	1.39
14	A	803	CLA	OBD-CAD	3.74	1.28	1.22
14	bA	812	CLA	C3D-C2D	3.74	1.49	1.39
14	B	809	CLA	CHD-C4C	3.74	1.47	1.39
14	bA	819	CLA	OBD-CAD	3.74	1.28	1.22
14	A	834	CLA	CHB-C1B	3.74	1.47	1.39
17	bI	101	BCR	C17-C18	3.74	1.40	1.35
14	cJ	102	CLA	C3D-C2D	3.74	1.49	1.39
14	B	811	CLA	C3B-C4B	3.74	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cA	834	CLA	C3D-C2D	3.74	1.49	1.39
14	A	807	CLA	CHB-C1B	3.74	1.47	1.39
14	X	201	CLA	C3D-C2D	3.74	1.49	1.39
14	cX	201	CLA	OBD-CAD	3.74	1.28	1.22
14	A	823	CLA	OBD-CAD	3.74	1.28	1.22
14	bA	842	CLA	OBD-CAD	3.74	1.28	1.22
14	B	826	CLA	CHB-C1B	3.74	1.47	1.39
14	bA	834	CLA	CHB-C1B	3.74	1.47	1.39
14	B	822	CLA	OBD-CAD	3.74	1.28	1.22
14	cB	850	CLA	OBD-CAD	3.74	1.28	1.22
14	bB	809	CLA	CHD-C4C	3.74	1.47	1.39
14	bA	807	CLA	CHB-C1B	3.74	1.47	1.39
14	bX	201	CLA	C3D-C2D	3.74	1.49	1.39
14	B	821	CLA	CHC-C4B	3.73	1.47	1.39
14	B	849	CLA	CHB-C1B	3.73	1.47	1.39
14	bB	833	CLA	OBD-CAD	3.73	1.28	1.22
14	bB	806	CLA	CHB-C1B	3.73	1.47	1.39
14	cA	807	CLA	CHB-C1B	3.73	1.47	1.39
14	A	829	CLA	CHC-C4B	3.73	1.47	1.39
14	bB	851	CLA	CHB-C1B	3.73	1.47	1.39
14	cB	835	CLA	CHC-C4B	3.73	1.47	1.39
14	A	816	CLA	OBD-CAD	3.73	1.28	1.22
14	B	833	CLA	OBD-CAD	3.73	1.28	1.22
14	bB	811	CLA	C3B-C4B	3.73	1.51	1.42
14	cJ	102	CLA	CHB-C1B	3.73	1.47	1.39
14	bB	802	CLA	CHC-C4B	3.73	1.47	1.39
14	B	821	CLA	C3D-C2D	3.73	1.49	1.39
14	bB	826	CLA	C4B-NB	-3.73	1.33	1.37
14	B	806	CLA	CHB-C1B	3.73	1.47	1.39
14	bB	820	CLA	OBD-CAD	3.73	1.28	1.22
14	cB	822	CLA	C3D-C2D	3.73	1.49	1.39
14	A	834	CLA	C3D-C2D	3.73	1.49	1.39
14	bB	821	CLA	C3D-C2D	3.73	1.49	1.39
14	B	838	CLA	CHB-C1B	3.73	1.47	1.39
14	bB	836	CLA	CHB-C1B	3.73	1.47	1.39
14	cL	202	CLA	CHC-C4B	3.73	1.47	1.39
14	bA	834	CLA	C3D-C2D	3.73	1.49	1.39
14	cX	201	CLA	C3D-C2D	3.73	1.49	1.39
14	cL	205	CLA	OBD-CAD	3.73	1.28	1.22
14	bJ	102	CLA	C3D-C2D	3.73	1.49	1.39
14	bB	822	CLA	OBD-CAD	3.73	1.28	1.22
14	B	802	CLA	CHC-C4B	3.73	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	851	CLA	CHB-C1B	3.73	1.47	1.39
14	B	836	CLA	CHB-C1B	3.73	1.47	1.39
14	cB	837	CLA	C3D-C2D	3.73	1.49	1.39
14	bB	801	CLA	OBD-CAD	3.73	1.28	1.22
14	cB	807	CLA	CHB-C1B	3.73	1.47	1.39
14	cB	803	CLA	CHC-C4B	3.73	1.47	1.39
14	bA	823	CLA	OBD-CAD	3.73	1.28	1.22
14	cB	821	CLA	C3D-C2D	3.73	1.49	1.39
14	L	203	CLA	OBD-CAD	3.73	1.28	1.22
14	bL	203	CLA	OBD-CAD	3.73	1.28	1.22
14	bL	202	CLA	CHB-C1B	3.73	1.47	1.39
14	cA	828	CLA	CHB-C1B	3.73	1.47	1.39
14	bA	819	CLA	C3D-C2D	3.73	1.49	1.39
14	bB	821	CLA	CHC-C4B	3.72	1.47	1.39
14	cB	839	CLA	CHB-C1B	3.72	1.47	1.39
14	cL	203	CLA	CHB-C1B	3.72	1.47	1.39
14	L	204	CLA	OBD-CAD	3.72	1.28	1.22
14	cX	201	CLA	CHB-C1B	3.72	1.47	1.39
14	bA	832	CLA	CHC-C4B	3.72	1.47	1.39
14	bB	838	CLA	CHB-C1B	3.72	1.47	1.39
14	cB	801	CLA	CHB-C1B	3.72	1.47	1.39
14	bA	824	CLA	OBD-CAD	3.72	1.28	1.22
14	bA	821	CLA	CHC-C4B	3.72	1.47	1.39
14	cL	204	CLA	OBD-CAD	3.72	1.28	1.22
14	A	811	CLA	C3D-C2D	3.72	1.49	1.39
14	A	811	CLA	OBD-CAD	3.72	1.28	1.22
14	bX	201	CLA	OBD-CAD	3.72	1.28	1.22
14	cA	816	CLA	OBD-CAD	3.72	1.28	1.22
14	bA	811	CLA	C3D-C2D	3.72	1.49	1.39
14	A	828	CLA	CHB-C1B	3.72	1.47	1.39
14	bA	806	CLA	C3D-C2D	3.72	1.49	1.39
14	X	201	CLA	CHB-C1B	3.72	1.47	1.39
14	cB	822	CLA	CHC-C4B	3.72	1.47	1.39
14	B	831	CLA	C3D-C2D	3.72	1.49	1.39
14	bB	851	CLA	C3D-C2D	3.72	1.49	1.39
14	cA	811	CLA	C3D-C2D	3.72	1.49	1.39
14	cB	827	CLA	C4B-NB	-3.72	1.33	1.37
14	bA	828	CLA	CHB-C1B	3.72	1.47	1.39
14	bX	201	CLA	CHB-C1B	3.72	1.47	1.39
14	B	820	CLA	C3D-C2D	3.72	1.49	1.39
14	cA	809	CLA	C3D-C2D	3.72	1.49	1.39
14	B	834	CLA	OBD-CAD	3.72	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cB	812	CLA	C3B-C4B	3.72	1.51	1.42
14	A	809	CLA	C3D-C2D	3.72	1.49	1.39
14	B	815	CLA	CHB-C1B	3.72	1.47	1.39
14	bB	826	CLA	CHB-C1B	3.72	1.47	1.39
14	cA	819	CLA	C3D-C2D	3.72	1.49	1.39
14	B	801	CLA	OBD-CAD	3.72	1.28	1.22
14	cB	830	CLA	OBD-CAD	3.72	1.28	1.22
14	cA	806	CLA	C3D-C2D	3.72	1.49	1.39
14	B	834	CLA	CHC-C4B	3.72	1.47	1.39
14	bJ	102	CLA	CHB-C1B	3.72	1.47	1.39
14	B	851	CLA	C3D-C2D	3.71	1.49	1.39
14	cB	823	CLA	OBD-CAD	3.71	1.28	1.22
14	bA	808	CLA	OBD-CAD	3.71	1.28	1.22
14	B	810	CLA	CHC-C4B	3.71	1.47	1.39
14	bB	815	CLA	CHB-C1B	3.71	1.47	1.39
14	bB	839	CLA	CHD-C4C	3.71	1.47	1.39
14	B	836	CLA	C3D-C2D	3.71	1.49	1.39
14	bB	820	CLA	C3D-C2D	3.71	1.49	1.39
14	cA	837	CLA	C3D-C2D	3.71	1.49	1.39
14	bA	823	CLA	CHB-C1B	3.71	1.47	1.39
14	cB	840	CLA	CHD-C4C	3.71	1.47	1.39
14	cA	842	CLA	OBD-CAD	3.71	1.28	1.22
14	B	839	CLA	CHD-C4C	3.71	1.47	1.39
14	bA	852	CLA	C1B-NB	-3.71	1.33	1.37
14	bA	842	CLA	CHB-C1B	3.71	1.47	1.39
14	bB	817	CLA	CHB-C1B	3.71	1.47	1.39
14	cB	801	CLA	C3D-C2D	3.71	1.49	1.39
14	cB	816	CLA	CHB-C1B	3.71	1.47	1.39
14	A	807	CLA	C3D-C2D	3.71	1.49	1.39
14	A	819	CLA	C3D-C2D	3.71	1.49	1.39
14	A	825	CLA	CHB-C1B	3.71	1.47	1.39
14	bB	819	CLA	CHB-C1B	3.71	1.47	1.39
14	cB	840	CLA	CHB-C1B	3.71	1.47	1.39
14	bA	809	CLA	C3D-C2D	3.71	1.49	1.39
14	cB	820	CLA	CHB-C1B	3.71	1.47	1.39
14	cA	811	CLA	OBD-CAD	3.71	1.28	1.22
14	cA	842	CLA	CHB-C1B	3.71	1.47	1.39
14	bB	849	CLA	OBD-CAD	3.71	1.28	1.22
14	B	819	CLA	CHB-C1B	3.71	1.47	1.39
14	bA	826	CLA	C3D-C2D	3.71	1.49	1.39
14	cB	818	CLA	CHB-C1B	3.71	1.47	1.39
14	bA	837	CLA	C3D-C2D	3.71	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cA	825	CLA	CHB-C1B	3.71	1.47	1.39
14	A	802	CLA	CHC-C1C	3.71	1.46	1.38
14	A	837	CLA	C3D-C2D	3.71	1.49	1.39
14	B	823	CLA	CHB-C1B	3.71	1.47	1.39
14	A	806	CLA	C3D-C2D	3.71	1.49	1.39
14	J	101	CLA	CHB-C1B	3.71	1.47	1.39
14	bB	831	CLA	C3D-C2D	3.71	1.49	1.39
14	A	825	CLA	CHC-C4B	3.71	1.47	1.39
14	A	826	CLA	C3D-C2D	3.71	1.49	1.39
14	A	808	CLA	OBD-CAD	3.71	1.28	1.22
14	B	829	CLA	OBD-CAD	3.71	1.28	1.22
14	bB	834	CLA	OBD-CAD	3.71	1.28	1.22
14	cA	852	CLA	C1B-NB	-3.71	1.33	1.37
14	B	807	CLA	CHC-C4B	3.71	1.47	1.39
14	bA	807	CLA	C3D-C2D	3.71	1.49	1.39
14	A	840	CLA	OBD-CAD	3.71	1.28	1.22
14	bA	836	CLA	CHC-C4B	3.71	1.47	1.39
14	cB	837	CLA	CHB-C1B	3.71	1.47	1.39
14	bA	812	CLA	CHB-C1B	3.70	1.47	1.39
14	cB	824	CLA	CHB-C1B	3.70	1.47	1.39
14	bB	810	CLA	CHC-C4B	3.70	1.47	1.39
14	B	832	CLA	C3D-C2D	3.70	1.49	1.39
14	cA	812	CLA	CHB-C1B	3.70	1.47	1.39
14	A	823	CLA	CHB-C1B	3.70	1.47	1.39
14	bA	839	CLA	CHB-C1B	3.70	1.47	1.39
14	cA	825	CLA	CHC-C4B	3.70	1.47	1.39
14	cA	840	CLA	OBD-CAD	3.70	1.28	1.22
14	B	817	CLA	CHB-C1B	3.70	1.47	1.39
14	cA	823	CLA	CHB-C1B	3.70	1.47	1.39
14	cB	827	CLA	CHB-C1B	3.70	1.47	1.39
14	cA	836	CLA	CHC-C4B	3.70	1.47	1.39
14	cA	839	CLA	CHB-C1B	3.70	1.47	1.39
14	bA	840	CLA	OBD-CAD	3.70	1.28	1.22
14	cB	835	CLA	OBD-CAD	3.70	1.28	1.22
14	cB	832	CLA	C3D-C2D	3.70	1.49	1.39
14	B	826	CLA	C4B-NB	-3.70	1.33	1.37
14	bJ	101	CLA	C3B-C4B	3.70	1.51	1.42
14	A	828	CLA	C4B-NB	-3.70	1.33	1.37
14	cB	811	CLA	CHC-C4B	3.70	1.47	1.39
14	bB	832	CLA	C3D-C2D	3.70	1.49	1.39
14	cB	834	CLA	OBD-CAD	3.70	1.28	1.22
14	bA	824	CLA	C3D-C2D	3.70	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bJ	101	CLA	CHB-C1B	3.70	1.47	1.39
14	cB	833	CLA	C3D-C2D	3.70	1.49	1.39
14	A	812	CLA	CHB-C1B	3.70	1.47	1.39
14	bA	825	CLA	CHC-C4B	3.70	1.47	1.39
14	A	820	CLA	C3B-C4B	3.70	1.51	1.42
14	bA	825	CLA	CHB-C1B	3.70	1.47	1.39
14	cA	807	CLA	C3D-C2D	3.70	1.49	1.39
14	bA	834	CLA	C3B-C4B	3.70	1.51	1.42
14	bA	831	CLA	OBD-CAD	3.70	1.28	1.22
14	bB	829	CLA	OBD-CAD	3.70	1.28	1.22
14	A	836	CLA	CHC-C4B	3.70	1.47	1.39
14	A	842	CLA	CHB-C1B	3.70	1.47	1.39
14	cA	802	CLA	CHC-C1C	3.70	1.46	1.38
14	A	852	CLA	C1B-NB	-3.70	1.33	1.37
14	bA	802	CLA	CHC-C1C	3.70	1.46	1.38
14	bB	810	CLA	OBD-CAD	3.69	1.28	1.22
14	cA	823	CLA	OBD-CAD	3.69	1.28	1.22
14	cJ	101	CLA	C3B-C4B	3.69	1.51	1.42
14	B	810	CLA	OBD-CAD	3.69	1.28	1.22
14	bB	823	CLA	CHB-C1B	3.69	1.47	1.39
14	A	839	CLA	CHB-C1B	3.69	1.47	1.39
14	B	839	CLA	CHB-C1B	3.69	1.47	1.39
14	cA	824	CLA	C3D-C2D	3.69	1.49	1.39
14	L	203	CLA	CHC-C4B	3.69	1.47	1.39
14	bA	824	CLA	CHC-C4B	3.69	1.47	1.39
14	bL	204	CLA	OBD-CAD	3.69	1.28	1.22
14	cA	808	CLA	OBD-CAD	3.69	1.28	1.22
14	A	824	CLA	C3D-C2D	3.69	1.49	1.39
14	J	101	CLA	C3B-C4B	3.69	1.51	1.42
14	A	824	CLA	CHC-C4B	3.69	1.47	1.39
14	bA	828	CLA	C4B-NB	-3.69	1.33	1.37
14	A	818	CLA	OBD-CAD	3.69	1.28	1.22
14	bA	808	CLA	C3D-C2D	3.69	1.49	1.39
14	cB	811	CLA	OBD-CAD	3.69	1.28	1.22
14	cA	834	CLA	C3B-C4B	3.69	1.51	1.42
14	cL	204	CLA	CHD-C1D	3.69	1.45	1.38
14	cB	808	CLA	CHC-C4B	3.69	1.47	1.39
14	cA	826	CLA	C3D-C2D	3.69	1.49	1.39
14	bB	807	CLA	CHC-C4B	3.69	1.47	1.39
14	L	203	CLA	CHD-C1D	3.69	1.45	1.38
14	cJ	101	CLA	CHB-C1B	3.69	1.47	1.39
14	A	808	CLA	C3D-C2D	3.69	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	836	CLA	C4B-NB	-3.69	1.33	1.37
14	A	834	CLA	C3B-C4B	3.69	1.51	1.42
14	B	815	CLA	C3D-C2D	3.69	1.49	1.39
14	bB	815	CLA	C3D-C2D	3.69	1.49	1.39
14	cB	816	CLA	C3D-C2D	3.69	1.49	1.39
14	cB	809	CLA	OBD-CAD	3.69	1.28	1.22
14	cA	824	CLA	CHC-C4B	3.69	1.47	1.39
14	bB	839	CLA	CHB-C1B	3.68	1.47	1.39
14	bA	836	CLA	C4B-NB	-3.68	1.33	1.37
14	bA	816	CLA	OBD-CAD	3.68	1.28	1.22
14	cA	813	CLA	C3D-C2D	3.68	1.49	1.39
14	bA	811	CLA	OBD-CAD	3.68	1.28	1.22
14	cB	802	CLA	OBD-CAD	3.68	1.28	1.22
14	cB	826	CLA	C3B-C4B	3.68	1.51	1.42
17	I	102	BCR	C17-C18	3.68	1.40	1.35
14	cA	828	CLA	C4B-NB	-3.68	1.33	1.37
14	B	823	CLA	C3D-C2D	3.68	1.49	1.39
14	A	813	CLA	C3D-C2D	3.68	1.49	1.39
14	cB	824	CLA	C3D-C2D	3.68	1.49	1.39
14	bA	813	CLA	C3D-C2D	3.68	1.49	1.39
14	bB	805	CLA	C3D-C2D	3.68	1.49	1.39
14	A	811	CLA	C3B-C4B	3.68	1.51	1.42
14	cA	813	CLA	CHB-C1B	3.68	1.47	1.39
14	A	805	CLA	C3D-C2D	3.68	1.49	1.39
14	cA	805	CLA	C3D-C2D	3.68	1.49	1.39
14	B	822	CLA	CHB-C1B	3.67	1.47	1.39
14	bB	822	CLA	CHB-C1B	3.67	1.47	1.39
14	A	819	CLA	C3B-C4B	3.67	1.51	1.42
14	cA	836	CLA	C4B-NB	-3.67	1.33	1.37
14	cB	817	CLA	C3B-C4B	3.67	1.51	1.42
14	cB	839	CLA	C3D-C2D	3.67	1.49	1.39
14	bB	825	CLA	CHB-C1B	3.67	1.47	1.39
14	B	825	CLA	C3B-C4B	3.67	1.51	1.42
14	bA	805	CLA	C3D-C2D	3.67	1.49	1.39
14	cB	826	CLA	CHB-C1B	3.67	1.47	1.39
14	B	805	CLA	C3D-C2D	3.67	1.49	1.39
14	cB	806	CLA	C3D-C2D	3.67	1.49	1.39
14	bL	203	CLA	CHD-C1D	3.67	1.45	1.38
14	B	825	CLA	CHB-C1B	3.67	1.47	1.39
14	cB	823	CLA	CHB-C1B	3.67	1.47	1.39
14	bB	823	CLA	C3D-C2D	3.67	1.49	1.39
14	bB	825	CLA	C3B-C4B	3.67	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cA	819	CLA	C3B-C4B	3.67	1.51	1.42
14	A	841	CLA	CHB-C1B	3.67	1.47	1.39
14	A	840	CLA	C3B-C4B	3.67	1.51	1.42
14	cA	808	CLA	C3D-C2D	3.67	1.49	1.39
14	bA	820	CLA	C3B-C4B	3.67	1.51	1.42
14	cB	836	CLA	OBD-CAD	3.67	1.28	1.22
13	bA	801	CL0	CHD-C4C	3.67	1.47	1.39
13	bA	801	CL0	C3D-C2D	3.67	1.49	1.39
14	bA	840	CLA	C3B-C4B	3.67	1.51	1.42
14	cA	820	CLA	C3B-C4B	3.67	1.51	1.42
14	A	821	CLA	OBD-CAD	3.67	1.28	1.22
14	A	839	CLA	CHC-C4B	3.66	1.47	1.39
14	cL	204	CLA	CHC-C4B	3.66	1.47	1.39
13	cA	801	CL0	CHD-C4C	3.66	1.47	1.39
14	bB	838	CLA	C3D-C2D	3.66	1.49	1.39
17	bI	102	BCR	C17-C18	3.66	1.40	1.35
14	bB	808	CLA	OBD-CAD	3.66	1.28	1.22
14	bB	835	CLA	OBD-CAD	3.66	1.28	1.22
14	bA	822	CLA	C3B-C4B	3.66	1.51	1.42
13	A	801	CL0	C3D-C2D	3.66	1.49	1.39
14	bB	808	CLA	CHD-C4C	3.66	1.47	1.39
14	cA	840	CLA	C3B-C4B	3.66	1.51	1.42
14	bL	203	CLA	CHC-C4B	3.66	1.47	1.39
14	bA	819	CLA	C3B-C4B	3.66	1.51	1.42
14	A	809	CLA	OBD-CAD	3.66	1.28	1.22
14	cA	831	CLA	OBD-CAD	3.66	1.28	1.22
14	bB	801	CLA	C3D-C2D	3.66	1.49	1.39
14	A	842	CLA	C3D-C2D	3.66	1.49	1.39
14	bB	816	CLA	C3B-C4B	3.66	1.51	1.42
17	cI	102	BCR	C17-C18	3.66	1.40	1.35
14	cF	201	CLA	CHB-C1B	3.66	1.47	1.39
14	B	838	CLA	C3D-C2D	3.66	1.49	1.39
14	bF	201	CLA	CHB-C1B	3.66	1.47	1.39
13	A	801	CL0	CHD-C4C	3.66	1.47	1.39
13	cA	801	CL0	C3D-C2D	3.66	1.49	1.39
14	cB	802	CLA	C3D-C2D	3.66	1.49	1.39
14	bB	808	CLA	C1B-NB	-3.66	1.33	1.37
14	cB	809	CLA	C1B-NB	-3.66	1.33	1.37
14	cA	818	CLA	OBD-CAD	3.66	1.28	1.22
14	bA	841	CLA	CHB-C1B	3.65	1.47	1.39
14	cA	802	CLA	C3D-C2D	3.65	1.49	1.39
17	B	844	BCR	C10-C9	3.65	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bA	821	CLA	OBD-CAD	3.65	1.28	1.22
14	cA	809	CLA	OBD-CAD	3.65	1.28	1.22
14	B	816	CLA	C3B-C4B	3.65	1.51	1.42
14	bA	842	CLA	C3D-C2D	3.65	1.49	1.39
14	A	831	CLA	OBD-CAD	3.65	1.28	1.22
14	cA	840	CLA	C3D-C2D	3.65	1.49	1.39
14	bA	840	CLA	C3D-C2D	3.65	1.49	1.39
14	cA	821	CLA	OBD-CAD	3.65	1.28	1.22
14	bA	802	CLA	C3D-C2D	3.65	1.49	1.39
14	B	808	CLA	OBD-CAD	3.65	1.28	1.22
14	cB	815	CLA	OBD-CAD	3.65	1.28	1.22
14	cA	841	CLA	CHB-C1B	3.65	1.47	1.39
14	A	840	CLA	C3D-C2D	3.65	1.49	1.39
14	bA	809	CLA	OBD-CAD	3.65	1.28	1.22
14	A	802	CLA	C3D-C2D	3.65	1.49	1.39
14	cF	201	CLA	OBD-CAD	3.65	1.28	1.22
14	B	819	CLA	C3B-C4B	3.65	1.51	1.42
14	cA	839	CLA	CHC-C4B	3.65	1.47	1.39
14	bB	819	CLA	C3B-C4B	3.65	1.51	1.42
14	bB	815	CLA	C3B-C4B	3.64	1.51	1.42
14	bA	824	CLA	C1B-NB	-3.64	1.33	1.37
14	A	813	CLA	CHB-C1B	3.64	1.47	1.39
14	B	801	CLA	C3D-C2D	3.64	1.49	1.39
14	B	835	CLA	OBD-CAD	3.64	1.28	1.22
14	bA	809	CLA	CHB-C1B	3.64	1.47	1.39
14	bA	818	CLA	OBD-CAD	3.64	1.28	1.22
14	cA	811	CLA	C3B-C4B	3.64	1.51	1.42
14	B	829	CLA	CHC-C4B	3.64	1.47	1.39
14	bA	827	CLA	C3D-C2D	3.64	1.49	1.39
14	A	809	CLA	CHB-C1B	3.64	1.47	1.39
14	bA	811	CLA	C3B-C4B	3.64	1.51	1.42
14	B	808	CLA	CHD-C4C	3.64	1.47	1.39
14	B	809	CLA	C1D-ND	3.64	1.42	1.37
14	cB	827	CLA	CHD-C1D	3.64	1.45	1.38
14	cB	809	CLA	CHD-C4C	3.64	1.47	1.39
14	bB	814	CLA	C3D-C2D	3.64	1.49	1.39
14	cA	824	CLA	C1B-NB	-3.64	1.33	1.37
14	B	831	CLA	CHB-C1B	3.64	1.47	1.39
14	bB	829	CLA	CHC-C4B	3.64	1.47	1.39
14	cA	822	CLA	C3B-C4B	3.63	1.51	1.42
14	B	814	CLA	C3D-C2D	3.63	1.49	1.39
14	bB	814	CLA	OBD-CAD	3.63	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bF	201	CLA	OBD-CAD	3.63	1.28	1.22
14	A	827	CLA	C3D-C2D	3.63	1.49	1.39
14	cA	827	CLA	C3D-C2D	3.63	1.49	1.39
14	cA	813	CLA	C3B-C4B	3.63	1.51	1.42
14	cB	820	CLA	C3B-C4B	3.63	1.51	1.42
14	A	822	CLA	C3B-C4B	3.63	1.51	1.42
14	bB	817	CLA	C3D-C2D	3.63	1.49	1.39
14	A	824	CLA	C1B-NB	-3.63	1.33	1.37
14	cA	842	CLA	C3D-C2D	3.63	1.49	1.39
14	bB	831	CLA	CHB-C1B	3.63	1.47	1.39
14	bA	804	CLA	OBD-CAD	3.63	1.28	1.22
14	cA	809	CLA	CHB-C1B	3.63	1.47	1.39
14	cB	830	CLA	CHC-C4B	3.63	1.47	1.39
14	cA	804	CLA	OBD-CAD	3.63	1.28	1.22
14	A	805	CLA	OBD-CAD	3.63	1.28	1.22
14	bB	809	CLA	C1D-ND	3.63	1.42	1.37
14	cB	850	CLA	C3B-C4B	3.63	1.51	1.42
14	B	814	CLA	OBD-CAD	3.63	1.28	1.22
14	F	201	CLA	CHB-C1B	3.63	1.47	1.39
14	bA	839	CLA	CHC-C4B	3.63	1.47	1.39
14	B	817	CLA	C3D-C2D	3.63	1.49	1.39
14	L	203	CLA	C3D-C2D	3.63	1.49	1.39
14	cB	832	CLA	CHB-C1B	3.63	1.47	1.39
14	cB	815	CLA	C3D-C2D	3.63	1.49	1.39
14	cB	818	CLA	C3D-C2D	3.63	1.49	1.39
14	bA	835	CLA	C3B-C4B	3.63	1.51	1.42
14	F	201	CLA	OBD-CAD	3.63	1.28	1.22
14	B	808	CLA	CHB-C1B	3.63	1.47	1.39
14	A	813	CLA	C3B-C4B	3.63	1.51	1.42
14	B	805	CLA	CHB-C1B	3.63	1.47	1.39
14	B	808	CLA	C1B-NB	-3.63	1.33	1.37
14	bA	813	CLA	C3B-C4B	3.63	1.51	1.42
14	B	827	CLA	C3D-C2D	3.62	1.49	1.39
14	B	849	CLA	C3B-C4B	3.62	1.51	1.42
14	cB	828	CLA	C3D-C2D	3.62	1.49	1.39
14	bB	827	CLA	C3D-C2D	3.62	1.49	1.39
14	bB	805	CLA	CHB-C1B	3.62	1.47	1.39
14	cA	835	CLA	CHB-C1B	3.62	1.47	1.39
14	bA	813	CLA	CHB-C1B	3.62	1.47	1.39
14	bB	817	CLA	CHC-C4B	3.62	1.47	1.39
14	cB	830	CLA	C3D-C2D	3.62	1.49	1.39
14	bA	835	CLA	CHB-C1B	3.62	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	826	CLA	CHD-C1D	3.62	1.45	1.38
14	bB	826	CLA	CHD-C1D	3.62	1.45	1.38
14	bB	808	CLA	CHB-C1B	3.62	1.47	1.39
17	cB	845	BCR	C10-C9	3.62	1.40	1.35
14	A	804	CLA	OBD-CAD	3.62	1.28	1.22
14	cB	806	CLA	CHB-C1B	3.62	1.47	1.39
14	B	803	CLA	CHB-C1B	3.62	1.47	1.39
14	B	815	CLA	C3B-C4B	3.62	1.51	1.42
17	bB	844	BCR	C10-C9	3.62	1.40	1.35
14	bB	849	CLA	C3B-C4B	3.62	1.51	1.42
14	bF	201	CLA	C3D-C2D	3.62	1.49	1.39
14	cA	835	CLA	C3B-C4B	3.62	1.51	1.42
14	A	835	CLA	C3B-C4B	3.62	1.51	1.42
14	bX	201	CLA	C3B-C4B	3.62	1.51	1.42
14	cB	816	CLA	C3B-C4B	3.62	1.51	1.42
14	A	832	CLA	C3D-C2D	3.62	1.49	1.39
14	bL	203	CLA	C3D-C2D	3.62	1.49	1.39
14	X	201	CLA	C3B-C4B	3.62	1.51	1.42
13	cA	801	CL0	OBD-CAD	3.61	1.28	1.22
14	A	835	CLA	CHB-C1B	3.61	1.47	1.39
14	cB	804	CLA	CHB-C1B	3.61	1.47	1.39
14	cL	204	CLA	C3D-C2D	3.61	1.49	1.39
14	B	803	CLA	CHC-C4B	3.61	1.47	1.39
14	cB	809	CLA	CHB-C1B	3.61	1.47	1.39
14	A	836	CLA	C3D-C2D	3.61	1.49	1.39
14	cB	840	CLA	CHC-C4B	3.61	1.47	1.39
14	cA	836	CLA	C3D-C2D	3.61	1.49	1.39
14	bB	839	CLA	CHC-C4B	3.61	1.47	1.39
14	bB	803	CLA	CHB-C1B	3.61	1.47	1.39
14	B	826	CLA	CHD-C4C	3.61	1.47	1.39
14	cA	831	CLA	CHC-C4B	3.61	1.47	1.39
14	B	839	CLA	CHC-C4B	3.61	1.47	1.39
14	bA	831	CLA	CHC-C4B	3.61	1.47	1.39
14	cB	818	CLA	CHC-C4B	3.61	1.47	1.39
14	cX	201	CLA	C3B-C4B	3.61	1.51	1.42
14	cA	832	CLA	C3D-C2D	3.61	1.49	1.39
14	bB	804	CLA	CHB-C1B	3.61	1.47	1.39
14	cB	810	CLA	C1D-ND	3.60	1.42	1.37
14	cA	837	CLA	CHC-C4B	3.60	1.47	1.39
14	F	201	CLA	C3D-C2D	3.60	1.49	1.39
14	bA	836	CLA	C3D-C2D	3.60	1.49	1.39
14	bA	832	CLA	C3D-C2D	3.60	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	828	CLA	CHC-C4B	3.60	1.47	1.39
14	A	838	CLA	CHC-C4B	3.60	1.47	1.39
14	B	817	CLA	CHC-C4B	3.60	1.47	1.39
13	bA	801	CL0	OBD-CAD	3.60	1.28	1.22
14	bA	808	CLA	C3B-C4B	3.60	1.51	1.42
14	A	806	CLA	CHB-C1B	3.60	1.47	1.39
14	bB	824	CLA	CHB-C1B	3.60	1.47	1.39
14	cB	804	CLA	CHC-C4B	3.60	1.47	1.39
14	cB	805	CLA	CHB-C1B	3.60	1.47	1.39
14	A	831	CLA	CHC-C4B	3.60	1.47	1.39
14	B	828	CLA	C1B-NB	-3.60	1.33	1.37
14	bB	828	CLA	C1B-NB	-3.60	1.33	1.37
14	cA	805	CLA	OBD-CAD	3.60	1.28	1.22
14	bB	829	CLA	C3D-C2D	3.60	1.48	1.39
14	bA	805	CLA	OBD-CAD	3.60	1.28	1.22
14	B	804	CLA	CHB-C1B	3.60	1.47	1.39
14	B	829	CLA	C3D-C2D	3.59	1.48	1.39
14	A	837	CLA	CHC-C4B	3.59	1.47	1.39
14	bA	806	CLA	CHB-C1B	3.59	1.47	1.39
14	bB	806	CLA	C3D-C2D	3.59	1.48	1.39
14	cA	806	CLA	CHB-C1B	3.59	1.47	1.39
14	cA	822	CLA	CHC-C4B	3.59	1.47	1.39
14	cB	807	CLA	C3D-C2D	3.59	1.48	1.39
14	A	804	CLA	CHB-C1B	3.59	1.47	1.39
14	cB	829	CLA	CHC-C4B	3.59	1.47	1.39
14	bB	826	CLA	CHD-C4C	3.59	1.47	1.39
14	bA	837	CLA	CHC-C4B	3.59	1.47	1.39
14	B	806	CLA	C3D-C2D	3.59	1.48	1.39
14	cA	804	CLA	CHB-C1B	3.59	1.47	1.39
14	bB	802	CLA	CHB-C1B	3.59	1.47	1.39
14	cB	829	CLA	C1B-NB	-3.59	1.33	1.37
14	bA	804	CLA	CHB-C1B	3.59	1.47	1.39
14	bA	826	CLA	OBD-CAD	3.58	1.28	1.22
14	cF	201	CLA	C3D-C2D	3.58	1.48	1.39
14	B	802	CLA	CHB-C1B	3.58	1.47	1.39
14	bA	838	CLA	CHC-C4B	3.58	1.47	1.39
14	cB	827	CLA	CHD-C4C	3.58	1.47	1.39
14	bB	828	CLA	CHC-C4B	3.58	1.47	1.39
14	cB	803	CLA	CHD-C4C	3.58	1.47	1.39
14	bB	809	CLA	C3D-C2D	3.58	1.48	1.39
14	A	822	CLA	CHC-C4B	3.58	1.47	1.39
14	bA	822	CLA	CHC-C4B	3.58	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	809	CLA	C3D-C2D	3.58	1.48	1.39
14	cB	810	CLA	C3D-C2D	3.58	1.48	1.39
14	bB	803	CLA	CHC-C4B	3.58	1.47	1.39
14	bJ	102	CLA	C3B-C4B	3.58	1.51	1.42
14	A	808	CLA	C3B-C4B	3.58	1.51	1.42
13	A	801	CL0	OBD-CAD	3.57	1.28	1.22
14	cJ	102	CLA	C3B-C4B	3.57	1.51	1.42
14	B	818	CLA	OBD-CAD	3.57	1.28	1.22
14	cB	825	CLA	CHB-C1B	3.57	1.47	1.39
14	J	102	CLA	C3B-C4B	3.57	1.51	1.42
14	cA	808	CLA	CHB-C1B	3.57	1.47	1.39
14	A	808	CLA	CHB-C1B	3.57	1.47	1.39
14	B	833	CLA	CHB-C1B	3.57	1.47	1.39
14	cA	808	CLA	C3B-C4B	3.57	1.51	1.42
14	cA	834	CLA	OBD-CAD	3.57	1.28	1.22
14	A	807	CLA	C3B-C4B	3.57	1.51	1.42
14	cB	803	CLA	CHB-C1B	3.57	1.47	1.39
14	cB	819	CLA	OBD-CAD	3.57	1.28	1.22
14	B	824	CLA	CHB-C1B	3.57	1.47	1.39
14	bB	833	CLA	CHB-C1B	3.57	1.47	1.39
14	cB	834	CLA	CHB-C1B	3.57	1.47	1.39
14	A	806	CLA	OBD-CAD	3.57	1.28	1.22
14	cA	805	CLA	C1B-NB	-3.57	1.33	1.37
14	A	826	CLA	OBD-CAD	3.57	1.28	1.22
14	cA	838	CLA	CHC-C4B	3.57	1.47	1.39
14	A	834	CLA	OBD-CAD	3.57	1.28	1.22
14	bA	807	CLA	C3B-C4B	3.56	1.51	1.42
14	cB	813	CLA	OBD-CAD	3.56	1.28	1.22
14	B	823	CLA	C1B-NB	-3.56	1.33	1.37
14	A	831	CLA	C3D-C2D	3.56	1.48	1.39
14	cA	837	CLA	C1B-NB	-3.56	1.33	1.37
14	bB	828	CLA	OBD-CAD	3.56	1.28	1.22
14	B	812	CLA	OBD-CAD	3.56	1.28	1.22
14	cA	826	CLA	OBD-CAD	3.56	1.28	1.22
14	B	802	CLA	CHD-C4C	3.56	1.47	1.39
14	B	818	CLA	C3B-C4B	3.56	1.51	1.42
14	bA	831	CLA	C3D-C2D	3.56	1.48	1.39
13	cA	801	CL0	CHB-C1B	3.56	1.47	1.39
14	bA	808	CLA	CHB-C1B	3.56	1.47	1.39
14	bB	816	CLA	CHB-C1B	3.56	1.47	1.39
14	cA	807	CLA	C3B-C4B	3.56	1.51	1.42
14	bB	804	CLA	OBD-CAD	3.56	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	828	CLA	OBD-CAD	3.55	1.28	1.22
14	bA	834	CLA	OBD-CAD	3.55	1.28	1.22
14	A	820	CLA	CHB-C1B	3.55	1.47	1.39
14	bB	818	CLA	C3B-C4B	3.55	1.51	1.42
14	bB	818	CLA	OBD-CAD	3.55	1.28	1.22
14	cB	829	CLA	CHB-C1B	3.55	1.47	1.39
14	cB	817	CLA	CHB-C1B	3.55	1.47	1.39
14	bB	827	CLA	OBD-CAD	3.55	1.28	1.22
14	cA	831	CLA	C3D-C2D	3.55	1.48	1.39
14	B	826	CLA	CHC-C4B	3.55	1.47	1.39
14	bA	820	CLA	CHB-C1B	3.55	1.47	1.39
14	bB	826	CLA	CHC-C4B	3.55	1.47	1.39
14	bB	828	CLA	CHB-C1B	3.55	1.47	1.39
14	cB	819	CLA	CHB-C1B	3.55	1.47	1.39
13	A	801	CL0	CHB-C1B	3.55	1.47	1.39
14	bB	807	CLA	OBD-CAD	3.55	1.28	1.22
14	bB	812	CLA	OBD-CAD	3.55	1.28	1.22
14	B	818	CLA	CHB-C1B	3.55	1.47	1.39
14	cA	828	CLA	C1B-NB	-3.55	1.33	1.37
14	cA	820	CLA	CHB-C1B	3.55	1.47	1.39
14	cB	827	CLA	CHC-C4B	3.55	1.47	1.39
14	B	804	CLA	OBD-CAD	3.54	1.28	1.22
14	bA	829	CLA	OBD-CAD	3.54	1.28	1.22
14	cA	830	CLA	C1B-NB	-3.54	1.33	1.37
14	cB	824	CLA	C1B-NB	-3.54	1.33	1.37
14	cA	812	CLA	OBD-CAD	3.54	1.28	1.22
13	bA	801	CL0	CHB-C1B	3.54	1.47	1.39
14	cA	836	CLA	CHB-C1B	3.54	1.47	1.39
14	bB	802	CLA	CHD-C4C	3.54	1.47	1.39
14	bB	818	CLA	CHB-C1B	3.54	1.47	1.39
14	cA	852	CLA	CHC-C4B	3.54	1.47	1.39
14	bA	810	CLA	C3B-C4B	3.54	1.51	1.42
14	bA	805	CLA	C1B-NB	-3.54	1.33	1.37
14	cB	829	CLA	OBD-CAD	3.54	1.28	1.22
14	cB	828	CLA	OBD-CAD	3.53	1.28	1.22
14	A	811	CLA	CHB-C1B	3.53	1.47	1.39
14	A	823	CLA	C3B-C4B	3.53	1.51	1.42
14	bA	823	CLA	C3B-C4B	3.53	1.51	1.42
14	A	830	CLA	C1B-NB	-3.53	1.33	1.37
14	B	828	CLA	CHB-C1B	3.53	1.47	1.39
14	cA	830	CLA	CHB-C1B	3.53	1.47	1.39
14	cB	840	CLA	OBD-CAD	3.53	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bB	823	CLA	C1B-NB	-3.53	1.33	1.37
14	cB	837	CLA	OBD-CAD	3.53	1.28	1.22
14	A	838	CLA	C3D-C2D	3.53	1.48	1.39
14	A	810	CLA	C3B-C4B	3.53	1.51	1.42
14	B	816	CLA	CHB-C1B	3.53	1.47	1.39
14	cB	805	CLA	OBD-CAD	3.53	1.28	1.22
14	bB	836	CLA	OBD-CAD	3.53	1.28	1.22
14	A	805	CLA	C1B-NB	-3.53	1.33	1.37
14	B	807	CLA	OBD-CAD	3.53	1.28	1.22
14	bA	811	CLA	CHB-C1B	3.53	1.47	1.39
14	A	837	CLA	C1B-NB	-3.53	1.33	1.37
14	B	836	CLA	OBD-CAD	3.53	1.28	1.22
14	cB	808	CLA	OBD-CAD	3.53	1.28	1.22
14	A	828	CLA	C1B-NB	-3.53	1.33	1.37
14	cA	841	CLA	CHD-C4C	3.53	1.47	1.39
14	B	839	CLA	OBD-CAD	3.53	1.28	1.22
14	bA	838	CLA	C3D-C2D	3.52	1.48	1.39
14	cA	838	CLA	C3D-C2D	3.52	1.48	1.39
14	cA	806	CLA	OBD-CAD	3.52	1.28	1.22
14	bA	805	CLA	CHB-C1B	3.52	1.47	1.39
14	bA	837	CLA	C1B-NB	-3.52	1.33	1.37
14	cB	819	CLA	C3B-C4B	3.52	1.51	1.42
14	cA	810	CLA	C3B-C4B	3.52	1.51	1.42
14	cA	823	CLA	C3B-C4B	3.52	1.51	1.42
14	A	805	CLA	CHB-C1B	3.52	1.47	1.39
14	cA	805	CLA	CHB-C1B	3.52	1.47	1.39
14	bA	852	CLA	CHC-C4B	3.52	1.47	1.39
14	cA	811	CLA	CHB-C1B	3.52	1.47	1.39
14	bA	806	CLA	OBD-CAD	3.52	1.28	1.22
14	B	827	CLA	OBD-CAD	3.52	1.28	1.22
14	A	830	CLA	CHB-C1B	3.52	1.47	1.39
14	bA	830	CLA	C1B-NB	-3.52	1.33	1.37
14	A	822	CLA	CHB-C1B	3.52	1.47	1.39
14	A	852	CLA	CHC-C4B	3.52	1.47	1.39
14	cA	829	CLA	OBD-CAD	3.52	1.28	1.22
14	bA	830	CLA	CHB-C1B	3.52	1.47	1.39
14	bB	839	CLA	OBD-CAD	3.52	1.28	1.22
14	cB	818	CLA	C1B-NB	-3.52	1.33	1.37
14	cB	820	CLA	C3D-C2D	3.51	1.48	1.39
14	A	812	CLA	OBD-CAD	3.51	1.28	1.22
14	bA	822	CLA	CHB-C1B	3.51	1.47	1.39
14	bA	806	CLA	C3B-C4B	3.51	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cB	833	CLA	CHB-C1B	3.51	1.47	1.39
14	cB	814	CLA	OBD-CAD	3.51	1.28	1.22
14	cB	833	CLA	C3B-C4B	3.51	1.51	1.42
14	bB	819	CLA	C3D-C2D	3.51	1.48	1.39
14	B	825	CLA	C3D-C2D	3.51	1.48	1.39
14	B	832	CLA	C3B-C4B	3.51	1.51	1.42
14	bB	825	CLA	C3D-C2D	3.51	1.48	1.39
14	B	806	CLA	OBD-CAD	3.51	1.28	1.22
14	cB	802	CLA	CHB-C1B	3.50	1.47	1.39
14	bA	824	CLA	CHB-C1B	3.50	1.47	1.39
14	bA	828	CLA	CHC-C4B	3.50	1.47	1.39
14	bB	832	CLA	C3B-C4B	3.50	1.50	1.42
14	A	833	CLA	C1B-NB	-3.50	1.33	1.37
14	A	829	CLA	OBD-CAD	3.50	1.28	1.22
14	bA	828	CLA	C1B-NB	-3.50	1.33	1.37
14	cA	833	CLA	C1B-NB	-3.50	1.33	1.37
14	cB	812	CLA	OBD-CAD	3.50	1.28	1.22
14	A	824	CLA	CHB-C1B	3.50	1.47	1.39
14	cA	822	CLA	CHB-C1B	3.50	1.47	1.39
14	bB	832	CLA	CHB-C1B	3.50	1.47	1.39
14	bA	818	CLA	C1B-NB	-3.50	1.33	1.37
14	B	819	CLA	C3D-C2D	3.50	1.48	1.39
14	cA	806	CLA	C3B-C4B	3.50	1.50	1.42
14	bA	831	CLA	C1B-NB	-3.50	1.33	1.37
14	bB	801	CLA	CHB-C1B	3.50	1.47	1.39
14	cB	826	CLA	C3D-C2D	3.50	1.48	1.39
14	bB	805	CLA	OBD-CAD	3.50	1.28	1.22
14	bB	806	CLA	OBD-CAD	3.50	1.28	1.22
14	A	841	CLA	CHD-C4C	3.50	1.47	1.39
14	A	836	CLA	CHB-C1B	3.49	1.47	1.39
14	cA	824	CLA	CHB-C1B	3.49	1.47	1.39
14	cA	828	CLA	CHC-C4B	3.49	1.47	1.39
14	bA	833	CLA	C1B-NB	-3.49	1.33	1.37
14	B	813	CLA	OBD-CAD	3.49	1.28	1.22
14	cA	834	CLA	C1B-NB	-3.49	1.33	1.37
14	L	201	CLA	C3D-C2D	3.49	1.48	1.39
14	B	817	CLA	C1B-NB	-3.49	1.33	1.37
14	B	805	CLA	OBD-CAD	3.49	1.28	1.22
14	A	828	CLA	CHC-C4B	3.49	1.47	1.39
14	cA	818	CLA	C1B-NB	-3.49	1.33	1.37
14	bB	813	CLA	OBD-CAD	3.49	1.28	1.22
14	A	841	CLA	CHC-C4B	3.49	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bA	836	CLA	CHB-C1B	3.49	1.47	1.39
14	A	818	CLA	C1B-NB	-3.49	1.33	1.37
14	A	806	CLA	C3B-C4B	3.49	1.50	1.42
14	bL	201	CLA	C3D-C2D	3.48	1.48	1.39
14	cL	202	CLA	C3D-C2D	3.48	1.48	1.39
14	cA	805	CLA	CHC-C4B	3.48	1.47	1.39
14	B	832	CLA	CHB-C1B	3.48	1.47	1.39
14	bA	812	CLA	OBD-CAD	3.48	1.28	1.22
14	bA	852	CLA	CHD-C4C	3.48	1.47	1.39
14	cA	831	CLA	C1B-NB	-3.48	1.33	1.37
14	B	834	CLA	C3B-C4B	3.48	1.50	1.42
14	bA	802	CLA	CHD-C4C	3.48	1.47	1.39
14	B	801	CLA	CHB-C1B	3.48	1.47	1.39
14	A	833	CLA	OBD-CAD	3.48	1.28	1.22
14	cA	838	CLA	C3B-C4B	3.48	1.50	1.42
14	cB	807	CLA	OBD-CAD	3.48	1.28	1.22
14	A	833	CLA	CHC-C4B	3.48	1.47	1.39
14	cA	833	CLA	OBD-CAD	3.48	1.28	1.22
14	cB	806	CLA	OBD-CAD	3.48	1.28	1.22
14	A	831	CLA	C1B-NB	-3.48	1.33	1.37
14	bB	817	CLA	C1B-NB	-3.48	1.33	1.37
14	A	852	CLA	CHD-C4C	3.47	1.47	1.39
14	bA	833	CLA	OBD-CAD	3.47	1.28	1.22
14	cF	201	CLA	C3B-C4B	3.47	1.50	1.42
14	A	802	CLA	CHD-C4C	3.47	1.47	1.39
14	B	806	CLA	C3B-C4B	3.47	1.50	1.42
14	bA	841	CLA	CHC-C4B	3.47	1.47	1.39
14	cA	802	CLA	CHD-C4C	3.47	1.47	1.39
14	cA	852	CLA	CHD-C4C	3.47	1.47	1.39
14	A	832	CLA	C1B-NB	-3.47	1.33	1.37
14	bA	833	CLA	CHC-C4B	3.47	1.47	1.39
14	bA	841	CLA	CHD-C4C	3.47	1.47	1.39
14	A	838	CLA	C3B-C4B	3.47	1.50	1.42
14	bA	805	CLA	CHC-C4B	3.47	1.47	1.39
14	cA	833	CLA	CHC-C4B	3.47	1.47	1.39
14	bF	201	CLA	C3B-C4B	3.47	1.50	1.42
14	A	805	CLA	CHC-C4B	3.47	1.47	1.39
14	bB	834	CLA	C3B-C4B	3.47	1.50	1.42
14	bL	201	CLA	CHD-C4C	3.46	1.47	1.39
14	F	201	CLA	C3B-C4B	3.46	1.50	1.42
14	cA	841	CLA	CHC-C4B	3.46	1.47	1.39
14	bA	838	CLA	C3B-C4B	3.46	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cL	202	CLA	CHD-C4C	3.46	1.47	1.39
14	bB	811	CLA	OBD-CAD	3.46	1.28	1.22
14	B	811	CLA	OBD-CAD	3.46	1.28	1.22
14	A	852	CLA	C4B-NB	-3.46	1.33	1.37
14	cB	807	CLA	C3B-C4B	3.46	1.50	1.42
14	cB	835	CLA	C3B-C4B	3.45	1.50	1.42
14	bL	202	CLA	C3D-C2D	3.45	1.48	1.39
14	A	829	CLA	C1B-NB	-3.45	1.33	1.37
14	L	202	CLA	C3D-C2D	3.45	1.48	1.39
14	cL	203	CLA	C3D-C2D	3.45	1.48	1.39
14	bB	806	CLA	C3B-C4B	3.45	1.50	1.42
14	bB	851	CLA	OBD-CAD	3.45	1.28	1.22
14	cA	809	CLA	C1B-NB	-3.44	1.33	1.37
14	A	834	CLA	C1B-NB	-3.44	1.33	1.37
14	cB	801	CLA	OBD-CAD	3.44	1.28	1.22
14	bA	829	CLA	C1B-NB	-3.44	1.33	1.37
14	bA	832	CLA	C1B-NB	-3.44	1.33	1.37
14	A	841	CLA	OBD-CAD	3.44	1.28	1.22
14	bA	806	CLA	C1B-NB	-3.44	1.33	1.37
14	cA	829	CLA	C1B-NB	-3.44	1.33	1.37
14	bA	841	CLA	OBD-CAD	3.44	1.28	1.22
14	L	203	CLA	C1B-NB	-3.44	1.33	1.37
14	L	201	CLA	CHD-C4C	3.44	1.47	1.39
14	cB	817	CLA	OBD-CAD	3.44	1.28	1.22
14	bA	813	CLA	OBD-CAD	3.43	1.28	1.22
14	cA	841	CLA	OBD-CAD	3.43	1.28	1.22
14	bL	201	CLA	CHD-C1D	3.43	1.45	1.38
14	B	816	CLA	OBD-CAD	3.43	1.28	1.22
14	bA	822	CLA	OBD-CAD	3.43	1.28	1.22
14	bB	838	CLA	OBD-CAD	3.43	1.28	1.22
14	bA	835	CLA	C1B-NB	-3.43	1.33	1.37
14	cB	839	CLA	CHC-C4B	3.43	1.47	1.39
14	B	830	CLA	OBD-CAD	3.43	1.28	1.22
14	A	835	CLA	C1B-NB	-3.43	1.33	1.37
14	cA	835	CLA	C1B-NB	-3.43	1.33	1.37
14	cL	202	CLA	CHD-C1D	3.43	1.45	1.38
14	B	851	CLA	OBD-CAD	3.43	1.28	1.22
14	bB	816	CLA	OBD-CAD	3.42	1.28	1.22
14	L	201	CLA	CHD-C1D	3.42	1.45	1.38
14	bA	834	CLA	C1B-NB	-3.42	1.33	1.37
14	bA	830	CLA	C3D-C2D	3.42	1.48	1.39
14	A	808	CLA	C1B-NB	-3.42	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cB	839	CLA	OBD-CAD	3.42	1.28	1.22
14	cA	852	CLA	C4B-NB	-3.42	1.33	1.37
14	bB	812	CLA	CHB-C1B	3.42	1.47	1.39
14	cA	822	CLA	OBD-CAD	3.42	1.28	1.22
14	cB	809	CLA	C3B-C4B	3.42	1.50	1.42
14	cB	813	CLA	CHB-C1B	3.42	1.47	1.39
14	cA	813	CLA	OBD-CAD	3.42	1.28	1.22
14	cL	204	CLA	C1B-NB	-3.41	1.33	1.37
14	B	838	CLA	CHC-C4B	3.41	1.47	1.39
14	bA	825	CLA	OBD-CAD	3.41	1.28	1.22
14	cA	825	CLA	OBD-CAD	3.41	1.28	1.22
14	bB	808	CLA	C3B-C4B	3.41	1.50	1.42
14	B	812	CLA	CHB-C1B	3.41	1.47	1.39
14	B	837	CLA	OBD-CAD	3.41	1.28	1.22
14	B	808	CLA	C3B-C4B	3.41	1.50	1.42
14	L	203	CLA	C4B-NB	-3.41	1.33	1.37
14	A	825	CLA	OBD-CAD	3.41	1.28	1.22
14	bA	820	CLA	OBD-CAD	3.41	1.28	1.22
14	bB	830	CLA	OBD-CAD	3.41	1.28	1.22
14	A	838	CLA	C1B-NB	-3.41	1.33	1.37
14	bB	837	CLA	OBD-CAD	3.41	1.28	1.22
14	A	809	CLA	C1B-NB	-3.41	1.33	1.37
14	bB	838	CLA	CHC-C4B	3.41	1.47	1.39
14	cB	831	CLA	OBD-CAD	3.41	1.28	1.22
14	A	830	CLA	C3D-C2D	3.41	1.48	1.39
14	cA	830	CLA	C3D-C2D	3.41	1.48	1.39
14	B	838	CLA	OBD-CAD	3.41	1.28	1.22
14	A	813	CLA	OBD-CAD	3.41	1.28	1.22
14	A	820	CLA	OBD-CAD	3.41	1.28	1.22
14	cB	838	CLA	OBD-CAD	3.40	1.28	1.22
14	bA	852	CLA	C4B-NB	-3.40	1.33	1.37
14	A	811	CLA	C1B-NB	-3.40	1.33	1.37
14	bA	808	CLA	C1B-NB	-3.40	1.33	1.37
14	cL	204	CLA	C4B-NB	-3.40	1.33	1.37
14	bL	203	CLA	C1B-NB	-3.40	1.33	1.37
14	cA	832	CLA	C1B-NB	-3.40	1.33	1.37
14	A	822	CLA	OBD-CAD	3.40	1.28	1.22
14	cA	820	CLA	OBD-CAD	3.39	1.28	1.22
14	A	806	CLA	C1B-NB	-3.39	1.33	1.37
14	B	802	CLA	OBD-CAD	3.39	1.28	1.22
14	cA	806	CLA	C1B-NB	-3.39	1.33	1.37
14	bB	834	CLA	C1B-NB	-3.39	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bA	809	CLA	C1B-NB	-3.38	1.33	1.37
14	bA	838	CLA	C1B-NB	-3.38	1.33	1.37
14	bA	830	CLA	OBD-CAD	3.38	1.28	1.22
14	cB	819	CLA	C1B-NB	-3.38	1.33	1.37
14	bL	203	CLA	C4B-NB	-3.38	1.33	1.37
14	cA	812	CLA	C1B-NB	-3.37	1.33	1.37
14	cA	811	CLA	C1B-NB	-3.37	1.33	1.37
14	bB	851	CLA	C1B-NB	-3.37	1.33	1.37
14	cA	808	CLA	C1B-NB	-3.37	1.33	1.37
14	B	818	CLA	C1B-NB	-3.37	1.33	1.37
14	A	842	CLA	C1B-NB	-3.37	1.33	1.37
14	bB	818	CLA	C1B-NB	-3.37	1.33	1.37
14	A	830	CLA	OBD-CAD	3.37	1.28	1.22
14	A	825	CLA	C3D-C2D	3.36	1.48	1.39
14	cB	801	CLA	C1B-NB	-3.36	1.33	1.37
14	bA	828	CLA	OBD-CAD	3.36	1.28	1.22
14	B	838	CLA	CHD-C4C	3.36	1.46	1.39
14	cB	803	CLA	OBD-CAD	3.36	1.28	1.22
14	cA	825	CLA	C3D-C2D	3.36	1.48	1.39
14	bA	811	CLA	C1B-NB	-3.36	1.33	1.37
14	cA	820	CLA	C1B-NB	-3.36	1.33	1.37
14	bA	842	CLA	C1B-NB	-3.36	1.33	1.37
14	cA	842	CLA	C1B-NB	-3.36	1.33	1.37
14	bA	812	CLA	C1B-NB	-3.35	1.33	1.37
14	cA	830	CLA	OBD-CAD	3.35	1.28	1.22
14	bB	802	CLA	OBD-CAD	3.35	1.28	1.22
14	bA	825	CLA	C3D-C2D	3.35	1.48	1.39
14	cA	838	CLA	C1B-NB	-3.34	1.33	1.37
14	bB	838	CLA	CHD-C4C	3.34	1.46	1.39
14	cB	809	CLA	CHC-C4B	3.34	1.46	1.39
14	A	837	CLA	C3B-C4B	3.34	1.50	1.42
14	A	820	CLA	C1B-NB	-3.34	1.33	1.37
14	A	812	CLA	C1B-NB	-3.34	1.33	1.37
14	bL	201	CLA	CHB-C1B	3.34	1.46	1.39
14	cA	828	CLA	OBD-CAD	3.34	1.28	1.22
14	B	851	CLA	C1B-NB	-3.34	1.33	1.37
14	cA	837	CLA	C3B-C4B	3.34	1.50	1.42
14	bA	837	CLA	C3B-C4B	3.34	1.50	1.42
14	B	834	CLA	C1B-NB	-3.33	1.33	1.37
14	bB	829	CLA	C4B-NB	-3.33	1.33	1.37
14	A	838	CLA	CHB-C1B	3.33	1.46	1.39
14	A	824	CLA	C3B-C4B	3.33	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bA	820	CLA	C1B-NB	-3.33	1.33	1.37
14	cB	839	CLA	CHD-C4C	3.33	1.46	1.39
14	B	808	CLA	CHC-C4B	3.33	1.46	1.39
14	L	201	CLA	CHB-C1B	3.33	1.46	1.39
14	cL	202	CLA	CHB-C1B	3.33	1.46	1.39
14	A	828	CLA	OBD-CAD	3.33	1.28	1.22
14	B	817	CLA	C4B-NB	-3.32	1.33	1.37
14	cA	838	CLA	CHB-C1B	3.32	1.46	1.39
14	cB	830	CLA	C4B-NB	-3.32	1.33	1.37
14	cB	826	CLA	OBD-CAD	3.32	1.28	1.22
14	cB	835	CLA	C1B-NB	-3.32	1.33	1.37
14	cF	201	CLA	C1B-NB	-3.32	1.33	1.37
14	bB	806	CLA	C1B-NB	-3.32	1.33	1.37
14	bF	201	CLA	C1B-NB	-3.32	1.33	1.37
14	A	823	CLA	C1B-NB	-3.31	1.33	1.37
14	B	832	CLA	C1B-NB	-3.31	1.33	1.37
14	bA	838	CLA	CHB-C1B	3.31	1.46	1.39
14	F	201	CLA	C1B-NB	-3.31	1.33	1.37
14	bB	808	CLA	CHC-C4B	3.31	1.46	1.39
14	bA	824	CLA	C3B-C4B	3.31	1.50	1.42
14	cA	824	CLA	C3B-C4B	3.31	1.50	1.42
14	cA	810	CLA	C1B-NB	-3.31	1.33	1.37
14	bB	817	CLA	C4B-NB	-3.30	1.33	1.37
14	cB	833	CLA	C1B-NB	-3.30	1.33	1.37
14	cB	807	CLA	C1B-NB	-3.30	1.33	1.37
14	cA	818	CLA	CHB-C1B	3.30	1.46	1.39
14	bB	825	CLA	OBD-CAD	3.30	1.28	1.22
14	A	814	CLA	C1B-NB	-3.30	1.33	1.37
14	cB	818	CLA	C4B-NB	-3.30	1.33	1.37
14	bB	824	CLA	C1B-NB	-3.30	1.33	1.37
14	B	825	CLA	OBD-CAD	3.30	1.28	1.22
14	bB	832	CLA	C1B-NB	-3.30	1.33	1.37
14	B	829	CLA	C4B-NB	-3.30	1.33	1.37
14	cA	823	CLA	C1B-NB	-3.30	1.33	1.37
14	B	833	CLA	C1B-NB	-3.29	1.33	1.37
14	cA	814	CLA	C1B-NB	-3.29	1.33	1.37
14	cA	837	CLA	OBD-CAD	3.29	1.28	1.22
14	bA	823	CLA	C1B-NB	-3.29	1.33	1.37
14	A	818	CLA	CHB-C1B	3.29	1.46	1.39
14	bA	837	CLA	OBD-CAD	3.29	1.28	1.22
14	B	824	CLA	C1B-NB	-3.29	1.33	1.37
14	cB	838	CLA	C4B-NB	-3.29	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bA	814	CLA	C1B-NB	-3.29	1.33	1.37
14	B	808	CLA	C3D-C2D	3.29	1.48	1.39
14	A	837	CLA	OBD-CAD	3.29	1.28	1.22
14	bA	827	CLA	OBD-CAD	3.28	1.28	1.22
14	B	806	CLA	C1B-NB	-3.28	1.33	1.37
14	bB	836	CLA	C1B-NB	-3.28	1.33	1.37
14	A	827	CLA	OBD-CAD	3.28	1.28	1.22
14	bA	818	CLA	CHB-C1B	3.28	1.46	1.39
14	bA	817	CLA	OBD-CAD	3.28	1.28	1.22
14	bB	808	CLA	C3D-C2D	3.27	1.48	1.39
14	bB	837	CLA	C4B-NB	-3.27	1.33	1.37
14	cB	827	CLA	C1B-NB	-3.27	1.33	1.37
14	bA	836	CLA	C1B-NB	-3.27	1.33	1.37
14	cA	819	CLA	C1B-NB	-3.27	1.33	1.37
14	cA	827	CLA	OBD-CAD	3.27	1.28	1.22
14	A	819	CLA	C1B-NB	-3.27	1.33	1.37
14	B	803	CLA	C1B-NB	-3.27	1.33	1.37
14	cA	804	CLA	C3B-C4B	3.27	1.50	1.42
14	bA	804	CLA	C3B-C4B	3.27	1.50	1.42
14	cB	806	CLA	C1B-NB	-3.27	1.33	1.37
14	B	837	CLA	C4B-NB	-3.27	1.33	1.37
14	bB	826	CLA	C1B-NB	-3.27	1.33	1.37
14	cA	830	CLA	CHC-C4B	3.27	1.46	1.39
14	bA	839	CLA	C4B-NB	-3.27	1.33	1.37
14	cA	836	CLA	C1B-NB	-3.27	1.33	1.37
14	bB	833	CLA	C1B-NB	-3.27	1.33	1.37
14	cB	834	CLA	C1B-NB	-3.27	1.33	1.37
14	A	817	CLA	OBD-CAD	3.27	1.28	1.22
14	cA	839	CLA	C4B-NB	-3.27	1.33	1.37
14	A	830	CLA	CHC-C4B	3.26	1.46	1.39
14	bB	803	CLA	C4B-NB	-3.26	1.33	1.37
14	A	804	CLA	C3B-C4B	3.26	1.50	1.42
14	cB	827	CLA	C3D-C2D	3.26	1.48	1.39
14	cA	817	CLA	OBD-CAD	3.26	1.28	1.22
14	B	836	CLA	C1B-NB	-3.26	1.33	1.37
14	cB	809	CLA	C3D-C2D	3.26	1.48	1.39
14	cB	804	CLA	C4B-NB	-3.26	1.33	1.37
14	A	817	CLA	C1B-NB	-3.26	1.33	1.37
14	bB	826	CLA	C3D-C2D	3.26	1.48	1.39
14	B	826	CLA	C1B-NB	-3.26	1.33	1.37
14	bB	803	CLA	C1B-NB	-3.26	1.33	1.37
14	B	826	CLA	C3D-C2D	3.26	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	810	CLA	C1B-NB	-3.26	1.33	1.37
14	cB	825	CLA	C1B-NB	-3.26	1.33	1.37
14	B	803	CLA	C4B-NB	-3.26	1.33	1.37
14	bA	817	CLA	C1B-NB	-3.25	1.33	1.37
14	bA	819	CLA	C1B-NB	-3.25	1.33	1.37
14	bB	805	CLA	C1B-NB	-3.25	1.33	1.37
14	A	827	CLA	C3B-C4B	3.25	1.50	1.42
14	bA	810	CLA	C1B-NB	-3.25	1.33	1.37
14	cA	817	CLA	C1B-NB	-3.25	1.33	1.37
14	bA	827	CLA	C3B-C4B	3.25	1.50	1.42
14	B	811	CLA	C1B-NB	-3.25	1.33	1.37
14	B	805	CLA	C1B-NB	-3.25	1.33	1.37
14	bJ	101	CLA	C1B-NB	-3.25	1.33	1.37
14	bA	833	CLA	CHB-C1B	3.25	1.46	1.39
14	A	836	CLA	C1B-NB	-3.25	1.33	1.37
14	B	838	CLA	C1B-NB	-3.25	1.33	1.37
14	B	849	CLA	C1B-NB	-3.25	1.33	1.37
14	cA	833	CLA	CHB-C1B	3.24	1.46	1.39
14	A	839	CLA	C4B-NB	-3.24	1.33	1.37
14	bA	830	CLA	CHC-C4B	3.24	1.46	1.39
14	B	810	CLA	C1B-NB	-3.24	1.33	1.37
14	cB	811	CLA	C1B-NB	-3.24	1.33	1.37
14	A	833	CLA	CHB-C1B	3.24	1.46	1.39
14	bB	831	CLA	OBD-CAD	3.24	1.28	1.22
13	bA	801	CL0	C3B-C4B	3.24	1.50	1.42
14	A	822	CLA	C1B-NB	-3.24	1.33	1.37
14	bA	812	CLA	C3B-C4B	3.24	1.50	1.42
14	cB	831	CLA	C1B-NB	-3.24	1.33	1.37
14	cA	827	CLA	C3B-C4B	3.24	1.50	1.42
14	B	831	CLA	OBD-CAD	3.24	1.28	1.22
14	A	812	CLA	C3B-C4B	3.24	1.50	1.42
14	cB	839	CLA	C1B-NB	-3.23	1.33	1.37
14	cB	812	CLA	C1B-NB	-3.23	1.33	1.37
14	bB	830	CLA	C1B-NB	-3.23	1.33	1.37
14	cB	804	CLA	C1B-NB	-3.23	1.33	1.37
14	cB	830	CLA	C1B-NB	-3.22	1.33	1.37
14	bB	849	CLA	C1B-NB	-3.22	1.33	1.37
14	bA	852	CLA	CHB-C1B	3.22	1.46	1.39
14	cB	832	CLA	OBD-CAD	3.22	1.28	1.22
14	bB	811	CLA	C1B-NB	-3.22	1.33	1.37
14	B	830	CLA	C1B-NB	-3.22	1.33	1.37
14	cB	850	CLA	C1B-NB	-3.22	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	J	101	CLA	C1B-NB	-3.22	1.33	1.37
14	A	852	CLA	CHB-C1B	3.21	1.46	1.39
13	A	801	CL0	C3B-C4B	3.21	1.50	1.42
13	cA	801	CL0	C3B-C4B	3.21	1.50	1.42
14	cB	840	CLA	C3B-C4B	3.21	1.50	1.42
14	B	816	CLA	C1B-NB	-3.21	1.33	1.37
14	B	827	CLA	C1B-NB	-3.21	1.33	1.37
14	bB	839	CLA	C3B-C4B	3.21	1.50	1.42
13	cA	801	CL0	C1B-NB	-3.21	1.33	1.37
14	B	839	CLA	C3B-C4B	3.21	1.50	1.42
13	bA	801	CL0	C1B-NB	-3.21	1.33	1.37
14	cA	813	CLA	C1B-NB	-3.21	1.33	1.37
14	bB	810	CLA	C1B-NB	-3.21	1.33	1.37
14	B	829	CLA	C1B-NB	-3.21	1.33	1.37
14	B	824	CLA	C3B-C4B	3.21	1.50	1.42
14	cA	852	CLA	CHB-C1B	3.21	1.46	1.39
14	bB	838	CLA	C1B-NB	-3.20	1.33	1.37
14	cA	812	CLA	C3B-C4B	3.20	1.50	1.42
13	A	801	CL0	C1B-NB	-3.20	1.33	1.37
14	cB	837	CLA	C1B-NB	-3.20	1.33	1.37
14	B	828	CLA	C3D-C2D	3.20	1.47	1.39
14	bA	813	CLA	C1B-NB	-3.20	1.33	1.37
14	cB	817	CLA	C1B-NB	-3.20	1.33	1.37
14	A	813	CLA	C1B-NB	-3.20	1.33	1.37
14	bB	816	CLA	C1B-NB	-3.20	1.33	1.37
14	cB	802	CLA	C3B-C4B	3.20	1.50	1.42
14	cB	825	CLA	C3B-C4B	3.20	1.50	1.42
14	bB	824	CLA	C3B-C4B	3.19	1.50	1.42
14	bB	801	CLA	C1B-NB	-3.19	1.33	1.37
14	bB	809	CLA	C4B-NB	-3.19	1.33	1.37
14	cA	822	CLA	C1B-NB	-3.19	1.33	1.37
14	bB	828	CLA	C3D-C2D	3.19	1.47	1.39
14	cB	826	CLA	C1B-NB	-3.19	1.33	1.37
14	cA	817	CLA	C4B-NB	-3.19	1.33	1.37
14	A	839	CLA	C1B-NB	-3.19	1.33	1.37
14	cB	829	CLA	C3D-C2D	3.18	1.47	1.39
14	bA	821	CLA	C4B-NB	-3.18	1.33	1.37
14	cA	826	CLA	C1B-NB	-3.18	1.33	1.37
14	cB	815	CLA	C4B-NB	-3.18	1.33	1.37
14	B	801	CLA	C3B-C4B	3.18	1.50	1.42
14	A	821	CLA	C4B-NB	-3.18	1.33	1.37
14	bA	822	CLA	C1B-NB	-3.18	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bB	825	CLA	C1B-NB	-3.18	1.33	1.37
14	cA	839	CLA	C1B-NB	-3.18	1.33	1.37
14	cB	828	CLA	C1B-NB	-3.18	1.33	1.37
14	B	825	CLA	C1B-NB	-3.18	1.33	1.37
14	L	204	CLA	C1B-NB	-3.18	1.33	1.37
14	bA	826	CLA	C1B-NB	-3.18	1.33	1.37
14	cA	821	CLA	C4B-NB	-3.18	1.33	1.37
14	L	201	CLA	C3B-C4B	3.18	1.50	1.42
14	A	826	CLA	C1B-NB	-3.17	1.33	1.37
14	bB	827	CLA	C1B-NB	-3.17	1.33	1.37
14	cA	805	CLA	C4B-NB	-3.17	1.33	1.37
14	cA	814	CLA	C4B-NB	-3.17	1.33	1.37
14	A	817	CLA	C4B-NB	-3.17	1.33	1.37
14	bA	805	CLA	C4B-NB	-3.17	1.33	1.37
14	bL	201	CLA	C3B-C4B	3.17	1.50	1.42
14	B	835	CLA	C1B-NB	-3.17	1.33	1.37
14	A	807	CLA	C1B-NB	-3.17	1.33	1.37
14	bL	204	CLA	C1B-NB	-3.17	1.33	1.37
14	cB	836	CLA	C1B-NB	-3.17	1.33	1.37
14	bB	801	CLA	C3B-C4B	3.17	1.50	1.42
14	cL	202	CLA	C3B-C4B	3.17	1.50	1.42
14	cL	205	CLA	C1B-NB	-3.17	1.33	1.37
14	cA	807	CLA	C1B-NB	-3.16	1.33	1.37
14	cJ	101	CLA	C1B-NB	-3.16	1.33	1.37
14	bA	814	CLA	C4B-NB	-3.16	1.33	1.37
14	cB	802	CLA	C1B-NB	-3.16	1.33	1.37
14	bB	829	CLA	C1B-NB	-3.16	1.33	1.37
14	bB	830	CLA	C3B-C4B	3.16	1.50	1.42
14	cA	802	CLA	CHC-C4B	3.16	1.46	1.39
14	bB	835	CLA	C1B-NB	-3.16	1.33	1.37
14	A	836	CLA	OBD-CAD	3.16	1.27	1.22
14	cA	815	CLA	C1B-NB	-3.16	1.33	1.37
14	bB	814	CLA	C4B-NB	-3.15	1.33	1.37
14	bA	802	CLA	CHC-C4B	3.15	1.46	1.39
14	bA	836	CLA	OBD-CAD	3.15	1.27	1.22
14	A	802	CLA	CHC-C4B	3.15	1.46	1.39
14	cB	823	CLA	C3B-C4B	3.15	1.50	1.42
14	cB	831	CLA	C3B-C4B	3.15	1.50	1.42
14	cL	202	CLA	C1B-NB	-3.15	1.33	1.37
14	B	822	CLA	C3B-C4B	3.15	1.50	1.42
14	A	805	CLA	C4B-NB	-3.15	1.33	1.37
14	B	801	CLA	C1B-NB	-3.15	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bA	807	CLA	C1B-NB	-3.15	1.33	1.37
14	L	201	CLA	C1B-NB	-3.15	1.33	1.37
14	cA	836	CLA	OBD-CAD	3.14	1.27	1.22
14	B	814	CLA	C4B-NB	-3.14	1.33	1.37
14	B	839	CLA	C1B-NB	-3.14	1.33	1.37
14	bB	822	CLA	C3B-C4B	3.14	1.50	1.42
14	cJ	102	CLA	C1B-NB	-3.14	1.33	1.37
14	cA	815	CLA	C3B-C4B	3.14	1.50	1.42
14	bA	839	CLA	C1B-NB	-3.14	1.33	1.37
14	bA	815	CLA	C3B-C4B	3.14	1.50	1.42
14	bB	814	CLA	C3B-C4B	3.14	1.50	1.42
14	B	809	CLA	C4B-NB	-3.13	1.33	1.37
14	B	830	CLA	C3B-C4B	3.13	1.50	1.42
14	B	823	CLA	C4B-NB	-3.13	1.33	1.37
14	A	815	CLA	C3B-C4B	3.13	1.50	1.42
14	cB	815	CLA	C3B-C4B	3.13	1.50	1.42
14	bA	817	CLA	C4B-NB	-3.13	1.33	1.37
14	bB	820	CLA	C1B-NB	-3.13	1.33	1.37
17	B	850	BCR	C8-C9	-3.13	1.39	1.45
14	bA	816	CLA	C3B-C4B	3.13	1.50	1.42
14	bA	815	CLA	C1B-NB	-3.13	1.33	1.37
14	cA	838	CLA	C4B-NB	-3.13	1.33	1.37
14	cB	840	CLA	C1B-NB	-3.13	1.33	1.37
14	bB	803	CLA	OBD-CAD	3.13	1.27	1.22
14	cB	820	CLA	C1B-NB	-3.13	1.33	1.37
14	bB	839	CLA	C1B-NB	-3.13	1.33	1.37
14	B	821	CLA	C1B-NB	-3.13	1.33	1.37
17	bB	850	BCR	C8-C9	-3.13	1.39	1.45
14	A	825	CLA	C4B-NB	-3.13	1.33	1.37
14	bB	836	CLA	C3B-C4B	3.13	1.50	1.42
14	cA	816	CLA	C3B-C4B	3.13	1.50	1.42
14	bL	201	CLA	C1B-NB	-3.13	1.33	1.37
14	cB	823	CLA	C4B-NB	-3.13	1.33	1.37
17	cB	851	BCR	C8-C9	-3.12	1.39	1.45
14	B	814	CLA	C3B-C4B	3.12	1.50	1.42
14	B	836	CLA	C3B-C4B	3.12	1.50	1.42
14	A	821	CLA	C1B-NB	-3.12	1.33	1.37
14	bA	838	CLA	C4B-NB	-3.12	1.33	1.37
14	cA	825	CLA	C4B-NB	-3.12	1.33	1.37
14	bB	813	CLA	C4B-NB	-3.12	1.33	1.37
14	A	838	CLA	C4B-NB	-3.12	1.33	1.37
14	bA	832	CLA	C3B-C4B	3.12	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bB	812	CLA	C1B-NB	-3.12	1.34	1.37
14	L	204	CLA	C4B-NB	-3.12	1.34	1.37
14	B	827	CLA	C3B-C4B	3.12	1.50	1.42
14	bA	825	CLA	C4B-NB	-3.12	1.34	1.37
14	bB	823	CLA	C3B-C4B	3.11	1.50	1.42
14	bB	802	CLA	C1B-NB	-3.11	1.34	1.37
14	cB	832	CLA	C1B-NB	-3.11	1.34	1.37
14	cB	837	CLA	C3B-C4B	3.11	1.50	1.42
14	B	802	CLA	C1B-NB	-3.11	1.34	1.37
14	cB	804	CLA	OBD-CAD	3.11	1.27	1.22
14	bB	823	CLA	C4B-NB	-3.11	1.34	1.37
14	cB	810	CLA	C4B-NB	-3.11	1.34	1.37
14	A	826	CLA	C3B-C4B	3.11	1.50	1.42
14	A	852	CLA	CHD-C1D	3.11	1.44	1.38
14	J	102	CLA	C1B-NB	-3.11	1.34	1.37
14	cB	803	CLA	C1B-NB	-3.11	1.34	1.37
14	cB	828	CLA	C3B-C4B	3.11	1.50	1.42
14	B	812	CLA	C1B-NB	-3.11	1.34	1.37
14	cB	813	CLA	C1B-NB	-3.11	1.34	1.37
14	cB	814	CLA	C4B-NB	-3.11	1.34	1.37
14	cB	824	CLA	C4B-NB	-3.11	1.34	1.37
14	cA	852	CLA	CHD-C1D	3.11	1.44	1.38
14	A	832	CLA	C3B-C4B	3.11	1.50	1.42
14	bB	827	CLA	C3B-C4B	3.11	1.50	1.42
14	bB	802	CLA	C4B-NB	-3.11	1.34	1.37
14	bA	826	CLA	C3B-C4B	3.11	1.50	1.42
14	A	814	CLA	C4B-NB	-3.11	1.34	1.37
14	cB	821	CLA	C1B-NB	-3.11	1.34	1.37
14	A	815	CLA	C1B-NB	-3.10	1.34	1.37
14	B	831	CLA	C1B-NB	-3.10	1.34	1.37
14	cL	205	CLA	C4B-NB	-3.10	1.34	1.37
14	cB	822	CLA	C1B-NB	-3.10	1.34	1.37
14	B	803	CLA	OBD-CAD	3.10	1.27	1.22
14	bB	826	CLA	OBD-CAD	3.10	1.27	1.22
14	cB	824	CLA	C3B-C4B	3.10	1.50	1.42
14	B	822	CLA	C4B-NB	-3.10	1.34	1.37
14	A	816	CLA	C3B-C4B	3.10	1.50	1.42
14	cA	821	CLA	C1B-NB	-3.10	1.34	1.37
14	B	813	CLA	C1B-NB	-3.09	1.34	1.37
14	bA	821	CLA	C1B-NB	-3.09	1.34	1.37
14	B	820	CLA	C1B-NB	-3.09	1.34	1.37
14	B	823	CLA	C3B-C4B	3.09	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bB	821	CLA	C1B-NB	-3.09	1.34	1.37
14	bB	822	CLA	C4B-NB	-3.09	1.34	1.37
14	A	838	CLA	OBD-CAD	3.09	1.27	1.22
14	B	813	CLA	C4B-NB	-3.09	1.34	1.37
14	bJ	102	CLA	C1B-NB	-3.09	1.34	1.37
14	cA	832	CLA	C3B-C4B	3.09	1.50	1.42
14	cA	838	CLA	OBD-CAD	3.09	1.27	1.22
14	bB	813	CLA	C1B-NB	-3.09	1.34	1.37
14	cB	821	CLA	C3B-C4B	3.08	1.50	1.42
14	A	803	CLA	C1B-NB	-3.08	1.34	1.37
14	bA	803	CLA	C1B-NB	-3.08	1.34	1.37
14	bB	831	CLA	C1B-NB	-3.08	1.34	1.37
14	bA	852	CLA	CHD-C1D	3.08	1.44	1.38
14	B	820	CLA	C3B-C4B	3.08	1.50	1.42
14	cA	826	CLA	C3B-C4B	3.08	1.50	1.42
14	bB	804	CLA	C3B-C4B	3.08	1.50	1.42
14	B	819	CLA	C1B-NB	-3.08	1.34	1.37
14	cA	803	CLA	C1B-NB	-3.08	1.34	1.37
14	bA	838	CLA	OBD-CAD	3.08	1.27	1.22
14	cB	827	CLA	OBD-CAD	3.08	1.27	1.22
14	A	809	CLA	C4B-NB	-3.08	1.34	1.37
14	bB	819	CLA	C1B-NB	-3.08	1.34	1.37
14	bL	204	CLA	C4B-NB	-3.07	1.34	1.37
14	cB	829	CLA	C4B-NB	-3.07	1.34	1.37
14	B	802	CLA	C4B-NB	-3.07	1.34	1.37
14	cB	802	CLA	C4B-NB	-3.07	1.34	1.37
14	B	821	CLA	C3B-C4B	3.07	1.49	1.42
14	bB	821	CLA	C3B-C4B	3.07	1.49	1.42
14	B	826	CLA	OBD-CAD	3.07	1.27	1.22
14	cB	822	CLA	C3B-C4B	3.07	1.49	1.42
14	bB	801	CLA	C4B-NB	-3.06	1.34	1.37
14	bB	809	CLA	CHC-C4B	3.06	1.46	1.39
14	B	801	CLA	C4B-NB	-3.06	1.34	1.37
14	B	828	CLA	C4B-NB	-3.06	1.34	1.37
14	B	804	CLA	C3B-C4B	3.06	1.49	1.42
14	bB	820	CLA	C3B-C4B	3.06	1.49	1.42
14	bB	828	CLA	C4B-NB	-3.05	1.34	1.37
14	cB	810	CLA	CHC-C4B	3.05	1.46	1.39
14	bA	809	CLA	C4B-NB	-3.05	1.34	1.37
14	bA	803	CLA	C3B-C4B	3.05	1.49	1.42
14	X	201	CLA	C1B-NB	-3.05	1.34	1.37
14	A	821	CLA	C3B-C4B	3.05	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cB	837	CLA	C4B-NB	-3.05	1.34	1.37
14	cA	809	CLA	C4B-NB	-3.05	1.34	1.37
14	cB	803	CLA	C4B-NB	-3.05	1.34	1.37
14	bA	852	CLA	C1D-ND	3.05	1.41	1.37
14	cA	803	CLA	C3B-C4B	3.05	1.49	1.42
14	A	803	CLA	C3B-C4B	3.05	1.49	1.42
14	cB	805	CLA	C3B-C4B	3.04	1.49	1.42
14	cB	806	CLA	C3B-C4B	3.04	1.49	1.42
14	cB	836	CLA	C3B-C4B	3.04	1.49	1.42
14	B	835	CLA	C3B-C4B	3.04	1.49	1.42
14	bA	836	CLA	C3B-C4B	3.04	1.49	1.42
14	cX	201	CLA	C1B-NB	-3.04	1.34	1.37
14	bB	835	CLA	C3B-C4B	3.04	1.49	1.42
14	A	836	CLA	C3B-C4B	3.04	1.49	1.42
14	cA	836	CLA	C3B-C4B	3.04	1.49	1.42
14	bA	803	CLA	C4B-NB	-3.04	1.34	1.37
14	B	805	CLA	C3B-C4B	3.04	1.49	1.42
14	B	809	CLA	CHC-C4B	3.03	1.46	1.39
14	bA	821	CLA	C3B-C4B	3.03	1.49	1.42
14	A	840	CLA	C1B-NB	-3.03	1.34	1.37
14	cB	814	CLA	C1B-NB	-3.03	1.34	1.37
14	cA	803	CLA	C4B-NB	-3.03	1.34	1.37
14	L	202	CLA	C1B-NB	-3.03	1.34	1.37
14	bB	836	CLA	C4B-NB	-3.03	1.34	1.37
14	bX	201	CLA	C1B-NB	-3.03	1.34	1.37
14	bA	802	CLA	C1B-NB	-3.02	1.34	1.37
14	bB	805	CLA	C3B-C4B	3.02	1.49	1.42
14	bB	810	CLA	C3B-C4B	3.02	1.49	1.42
14	cA	821	CLA	C3B-C4B	3.02	1.49	1.42
14	bA	840	CLA	C1B-NB	-3.02	1.34	1.37
14	B	807	CLA	C4B-NB	-3.02	1.34	1.37
14	cA	840	CLA	C1B-NB	-3.02	1.34	1.37
14	A	852	CLA	C1D-ND	3.02	1.41	1.37
14	A	802	CLA	C1B-NB	-3.01	1.34	1.37
14	cA	816	CLA	C1B-NB	-3.01	1.34	1.37
14	cL	203	CLA	C1B-NB	-3.01	1.34	1.37
14	cB	808	CLA	C4B-NB	-3.01	1.34	1.37
14	bA	825	CLA	C3B-C4B	3.01	1.49	1.42
14	A	804	CLA	C4B-NB	-3.00	1.34	1.37
14	A	803	CLA	C4B-NB	-3.00	1.34	1.37
14	B	836	CLA	C4B-NB	-3.00	1.34	1.37
14	cB	811	CLA	C3B-C4B	3.00	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	822	CLA	C1B-NB	-3.00	1.34	1.37
14	bL	202	CLA	C1B-NB	-3.00	1.34	1.37
14	B	810	CLA	C3B-C4B	3.00	1.49	1.42
14	bB	815	CLA	C1B-NB	-3.00	1.34	1.37
14	bB	822	CLA	C1B-NB	-3.00	1.34	1.37
14	cA	825	CLA	C3B-C4B	3.00	1.49	1.42
17	cB	845	BCR	C8-C9	-3.00	1.39	1.45
14	A	816	CLA	C1B-NB	-3.00	1.34	1.37
14	bA	804	CLA	C4B-NB	-3.00	1.34	1.37
14	cA	852	CLA	C1D-ND	2.99	1.41	1.37
14	cB	825	CLA	C4B-NB	-2.99	1.34	1.37
14	B	813	CLA	C3B-C4B	2.99	1.49	1.42
14	cA	814	CLA	C3B-C4B	2.99	1.49	1.42
14	cA	802	CLA	C1B-NB	-2.99	1.34	1.37
14	A	825	CLA	C3B-C4B	2.99	1.49	1.42
14	cB	839	CLA	C3B-C4B	2.99	1.49	1.42
14	B	838	CLA	C3B-C4B	2.99	1.49	1.42
14	B	815	CLA	C1B-NB	-2.99	1.34	1.37
14	bA	812	CLA	C4B-NB	-2.99	1.34	1.37
14	B	831	CLA	C1C-C2C	2.99	1.50	1.44
14	bB	835	CLA	C4B-NB	-2.99	1.34	1.37
14	cB	831	CLA	C4B-NB	-2.99	1.34	1.37
14	A	802	CLA	OBD-CAD	2.99	1.27	1.22
14	cB	832	CLA	C1C-C2C	2.99	1.50	1.44
14	A	814	CLA	C3B-C4B	2.99	1.49	1.42
14	cA	804	CLA	C4B-NB	-2.98	1.34	1.37
14	bB	804	CLA	C4B-NB	-2.98	1.34	1.37
14	B	804	CLA	C4B-NB	-2.98	1.34	1.37
14	bB	830	CLA	C4B-NB	-2.98	1.34	1.37
14	cB	805	CLA	C4B-NB	-2.98	1.34	1.37
14	cA	809	CLA	C3B-C4B	2.98	1.49	1.42
14	B	830	CLA	C4B-NB	-2.98	1.34	1.37
17	B	844	BCR	C8-C9	-2.98	1.39	1.45
14	bA	809	CLA	C3B-C4B	2.98	1.49	1.42
14	bB	838	CLA	C3B-C4B	2.98	1.49	1.42
14	cB	814	CLA	C3B-C4B	2.98	1.49	1.42
14	cA	812	CLA	C4B-NB	-2.98	1.34	1.37
14	bA	802	CLA	OBD-CAD	2.98	1.27	1.22
14	A	812	CLA	C4B-NB	-2.98	1.34	1.37
14	A	827	CLA	C4B-NB	-2.98	1.34	1.37
14	cA	802	CLA	OBD-CAD	2.97	1.27	1.22
14	cB	805	CLA	C1B-NB	-2.97	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	809	CLA	C3B-C4B	2.97	1.49	1.42
14	B	817	CLA	C3B-C4B	2.97	1.49	1.42
14	bB	813	CLA	C3B-C4B	2.97	1.49	1.42
14	bB	817	CLA	C3B-C4B	2.97	1.49	1.42
14	bB	824	CLA	C4B-NB	-2.97	1.34	1.37
14	bA	814	CLA	C3B-C4B	2.97	1.49	1.42
14	cB	816	CLA	C1B-NB	-2.97	1.34	1.37
14	cB	823	CLA	C1B-NB	-2.97	1.34	1.37
14	cB	836	CLA	C4B-NB	-2.97	1.34	1.37
14	bA	827	CLA	C4B-NB	-2.96	1.34	1.37
14	B	824	CLA	C4B-NB	-2.96	1.34	1.37
14	bB	809	CLA	OBD-CAD	2.96	1.27	1.22
14	bB	807	CLA	C4B-NB	-2.96	1.34	1.37
14	cB	818	CLA	C3B-C4B	2.96	1.49	1.42
14	A	825	CLA	C1B-NB	-2.96	1.34	1.37
14	bA	816	CLA	C1B-NB	-2.96	1.34	1.37
14	B	805	CLA	C4B-NB	-2.96	1.34	1.37
14	bB	820	CLA	C4B-NB	-2.96	1.34	1.37
14	bA	829	CLA	C3B-C4B	2.96	1.49	1.42
14	bB	831	CLA	C1C-C2C	2.96	1.50	1.44
14	cA	827	CLA	C4B-NB	-2.96	1.34	1.37
14	cB	821	CLA	C4B-NB	-2.95	1.34	1.37
14	B	835	CLA	C4B-NB	-2.95	1.34	1.37
14	A	842	CLA	C3B-C4B	2.95	1.49	1.42
14	A	829	CLA	C3B-C4B	2.95	1.49	1.42
14	cB	806	CLA	C4B-NB	-2.94	1.34	1.37
14	A	827	CLA	C1B-NB	-2.94	1.34	1.37
14	B	809	CLA	OBD-CAD	2.94	1.27	1.22
14	bA	827	CLA	C1B-NB	-2.94	1.34	1.37
14	cA	827	CLA	C1B-NB	-2.94	1.34	1.37
14	bA	842	CLA	C3B-C4B	2.94	1.49	1.42
14	A	815	CLA	C4B-NB	-2.94	1.34	1.37
14	B	837	CLA	C1B-NB	-2.94	1.34	1.37
14	bA	831	CLA	C4B-NB	-2.94	1.34	1.37
14	cA	815	CLA	C4B-NB	-2.94	1.34	1.37
14	cA	842	CLA	C3B-C4B	2.94	1.49	1.42
17	bB	844	BCR	C8-C9	-2.94	1.39	1.45
14	B	814	CLA	C1B-NB	-2.94	1.34	1.37
14	bB	814	CLA	C1B-NB	-2.94	1.34	1.37
14	cA	804	CLA	C1B-NB	-2.94	1.34	1.37
14	cA	829	CLA	C3B-C4B	2.94	1.49	1.42
14	bA	825	CLA	C1B-NB	-2.94	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cA	831	CLA	C4B-NB	-2.94	1.34	1.37
14	bA	804	CLA	C1B-NB	-2.93	1.34	1.37
14	B	820	CLA	C4B-NB	-2.93	1.34	1.37
14	B	807	CLA	C1B-C2B	2.93	1.50	1.43
14	L	202	CLA	C3B-C4B	2.93	1.49	1.42
14	cB	810	CLA	OBD-CAD	2.93	1.27	1.22
14	B	804	CLA	C1B-NB	-2.93	1.34	1.37
14	cA	825	CLA	C1B-NB	-2.93	1.34	1.37
14	A	831	CLA	C4B-NB	-2.93	1.34	1.37
14	cA	816	CLA	C4B-NB	-2.93	1.34	1.37
14	bA	816	CLA	C4B-NB	-2.93	1.34	1.37
14	cB	808	CLA	C1B-NB	-2.92	1.34	1.37
14	bL	202	CLA	C3B-C4B	2.92	1.49	1.42
14	A	816	CLA	C4B-NB	-2.92	1.34	1.37
14	cB	811	CLA	C4B-NB	-2.92	1.34	1.37
14	bB	837	CLA	C1B-NB	-2.92	1.34	1.37
14	bB	807	CLA	C1B-C2B	2.92	1.50	1.43
14	bB	804	CLA	C1B-NB	-2.92	1.34	1.37
14	cL	203	CLA	C3B-C4B	2.92	1.49	1.42
14	cB	808	CLA	C1B-C2B	2.92	1.50	1.43
14	cB	830	CLA	C3B-C4B	2.91	1.49	1.42
14	cA	842	CLA	C4B-NB	-2.91	1.34	1.37
14	bA	842	CLA	C4B-NB	-2.91	1.34	1.37
14	cL	202	CLA	OBD-CAD	2.91	1.27	1.22
14	bB	829	CLA	C3B-C4B	2.91	1.49	1.42
14	B	810	CLA	C4B-NB	-2.91	1.34	1.37
14	bA	832	CLA	C4B-NB	-2.91	1.34	1.37
14	bB	810	CLA	C4B-NB	-2.91	1.34	1.37
14	cB	803	CLA	C1B-C2B	2.90	1.50	1.43
14	bB	805	CLA	C4B-NB	-2.90	1.34	1.37
14	cB	815	CLA	C1B-NB	-2.90	1.34	1.37
14	B	839	CLA	C4C-C3C	2.90	1.50	1.45
14	bB	837	CLA	C3B-C4B	2.90	1.49	1.42
14	J	102	CLA	C1C-C2C	2.90	1.50	1.44
14	cB	840	CLA	C4B-NB	-2.90	1.34	1.37
14	bB	839	CLA	C4C-C3C	2.90	1.50	1.45
14	B	829	CLA	C3B-C4B	2.90	1.49	1.42
14	bA	834	CLA	C4C-C3C	2.90	1.50	1.45
14	L	204	CLA	C3B-C4B	2.90	1.49	1.42
14	cA	832	CLA	C4B-NB	-2.90	1.34	1.37
14	bA	805	CLA	C3B-C4B	2.90	1.49	1.42
14	L	201	CLA	OBD-CAD	2.90	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	804	CLA	C1B-NB	-2.90	1.34	1.37
14	B	837	CLA	C3B-C4B	2.90	1.49	1.42
14	cA	852	CLA	OBD-CAD	2.89	1.27	1.22
14	cJ	102	CLA	C1C-C2C	2.89	1.50	1.44
14	A	852	CLA	OBD-CAD	2.89	1.27	1.22
14	cB	838	CLA	C3B-C4B	2.89	1.49	1.42
14	cL	205	CLA	C3B-C4B	2.89	1.49	1.42
14	B	802	CLA	C1B-C2B	2.89	1.50	1.43
14	cA	814	CLA	C1B-C2B	2.89	1.50	1.43
14	A	805	CLA	C3B-C4B	2.89	1.49	1.42
14	bB	807	CLA	C1B-NB	-2.89	1.34	1.37
14	bB	821	CLA	C4B-NB	-2.89	1.34	1.37
14	bA	852	CLA	OBD-CAD	2.89	1.27	1.22
14	A	814	CLA	C1B-C2B	2.89	1.50	1.43
14	B	820	CLA	C1B-C2B	2.89	1.50	1.43
14	cA	834	CLA	C4C-C3C	2.89	1.50	1.45
14	bB	839	CLA	C4B-NB	-2.89	1.34	1.37
14	B	821	CLA	C1B-C2B	2.88	1.50	1.43
14	cB	838	CLA	C1B-NB	-2.88	1.34	1.37
14	cB	840	CLA	C4C-C3C	2.88	1.50	1.45
14	bB	802	CLA	C1B-C2B	2.88	1.50	1.43
14	cB	822	CLA	C4B-NB	-2.88	1.34	1.37
14	cA	805	CLA	C3B-C4B	2.88	1.49	1.42
14	bL	201	CLA	OBD-CAD	2.88	1.27	1.22
14	B	821	CLA	C4B-NB	-2.88	1.34	1.37
14	bL	204	CLA	C3B-C4B	2.88	1.49	1.42
14	A	842	CLA	C4B-NB	-2.88	1.34	1.37
14	B	839	CLA	C4B-NB	-2.88	1.34	1.37
14	A	832	CLA	C4B-NB	-2.88	1.34	1.37
14	cB	822	CLA	C1B-C2B	2.87	1.50	1.43
14	bB	820	CLA	C1B-C2B	2.87	1.50	1.43
14	bB	821	CLA	C1B-C2B	2.87	1.50	1.43
14	A	816	CLA	C1B-C2B	2.87	1.50	1.43
14	B	807	CLA	C1B-NB	-2.87	1.34	1.37
14	bJ	102	CLA	C1C-C2C	2.87	1.50	1.44
14	B	827	CLA	C4B-NB	-2.87	1.34	1.37
14	bA	814	CLA	C1B-C2B	2.87	1.50	1.43
14	bA	816	CLA	C1B-C2B	2.86	1.50	1.43
14	cJ	101	CLA	C1C-C2C	2.86	1.50	1.44
14	bA	815	CLA	C4B-NB	-2.86	1.34	1.37
14	bB	827	CLA	C4B-NB	-2.86	1.34	1.37
14	cB	821	CLA	C1B-C2B	2.86	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cA	816	CLA	C1B-C2B	2.86	1.50	1.43
14	cB	828	CLA	C4B-NB	-2.86	1.34	1.37
14	A	834	CLA	C4C-C3C	2.86	1.50	1.45
14	cA	852	CLA	C1B-C2B	2.86	1.50	1.43
14	bL	201	CLA	C4B-NB	-2.86	1.34	1.37
14	B	827	CLA	C1C-C2C	2.86	1.50	1.44
14	bA	852	CLA	C1B-C2B	2.85	1.50	1.43
14	cL	202	CLA	C4B-NB	-2.85	1.34	1.37
14	cB	839	CLA	C4B-NB	-2.85	1.34	1.37
14	bB	812	CLA	C1C-C2C	2.85	1.50	1.44
14	B	814	CLA	C1B-C2B	2.85	1.50	1.43
14	X	201	CLA	C1C-C2C	2.85	1.50	1.44
14	cA	831	CLA	C3B-C4B	2.84	1.49	1.42
14	B	812	CLA	C1C-C2C	2.84	1.50	1.44
14	A	852	CLA	C1B-C2B	2.84	1.50	1.43
14	A	831	CLA	C1B-C2B	2.84	1.50	1.43
14	bB	829	CLA	C4C-C3C	2.84	1.49	1.45
14	A	803	CLA	C1B-C2B	2.84	1.49	1.43
14	cA	803	CLA	C1B-C2B	2.84	1.49	1.43
14	J	101	CLA	C1C-C2C	2.84	1.50	1.44
14	bB	814	CLA	C1B-C2B	2.84	1.49	1.43
14	cA	831	CLA	C1B-C2B	2.84	1.49	1.43
14	bA	803	CLA	C1B-C2B	2.84	1.49	1.43
14	bB	827	CLA	C1C-C2C	2.84	1.50	1.44
14	bJ	101	CLA	C1C-C2C	2.84	1.50	1.44
14	cB	813	CLA	C1C-C2C	2.84	1.50	1.44
14	cB	815	CLA	C1B-C2B	2.84	1.49	1.43
14	bA	831	CLA	C3B-C4B	2.83	1.49	1.42
14	A	815	CLA	C1B-C2B	2.83	1.49	1.43
14	cA	839	CLA	C1B-C2B	2.83	1.49	1.43
14	bA	831	CLA	C1B-C2B	2.83	1.49	1.43
14	cA	821	CLA	C1B-C2B	2.83	1.49	1.43
14	cB	821	CLA	C4C-C3C	2.83	1.49	1.45
14	cB	828	CLA	C1C-C2C	2.83	1.50	1.44
14	B	838	CLA	C4B-NB	-2.83	1.34	1.37
14	bB	813	CLA	C1B-C2B	2.82	1.49	1.43
14	bB	837	CLA	C1B-C2B	2.82	1.49	1.43
14	L	201	CLA	C4B-NB	-2.82	1.34	1.37
14	B	828	CLA	C3B-C4B	2.82	1.49	1.42
14	cX	201	CLA	C1C-C2C	2.82	1.50	1.44
14	bB	828	CLA	C3B-C4B	2.82	1.49	1.42
14	B	813	CLA	C1B-C2B	2.82	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	837	CLA	C1B-C2B	2.82	1.49	1.43
14	bX	201	CLA	C1C-C2C	2.82	1.50	1.44
14	B	810	CLA	C1B-C2B	2.82	1.49	1.43
14	B	829	CLA	C4C-C3C	2.82	1.49	1.45
14	A	839	CLA	C1B-C2B	2.82	1.49	1.43
14	cB	838	CLA	C1B-C2B	2.82	1.49	1.43
14	bB	835	CLA	C1B-C2B	2.82	1.49	1.43
14	A	831	CLA	C3B-C4B	2.82	1.49	1.42
14	bB	838	CLA	C4B-NB	-2.82	1.34	1.37
14	cA	826	CLA	C1B-C2B	2.81	1.49	1.43
14	cB	834	CLA	C1C-C2C	2.81	1.50	1.44
14	A	829	CLA	C4B-NB	-2.81	1.34	1.37
14	cB	830	CLA	C4C-C3C	2.81	1.49	1.45
14	cA	827	CLA	C1B-C2B	2.81	1.49	1.43
14	cB	836	CLA	C1C-C2C	2.81	1.50	1.44
14	bA	826	CLA	C1B-C2B	2.81	1.49	1.43
14	cA	815	CLA	C1B-C2B	2.81	1.49	1.43
14	cB	811	CLA	C1B-C2B	2.81	1.49	1.43
14	bB	820	CLA	C4C-C3C	2.81	1.49	1.45
14	B	820	CLA	C4C-C3C	2.81	1.49	1.45
14	L	202	CLA	C4B-NB	-2.81	1.34	1.37
14	bB	827	CLA	C1B-C2B	2.81	1.49	1.43
14	cB	836	CLA	C1B-C2B	2.81	1.49	1.43
14	bA	839	CLA	C1B-C2B	2.81	1.49	1.43
14	cB	814	CLA	C1B-C2B	2.81	1.49	1.43
14	cB	829	CLA	C3B-C4B	2.81	1.49	1.42
14	bB	803	CLA	C3B-C4B	2.81	1.49	1.42
17	cL	207	BCR	C8-C9	-2.81	1.39	1.45
14	bA	827	CLA	C1B-C2B	2.80	1.49	1.43
14	B	833	CLA	C1C-C2C	2.80	1.50	1.44
14	bA	815	CLA	C1B-C2B	2.80	1.49	1.43
14	bA	821	CLA	C1B-C2B	2.80	1.49	1.43
14	bB	833	CLA	C1C-C2C	2.80	1.50	1.44
17	bL	206	BCR	C8-C9	-2.80	1.39	1.45
14	B	835	CLA	C1B-C2B	2.80	1.49	1.43
14	A	821	CLA	C1B-C2B	2.80	1.49	1.43
17	bL	205	BCR	C23-C22	-2.80	1.39	1.45
17	bB	844	BCR	C23-C22	-2.80	1.39	1.45
17	cL	206	BCR	C23-C22	-2.80	1.39	1.45
14	cB	804	CLA	C3B-C4B	2.80	1.49	1.42
14	B	827	CLA	C1B-C2B	2.80	1.49	1.43
14	cA	818	CLA	C1C-C2C	2.80	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bB	810	CLA	C1B-C2B	2.80	1.49	1.43
14	cA	807	CLA	C4C-C3C	2.80	1.49	1.45
17	L	205	BCR	C23-C22	-2.80	1.39	1.45
14	bB	806	CLA	C1C-C2C	2.80	1.50	1.44
14	cB	828	CLA	C1B-C2B	2.80	1.49	1.43
14	bA	818	CLA	C1C-C2C	2.80	1.50	1.44
14	cB	807	CLA	C1C-C2C	2.80	1.50	1.44
14	cA	829	CLA	C4B-NB	-2.80	1.34	1.37
14	bA	829	CLA	C4B-NB	-2.79	1.34	1.37
14	B	835	CLA	C1C-C2C	2.79	1.50	1.44
17	cB	845	BCR	C23-C22	-2.79	1.39	1.45
14	cA	808	CLA	C1C-C2C	2.79	1.50	1.44
14	cA	814	CLA	C1C-C2C	2.79	1.50	1.44
17	B	844	BCR	C23-C22	-2.79	1.39	1.45
14	cB	820	CLA	C1C-C2C	2.79	1.50	1.44
14	cL	203	CLA	C4B-NB	-2.79	1.34	1.37
14	bA	814	CLA	C1C-C2C	2.79	1.50	1.44
14	cB	831	CLA	C1B-C2B	2.79	1.49	1.43
14	cA	825	CLA	C1C-C2C	2.79	1.50	1.44
14	bA	825	CLA	C1C-C2C	2.79	1.50	1.44
14	A	827	CLA	C1B-C2B	2.79	1.49	1.43
14	cB	830	CLA	C1B-C2B	2.79	1.49	1.43
17	cB	842	BCR	C23-C22	-2.79	1.40	1.45
14	A	832	CLA	OBD-CAD	2.79	1.27	1.22
14	bB	830	CLA	C1B-C2B	2.79	1.49	1.43
17	L	206	BCR	C8-C9	-2.79	1.40	1.45
14	A	826	CLA	C1B-C2B	2.78	1.49	1.43
14	bB	835	CLA	C1C-C2C	2.78	1.50	1.44
14	bB	851	CLA	C1C-C2C	2.78	1.50	1.44
14	bA	807	CLA	C4C-C3C	2.78	1.49	1.45
14	B	803	CLA	C3B-C4B	2.78	1.49	1.42
14	A	818	CLA	C1C-C2C	2.78	1.49	1.44
14	cA	817	CLA	C3B-C4B	2.78	1.49	1.42
14	cL	204	CLA	C3B-C4B	2.78	1.49	1.42
14	B	851	CLA	C1C-C2C	2.78	1.49	1.44
14	A	825	CLA	C1C-C2C	2.78	1.49	1.44
14	A	807	CLA	C4C-C3C	2.78	1.49	1.45
14	B	806	CLA	C1C-C2C	2.78	1.49	1.44
14	B	829	CLA	C1B-C2B	2.78	1.49	1.43
14	A	826	CLA	C4B-NB	-2.78	1.34	1.37
14	cB	801	CLA	C1C-C2C	2.78	1.49	1.44
14	bL	204	CLA	C4C-C3C	2.78	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	808	CLA	C1C-C2C	2.78	1.49	1.44
14	A	814	CLA	C1C-C2C	2.78	1.49	1.44
14	cA	806	CLA	C1C-C2C	2.78	1.49	1.44
14	L	204	CLA	C4C-C3C	2.78	1.49	1.45
14	cA	832	CLA	OBD-CAD	2.78	1.27	1.22
14	B	830	CLA	C1B-C2B	2.78	1.49	1.43
14	cL	205	CLA	C4C-C3C	2.78	1.49	1.45
14	cB	815	CLA	C4C-C3C	2.77	1.49	1.45
14	B	819	CLA	C1C-C2C	2.77	1.49	1.44
14	bA	826	CLA	C4B-NB	-2.77	1.34	1.37
14	cA	803	CLA	C1C-C2C	2.77	1.49	1.44
14	L	203	CLA	C3B-C4B	2.77	1.49	1.42
14	bL	203	CLA	C3B-C4B	2.77	1.49	1.42
14	bB	814	CLA	C4C-C3C	2.77	1.49	1.45
14	bB	829	CLA	C1B-C2B	2.77	1.49	1.43
14	B	804	CLA	C1B-C2B	2.77	1.49	1.43
14	bB	807	CLA	C1C-C2C	2.77	1.49	1.44
14	bA	806	CLA	C1C-C2C	2.77	1.49	1.44
14	bA	832	CLA	OBD-CAD	2.77	1.27	1.22
17	cA	845	BCR	C8-C9	-2.77	1.40	1.45
14	cB	805	CLA	C1B-C2B	2.77	1.49	1.43
14	A	806	CLA	C1C-C2C	2.77	1.49	1.44
14	bB	824	CLA	C1C-C2C	2.77	1.49	1.44
14	bB	815	CLA	C1C-C2C	2.76	1.49	1.44
17	B	841	BCR	C23-C22	-2.76	1.40	1.45
14	F	201	CLA	C1C-C2C	2.76	1.49	1.44
14	bA	803	CLA	C1C-C2C	2.76	1.49	1.44
14	bA	808	CLA	C1C-C2C	2.76	1.49	1.44
17	bA	845	BCR	C8-C9	-2.76	1.40	1.45
14	bB	804	CLA	C1B-C2B	2.76	1.49	1.43
14	A	817	CLA	C3B-C4B	2.76	1.49	1.42
14	bA	817	CLA	C3B-C4B	2.76	1.49	1.42
14	bB	819	CLA	C1C-C2C	2.76	1.49	1.44
14	cB	816	CLA	C1C-C2C	2.76	1.49	1.44
14	cA	825	CLA	C1B-C2B	2.76	1.49	1.43
14	A	825	CLA	C1B-C2B	2.76	1.49	1.43
14	cB	808	CLA	C1C-C2C	2.76	1.49	1.44
14	cA	826	CLA	C4B-NB	-2.76	1.34	1.37
14	bA	817	CLA	C1B-C2B	2.76	1.49	1.43
14	cA	817	CLA	C1B-C2B	2.76	1.49	1.43
14	bA	825	CLA	C1B-C2B	2.76	1.49	1.43
14	B	815	CLA	C1C-C2C	2.76	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bA	842	CLA	C1B-C2B	2.76	1.49	1.43
17	bB	841	BCR	C23-C22	-2.76	1.40	1.45
14	A	817	CLA	C1B-C2B	2.76	1.49	1.43
14	A	842	CLA	C1B-C2B	2.76	1.49	1.43
14	A	827	CLA	C1C-C2C	2.75	1.49	1.44
14	cA	822	CLA	C4B-NB	-2.75	1.34	1.37
14	bA	827	CLA	C1C-C2C	2.75	1.49	1.44
14	A	836	CLA	C1B-C2B	2.75	1.49	1.43
14	bL	202	CLA	C4B-NB	-2.75	1.34	1.37
14	bB	816	CLA	C1C-C2C	2.75	1.49	1.44
14	B	816	CLA	C1C-C2C	2.75	1.49	1.44
14	bA	836	CLA	C1B-C2B	2.75	1.49	1.43
14	cA	842	CLA	C1B-C2B	2.75	1.49	1.43
14	cA	827	CLA	C1C-C2C	2.75	1.49	1.44
14	B	814	CLA	C4C-C3C	2.75	1.49	1.45
14	cA	836	CLA	C1B-C2B	2.75	1.49	1.43
14	B	807	CLA	C1C-C2C	2.75	1.49	1.44
14	cB	825	CLA	C1C-C2C	2.75	1.49	1.44
14	bA	826	CLA	C1C-C2C	2.75	1.49	1.44
14	cB	817	CLA	C1C-C2C	2.74	1.49	1.44
14	A	802	CLA	C1C-C2C	2.74	1.49	1.44
14	cF	201	CLA	C1C-C2C	2.74	1.49	1.44
14	B	822	CLA	C1B-C2B	2.74	1.49	1.43
14	cA	802	CLA	C1C-C2C	2.74	1.49	1.44
14	cA	826	CLA	C1C-C2C	2.74	1.49	1.44
17	A	845	BCR	C8-C9	-2.73	1.40	1.45
14	A	803	CLA	C1C-C2C	2.73	1.49	1.44
14	B	813	CLA	C4C-C3C	2.73	1.49	1.45
14	cB	814	CLA	C4C-C3C	2.73	1.49	1.45
14	bB	822	CLA	C1B-C2B	2.73	1.49	1.43
14	bA	832	CLA	C1C-C2C	2.73	1.49	1.44
14	cB	822	CLA	C4C-C3C	2.73	1.49	1.45
14	bF	201	CLA	C1C-C2C	2.73	1.49	1.44
14	A	826	CLA	C1C-C2C	2.73	1.49	1.44
14	bA	802	CLA	C1C-C2C	2.73	1.49	1.44
14	cB	823	CLA	C1B-C2B	2.73	1.49	1.43
14	bB	826	CLA	C1C-NC	-2.73	1.33	1.37
14	B	821	CLA	C4C-C3C	2.73	1.49	1.45
14	cB	827	CLA	C1C-NC	-2.73	1.33	1.37
14	B	826	CLA	C1C-NC	-2.72	1.33	1.37
14	bA	804	CLA	C1B-C2B	2.72	1.49	1.43
14	bB	813	CLA	C4C-C3C	2.72	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bA	839	CLA	C3B-C4B	2.72	1.49	1.42
14	bB	825	CLA	C1C-C2C	2.72	1.49	1.44
14	cL	203	CLA	C1B-C2B	2.72	1.49	1.43
14	B	823	CLA	C1B-C2B	2.72	1.49	1.43
14	B	802	CLA	C3B-C4B	2.72	1.49	1.42
14	cA	839	CLA	C3B-C4B	2.72	1.49	1.42
14	bB	802	CLA	C3B-C4B	2.72	1.49	1.42
14	cB	802	CLA	C1C-C2C	2.72	1.49	1.44
14	B	824	CLA	C1C-C2C	2.71	1.49	1.44
14	A	832	CLA	C1C-C2C	2.71	1.49	1.44
14	cA	832	CLA	C1C-C2C	2.71	1.49	1.44
14	cA	804	CLA	C1B-C2B	2.71	1.49	1.43
14	bB	821	CLA	C4C-C3C	2.71	1.49	1.45
14	bB	823	CLA	C1B-C2B	2.71	1.49	1.43
14	cB	826	CLA	C1C-C2C	2.71	1.49	1.44
14	A	804	CLA	C1B-C2B	2.71	1.49	1.43
14	A	839	CLA	C3B-C4B	2.71	1.49	1.42
14	cB	803	CLA	C3B-C4B	2.71	1.49	1.42
14	B	825	CLA	C1C-C2C	2.71	1.49	1.44
14	bB	801	CLA	C1C-C2C	2.70	1.49	1.44
14	bA	812	CLA	C4C-C3C	2.70	1.49	1.45
14	cB	808	CLA	C3B-C4B	2.70	1.49	1.42
14	bA	822	CLA	C4B-NB	-2.70	1.34	1.37
14	A	811	CLA	C1C-C2C	2.70	1.49	1.44
14	cA	811	CLA	C1C-C2C	2.70	1.49	1.44
14	cA	812	CLA	C4C-C3C	2.70	1.49	1.45
14	B	801	CLA	C1C-C2C	2.70	1.49	1.44
14	bB	824	CLA	C1B-C2B	2.70	1.49	1.43
14	cA	833	CLA	C1B-C2B	2.70	1.49	1.43
14	A	822	CLA	C4B-NB	-2.70	1.34	1.37
14	bA	840	CLA	C1C-C2C	2.70	1.49	1.44
14	bB	849	CLA	C1C-C2C	2.70	1.49	1.44
14	bF	201	CLA	C4B-NB	-2.70	1.34	1.37
14	A	840	CLA	C1C-C2C	2.70	1.49	1.44
14	A	841	CLA	C4D-CHA	2.70	1.48	1.38
14	B	824	CLA	C1B-C2B	2.70	1.49	1.43
14	cA	820	CLA	C1C-C2C	2.70	1.49	1.44
14	cB	825	CLA	C1B-C2B	2.70	1.49	1.43
14	A	820	CLA	C1C-C2C	2.70	1.49	1.44
14	bL	202	CLA	C1C-C2C	2.70	1.49	1.44
14	A	812	CLA	C4C-C3C	2.70	1.49	1.45
14	bL	203	CLA	C1B-C2B	2.70	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cF	201	CLA	C4B-NB	-2.70	1.34	1.37
14	bB	823	CLA	C1C-C2C	2.69	1.49	1.44
14	B	823	CLA	C1C-C2C	2.69	1.49	1.44
14	bA	811	CLA	C1C-C2C	2.69	1.49	1.44
14	cA	824	CLA	C1C-C2C	2.69	1.49	1.44
14	bA	833	CLA	C1B-C2B	2.69	1.49	1.43
14	L	202	CLA	C1C-C2C	2.69	1.49	1.44
14	B	807	CLA	C3B-C4B	2.69	1.49	1.42
14	bA	833	CLA	C3B-C4B	2.69	1.49	1.42
14	bB	807	CLA	C3B-C4B	2.69	1.49	1.42
14	A	823	CLA	C4C-C3C	2.69	1.49	1.45
14	cA	823	CLA	C4C-C3C	2.69	1.49	1.45
14	cB	824	CLA	C1C-C2C	2.69	1.49	1.44
14	cB	850	CLA	C1C-C2C	2.69	1.49	1.44
14	L	203	CLA	C1B-C2B	2.69	1.49	1.43
14	bL	202	CLA	C1B-C2B	2.69	1.49	1.43
14	A	833	CLA	C1B-C2B	2.69	1.49	1.43
14	L	202	CLA	C1B-C2B	2.68	1.49	1.43
14	cA	812	CLA	C1B-C2B	2.68	1.49	1.43
14	bA	820	CLA	C1C-C2C	2.68	1.49	1.44
14	cL	203	CLA	C1C-C2C	2.68	1.49	1.44
14	bA	841	CLA	C4D-CHA	2.68	1.47	1.38
14	bA	816	CLA	C1C-C2C	2.68	1.49	1.44
14	cA	841	CLA	C4D-CHA	2.68	1.47	1.38
14	cB	824	CLA	C1B-C2B	2.68	1.49	1.43
14	cA	831	CLA	C1C-C2C	2.68	1.49	1.44
14	A	833	CLA	C3B-C4B	2.68	1.49	1.42
14	bB	830	CLA	C1C-C2C	2.68	1.49	1.44
14	A	816	CLA	C1C-C2C	2.68	1.49	1.44
14	bA	824	CLA	C1C-C2C	2.68	1.49	1.44
14	bA	819	CLA	C4C-C3C	2.68	1.49	1.45
14	cA	833	CLA	C3B-C4B	2.67	1.49	1.42
14	A	817	CLA	C1C-C2C	2.67	1.49	1.44
14	A	828	CLA	C3B-C4B	2.67	1.49	1.42
17	J	103	BCR	C8-C9	-2.67	1.40	1.45
14	cL	204	CLA	C1B-C2B	2.67	1.49	1.43
14	A	824	CLA	C1C-C2C	2.67	1.49	1.44
14	cA	816	CLA	C1C-C2C	2.67	1.49	1.44
14	bL	204	CLA	C4D-CHA	2.67	1.47	1.38
14	A	809	CLA	C1B-C2B	2.67	1.49	1.43
17	cJ	103	BCR	C8-C9	-2.67	1.40	1.45
14	B	849	CLA	C1C-C2C	2.67	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cB	831	CLA	C1C-C2C	2.67	1.49	1.44
14	cA	817	CLA	C1C-C2C	2.67	1.49	1.44
14	cA	840	CLA	C1C-C2C	2.67	1.49	1.44
14	A	821	CLA	C1C-C2C	2.67	1.49	1.44
14	A	831	CLA	C1C-C2C	2.66	1.49	1.44
14	bA	828	CLA	C3B-C4B	2.66	1.49	1.42
14	bA	817	CLA	C1C-C2C	2.66	1.49	1.44
14	L	204	CLA	C4D-CHA	2.66	1.47	1.38
14	cL	205	CLA	C4D-CHA	2.66	1.47	1.38
14	B	830	CLA	C1C-C2C	2.66	1.49	1.44
14	cA	828	CLA	C3B-C4B	2.66	1.49	1.42
14	B	811	CLA	C4C-C3C	2.66	1.49	1.45
14	B	834	CLA	C4C-C3C	2.66	1.49	1.45
14	bB	834	CLA	C4C-C3C	2.66	1.49	1.45
14	cA	819	CLA	C4C-C3C	2.66	1.49	1.45
14	bB	811	CLA	C4C-C3C	2.66	1.49	1.45
14	cA	809	CLA	C1B-C2B	2.66	1.49	1.43
14	bA	812	CLA	C1B-C2B	2.66	1.49	1.43
14	cB	812	CLA	C4C-C3C	2.66	1.49	1.45
14	A	819	CLA	C4C-C3C	2.65	1.49	1.45
14	A	836	CLA	C3D-C4D	-2.65	1.38	1.44
14	A	812	CLA	C1B-C2B	2.65	1.49	1.43
14	bA	823	CLA	C4C-C3C	2.65	1.49	1.45
14	bA	835	CLA	C1C-C2C	2.65	1.49	1.44
14	bA	834	CLA	C4B-NB	-2.65	1.34	1.37
14	cA	836	CLA	C3D-C4D	-2.65	1.38	1.44
14	bB	808	CLA	C3D-C4D	-2.65	1.38	1.44
14	F	201	CLA	C4B-NB	-2.65	1.34	1.37
13	cA	801	CL0	C1C-C2C	2.65	1.49	1.44
14	bA	831	CLA	C1C-C2C	2.65	1.49	1.44
14	bA	802	CLA	C1B-C2B	2.65	1.49	1.43
14	cA	835	CLA	C1C-C2C	2.65	1.49	1.44
14	cB	809	CLA	C3D-C4D	-2.65	1.38	1.44
14	cA	805	CLA	C1C-C2C	2.65	1.49	1.44
13	A	801	CL0	C1C-C2C	2.65	1.49	1.44
14	bA	836	CLA	C3D-C4D	-2.65	1.38	1.44
17	bJ	103	BCR	C8-C9	-2.65	1.40	1.45
14	bB	839	CLA	C4D-CHA	2.65	1.47	1.38
14	cB	835	CLA	C4C-C3C	2.65	1.49	1.45
14	A	835	CLA	C1C-C2C	2.64	1.49	1.44
14	bA	821	CLA	C1C-C2C	2.64	1.49	1.44
14	bL	204	CLA	C1C-C2C	2.64	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	L	204	CLA	C1B-C2B	2.64	1.49	1.43
14	B	805	CLA	C1C-C2C	2.64	1.49	1.44
14	L	204	CLA	C1C-C2C	2.64	1.49	1.44
14	A	834	CLA	C4B-NB	-2.64	1.34	1.37
13	bA	801	CL0	C1C-C2C	2.64	1.49	1.44
14	cA	821	CLA	C1C-C2C	2.64	1.49	1.44
14	cL	205	CLA	C1C-C2C	2.64	1.49	1.44
14	B	839	CLA	C4D-CHA	2.64	1.47	1.38
14	bA	809	CLA	C1B-C2B	2.64	1.49	1.43
13	cA	801	CL0	C4D-CHA	2.64	1.47	1.38
14	bB	802	CLA	C1C-C2C	2.64	1.49	1.44
14	B	802	CLA	C1C-C2C	2.64	1.49	1.44
14	cB	806	CLA	C1C-C2C	2.64	1.49	1.44
14	bA	810	CLA	C1C-C2C	2.64	1.49	1.44
13	bA	801	CL0	C4D-CHA	2.64	1.47	1.38
14	cA	802	CLA	C1B-C2B	2.63	1.49	1.43
13	A	801	CL0	C4D-CHA	2.63	1.47	1.38
14	bA	805	CLA	C1C-C2C	2.63	1.49	1.44
14	cB	806	CLA	C1B-C2B	2.63	1.49	1.43
14	bB	836	CLA	C1B-C2B	2.63	1.49	1.43
14	bB	805	CLA	C1C-C2C	2.63	1.49	1.44
14	A	837	CLA	C1B-C2B	2.63	1.49	1.43
14	cA	837	CLA	C1B-C2B	2.63	1.49	1.43
14	A	802	CLA	C1B-C2B	2.63	1.49	1.43
14	A	805	CLA	C1C-C2C	2.63	1.49	1.44
14	B	822	CLA	C1C-C2C	2.63	1.49	1.44
14	B	805	CLA	C1B-C2B	2.63	1.49	1.43
17	cB	847	BCR	C8-C9	-2.63	1.40	1.45
14	bB	824	CLA	C4D-CHA	2.63	1.47	1.38
14	bA	809	CLA	C1C-C2C	2.63	1.49	1.44
14	cA	809	CLA	C1C-C2C	2.63	1.49	1.44
14	cB	803	CLA	C1C-C2C	2.63	1.49	1.44
14	B	824	CLA	C4D-CHA	2.63	1.47	1.38
14	bB	805	CLA	C1B-C2B	2.63	1.49	1.43
14	cL	205	CLA	C1B-C2B	2.63	1.49	1.43
14	cB	840	CLA	C4D-CHA	2.62	1.47	1.38
14	bA	837	CLA	C1B-C2B	2.62	1.49	1.43
14	cA	834	CLA	C4B-NB	-2.62	1.34	1.37
14	bL	204	CLA	C1B-C2B	2.62	1.49	1.43
14	cB	837	CLA	C1B-C2B	2.62	1.49	1.43
14	B	836	CLA	C1B-C2B	2.62	1.49	1.43
14	bB	817	CLA	C1B-C2B	2.62	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	808	CLA	C3D-C4D	-2.62	1.38	1.44
17	bI	101	BCR	C8-C9	-2.62	1.40	1.45
17	B	845	BCR	C8-C9	-2.62	1.40	1.45
14	bA	802	CLA	C4B-NB	-2.62	1.34	1.37
14	cB	818	CLA	C1B-C2B	2.62	1.49	1.43
14	cA	817	CLA	C4C-C3C	2.62	1.49	1.45
14	A	815	CLA	C1C-C2C	2.62	1.49	1.44
14	A	810	CLA	C1C-C2C	2.62	1.49	1.44
14	B	817	CLA	C1B-C2B	2.62	1.49	1.43
14	cB	817	CLA	C4B-NB	-2.62	1.34	1.37
14	A	817	CLA	C4C-C3C	2.61	1.49	1.45
17	bB	845	BCR	C8-C9	-2.61	1.40	1.45
14	cB	805	CLA	C1C-C2C	2.61	1.49	1.44
17	B	846	BCR	C8-C9	-2.61	1.40	1.45
14	cB	823	CLA	C1C-C2C	2.61	1.49	1.44
14	A	804	CLA	C1C-C2C	2.61	1.49	1.44
14	bA	804	CLA	C1C-C2C	2.61	1.49	1.44
14	bA	822	CLA	C1C-C2C	2.61	1.49	1.44
14	bB	822	CLA	C1C-C2C	2.61	1.49	1.44
14	cA	802	CLA	C4B-NB	-2.61	1.34	1.37
17	cB	846	BCR	C8-C9	-2.61	1.40	1.45
14	A	809	CLA	C1C-C2C	2.61	1.49	1.44
14	A	822	CLA	C1C-C2C	2.61	1.49	1.44
14	cA	810	CLA	C1C-C2C	2.61	1.49	1.44
14	cA	822	CLA	C1C-C2C	2.61	1.49	1.44
14	cB	825	CLA	C4D-CHA	2.61	1.47	1.38
17	cI	101	BCR	C8-C9	-2.60	1.40	1.45
17	I	101	BCR	C8-C9	-2.60	1.40	1.45
17	bB	846	BCR	C8-C9	-2.60	1.40	1.45
14	cA	815	CLA	C1C-C2C	2.60	1.49	1.44
17	bA	848	BCR	C8-C9	-2.60	1.40	1.45
14	bA	832	CLA	C4D-CHA	2.60	1.47	1.38
14	cL	202	CLA	C1C-C2C	2.60	1.49	1.44
14	B	816	CLA	C4C-C3C	2.60	1.49	1.45
14	bA	819	CLA	C4D-CHA	2.60	1.47	1.38
14	bB	803	CLA	C1B-C2B	2.60	1.49	1.43
14	cA	804	CLA	C1C-C2C	2.60	1.49	1.44
17	cA	848	BCR	C8-C9	-2.60	1.40	1.45
14	cA	819	CLA	C4D-CHA	2.60	1.47	1.38
14	A	802	CLA	C4B-NB	-2.59	1.34	1.37
17	B	843	BCR	C8-C9	-2.59	1.40	1.45
14	bA	817	CLA	C4C-C3C	2.59	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	804	CLA	C1C-C2C	2.59	1.49	1.44
14	A	802	CLA	C3D-C4D	-2.59	1.38	1.44
14	A	835	CLA	C4D-CHA	2.59	1.47	1.38
17	A	848	BCR	C8-C9	-2.59	1.40	1.45
14	bA	823	CLA	C1C-C2C	2.59	1.49	1.44
14	cB	824	CLA	C4D-CHA	2.59	1.47	1.38
14	bB	823	CLA	C4D-CHA	2.59	1.47	1.38
14	A	823	CLA	C1C-C2C	2.59	1.49	1.44
14	cB	817	CLA	C4C-C3C	2.59	1.49	1.45
14	bX	201	CLA	C4D-CHA	2.59	1.47	1.38
14	cA	835	CLA	C4D-CHA	2.59	1.47	1.38
14	B	820	CLA	C1C-C2C	2.59	1.49	1.44
14	cB	804	CLA	C1B-C2B	2.59	1.49	1.43
14	cA	824	CLA	C4D-CHA	2.59	1.47	1.38
14	bB	804	CLA	C1C-C2C	2.59	1.49	1.44
14	bB	816	CLA	C4C-C3C	2.59	1.49	1.45
14	B	823	CLA	C4D-CHA	2.59	1.47	1.38
14	A	820	CLA	C4C-C3C	2.59	1.49	1.45
14	bL	201	CLA	C1C-C2C	2.59	1.49	1.44
14	cX	201	CLA	C4D-CHA	2.59	1.47	1.38
14	bB	829	CLA	C1C-C2C	2.59	1.49	1.44
14	bB	832	CLA	C1C-C2C	2.59	1.49	1.44
14	cB	830	CLA	C1C-C2C	2.59	1.49	1.44
14	X	201	CLA	C4D-CHA	2.59	1.47	1.38
14	L	201	CLA	C1C-C2C	2.59	1.49	1.44
14	cA	832	CLA	C3D-C4D	-2.58	1.38	1.44
14	A	824	CLA	C4D-CHA	2.58	1.47	1.38
14	A	832	CLA	C4D-CHA	2.58	1.47	1.38
14	B	832	CLA	C1C-C2C	2.58	1.49	1.44
17	cA	847	BCR	C23-C22	-2.58	1.40	1.45
14	bA	824	CLA	C4D-CHA	2.58	1.47	1.38
17	cB	847	BCR	C23-C22	-2.58	1.40	1.45
14	bB	835	CLA	C4C-C3C	2.58	1.49	1.45
14	cJ	101	CLA	C4D-CHA	2.58	1.47	1.38
14	cB	833	CLA	C1C-C2C	2.58	1.49	1.44
14	cA	832	CLA	C4D-CHA	2.58	1.47	1.38
14	bA	815	CLA	C1C-C2C	2.58	1.49	1.44
17	bL	206	BCR	C23-C22	-2.58	1.40	1.45
14	bA	832	CLA	C3D-C4D	-2.58	1.38	1.44
14	B	803	CLA	C1B-C2B	2.58	1.49	1.43
14	A	819	CLA	C4D-CHA	2.58	1.47	1.38
17	A	847	BCR	C23-C22	-2.58	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	846	BCR	C23-C22	-2.58	1.40	1.45
14	bA	835	CLA	C4D-CHA	2.58	1.47	1.38
14	cA	820	CLA	C4C-C3C	2.58	1.49	1.45
14	B	811	CLA	C1C-C2C	2.58	1.49	1.44
14	cB	812	CLA	C1C-C2C	2.58	1.49	1.44
17	bB	843	BCR	C8-C9	-2.58	1.40	1.45
14	bA	813	CLA	C1C-C2C	2.58	1.49	1.44
14	cA	813	CLA	C1C-C2C	2.58	1.49	1.44
14	bB	820	CLA	C1C-C2C	2.57	1.49	1.44
17	bA	847	BCR	C23-C22	-2.57	1.40	1.45
14	bA	820	CLA	C4C-C3C	2.57	1.49	1.45
17	J	103	BCR	C23-C22	-2.57	1.40	1.45
17	cJ	103	BCR	C23-C22	-2.57	1.40	1.45
14	A	813	CLA	C1C-C2C	2.57	1.49	1.44
14	bJ	101	CLA	C4D-CHA	2.57	1.47	1.38
17	bB	846	BCR	C23-C22	-2.57	1.40	1.45
14	cB	840	CLA	C1C-C2C	2.57	1.49	1.44
17	cB	844	BCR	C8-C9	-2.57	1.40	1.45
14	A	832	CLA	C3D-C4D	-2.57	1.38	1.44
14	cA	813	CLA	C4B-NB	-2.57	1.34	1.37
14	cB	832	CLA	C4C-C3C	2.57	1.49	1.45
14	B	829	CLA	C1C-C2C	2.57	1.49	1.44
14	bB	811	CLA	C1C-C2C	2.57	1.49	1.44
14	bA	814	CLA	C4D-CHA	2.57	1.47	1.38
14	B	835	CLA	C4C-C3C	2.57	1.49	1.45
14	bB	825	CLA	C4D-CHA	2.57	1.47	1.38
14	bB	831	CLA	C4C-C3C	2.57	1.49	1.45
14	cB	826	CLA	C4D-CHA	2.57	1.47	1.38
14	B	839	CLA	C1C-C2C	2.57	1.49	1.44
14	bA	802	CLA	C3D-C4D	-2.56	1.38	1.44
14	cA	823	CLA	C1C-C2C	2.56	1.49	1.44
14	cB	840	CLA	C1B-C2B	2.56	1.49	1.43
14	cA	802	CLA	C3D-C4D	-2.56	1.38	1.44
14	cA	826	CLA	C4D-CHA	2.56	1.47	1.38
14	cB	827	CLA	C4C-C3C	2.56	1.49	1.45
14	B	832	CLA	C4B-NB	-2.56	1.34	1.37
14	cB	821	CLA	C1C-C2C	2.56	1.49	1.44
17	bA	848	BCR	C23-C22	-2.56	1.40	1.45
14	B	805	CLA	C4D-CHA	2.56	1.47	1.38
14	B	832	CLA	C4D-CHA	2.56	1.47	1.38
14	J	101	CLA	C4D-CHA	2.56	1.47	1.38
17	bA	846	BCR	C8-C9	-2.56	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bB	832	CLA	C4B-NB	-2.56	1.34	1.37
14	cL	202	CLA	C4D-CHA	2.56	1.47	1.38
14	bA	813	CLA	C4C-C3C	2.56	1.49	1.45
14	bB	805	CLA	C4D-CHA	2.56	1.47	1.38
14	bB	839	CLA	C1C-C2C	2.56	1.49	1.44
14	bL	201	CLA	C4D-CHA	2.56	1.47	1.38
14	B	825	CLA	C4D-CHA	2.56	1.47	1.38
14	cB	806	CLA	C4D-CHA	2.56	1.47	1.38
17	cA	848	BCR	C23-C22	-2.56	1.40	1.45
14	bA	826	CLA	C4D-CHA	2.56	1.47	1.38
14	B	839	CLA	C1B-C2B	2.56	1.49	1.43
17	L	206	BCR	C23-C22	-2.56	1.40	1.45
14	L	201	CLA	C4D-CHA	2.56	1.47	1.38
14	bA	841	CLA	C3B-C4B	2.56	1.48	1.42
14	A	826	CLA	C4D-CHA	2.55	1.47	1.38
14	bB	839	CLA	C1B-C2B	2.55	1.49	1.43
14	B	816	CLA	C4B-NB	-2.55	1.34	1.37
14	bB	826	CLA	C4C-C3C	2.55	1.49	1.45
14	B	849	CLA	C4D-CHA	2.55	1.47	1.38
14	cB	833	CLA	C4D-CHA	2.55	1.47	1.38
14	cB	850	CLA	C4C-C3C	2.55	1.49	1.45
14	cB	833	CLA	C4B-NB	-2.55	1.34	1.37
14	J	102	CLA	C1B-C2B	2.55	1.49	1.43
17	A	848	BCR	C23-C22	-2.55	1.40	1.45
17	A	846	BCR	C8-C9	-2.55	1.40	1.45
17	bI	102	BCR	C8-C9	-2.55	1.40	1.45
14	B	831	CLA	C4C-C3C	2.55	1.49	1.45
17	A	847	BCR	C8-C9	-2.55	1.40	1.45
14	bB	849	CLA	C4C-C3C	2.55	1.49	1.45
14	B	802	CLA	C4D-CHA	2.55	1.47	1.38
14	bB	832	CLA	C4D-CHA	2.55	1.47	1.38
14	bX	201	CLA	C1B-C2B	2.55	1.49	1.43
14	cX	201	CLA	C1B-C2B	2.55	1.49	1.43
14	cB	803	CLA	C4D-CHA	2.55	1.47	1.38
14	bJ	102	CLA	C1B-C2B	2.55	1.49	1.43
14	cJ	102	CLA	C1B-C2B	2.55	1.49	1.43
17	bJ	103	BCR	C23-C22	-2.55	1.40	1.45
14	cA	807	CLA	C1B-C2B	2.55	1.49	1.43
14	J	102	CLA	C4D-CHA	2.55	1.47	1.38
14	bB	802	CLA	C4D-CHA	2.55	1.47	1.38
14	bA	830	CLA	C3B-C4B	2.55	1.48	1.42
14	bA	830	CLA	C3D-C4D	-2.55	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cA	830	CLA	C3D-C4D	-2.55	1.38	1.44
14	cA	814	CLA	C4D-CHA	2.55	1.47	1.38
14	cB	850	CLA	C4D-CHA	2.55	1.47	1.38
14	bB	816	CLA	C4B-NB	-2.55	1.34	1.37
14	bB	836	CLA	C1C-C2C	2.55	1.49	1.44
14	X	201	CLA	C1B-C2B	2.54	1.49	1.43
14	bA	808	CLA	C1B-C2B	2.54	1.49	1.43
14	cB	807	CLA	C4D-CHA	2.54	1.47	1.38
14	bB	803	CLA	C1C-C2C	2.54	1.49	1.44
14	cA	813	CLA	C4C-C3C	2.54	1.49	1.45
14	cB	809	CLA	C1B-C2B	2.54	1.49	1.43
14	bB	810	CLA	C1C-C2C	2.54	1.49	1.44
14	cA	818	CLA	C4C-C3C	2.54	1.49	1.45
14	A	814	CLA	C4D-CHA	2.54	1.47	1.38
14	cA	812	CLA	C3B-C2B	2.54	1.49	1.41
14	cA	808	CLA	C1B-C2B	2.54	1.49	1.43
14	A	830	CLA	C3B-C4B	2.54	1.48	1.42
14	cB	836	CLA	C4C-C3C	2.54	1.49	1.45
14	bA	814	CLA	C3B-C2B	2.54	1.49	1.41
14	bB	835	CLA	C4D-CHA	2.54	1.47	1.38
17	cI	102	BCR	C8-C9	-2.54	1.40	1.45
14	A	821	CLA	C4C-C3C	2.54	1.49	1.45
14	bA	818	CLA	C4C-C3C	2.54	1.49	1.45
14	bB	808	CLA	C1B-C2B	2.54	1.49	1.43
14	bA	812	CLA	C3B-C2B	2.54	1.49	1.41
14	bB	806	CLA	C4D-CHA	2.54	1.47	1.38
14	A	808	CLA	C1B-C2B	2.54	1.49	1.43
14	cA	841	CLA	C3B-C4B	2.54	1.48	1.42
17	bA	849	BCR	C8-C9	-2.54	1.40	1.45
14	B	849	CLA	C4C-C3C	2.54	1.49	1.45
14	B	806	CLA	C4D-CHA	2.54	1.47	1.38
14	cJ	102	CLA	C4D-CHA	2.53	1.47	1.38
14	A	818	CLA	C4C-C3C	2.53	1.49	1.45
14	bA	821	CLA	C4C-C3C	2.53	1.49	1.45
14	A	830	CLA	C3D-C4D	-2.53	1.38	1.44
17	I	102	BCR	C8-C9	-2.53	1.40	1.45
17	cL	207	BCR	C23-C22	-2.53	1.40	1.45
14	B	818	CLA	C1C-C2C	2.53	1.49	1.44
14	A	813	CLA	C4C-C3C	2.53	1.49	1.45
14	A	852	CLA	C3B-C4B	2.53	1.48	1.42
14	B	826	CLA	C4C-C3C	2.53	1.49	1.45
14	bA	852	CLA	C3B-C4B	2.53	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cB	837	CLA	C1C-C2C	2.53	1.49	1.44
14	A	813	CLA	C4D-CHA	2.53	1.47	1.38
14	cB	804	CLA	C1C-C2C	2.53	1.49	1.44
14	B	808	CLA	C1B-C2B	2.53	1.49	1.43
14	cA	852	CLA	C3B-C4B	2.53	1.48	1.42
14	A	815	CLA	C4D-CHA	2.53	1.47	1.38
14	bA	819	CLA	C1C-C2C	2.53	1.49	1.44
14	bB	818	CLA	C1C-C2C	2.53	1.49	1.44
17	cA	847	BCR	C8-C9	-2.53	1.40	1.45
14	B	803	CLA	C1C-C2C	2.53	1.49	1.44
14	bA	803	CLA	C4C-C3C	2.53	1.49	1.45
14	bB	814	CLA	C1C-C2C	2.53	1.49	1.44
14	bB	849	CLA	C4D-CHA	2.53	1.47	1.38
14	cA	813	CLA	C4D-CHA	2.53	1.47	1.38
14	bJ	102	CLA	C4D-CHA	2.53	1.47	1.38
14	B	804	CLA	C4D-CHA	2.53	1.47	1.38
14	B	833	CLA	C4D-CHA	2.53	1.47	1.38
17	bA	847	BCR	C8-C9	-2.53	1.40	1.45
14	cA	807	CLA	C1C-C2C	2.53	1.49	1.44
14	A	812	CLA	C3B-C2B	2.53	1.49	1.41
14	cB	824	CLA	C3B-C2B	2.53	1.49	1.41
14	cA	817	CLA	C4D-CHA	2.53	1.47	1.38
14	bA	817	CLA	C3B-C2B	2.53	1.49	1.41
14	B	814	CLA	C1C-C2C	2.53	1.49	1.44
14	bB	818	CLA	C4D-CHA	2.53	1.47	1.38
14	cB	834	CLA	C4D-CHA	2.53	1.47	1.38
14	bA	807	CLA	C1B-C2B	2.52	1.49	1.43
14	cB	827	CLA	C1B-C2B	2.52	1.49	1.43
14	bA	813	CLA	C4D-CHA	2.52	1.47	1.38
14	bA	815	CLA	C4D-CHA	2.52	1.47	1.38
14	A	829	CLA	C4D-CHA	2.52	1.47	1.38
14	bA	817	CLA	C4D-CHA	2.52	1.47	1.38
14	A	822	CLA	C1B-C2B	2.52	1.49	1.43
14	bB	821	CLA	C4D-CHA	2.52	1.47	1.38
14	cA	817	CLA	C3B-C2B	2.52	1.49	1.41
14	cB	822	CLA	C4D-CHA	2.52	1.47	1.38
14	B	821	CLA	C4D-CHA	2.52	1.47	1.38
14	A	817	CLA	C4D-CHA	2.52	1.47	1.38
14	cB	811	CLA	C4C-C3C	2.52	1.49	1.45
17	cA	849	BCR	C8-C9	-2.52	1.40	1.45
14	cA	822	CLA	C1B-C2B	2.52	1.49	1.43
14	B	835	CLA	C4D-CHA	2.52	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	cL	207	BCR	C12-C13	-2.52	1.40	1.45
14	A	841	CLA	C3B-C4B	2.52	1.48	1.42
14	A	817	CLA	C3B-C2B	2.52	1.49	1.41
14	cA	829	CLA	C4D-CHA	2.52	1.47	1.38
14	B	809	CLA	C3B-C4B	2.52	1.48	1.42
14	cA	821	CLA	C4C-C3C	2.52	1.49	1.45
14	bB	833	CLA	C4D-CHA	2.52	1.47	1.38
14	cB	811	CLA	C1C-C2C	2.52	1.49	1.44
14	A	814	CLA	C3B-C2B	2.52	1.49	1.41
17	cA	846	BCR	C8-C9	-2.52	1.40	1.45
14	cA	815	CLA	C4D-CHA	2.52	1.47	1.38
14	bB	812	CLA	C4B-NB	-2.52	1.34	1.37
14	bB	809	CLA	C3B-C4B	2.52	1.48	1.42
14	bB	815	CLA	C1B-C2B	2.52	1.49	1.43
14	cB	815	CLA	C1C-C2C	2.52	1.49	1.44
14	cB	819	CLA	C4D-CHA	2.52	1.47	1.38
14	A	807	CLA	C1B-C2B	2.52	1.49	1.43
14	bB	810	CLA	C4C-C3C	2.52	1.49	1.45
14	B	823	CLA	C3B-C2B	2.52	1.49	1.41
14	cA	830	CLA	C3B-C4B	2.52	1.48	1.42
14	B	810	CLA	C1C-C2C	2.52	1.49	1.44
14	B	834	CLA	C4D-CHA	2.52	1.47	1.38
14	bB	823	CLA	C3B-C2B	2.52	1.49	1.41
14	cB	826	CLA	C4B-NB	-2.52	1.34	1.37
14	A	821	CLA	C4D-CHA	2.51	1.47	1.38
14	B	837	CLA	C1C-C2C	2.51	1.49	1.44
14	B	818	CLA	C4D-CHA	2.51	1.47	1.38
14	bB	814	CLA	C4D-CHA	2.51	1.47	1.38
14	bA	821	CLA	C4D-CHA	2.51	1.47	1.38
14	A	823	CLA	C1B-C2B	2.51	1.49	1.43
14	B	851	CLA	C4D-CHA	2.51	1.47	1.38
14	bB	851	CLA	C4D-CHA	2.51	1.47	1.38
14	B	826	CLA	C1B-C2B	2.51	1.49	1.43
14	B	836	CLA	C1C-C2C	2.51	1.49	1.44
14	cB	815	CLA	C4D-CHA	2.51	1.47	1.38
14	A	834	CLA	C4D-CHA	2.51	1.47	1.38
14	A	816	CLA	C3B-C2B	2.51	1.49	1.41
14	A	813	CLA	C4B-NB	-2.51	1.34	1.37
14	A	807	CLA	C1C-C2C	2.51	1.49	1.44
14	cB	801	CLA	C4D-CHA	2.51	1.47	1.38
14	cB	835	CLA	C4D-CHA	2.51	1.47	1.38
14	bA	822	CLA	C1B-C2B	2.51	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	803	CLA	C4C-C3C	2.51	1.49	1.45
14	B	810	CLA	C4C-C3C	2.51	1.49	1.45
14	bB	804	CLA	C4D-CHA	2.51	1.47	1.38
14	bB	834	CLA	C4D-CHA	2.51	1.47	1.38
14	bB	826	CLA	C1B-C2B	2.51	1.49	1.43
14	cA	823	CLA	C1B-C2B	2.51	1.49	1.43
14	bA	829	CLA	C4D-CHA	2.51	1.47	1.38
14	cA	821	CLA	C4D-CHA	2.51	1.47	1.38
14	bB	837	CLA	C1C-C2C	2.51	1.49	1.44
14	bA	815	CLA	C4C-C3C	2.51	1.49	1.45
17	bL	206	BCR	C12-C13	-2.51	1.40	1.45
14	A	815	CLA	C4C-C3C	2.51	1.49	1.45
14	bA	807	CLA	C4D-CHA	2.51	1.47	1.38
14	cB	805	CLA	C4D-CHA	2.51	1.47	1.38
14	cB	819	CLA	C1C-C2C	2.51	1.49	1.44
14	bJ	101	CLA	C1B-C2B	2.51	1.49	1.43
14	B	814	CLA	C4D-CHA	2.51	1.47	1.38
14	cA	842	CLA	C1C-C2C	2.51	1.49	1.44
14	bB	807	CLA	C4D-CHA	2.51	1.47	1.38
14	A	842	CLA	C1C-C2C	2.51	1.49	1.44
14	B	822	CLA	C4D-CHA	2.51	1.47	1.38
14	bA	807	CLA	C1C-C2C	2.51	1.49	1.44
14	cA	834	CLA	C4D-CHA	2.51	1.47	1.38
14	bA	816	CLA	C3B-C2B	2.50	1.49	1.41
14	bB	822	CLA	C4D-CHA	2.50	1.47	1.38
17	bF	202	BCR	C8-C9	-2.50	1.40	1.45
14	cB	811	CLA	C4D-CHA	2.50	1.47	1.38
14	cA	803	CLA	C4C-C3C	2.50	1.49	1.45
14	bA	842	CLA	C1C-C2C	2.50	1.49	1.44
14	cB	823	CLA	C4D-CHA	2.50	1.47	1.38
14	cB	836	CLA	C4D-CHA	2.50	1.47	1.38
14	cA	816	CLA	C3B-C2B	2.50	1.49	1.41
14	bB	801	CLA	C1B-C2B	2.50	1.49	1.43
14	cA	810	CLA	C1B-C2B	2.50	1.49	1.43
14	cB	808	CLA	C4D-CHA	2.50	1.47	1.38
14	A	807	CLA	C4D-CHA	2.50	1.47	1.38
14	bA	832	CLA	C1B-C2B	2.50	1.49	1.43
14	B	812	CLA	C4B-NB	-2.50	1.34	1.37
14	B	825	CLA	C4B-NB	-2.50	1.34	1.37
14	cB	807	CLA	C1B-C2B	2.50	1.49	1.43
14	bA	819	CLA	C1B-C2B	2.50	1.49	1.43
14	B	837	CLA	C4C-C3C	2.50	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	819	CLA	C1C-C2C	2.50	1.49	1.44
17	F	202	BCR	C8-C9	-2.50	1.40	1.45
17	bM	101	BCR	C8-C9	-2.50	1.40	1.45
14	cB	838	CLA	C1C-C2C	2.50	1.49	1.44
14	B	816	CLA	C4D-CHA	2.50	1.47	1.38
14	B	815	CLA	C1B-C2B	2.50	1.49	1.43
14	A	840	CLA	C4D-CHA	2.50	1.47	1.38
14	A	822	CLA	C4C-C3C	2.50	1.49	1.45
14	cB	817	CLA	C4D-CHA	2.50	1.47	1.38
14	bA	810	CLA	C1B-C2B	2.50	1.49	1.43
14	A	805	CLA	C4D-CHA	2.50	1.47	1.38
14	bB	810	CLA	C4D-CHA	2.50	1.47	1.38
14	cA	814	CLA	C3B-C2B	2.50	1.49	1.41
17	A	849	BCR	C8-C9	-2.50	1.40	1.45
14	bB	816	CLA	C4D-CHA	2.50	1.47	1.38
14	cA	807	CLA	C4D-CHA	2.50	1.47	1.38
17	cF	202	BCR	C8-C9	-2.50	1.40	1.45
14	B	801	CLA	C1B-C2B	2.50	1.49	1.43
14	cA	819	CLA	C1B-C2B	2.50	1.49	1.43
14	cA	829	CLA	C1B-C2B	2.50	1.49	1.43
14	B	810	CLA	C4D-CHA	2.49	1.47	1.38
14	bA	829	CLA	C1B-C2B	2.49	1.49	1.43
14	cB	802	CLA	C1B-C2B	2.49	1.49	1.43
14	cB	814	CLA	C4D-CHA	2.49	1.47	1.38
14	bA	822	CLA	C4C-C3C	2.49	1.49	1.45
14	cB	805	CLA	C4C-C3C	2.49	1.49	1.45
14	B	807	CLA	C4D-CHA	2.49	1.47	1.38
14	cA	837	CLA	C1C-C2C	2.49	1.49	1.44
14	cA	805	CLA	C4D-CHA	2.49	1.47	1.38
14	cB	820	CLA	C1B-C2B	2.49	1.49	1.43
14	bA	805	CLA	C4D-CHA	2.49	1.47	1.38
14	bB	804	CLA	C4C-C3C	2.49	1.49	1.45
14	bB	837	CLA	C4C-C3C	2.49	1.49	1.45
14	bA	834	CLA	C4D-CHA	2.49	1.47	1.38
14	cB	810	CLA	C3B-C4B	2.49	1.48	1.42
14	bA	803	CLA	C4D-CHA	2.49	1.47	1.38
14	A	809	CLA	C4D-CHA	2.49	1.47	1.38
14	A	833	CLA	C4D-CHA	2.49	1.47	1.38
14	A	841	CLA	C1C-C2C	2.49	1.49	1.44
14	bB	828	CLA	C1B-C2B	2.49	1.49	1.43
14	bB	812	CLA	C4D-CHA	2.49	1.47	1.38
14	bA	837	CLA	C1C-C2C	2.49	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cA	819	CLA	C1C-C2C	2.49	1.49	1.44
14	bA	809	CLA	C4D-CHA	2.49	1.47	1.38
14	bB	813	CLA	C4D-CHA	2.49	1.47	1.38
14	A	819	CLA	C1B-C2B	2.49	1.49	1.43
14	cB	816	CLA	C1B-C2B	2.49	1.49	1.43
14	cJ	101	CLA	C1B-C2B	2.49	1.49	1.43
14	A	837	CLA	C1C-C2C	2.49	1.49	1.44
14	bA	816	CLA	C4D-CHA	2.49	1.47	1.38
14	bA	840	CLA	C4D-CHA	2.49	1.47	1.38
14	J	101	CLA	C1B-C2B	2.49	1.49	1.43
14	bA	840	CLA	C1B-C2B	2.49	1.49	1.43
14	cA	832	CLA	C1B-C2B	2.49	1.49	1.43
14	A	816	CLA	C4D-CHA	2.49	1.47	1.38
14	bA	833	CLA	C4D-CHA	2.49	1.47	1.38
14	cA	833	CLA	C4D-CHA	2.49	1.47	1.38
14	cA	840	CLA	C4D-CHA	2.49	1.47	1.38
14	bA	837	CLA	C4B-NB	-2.49	1.34	1.37
14	cA	809	CLA	C4D-CHA	2.49	1.47	1.38
14	cB	813	CLA	C4D-CHA	2.49	1.47	1.38
14	B	812	CLA	C4D-CHA	2.49	1.47	1.38
14	B	819	CLA	C1B-C2B	2.49	1.49	1.43
14	bB	825	CLA	C4B-NB	-2.49	1.34	1.37
14	cB	813	CLA	C4B-NB	-2.49	1.34	1.37
14	A	832	CLA	C1B-C2B	2.49	1.49	1.43
14	B	804	CLA	C4C-C3C	2.49	1.49	1.45
14	cA	816	CLA	C4D-CHA	2.49	1.47	1.38
14	bA	823	CLA	C1B-C2B	2.49	1.49	1.43
17	M	101	BCR	C8-C9	-2.48	1.40	1.45
14	bB	825	CLA	C3D-C4D	-2.48	1.38	1.44
14	A	829	CLA	C1B-C2B	2.48	1.49	1.43
14	bB	826	CLA	C3B-C2B	2.48	1.49	1.41
14	B	806	CLA	C1B-C2B	2.48	1.49	1.43
14	cA	815	CLA	C4C-C3C	2.48	1.49	1.45
14	cB	815	CLA	C3B-C2B	2.48	1.49	1.41
14	bA	804	CLA	C4D-CHA	2.48	1.47	1.38
14	cA	805	CLA	C1B-C2B	2.48	1.49	1.43
14	cA	840	CLA	C1B-C2B	2.48	1.49	1.43
17	cM	101	BCR	C8-C9	-2.48	1.40	1.45
14	bB	819	CLA	C1B-C2B	2.48	1.49	1.43
14	bB	838	CLA	C4D-CHA	2.48	1.47	1.38
17	bB	847	BCR	C23-C22	-2.48	1.40	1.45
17	cB	848	BCR	C23-C22	-2.48	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bB	820	CLA	C3B-C2B	2.48	1.49	1.41
14	bB	806	CLA	C1B-C2B	2.48	1.49	1.43
14	B	813	CLA	C4D-CHA	2.48	1.47	1.38
14	A	840	CLA	C1B-C2B	2.48	1.49	1.43
14	cB	821	CLA	C3B-C2B	2.48	1.49	1.41
14	cB	827	CLA	C1C-C2C	2.48	1.49	1.44
14	A	803	CLA	C4D-CHA	2.48	1.47	1.38
14	B	820	CLA	C3B-C2B	2.48	1.49	1.41
14	cB	838	CLA	C4C-C3C	2.48	1.49	1.45
14	bA	833	CLA	C3D-C4D	-2.48	1.38	1.44
14	cA	822	CLA	C4C-C3C	2.48	1.49	1.45
14	cA	803	CLA	C4D-CHA	2.48	1.47	1.38
14	cB	831	CLA	C3B-C2B	2.48	1.49	1.41
14	B	838	CLA	C4D-CHA	2.48	1.47	1.38
14	bA	834	CLA	C1C-C2C	2.48	1.49	1.44
14	cA	841	CLA	C1C-C2C	2.48	1.49	1.44
14	B	830	CLA	C3B-C2B	2.48	1.49	1.41
14	bA	841	CLA	C1C-C2C	2.48	1.49	1.44
17	cB	842	BCR	C8-C9	-2.48	1.40	1.45
14	bA	836	CLA	C4D-CHA	2.48	1.47	1.38
14	bA	810	CLA	C4D-CHA	2.48	1.47	1.38
14	B	826	CLA	C1C-C2C	2.47	1.49	1.44
14	cB	827	CLA	C3B-C2B	2.47	1.49	1.41
14	bA	813	CLA	C4B-NB	-2.47	1.34	1.37
14	B	826	CLA	C3B-C2B	2.47	1.49	1.41
14	bB	826	CLA	C3D-C4D	-2.47	1.38	1.44
14	bA	805	CLA	C1B-C2B	2.47	1.49	1.43
17	B	841	BCR	C8-C9	-2.47	1.40	1.45
17	B	847	BCR	C23-C22	-2.47	1.40	1.45
14	A	836	CLA	C4D-CHA	2.47	1.47	1.38
14	bB	830	CLA	C3B-C2B	2.47	1.49	1.41
17	L	206	BCR	C12-C13	-2.47	1.40	1.45
14	bB	830	CLA	C4C-C3C	2.47	1.49	1.45
14	A	810	CLA	C4D-CHA	2.47	1.47	1.38
14	cA	810	CLA	C4D-CHA	2.47	1.47	1.38
14	B	826	CLA	C3D-C4D	-2.47	1.38	1.44
14	cA	837	CLA	C4B-NB	-2.47	1.34	1.37
14	A	810	CLA	C1B-C2B	2.47	1.49	1.43
14	B	811	CLA	C4D-CHA	2.47	1.47	1.38
14	cB	839	CLA	C4D-CHA	2.47	1.47	1.38
14	cB	831	CLA	C4C-C3C	2.47	1.49	1.45
14	B	814	CLA	C3B-C2B	2.47	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bB	821	CLA	C1C-C2C	2.47	1.49	1.44
17	A	849	BCR	C23-C22	-2.47	1.40	1.45
14	bB	826	CLA	C1C-C2C	2.47	1.49	1.44
14	cB	822	CLA	C1C-C2C	2.47	1.49	1.44
14	bB	811	CLA	C4D-CHA	2.47	1.47	1.38
14	A	804	CLA	C4D-CHA	2.47	1.47	1.38
14	A	805	CLA	C1B-C2B	2.47	1.49	1.43
14	B	830	CLA	C4C-C3C	2.47	1.49	1.45
17	bA	849	BCR	C23-C22	-2.47	1.40	1.45
14	A	828	CLA	C1C-C2C	2.46	1.49	1.44
14	cB	850	CLA	C1B-C2B	2.46	1.49	1.43
17	cB	845	BCR	C12-C13	-2.46	1.40	1.45
14	A	833	CLA	C3D-C4D	-2.46	1.38	1.44
14	B	825	CLA	C3D-C4D	-2.46	1.38	1.44
14	cA	836	CLA	C4D-CHA	2.46	1.47	1.38
14	cA	829	CLA	C1C-C2C	2.46	1.49	1.44
14	A	825	CLA	C3B-C2B	2.46	1.49	1.41
14	B	828	CLA	C1B-C2B	2.46	1.49	1.43
14	cA	825	CLA	C3B-C2B	2.46	1.49	1.41
14	A	837	CLA	C4B-NB	-2.46	1.34	1.37
14	J	101	CLA	C4C-C3C	2.46	1.49	1.45
14	bA	825	CLA	C3B-C2B	2.46	1.49	1.41
14	bB	814	CLA	C3B-C2B	2.46	1.49	1.41
14	cB	809	CLA	C4C-C3C	2.46	1.49	1.45
14	A	808	CLA	C4D-CHA	2.46	1.47	1.38
14	B	821	CLA	C1C-C2C	2.46	1.49	1.44
14	cA	804	CLA	C4D-CHA	2.46	1.47	1.38
14	cB	826	CLA	C3D-C4D	-2.46	1.38	1.44
14	cJ	101	CLA	C4C-C3C	2.46	1.49	1.45
14	bL	202	CLA	C4D-CHA	2.46	1.47	1.38
17	bB	844	BCR	C12-C13	-2.46	1.40	1.45
14	cB	831	CLA	C4D-CHA	2.46	1.47	1.38
17	bB	841	BCR	C8-C9	-2.46	1.40	1.45
14	B	818	CLA	C4B-NB	-2.46	1.34	1.37
14	A	831	CLA	C3B-C2B	2.46	1.49	1.41
14	A	829	CLA	C1C-C2C	2.46	1.49	1.44
14	bB	849	CLA	C1B-C2B	2.46	1.49	1.43
14	bA	828	CLA	C1C-C2C	2.46	1.49	1.44
14	A	811	CLA	C4D-CHA	2.46	1.47	1.38
14	cA	808	CLA	C4D-CHA	2.46	1.47	1.38
14	A	823	CLA	C4D-CHA	2.46	1.47	1.38
14	bA	811	CLA	C4D-CHA	2.46	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bB	830	CLA	C4D-CHA	2.46	1.47	1.38
14	cB	812	CLA	C4D-CHA	2.46	1.47	1.38
14	L	202	CLA	C4D-CHA	2.46	1.47	1.38
14	cA	811	CLA	C4D-CHA	2.46	1.47	1.38
17	B	844	BCR	C12-C13	-2.46	1.40	1.45
14	bA	808	CLA	C4D-CHA	2.46	1.47	1.38
14	cA	823	CLA	C4D-CHA	2.46	1.47	1.38
14	B	849	CLA	C1B-C2B	2.46	1.49	1.43
14	bJ	101	CLA	C4C-C3C	2.45	1.49	1.45
14	B	827	CLA	C4D-CHA	2.45	1.47	1.38
14	bA	825	CLA	C4D-CHA	2.45	1.47	1.38
14	A	842	CLA	C4D-CHA	2.45	1.47	1.38
14	A	827	CLA	C3B-C2B	2.45	1.49	1.41
14	bB	827	CLA	C3B-C2B	2.45	1.49	1.41
14	bA	823	CLA	C4D-CHA	2.45	1.47	1.38
14	A	828	CLA	C4D-CHA	2.45	1.47	1.38
17	B	850	BCR	C23-C22	-2.45	1.40	1.45
14	cB	812	CLA	C1B-C2B	2.45	1.49	1.43
14	cB	820	CLA	C4D-CHA	2.45	1.47	1.38
14	cA	833	CLA	C1C-NC	-2.45	1.34	1.37
14	B	830	CLA	C4D-CHA	2.45	1.47	1.38
14	bA	803	CLA	C3B-C2B	2.45	1.49	1.41
14	bA	831	CLA	C3B-C2B	2.45	1.49	1.41
14	cA	803	CLA	C3B-C2B	2.45	1.49	1.41
14	cA	831	CLA	C3B-C2B	2.45	1.49	1.41
14	B	811	CLA	C1B-C2B	2.45	1.49	1.43
17	cA	849	BCR	C23-C22	-2.45	1.40	1.45
14	bB	820	CLA	C4D-CHA	2.45	1.47	1.38
14	A	803	CLA	C3B-C2B	2.45	1.49	1.41
14	cA	828	CLA	C1C-C2C	2.45	1.49	1.44
14	cB	829	CLA	C1B-C2B	2.45	1.49	1.43
14	cA	833	CLA	C3D-C4D	-2.45	1.38	1.44
14	bL	203	CLA	C1C-C2C	2.45	1.49	1.44
14	B	820	CLA	C4D-CHA	2.45	1.47	1.38
14	cB	821	CLA	C4D-CHA	2.45	1.47	1.38
17	cB	851	BCR	C23-C22	-2.45	1.40	1.45
14	bB	819	CLA	C4D-CHA	2.45	1.47	1.38
14	A	827	CLA	C4C-C3C	2.45	1.49	1.45
14	cA	812	CLA	C4D-CHA	2.45	1.47	1.38
14	B	808	CLA	C4C-C3C	2.45	1.49	1.45
14	B	835	CLA	C3B-C2B	2.45	1.49	1.41
14	bA	842	CLA	C4D-CHA	2.45	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cB	836	CLA	C3B-C2B	2.45	1.49	1.41
14	bA	827	CLA	C3B-C2B	2.45	1.49	1.41
14	cB	839	CLA	C4C-C3C	2.45	1.49	1.45
14	bA	836	CLA	C1C-C2C	2.45	1.49	1.44
14	cA	815	CLA	C3B-C2B	2.45	1.49	1.41
14	bA	835	CLA	C4C-C3C	2.45	1.49	1.45
14	cB	827	CLA	C4D-CHA	2.45	1.47	1.38
14	bA	827	CLA	C4D-CHA	2.45	1.47	1.38
14	B	827	CLA	C3B-C2B	2.44	1.49	1.41
14	cB	828	CLA	C3B-C2B	2.44	1.49	1.41
14	bA	812	CLA	C4D-CHA	2.44	1.47	1.38
14	bB	826	CLA	C4D-CHA	2.44	1.47	1.38
14	cB	828	CLA	C4D-CHA	2.44	1.47	1.38
14	cL	203	CLA	C4D-CHA	2.44	1.47	1.38
14	A	827	CLA	C4D-CHA	2.44	1.47	1.38
14	B	819	CLA	C4D-CHA	2.44	1.47	1.38
14	bA	826	CLA	C3B-C2B	2.44	1.49	1.41
14	cB	827	CLA	C3D-C4D	-2.44	1.38	1.44
14	cA	827	CLA	C4D-CHA	2.44	1.47	1.38
14	A	822	CLA	C4D-CHA	2.44	1.47	1.38
14	bA	828	CLA	C4D-CHA	2.44	1.47	1.38
14	bB	838	CLA	C4C-C3C	2.44	1.49	1.45
14	A	834	CLA	C1C-C2C	2.44	1.49	1.44
14	A	834	CLA	C1B-C2B	2.44	1.49	1.43
14	A	825	CLA	C4D-CHA	2.44	1.47	1.38
14	cB	819	CLA	C4B-NB	-2.44	1.34	1.37
14	cA	826	CLA	C3B-C2B	2.44	1.49	1.41
14	bB	838	CLA	C3D-C4D	-2.44	1.38	1.44
14	bB	815	CLA	C4D-CHA	2.44	1.47	1.38
14	cA	827	CLA	C3B-C2B	2.44	1.49	1.41
14	L	203	CLA	C1C-C2C	2.44	1.49	1.44
14	F	201	CLA	C1B-C2B	2.44	1.49	1.43
14	cA	828	CLA	C4D-CHA	2.44	1.47	1.38
14	B	815	CLA	C4D-CHA	2.44	1.47	1.38
17	bB	850	BCR	C23-C22	-2.44	1.40	1.45
14	bB	818	CLA	C4B-NB	-2.44	1.34	1.37
14	bB	808	CLA	C4C-C3C	2.44	1.49	1.45
14	cB	816	CLA	C4D-CHA	2.44	1.47	1.38
14	cB	839	CLA	C3D-C4D	-2.44	1.38	1.44
14	bA	824	CLA	C4B-NB	-2.44	1.34	1.37
14	cA	842	CLA	C4D-CHA	2.44	1.47	1.38
14	bA	829	CLA	C1C-C2C	2.44	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bB	813	CLA	C1C-C2C	2.44	1.49	1.44
14	B	826	CLA	C4D-CHA	2.44	1.47	1.38
14	bA	815	CLA	C3B-C2B	2.44	1.49	1.41
14	bA	822	CLA	C4D-CHA	2.44	1.47	1.38
14	cX	201	CLA	C4C-C3C	2.44	1.49	1.45
14	bB	827	CLA	C4D-CHA	2.44	1.47	1.38
14	cA	834	CLA	C1B-C2B	2.43	1.49	1.43
14	cB	830	CLA	C3D-C4D	-2.43	1.38	1.44
14	A	812	CLA	C4D-CHA	2.43	1.47	1.38
14	A	826	CLA	C3B-C2B	2.43	1.49	1.41
14	cB	814	CLA	C1C-C2C	2.43	1.49	1.44
14	bB	822	CLA	C3B-C2B	2.43	1.49	1.41
14	B	813	CLA	C1C-C2C	2.43	1.49	1.44
14	cB	823	CLA	C3B-C2B	2.43	1.49	1.41
14	bB	811	CLA	C1B-C2B	2.43	1.49	1.43
14	cA	825	CLA	C4D-CHA	2.43	1.47	1.38
14	cA	836	CLA	C1C-C2C	2.43	1.49	1.44
14	A	835	CLA	C4C-C3C	2.43	1.49	1.45
14	cF	201	CLA	C1B-C2B	2.43	1.49	1.43
14	A	836	CLA	C1C-C2C	2.43	1.49	1.44
14	B	822	CLA	C3B-C2B	2.43	1.49	1.41
14	B	838	CLA	C3D-C4D	-2.43	1.38	1.44
14	A	811	CLA	C1B-C2B	2.43	1.49	1.43
14	cB	829	CLA	C3D-C4D	-2.43	1.38	1.44
14	bB	835	CLA	C3B-C2B	2.43	1.49	1.41
14	cA	822	CLA	C4D-CHA	2.43	1.47	1.38
14	bB	818	CLA	C4C-C3C	2.43	1.49	1.45
14	cA	809	CLA	C3B-C2B	2.43	1.49	1.41
14	bB	828	CLA	C3D-C4D	-2.43	1.38	1.44
14	bF	201	CLA	C1B-C2B	2.43	1.49	1.43
14	cA	834	CLA	C1C-C2C	2.43	1.49	1.44
14	cA	811	CLA	C1B-C2B	2.43	1.49	1.43
14	bA	813	CLA	C1B-C2B	2.43	1.49	1.43
14	B	836	CLA	C4D-CHA	2.43	1.47	1.38
14	B	828	CLA	C3D-C4D	-2.43	1.38	1.44
14	A	815	CLA	C3B-C2B	2.43	1.49	1.41
14	bJ	102	CLA	C4C-C3C	2.43	1.49	1.45
14	bA	813	CLA	C3D-C4D	-2.42	1.38	1.44
14	cB	838	CLA	C4D-CHA	2.42	1.47	1.38
14	cB	829	CLA	C1C-C2C	2.42	1.49	1.44
14	cA	810	CLA	C4C-C3C	2.42	1.49	1.45
14	cA	827	CLA	C4C-C3C	2.42	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	M	101	BCR	C23-C22	-2.42	1.40	1.45
14	bA	814	CLA	C4C-C3C	2.42	1.49	1.45
14	cA	813	CLA	C3D-C4D	-2.42	1.38	1.44
14	A	813	CLA	C1B-C2B	2.42	1.49	1.43
14	cB	825	CLA	C4C-C3C	2.42	1.49	1.45
17	cM	101	BCR	C23-C22	-2.42	1.40	1.45
14	cB	819	CLA	C4C-C3C	2.42	1.49	1.45
14	cJ	102	CLA	C4C-C3C	2.42	1.49	1.45
14	A	809	CLA	C3B-C2B	2.42	1.49	1.41
14	bA	809	CLA	C3B-C2B	2.42	1.49	1.41
14	cB	837	CLA	C3B-C2B	2.42	1.49	1.41
14	cB	810	CLA	C1B-C2B	2.42	1.49	1.43
14	B	836	CLA	C3B-C2B	2.42	1.49	1.41
14	A	814	CLA	C4C-C3C	2.42	1.49	1.45
14	cA	814	CLA	C4C-C3C	2.42	1.49	1.45
14	B	818	CLA	C4C-C3C	2.42	1.49	1.45
14	bA	842	CLA	C4C-C3C	2.42	1.49	1.45
17	bM	101	BCR	C23-C22	-2.42	1.40	1.45
14	cA	835	CLA	C4C-C3C	2.42	1.49	1.45
14	A	810	CLA	C4C-C3C	2.42	1.49	1.45
14	bB	824	CLA	C4C-C3C	2.42	1.49	1.45
14	bB	809	CLA	C4D-CHA	2.42	1.47	1.38
14	B	825	CLA	C1B-C2B	2.42	1.48	1.43
14	bA	811	CLA	C1B-C2B	2.41	1.48	1.43
14	cB	837	CLA	C4D-CHA	2.41	1.47	1.38
14	cA	824	CLA	C4B-NB	-2.41	1.34	1.37
14	B	832	CLA	C1B-C2B	2.41	1.48	1.43
14	cB	826	CLA	C1B-C2B	2.41	1.48	1.43
14	A	824	CLA	C4B-NB	-2.41	1.34	1.37
14	bB	829	CLA	C3D-C4D	-2.41	1.38	1.44
14	A	842	CLA	C4C-C3C	2.41	1.49	1.45
14	L	202	CLA	C4C-C3C	2.41	1.49	1.45
14	cB	822	CLA	C3B-C2B	2.41	1.49	1.41
14	bA	827	CLA	C4C-C3C	2.41	1.49	1.45
14	cL	204	CLA	C1C-C2C	2.41	1.49	1.44
14	B	837	CLA	C4D-CHA	2.41	1.47	1.38
14	J	102	CLA	C4C-C3C	2.41	1.49	1.45
14	bB	836	CLA	C4D-CHA	2.41	1.47	1.38
14	A	813	CLA	C3D-C4D	-2.41	1.38	1.44
14	bA	834	CLA	C1B-C2B	2.41	1.48	1.43
14	bL	202	CLA	C4C-C3C	2.41	1.49	1.45
14	A	802	CLA	C1C-NC	-2.41	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	833	CLA	C1C-NC	-2.41	1.34	1.37
14	cB	833	CLA	C1B-C2B	2.41	1.48	1.43
14	B	809	CLA	C4D-CHA	2.41	1.47	1.38
14	cB	806	CLA	C3B-C2B	2.41	1.49	1.41
14	bB	807	CLA	C4C-C3C	2.41	1.49	1.45
14	bX	201	CLA	C4C-C3C	2.41	1.49	1.45
14	bB	836	CLA	C3B-C2B	2.41	1.49	1.41
14	B	807	CLA	C4C-C3C	2.41	1.49	1.45
14	bA	810	CLA	C4C-C3C	2.41	1.49	1.45
14	B	821	CLA	C3B-C2B	2.41	1.49	1.41
14	bB	821	CLA	C3B-C2B	2.41	1.49	1.41
14	cA	821	CLA	C3B-C2B	2.41	1.49	1.41
14	B	805	CLA	C3B-C2B	2.41	1.49	1.41
14	B	829	CLA	C3D-C4D	-2.41	1.38	1.44
14	bB	809	CLA	C1B-C2B	2.41	1.48	1.43
14	bB	805	CLA	C3B-C2B	2.41	1.49	1.41
14	B	833	CLA	C4C-C3C	2.40	1.49	1.45
14	bB	824	CLA	C3B-C2B	2.40	1.49	1.41
14	B	802	CLA	C3B-C2B	2.40	1.49	1.41
14	L	202	CLA	C3B-C2B	2.40	1.49	1.41
14	cB	825	CLA	C3B-C2B	2.40	1.49	1.41
14	A	839	CLA	C1C-C2C	2.40	1.49	1.44
14	cA	802	CLA	C4D-CHA	2.40	1.46	1.38
14	cA	802	CLA	C1C-NC	-2.40	1.34	1.37
14	B	810	CLA	C3B-C2B	2.40	1.49	1.41
14	bB	825	CLA	C1B-C2B	2.40	1.48	1.43
14	cL	203	CLA	C4C-C3C	2.40	1.49	1.45
14	A	821	CLA	C3B-C2B	2.40	1.49	1.41
14	cB	809	CLA	C1C-C2C	2.40	1.49	1.44
14	B	824	CLA	C4C-C3C	2.40	1.49	1.45
14	B	838	CLA	C4C-C3C	2.40	1.49	1.45
14	bB	851	CLA	C4C-C3C	2.40	1.49	1.45
14	B	834	CLA	C1C-C2C	2.40	1.49	1.44
14	cA	842	CLA	C4C-C3C	2.40	1.49	1.45
14	bB	837	CLA	C4D-CHA	2.40	1.46	1.38
14	bB	807	CLA	C3D-C4D	-2.40	1.38	1.44
14	B	824	CLA	C3B-C2B	2.40	1.49	1.41
14	B	828	CLA	C1C-C2C	2.40	1.49	1.44
14	bB	802	CLA	C3B-C2B	2.40	1.49	1.41
14	cA	839	CLA	C4D-CHA	2.40	1.46	1.38
14	bA	821	CLA	C3B-C2B	2.40	1.49	1.41
14	cB	810	CLA	C4D-CHA	2.40	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	802	CLA	C4D-CHA	2.40	1.46	1.38
14	bA	838	CLA	C1C-C2C	2.40	1.49	1.44
14	cB	810	CLA	C1C-C2C	2.40	1.49	1.44
14	X	201	CLA	C4C-C3C	2.40	1.49	1.45
14	bB	832	CLA	C1B-C2B	2.40	1.48	1.43
14	cB	803	CLA	C3B-C2B	2.39	1.49	1.41
14	A	839	CLA	C4D-CHA	2.39	1.46	1.38
14	bL	202	CLA	C3B-C2B	2.39	1.49	1.41
14	cB	839	CLA	C1C-NC	-2.39	1.34	1.37
14	cA	813	CLA	C1B-C2B	2.39	1.48	1.43
14	bB	810	CLA	C3B-C2B	2.39	1.49	1.41
14	cA	812	CLA	C3D-C4D	-2.39	1.38	1.44
14	bB	808	CLA	C4D-CHA	2.39	1.46	1.38
14	B	809	CLA	C1B-C2B	2.39	1.48	1.43
14	cL	203	CLA	C3B-C2B	2.39	1.49	1.41
14	bA	833	CLA	C1C-NC	-2.39	1.34	1.37
14	bB	808	CLA	C1C-NC	-2.39	1.34	1.37
14	cA	839	CLA	C1C-C2C	2.39	1.49	1.44
14	bB	833	CLA	C1B-C2B	2.39	1.48	1.43
17	cI	101	BCR	C23-C22	-2.39	1.40	1.45
14	bA	802	CLA	C4D-CHA	2.39	1.46	1.38
14	bA	839	CLA	C4D-CHA	2.39	1.46	1.38
14	cL	204	CLA	C3B-C2B	2.39	1.49	1.41
14	bA	811	CLA	C4C-C3C	2.39	1.49	1.45
14	cB	804	CLA	C4D-CHA	2.39	1.46	1.38
14	bA	839	CLA	C1C-C2C	2.39	1.49	1.44
14	bA	808	CLA	C4B-NB	-2.39	1.34	1.37
17	cB	844	BCR	C23-C22	-2.39	1.40	1.45
14	B	809	CLA	C1C-C2C	2.39	1.49	1.44
14	bB	808	CLA	C1C-C2C	2.39	1.49	1.44
14	cB	811	CLA	C3B-C2B	2.39	1.49	1.41
14	B	851	CLA	C4C-C3C	2.39	1.49	1.45
14	cA	811	CLA	C4C-C3C	2.39	1.49	1.45
14	cB	806	CLA	C4C-C3C	2.39	1.49	1.45
14	cB	808	CLA	C4C-C3C	2.39	1.49	1.45
14	L	203	CLA	C3B-C2B	2.39	1.49	1.41
17	bI	101	BCR	C23-C22	-2.39	1.40	1.45
14	F	201	CLA	C4D-CHA	2.39	1.46	1.38
14	B	833	CLA	C1B-C2B	2.39	1.48	1.43
14	cB	809	CLA	C4D-CHA	2.38	1.46	1.38
14	bB	828	CLA	C1C-C2C	2.38	1.49	1.44
17	I	101	BCR	C23-C22	-2.38	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	bB	842	BCR	C23-C22	-2.38	1.40	1.45
14	cA	827	CLA	C3D-C4D	-2.38	1.38	1.44
14	cB	808	CLA	C3D-C4D	-2.38	1.38	1.44
14	bL	203	CLA	C1C-NC	-2.38	1.34	1.37
14	B	838	CLA	C1C-NC	-2.38	1.34	1.37
14	cB	834	CLA	C1B-C2B	2.38	1.48	1.43
17	bB	843	BCR	C23-C22	-2.38	1.40	1.45
14	A	828	CLA	C1B-C2B	2.38	1.48	1.43
14	cA	812	CLA	C1C-C2C	2.38	1.49	1.44
14	cB	839	CLA	C1C-C2C	2.38	1.49	1.44
14	bA	802	CLA	C1C-NC	-2.38	1.34	1.37
14	bB	803	CLA	C4D-CHA	2.38	1.46	1.38
14	B	808	CLA	C4D-CHA	2.38	1.46	1.38
14	bA	812	CLA	C1C-C2C	2.38	1.49	1.44
17	L	205	BCR	C8-C9	-2.38	1.40	1.45
14	cB	801	CLA	C4C-C3C	2.38	1.49	1.45
14	B	829	CLA	C4D-CHA	2.38	1.46	1.38
17	B	843	BCR	C23-C22	-2.38	1.40	1.45
14	A	811	CLA	C4C-C3C	2.38	1.49	1.45
17	bB	842	BCR	C8-C9	-2.38	1.40	1.45
14	B	803	CLA	C4D-CHA	2.38	1.46	1.38
14	bL	203	CLA	C3B-C2B	2.38	1.49	1.41
14	cA	820	CLA	C4D-CHA	2.38	1.46	1.38
14	B	819	CLA	C4C-C3C	2.38	1.49	1.45
14	A	812	CLA	C1C-C2C	2.38	1.49	1.44
14	A	838	CLA	C1C-C2C	2.38	1.49	1.44
14	cB	820	CLA	C3D-C4D	-2.38	1.38	1.44
14	cF	201	CLA	C4D-CHA	2.38	1.46	1.38
14	bB	819	CLA	C4C-C3C	2.37	1.49	1.45
14	bA	806	CLA	C3D-C4D	-2.37	1.38	1.44
14	bA	820	CLA	C3D-C4D	-2.37	1.38	1.44
14	cA	820	CLA	C3D-C4D	-2.37	1.38	1.44
14	bA	818	CLA	C4B-NB	-2.37	1.34	1.37
14	cA	808	CLA	C4B-NB	-2.37	1.34	1.37
14	cB	830	CLA	C4D-CHA	2.37	1.46	1.38
14	cB	820	CLA	C4C-C3C	2.37	1.49	1.45
14	bA	840	CLA	C3D-C4D	-2.37	1.38	1.44
17	cL	206	BCR	C8-C9	-2.37	1.40	1.45
14	cA	838	CLA	C1C-C2C	2.37	1.49	1.44
14	cA	840	CLA	C3D-C4D	-2.37	1.38	1.44
14	cB	809	CLA	C1C-NC	-2.37	1.34	1.37
14	cA	828	CLA	C1B-C2B	2.37	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	840	CLA	C3D-C4D	-2.37	1.38	1.44
14	bB	831	CLA	C4D-CHA	2.37	1.46	1.38
14	A	818	CLA	C4B-NB	-2.37	1.34	1.37
14	bA	804	CLA	C3B-C2B	2.37	1.49	1.41
14	bA	806	CLA	C4D-CHA	2.37	1.46	1.38
14	A	806	CLA	C4D-CHA	2.37	1.46	1.38
14	bB	826	CLA	C3B-C4B	2.37	1.48	1.42
17	B	842	BCR	C23-C22	-2.37	1.40	1.45
14	bB	813	CLA	C3B-C2B	2.37	1.49	1.41
14	bB	838	CLA	C1C-NC	-2.37	1.34	1.37
14	bA	820	CLA	C4D-CHA	2.37	1.46	1.38
14	B	829	CLA	C3B-C2B	2.37	1.49	1.41
14	B	813	CLA	C3B-C2B	2.37	1.49	1.41
14	cA	818	CLA	C4D-CHA	2.37	1.46	1.38
14	cB	834	CLA	C4C-C3C	2.37	1.49	1.45
14	A	827	CLA	C3D-C4D	-2.37	1.38	1.44
14	bB	809	CLA	C1C-C2C	2.37	1.49	1.44
14	bB	838	CLA	C1C-C2C	2.37	1.49	1.44
14	cB	835	CLA	C1C-C2C	2.37	1.49	1.44
14	bF	201	CLA	C4D-CHA	2.37	1.46	1.38
14	J	102	CLA	C4B-NB	-2.37	1.34	1.37
14	B	838	CLA	C1C-C2C	2.37	1.49	1.44
14	bB	831	CLA	C1B-C2B	2.37	1.48	1.43
14	cB	835	CLA	C1B-C2B	2.37	1.48	1.43
14	B	831	CLA	C4D-CHA	2.37	1.46	1.38
17	bL	205	BCR	C8-C9	-2.37	1.40	1.45
14	cB	832	CLA	C4D-CHA	2.37	1.46	1.38
14	cB	828	CLA	C3D-C4D	-2.37	1.38	1.44
14	bA	818	CLA	C4D-CHA	2.37	1.46	1.38
14	B	834	CLA	C1B-C2B	2.37	1.48	1.43
14	cL	204	CLA	C1C-NC	-2.37	1.34	1.37
14	bB	802	CLA	C4C-C3C	2.37	1.49	1.45
14	cA	804	CLA	C3B-C2B	2.37	1.49	1.41
14	bB	829	CLA	C3B-C2B	2.36	1.49	1.41
14	bA	827	CLA	C3D-C4D	-2.36	1.38	1.44
14	A	818	CLA	C4D-CHA	2.36	1.46	1.38
14	bB	833	CLA	C4C-C3C	2.36	1.49	1.45
14	bA	840	CLA	C4C-C3C	2.36	1.49	1.45
14	B	837	CLA	C3D-C4D	-2.36	1.38	1.44
14	bB	819	CLA	C3D-C4D	-2.36	1.38	1.44
14	cB	838	CLA	C3D-C4D	-2.36	1.38	1.44
14	cB	814	CLA	C3B-C2B	2.36	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	820	CLA	C4D-CHA	2.36	1.46	1.38
14	bB	829	CLA	C4D-CHA	2.36	1.46	1.38
14	B	805	CLA	C4C-C3C	2.36	1.49	1.45
14	cA	828	CLA	C3B-C2B	2.36	1.49	1.41
14	cB	830	CLA	C3B-C2B	2.36	1.49	1.41
14	bA	828	CLA	C1B-C2B	2.36	1.48	1.43
17	I	101	BCR	C12-C13	-2.36	1.40	1.45
14	B	807	CLA	C3D-C4D	-2.36	1.38	1.44
14	cB	834	CLA	C4B-NB	-2.36	1.34	1.37
14	bB	834	CLA	C1B-C2B	2.36	1.48	1.43
14	bA	817	CLA	C3D-C4D	-2.36	1.38	1.44
14	cB	832	CLA	C1B-C2B	2.36	1.48	1.43
14	cA	806	CLA	C4D-CHA	2.36	1.46	1.38
14	A	820	CLA	C3D-C4D	-2.36	1.38	1.44
14	cA	831	CLA	C4D-CHA	2.36	1.46	1.38
14	B	819	CLA	C3D-C4D	-2.36	1.38	1.44
17	B	842	BCR	C8-C9	-2.36	1.40	1.45
14	bB	805	CLA	C4C-C3C	2.36	1.49	1.45
14	B	831	CLA	C1B-C2B	2.36	1.48	1.43
14	A	828	CLA	C3B-C2B	2.36	1.49	1.41
14	B	827	CLA	C3D-C4D	-2.36	1.38	1.44
14	bA	826	CLA	C3D-C4D	-2.36	1.38	1.44
14	A	804	CLA	C3B-C2B	2.36	1.49	1.41
14	B	808	CLA	C1C-C2C	2.36	1.49	1.44
14	B	817	CLA	C3B-C2B	2.36	1.49	1.41
14	bB	834	CLA	C1C-C2C	2.36	1.49	1.44
17	cB	843	BCR	C23-C22	-2.36	1.40	1.45
14	B	804	CLA	C3D-C4D	-2.36	1.38	1.44
14	bA	837	CLA	C4D-CHA	2.35	1.46	1.38
14	B	808	CLA	C1C-NC	-2.35	1.34	1.37
14	cA	818	CLA	C4B-NB	-2.35	1.34	1.37
14	cA	840	CLA	C4C-C3C	2.35	1.49	1.45
14	A	837	CLA	C4D-CHA	2.35	1.46	1.38
14	cB	818	CLA	C3B-C2B	2.35	1.49	1.41
17	cI	101	BCR	C12-C13	-2.35	1.40	1.45
14	L	203	CLA	C1C-NC	-2.35	1.34	1.37
14	B	804	CLA	C3B-C2B	2.35	1.49	1.41
14	bA	831	CLA	C4D-CHA	2.35	1.46	1.38
14	cA	837	CLA	C4D-CHA	2.35	1.46	1.38
14	bB	837	CLA	C3D-C4D	-2.35	1.38	1.44
14	bB	817	CLA	C3B-C2B	2.35	1.49	1.41
14	A	812	CLA	C3D-C4D	-2.35	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	840	CLA	C4C-C3C	2.35	1.49	1.45
14	B	812	CLA	C4C-C3C	2.35	1.49	1.45
14	cA	806	CLA	C3D-C4D	-2.35	1.38	1.44
14	bA	828	CLA	C3B-C2B	2.35	1.49	1.41
14	A	826	CLA	C3D-C4D	-2.35	1.38	1.44
14	A	831	CLA	C4D-CHA	2.35	1.46	1.38
14	cA	817	CLA	C3D-C4D	-2.35	1.38	1.44
14	cB	805	CLA	C3D-C4D	-2.35	1.38	1.44
14	B	826	CLA	C3B-C4B	2.35	1.48	1.42
14	B	833	CLA	C4B-NB	-2.35	1.34	1.37
14	cA	806	CLA	C1B-C2B	2.35	1.48	1.43
14	B	816	CLA	C3D-C4D	-2.35	1.38	1.44
17	cB	843	BCR	C8-C9	-2.35	1.40	1.45
14	A	804	CLA	C4C-C3C	2.35	1.49	1.45
14	cB	827	CLA	C3B-C4B	2.35	1.48	1.42
14	bB	804	CLA	C3D-C4D	-2.34	1.38	1.44
14	cA	816	CLA	C4C-C3C	2.34	1.49	1.45
14	cA	824	CLA	C4C-C3C	2.34	1.49	1.45
14	cB	804	CLA	C3D-C4D	-2.34	1.38	1.44
14	cA	809	CLA	C3D-C4D	-2.34	1.38	1.44
14	B	802	CLA	C4C-C3C	2.34	1.49	1.45
14	bA	816	CLA	C4C-C3C	2.34	1.49	1.45
14	cB	813	CLA	C4C-C3C	2.34	1.49	1.45
14	L	202	CLA	C3D-C4D	-2.34	1.38	1.44
14	bA	806	CLA	C1B-C2B	2.34	1.48	1.43
14	A	816	CLA	C4C-C3C	2.34	1.49	1.45
14	B	801	CLA	C3B-C2B	2.34	1.49	1.41
14	bB	812	CLA	C4C-C3C	2.34	1.49	1.45
14	bB	827	CLA	C3D-C4D	-2.34	1.38	1.44
14	bB	822	CLA	C4C-C3C	2.34	1.49	1.45
14	bA	809	CLA	C3D-C4D	-2.34	1.38	1.44
14	bB	804	CLA	C3B-C2B	2.34	1.49	1.41
14	A	819	CLA	C4B-NB	-2.34	1.34	1.37
14	B	837	CLA	C3B-C2B	2.34	1.49	1.41
14	bB	816	CLA	C3D-C4D	-2.34	1.38	1.44
14	cA	803	CLA	C3D-C4D	-2.34	1.38	1.44
17	bI	101	BCR	C12-C13	-2.34	1.40	1.45
14	bB	837	CLA	C3B-C2B	2.34	1.49	1.41
14	A	806	CLA	C3D-C4D	-2.34	1.38	1.44
14	A	817	CLA	C3D-C4D	-2.34	1.38	1.44
14	bB	801	CLA	C3B-C2B	2.34	1.49	1.41
13	bA	801	CL0	C4C-C3C	2.34	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bB	851	CLA	C3B-C2B	2.34	1.49	1.41
14	A	806	CLA	C1B-C2B	2.34	1.48	1.43
14	bA	819	CLA	C4B-NB	-2.34	1.34	1.37
14	cB	801	CLA	C3B-C2B	2.34	1.49	1.41
14	cB	805	CLA	C3B-C2B	2.34	1.49	1.41
14	bA	812	CLA	C3D-C4D	-2.33	1.38	1.44
14	A	811	CLA	C4B-NB	-2.33	1.34	1.37
14	cA	811	CLA	C4B-NB	-2.33	1.34	1.37
14	cA	826	CLA	C3D-C4D	-2.33	1.38	1.44
14	B	817	CLA	C4D-CHA	2.33	1.46	1.38
14	bB	815	CLA	C4C-C3C	2.33	1.49	1.45
14	cB	838	CLA	C3B-C2B	2.33	1.49	1.41
14	B	815	CLA	C4C-C3C	2.33	1.49	1.45
14	B	822	CLA	C4C-C3C	2.33	1.49	1.45
14	cB	818	CLA	C4D-CHA	2.33	1.46	1.38
14	A	824	CLA	C4C-C3C	2.33	1.49	1.45
14	bB	811	CLA	C3D-C4D	-2.33	1.38	1.44
14	bA	840	CLA	C4B-NB	-2.33	1.34	1.37
17	bI	102	BCR	C12-C13	-2.33	1.40	1.45
14	B	806	CLA	C3D-C4D	-2.33	1.38	1.44
14	cB	807	CLA	C3D-C4D	-2.33	1.38	1.44
14	cL	202	CLA	C3D-C4D	-2.33	1.38	1.44
14	cA	804	CLA	C4C-C3C	2.33	1.49	1.45
13	A	801	CL0	C4C-C3C	2.33	1.49	1.45
17	cI	102	BCR	C12-C13	-2.33	1.40	1.45
14	A	803	CLA	C3D-C4D	-2.33	1.38	1.44
14	cL	203	CLA	C3D-C4D	-2.33	1.38	1.44
14	A	839	CLA	C3B-C2B	2.33	1.49	1.41
17	B	845	BCR	C23-C22	-2.33	1.40	1.45
14	B	851	CLA	C3B-C2B	2.33	1.49	1.41
14	A	809	CLA	C3D-C4D	-2.33	1.38	1.44
14	bB	851	CLA	C3D-C4D	-2.33	1.38	1.44
14	B	817	CLA	C3D-C4D	-2.33	1.38	1.44
14	bA	833	CLA	C4C-C3C	2.33	1.49	1.45
14	cB	824	CLA	C4C-C3C	2.33	1.49	1.45
14	cB	817	CLA	C3D-C4D	-2.32	1.38	1.44
14	cA	840	CLA	C4B-NB	-2.32	1.34	1.37
14	bA	839	CLA	C3B-C2B	2.32	1.49	1.41
14	A	822	CLA	C3D-C4D	-2.32	1.38	1.44
14	cB	816	CLA	C4C-C3C	2.32	1.49	1.45
14	cA	819	CLA	C4B-NB	-2.32	1.34	1.37
14	cB	802	CLA	C3B-C2B	2.32	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	bB	845	BCR	C23-C22	-2.32	1.41	1.45
17	cB	846	BCR	C23-C22	-2.32	1.41	1.45
17	bB	846	BCR	C12-C13	-2.32	1.41	1.45
14	bA	803	CLA	C3D-C4D	-2.32	1.38	1.44
14	B	811	CLA	C3D-C4D	-2.32	1.38	1.44
14	A	840	CLA	C4B-NB	-2.32	1.34	1.37
14	bB	833	CLA	C4B-NB	-2.32	1.34	1.37
14	cB	812	CLA	C3D-C4D	-2.32	1.38	1.44
14	bA	824	CLA	C4C-C3C	2.32	1.49	1.45
14	bB	817	CLA	C4D-CHA	2.32	1.46	1.38
14	bA	825	CLA	C4C-C3C	2.32	1.49	1.45
14	B	806	CLA	C4C-C3C	2.32	1.49	1.45
14	bA	804	CLA	C4C-C3C	2.32	1.49	1.45
14	A	808	CLA	C4B-NB	-2.32	1.34	1.37
13	cA	801	CL0	C4C-C3C	2.32	1.49	1.45
14	bB	823	CLA	C4C-C3C	2.32	1.49	1.45
14	cB	803	CLA	C4C-C3C	2.32	1.49	1.45
14	cB	823	CLA	C4C-C3C	2.32	1.49	1.45
14	B	801	CLA	C4D-CHA	2.32	1.46	1.38
14	cJ	102	CLA	C4B-NB	-2.32	1.34	1.37
14	cA	839	CLA	C3B-C2B	2.31	1.49	1.41
14	bB	831	CLA	C3D-C4D	-2.31	1.38	1.44
14	bA	830	CLA	C1B-C2B	2.31	1.48	1.43
14	B	827	CLA	C4C-C3C	2.31	1.49	1.45
14	bB	827	CLA	C4C-C3C	2.31	1.49	1.45
14	B	823	CLA	C4C-C3C	2.31	1.49	1.45
14	bA	831	CLA	C4C-C3C	2.31	1.49	1.45
14	bB	814	CLA	C3D-C4D	-2.31	1.39	1.44
14	cA	822	CLA	C3D-C4D	-2.31	1.39	1.44
14	bB	806	CLA	C4C-C3C	2.31	1.49	1.45
14	cB	801	CLA	C3D-C4D	-2.31	1.39	1.44
14	cL	202	CLA	C1C-NC	-2.31	1.34	1.37
14	B	831	CLA	C3D-C4D	-2.31	1.39	1.44
14	bB	803	CLA	C3D-C4D	-2.31	1.39	1.44
14	B	851	CLA	C1B-C2B	2.31	1.48	1.43
14	cB	839	CLA	C1B-C2B	2.31	1.48	1.43
14	A	831	CLA	C4C-C3C	2.31	1.49	1.45
14	cB	807	CLA	C4C-C3C	2.31	1.49	1.45
17	B	846	BCR	C12-C13	-2.31	1.41	1.45
14	bL	202	CLA	C3D-C4D	-2.31	1.39	1.44
14	bB	801	CLA	C4D-CHA	2.31	1.46	1.38
14	bA	832	CLA	C4C-C3C	2.31	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cA	806	CLA	C4B-NB	-2.31	1.34	1.37
14	bL	201	CLA	C1C-NC	-2.31	1.34	1.37
14	cB	801	CLA	C1B-C2B	2.31	1.48	1.43
14	cB	802	CLA	C4D-CHA	2.31	1.46	1.38
14	bA	835	CLA	C3D-C4D	-2.31	1.39	1.44
14	bA	811	CLA	C4B-NB	-2.31	1.34	1.37
14	bJ	102	CLA	C4B-NB	-2.31	1.34	1.37
17	cB	848	BCR	C8-C9	-2.30	1.41	1.45
14	bL	201	CLA	C3D-C4D	-2.30	1.39	1.44
17	I	102	BCR	C12-C13	-2.30	1.41	1.45
14	cB	818	CLA	C3D-C4D	-2.30	1.39	1.44
14	A	833	CLA	C4C-C3C	2.30	1.49	1.45
14	cB	810	CLA	C3D-C4D	-2.30	1.39	1.44
17	B	847	BCR	C8-C9	-2.30	1.41	1.45
14	bB	817	CLA	C1C-C2C	2.30	1.49	1.44
14	cA	831	CLA	C4C-C3C	2.30	1.49	1.45
14	bA	837	CLA	C3D-C4D	-2.30	1.39	1.44
14	A	837	CLA	C3D-C4D	-2.30	1.39	1.44
14	bB	806	CLA	C3D-C4D	-2.30	1.39	1.44
14	bB	809	CLA	C3D-C4D	-2.30	1.39	1.44
14	cB	828	CLA	C4C-C3C	2.30	1.49	1.45
17	bB	847	BCR	C8-C9	-2.30	1.41	1.45
14	A	835	CLA	C3D-C4D	-2.30	1.39	1.44
14	L	201	CLA	C3D-C4D	-2.30	1.39	1.44
17	bB	850	BCR	C12-C13	-2.30	1.41	1.45
13	A	801	CL0	C3D-C4D	-2.30	1.39	1.44
14	cA	837	CLA	C3D-C4D	-2.30	1.39	1.44
17	cB	847	BCR	C12-C13	-2.30	1.41	1.45
14	B	803	CLA	C3D-C4D	-2.30	1.39	1.44
14	cB	815	CLA	C3D-C4D	-2.30	1.39	1.44
13	cA	801	CL0	C3D-C4D	-2.30	1.39	1.44
14	B	814	CLA	C3D-C4D	-2.30	1.39	1.44
17	bF	202	BCR	C23-C22	-2.30	1.41	1.45
14	bB	851	CLA	C1B-C2B	2.30	1.48	1.43
14	L	201	CLA	C1C-NC	-2.30	1.34	1.37
14	cB	831	CLA	C3D-C4D	-2.30	1.39	1.44
14	bJ	101	CLA	C4B-NB	-2.30	1.35	1.37
14	cA	833	CLA	C4C-C3C	2.30	1.49	1.45
17	F	202	BCR	C23-C22	-2.30	1.41	1.45
14	A	825	CLA	C4C-C3C	2.30	1.49	1.45
14	bB	838	CLA	C1B-C2B	2.30	1.48	1.43
14	cA	830	CLA	C1B-C2B	2.30	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bA	822	CLA	C3D-C4D	-2.29	1.39	1.44
17	B	850	BCR	C12-C13	-2.29	1.41	1.45
14	bB	817	CLA	C3D-C4D	-2.29	1.39	1.44
14	cA	825	CLA	C4C-C3C	2.29	1.49	1.45
14	bB	811	CLA	C4B-NB	-2.29	1.35	1.37
14	B	838	CLA	C1B-C2B	2.29	1.48	1.43
14	B	809	CLA	C3D-C4D	-2.29	1.39	1.44
14	bB	805	CLA	C3D-C4D	-2.29	1.39	1.44
14	cA	841	CLA	C4C-C3C	2.29	1.49	1.45
14	B	830	CLA	C3D-C4D	-2.29	1.39	1.44
14	A	841	CLA	C4C-C3C	2.29	1.49	1.45
14	B	851	CLA	C3D-C4D	-2.29	1.39	1.44
14	bA	805	CLA	C3B-C2B	2.29	1.48	1.41
14	bA	810	CLA	C3D-C4D	-2.29	1.39	1.44
14	A	805	CLA	C3B-C2B	2.29	1.48	1.41
14	A	830	CLA	C1B-C2B	2.29	1.48	1.43
14	J	101	CLA	C4B-NB	-2.29	1.35	1.37
14	bA	807	CLA	C4B-NB	-2.29	1.35	1.37
14	A	832	CLA	C4C-C3C	2.29	1.49	1.45
14	cA	835	CLA	C3D-C4D	-2.29	1.39	1.44
14	cB	832	CLA	C3D-C4D	-2.29	1.39	1.44
17	cA	845	BCR	C23-C22	-2.29	1.41	1.45
17	cF	202	BCR	C23-C22	-2.29	1.41	1.45
17	cB	851	BCR	C12-C13	-2.28	1.41	1.45
14	cA	805	CLA	C3B-C2B	2.28	1.48	1.41
14	A	830	CLA	C4D-CHA	2.28	1.46	1.38
14	cA	807	CLA	C4B-NB	-2.28	1.35	1.37
14	B	817	CLA	C1C-C2C	2.28	1.49	1.44
14	B	811	CLA	C4B-NB	-2.28	1.35	1.37
14	cA	832	CLA	C4C-C3C	2.28	1.49	1.45
14	bA	830	CLA	C4D-CHA	2.28	1.46	1.38
14	A	807	CLA	C4B-NB	-2.28	1.35	1.37
14	B	813	CLA	C3D-C4D	-2.28	1.39	1.44
14	bB	830	CLA	C3D-C4D	-2.28	1.39	1.44
14	cA	819	CLA	C3D-C4D	-2.28	1.39	1.44
13	bA	801	CL0	C3D-C4D	-2.28	1.39	1.44
14	cB	812	CLA	C4B-NB	-2.28	1.35	1.37
14	cJ	101	CLA	C4B-NB	-2.28	1.35	1.37
17	cI	102	BCR	C23-C22	-2.28	1.41	1.45
14	bB	818	CLA	C3D-C4D	-2.28	1.39	1.44
14	bB	811	CLA	C3B-C2B	2.28	1.48	1.41
14	cB	818	CLA	C1C-C2C	2.28	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cB	806	CLA	C3D-C4D	-2.28	1.39	1.44
14	bL	203	CLA	C3D-C4D	-2.28	1.39	1.44
14	cA	810	CLA	C3D-C4D	-2.28	1.39	1.44
14	cA	811	CLA	C3D-C4D	-2.28	1.39	1.44
14	bB	803	CLA	C4C-C3C	2.28	1.49	1.45
14	bA	811	CLA	C3D-C4D	-2.27	1.39	1.44
14	cB	814	CLA	C3D-C4D	-2.27	1.39	1.44
14	cA	842	CLA	C3B-C2B	2.27	1.48	1.41
14	cB	819	CLA	C3D-C4D	-2.27	1.39	1.44
14	B	819	CLA	C4B-NB	-2.27	1.35	1.37
14	bA	816	CLA	C3D-C4D	-2.27	1.39	1.44
14	cB	812	CLA	C3B-C2B	2.27	1.48	1.41
14	cA	824	CLA	C1B-C2B	2.27	1.48	1.43
14	cA	830	CLA	C4D-CHA	2.27	1.46	1.38
14	bB	836	CLA	C3D-C4D	-2.27	1.39	1.44
14	cB	837	CLA	C3D-C4D	-2.27	1.39	1.44
14	bA	841	CLA	C4C-C3C	2.27	1.49	1.45
14	bB	813	CLA	C3D-C4D	-2.27	1.39	1.44
14	B	818	CLA	C3D-C4D	-2.27	1.39	1.44
14	cB	820	CLA	C4B-NB	-2.27	1.35	1.37
14	cB	824	CLA	C3D-C4D	-2.27	1.39	1.44
14	A	842	CLA	C3B-C2B	2.27	1.48	1.41
14	B	811	CLA	C3B-C2B	2.27	1.48	1.41
14	bA	806	CLA	C4B-NB	-2.27	1.35	1.37
14	B	823	CLA	C3D-C4D	-2.27	1.39	1.44
14	bA	819	CLA	C3D-C4D	-2.27	1.39	1.44
14	bX	201	CLA	C4B-NB	-2.27	1.35	1.37
14	A	810	CLA	C3D-C4D	-2.27	1.39	1.44
14	L	203	CLA	C3D-C4D	-2.27	1.39	1.44
14	cB	840	CLA	C3D-C4D	-2.27	1.39	1.44
14	cA	831	CLA	C3D-C4D	-2.27	1.39	1.44
14	A	821	CLA	C3D-C4D	-2.27	1.39	1.44
14	B	839	CLA	C3D-C4D	-2.27	1.39	1.44
14	bB	839	CLA	C3D-C4D	-2.27	1.39	1.44
14	cB	804	CLA	C4C-C3C	2.27	1.48	1.45
14	A	825	CLA	C3D-C4D	-2.27	1.39	1.44
14	cA	835	CLA	C1B-C2B	2.27	1.48	1.43
14	bA	802	CLA	C4C-C3C	2.27	1.48	1.45
14	A	806	CLA	C4B-NB	-2.27	1.35	1.37
14	bB	819	CLA	C4B-NB	-2.27	1.35	1.37
14	A	802	CLA	C4C-C3C	2.27	1.48	1.45
14	A	831	CLA	C3D-C4D	-2.27	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cL	204	CLA	C3D-C4D	-2.27	1.39	1.44
14	cA	829	CLA	C4C-C3C	2.27	1.48	1.45
14	A	811	CLA	C3D-C4D	-2.26	1.39	1.44
14	bA	825	CLA	C3D-C4D	-2.26	1.39	1.44
14	B	836	CLA	C3D-C4D	-2.26	1.39	1.44
14	bA	821	CLA	C3D-C4D	-2.26	1.39	1.44
17	A	845	BCR	C23-C22	-2.26	1.41	1.45
14	B	831	CLA	C4B-NB	-2.26	1.35	1.37
14	A	842	CLA	C3D-C4D	-2.26	1.39	1.44
17	bI	102	BCR	C23-C22	-2.26	1.41	1.45
14	bA	829	CLA	C3D-C4D	-2.26	1.39	1.44
14	bA	808	CLA	C4C-C3C	2.26	1.48	1.45
14	bA	829	CLA	C4C-C3C	2.26	1.48	1.45
14	B	810	CLA	C3D-C4D	-2.26	1.39	1.44
14	cB	821	CLA	C3D-C4D	-2.26	1.39	1.44
14	cB	835	CLA	C3D-C4D	-2.26	1.39	1.44
14	A	835	CLA	C1B-C2B	2.26	1.48	1.43
14	bA	835	CLA	C1B-C2B	2.26	1.48	1.43
14	bB	810	CLA	C3D-C4D	-2.26	1.39	1.44
14	cA	802	CLA	C4C-C3C	2.26	1.48	1.45
17	I	102	BCR	C23-C22	-2.26	1.41	1.45
14	A	819	CLA	C3D-C4D	-2.26	1.39	1.44
14	bB	823	CLA	C3D-C4D	-2.26	1.39	1.44
14	cA	829	CLA	C3B-C2B	2.26	1.48	1.41
14	cA	825	CLA	C3D-C4D	-2.26	1.39	1.44
14	bL	203	CLA	C4D-CHA	2.26	1.46	1.38
14	B	820	CLA	C3D-C4D	-2.26	1.39	1.44
14	cA	842	CLA	C3D-C4D	-2.26	1.39	1.44
14	bB	820	CLA	C3D-C4D	-2.26	1.39	1.44
14	A	829	CLA	C3B-C2B	2.26	1.48	1.41
14	cB	829	CLA	C3B-C2B	2.26	1.48	1.41
14	cL	204	CLA	C4D-CHA	2.26	1.46	1.38
14	A	829	CLA	C4C-C3C	2.26	1.48	1.45
14	bA	829	CLA	C3B-C2B	2.26	1.48	1.41
14	bB	834	CLA	C3D-C4D	-2.26	1.39	1.44
14	cA	829	CLA	C3D-C4D	-2.26	1.39	1.44
14	cA	852	CLA	C4D-CHA	2.26	1.46	1.38
14	B	807	CLA	C3B-C2B	2.26	1.48	1.41
14	bA	838	CLA	C1B-C2B	2.26	1.48	1.43
14	bA	814	CLA	C3D-C4D	-2.26	1.39	1.44
14	bA	842	CLA	C3B-C2B	2.26	1.48	1.41
14	B	805	CLA	C3D-C4D	-2.25	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bA	815	CLA	C3D-C4D	-2.25	1.39	1.44
14	A	852	CLA	C4D-CHA	2.25	1.46	1.38
14	B	834	CLA	C3D-C4D	-2.25	1.39	1.44
14	bB	849	CLA	C3B-C2B	2.25	1.48	1.41
14	A	829	CLA	C3D-C4D	-2.25	1.39	1.44
14	cB	813	CLA	C3D-C4D	-2.25	1.39	1.44
14	A	824	CLA	C1B-C2B	2.25	1.48	1.43
14	B	849	CLA	C3B-C2B	2.25	1.48	1.41
14	B	803	CLA	C4C-C3C	2.25	1.48	1.45
14	L	203	CLA	C4D-CHA	2.25	1.46	1.38
14	A	838	CLA	C1B-C2B	2.25	1.48	1.43
14	bB	828	CLA	C3B-C2B	2.25	1.48	1.41
14	cB	808	CLA	C3B-C2B	2.25	1.48	1.41
14	cB	811	CLA	C3D-C4D	-2.25	1.39	1.44
14	cA	808	CLA	C4C-C3C	2.25	1.48	1.45
14	bA	831	CLA	C3D-C4D	-2.25	1.39	1.44
14	bB	812	CLA	C3D-C4D	-2.25	1.39	1.44
14	bB	833	CLA	C3D-C4D	-2.25	1.39	1.44
14	cA	838	CLA	C1B-C2B	2.25	1.48	1.43
14	cB	850	CLA	C3B-C2B	2.25	1.48	1.41
14	B	833	CLA	C3D-C4D	-2.25	1.39	1.44
14	B	828	CLA	C3B-C2B	2.25	1.48	1.41
14	bB	831	CLA	C4B-NB	-2.25	1.35	1.37
17	bA	845	BCR	C23-C22	-2.25	1.41	1.45
14	bB	807	CLA	C3B-C2B	2.25	1.48	1.41
14	bA	818	CLA	C3D-C4D	-2.25	1.39	1.44
17	A	848	BCR	C19-C18	-2.25	1.41	1.45
14	cA	814	CLA	C3D-C4D	-2.25	1.39	1.44
14	A	808	CLA	C4C-C3C	2.25	1.48	1.45
14	bA	852	CLA	C4D-CHA	2.24	1.46	1.38
14	cA	821	CLA	C3D-C4D	-2.24	1.39	1.44
14	A	839	CLA	C4C-C3C	2.24	1.48	1.45
14	A	839	CLA	C3D-C4D	-2.24	1.39	1.44
14	B	812	CLA	C3D-C4D	-2.24	1.39	1.44
14	bB	803	CLA	C3B-C2B	2.24	1.48	1.41
14	cB	804	CLA	C3B-C2B	2.24	1.48	1.41
14	bA	824	CLA	C1B-C2B	2.24	1.48	1.43
14	A	816	CLA	C3D-C4D	-2.24	1.39	1.44
14	cB	850	CLA	C3D-C4D	-2.24	1.39	1.44
14	A	836	CLA	C3B-C2B	2.24	1.48	1.41
14	bA	842	CLA	C3D-C4D	-2.24	1.39	1.44
14	cA	816	CLA	C3D-C4D	-2.24	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	L	206	BCR	C19-C18	-2.24	1.41	1.45
14	B	803	CLA	C3B-C2B	2.24	1.48	1.41
14	cA	822	CLA	C1D-C2D	2.24	1.49	1.45
14	cB	832	CLA	C4B-NB	-2.24	1.35	1.37
14	A	818	CLA	C3D-C4D	-2.24	1.39	1.44
14	A	815	CLA	C3D-C4D	-2.24	1.39	1.44
14	bA	839	CLA	C3D-C4D	-2.24	1.39	1.44
14	cB	820	CLA	C3B-C2B	2.23	1.48	1.41
13	bA	801	CL0	C1B-C2B	2.23	1.48	1.43
14	A	822	CLA	C1D-C2D	2.23	1.49	1.45
14	cA	815	CLA	C3D-C4D	-2.23	1.39	1.44
14	cB	836	CLA	C3D-C4D	-2.23	1.39	1.44
14	bA	836	CLA	C3B-C2B	2.23	1.48	1.41
14	bB	816	CLA	C1B-C2B	2.23	1.48	1.43
14	cA	839	CLA	C3D-C4D	-2.23	1.39	1.44
14	A	809	CLA	C4C-C3C	2.23	1.48	1.45
17	cA	848	BCR	C19-C18	-2.23	1.41	1.45
14	bB	825	CLA	C4C-C3C	2.23	1.48	1.45
14	bB	819	CLA	C3B-C2B	2.23	1.48	1.41
14	bA	804	CLA	C3D-C4D	-2.23	1.39	1.44
17	bA	848	BCR	C19-C18	-2.23	1.41	1.45
14	cA	818	CLA	C3D-C4D	-2.23	1.39	1.44
14	cB	834	CLA	C3D-C4D	-2.23	1.39	1.44
14	bA	819	CLA	C3B-C2B	2.23	1.48	1.41
14	cB	826	CLA	C4C-C3C	2.23	1.48	1.45
14	A	814	CLA	C3D-C4D	-2.23	1.39	1.44
14	B	819	CLA	C3B-C2B	2.23	1.48	1.41
14	B	825	CLA	C4C-C3C	2.23	1.48	1.45
14	B	835	CLA	C3D-C4D	-2.23	1.39	1.44
14	X	201	CLA	C4B-NB	-2.23	1.35	1.37
13	A	801	CL0	C1B-C2B	2.23	1.48	1.43
17	bL	206	BCR	C19-C18	-2.23	1.41	1.45
14	bJ	102	CLA	C3B-C2B	2.22	1.48	1.41
14	cA	836	CLA	C3B-C2B	2.22	1.48	1.41
14	cL	205	CLA	C3B-C2B	2.22	1.48	1.41
14	bA	807	CLA	C3D-C4D	-2.22	1.39	1.44
14	bB	835	CLA	C3D-C4D	-2.22	1.39	1.44
14	cA	804	CLA	C3D-C4D	-2.22	1.39	1.44
14	bL	204	CLA	C3B-C2B	2.22	1.48	1.41
14	cA	819	CLA	C3B-C2B	2.22	1.48	1.41
14	cA	807	CLA	C3D-C4D	-2.22	1.39	1.44
14	bB	833	CLA	C3B-C2B	2.22	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	833	CLA	C3B-C2B	2.22	1.48	1.41
13	bA	801	CL0	C4B-NB	-2.22	1.35	1.37
14	cX	201	CLA	C4B-NB	-2.22	1.35	1.37
14	A	819	CLA	C3B-C2B	2.22	1.48	1.41
14	L	204	CLA	C3B-C2B	2.22	1.48	1.41
14	B	849	CLA	C3D-C4D	-2.22	1.39	1.44
14	bA	809	CLA	C4C-C3C	2.22	1.48	1.45
14	A	804	CLA	C3D-C4D	-2.22	1.39	1.44
14	B	816	CLA	C1B-C2B	2.22	1.48	1.43
14	bB	849	CLA	C3D-C4D	-2.22	1.39	1.44
14	bA	810	CLA	C4B-NB	-2.22	1.35	1.37
14	cB	817	CLA	C1B-C2B	2.22	1.48	1.43
14	B	809	CLA	C4C-C3C	2.22	1.48	1.45
13	cA	801	CL0	C1B-C2B	2.21	1.48	1.43
17	cL	207	BCR	C19-C18	-2.21	1.41	1.45
14	cF	201	CLA	C3D-C4D	-2.21	1.39	1.44
14	bA	839	CLA	C4C-C3C	2.21	1.48	1.45
14	B	821	CLA	C3D-C4D	-2.21	1.39	1.44
14	bB	809	CLA	C4C-C3C	2.21	1.48	1.45
14	cA	805	CLA	C4C-C3C	2.21	1.48	1.45
14	A	834	CLA	C3D-C4D	-2.21	1.39	1.44
14	B	812	CLA	C1B-C2B	2.21	1.48	1.43
14	bB	802	CLA	C3D-C4D	-2.21	1.39	1.44
14	A	852	CLA	C3B-C2B	2.21	1.48	1.41
14	cB	822	CLA	C3D-C4D	-2.21	1.39	1.44
14	cA	852	CLA	C3B-C2B	2.21	1.48	1.41
14	bA	822	CLA	C1D-C2D	2.21	1.49	1.45
14	A	805	CLA	C4C-C3C	2.21	1.48	1.45
14	bA	805	CLA	C4C-C3C	2.21	1.48	1.45
14	J	102	CLA	C3B-C2B	2.21	1.48	1.41
14	bA	852	CLA	C3B-C2B	2.21	1.48	1.41
14	A	807	CLA	C3D-C4D	-2.21	1.39	1.44
14	cA	811	CLA	C3B-C2B	2.21	1.48	1.41
14	cA	834	CLA	C3D-C4D	-2.20	1.39	1.44
14	cB	834	CLA	C3B-C2B	2.20	1.48	1.41
14	cJ	102	CLA	C3B-C2B	2.20	1.48	1.41
14	B	802	CLA	C3D-C4D	-2.20	1.39	1.44
14	bA	834	CLA	C3D-C4D	-2.20	1.39	1.44
14	bX	201	CLA	C3B-C2B	2.20	1.48	1.41
14	bA	808	CLA	C3D-C4D	-2.20	1.39	1.44
17	bB	845	BCR	C12-C13	-2.20	1.41	1.45
14	X	201	CLA	C3B-C2B	2.20	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bA	838	CLA	C4D-CHA	2.20	1.46	1.38
14	bB	849	CLA	C4B-NB	-2.20	1.35	1.37
14	F	201	CLA	C3D-C4D	-2.20	1.39	1.44
14	cA	838	CLA	C3D-C4D	-2.20	1.39	1.44
14	cA	839	CLA	C4C-C3C	2.20	1.48	1.45
14	cB	810	CLA	C4C-C3C	2.20	1.48	1.45
14	bB	821	CLA	C3D-C4D	-2.20	1.39	1.44
14	bA	837	CLA	C4C-C3C	2.20	1.48	1.45
14	cJ	101	CLA	C3D-C4D	-2.20	1.39	1.44
14	cA	820	CLA	C4B-NB	-2.20	1.35	1.37
14	A	811	CLA	C3B-C2B	2.20	1.48	1.41
14	B	815	CLA	C3D-C4D	-2.20	1.39	1.44
14	cB	817	CLA	C3B-C2B	2.20	1.48	1.41
14	bA	838	CLA	C3D-C4D	-2.20	1.39	1.44
14	bJ	101	CLA	C3D-C4D	-2.20	1.39	1.44
14	bA	811	CLA	C3B-C2B	2.20	1.48	1.41
17	A	849	BCR	C12-C13	-2.20	1.41	1.45
14	J	101	CLA	C3B-C2B	2.20	1.48	1.41
14	cB	801	CLA	C4B-NB	-2.20	1.35	1.37
14	A	838	CLA	C3D-C4D	-2.20	1.39	1.44
14	bB	815	CLA	C3D-C4D	-2.20	1.39	1.44
14	A	838	CLA	C4D-CHA	2.20	1.46	1.38
13	cA	801	CL0	C4B-NB	-2.19	1.35	1.37
14	cA	810	CLA	C4B-NB	-2.19	1.35	1.37
14	bB	816	CLA	C3B-C2B	2.19	1.48	1.41
14	B	816	CLA	C3B-C2B	2.19	1.48	1.41
17	bL	205	BCR	C12-C13	-2.19	1.41	1.45
14	bJ	101	CLA	C3B-C2B	2.19	1.48	1.41
14	bA	820	CLA	C1D-C2D	2.19	1.49	1.45
17	B	845	BCR	C12-C13	-2.19	1.41	1.45
14	bF	201	CLA	C3D-C4D	-2.19	1.39	1.44
17	bA	849	BCR	C12-C13	-2.19	1.41	1.45
14	cJ	101	CLA	C3B-C2B	2.19	1.48	1.41
13	A	801	CL0	C4B-NB	-2.19	1.35	1.37
14	B	849	CLA	C4B-NB	-2.19	1.35	1.37
14	A	820	CLA	C4B-NB	-2.19	1.35	1.37
14	cA	838	CLA	C4D-CHA	2.19	1.46	1.38
14	cA	808	CLA	C3D-C4D	-2.19	1.39	1.44
14	bB	812	CLA	C1B-C2B	2.19	1.48	1.43
14	cB	813	CLA	C1B-C2B	2.19	1.48	1.43
17	cB	846	BCR	C12-C13	-2.19	1.41	1.45
14	cB	803	CLA	C3D-C4D	-2.19	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bA	820	CLA	C4B-NB	-2.19	1.35	1.37
14	J	101	CLA	C3D-C4D	-2.19	1.39	1.44
17	cL	206	BCR	C12-C13	-2.19	1.41	1.45
14	cA	834	CLA	C3B-C2B	2.18	1.48	1.41
14	L	201	CLA	C4C-C3C	2.18	1.48	1.45
14	bB	815	CLA	C4B-NB	-2.18	1.35	1.37
17	L	205	BCR	C12-C13	-2.18	1.41	1.45
14	bB	806	CLA	C3B-C2B	2.18	1.48	1.41
14	A	810	CLA	C4B-NB	-2.18	1.35	1.37
14	cA	809	CLA	C4C-C3C	2.18	1.48	1.45
14	cL	202	CLA	C4C-C3C	2.18	1.48	1.45
14	cX	201	CLA	C3B-C2B	2.18	1.48	1.41
14	cA	820	CLA	C1D-C2D	2.18	1.49	1.45
14	bB	834	CLA	C4B-NB	-2.18	1.35	1.37
17	cA	849	BCR	C12-C13	-2.18	1.41	1.45
14	A	808	CLA	C3D-C4D	-2.18	1.39	1.44
14	A	837	CLA	C4C-C3C	2.18	1.48	1.45
14	bA	830	CLA	C1C-C2C	2.18	1.48	1.44
14	cA	805	CLA	C3D-C4D	-2.18	1.39	1.44
14	cB	807	CLA	C3B-C2B	2.18	1.48	1.41
14	A	834	CLA	C3B-C2B	2.18	1.48	1.41
14	B	834	CLA	C4B-NB	-2.18	1.35	1.37
14	A	805	CLA	C3D-C4D	-2.18	1.39	1.44
14	bX	201	CLA	C3D-C4D	-2.18	1.39	1.44
14	A	835	CLA	C4B-NB	-2.18	1.35	1.37
14	B	806	CLA	C3B-C2B	2.18	1.48	1.41
14	bL	201	CLA	C1B-C2B	2.18	1.48	1.43
14	X	201	CLA	C3D-C4D	-2.18	1.39	1.44
14	bA	805	CLA	C3D-C4D	-2.18	1.39	1.44
14	bA	824	CLA	C3D-C4D	-2.18	1.39	1.44
14	B	815	CLA	C4B-NB	-2.18	1.35	1.37
14	L	201	CLA	C1B-C2B	2.17	1.48	1.43
14	cX	201	CLA	C3D-C4D	-2.17	1.39	1.44
14	A	820	CLA	C1D-C2D	2.17	1.49	1.45
14	bA	835	CLA	C3B-C2B	2.17	1.48	1.41
14	bA	834	CLA	C3B-C2B	2.17	1.48	1.41
14	B	824	CLA	C3D-C4D	-2.17	1.39	1.44
17	cA	846	BCR	C23-C22	-2.17	1.41	1.45
14	cB	850	CLA	C4B-NB	-2.17	1.35	1.37
14	A	830	CLA	C1C-C2C	2.17	1.48	1.44
14	B	801	CLA	C3D-C4D	-2.17	1.39	1.44
14	bB	824	CLA	C3D-C4D	-2.17	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cB	802	CLA	C3D-C4D	-2.17	1.39	1.44
14	cL	202	CLA	C1B-C2B	2.17	1.48	1.43
14	A	822	CLA	C3B-C2B	2.17	1.48	1.41
14	cB	816	CLA	C3D-C4D	-2.17	1.39	1.44
17	L	205	BCR	C19-C18	-2.17	1.41	1.45
14	cA	822	CLA	C3B-C2B	2.16	1.48	1.41
14	cA	833	CLA	C3B-C2B	2.16	1.48	1.41
14	cB	816	CLA	C4B-NB	-2.16	1.35	1.37
14	cA	837	CLA	C4C-C3C	2.16	1.48	1.45
14	bB	801	CLA	C3D-C4D	-2.16	1.39	1.44
14	B	851	CLA	C4B-NB	-2.16	1.35	1.37
17	cM	101	BCR	C12-C13	-2.16	1.41	1.45
14	bB	851	CLA	C4B-NB	-2.16	1.35	1.37
14	B	822	CLA	C3D-C4D	-2.16	1.39	1.44
14	bA	833	CLA	C3B-C2B	2.16	1.48	1.41
14	A	824	CLA	C3D-C4D	-2.16	1.39	1.44
14	cA	840	CLA	C3B-C2B	2.16	1.48	1.41
17	M	101	BCR	C12-C13	-2.16	1.41	1.45
14	A	806	CLA	C4C-C3C	2.16	1.48	1.45
14	bA	806	CLA	C4C-C3C	2.16	1.48	1.45
14	bA	822	CLA	C3B-C2B	2.16	1.48	1.41
14	A	835	CLA	C3B-C2B	2.16	1.48	1.41
17	A	846	BCR	C23-C22	-2.16	1.41	1.45
14	bB	832	CLA	C3D-C4D	-2.16	1.39	1.44
14	bL	201	CLA	C4C-C3C	2.15	1.48	1.45
14	bB	822	CLA	C3D-C4D	-2.15	1.39	1.44
14	cB	825	CLA	C3D-C4D	-2.15	1.39	1.44
14	A	840	CLA	C3B-C2B	2.15	1.48	1.41
14	B	832	CLA	C3D-C4D	-2.15	1.39	1.44
14	cA	830	CLA	C1C-C2C	2.15	1.48	1.44
14	cA	841	CLA	C3D-C4D	-2.15	1.39	1.44
14	bB	817	CLA	C1D-C2D	2.15	1.49	1.45
14	cB	823	CLA	C3D-C4D	-2.15	1.39	1.44
14	bA	840	CLA	C3B-C2B	2.14	1.48	1.41
17	bM	101	BCR	C12-C13	-2.14	1.41	1.45
14	A	833	CLA	C3B-C2B	2.14	1.48	1.41
14	cA	824	CLA	C3D-C4D	-2.14	1.39	1.44
14	cA	806	CLA	C4C-C3C	2.14	1.48	1.45
14	cB	826	CLA	C3B-C2B	2.14	1.48	1.41
17	B	844	BCR	C19-C18	-2.14	1.41	1.45
14	bA	832	CLA	C3B-C2B	2.14	1.48	1.41
14	cA	832	CLA	C3B-C2B	2.14	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	bA	846	BCR	C23-C22	-2.14	1.41	1.45
17	cL	206	BCR	C19-C18	-2.14	1.41	1.45
14	B	825	CLA	C3B-C2B	2.14	1.48	1.41
17	bB	844	BCR	C19-C18	-2.14	1.41	1.45
17	cA	848	BCR	C12-C13	-2.14	1.41	1.45
14	cA	835	CLA	C3B-C2B	2.14	1.48	1.41
14	J	102	CLA	C3D-C4D	-2.14	1.39	1.44
14	A	823	CLA	C3B-C2B	2.14	1.48	1.41
14	bA	824	CLA	C3B-C2B	2.14	1.48	1.41
14	bB	825	CLA	C3B-C2B	2.14	1.48	1.41
17	bL	205	BCR	C19-C18	-2.14	1.41	1.45
14	B	831	CLA	C3B-C2B	2.14	1.48	1.41
14	cA	826	CLA	C4C-C3C	2.14	1.48	1.45
14	cB	819	CLA	C1B-C2B	2.14	1.48	1.43
17	bA	848	BCR	C12-C13	-2.14	1.41	1.45
15	B	840	PQN	C3-C2	2.13	1.39	1.35
15	cB	841	PQN	C3-C2	2.13	1.39	1.35
14	bB	818	CLA	C1B-C2B	2.13	1.48	1.43
14	B	817	CLA	C1D-C2D	2.13	1.49	1.45
14	cL	202	CLA	C3B-C2B	2.13	1.48	1.41
14	A	826	CLA	C4C-C3C	2.13	1.48	1.45
14	bB	831	CLA	C3B-C2B	2.13	1.48	1.41
14	cB	832	CLA	C3B-C2B	2.13	1.48	1.41
14	cB	818	CLA	C1D-C2D	2.13	1.49	1.45
14	bA	826	CLA	C4C-C3C	2.13	1.48	1.45
14	cB	840	CLA	C1C-NC	-2.13	1.34	1.37
14	A	832	CLA	C3B-C2B	2.13	1.48	1.41
14	B	818	CLA	C1B-C2B	2.13	1.48	1.43
17	A	848	BCR	C12-C13	-2.13	1.41	1.45
17	cB	845	BCR	C19-C18	-2.13	1.41	1.45
14	A	841	CLA	C3D-C4D	-2.13	1.39	1.44
14	A	824	CLA	C3B-C2B	2.13	1.48	1.41
14	cB	835	CLA	C4B-NB	-2.13	1.35	1.37
14	A	823	CLA	C3D-C4D	-2.13	1.39	1.44
14	cA	823	CLA	C3B-C2B	2.13	1.48	1.41
14	L	201	CLA	C3B-C2B	2.13	1.48	1.41
14	cB	833	CLA	C3D-C4D	-2.13	1.39	1.44
14	bL	201	CLA	C3B-C2B	2.12	1.48	1.41
14	cA	824	CLA	C3B-C2B	2.12	1.48	1.41
14	bA	841	CLA	C3D-C4D	-2.12	1.39	1.44
14	cL	205	CLA	C3D-C4D	-2.12	1.39	1.44
14	B	832	CLA	C4C-C3C	2.12	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cB	829	CLA	C4D-CHA	2.12	1.45	1.38
14	L	204	CLA	C3D-C4D	-2.12	1.39	1.44
14	cB	811	CLA	C1D-C2D	2.12	1.49	1.45
14	bB	828	CLA	C4D-CHA	2.12	1.45	1.38
14	B	828	CLA	C4D-CHA	2.12	1.45	1.38
15	bB	840	PQN	C3-C2	2.12	1.39	1.35
14	bA	823	CLA	C3B-C2B	2.12	1.48	1.41
14	cA	820	CLA	C1B-C2B	2.12	1.48	1.43
14	bA	833	CLA	C1C-C2C	2.12	1.48	1.44
14	cJ	102	CLA	C3D-C4D	-2.12	1.39	1.44
14	B	839	CLA	C1C-NC	-2.12	1.34	1.37
14	B	815	CLA	C3B-C2B	2.12	1.48	1.41
14	cA	835	CLA	C4B-NB	-2.12	1.35	1.37
14	cB	816	CLA	C3B-C2B	2.12	1.48	1.41
14	cA	833	CLA	C1C-C2C	2.11	1.48	1.44
14	bJ	102	CLA	C3D-C4D	-2.11	1.39	1.44
14	cA	823	CLA	C3D-C4D	-2.11	1.39	1.44
14	cA	810	CLA	C3B-C2B	2.11	1.48	1.41
14	bB	815	CLA	C3B-C2B	2.11	1.48	1.41
14	B	810	CLA	C1D-C2D	2.11	1.49	1.45
14	cA	813	CLA	C3B-C2B	2.11	1.48	1.41
14	bA	835	CLA	C4B-NB	-2.11	1.35	1.37
14	A	820	CLA	C1B-C2B	2.11	1.48	1.43
15	bA	843	PQN	C3-C2	2.11	1.39	1.35
14	L	203	CLA	C4C-C3C	2.11	1.48	1.45
14	cA	806	CLA	C3B-C2B	2.10	1.48	1.41
14	B	817	CLA	C1C-NC	-2.10	1.34	1.37
14	A	810	CLA	C3B-C2B	2.10	1.48	1.41
14	cB	818	CLA	C1C-NC	-2.10	1.34	1.37
14	A	806	CLA	C3B-C2B	2.10	1.48	1.41
14	bL	204	CLA	C3D-C4D	-2.10	1.39	1.44
14	bB	810	CLA	C1D-C2D	2.10	1.49	1.45
14	bA	806	CLA	C3B-C2B	2.10	1.48	1.41
14	A	833	CLA	C1C-C2C	2.10	1.48	1.44
14	bB	839	CLA	C1C-NC	-2.10	1.34	1.37
14	A	815	CLA	C1D-C2D	2.10	1.49	1.45
14	bA	813	CLA	C3B-C2B	2.10	1.48	1.41
14	bB	805	CLA	C1D-C2D	2.10	1.49	1.45
14	cB	833	CLA	C4C-C3C	2.10	1.48	1.45
14	bA	823	CLA	C3D-C4D	-2.10	1.39	1.44
14	cA	838	CLA	C4C-C3C	2.10	1.48	1.45
14	bA	820	CLA	C1B-C2B	2.10	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bA	810	CLA	C3B-C2B	2.10	1.48	1.41
14	bA	838	CLA	C4C-C3C	2.10	1.48	1.45
14	bL	202	CLA	C1D-C2D	2.10	1.49	1.45
14	A	813	CLA	C3B-C2B	2.09	1.48	1.41
17	I	101	BCR	C19-C18	-2.09	1.41	1.45
14	bB	832	CLA	C4C-C3C	2.09	1.48	1.45
17	bJ	103	BCR	C19-C18	-2.09	1.41	1.45
17	cB	848	BCR	C12-C13	-2.09	1.41	1.45
17	A	847	BCR	C12-C13	-2.09	1.41	1.45
17	J	103	BCR	C19-C18	-2.09	1.41	1.45
17	cJ	103	BCR	C19-C18	-2.09	1.41	1.45
14	A	852	CLA	C1C-C2C	2.09	1.48	1.44
14	A	818	CLA	C1B-C2B	2.09	1.48	1.43
14	cB	806	CLA	C1D-C2D	2.09	1.49	1.45
17	cB	848	BCR	C19-C18	-2.09	1.41	1.45
14	bA	818	CLA	C1B-C2B	2.09	1.48	1.43
14	A	828	CLA	C3D-C4D	-2.09	1.39	1.44
14	bL	203	CLA	C4C-C3C	2.09	1.48	1.45
14	cA	810	CLA	C1D-C2D	2.09	1.49	1.45
14	cA	828	CLA	C3D-C4D	-2.09	1.39	1.44
14	L	202	CLA	C1D-C2D	2.09	1.49	1.45
14	cB	837	CLA	C4C-C3C	2.09	1.48	1.45
15	A	843	PQN	C3-C2	2.09	1.39	1.35
14	bB	817	CLA	C1C-NC	-2.08	1.34	1.37
14	A	841	CLA	C1B-C2B	2.08	1.48	1.43
14	cB	822	CLA	C1D-C2D	2.08	1.49	1.45
17	B	847	BCR	C12-C13	-2.08	1.41	1.45
17	cI	101	BCR	C19-C18	-2.08	1.41	1.45
14	A	810	CLA	C1D-C2D	2.08	1.49	1.45
14	cA	802	CLA	C3B-C4B	2.08	1.47	1.42
14	bA	810	CLA	C1D-C2D	2.08	1.49	1.45
14	cJ	101	CLA	C1D-C2D	2.08	1.49	1.45
17	bB	847	BCR	C12-C13	-2.08	1.41	1.45
17	bB	847	BCR	C19-C18	-2.08	1.41	1.45
14	B	836	CLA	C4C-C3C	2.08	1.48	1.45
14	cB	813	CLA	C3B-C2B	2.08	1.48	1.41
17	B	847	BCR	C19-C18	-2.08	1.41	1.45
14	bB	812	CLA	C3B-C2B	2.08	1.48	1.41
14	cA	815	CLA	C1D-C2D	2.08	1.49	1.45
14	bJ	101	CLA	C1D-C2D	2.08	1.49	1.45
14	B	805	CLA	C1D-C2D	2.08	1.49	1.45
14	bB	836	CLA	C4C-C3C	2.08	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bA	815	CLA	C1D-C2D	2.08	1.49	1.45
14	B	812	CLA	C3B-C2B	2.08	1.48	1.41
14	J	101	CLA	C1D-C2D	2.08	1.49	1.45
14	cA	841	CLA	C1B-C2B	2.08	1.48	1.43
14	A	802	CLA	C3B-C4B	2.07	1.47	1.42
14	bA	802	CLA	C3B-C4B	2.07	1.47	1.42
15	cA	843	PQN	C3-C2	2.07	1.39	1.35
14	bA	807	CLA	C3B-C2B	2.07	1.48	1.41
14	cB	835	CLA	C3B-C2B	2.07	1.48	1.41
14	B	816	CLA	C1D-C2D	2.07	1.49	1.45
14	B	821	CLA	C1D-C2D	2.07	1.49	1.45
14	bA	852	CLA	C1C-C2C	2.07	1.48	1.44
13	bA	801	CL0	C3B-C2B	2.07	1.48	1.41
13	cA	801	CL0	C3B-C2B	2.07	1.48	1.41
14	bB	816	CLA	C1D-C2D	2.07	1.49	1.45
14	bA	837	CLA	C3B-C2B	2.07	1.48	1.41
14	A	838	CLA	C4C-C3C	2.07	1.48	1.45
14	bB	834	CLA	C3B-C2B	2.07	1.48	1.41
14	B	814	CLA	C1D-C2D	2.07	1.49	1.45
14	cA	818	CLA	C1B-C2B	2.07	1.48	1.43
14	cA	807	CLA	C3B-C2B	2.07	1.48	1.41
14	cL	204	CLA	C4C-C3C	2.07	1.48	1.45
14	bA	828	CLA	C3D-C4D	-2.07	1.39	1.44
17	bA	847	BCR	C12-C13	-2.07	1.41	1.45
14	bA	823	CLA	C4B-NB	-2.07	1.35	1.37
14	A	837	CLA	C3B-C2B	2.06	1.48	1.41
14	cA	837	CLA	C3B-C2B	2.06	1.48	1.41
14	bA	802	CLA	C3B-C2B	2.06	1.48	1.41
14	bB	821	CLA	C1D-C2D	2.06	1.49	1.45
14	B	834	CLA	C3B-C2B	2.06	1.48	1.41
14	bA	805	CLA	C1D-C2D	2.06	1.49	1.45
14	cB	815	CLA	C1D-C2D	2.06	1.49	1.45
14	bA	841	CLA	C1B-C2B	2.06	1.48	1.43
13	A	801	CL0	C3B-C2B	2.06	1.48	1.41
14	B	839	CLA	C3B-C2B	2.06	1.48	1.41
14	A	802	CLA	C3B-C2B	2.06	1.48	1.41
14	A	805	CLA	C1D-C2D	2.06	1.49	1.45
14	cA	818	CLA	C1D-C2D	2.06	1.49	1.45
14	bB	839	CLA	C3B-C2B	2.06	1.48	1.41
14	B	830	CLA	C1D-C2D	2.06	1.49	1.45
17	cA	847	BCR	C12-C13	-2.06	1.41	1.45
14	cB	840	CLA	C3B-C2B	2.06	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bB	814	CLA	C1D-C2D	2.06	1.49	1.45
14	cB	817	CLA	C1D-C2D	2.06	1.49	1.45
14	cL	203	CLA	C1D-C2D	2.06	1.49	1.45
14	cA	823	CLA	C4B-NB	-2.06	1.35	1.37
14	B	808	CLA	C4B-NB	-2.06	1.35	1.37
14	cB	835	CLA	C1D-C2D	2.06	1.49	1.45
14	cB	809	CLA	C4B-NB	-2.05	1.35	1.37
14	cA	852	CLA	C1C-C2C	2.05	1.48	1.44
14	A	807	CLA	C3B-C2B	2.05	1.48	1.41
17	bB	843	BCR	C20-C19	2.05	1.39	1.34
17	bI	101	BCR	C19-C18	-2.05	1.41	1.45
17	B	842	BCR	C20-C19	2.05	1.39	1.34
14	A	818	CLA	C1D-C2D	2.05	1.49	1.45
14	cA	802	CLA	C3B-C2B	2.05	1.48	1.41
17	M	101	BCR	C19-C18	-2.05	1.41	1.45
14	bA	841	CLA	C4B-NB	-2.05	1.35	1.37
14	bB	830	CLA	C1D-C2D	2.05	1.49	1.45
14	B	817	CLA	C4C-C3C	2.05	1.48	1.45
14	bA	818	CLA	C1D-C2D	2.05	1.49	1.45
17	bI	102	BCR	C19-C18	-2.05	1.41	1.45
14	cA	805	CLA	C1D-C2D	2.05	1.49	1.45
14	cA	808	CLA	C3B-C2B	2.05	1.48	1.41
17	bB	842	BCR	C20-C19	2.05	1.39	1.34
17	I	102	BCR	C19-C18	-2.04	1.41	1.45
14	bB	817	CLA	C4C-C3C	2.04	1.48	1.45
14	bB	834	CLA	C1D-C2D	2.04	1.49	1.45
14	cB	818	CLA	C4C-C3C	2.04	1.48	1.45
14	cB	831	CLA	C1D-C2D	2.04	1.49	1.45
17	bM	101	BCR	C19-C18	-2.04	1.41	1.45
14	cB	816	CLA	C1D-C2D	2.04	1.49	1.45
14	cA	841	CLA	C4B-NB	-2.03	1.35	1.37
14	A	823	CLA	C4B-NB	-2.03	1.35	1.37
17	bB	850	BCR	C19-C18	-2.03	1.41	1.45
14	cA	828	CLA	C4C-C3C	2.03	1.48	1.45
17	cM	101	BCR	C19-C18	-2.03	1.41	1.45
14	cB	807	CLA	C4B-NB	-2.03	1.35	1.37
14	cX	201	CLA	C1D-C2D	2.03	1.49	1.45
14	A	828	CLA	C4C-C3C	2.03	1.48	1.45
17	cB	851	BCR	C19-C18	-2.02	1.41	1.45
14	bA	828	CLA	C4C-C3C	2.02	1.48	1.45
14	bB	815	CLA	C1D-C2D	2.02	1.49	1.45
14	A	808	CLA	C3B-C2B	2.02	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cB	819	CLA	C3B-C2B	2.02	1.48	1.41
14	bB	808	CLA	C4B-NB	-2.02	1.35	1.37
14	bB	818	CLA	C3B-C2B	2.02	1.48	1.41
17	B	843	BCR	C20-C19	2.02	1.39	1.34
14	B	818	CLA	C3B-C2B	2.02	1.48	1.41
17	cB	843	BCR	C20-C19	2.02	1.39	1.34
17	cB	844	BCR	C20-C19	2.02	1.39	1.34
14	cB	813	CLA	C1D-C2D	2.02	1.49	1.45
17	cA	845	BCR	C12-C13	-2.02	1.41	1.45
14	B	812	CLA	C1D-C2D	2.02	1.49	1.45
14	A	818	CLA	C3B-C2B	2.02	1.48	1.41
14	bA	820	CLA	C3B-C2B	2.02	1.48	1.41
14	cA	818	CLA	C3B-C2B	2.02	1.48	1.41
14	F	201	CLA	C3B-C2B	2.02	1.48	1.41
14	bA	808	CLA	C3B-C2B	2.02	1.48	1.41
17	B	850	BCR	C19-C18	-2.02	1.41	1.45
14	A	841	CLA	C4B-NB	-2.02	1.35	1.37
17	cI	102	BCR	C19-C18	-2.02	1.41	1.45
14	B	815	CLA	C1D-C2D	2.02	1.49	1.45
14	X	201	CLA	C1D-C2D	2.02	1.49	1.45
14	bJ	102	CLA	C1D-C2D	2.01	1.49	1.45
14	A	820	CLA	C3B-C2B	2.01	1.48	1.41
14	cA	820	CLA	C3B-C2B	2.01	1.48	1.41
14	A	804	CLA	C1D-C2D	2.01	1.49	1.45
14	B	849	CLA	C1D-C2D	2.01	1.49	1.45
14	bA	818	CLA	C3B-C2B	2.01	1.48	1.41
14	bB	806	CLA	C4B-NB	-2.01	1.35	1.37
17	bA	845	BCR	C12-C13	-2.01	1.41	1.45
14	bX	201	CLA	C1D-C2D	2.01	1.49	1.45
17	bA	846	BCR	C12-C13	-2.01	1.41	1.45
14	bA	804	CLA	C1D-C2D	2.01	1.49	1.45
14	bB	833	CLA	C1D-C2D	2.01	1.49	1.45
14	B	806	CLA	C4B-NB	-2.01	1.35	1.37
14	A	812	CLA	C1D-C2D	2.01	1.49	1.45
14	cA	804	CLA	C1D-C2D	2.01	1.49	1.45
14	A	807	CLA	C1D-C2D	2.01	1.49	1.45
14	B	834	CLA	C1D-C2D	2.01	1.49	1.45
14	J	102	CLA	C1D-C2D	2.01	1.49	1.45
17	B	841	BCR	C12-C13	-2.01	1.41	1.45
14	cB	850	CLA	C1D-C2D	2.01	1.49	1.45
17	cB	842	BCR	C12-C13	-2.01	1.41	1.45
14	bF	201	CLA	C3B-C2B	2.01	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	cA	807	CLA	C1D-C2D	2.01	1.49	1.45
14	bA	811	CLA	C1D-C2D	2.01	1.49	1.45
17	A	845	BCR	C12-C13	-2.01	1.41	1.45
17	B	843	BCR	C12-C13	-2.01	1.41	1.45
14	cF	201	CLA	C3B-C2B	2.00	1.48	1.41
14	bA	830	CLA	C4C-C3C	2.00	1.48	1.45
14	cJ	102	CLA	C1D-C2D	2.00	1.49	1.45
14	B	833	CLA	C1D-C2D	2.00	1.49	1.45

All (8404) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cL	203	CLA	O2A-CGA-O1A	-18.70	76.39	123.59
14	bL	202	CLA	O2A-CGA-O1A	-18.70	76.40	123.59
14	L	202	CLA	O2A-CGA-O1A	-18.70	76.40	123.59
14	cL	203	CLA	O2A-CGA-CBA	15.63	160.95	111.91
14	L	202	CLA	O2A-CGA-CBA	15.62	160.94	111.91
14	bL	202	CLA	O2A-CGA-CBA	15.62	160.93	111.91
14	bL	203	CLA	C1D-ND-C4D	-10.59	98.81	106.33
14	cL	204	CLA	C1D-ND-C4D	-10.59	98.82	106.33
14	L	203	CLA	C1D-ND-C4D	-10.58	98.82	106.33
14	bB	828	CLA	C1D-ND-C4D	-10.56	98.83	106.33
14	B	828	CLA	C1D-ND-C4D	-10.56	98.83	106.33
14	cB	829	CLA	C1D-ND-C4D	-10.56	98.83	106.33
14	bB	831	CLA	C1D-ND-C4D	-10.20	99.09	106.33
14	B	831	CLA	C1D-ND-C4D	-10.19	99.10	106.33
14	cB	832	CLA	C1D-ND-C4D	-10.18	99.10	106.33
14	bL	202	CLA	O1A-CGA-CBA	-10.04	84.56	123.73
14	L	202	CLA	O1A-CGA-CBA	-10.04	84.56	123.73
14	cL	203	CLA	O1A-CGA-CBA	-10.03	84.58	123.73
14	bB	815	CLA	C1D-ND-C4D	-10.03	99.21	106.33
14	B	815	CLA	C1D-ND-C4D	-10.02	99.22	106.33
14	B	820	CLA	C1D-ND-C4D	-10.01	99.22	106.33
14	bA	825	CLA	C1D-ND-C4D	-9.99	99.24	106.33
14	bB	820	CLA	C1D-ND-C4D	-9.99	99.24	106.33
14	A	825	CLA	C1D-ND-C4D	-9.98	99.25	106.33
14	cA	825	CLA	C1D-ND-C4D	-9.98	99.25	106.33
14	cB	816	CLA	C1D-ND-C4D	-9.97	99.25	106.33
14	cB	821	CLA	C1D-ND-C4D	-9.97	99.25	106.33
14	bA	838	CLA	C1D-ND-C4D	-9.96	99.26	106.33
14	bB	812	CLA	C1D-ND-C4D	-9.95	99.27	106.33
14	cA	838	CLA	C1D-ND-C4D	-9.95	99.27	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cB	813	CLA	C1D-ND-C4D	-9.94	99.27	106.33
14	A	838	CLA	C1D-ND-C4D	-9.94	99.28	106.33
14	B	812	CLA	C1D-ND-C4D	-9.93	99.28	106.33
14	cA	831	CLA	C1D-ND-C4D	-9.93	99.28	106.33
14	bA	831	CLA	C1D-ND-C4D	-9.92	99.29	106.33
14	A	831	CLA	C1D-ND-C4D	-9.90	99.30	106.33
14	A	823	CLA	C1D-ND-C4D	-9.90	99.30	106.33
14	cA	823	CLA	C1D-ND-C4D	-9.88	99.32	106.33
14	bA	823	CLA	C1D-ND-C4D	-9.87	99.33	106.33
14	B	836	CLA	C1D-ND-C4D	-9.76	99.40	106.33
14	cB	820	CLA	C1D-ND-C4D	-9.76	99.40	106.33
14	cA	811	CLA	C1D-ND-C4D	-9.75	99.41	106.33
14	cB	837	CLA	C1D-ND-C4D	-9.74	99.41	106.33
14	B	801	CLA	C1D-ND-C4D	-9.74	99.42	106.33
14	bB	836	CLA	C1D-ND-C4D	-9.74	99.42	106.33
14	bB	819	CLA	C1D-ND-C4D	-9.73	99.42	106.33
14	A	811	CLA	C1D-ND-C4D	-9.73	99.42	106.33
14	cL	203	CLA	C1D-ND-C4D	-9.73	99.42	106.33
14	cA	812	CLA	C1D-ND-C4D	-9.73	99.42	106.33
14	B	819	CLA	C1D-ND-C4D	-9.72	99.43	106.33
14	bA	811	CLA	C1D-ND-C4D	-9.72	99.43	106.33
14	cB	802	CLA	C1D-ND-C4D	-9.72	99.43	106.33
14	bB	822	CLA	C1D-ND-C4D	-9.70	99.44	106.33
14	A	808	CLA	C1D-ND-C4D	-9.70	99.45	106.33
14	bA	816	CLA	C1D-ND-C4D	-9.70	99.45	106.33
14	L	202	CLA	C1D-ND-C4D	-9.70	99.45	106.33
14	bA	812	CLA	C1D-ND-C4D	-9.70	99.45	106.33
14	bB	801	CLA	C1D-ND-C4D	-9.69	99.45	106.33
14	cA	808	CLA	C1D-ND-C4D	-9.68	99.46	106.33
14	bA	804	CLA	C1D-ND-C4D	-9.68	99.46	106.33
14	bL	202	CLA	C1D-ND-C4D	-9.67	99.46	106.33
14	B	806	CLA	C1D-ND-C4D	-9.67	99.47	106.33
14	bL	201	CLA	C1D-ND-C4D	-9.66	99.47	106.33
14	bB	851	CLA	C1D-ND-C4D	-9.66	99.47	106.33
14	bA	808	CLA	C1D-ND-C4D	-9.66	99.47	106.33
14	cL	202	CLA	C1D-ND-C4D	-9.66	99.47	106.33
14	A	812	CLA	C1D-ND-C4D	-9.66	99.48	106.33
14	cA	804	CLA	C1D-ND-C4D	-9.66	99.48	106.33
14	cB	823	CLA	C1D-ND-C4D	-9.65	99.48	106.33
14	bA	837	CLA	C1D-ND-C4D	-9.65	99.48	106.33
14	A	816	CLA	C1D-ND-C4D	-9.64	99.48	106.33
14	A	804	CLA	C1D-ND-C4D	-9.64	99.48	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bB	806	CLA	C1D-ND-C4D	-9.64	99.49	106.33
14	cB	807	CLA	C1D-ND-C4D	-9.64	99.49	106.33
14	A	820	CLA	C1D-ND-C4D	-9.64	99.49	106.33
14	bA	840	CLA	C1D-ND-C4D	-9.64	99.49	106.33
14	bA	818	CLA	C1D-ND-C4D	-9.64	99.49	106.33
14	A	807	CLA	C1D-ND-C4D	-9.64	99.49	106.33
14	cA	816	CLA	C1D-ND-C4D	-9.64	99.49	106.33
14	B	822	CLA	C1D-ND-C4D	-9.63	99.49	106.33
14	A	840	CLA	C1D-ND-C4D	-9.63	99.50	106.33
14	bA	807	CLA	C1D-ND-C4D	-9.63	99.50	106.33
14	A	839	CLA	C1D-ND-C4D	-9.63	99.50	106.33
14	cA	840	CLA	C1D-ND-C4D	-9.63	99.50	106.33
14	A	837	CLA	C1D-ND-C4D	-9.63	99.50	106.33
14	cA	820	CLA	C1D-ND-C4D	-9.62	99.50	106.33
14	cA	837	CLA	C1D-ND-C4D	-9.62	99.50	106.33
14	bA	820	CLA	C1D-ND-C4D	-9.62	99.50	106.33
14	A	818	CLA	C1D-ND-C4D	-9.62	99.50	106.33
14	cB	801	CLA	C1D-ND-C4D	-9.61	99.50	106.33
14	L	201	CLA	C1D-ND-C4D	-9.61	99.51	106.33
14	bA	839	CLA	C1D-ND-C4D	-9.61	99.51	106.33
14	F	201	CLA	C1D-ND-C4D	-9.61	99.51	106.33
14	cA	818	CLA	C1D-ND-C4D	-9.60	99.51	106.33
14	A	842	CLA	C1D-ND-C4D	-9.60	99.51	106.33
14	B	851	CLA	C1D-ND-C4D	-9.60	99.51	106.33
14	cA	807	CLA	C1D-ND-C4D	-9.60	99.52	106.33
14	cX	201	CLA	C1D-ND-C4D	-9.59	99.52	106.33
14	B	821	CLA	C1D-ND-C4D	-9.59	99.52	106.33
14	A	810	CLA	C1D-ND-C4D	-9.58	99.53	106.33
14	cB	838	CLA	C1D-ND-C4D	-9.58	99.53	106.33
14	cA	839	CLA	C1D-ND-C4D	-9.58	99.53	106.33
14	bA	805	CLA	C1D-ND-C4D	-9.58	99.53	106.33
14	bA	810	CLA	C1D-ND-C4D	-9.58	99.53	106.33
14	cA	842	CLA	C1D-ND-C4D	-9.58	99.53	106.33
14	X	201	CLA	C1D-ND-C4D	-9.58	99.53	106.33
14	cA	810	CLA	C1D-ND-C4D	-9.57	99.53	106.33
14	bA	842	CLA	C1D-ND-C4D	-9.57	99.53	106.33
14	bX	201	CLA	C1D-ND-C4D	-9.57	99.54	106.33
14	cA	819	CLA	C1D-ND-C4D	-9.56	99.54	106.33
14	bB	814	CLA	C1D-ND-C4D	-9.56	99.55	106.33
14	B	814	CLA	C1D-ND-C4D	-9.56	99.55	106.33
14	A	821	CLA	C1D-ND-C4D	-9.55	99.55	106.33
14	bB	821	CLA	C1D-ND-C4D	-9.55	99.55	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bB	805	CLA	C1D-ND-C4D	-9.55	99.55	106.33
14	cB	822	CLA	C1D-ND-C4D	-9.55	99.55	106.33
14	cB	815	CLA	C1D-ND-C4D	-9.55	99.55	106.33
14	B	837	CLA	C1D-ND-C4D	-9.55	99.55	106.33
14	A	805	CLA	C1D-ND-C4D	-9.54	99.56	106.33
14	bA	827	CLA	C1D-ND-C4D	-9.54	99.56	106.33
14	cA	805	CLA	C1D-ND-C4D	-9.54	99.56	106.33
14	cF	201	CLA	C1D-ND-C4D	-9.54	99.56	106.33
14	cJ	102	CLA	C1D-ND-C4D	-9.54	99.56	106.33
14	B	811	CLA	C1D-ND-C4D	-9.53	99.56	106.33
14	bB	835	CLA	C1D-ND-C4D	-9.53	99.56	106.33
14	bF	201	CLA	C1D-ND-C4D	-9.53	99.56	106.33
14	bB	811	CLA	C1D-ND-C4D	-9.53	99.56	106.33
14	bA	819	CLA	C1D-ND-C4D	-9.53	99.57	106.33
14	cA	827	CLA	C1D-ND-C4D	-9.53	99.57	106.33
14	cB	806	CLA	C1D-ND-C4D	-9.53	99.57	106.33
14	A	802	CLA	C1D-ND-C4D	-9.53	99.57	106.33
14	B	805	CLA	C1D-ND-C4D	-9.52	99.57	106.33
14	bA	821	CLA	C1D-ND-C4D	-9.52	99.57	106.33
14	cA	802	CLA	C1D-ND-C4D	-9.52	99.57	106.33
14	cA	821	CLA	C1D-ND-C4D	-9.52	99.57	106.33
14	cB	836	CLA	C1D-ND-C4D	-9.52	99.57	106.33
14	J	102	CLA	C1D-ND-C4D	-9.51	99.58	106.33
14	bB	830	CLA	C1D-ND-C4D	-9.51	99.58	106.33
14	bB	837	CLA	C1D-ND-C4D	-9.51	99.58	106.33
14	bJ	102	CLA	C1D-ND-C4D	-9.51	99.58	106.33
14	B	835	CLA	C1D-ND-C4D	-9.51	99.58	106.33
14	cJ	101	CLA	C1D-ND-C4D	-9.51	99.58	106.33
14	J	101	CLA	C1D-ND-C4D	-9.51	99.58	106.33
14	bA	809	CLA	C1D-ND-C4D	-9.51	99.58	106.33
14	A	819	CLA	C1D-ND-C4D	-9.50	99.58	106.33
14	cB	850	CLA	C1D-ND-C4D	-9.50	99.58	106.33
14	cB	812	CLA	C1D-ND-C4D	-9.50	99.58	106.33
14	bA	826	CLA	C1D-ND-C4D	-9.50	99.58	106.33
14	cB	805	CLA	C1D-ND-C4D	-9.50	99.59	106.33
14	B	830	CLA	C1D-ND-C4D	-9.50	99.59	106.33
14	bA	802	CLA	C1D-ND-C4D	-9.50	99.59	106.33
14	bB	818	CLA	C1D-ND-C4D	-9.50	99.59	106.33
14	bJ	101	CLA	C1D-ND-C4D	-9.50	99.59	106.33
14	B	804	CLA	C1D-ND-C4D	-9.50	99.59	106.33
14	bB	804	CLA	C1D-ND-C4D	-9.49	99.59	106.33
14	cB	831	CLA	C1D-ND-C4D	-9.49	99.59	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	817	CLA	C1D-ND-C4D	-9.49	99.59	106.33
14	bB	816	CLA	C1D-ND-C4D	-9.49	99.60	106.33
14	B	816	CLA	C1D-ND-C4D	-9.48	99.60	106.33
14	B	849	CLA	C1D-ND-C4D	-9.48	99.60	106.33
14	bB	839	CLA	C1D-ND-C4D	-9.48	99.60	106.33
14	A	827	CLA	C1D-ND-C4D	-9.48	99.60	106.33
14	cB	818	CLA	C1D-ND-C4D	-9.48	99.60	106.33
14	bB	849	CLA	C1D-ND-C4D	-9.48	99.60	106.33
14	bB	832	CLA	C1D-ND-C4D	-9.48	99.60	106.33
14	cB	817	CLA	C1D-ND-C4D	-9.47	99.61	106.33
14	cB	819	CLA	C1D-ND-C4D	-9.47	99.61	106.33
14	cA	809	CLA	C1D-ND-C4D	-9.47	99.61	106.33
14	A	826	CLA	C1D-ND-C4D	-9.46	99.61	106.33
14	cA	826	CLA	C1D-ND-C4D	-9.46	99.61	106.33
14	B	832	CLA	C1D-ND-C4D	-9.46	99.61	106.33
14	B	827	CLA	C1D-ND-C4D	-9.46	99.61	106.33
14	B	839	CLA	C1D-ND-C4D	-9.46	99.62	106.33
14	A	806	CLA	C1D-ND-C4D	-9.45	99.62	106.33
14	bA	806	CLA	C1D-ND-C4D	-9.45	99.62	106.33
14	bA	815	CLA	C1D-ND-C4D	-9.45	99.62	106.33
14	cB	840	CLA	C1D-ND-C4D	-9.45	99.62	106.33
14	A	809	CLA	C1D-ND-C4D	-9.45	99.62	106.33
14	cB	809	CLA	C1D-ND-C4D	-9.44	99.63	106.33
14	B	808	CLA	C1D-ND-C4D	-9.44	99.63	106.33
14	cA	815	CLA	C1D-ND-C4D	-9.43	99.63	106.33
14	bB	817	CLA	C1D-ND-C4D	-9.43	99.64	106.33
14	bB	808	CLA	C1D-ND-C4D	-9.43	99.64	106.33
14	cB	830	CLA	C1D-ND-C4D	-9.43	99.64	106.33
14	B	818	CLA	C1D-ND-C4D	-9.43	99.64	106.33
14	bA	814	CLA	C1D-ND-C4D	-9.42	99.64	106.33
14	cB	828	CLA	C1D-ND-C4D	-9.42	99.64	106.33
14	B	829	CLA	C1D-ND-C4D	-9.42	99.64	106.33
14	cB	814	CLA	C1D-ND-C4D	-9.42	99.64	106.33
14	bB	810	CLA	C1D-ND-C4D	-9.42	99.64	106.33
14	bB	825	CLA	C1D-ND-C4D	-9.42	99.64	106.33
14	A	815	CLA	C1D-ND-C4D	-9.42	99.65	106.33
14	cB	833	CLA	C1D-ND-C4D	-9.41	99.65	106.33
14	cA	806	CLA	C1D-ND-C4D	-9.41	99.65	106.33
14	A	814	CLA	C1D-ND-C4D	-9.40	99.66	106.33
14	bB	827	CLA	C1D-ND-C4D	-9.40	99.66	106.33
14	B	813	CLA	C1D-ND-C4D	-9.39	99.66	106.33
14	bB	813	CLA	C1D-ND-C4D	-9.39	99.67	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bB	829	CLA	C1D-ND-C4D	-9.38	99.67	106.33
14	cA	813	CLA	C1D-ND-C4D	-9.38	99.67	106.33
14	B	825	CLA	C1D-ND-C4D	-9.38	99.67	106.33
14	cB	826	CLA	C1D-ND-C4D	-9.38	99.67	106.33
14	cB	827	CLA	C1D-ND-C4D	-9.38	99.67	106.33
14	A	813	CLA	C1D-ND-C4D	-9.37	99.68	106.33
14	cA	834	CLA	C1D-ND-C4D	-9.37	99.68	106.33
14	cA	814	CLA	C1D-ND-C4D	-9.37	99.68	106.33
14	cB	811	CLA	C1D-ND-C4D	-9.37	99.68	106.33
14	B	810	CLA	C1D-ND-C4D	-9.37	99.68	106.33
14	bA	813	CLA	C1D-ND-C4D	-9.37	99.68	106.33
14	bA	835	CLA	C1D-ND-C4D	-9.36	99.68	106.33
14	bA	829	CLA	C1D-ND-C4D	-9.34	99.70	106.33
14	cA	829	CLA	C1D-ND-C4D	-9.34	99.70	106.33
14	B	826	CLA	C1D-ND-C4D	-9.33	99.70	106.33
14	A	835	CLA	C1D-ND-C4D	-9.33	99.71	106.33
14	A	829	CLA	C1D-ND-C4D	-9.33	99.71	106.33
14	cA	817	CLA	C1D-ND-C4D	-9.33	99.71	106.33
14	A	822	CLA	C1D-ND-C4D	-9.32	99.71	106.33
14	bA	834	CLA	C1D-ND-C4D	-9.32	99.71	106.33
14	A	834	CLA	C1D-ND-C4D	-9.32	99.72	106.33
14	bA	817	CLA	C1D-ND-C4D	-9.31	99.72	106.33
14	A	817	CLA	C1D-ND-C4D	-9.30	99.73	106.33
14	bL	201	CLA	C2D-C1D-ND	9.30	116.95	110.10
14	cA	822	CLA	C1D-ND-C4D	-9.29	99.73	106.33
14	bA	803	CLA	C1D-ND-C4D	-9.28	99.74	106.33
14	bB	826	CLA	C1D-ND-C4D	-9.27	99.75	106.33
14	A	803	CLA	C1D-ND-C4D	-9.27	99.75	106.33
14	cA	803	CLA	C1D-ND-C4D	-9.27	99.75	106.33
14	cL	204	CLA	C2D-C1D-ND	9.27	116.93	110.10
14	cA	835	CLA	C1D-ND-C4D	-9.27	99.75	106.33
14	bA	822	CLA	C1D-ND-C4D	-9.26	99.76	106.33
14	L	203	CLA	C2D-C1D-ND	9.25	116.92	110.10
14	L	201	CLA	C2D-C1D-ND	9.25	116.92	110.10
14	bL	203	CLA	C2D-C1D-ND	9.25	116.92	110.10
14	cL	202	CLA	C2D-C1D-ND	9.24	116.91	110.10
14	B	807	CLA	C1D-ND-C4D	-9.24	99.77	106.33
14	bB	833	CLA	C1D-ND-C4D	-9.23	99.78	106.33
13	cA	801	CL0	C1D-ND-C4D	-9.22	99.78	106.33
14	cB	834	CLA	C1D-ND-C4D	-9.22	99.79	106.33
14	bB	807	CLA	C1D-ND-C4D	-9.21	99.79	106.33
14	bB	838	CLA	C1D-ND-C4D	-9.21	99.79	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	833	CLA	C1D-ND-C4D	-9.21	99.79	106.33
14	bB	824	CLA	C1D-ND-C4D	-9.19	99.81	106.33
13	A	801	CL0	C1D-ND-C4D	-9.18	99.81	106.33
14	cB	839	CLA	C1D-ND-C4D	-9.18	99.81	106.33
14	cB	808	CLA	C1D-ND-C4D	-9.18	99.82	106.33
13	bA	801	CL0	C1D-ND-C4D	-9.18	99.82	106.33
14	B	824	CLA	C1D-ND-C4D	-9.18	99.82	106.33
14	bB	834	CLA	C1D-ND-C4D	-9.17	99.82	106.33
14	B	834	CLA	C1D-ND-C4D	-9.16	99.82	106.33
14	B	838	CLA	C1D-ND-C4D	-9.16	99.83	106.33
14	cB	825	CLA	C1D-ND-C4D	-9.15	99.83	106.33
14	cB	835	CLA	C1D-ND-C4D	-9.12	99.86	106.33
14	A	830	CLA	C1D-ND-C4D	-9.12	99.86	106.33
14	bA	830	CLA	C1D-ND-C4D	-9.11	99.86	106.33
14	cA	824	CLA	C1D-ND-C4D	-9.11	99.86	106.33
14	A	836	CLA	C1D-ND-C4D	-9.11	99.86	106.33
14	A	824	CLA	C1D-ND-C4D	-9.10	99.87	106.33
14	bA	836	CLA	C1D-ND-C4D	-9.10	99.87	106.33
14	cA	830	CLA	C1D-ND-C4D	-9.10	99.87	106.33
14	bA	824	CLA	C1D-ND-C4D	-9.08	99.88	106.33
14	cA	836	CLA	C1D-ND-C4D	-9.08	99.89	106.33
14	bL	204	CLA	C1D-ND-C4D	-9.06	99.90	106.33
14	L	204	CLA	C1D-ND-C4D	-9.06	99.90	106.33
14	bA	841	CLA	C1D-ND-C4D	-9.06	99.90	106.33
14	cL	205	CLA	C1D-ND-C4D	-9.05	99.91	106.33
14	A	841	CLA	C1D-ND-C4D	-9.04	99.91	106.33
14	cA	841	CLA	C1D-ND-C4D	-9.03	99.92	106.33
14	bA	828	CLA	C1D-ND-C4D	-9.02	99.93	106.33
14	A	828	CLA	C1D-ND-C4D	-9.01	99.94	106.33
14	cA	828	CLA	C1D-ND-C4D	-9.01	99.94	106.33
14	bB	809	CLA	C1D-ND-C4D	-8.99	99.95	106.33
14	B	809	CLA	C1D-ND-C4D	-8.95	99.98	106.33
14	cB	810	CLA	C1D-ND-C4D	-8.94	99.99	106.33
14	bA	832	CLA	C1D-ND-C4D	-8.85	100.05	106.33
14	cA	832	CLA	C1D-ND-C4D	-8.84	100.05	106.33
14	cB	824	CLA	C1D-ND-C4D	-8.83	100.06	106.33
14	B	823	CLA	C1D-ND-C4D	-8.82	100.07	106.33
14	A	832	CLA	C1D-ND-C4D	-8.82	100.07	106.33
14	bB	823	CLA	C1D-ND-C4D	-8.81	100.08	106.33
14	B	803	CLA	C1D-ND-C4D	-8.81	100.08	106.33
14	cB	804	CLA	C1D-ND-C4D	-8.78	100.09	106.33
14	bB	803	CLA	C1D-ND-C4D	-8.76	100.11	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	801	CLA	C2D-C1D-ND	8.76	116.56	110.10
14	bB	801	CLA	C2D-C1D-ND	8.75	116.55	110.10
14	cB	802	CLA	C2D-C1D-ND	8.73	116.54	110.10
14	B	802	CLA	C1D-ND-C4D	-8.70	100.15	106.33
14	A	825	CLA	C2D-C1D-ND	8.69	116.51	110.10
14	bB	802	CLA	C1D-ND-C4D	-8.67	100.17	106.33
14	cB	803	CLA	C1D-ND-C4D	-8.67	100.17	106.33
14	bA	825	CLA	C2D-C1D-ND	8.67	116.49	110.10
14	cA	825	CLA	C2D-C1D-ND	8.64	116.47	110.10
14	B	831	CLA	C2D-C1D-ND	8.56	116.42	110.10
14	B	828	CLA	C2D-C1D-ND	8.55	116.40	110.10
14	bB	839	CLA	C2D-C1D-ND	8.55	116.40	110.10
14	cB	832	CLA	C2D-C1D-ND	8.54	116.40	110.10
14	bB	831	CLA	C2D-C1D-ND	8.54	116.39	110.10
14	bB	828	CLA	C2D-C1D-ND	8.53	116.39	110.10
14	bB	812	CLA	C2D-C1D-ND	8.53	116.39	110.10
14	cB	829	CLA	C2D-C1D-ND	8.51	116.38	110.10
14	B	839	CLA	C2D-C1D-ND	8.50	116.37	110.10
14	bA	838	CLA	C2D-C1D-ND	8.50	116.37	110.10
14	cB	813	CLA	C2D-C1D-ND	8.50	116.37	110.10
14	cB	840	CLA	C2D-C1D-ND	8.50	116.37	110.10
14	bB	803	CLA	C2D-C1D-ND	8.50	116.37	110.10
14	B	812	CLA	C2D-C1D-ND	8.50	116.37	110.10
14	B	803	CLA	C2D-C1D-ND	8.49	116.36	110.10
14	bA	841	CLA	C2D-C1D-ND	8.49	116.36	110.10
14	A	838	CLA	C2D-C1D-ND	8.48	116.35	110.10
14	A	841	CLA	C2D-C1D-ND	8.47	116.35	110.10
14	cA	838	CLA	C2D-C1D-ND	8.47	116.34	110.10
14	cA	841	CLA	C2D-C1D-ND	8.45	116.33	110.10
14	cB	804	CLA	C2D-C1D-ND	8.43	116.32	110.10
14	A	852	CLA	C2D-C1D-ND	8.37	116.28	110.10
14	bA	802	CLA	C2D-C1D-ND	8.36	116.27	110.10
14	cA	852	CLA	C2D-C1D-ND	8.36	116.26	110.10
14	cA	802	CLA	C2D-C1D-ND	8.36	116.26	110.10
14	bB	809	CLA	C2D-C1D-ND	8.35	116.26	110.10
14	cA	804	CLA	C2B-C1B-NB	8.35	115.83	110.23
14	A	802	CLA	C2D-C1D-ND	8.35	116.26	110.10
14	bA	804	CLA	C2B-C1B-NB	8.34	115.82	110.23
14	cA	823	CLA	C2D-C1D-ND	8.34	116.25	110.10
14	cA	828	CLA	C2D-C1D-ND	8.33	116.24	110.10
14	cB	810	CLA	C2D-C1D-ND	8.32	116.24	110.10
14	B	809	CLA	C2D-C1D-ND	8.32	116.23	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bA	852	CLA	C2D-C1D-ND	8.32	116.23	110.10
14	A	804	CLA	C2B-C1B-NB	8.31	115.81	110.23
14	A	823	CLA	C2D-C1D-ND	8.31	116.23	110.10
14	bA	828	CLA	C2D-C1D-ND	8.31	116.23	110.10
14	bB	832	CLA	C2D-C1D-ND	8.31	116.22	110.10
14	bA	823	CLA	C2D-C1D-ND	8.30	116.22	110.10
14	bB	838	CLA	C2D-C1D-ND	8.30	116.22	110.10
14	A	828	CLA	C2D-C1D-ND	8.30	116.22	110.10
14	bB	824	CLA	C2B-C1B-NB	8.30	115.79	110.23
14	bA	826	CLA	C2D-C1D-ND	8.29	116.21	110.10
14	cB	825	CLA	C2B-C1B-NB	8.28	115.78	110.23
14	bB	817	CLA	C2B-C1B-NB	8.28	115.78	110.23
14	B	824	CLA	C2B-C1B-NB	8.27	115.78	110.23
14	cB	833	CLA	C2D-C1D-ND	8.27	116.20	110.10
14	cB	839	CLA	C2D-C1D-ND	8.27	116.20	110.10
14	F	201	CLA	C2D-C1D-ND	8.26	116.19	110.10
14	A	826	CLA	C2D-C1D-ND	8.26	116.19	110.10
14	B	832	CLA	C2D-C1D-ND	8.26	116.19	110.10
14	B	838	CLA	C2D-C1D-ND	8.26	116.19	110.10
14	cA	826	CLA	C2D-C1D-ND	8.25	116.19	110.10
14	bF	201	CLA	C2D-C1D-ND	8.25	116.19	110.10
14	B	817	CLA	C2B-C1B-NB	8.25	115.76	110.23
14	cB	818	CLA	C2B-C1B-NB	8.25	115.76	110.23
14	bA	831	CLA	C2D-C1D-ND	8.25	116.18	110.10
14	cA	818	CLA	C2B-C1B-NB	8.24	115.76	110.23
14	bA	833	CLA	C1D-ND-C4D	-8.24	100.48	106.33
14	A	831	CLA	C2D-C1D-ND	8.23	116.17	110.10
14	B	804	CLA	C2D-C1D-ND	8.23	116.17	110.10
14	bA	837	CLA	C2D-C1D-ND	8.23	116.17	110.10
14	bB	815	CLA	C2D-C1D-ND	8.22	116.17	110.10
14	cA	837	CLA	C2D-C1D-ND	8.22	116.17	110.10
14	A	852	CLA	C1D-ND-C4D	-8.22	100.49	106.33
14	cB	805	CLA	C2D-C1D-ND	8.22	116.16	110.10
14	A	833	CLA	C1D-ND-C4D	-8.22	100.50	106.33
14	cA	831	CLA	C2D-C1D-ND	8.22	116.16	110.10
14	bA	806	CLA	C2D-C1D-ND	8.22	116.16	110.10
14	bB	804	CLA	C2D-C1D-ND	8.22	116.16	110.10
14	A	818	CLA	C2B-C1B-NB	8.22	115.74	110.23
14	A	806	CLA	C2D-C1D-ND	8.21	116.16	110.10
14	cB	816	CLA	C2D-C1D-ND	8.21	116.16	110.10
14	bA	852	CLA	C1D-ND-C4D	-8.21	100.50	106.33
14	B	815	CLA	C2D-C1D-ND	8.21	116.15	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cF	201	CLA	C2D-C1D-ND	8.21	116.15	110.10
14	cA	806	CLA	C2D-C1D-ND	8.20	116.15	110.10
14	bB	822	CLA	C2D-C1D-ND	8.20	116.15	110.10
14	cA	852	CLA	C1D-ND-C4D	-8.20	100.51	106.33
14	bB	812	CLA	C2B-C1B-NB	8.20	115.73	110.23
14	A	837	CLA	C2D-C1D-ND	8.20	116.14	110.10
14	bA	818	CLA	C2B-C1B-NB	8.19	115.72	110.23
14	cA	833	CLA	C1D-ND-C4D	-8.19	100.52	106.33
14	cB	813	CLA	C2B-C1B-NB	8.18	115.72	110.23
14	cL	203	CLA	CMD-C2D-C1D	8.16	139.10	124.71
14	cA	834	CLA	C2B-C1B-NB	8.16	115.70	110.23
14	cA	813	CLA	C2D-C1D-ND	8.16	116.11	110.10
14	B	822	CLA	C2D-C1D-ND	8.15	116.11	110.10
14	bL	202	CLA	CMD-C2D-C1D	8.15	139.08	124.71
14	L	202	CLA	CMD-C2D-C1D	8.15	139.07	124.71
14	bB	816	CLA	C2B-C1B-NB	8.15	115.69	110.23
14	A	813	CLA	C2D-C1D-ND	8.15	116.11	110.10
14	B	836	CLA	C2D-C1D-ND	8.15	116.11	110.10
14	cB	823	CLA	C2D-C1D-ND	8.15	116.11	110.10
14	bA	813	CLA	C2D-C1D-ND	8.14	116.11	110.10
14	cB	821	CLA	C2D-C1D-ND	8.14	116.11	110.10
14	A	839	CLA	C2D-C1D-ND	8.14	116.11	110.10
14	B	812	CLA	C2B-C1B-NB	8.14	115.69	110.23
14	B	820	CLA	C2D-C1D-ND	8.14	116.10	110.10
13	cA	801	CL0	C2D-C1D-ND	8.14	116.10	110.10
14	B	823	CLA	C2D-C1D-ND	8.13	116.10	110.10
14	bA	834	CLA	C2B-C1B-NB	8.13	115.69	110.23
14	B	816	CLA	C2B-C1B-NB	8.13	115.68	110.23
14	bA	829	CLA	C2D-C1D-ND	8.13	116.09	110.10
14	cB	817	CLA	C2B-C1B-NB	8.13	115.68	110.23
14	bB	836	CLA	C2D-C1D-ND	8.12	116.09	110.10
14	bB	823	CLA	C2D-C1D-ND	8.12	116.09	110.10
14	A	829	CLA	C2D-C1D-ND	8.12	116.09	110.10
14	bB	820	CLA	C2D-C1D-ND	8.12	116.09	110.10
14	cA	829	CLA	C2D-C1D-ND	8.12	116.08	110.10
14	cB	837	CLA	C2D-C1D-ND	8.11	116.08	110.10
14	cB	824	CLA	C2D-C1D-ND	8.11	116.08	110.10
13	bA	801	CL0	C2D-C1D-ND	8.11	116.08	110.10
13	A	801	CL0	C2D-C1D-ND	8.10	116.08	110.10
14	bA	812	CLA	C2B-C1B-NB	8.10	115.66	110.23
14	cA	812	CLA	C2B-C1B-NB	8.10	115.66	110.23
14	cB	836	CLA	C2D-C1D-ND	8.10	116.07	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bA	839	CLA	C2D-C1D-ND	8.09	116.07	110.10
14	cA	839	CLA	C2D-C1D-ND	8.09	116.06	110.10
14	bB	835	CLA	C2D-C1D-ND	8.09	116.06	110.10
14	A	834	CLA	C2B-C1B-NB	8.08	115.65	110.23
14	A	812	CLA	C2B-C1B-NB	8.08	115.65	110.23
14	B	835	CLA	C2D-C1D-ND	8.07	116.05	110.10
14	bB	806	CLA	C2D-C1D-ND	8.07	116.05	110.10
14	B	806	CLA	C2D-C1D-ND	8.05	116.04	110.10
14	cB	807	CLA	C2D-C1D-ND	8.05	116.03	110.10
14	A	832	CLA	C2D-C1D-ND	8.04	116.03	110.10
14	cB	827	CLA	C2D-C1D-ND	8.03	116.03	110.10
14	bA	832	CLA	C2D-C1D-ND	8.03	116.02	110.10
14	cA	832	CLA	C2D-C1D-ND	8.02	116.02	110.10
14	bB	851	CLA	C2D-C1D-ND	8.01	116.01	110.10
14	B	802	CLA	C2D-C1D-ND	8.01	116.01	110.10
14	cB	801	CLA	C2D-C1D-ND	8.00	116.00	110.10
14	B	826	CLA	C2D-C1D-ND	7.99	115.99	110.10
14	B	817	CLA	C2D-C1D-ND	7.99	115.99	110.10
14	bB	802	CLA	C2D-C1D-ND	7.99	115.99	110.10
14	bB	817	CLA	C2D-C1D-ND	7.99	115.99	110.10
14	cB	803	CLA	C2D-C1D-ND	7.99	115.99	110.10
14	B	851	CLA	C2D-C1D-ND	7.98	115.99	110.10
14	bA	827	CLA	C2D-C1D-ND	7.97	115.98	110.10
14	cA	816	CLA	C2D-C1D-ND	7.97	115.98	110.10
14	B	821	CLA	C2D-C1D-ND	7.97	115.98	110.10
14	bA	816	CLA	C2D-C1D-ND	7.97	115.98	110.10
14	A	808	CLA	C2D-C1D-ND	7.97	115.97	110.10
14	cB	818	CLA	C2D-C1D-ND	7.97	115.97	110.10
14	A	816	CLA	C2D-C1D-ND	7.96	115.97	110.10
14	bB	821	CLA	C2D-C1D-ND	7.95	115.97	110.10
14	bB	826	CLA	C2D-C1D-ND	7.95	115.96	110.10
14	cB	822	CLA	C2D-C1D-ND	7.95	115.96	110.10
14	cX	201	CLA	C2D-C1D-ND	7.95	115.96	110.10
14	bB	824	CLA	C2D-C1D-ND	7.95	115.96	110.10
14	B	807	CLA	C2D-C1D-ND	7.94	115.96	110.10
14	X	201	CLA	C2D-C1D-ND	7.94	115.96	110.10
14	B	824	CLA	C2D-C1D-ND	7.94	115.96	110.10
14	cA	827	CLA	C2D-C1D-ND	7.94	115.96	110.10
14	bX	201	CLA	C2D-C1D-ND	7.94	115.95	110.10
14	B	825	CLA	C2D-C1D-ND	7.94	115.95	110.10
14	bB	825	CLA	C2D-C1D-ND	7.94	115.95	110.10
14	bB	807	CLA	C2D-C1D-ND	7.93	115.95	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cB	826	CLA	C2D-C1D-ND	7.93	115.95	110.10
14	cB	825	CLA	C2D-C1D-ND	7.93	115.95	110.10
14	J	102	CLA	C2D-C1D-ND	7.92	115.94	110.10
14	cJ	102	CLA	C2D-C1D-ND	7.92	115.94	110.10
14	bA	805	CLA	C2D-C1D-ND	7.92	115.94	110.10
14	cA	808	CLA	C2D-C1D-ND	7.92	115.94	110.10
14	A	805	CLA	C2D-C1D-ND	7.92	115.94	110.10
14	bA	808	CLA	C2D-C1D-ND	7.92	115.94	110.10
14	A	827	CLA	C2D-C1D-ND	7.91	115.94	110.10
14	bA	804	CLA	C2D-C1D-ND	7.91	115.93	110.10
14	cA	805	CLA	C2D-C1D-ND	7.91	115.93	110.10
14	A	821	CLA	C2D-C1D-ND	7.90	115.92	110.10
14	cA	821	CLA	C2D-C1D-ND	7.90	115.92	110.10
14	bJ	102	CLA	C2D-C1D-ND	7.90	115.92	110.10
14	bA	821	CLA	C2D-C1D-ND	7.89	115.92	110.10
14	cA	811	CLA	C2D-C1D-ND	7.89	115.92	110.10
14	bA	811	CLA	C2D-C1D-ND	7.88	115.91	110.10
14	A	811	CLA	C2D-C1D-ND	7.88	115.91	110.10
14	cB	808	CLA	C2D-C1D-ND	7.88	115.91	110.10
14	bJ	101	CLA	C2D-C1D-ND	7.88	115.91	110.10
14	J	101	CLA	C2D-C1D-ND	7.87	115.91	110.10
14	A	804	CLA	C2D-C1D-ND	7.87	115.90	110.10
14	B	837	CLA	C2D-C1D-ND	7.86	115.90	110.10
14	A	807	CLA	C2D-C1D-ND	7.85	115.89	110.10
14	cA	804	CLA	C2D-C1D-ND	7.85	115.89	110.10
14	cJ	101	CLA	C2D-C1D-ND	7.85	115.89	110.10
14	bB	822	CLA	C2B-C1B-NB	7.85	115.49	110.23
14	cB	824	CLA	C2B-C1B-NB	7.84	115.49	110.23
14	bA	807	CLA	C2D-C1D-ND	7.84	115.88	110.10
14	B	808	CLA	C2D-C1D-ND	7.84	115.88	110.10
14	cB	838	CLA	C2D-C1D-ND	7.84	115.88	110.10
14	A	812	CLA	C2D-C1D-ND	7.83	115.88	110.10
14	cA	812	CLA	C2D-C1D-ND	7.83	115.88	110.10
14	A	842	CLA	C2D-C1D-ND	7.83	115.88	110.10
14	B	833	CLA	C2B-C1B-NB	7.83	115.48	110.23
14	bA	812	CLA	C2D-C1D-ND	7.83	115.87	110.10
14	cB	834	CLA	C2B-C1B-NB	7.82	115.48	110.23
14	cB	823	CLA	C2B-C1B-NB	7.81	115.47	110.23
14	bB	837	CLA	C2D-C1D-ND	7.81	115.86	110.10
14	bB	833	CLA	C2B-C1B-NB	7.81	115.47	110.23
14	B	823	CLA	C2B-C1B-NB	7.80	115.46	110.23
14	B	822	CLA	C2B-C1B-NB	7.80	115.46	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bA	842	CLA	C2D-C1D-ND	7.80	115.85	110.10
14	bB	823	CLA	C2B-C1B-NB	7.80	115.46	110.23
14	A	810	CLA	C2D-C1D-ND	7.79	115.85	110.10
14	bA	818	CLA	C2D-C1D-ND	7.79	115.84	110.10
14	A	814	CLA	C2D-C1D-ND	7.79	115.84	110.10
14	bB	808	CLA	C2D-C1D-ND	7.79	115.84	110.10
14	cA	810	CLA	C2D-C1D-ND	7.79	115.84	110.10
14	bA	810	CLA	C2D-C1D-ND	7.79	115.84	110.10
14	bL	204	CLA	C2D-C1D-ND	7.78	115.84	110.10
14	cA	842	CLA	C2D-C1D-ND	7.78	115.84	110.10
14	cB	809	CLA	C2D-C1D-ND	7.78	115.84	110.10
14	cL	205	CLA	C2D-C1D-ND	7.78	115.84	110.10
14	cA	818	CLA	C2D-C1D-ND	7.78	115.84	110.10
14	A	818	CLA	C2D-C1D-ND	7.78	115.84	110.10
14	L	204	CLA	C2D-C1D-ND	7.78	115.84	110.10
14	bA	814	CLA	C2D-C1D-ND	7.78	115.83	110.10
14	cB	850	CLA	C2D-C1D-ND	7.78	115.83	110.10
14	bA	811	CLA	C2B-C1B-NB	7.77	115.44	110.23
14	cA	807	CLA	C2D-C1D-ND	7.77	115.83	110.10
14	bB	849	CLA	C2D-C1D-ND	7.77	115.83	110.10
14	cA	828	CLA	C2B-C1B-NB	7.76	115.44	110.23
14	B	851	CLA	C2B-C1B-NB	7.76	115.43	110.23
14	A	811	CLA	C2B-C1B-NB	7.76	115.43	110.23
14	bB	818	CLA	C2D-C1D-ND	7.76	115.82	110.10
14	A	828	CLA	C2B-C1B-NB	7.75	115.43	110.23
14	bB	851	CLA	C2B-C1B-NB	7.75	115.43	110.23
14	bA	828	CLA	C2B-C1B-NB	7.75	115.42	110.23
14	cA	811	CLA	C2B-C1B-NB	7.74	115.42	110.23
14	cA	814	CLA	C2D-C1D-ND	7.74	115.81	110.10
14	bA	805	CLA	C2B-C1B-NB	7.73	115.42	110.23
14	bA	809	CLA	C2D-C1D-ND	7.73	115.80	110.10
14	cB	801	CLA	C2B-C1B-NB	7.73	115.41	110.23
14	B	849	CLA	C2D-C1D-ND	7.73	115.80	110.10
14	cB	819	CLA	C2D-C1D-ND	7.73	115.80	110.10
14	cB	834	CLA	C2D-C1D-ND	7.73	115.80	110.10
14	B	818	CLA	C2D-C1D-ND	7.72	115.80	110.10
14	cA	809	CLA	C2D-C1D-ND	7.72	115.79	110.10
14	bB	833	CLA	C2D-C1D-ND	7.71	115.79	110.10
14	A	805	CLA	C2B-C1B-NB	7.71	115.40	110.23
14	bA	817	CLA	C2D-C1D-ND	7.71	115.79	110.10
14	B	833	CLA	C2D-C1D-ND	7.71	115.79	110.10
14	cA	817	CLA	C2D-C1D-ND	7.71	115.78	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	817	CLA	C2D-C1D-ND	7.70	115.78	110.10
14	bB	830	CLA	C2D-C1D-ND	7.70	115.78	110.10
14	B	830	CLA	C2D-C1D-ND	7.70	115.78	110.10
14	A	827	CLA	C2B-C1B-NB	7.69	115.39	110.23
14	bA	827	CLA	C2B-C1B-NB	7.69	115.39	110.23
14	cA	805	CLA	C2B-C1B-NB	7.69	115.39	110.23
14	cA	827	CLA	C2B-C1B-NB	7.69	115.39	110.23
14	cB	815	CLA	C2D-C1D-ND	7.68	115.77	110.10
14	A	809	CLA	C2D-C1D-ND	7.68	115.77	110.10
14	cB	831	CLA	C2D-C1D-ND	7.68	115.76	110.10
14	bA	835	CLA	C2D-C1D-ND	7.68	115.76	110.10
14	bA	822	CLA	C2B-C1B-NB	7.68	115.38	110.23
14	bB	805	CLA	C2B-C1B-NB	7.67	115.38	110.23
14	B	811	CLA	C2D-C1D-ND	7.67	115.76	110.10
14	bB	816	CLA	C2D-C1D-ND	7.67	115.76	110.10
14	bB	814	CLA	C2D-C1D-ND	7.67	115.76	110.10
14	cA	815	CLA	C2D-C1D-ND	7.67	115.76	110.10
14	A	836	CLA	C2D-C1D-ND	7.67	115.75	110.10
14	A	824	CLA	C2D-C1D-ND	7.66	115.75	110.10
14	B	814	CLA	C2D-C1D-ND	7.66	115.75	110.10
14	cB	817	CLA	C2D-C1D-ND	7.66	115.75	110.10
14	B	816	CLA	C2D-C1D-ND	7.66	115.75	110.10
14	cA	824	CLA	C2D-C1D-ND	7.66	115.75	110.10
14	cB	812	CLA	C2D-C1D-ND	7.66	115.75	110.10
14	B	805	CLA	C2B-C1B-NB	7.66	115.37	110.23
14	A	822	CLA	C2B-C1B-NB	7.65	115.36	110.23
14	bB	811	CLA	C2D-C1D-ND	7.65	115.74	110.10
14	bA	824	CLA	C2D-C1D-ND	7.65	115.74	110.10
14	cB	806	CLA	C2B-C1B-NB	7.65	115.36	110.23
14	cA	819	CLA	C2D-C1D-ND	7.65	115.74	110.10
14	bA	836	CLA	C2D-C1D-ND	7.64	115.73	110.10
14	bA	816	CLA	C2B-C1B-NB	7.64	115.35	110.23
14	A	821	CLA	C2B-C1B-NB	7.63	115.35	110.23
14	bB	827	CLA	C2B-C1B-NB	7.63	115.34	110.23
14	cA	836	CLA	C2D-C1D-ND	7.63	115.72	110.10
14	cA	822	CLA	C2B-C1B-NB	7.62	115.34	110.23
14	bA	815	CLA	C2D-C1D-ND	7.62	115.72	110.10
14	cB	828	CLA	C2B-C1B-NB	7.62	115.34	110.23
14	A	819	CLA	C2D-C1D-ND	7.62	115.72	110.10
14	B	804	CLA	C2B-C1B-NB	7.62	115.34	110.23
14	B	827	CLA	C2B-C1B-NB	7.62	115.34	110.23
14	bA	819	CLA	C2D-C1D-ND	7.62	115.72	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	815	CLA	C2D-C1D-ND	7.62	115.72	110.10
14	bA	840	CLA	C2D-C1D-ND	7.62	115.72	110.10
14	B	836	CLA	C2B-C1B-NB	7.61	115.34	110.23
14	bA	803	CLA	C2D-C1D-ND	7.61	115.72	110.10
14	bB	830	CLA	C2B-C1B-NB	7.61	115.34	110.23
14	cA	816	CLA	C2B-C1B-NB	7.61	115.34	110.23
14	cB	831	CLA	C2B-C1B-NB	7.61	115.34	110.23
14	A	835	CLA	C2D-C1D-ND	7.61	115.71	110.10
14	A	816	CLA	C2B-C1B-NB	7.61	115.33	110.23
14	B	830	CLA	C2B-C1B-NB	7.61	115.33	110.23
14	cA	821	CLA	C2B-C1B-NB	7.60	115.33	110.23
14	cA	803	CLA	C2D-C1D-ND	7.60	115.70	110.10
14	cB	820	CLA	C2D-C1D-ND	7.60	115.70	110.10
14	cA	836	CLA	C2B-C1B-NB	7.60	115.33	110.23
14	A	803	CLA	C2D-C1D-ND	7.60	115.70	110.10
14	B	810	CLA	C2D-C1D-ND	7.60	115.70	110.10
14	bB	804	CLA	C2B-C1B-NB	7.59	115.32	110.23
14	bA	836	CLA	C2B-C1B-NB	7.59	115.32	110.23
14	bB	810	CLA	C2D-C1D-ND	7.59	115.70	110.10
14	cB	805	CLA	C2B-C1B-NB	7.59	115.32	110.23
14	A	822	CLA	C2D-C1D-ND	7.59	115.69	110.10
14	bB	819	CLA	C2D-C1D-ND	7.58	115.69	110.10
14	bA	826	CLA	C2B-C1B-NB	7.58	115.31	110.23
14	cA	815	CLA	C2B-C1B-NB	7.58	115.31	110.23
14	B	825	CLA	CMD-C2D-C1D	7.58	138.07	124.71
14	cB	830	CLA	C2D-C1D-ND	7.58	115.69	110.10
14	cB	826	CLA	CMD-C2D-C1D	7.58	138.07	124.71
14	bB	825	CLA	CMD-C2D-C1D	7.57	138.06	124.71
14	cB	811	CLA	C2D-C1D-ND	7.57	115.69	110.10
14	bB	836	CLA	C2B-C1B-NB	7.57	115.31	110.23
14	A	840	CLA	C2D-C1D-ND	7.57	115.68	110.10
14	cA	826	CLA	C2B-C1B-NB	7.57	115.30	110.23
14	cA	840	CLA	C2D-C1D-ND	7.56	115.68	110.10
14	bA	815	CLA	C2B-C1B-NB	7.56	115.30	110.23
14	B	819	CLA	C2D-C1D-ND	7.56	115.68	110.10
14	cA	822	CLA	C2D-C1D-ND	7.56	115.68	110.10
14	bA	821	CLA	C2B-C1B-NB	7.56	115.30	110.23
14	cB	812	CLA	C2B-C1B-NB	7.56	115.30	110.23
14	cA	835	CLA	C2D-C1D-ND	7.56	115.67	110.10
14	A	826	CLA	C2B-C1B-NB	7.56	115.30	110.23
14	bB	821	CLA	C2B-C1B-NB	7.56	115.30	110.23
14	bA	822	CLA	C2D-C1D-ND	7.55	115.67	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	836	CLA	C2B-C1B-NB	7.55	115.30	110.23
14	J	101	CLA	C2B-C1B-NB	7.55	115.30	110.23
14	bB	829	CLA	C2D-C1D-ND	7.55	115.67	110.10
14	A	830	CLA	C2D-C1D-ND	7.55	115.67	110.10
14	cB	802	CLA	C2B-C1B-NB	7.55	115.29	110.23
14	B	813	CLA	C2B-C1B-NB	7.55	115.29	110.23
14	bB	811	CLA	C2B-C1B-NB	7.54	115.28	110.23
14	B	811	CLA	C2B-C1B-NB	7.53	115.28	110.23
14	A	815	CLA	C2B-C1B-NB	7.53	115.28	110.23
14	cB	837	CLA	C2B-C1B-NB	7.53	115.28	110.23
14	bB	801	CLA	C2B-C1B-NB	7.53	115.28	110.23
14	bA	830	CLA	C2D-C1D-ND	7.53	115.65	110.10
14	cB	804	CLA	C2B-C1B-NB	7.53	115.28	110.23
14	bB	834	CLA	C2D-C1D-ND	7.53	115.65	110.10
14	bB	826	CLA	CMD-C2D-C1D	7.53	137.98	124.71
14	cB	833	CLA	C2B-C1B-NB	7.53	115.28	110.23
14	cB	827	CLA	CMD-C2D-C1D	7.52	137.97	124.71
14	bB	803	CLA	C2B-C1B-NB	7.52	115.28	110.23
14	B	826	CLA	CMD-C2D-C1D	7.52	137.97	124.71
14	B	803	CLA	C2B-C1B-NB	7.52	115.28	110.23
14	cJ	101	CLA	C2B-C1B-NB	7.52	115.27	110.23
14	B	829	CLA	C2D-C1D-ND	7.52	115.65	110.10
14	bJ	101	CLA	C2B-C1B-NB	7.52	115.27	110.23
14	cA	809	CLA	C2B-C1B-NB	7.52	115.27	110.23
14	bA	819	CLA	C2B-C1B-NB	7.52	115.27	110.23
14	B	821	CLA	C2B-C1B-NB	7.52	115.27	110.23
14	cB	822	CLA	C2B-C1B-NB	7.51	115.27	110.23
14	bB	805	CLA	C2D-C1D-ND	7.51	115.64	110.10
14	cB	806	CLA	C2D-C1D-ND	7.51	115.64	110.10
14	B	805	CLA	C2D-C1D-ND	7.51	115.64	110.10
14	B	827	CLA	C2D-C1D-ND	7.50	115.63	110.10
14	cA	819	CLA	C2B-C1B-NB	7.50	115.26	110.23
14	cB	814	CLA	C2B-C1B-NB	7.50	115.26	110.23
14	B	814	CLA	C2B-C1B-NB	7.50	115.26	110.23
14	B	801	CLA	C2B-C1B-NB	7.50	115.26	110.23
14	A	819	CLA	C2B-C1B-NB	7.50	115.26	110.23
14	cL	203	CLA	C2D-C1D-ND	7.50	115.63	110.10
14	cA	835	CLA	C2B-C1B-NB	7.50	115.26	110.23
14	bB	827	CLA	C2D-C1D-ND	7.50	115.63	110.10
14	cA	830	CLA	C2D-C1D-ND	7.50	115.63	110.10
14	bA	809	CLA	C2B-C1B-NB	7.50	115.26	110.23
14	bA	835	CLA	C2B-C1B-NB	7.49	115.25	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bB	832	CLA	C2B-C1B-NB	7.49	115.25	110.23
14	cB	815	CLA	C2B-C1B-NB	7.49	115.25	110.23
14	B	832	CLA	C2B-C1B-NB	7.49	115.25	110.23
14	bB	831	CLA	C2B-C1B-NB	7.49	115.25	110.23
14	bB	813	CLA	C2B-C1B-NB	7.48	115.25	110.23
14	cB	832	CLA	C2B-C1B-NB	7.47	115.24	110.23
14	B	834	CLA	C2D-C1D-ND	7.47	115.61	110.10
14	B	831	CLA	C2B-C1B-NB	7.47	115.24	110.23
14	bB	814	CLA	C2B-C1B-NB	7.46	115.24	110.23
14	bL	202	CLA	C2D-C1D-ND	7.46	115.60	110.10
14	cB	828	CLA	C2D-C1D-ND	7.46	115.60	110.10
14	cB	850	CLA	C2B-C1B-NB	7.45	115.23	110.23
14	A	809	CLA	C2B-C1B-NB	7.44	115.22	110.23
14	cB	835	CLA	C2D-C1D-ND	7.44	115.58	110.10
14	B	849	CLA	C2B-C1B-NB	7.44	115.22	110.23
14	bB	849	CLA	C2B-C1B-NB	7.44	115.22	110.23
14	L	202	CLA	C2D-C1D-ND	7.43	115.58	110.10
14	A	835	CLA	C2B-C1B-NB	7.43	115.21	110.23
14	cA	820	CLA	C2D-C1D-ND	7.42	115.57	110.10
14	A	838	CLA	C2B-C1B-NB	7.41	115.20	110.23
14	A	825	CLA	C2B-C1B-NB	7.41	115.20	110.23
14	cA	834	CLA	C2D-C1D-ND	7.41	115.56	110.10
14	A	820	CLA	C2D-C1D-ND	7.41	115.56	110.10
14	bA	820	CLA	C2D-C1D-ND	7.40	115.56	110.10
14	bA	825	CLA	C2B-C1B-NB	7.40	115.19	110.23
14	cA	825	CLA	C2B-C1B-NB	7.40	115.19	110.23
14	bA	838	CLA	C2B-C1B-NB	7.38	115.18	110.23
14	B	837	CLA	C2B-C1B-NB	7.38	115.18	110.23
14	B	818	CLA	C2B-C1B-NB	7.37	115.17	110.23
14	cB	819	CLA	C2B-C1B-NB	7.37	115.17	110.23
14	bB	818	CLA	C2B-C1B-NB	7.37	115.17	110.23
14	bA	834	CLA	C2D-C1D-ND	7.37	115.53	110.10
14	A	834	CLA	C2D-C1D-ND	7.37	115.53	110.10
14	cB	820	CLA	CMD-C2D-C1D	7.37	137.69	124.71
14	bB	819	CLA	CMD-C2D-C1D	7.36	137.69	124.71
14	cB	814	CLA	C2D-C1D-ND	7.36	115.53	110.10
14	bB	837	CLA	C2B-C1B-NB	7.36	115.16	110.23
14	cA	838	CLA	C2B-C1B-NB	7.36	115.16	110.23
14	B	825	CLA	C2B-C1B-NB	7.35	115.16	110.23
14	B	813	CLA	C2D-C1D-ND	7.35	115.52	110.10
14	cB	826	CLA	C2B-C1B-NB	7.35	115.16	110.23
14	A	823	CLA	C2B-C1B-NB	7.35	115.16	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	819	CLA	CMD-C2D-C1D	7.35	137.66	124.71
14	bB	825	CLA	C2B-C1B-NB	7.34	115.16	110.23
14	bA	823	CLA	C2B-C1B-NB	7.34	115.16	110.23
14	bB	813	CLA	C2D-C1D-ND	7.34	115.51	110.10
14	cA	813	CLA	C2B-C1B-NB	7.34	115.15	110.23
14	bA	813	CLA	C2B-C1B-NB	7.33	115.14	110.23
14	cB	820	CLA	C2B-C1B-NB	7.32	115.14	110.23
14	bA	814	CLA	C2B-C1B-NB	7.32	115.14	110.23
14	bL	204	CLA	C2B-C1B-NB	7.32	115.14	110.23
14	cJ	102	CLA	C2B-C1B-NB	7.32	115.14	110.23
14	bB	819	CLA	C2B-C1B-NB	7.32	115.14	110.23
14	A	813	CLA	C2B-C1B-NB	7.32	115.14	110.23
14	cB	838	CLA	C2B-C1B-NB	7.32	115.14	110.23
14	B	819	CLA	C2B-C1B-NB	7.31	115.14	110.23
14	bJ	102	CLA	C2B-C1B-NB	7.30	115.13	110.23
14	bB	817	CLA	CMD-C2D-C1D	7.30	137.58	124.71
14	B	835	CLA	C2B-C1B-NB	7.30	115.13	110.23
14	cA	823	CLA	C2B-C1B-NB	7.30	115.13	110.23
14	cL	205	CLA	C2B-C1B-NB	7.30	115.12	110.23
14	A	820	CLA	C2B-C1B-NB	7.29	115.12	110.23
14	J	102	CLA	C2B-C1B-NB	7.29	115.12	110.23
14	A	814	CLA	C2B-C1B-NB	7.29	115.12	110.23
14	bA	820	CLA	C2B-C1B-NB	7.29	115.12	110.23
14	cA	814	CLA	C2B-C1B-NB	7.29	115.12	110.23
14	B	817	CLA	CMD-C2D-C1D	7.29	137.56	124.71
14	cB	836	CLA	C2B-C1B-NB	7.29	115.12	110.23
14	cB	818	CLA	CMD-C2D-C1D	7.29	137.55	124.71
14	L	204	CLA	C2B-C1B-NB	7.29	115.12	110.23
14	A	806	CLA	C2B-C1B-NB	7.27	115.11	110.23
14	cA	820	CLA	C2B-C1B-NB	7.26	115.10	110.23
14	A	808	CLA	C2B-C1B-NB	7.25	115.09	110.23
14	bB	835	CLA	C2B-C1B-NB	7.25	115.09	110.23
14	B	829	CLA	C2B-C1B-NB	7.25	115.09	110.23
14	cA	808	CLA	C2B-C1B-NB	7.25	115.09	110.23
14	A	803	CLA	C2B-C1B-NB	7.22	115.07	110.23
14	B	820	CLA	C2B-C1B-NB	7.22	115.07	110.23
14	bA	803	CLA	C2B-C1B-NB	7.22	115.07	110.23
14	cA	803	CLA	C2B-C1B-NB	7.22	115.07	110.23
14	cB	821	CLA	C2B-C1B-NB	7.22	115.07	110.23
14	B	810	CLA	C2B-C1B-NB	7.21	115.07	110.23
14	bA	806	CLA	C2B-C1B-NB	7.21	115.07	110.23
14	cA	806	CLA	C2B-C1B-NB	7.21	115.07	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bB	820	CLA	C2B-C1B-NB	7.21	115.07	110.23
14	bB	829	CLA	C2B-C1B-NB	7.21	115.06	110.23
14	bB	810	CLA	C2B-C1B-NB	7.20	115.06	110.23
14	cB	830	CLA	C2B-C1B-NB	7.20	115.06	110.23
14	X	201	CLA	C2B-C1B-NB	7.20	115.06	110.23
14	cB	815	CLA	CMD-C2D-C1D	7.19	137.38	124.71
14	B	814	CLA	CMD-C2D-C1D	7.18	137.37	124.71
14	bB	814	CLA	CMD-C2D-C1D	7.18	137.37	124.71
14	L	203	CLA	C2B-C1B-NB	7.18	115.04	110.23
14	cB	811	CLA	C2B-C1B-NB	7.18	115.04	110.23
14	cX	201	CLA	C2B-C1B-NB	7.17	115.04	110.23
14	cL	204	CLA	C2B-C1B-NB	7.17	115.04	110.23
14	bA	808	CLA	C2B-C1B-NB	7.16	115.03	110.23
14	bX	201	CLA	C2B-C1B-NB	7.15	115.02	110.23
14	bB	805	CLA	CMD-C2D-C1D	7.14	137.30	124.71
14	B	805	CLA	CMD-C2D-C1D	7.14	137.29	124.71
14	cB	824	CLA	CMD-C2D-C1D	7.13	137.28	124.71
14	bB	823	CLA	CMD-C2D-C1D	7.13	137.28	124.71
14	B	823	CLA	CMD-C2D-C1D	7.13	137.28	124.71
14	cB	806	CLA	CMD-C2D-C1D	7.13	137.28	124.71
14	A	807	CLA	C2B-C1B-NB	7.13	115.01	110.23
14	B	815	CLA	C2B-C1B-NB	7.13	115.01	110.23
14	cB	816	CLA	C2B-C1B-NB	7.11	115.00	110.23
14	bB	806	CLA	CMD-C2D-C1D	7.11	137.25	124.71
14	bB	815	CLA	C2B-C1B-NB	7.11	115.00	110.23
14	cB	807	CLA	CMD-C2D-C1D	7.11	137.24	124.71
14	B	806	CLA	CMD-C2D-C1D	7.10	137.23	124.71
14	bL	203	CLA	C2B-C1B-NB	7.10	114.99	110.23
14	cA	807	CLA	C2B-C1B-NB	7.10	114.99	110.23
14	cA	805	CLA	CMD-C2D-C1D	7.09	137.21	124.71
14	bA	807	CLA	C2B-C1B-NB	7.08	114.98	110.23
14	A	805	CLA	CMD-C2D-C1D	7.08	137.19	124.71
14	cA	802	CLA	CHD-C1D-ND	-7.08	117.95	124.45
14	bA	805	CLA	CMD-C2D-C1D	7.08	137.18	124.71
14	A	839	CLA	C2B-C1B-NB	7.07	114.97	110.23
14	A	802	CLA	CHD-C1D-ND	-7.07	117.96	124.45
14	bA	802	CLA	CHD-C1D-ND	-7.06	117.96	124.45
14	B	806	CLA	C2B-C1B-NB	7.06	114.96	110.23
14	bB	808	CLA	C2B-C1B-NB	7.06	114.96	110.23
14	bB	806	CLA	C2B-C1B-NB	7.05	114.96	110.23
14	cB	807	CLA	C2B-C1B-NB	7.04	114.95	110.23
14	bA	839	CLA	C2B-C1B-NB	7.03	114.94	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bF	201	CLA	C2B-C1B-NB	7.03	114.94	110.23
14	F	201	CLA	C2B-C1B-NB	7.03	114.94	110.23
14	cF	201	CLA	C2B-C1B-NB	7.02	114.94	110.23
14	A	833	CLA	C2D-C1D-ND	7.00	115.26	110.10
14	cA	839	CLA	C2B-C1B-NB	7.00	114.93	110.23
14	cA	833	CLA	C2D-C1D-ND	6.99	115.25	110.10
14	B	808	CLA	C2B-C1B-NB	6.99	114.92	110.23
14	bA	833	CLA	C2D-C1D-ND	6.98	115.25	110.10
14	bA	827	CLA	CMD-C2D-C1D	6.97	137.00	124.71
14	bA	833	CLA	C2B-C1B-NB	6.96	114.90	110.23
14	cB	809	CLA	C2B-C1B-NB	6.96	114.90	110.23
14	A	827	CLA	CMD-C2D-C1D	6.96	136.97	124.71
14	cA	827	CLA	CMD-C2D-C1D	6.96	136.97	124.71
14	cB	803	CLA	C2B-C1B-NB	6.95	114.89	110.23
14	A	831	CLA	C2B-C1B-NB	6.94	114.89	110.23
14	cA	833	CLA	C2B-C1B-NB	6.94	114.89	110.23
14	bB	802	CLA	C2B-C1B-NB	6.94	114.89	110.23
14	B	802	CLA	C2B-C1B-NB	6.94	114.88	110.23
14	cA	831	CLA	C2B-C1B-NB	6.94	114.88	110.23
14	A	825	CLA	CMD-C2D-C1D	6.94	136.94	124.71
14	A	833	CLA	C2B-C1B-NB	6.93	114.88	110.23
14	bB	851	CLA	CMD-C2D-C1D	6.93	136.93	124.71
14	cB	801	CLA	CMD-C2D-C1D	6.93	136.92	124.71
14	B	851	CLA	CMD-C2D-C1D	6.93	136.92	124.71
14	bA	831	CLA	C2B-C1B-NB	6.92	114.87	110.23
14	bA	825	CLA	CMD-C2D-C1D	6.92	136.91	124.71
14	bA	842	CLA	CMD-C2D-C1D	6.92	136.90	124.71
14	B	821	CLA	CMD-C2D-C1D	6.92	136.90	124.71
14	cA	825	CLA	CMD-C2D-C1D	6.92	136.90	124.71
14	cA	830	CLA	C2B-C1B-NB	6.91	114.87	110.23
14	cB	822	CLA	CMD-C2D-C1D	6.91	136.90	124.71
14	A	842	CLA	CMD-C2D-C1D	6.91	136.89	124.71
14	bB	821	CLA	CMD-C2D-C1D	6.91	136.89	124.71
14	bB	829	CLA	CMD-C2D-C1D	6.91	136.89	124.71
14	L	202	CLA	C2B-C1B-NB	6.91	114.86	110.23
14	cB	830	CLA	CMD-C2D-C1D	6.91	136.88	124.71
14	bB	828	CLA	C2B-C1B-NB	6.90	114.86	110.23
14	bA	830	CLA	C2B-C1B-NB	6.90	114.86	110.23
14	bA	824	CLA	C2B-C1B-NB	6.90	114.86	110.23
14	cA	842	CLA	CMD-C2D-C1D	6.90	136.87	124.71
14	bL	202	CLA	C2B-C1B-NB	6.89	114.85	110.23
14	B	829	CLA	CMD-C2D-C1D	6.89	136.85	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bA	842	CLA	C2B-C1B-NB	6.89	114.85	110.23
14	A	824	CLA	C2B-C1B-NB	6.88	114.85	110.23
14	cB	829	CLA	C2B-C1B-NB	6.88	114.85	110.23
14	A	830	CLA	C2B-C1B-NB	6.88	114.84	110.23
14	A	842	CLA	C2B-C1B-NB	6.88	114.84	110.23
14	cA	824	CLA	C2B-C1B-NB	6.88	114.84	110.23
14	cA	842	CLA	C2B-C1B-NB	6.88	114.84	110.23
14	A	840	CLA	C2B-C1B-NB	6.87	114.84	110.23
14	bB	815	CLA	CMD-C2D-C1D	6.86	136.81	124.71
14	cB	816	CLA	CMD-C2D-C1D	6.86	136.81	124.71
14	B	815	CLA	CMD-C2D-C1D	6.86	136.81	124.71
14	cL	203	CLA	C2B-C1B-NB	6.86	114.83	110.23
14	B	828	CLA	C2B-C1B-NB	6.85	114.83	110.23
14	cA	840	CLA	C2B-C1B-NB	6.83	114.81	110.23
14	A	818	CLA	CMD-C2D-C1D	6.83	136.75	124.71
14	cA	818	CLA	CMD-C2D-C1D	6.82	136.74	124.71
14	cA	822	CLA	CHD-C1D-ND	-6.82	118.18	124.45
14	bA	818	CLA	CMD-C2D-C1D	6.82	136.74	124.71
14	bA	806	CLA	CMD-C2D-C1D	6.82	136.74	124.71
14	cA	806	CLA	CMD-C2D-C1D	6.82	136.74	124.71
14	A	822	CLA	CHD-C1D-ND	-6.82	118.19	124.45
14	A	806	CLA	CMD-C2D-C1D	6.82	136.73	124.71
14	cB	817	CLA	CMD-C2D-C1D	6.82	136.73	124.71
14	bA	822	CLA	CHD-C1D-ND	-6.82	118.19	124.45
14	B	816	CLA	CMD-C2D-C1D	6.81	136.71	124.71
14	bA	826	CLA	CMD-C2D-C1D	6.81	136.71	124.71
14	bJ	101	CLA	CMD-C2D-C1D	6.81	136.71	124.71
14	bB	816	CLA	CMD-C2D-C1D	6.81	136.71	124.71
14	cA	819	CLA	CMD-C2D-C1D	6.81	136.71	124.71
14	bA	840	CLA	C2B-C1B-NB	6.81	114.80	110.23
14	J	101	CLA	CMD-C2D-C1D	6.80	136.70	124.71
14	bA	819	CLA	CMD-C2D-C1D	6.80	136.70	124.71
14	A	819	CLA	CMD-C2D-C1D	6.80	136.70	124.71
14	cJ	101	CLA	CMD-C2D-C1D	6.80	136.70	124.71
14	A	826	CLA	CMD-C2D-C1D	6.80	136.69	124.71
14	cA	826	CLA	CMD-C2D-C1D	6.79	136.69	124.71
14	cA	815	CLA	CMD-C2D-C1D	6.78	136.66	124.71
14	bX	201	CLA	CMD-C2D-C1D	6.78	136.66	124.71
14	X	201	CLA	CMD-C2D-C1D	6.78	136.66	124.71
14	A	807	CLA	CMD-C2D-C1D	6.78	136.66	124.71
14	cA	813	CLA	CMD-C2D-C1D	6.78	136.66	124.71
14	cX	201	CLA	CMD-C2D-C1D	6.77	136.65	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bA	824	CLA	CMD-C2D-C1D	6.77	136.64	124.71
14	bA	813	CLA	CMD-C2D-C1D	6.77	136.64	124.71
14	cA	807	CLA	CMD-C2D-C1D	6.77	136.64	124.71
14	bA	815	CLA	CMD-C2D-C1D	6.77	136.64	124.71
14	A	824	CLA	CMD-C2D-C1D	6.76	136.63	124.71
14	A	815	CLA	CMD-C2D-C1D	6.76	136.63	124.71
14	bA	807	CLA	CMD-C2D-C1D	6.76	136.63	124.71
14	A	813	CLA	CMD-C2D-C1D	6.76	136.63	124.71
14	cA	824	CLA	CMD-C2D-C1D	6.76	136.62	124.71
14	J	102	CLA	CMD-C2D-C1D	6.75	136.62	124.71
14	cB	823	CLA	CMD-C2D-C1D	6.75	136.61	124.71
14	bJ	102	CLA	CMD-C2D-C1D	6.74	136.59	124.71
14	B	830	CLA	CMD-C2D-C1D	6.74	136.59	124.71
14	bB	822	CLA	CMD-C2D-C1D	6.74	136.59	124.71
14	cJ	102	CLA	CMD-C2D-C1D	6.74	136.58	124.71
14	B	822	CLA	CMD-C2D-C1D	6.73	136.58	124.71
14	bB	830	CLA	CMD-C2D-C1D	6.73	136.58	124.71
14	bA	817	CLA	C2B-C1B-NB	6.73	114.74	110.23
14	cB	850	CLA	CMD-C2D-C1D	6.73	136.57	124.71
14	cB	831	CLA	CMD-C2D-C1D	6.73	136.57	124.71
14	bB	831	CLA	CHD-C1D-ND	-6.73	118.27	124.45
14	bB	849	CLA	CMD-C2D-C1D	6.72	136.56	124.71
14	cB	835	CLA	C2B-C1B-NB	6.72	114.74	110.23
14	B	831	CLA	CHD-C1D-ND	-6.72	118.28	124.45
14	cA	817	CLA	C2B-C1B-NB	6.72	114.73	110.23
14	cB	832	CLA	CHD-C1D-ND	-6.71	118.28	124.45
14	A	817	CLA	C2B-C1B-NB	6.71	114.73	110.23
14	bA	835	CLA	CMD-C2D-C1D	6.71	136.54	124.71
14	A	810	CLA	CMD-C2D-C1D	6.71	136.53	124.71
14	B	849	CLA	CMD-C2D-C1D	6.71	136.53	124.71
14	cA	810	CLA	CMD-C2D-C1D	6.71	136.53	124.71
14	bA	810	CLA	CMD-C2D-C1D	6.70	136.53	124.71
14	B	831	CLA	CMD-C2D-C1D	6.70	136.53	124.71
14	bB	834	CLA	C2B-C1B-NB	6.70	114.72	110.23
14	cB	832	CLA	CMD-C2D-C1D	6.70	136.52	124.71
14	B	834	CLA	C2B-C1B-NB	6.70	114.72	110.23
14	bB	831	CLA	CMD-C2D-C1D	6.69	136.51	124.71
14	cA	821	CLA	CMD-C2D-C1D	6.69	136.50	124.71
14	A	822	CLA	CMD-C2D-C1D	6.69	136.50	124.71
14	bA	821	CLA	CMD-C2D-C1D	6.69	136.50	124.71
14	A	821	CLA	CMD-C2D-C1D	6.68	136.49	124.71
14	cA	812	CLA	CMD-C2D-C1D	6.68	136.49	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bA	840	CLA	CMD-C2D-C1D	6.68	136.49	124.71
14	A	812	CLA	CMD-C2D-C1D	6.68	136.49	124.71
14	A	835	CLA	CMD-C2D-C1D	6.68	136.49	124.71
14	bA	822	CLA	CMD-C2D-C1D	6.68	136.49	124.71
14	cB	808	CLA	C2B-C1B-NB	6.68	114.71	110.23
14	bA	812	CLA	CMD-C2D-C1D	6.68	136.48	124.71
14	cA	835	CLA	CMD-C2D-C1D	6.68	136.48	124.71
14	bB	807	CLA	C2B-C1B-NB	6.67	114.71	110.23
14	bL	201	CLA	C2B-C1B-NB	6.67	114.70	110.23
14	A	840	CLA	CMD-C2D-C1D	6.67	136.47	124.71
14	L	201	CLA	C2B-C1B-NB	6.67	114.70	110.23
14	cA	822	CLA	CMD-C2D-C1D	6.67	136.46	124.71
14	B	807	CLA	C2B-C1B-NB	6.66	114.70	110.23
14	cA	809	CLA	CMD-C2D-C1D	6.66	136.44	124.71
13	A	801	CL0	C2B-C1B-NB	6.66	114.69	110.23
14	cL	202	CLA	C2B-C1B-NB	6.65	114.69	110.23
14	cA	840	CLA	CMD-C2D-C1D	6.65	136.43	124.71
14	bB	834	CLA	CMD-C2D-C1D	6.65	136.43	124.71
14	bA	809	CLA	CMD-C2D-C1D	6.64	136.42	124.71
14	B	834	CLA	CMD-C2D-C1D	6.64	136.41	124.71
14	A	811	CLA	CMD-C2D-C1D	6.64	136.41	124.71
14	bA	811	CLA	CMD-C2D-C1D	6.63	136.41	124.71
14	A	809	CLA	CMD-C2D-C1D	6.63	136.40	124.71
14	cA	811	CLA	CMD-C2D-C1D	6.63	136.40	124.71
14	A	820	CLA	CHD-C1D-ND	-6.63	118.36	124.45
13	cA	801	CL0	C2B-C1B-NB	6.63	114.67	110.23
13	bA	801	CL0	C2B-C1B-NB	6.62	114.67	110.23
14	cB	835	CLA	CMD-C2D-C1D	6.62	136.38	124.71
14	cA	829	CLA	C2B-C1B-NB	6.62	114.67	110.23
14	cA	820	CLA	CMD-C2D-C1D	6.61	136.37	124.71
14	bA	829	CLA	C2B-C1B-NB	6.61	114.66	110.23
14	bA	820	CLA	CMD-C2D-C1D	6.61	136.36	124.71
14	B	833	CLA	CMD-C2D-C1D	6.61	136.36	124.71
14	bA	804	CLA	CMD-C2D-C1D	6.61	136.36	124.71
14	B	810	CLA	CMD-C2D-C1D	6.61	136.36	124.71
14	A	820	CLA	CMD-C2D-C1D	6.61	136.35	124.71
14	cB	811	CLA	CMD-C2D-C1D	6.60	136.35	124.71
14	bA	820	CLA	CHD-C1D-ND	-6.60	118.39	124.45
14	bA	831	CLA	CMD-C2D-C1D	6.60	136.35	124.71
14	A	829	CLA	C2B-C1B-NB	6.60	114.66	110.23
14	bB	810	CLA	CMD-C2D-C1D	6.60	136.34	124.71
14	cA	820	CLA	CHD-C1D-ND	-6.60	118.39	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	831	CLA	CMD-C2D-C1D	6.59	136.34	124.71
14	bB	833	CLA	CMD-C2D-C1D	6.59	136.33	124.71
14	cB	834	CLA	CMD-C2D-C1D	6.59	136.33	124.71
14	A	804	CLA	CMD-C2D-C1D	6.59	136.32	124.71
14	cA	831	CLA	CMD-C2D-C1D	6.59	136.32	124.71
14	B	812	CLA	CMD-C2D-C1D	6.59	136.32	124.71
14	cB	821	CLA	CMD-C2D-C1D	6.59	136.32	124.71
14	bA	834	CLA	CMD-C2D-C1D	6.58	136.31	124.71
14	bB	812	CLA	CMD-C2D-C1D	6.58	136.31	124.71
14	B	820	CLA	CMD-C2D-C1D	6.58	136.31	124.71
14	A	834	CLA	CMD-C2D-C1D	6.58	136.31	124.71
14	cB	813	CLA	CMD-C2D-C1D	6.58	136.31	124.71
14	cA	834	CLA	CMD-C2D-C1D	6.58	136.30	124.71
14	B	804	CLA	CMD-C2D-C1D	6.57	136.29	124.71
14	bB	820	CLA	CMD-C2D-C1D	6.57	136.29	124.71
14	cA	804	CLA	CMD-C2D-C1D	6.57	136.28	124.71
14	cB	805	CLA	CMD-C2D-C1D	6.56	136.28	124.71
14	bB	804	CLA	CMD-C2D-C1D	6.55	136.26	124.71
14	bB	812	CLA	CHD-C1D-ND	-6.55	118.43	124.45
14	cB	813	CLA	CHD-C1D-ND	-6.54	118.44	124.45
14	B	835	CLA	CMD-C2D-C1D	6.53	136.22	124.71
14	B	812	CLA	CHD-C1D-ND	-6.53	118.46	124.45
14	B	826	CLA	C2B-C1B-NB	6.53	114.61	110.23
14	B	837	CLA	CMD-C2D-C1D	6.53	136.21	124.71
14	cB	836	CLA	CMD-C2D-C1D	6.52	136.20	124.71
14	cL	203	CLA	CHD-C1D-ND	-6.52	118.46	124.45
14	A	805	CLA	CHD-C1D-ND	-6.52	118.46	124.45
14	bA	805	CLA	CHD-C1D-ND	-6.51	118.47	124.45
14	bB	835	CLA	CMD-C2D-C1D	6.51	136.19	124.71
14	cB	838	CLA	CMD-C2D-C1D	6.51	136.18	124.71
14	bB	836	CLA	CMD-C2D-C1D	6.50	136.17	124.71
14	bB	837	CLA	CMD-C2D-C1D	6.50	136.17	124.71
14	cA	805	CLA	CHD-C1D-ND	-6.50	118.48	124.45
14	B	836	CLA	CMD-C2D-C1D	6.50	136.16	124.71
14	cB	837	CLA	CMD-C2D-C1D	6.49	136.16	124.71
14	A	810	CLA	C2B-C1B-NB	6.49	114.58	110.23
14	bB	826	CLA	C2B-C1B-NB	6.49	114.58	110.23
14	L	202	CLA	CHD-C1D-ND	-6.49	118.49	124.45
14	cA	810	CLA	C2B-C1B-NB	6.49	114.58	110.23
14	A	832	CLA	CMD-C2D-C1D	6.48	136.13	124.71
14	bA	832	CLA	CMD-C2D-C1D	6.47	136.12	124.71
14	bB	810	CLA	CHD-C1D-ND	-6.47	118.50	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bL	202	CLA	CHD-C1D-ND	-6.47	118.50	124.45
14	cA	832	CLA	CMD-C2D-C1D	6.47	136.12	124.71
14	cB	827	CLA	C2B-C1B-NB	6.47	114.57	110.23
14	A	808	CLA	CMD-C2D-C1D	6.47	136.11	124.71
14	bA	808	CLA	CMD-C2D-C1D	6.47	136.11	124.71
14	bA	802	CLA	CMD-C2D-C1D	6.46	136.10	124.71
14	B	839	CLA	C2B-C1B-NB	6.46	114.56	110.23
14	cA	802	CLA	CMD-C2D-C1D	6.45	136.09	124.71
14	bA	810	CLA	C2B-C1B-NB	6.45	114.56	110.23
14	B	810	CLA	CHD-C1D-ND	-6.45	118.52	124.45
14	bB	839	CLA	C2B-C1B-NB	6.45	114.56	110.23
14	cB	811	CLA	CHD-C1D-ND	-6.45	118.53	124.45
14	A	802	CLA	CMD-C2D-C1D	6.45	136.07	124.71
14	B	817	CLA	CHD-C1D-ND	-6.44	118.53	124.45
14	cA	808	CLA	CMD-C2D-C1D	6.44	136.07	124.71
14	bA	833	CLA	O2D-CGD-CBD	6.44	122.71	111.27
14	cA	833	CLA	O2D-CGD-CBD	6.44	122.71	111.27
14	A	833	CLA	O2D-CGD-CBD	6.43	122.70	111.27
14	cB	817	CLA	CHD-C1D-ND	-6.43	118.54	124.45
14	cB	840	CLA	C2B-C1B-NB	6.43	114.54	110.23
14	bB	816	CLA	CHD-C1D-ND	-6.43	118.55	124.45
14	bA	803	CLA	CMD-C2D-C1D	6.43	136.04	124.71
14	cA	803	CLA	CMD-C2D-C1D	6.42	136.04	124.71
14	B	816	CLA	CHD-C1D-ND	-6.42	118.55	124.45
14	B	827	CLA	CMD-C2D-C1D	6.42	136.02	124.71
14	bB	827	CLA	CMD-C2D-C1D	6.42	136.02	124.71
14	A	803	CLA	CMD-C2D-C1D	6.41	136.02	124.71
14	cB	818	CLA	CHD-C1D-ND	-6.41	118.56	124.45
14	cB	828	CLA	CMD-C2D-C1D	6.40	136.00	124.71
14	B	811	CLA	CMD-C2D-C1D	6.40	136.00	124.71
14	cB	831	CLA	CHD-C1D-ND	-6.40	118.58	124.45
14	cB	812	CLA	CMD-C2D-C1D	6.39	135.98	124.71
14	bB	811	CLA	CMD-C2D-C1D	6.39	135.98	124.71
14	bF	201	CLA	CMD-C2D-C1D	6.39	135.98	124.71
14	bB	817	CLA	CHD-C1D-ND	-6.39	118.58	124.45
14	bA	818	CLA	CHD-C1D-ND	-6.39	118.58	124.45
14	bB	830	CLA	CHD-C1D-ND	-6.39	118.58	124.45
14	bB	839	CLA	CMD-C2D-C1D	6.39	135.97	124.71
14	A	832	CLA	C2B-C1B-NB	6.38	114.51	110.23
14	B	839	CLA	CMD-C2D-C1D	6.38	135.96	124.71
14	cB	840	CLA	CMD-C2D-C1D	6.38	135.95	124.71
14	bA	832	CLA	C2B-C1B-NB	6.38	114.51	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	F	201	CLA	CMD-C2D-C1D	6.37	135.94	124.71
14	A	818	CLA	CHD-C1D-ND	-6.37	118.60	124.45
14	cA	818	CLA	CHD-C1D-ND	-6.37	118.60	124.45
14	cB	806	CLA	CHD-C1D-ND	-6.37	118.60	124.45
14	cA	832	CLA	C2B-C1B-NB	6.36	114.50	110.23
14	cB	833	CLA	O2D-CGD-CBD	6.36	122.57	111.27
14	cF	201	CLA	CMD-C2D-C1D	6.36	135.92	124.71
14	B	830	CLA	CHD-C1D-ND	-6.36	118.61	124.45
14	A	814	CLA	CMD-C2D-C1D	6.36	135.92	124.71
14	B	805	CLA	CHD-C1D-ND	-6.35	118.61	124.45
14	B	832	CLA	O2D-CGD-CBD	6.35	122.56	111.27
14	B	808	CLA	CMD-C2D-C1D	6.35	135.91	124.71
14	B	828	CLA	CMD-C2D-C1D	6.35	135.91	124.71
14	bA	814	CLA	CMD-C2D-C1D	6.35	135.91	124.71
14	cL	205	CLA	CMD-C2D-C1D	6.35	135.90	124.71
14	cA	817	CLA	CMD-C2D-C1D	6.35	135.90	124.71
14	bA	817	CLA	CMD-C2D-C1D	6.34	135.89	124.71
14	bA	839	CLA	CMD-C2D-C1D	6.34	135.89	124.71
14	bL	204	CLA	CMD-C2D-C1D	6.34	135.89	124.71
14	bB	832	CLA	O2D-CGD-CBD	6.34	122.54	111.27
14	cB	809	CLA	CMD-C2D-C1D	6.34	135.89	124.71
14	bB	828	CLA	CMD-C2D-C1D	6.34	135.89	124.71
14	cA	823	CLA	CMD-C2D-C1D	6.34	135.89	124.71
14	cA	814	CLA	CMD-C2D-C1D	6.34	135.88	124.71
14	L	204	CLA	CMD-C2D-C1D	6.34	135.88	124.71
14	A	839	CLA	CMD-C2D-C1D	6.34	135.88	124.71
14	cA	816	CLA	CMD-C2D-C1D	6.34	135.88	124.71
14	A	817	CLA	CMD-C2D-C1D	6.33	135.88	124.71
14	bB	805	CLA	CHD-C1D-ND	-6.33	118.63	124.45
14	A	816	CLA	CMD-C2D-C1D	6.33	135.87	124.71
14	A	823	CLA	CMD-C2D-C1D	6.33	135.87	124.71
14	bA	823	CLA	CMD-C2D-C1D	6.33	135.87	124.71
14	bB	808	CLA	CMD-C2D-C1D	6.33	135.87	124.71
14	bA	816	CLA	CMD-C2D-C1D	6.33	135.87	124.71
14	cB	829	CLA	CMD-C2D-C1D	6.33	135.87	124.71
14	cA	839	CLA	CMD-C2D-C1D	6.32	135.86	124.71
14	cA	804	CLA	CHD-C1D-ND	-6.32	118.64	124.45
14	A	804	CLA	CHD-C1D-ND	-6.31	118.66	124.45
14	bB	821	CLA	CHD-C1D-ND	-6.31	118.66	124.45
14	B	821	CLA	CHD-C1D-ND	-6.31	118.66	124.45
14	bA	810	CLA	CHD-C1D-ND	-6.30	118.66	124.45
14	bA	804	CLA	CHD-C1D-ND	-6.30	118.66	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	806	CLA	CHD-C1D-ND	-6.30	118.67	124.45
14	cA	811	CLA	CHD-C1D-ND	-6.29	118.68	124.45
14	bA	806	CLA	CHD-C1D-ND	-6.29	118.68	124.45
14	A	810	CLA	CHD-C1D-ND	-6.28	118.68	124.45
14	cA	806	CLA	CHD-C1D-ND	-6.28	118.68	124.45
14	bA	830	CLA	CMD-C2D-C1D	6.28	135.78	124.71
14	cA	810	CLA	CHD-C1D-ND	-6.28	118.68	124.45
14	A	830	CLA	CMD-C2D-C1D	6.27	135.77	124.71
14	cA	815	CLA	CHD-C1D-ND	-6.27	118.69	124.45
14	cB	822	CLA	CHD-C1D-ND	-6.27	118.69	124.45
14	cA	830	CLA	CMD-C2D-C1D	6.27	135.75	124.71
14	bB	851	CLA	CHD-C1D-ND	-6.26	118.70	124.45
14	A	836	CLA	CMD-C2D-C1D	6.26	135.75	124.71
14	cA	836	CLA	CMD-C2D-C1D	6.26	135.74	124.71
14	bB	807	CLA	CMD-C2D-C1D	6.26	135.74	124.71
14	A	811	CLA	CHD-C1D-ND	-6.26	118.70	124.45
14	bA	815	CLA	CHD-C1D-ND	-6.26	118.70	124.45
14	cB	808	CLA	CMD-C2D-C1D	6.25	135.74	124.71
14	B	807	CLA	CMD-C2D-C1D	6.25	135.73	124.71
14	bA	836	CLA	CMD-C2D-C1D	6.25	135.73	124.71
14	A	815	CLA	CHD-C1D-ND	-6.25	118.71	124.45
14	B	815	CLA	CHD-C1D-ND	-6.25	118.71	124.45
14	A	823	CLA	CHD-C1D-ND	-6.24	118.72	124.45
14	bB	837	CLA	CHD-C1D-ND	-6.24	118.72	124.45
14	cB	816	CLA	CHD-C1D-ND	-6.24	118.72	124.45
14	bB	815	CLA	CHD-C1D-ND	-6.24	118.72	124.45
14	cB	801	CLA	CHD-C1D-ND	-6.24	118.72	124.45
14	B	837	CLA	CHD-C1D-ND	-6.23	118.73	124.45
14	cB	838	CLA	CHD-C1D-ND	-6.23	118.73	124.45
14	bB	814	CLA	CHD-C1D-ND	-6.22	118.73	124.45
14	B	836	CLA	CHD-C1D-ND	-6.22	118.74	124.45
14	bA	811	CLA	CHD-C1D-ND	-6.22	118.74	124.45
14	cB	815	CLA	CHD-C1D-ND	-6.22	118.74	124.45
14	cB	837	CLA	CHD-C1D-ND	-6.22	118.74	124.45
14	B	851	CLA	CHD-C1D-ND	-6.21	118.74	124.45
14	bA	821	CLA	CHD-C1D-ND	-6.21	118.75	124.45
14	cA	823	CLA	CHD-C1D-ND	-6.21	118.75	124.45
14	B	814	CLA	CHD-C1D-ND	-6.21	118.75	124.45
14	bB	832	CLA	CMD-C2D-C1D	6.20	135.64	124.71
14	bB	822	CLA	CHD-C1D-ND	-6.20	118.75	124.45
14	cB	833	CLA	CMD-C2D-C1D	6.20	135.64	124.71
14	bB	836	CLA	CHD-C1D-ND	-6.20	118.76	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	821	CLA	CHD-C1D-ND	-6.20	118.76	124.45
14	bB	818	CLA	CMD-C2D-C1D	6.20	135.63	124.71
14	bB	806	CLA	CHD-C1D-ND	-6.19	118.76	124.45
14	cB	819	CLA	CMD-C2D-C1D	6.19	135.62	124.71
14	bA	823	CLA	CHD-C1D-ND	-6.19	118.77	124.45
14	B	832	CLA	CMD-C2D-C1D	6.19	135.62	124.71
14	B	818	CLA	CMD-C2D-C1D	6.19	135.62	124.71
14	A	821	CLA	CHD-C1D-ND	-6.19	118.77	124.45
14	bA	827	CLA	CHD-C1D-ND	-6.18	118.77	124.45
14	B	806	CLA	CHD-C1D-ND	-6.18	118.78	124.45
14	cB	819	CLA	CHD-C1D-ND	-6.18	118.78	124.45
14	bB	824	CLA	CMD-C2D-C1D	6.17	135.59	124.71
14	A	807	CLA	CHD-C1D-ND	-6.17	118.79	124.45
14	bB	818	CLA	CHD-C1D-ND	-6.17	118.79	124.45
14	B	824	CLA	CMD-C2D-C1D	6.17	135.58	124.71
14	B	826	CLA	C2C-C1C-NC	6.16	115.75	109.97
14	cB	825	CLA	CMD-C2D-C1D	6.16	135.58	124.71
14	cA	827	CLA	CHD-C1D-ND	-6.16	118.79	124.45
14	bA	807	CLA	CHD-C1D-ND	-6.16	118.79	124.45
14	cB	823	CLA	CHD-C1D-ND	-6.16	118.79	124.45
14	B	822	CLA	CHD-C1D-ND	-6.16	118.80	124.45
14	cB	807	CLA	CHD-C1D-ND	-6.16	118.80	124.45
14	cB	827	CLA	C2C-C1C-NC	6.15	115.74	109.97
14	cA	812	CLA	CHD-C1D-ND	-6.15	118.80	124.45
14	bB	849	CLA	CHD-C1D-ND	-6.15	118.80	124.45
14	bA	812	CLA	CHD-C1D-ND	-6.14	118.81	124.45
14	cB	850	CLA	CHD-C1D-ND	-6.14	118.81	124.45
14	cB	834	CLA	CHD-C1D-ND	-6.14	118.81	124.45
14	B	818	CLA	CHD-C1D-ND	-6.14	118.81	124.45
14	bB	826	CLA	C2C-C1C-NC	6.14	115.72	109.97
14	bB	833	CLA	CHD-C1D-ND	-6.13	118.82	124.45
14	B	820	CLA	CHD-C1D-ND	-6.13	118.82	124.45
14	A	827	CLA	CHD-C1D-ND	-6.13	118.82	124.45
14	cJ	102	CLA	CHD-C1D-ND	-6.13	118.82	124.45
14	A	812	CLA	CHD-C1D-ND	-6.12	118.83	124.45
14	B	849	CLA	CHD-C1D-ND	-6.12	118.83	124.45
14	B	833	CLA	CHD-C1D-ND	-6.12	118.83	124.45
14	cA	807	CLA	CHD-C1D-ND	-6.11	118.84	124.45
14	J	102	CLA	CHD-C1D-ND	-6.11	118.84	124.45
14	bB	819	CLA	CHD-C1D-ND	-6.11	118.84	124.45
14	bJ	102	CLA	CHD-C1D-ND	-6.11	118.84	124.45
14	bB	835	CLA	CHD-C1D-ND	-6.11	118.84	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cB	836	CLA	CHD-C1D-ND	-6.10	118.84	124.45
14	cX	201	CLA	CHD-C1D-ND	-6.10	118.85	124.45
14	bB	820	CLA	CHD-C1D-ND	-6.10	118.85	124.45
14	B	819	CLA	CHD-C1D-ND	-6.10	118.85	124.45
14	cB	820	CLA	CHD-C1D-ND	-6.10	118.85	124.45
14	J	101	CLA	CHD-C1D-ND	-6.10	118.85	124.45
14	B	835	CLA	CHD-C1D-ND	-6.09	118.85	124.45
14	X	201	CLA	CHD-C1D-ND	-6.09	118.85	124.45
14	B	838	CLA	C2B-C1B-NB	6.09	114.31	110.23
14	bX	201	CLA	CHD-C1D-ND	-6.09	118.86	124.45
14	cB	821	CLA	CHD-C1D-ND	-6.09	118.86	124.45
14	bB	839	CLA	C2C-C1C-NC	6.09	115.67	109.97
14	B	839	CLA	C2C-C1C-NC	6.08	115.67	109.97
14	bA	842	CLA	CHD-C1D-ND	-6.08	118.87	124.45
14	A	842	CLA	CHD-C1D-ND	-6.08	118.87	124.45
14	bJ	101	CLA	CHD-C1D-ND	-6.08	118.87	124.45
14	cB	840	CLA	C2C-C1C-NC	6.07	115.66	109.97
14	cJ	101	CLA	CHD-C1D-ND	-6.07	118.87	124.45
13	bA	801	CL0	CMD-C2D-C1D	6.07	135.41	124.71
14	cA	842	CLA	CHD-C1D-ND	-6.07	118.87	124.45
14	A	835	CLA	CHD-C1D-ND	-6.07	118.88	124.45
14	bB	834	CLA	CHD-C1D-ND	-6.07	118.88	124.45
14	bA	835	CLA	CHD-C1D-ND	-6.07	118.88	124.45
14	B	838	CLA	C2C-C1C-NC	6.07	115.66	109.97
13	A	801	CL0	CMD-C2D-C1D	6.06	135.40	124.71
14	cA	835	CLA	CHD-C1D-ND	-6.06	118.88	124.45
13	cA	801	CL0	CMD-C2D-C1D	6.06	135.40	124.71
14	bA	809	CLA	CHD-C1D-ND	-6.06	118.89	124.45
14	bB	838	CLA	C2B-C1B-NB	6.06	114.29	110.23
14	B	834	CLA	CHD-C1D-ND	-6.05	118.89	124.45
14	bA	819	CLA	CHD-C1D-ND	-6.05	118.89	124.45
14	cB	839	CLA	C2B-C1B-NB	6.05	114.29	110.23
14	cB	839	CLA	C2C-C1C-NC	6.05	115.64	109.97
14	bB	838	CLA	C2C-C1C-NC	6.04	115.63	109.97
14	bA	829	CLA	O2D-CGD-CBD	6.04	122.00	111.27
14	cA	834	CLA	CHD-C1D-ND	-6.04	118.91	124.45
14	A	819	CLA	CHD-C1D-ND	-6.04	118.91	124.45
14	cA	829	CLA	O2D-CGD-CBD	6.03	121.99	111.27
14	cA	831	CLA	CHD-C1D-ND	-6.03	118.91	124.45
14	cA	819	CLA	CHD-C1D-ND	-6.03	118.92	124.45
14	cA	837	CLA	C2B-C1B-NB	6.02	114.27	110.23
14	A	829	CLA	O2D-CGD-CBD	6.02	121.97	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bA	837	CLA	CMD-C2D-C1D	6.02	135.32	124.71
14	cA	837	CLA	CMD-C2D-C1D	6.02	135.32	124.71
14	bA	834	CLA	CHD-C1D-ND	-6.02	118.92	124.45
14	cB	835	CLA	CHD-C1D-ND	-6.02	118.92	124.45
14	A	809	CLA	CHD-C1D-ND	-6.01	118.93	124.45
14	bB	825	CLA	CHD-C1D-ND	-6.01	118.93	124.45
14	A	837	CLA	CMD-C2D-C1D	6.01	135.31	124.71
14	cA	809	CLA	CHD-C1D-ND	-6.01	118.93	124.45
14	bA	837	CLA	C2B-C1B-NB	6.00	114.26	110.23
14	A	834	CLA	CHD-C1D-ND	-6.00	118.94	124.45
14	A	839	CLA	CHD-C1D-ND	-6.00	118.94	124.45
14	bA	831	CLA	CHD-C1D-ND	-6.00	118.94	124.45
14	A	831	CLA	CHD-C1D-ND	-6.00	118.94	124.45
14	B	825	CLA	CHD-C1D-ND	-5.99	118.95	124.45
14	bA	817	CLA	CHD-C1D-ND	-5.98	118.96	124.45
14	cB	826	CLA	CHD-C1D-ND	-5.97	118.96	124.45
14	cA	833	CLA	CHD-C1D-ND	-5.97	118.97	124.45
14	bA	833	CLA	CHD-C1D-ND	-5.97	118.97	124.45
14	bA	839	CLA	CHD-C1D-ND	-5.97	118.97	124.45
14	A	837	CLA	C2B-C1B-NB	5.97	114.23	110.23
14	A	817	CLA	CHD-C1D-ND	-5.97	118.97	124.45
14	A	833	CLA	CHD-C1D-ND	-5.96	118.98	124.45
14	cA	817	CLA	CHD-C1D-ND	-5.96	118.98	124.45
14	bA	816	CLA	CHD-C1D-ND	-5.95	118.98	124.45
14	cA	839	CLA	CHD-C1D-ND	-5.95	118.98	124.45
14	A	814	CLA	CHD-C1D-ND	-5.94	119.00	124.45
14	A	803	CLA	CHD-C1D-ND	-5.93	119.00	124.45
14	bA	803	CLA	CHD-C1D-ND	-5.93	119.01	124.45
14	B	824	CLA	CHD-C1D-ND	-5.93	119.01	124.45
14	cA	816	CLA	CHD-C1D-ND	-5.93	119.01	124.45
14	A	808	CLA	CHD-C1D-ND	-5.92	119.01	124.45
14	bB	824	CLA	CHD-C1D-ND	-5.92	119.01	124.45
14	cB	830	CLA	CHD-C1D-ND	-5.92	119.01	124.45
14	A	816	CLA	CHD-C1D-ND	-5.92	119.01	124.45
14	bA	814	CLA	CHD-C1D-ND	-5.92	119.01	124.45
14	cB	825	CLA	CHD-C1D-ND	-5.92	119.01	124.45
14	cA	814	CLA	CHD-C1D-ND	-5.92	119.02	124.45
14	A	838	CLA	O2D-CGD-CBD	5.92	121.78	111.27
14	cA	838	CLA	O2D-CGD-CBD	5.92	121.78	111.27
14	B	804	CLA	CHD-C1D-ND	-5.91	119.02	124.45
14	bA	838	CLA	O2D-CGD-CBD	5.91	121.77	111.27
14	cL	205	CLA	CHD-C1D-ND	-5.91	119.02	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	803	CLA	CHD-C1D-ND	-5.91	119.03	124.45
14	bB	804	CLA	CHD-C1D-ND	-5.91	119.03	124.45
14	B	829	CLA	CHD-C1D-ND	-5.90	119.03	124.45
14	cB	805	CLA	CHD-C1D-ND	-5.90	119.03	124.45
14	bA	825	CLA	CHD-C1D-ND	-5.90	119.03	124.45
14	cA	825	CLA	CHD-C1D-ND	-5.90	119.03	124.45
14	L	204	CLA	CHD-C1D-ND	-5.90	119.03	124.45
14	cA	808	CLA	CHD-C1D-ND	-5.89	119.04	124.45
14	cB	812	CLA	CHD-C1D-ND	-5.89	119.04	124.45
14	A	825	CLA	CHD-C1D-ND	-5.89	119.04	124.45
14	L	201	CLA	C2C-C1C-NC	5.89	115.49	109.97
14	cL	202	CLA	C2C-C1C-NC	5.88	115.48	109.97
14	A	826	CLA	CHD-C1D-ND	-5.88	119.05	124.45
14	bA	826	CLA	CHD-C1D-ND	-5.88	119.05	124.45
14	bA	808	CLA	CHD-C1D-ND	-5.88	119.05	124.45
14	bL	204	CLA	CHD-C1D-ND	-5.88	119.05	124.45
14	bB	829	CLA	CHD-C1D-ND	-5.87	119.06	124.45
14	bL	201	CLA	C2C-C1C-NC	5.87	115.47	109.97
14	B	804	CLA	O2D-CGD-CBD	5.86	121.69	111.27
14	bB	811	CLA	CHD-C1D-ND	-5.86	119.07	124.45
14	bA	838	CLA	CMD-C2D-C1D	5.86	135.04	124.71
14	cA	826	CLA	CHD-C1D-ND	-5.86	119.07	124.45
14	cA	838	CLA	CMD-C2D-C1D	5.86	135.03	124.71
14	A	838	CLA	CMD-C2D-C1D	5.86	135.03	124.71
14	bB	804	CLA	O2D-CGD-CBD	5.86	121.67	111.27
14	B	828	CLA	O2D-CGD-CBD	5.85	121.67	111.27
14	cB	805	CLA	O2D-CGD-CBD	5.85	121.66	111.27
14	B	811	CLA	CHD-C1D-ND	-5.85	119.08	124.45
14	bB	828	CLA	O2D-CGD-CBD	5.85	121.66	111.27
14	cB	829	CLA	O2D-CGD-CBD	5.84	121.64	111.27
14	bL	201	CLA	CMD-C2D-C1D	5.83	134.99	124.71
14	A	832	CLA	C2C-C1C-NC	5.83	115.43	109.97
14	A	802	CLA	C2B-C1B-NB	5.83	114.14	110.23
14	B	823	CLA	CHD-C1D-ND	-5.83	119.10	124.45
14	L	201	CLA	CMD-C2D-C1D	5.83	134.98	124.71
14	bA	840	CLA	CHD-C1D-ND	-5.82	119.10	124.45
14	bA	802	CLA	C2B-C1B-NB	5.82	114.14	110.23
14	bA	802	CLA	O2D-CGD-CBD	5.82	121.61	111.27
14	bB	803	CLA	O2D-CGD-CBD	5.82	121.61	111.27
14	cA	802	CLA	C2B-C1B-NB	5.82	114.13	110.23
14	cB	804	CLA	O2D-CGD-CBD	5.82	121.61	111.27
14	cA	802	CLA	O2D-CGD-CBD	5.82	121.61	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	840	CLA	CHD-C1D-ND	-5.82	119.11	124.45
14	B	803	CLA	O2D-CGD-CBD	5.82	121.60	111.27
14	cL	202	CLA	CMD-C2D-C1D	5.81	134.96	124.71
14	A	840	CLA	CHD-C1D-ND	-5.81	119.11	124.45
14	bB	823	CLA	CHD-C1D-ND	-5.81	119.11	124.45
14	cA	832	CLA	C2C-C1C-NC	5.81	115.42	109.97
14	cB	824	CLA	CHD-C1D-ND	-5.81	119.12	124.45
14	bA	832	CLA	C2C-C1C-NC	5.81	115.41	109.97
14	A	802	CLA	O2D-CGD-CBD	5.80	121.58	111.27
14	bA	826	CLA	O2D-CGD-CBD	5.80	121.57	111.27
14	cL	204	CLA	CHD-C1D-ND	-5.80	119.13	124.45
14	cA	826	CLA	O2D-CGD-CBD	5.79	121.56	111.27
14	A	826	CLA	O2D-CGD-CBD	5.79	121.56	111.27
14	bL	203	CLA	CHD-C1D-ND	-5.78	119.14	124.45
14	A	838	CLA	CHD-C1D-ND	-5.78	119.14	124.45
14	bA	838	CLA	CHD-C1D-ND	-5.78	119.14	124.45
14	cA	838	CLA	CHD-C1D-ND	-5.78	119.15	124.45
14	cB	814	CLA	CHD-C1D-ND	-5.78	119.15	124.45
14	cA	813	CLA	CHD-C1D-ND	-5.77	119.15	124.45
14	B	813	CLA	CHD-C1D-ND	-5.77	119.15	124.45
14	L	203	CLA	CHD-C1D-ND	-5.77	119.15	124.45
14	bA	825	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
14	A	813	CLA	CHD-C1D-ND	-5.77	119.16	124.45
14	cA	802	CLA	C2C-C1C-NC	5.76	115.37	109.97
14	bA	813	CLA	CHD-C1D-ND	-5.76	119.16	124.45
14	bB	813	CLA	CHD-C1D-ND	-5.76	119.16	124.45
14	cB	810	CLA	C2C-C1C-NC	5.76	115.37	109.97
14	A	841	CLA	C2C-C1C-NC	5.76	115.36	109.97
14	A	825	CLA	CHD-C4C-C3C	-5.75	116.38	124.84
14	bB	809	CLA	C2C-C1C-NC	5.75	115.36	109.97
14	bA	841	CLA	C2C-C1C-NC	5.75	115.36	109.97
14	B	807	CLA	CHD-C1D-ND	-5.74	119.18	124.45
14	B	823	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
14	cA	825	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
14	cB	824	CLA	CHD-C4C-C3C	-5.74	116.41	124.84
14	bA	802	CLA	C2C-C1C-NC	5.73	115.34	109.97
14	bB	823	CLA	CHD-C4C-C3C	-5.73	116.42	124.84
14	A	802	CLA	C2C-C1C-NC	5.73	115.34	109.97
14	bB	807	CLA	CHD-C1D-ND	-5.73	119.19	124.45
14	B	809	CLA	C2C-C1C-NC	5.73	115.34	109.97
14	F	201	CLA	CHD-C1D-ND	-5.73	119.19	124.45
14	cA	841	CLA	C2C-C1C-NC	5.72	115.33	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bF	201	CLA	CHD-C1D-ND	-5.72	119.20	124.45
14	cB	802	CLA	CHD-C4C-C3C	-5.71	116.44	124.84
14	bA	837	CLA	CHD-C1D-ND	-5.71	119.20	124.45
14	B	801	CLA	CHD-C4C-C3C	-5.71	116.44	124.84
14	cB	803	CLA	CMD-C2D-C1D	5.71	134.77	124.71
14	bB	801	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
14	bB	802	CLA	C2C-C1C-NC	5.71	115.32	109.97
14	B	824	CLA	O2D-CGD-CBD	5.71	121.41	111.27
14	bB	824	CLA	O2D-CGD-CBD	5.71	121.41	111.27
14	B	802	CLA	CMD-C2D-C1D	5.70	134.76	124.71
14	B	802	CLA	C2C-C1C-NC	5.70	115.31	109.97
14	cB	825	CLA	O2D-CGD-CBD	5.70	121.40	111.27
14	bB	802	CLA	CMD-C2D-C1D	5.70	134.76	124.71
14	cB	804	CLA	CHD-C4C-C3C	-5.70	116.47	124.84
14	cA	837	CLA	CHD-C1D-ND	-5.70	119.22	124.45
14	B	827	CLA	CHD-C1D-ND	-5.69	119.22	124.45
14	cB	808	CLA	CHD-C1D-ND	-5.69	119.22	124.45
14	A	837	CLA	CHD-C1D-ND	-5.69	119.22	124.45
14	bB	839	CLA	CHD-C1D-ND	-5.68	119.23	124.45
14	cB	828	CLA	CHD-C1D-ND	-5.68	119.23	124.45
14	bB	803	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
14	cB	803	CLA	C2C-C1C-NC	5.68	115.29	109.97
14	A	808	CLA	O2D-CGD-CBD	5.68	121.35	111.27
14	cF	201	CLA	CHD-C1D-ND	-5.67	119.24	124.45
14	bB	827	CLA	CHD-C1D-ND	-5.67	119.24	124.45
14	B	803	CLA	CHD-C4C-C3C	-5.67	116.51	124.84
14	cB	840	CLA	CHD-C1D-ND	-5.67	119.25	124.45
14	bA	808	CLA	O2D-CGD-CBD	5.67	121.34	111.27
14	B	839	CLA	CHD-C1D-ND	-5.66	119.25	124.45
14	cA	824	CLA	CHD-C1D-ND	-5.66	119.25	124.45
14	cA	808	CLA	O2D-CGD-CBD	5.66	121.32	111.27
14	A	824	CLA	CHD-C1D-ND	-5.65	119.26	124.45
14	cA	803	CLA	O2D-CGD-CBD	5.65	121.31	111.27
14	A	830	CLA	CHD-C1D-ND	-5.65	119.26	124.45
14	cA	826	CLA	CHD-C4C-C3C	-5.65	116.53	124.84
14	bA	833	CLA	C2C-C1C-NC	5.65	115.26	109.97
14	A	826	CLA	CHD-C4C-C3C	-5.65	116.54	124.84
14	A	833	CLA	CMD-C2D-C1D	5.65	134.67	124.71
14	A	833	CLA	C2C-C1C-NC	5.65	115.26	109.97
14	bA	830	CLA	CHD-C1D-ND	-5.65	119.27	124.45
14	bA	803	CLA	O2D-CGD-CBD	5.64	121.29	111.27
14	A	803	CLA	O2D-CGD-CBD	5.64	121.29	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bA	826	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
14	bB	813	CLA	CMD-C2D-C1D	5.64	134.65	124.71
14	cA	833	CLA	C2C-C1C-NC	5.64	115.25	109.97
14	cB	814	CLA	CMD-C2D-C1D	5.64	134.65	124.71
14	bA	802	CLA	CHD-C4C-C3C	-5.64	116.56	124.84
14	cA	833	CLA	CMD-C2D-C1D	5.63	134.64	124.71
14	cA	802	CLA	CHD-C4C-C3C	-5.63	116.56	124.84
14	A	802	CLA	CHD-C4C-C3C	-5.63	116.57	124.84
14	bA	833	CLA	CMD-C2D-C1D	5.63	134.63	124.71
14	B	813	CLA	CMD-C2D-C1D	5.63	134.63	124.71
14	bA	824	CLA	CHD-C1D-ND	-5.62	119.28	124.45
14	cA	830	CLA	CHD-C1D-ND	-5.62	119.29	124.45
14	cB	838	CLA	O2D-CGD-CBD	5.62	121.26	111.27
14	cB	826	CLA	CHD-C4C-C3C	-5.62	116.58	124.84
14	bA	836	CLA	CHD-C4C-C3C	-5.62	116.58	124.84
14	cB	829	CLA	CHD-C1D-ND	-5.62	119.29	124.45
14	cA	836	CLA	CHD-C4C-C3C	-5.62	116.58	124.84
14	A	836	CLA	CHD-C4C-C3C	-5.62	116.58	124.84
14	bA	806	CLA	CHD-C4C-C3C	-5.61	116.59	124.84
14	B	837	CLA	O2D-CGD-CBD	5.61	121.25	111.27
14	bB	825	CLA	CHD-C4C-C3C	-5.61	116.59	124.84
14	bB	837	CLA	O2D-CGD-CBD	5.61	121.24	111.27
14	cA	806	CLA	CHD-C4C-C3C	-5.61	116.60	124.84
14	cB	827	CLA	CHD-C1D-ND	-5.61	119.30	124.45
14	B	825	CLA	CHD-C4C-C3C	-5.61	116.60	124.84
14	bA	829	CLA	CHD-C1D-ND	-5.61	119.30	124.45
14	cA	804	CLA	O2D-CGD-CBD	5.60	121.22	111.27
14	A	806	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
14	B	814	CLA	O2D-CGD-CBD	5.60	121.22	111.27
14	A	804	CLA	O2D-CGD-CBD	5.60	121.22	111.27
14	bB	828	CLA	CHD-C1D-ND	-5.60	119.31	124.45
14	cA	829	CLA	CHD-C1D-ND	-5.60	119.31	124.45
14	B	812	CLA	C4A-NA-C1A	-5.60	104.19	106.71
14	A	832	CLA	CHD-C1D-ND	-5.59	119.31	124.45
14	B	828	CLA	CHD-C1D-ND	-5.59	119.31	124.45
14	bA	804	CLA	O2D-CGD-CBD	5.59	121.20	111.27
14	A	829	CLA	CHD-C1D-ND	-5.59	119.32	124.45
14	cA	832	CLA	CHD-C1D-ND	-5.59	119.32	124.45
14	cB	815	CLA	O2D-CGD-CBD	5.58	121.19	111.27
14	bB	814	CLA	O2D-CGD-CBD	5.58	121.19	111.27
14	bA	836	CLA	CHD-C1D-ND	-5.58	119.32	124.45
14	bB	817	CLA	CHD-C4C-C3C	-5.58	116.64	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	836	CLA	CHD-C1D-ND	-5.58	119.33	124.45
14	bA	832	CLA	CHD-C1D-ND	-5.58	119.33	124.45
14	B	817	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
14	B	831	CLA	C4A-NA-C1A	-5.58	104.20	106.71
14	bB	820	CLA	O2D-CGD-CBD	5.57	121.17	111.27
14	cB	821	CLA	O2D-CGD-CBD	5.57	121.17	111.27
14	cB	808	CLA	O2D-CGD-CBD	5.57	121.17	111.27
14	bB	831	CLA	C4A-NA-C1A	-5.57	104.20	106.71
14	cB	832	CLA	C4A-NA-C1A	-5.57	104.20	106.71
14	B	820	CLA	O2D-CGD-CBD	5.57	121.16	111.27
14	cB	818	CLA	CHD-C4C-C3C	-5.57	116.66	124.84
14	B	807	CLA	O2D-CGD-CBD	5.56	121.15	111.27
14	B	826	CLA	CHD-C1D-ND	-5.56	119.34	124.45
14	cA	836	CLA	CHD-C1D-ND	-5.56	119.35	124.45
14	F	201	CLA	CHD-C4C-C3C	-5.56	116.67	124.84
14	L	203	CLA	CMD-C2D-C1D	5.55	134.50	124.71
13	cA	801	CL0	C2C-C1C-NC	5.55	115.17	109.97
14	cL	204	CLA	CMD-C2D-C1D	5.55	134.49	124.71
14	bL	203	CLA	CMD-C2D-C1D	5.55	134.49	124.71
14	bB	807	CLA	O2D-CGD-CBD	5.55	121.12	111.27
13	A	801	CL0	C2C-C1C-NC	5.54	115.17	109.97
14	cB	813	CLA	C4A-NA-C1A	-5.54	104.21	106.71
14	bB	812	CLA	C4A-NA-C1A	-5.54	104.22	106.71
14	bB	801	CLA	CHD-C1D-ND	-5.54	119.36	124.45
14	cB	802	CLA	CHD-C1D-ND	-5.53	119.37	124.45
14	B	805	CLA	O2D-CGD-CBD	5.53	121.09	111.27
14	A	829	CLA	CMD-C2D-C1D	5.53	134.46	124.71
14	A	828	CLA	CHD-C1D-ND	-5.53	119.37	124.45
13	bA	801	CL0	C2C-C1C-NC	5.53	115.15	109.97
14	bB	805	CLA	O2D-CGD-CBD	5.53	121.09	111.27
14	cA	829	CLA	CMD-C2D-C1D	5.53	134.45	124.71
14	cF	201	CLA	CHD-C4C-C3C	-5.53	116.72	124.84
14	B	801	CLA	CHD-C1D-ND	-5.53	119.38	124.45
14	bA	829	CLA	CMD-C2D-C1D	5.52	134.45	124.71
14	bL	204	CLA	C2C-C1C-NC	5.52	115.14	109.97
14	bF	201	CLA	CHD-C4C-C3C	-5.52	116.73	124.84
14	cL	205	CLA	C2C-C1C-NC	5.52	115.14	109.97
14	bB	826	CLA	CHD-C1D-ND	-5.52	119.38	124.45
14	bB	828	CLA	CHD-C4C-C3C	-5.52	116.73	124.84
14	L	204	CLA	C2C-C1C-NC	5.52	115.14	109.97
14	cB	806	CLA	O2D-CGD-CBD	5.52	121.07	111.27
14	L	203	CLA	CHD-C4C-C3C	-5.51	116.74	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bL	203	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
14	bA	828	CLA	CHD-C1D-ND	-5.51	119.39	124.45
14	cL	204	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
14	bB	832	CLA	CHD-C1D-ND	-5.50	119.40	124.45
14	B	828	CLA	CHD-C4C-C3C	-5.50	116.76	124.84
14	cA	828	CLA	CHD-C1D-ND	-5.50	119.40	124.45
14	cB	829	CLA	CHD-C4C-C3C	-5.49	116.76	124.84
14	A	828	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
14	cA	828	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
14	B	832	CLA	CHD-C1D-ND	-5.49	119.41	124.45
14	bA	828	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
14	B	832	CLA	CHD-C4C-C3C	-5.48	116.78	124.84
14	bB	832	CLA	CHD-C4C-C3C	-5.48	116.79	124.84
14	cB	833	CLA	CHD-C1D-ND	-5.47	119.43	124.45
14	cB	833	CLA	CHD-C4C-C3C	-5.47	116.81	124.84
14	B	807	CLA	C2C-C1C-NC	5.46	115.09	109.97
14	bA	830	CLA	O2D-CGD-CBD	5.46	120.96	111.27
14	bA	832	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
14	bA	841	CLA	CMD-C2D-C1D	5.45	134.31	124.71
14	A	815	CLA	O2D-CGD-CBD	5.45	120.95	111.27
14	B	803	CLA	C2C-C1C-NC	5.45	115.08	109.97
14	cA	841	CLA	CMD-C2D-C1D	5.45	134.31	124.71
14	A	817	CLA	C2C-C1C-NC	5.45	115.07	109.97
14	cA	830	CLA	O2D-CGD-CBD	5.44	120.93	111.27
14	A	841	CLA	CAA-C2A-C3A	-5.44	97.89	112.78
14	A	841	CLA	CMD-C2D-C1D	5.44	134.30	124.71
14	bA	817	CLA	C2C-C1C-NC	5.44	115.06	109.97
14	bB	803	CLA	C2C-C1C-NC	5.43	115.06	109.97
14	cA	832	CLA	CHD-C4C-C3C	-5.43	116.86	124.84
14	cA	815	CLA	O2D-CGD-CBD	5.43	120.92	111.27
14	bA	831	CLA	C2C-C1C-NC	5.43	115.06	109.97
14	bA	841	CLA	CAA-C2A-C3A	-5.43	97.91	112.78
14	cA	817	CLA	C2C-C1C-NC	5.43	115.06	109.97
14	cX	201	CLA	O2D-CGD-CBD	5.43	120.92	111.27
14	B	813	CLA	O2D-CGD-CBD	5.43	120.92	111.27
14	cA	841	CLA	CAA-C2A-C3A	-5.43	97.92	112.78
14	cB	808	CLA	C2C-C1C-NC	5.43	115.06	109.97
14	A	830	CLA	O2D-CGD-CBD	5.43	120.91	111.27
14	bA	833	CLA	C4A-NA-C1A	-5.42	104.27	106.71
14	cB	814	CLA	O2D-CGD-CBD	5.42	120.90	111.27
14	cB	804	CLA	C2C-C1C-NC	5.42	115.05	109.97
14	bX	201	CLA	O2D-CGD-CBD	5.42	120.90	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bA	815	CLA	O2D-CGD-CBD	5.42	120.90	111.27
14	A	832	CLA	CHD-C4C-C3C	-5.42	116.88	124.84
14	B	822	CLA	CHD-C4C-C3C	-5.42	116.88	124.84
14	bB	813	CLA	O2D-CGD-CBD	5.42	120.89	111.27
14	bB	807	CLA	C2C-C1C-NC	5.41	115.04	109.97
14	A	833	CLA	C4A-NA-C1A	-5.41	104.27	106.71
14	cB	823	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
14	bB	822	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
14	X	201	CLA	O2D-CGD-CBD	5.41	120.88	111.27
14	bB	838	CLA	CHD-C4C-C3C	-5.40	116.90	124.84
14	cB	801	CLA	CHD-C4C-C3C	-5.40	116.90	124.84
14	cB	839	CLA	CMD-C2D-C1D	5.40	134.22	124.71
14	cA	833	CLA	C4A-NA-C1A	-5.39	104.28	106.71
14	cA	830	CLA	C2C-C1C-NC	5.39	115.02	109.97
14	B	838	CLA	CMD-C2D-C1D	5.39	134.21	124.71
14	bB	851	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
14	bB	838	CLA	CMD-C2D-C1D	5.39	134.20	124.71
14	A	831	CLA	C2C-C1C-NC	5.38	115.02	109.97
14	B	851	CLA	CHD-C4C-C3C	-5.38	116.93	124.84
14	A	820	CLA	C4A-NA-C1A	-5.38	104.29	106.71
14	bA	830	CLA	C2C-C1C-NC	5.38	115.01	109.97
14	cB	824	CLA	O2D-CGD-CBD	5.38	120.83	111.27
14	B	823	CLA	O2D-CGD-CBD	5.38	120.82	111.27
14	B	838	CLA	CHD-C4C-C3C	-5.37	116.94	124.84
14	A	818	CLA	O2D-CGD-CBD	5.37	120.81	111.27
14	bB	815	CLA	CHD-C4C-C3C	-5.37	116.95	124.84
14	cA	831	CLA	C2C-C1C-NC	5.36	115.00	109.97
14	B	808	CLA	O2D-CGD-CBD	5.36	120.80	111.27
14	cB	839	CLA	CHD-C4C-C3C	-5.36	116.96	124.84
14	bB	808	CLA	O2D-CGD-CBD	5.36	120.80	111.27
14	bB	823	CLA	O2D-CGD-CBD	5.36	120.79	111.27
14	bA	818	CLA	O2D-CGD-CBD	5.36	120.79	111.27
14	cB	816	CLA	CHD-C4C-C3C	-5.36	116.97	124.84
14	bB	827	CLA	CHD-C4C-C3C	-5.35	116.97	124.84
14	cA	820	CLA	C4A-NA-C1A	-5.35	104.30	106.71
14	B	809	CLA	C2B-C1B-NB	5.35	113.82	110.23
14	cA	818	CLA	O2D-CGD-CBD	5.35	120.77	111.27
14	bB	806	CLA	CHD-C4C-C3C	-5.35	116.98	124.84
14	B	829	CLA	C2C-C1C-NC	5.35	114.98	109.97
14	B	815	CLA	CHD-C4C-C3C	-5.34	116.98	124.84
14	cB	809	CLA	O2D-CGD-CBD	5.34	120.76	111.27
14	B	827	CLA	CHD-C4C-C3C	-5.34	116.99	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	830	CLA	C2C-C1C-NC	5.34	114.98	109.97
14	bB	831	CLA	O2D-CGD-CBD	5.34	120.76	111.27
13	bA	801	CL0	O2D-CGD-CBD	5.34	120.76	111.27
14	A	824	CLA	CHD-C4C-C3C	-5.34	116.99	124.84
14	cA	810	CLA	C2C-C1C-NC	5.34	114.97	109.97
14	B	806	CLA	CHD-C4C-C3C	-5.34	117.00	124.84
14	cB	807	CLA	CHD-C4C-C3C	-5.34	117.00	124.84
14	cB	828	CLA	CHD-C4C-C3C	-5.34	117.00	124.84
14	B	831	CLA	O2D-CGD-CBD	5.33	120.75	111.27
14	bA	820	CLA	C4A-NA-C1A	-5.33	104.31	106.71
14	bA	852	CLA	CHD-C4C-C3C	-5.33	117.00	124.84
14	cB	832	CLA	O2D-CGD-CBD	5.33	120.74	111.27
14	bB	830	CLA	CHD-C4C-C3C	-5.33	117.01	124.84
14	B	819	CLA	CHD-C4C-C3C	-5.33	117.01	124.84
14	cA	824	CLA	CHD-C4C-C3C	-5.33	117.01	124.84
14	cB	817	CLA	C4A-NA-C1A	-5.33	104.31	106.71
14	cA	852	CLA	CHD-C4C-C3C	-5.33	117.01	124.84
14	bB	809	CLA	C2B-C1B-NB	5.33	113.80	110.23
14	A	852	CLA	CHD-C4C-C3C	-5.33	117.01	124.84
14	bA	824	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
14	bB	819	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
14	cB	820	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
14	cB	831	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
14	bA	837	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
14	bA	810	CLA	C2C-C1C-NC	5.32	114.95	109.97
14	cB	810	CLA	C2B-C1B-NB	5.32	113.80	110.23
13	A	801	CL0	O2D-CGD-CBD	5.32	120.72	111.27
14	A	810	CLA	C2C-C1C-NC	5.32	114.95	109.97
14	bA	808	CLA	CHD-C4C-C3C	-5.32	117.03	124.84
14	cA	852	CLA	C2B-C1B-NB	5.31	113.80	110.23
14	bB	808	CLA	C2C-C1C-NC	5.31	114.95	109.97
13	cA	801	CL0	O2D-CGD-CBD	5.31	120.71	111.27
14	cB	830	CLA	O2D-CGD-CBD	5.31	120.71	111.27
14	B	830	CLA	CHD-C4C-C3C	-5.31	117.03	124.84
14	A	831	CLA	CHD-C4C-C3C	-5.31	117.03	124.84
14	A	816	CLA	CHD-C4C-C3C	-5.31	117.03	124.84
14	cA	837	CLA	CHD-C4C-C3C	-5.31	117.03	124.84
14	bB	829	CLA	C2C-C1C-NC	5.31	114.95	109.97
14	A	837	CLA	CHD-C4C-C3C	-5.31	117.04	124.84
14	cA	816	CLA	CHD-C4C-C3C	-5.31	117.04	124.84
14	A	808	CLA	CHD-C4C-C3C	-5.31	117.04	124.84
14	A	852	CLA	C2B-C1B-NB	5.31	113.79	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bA	816	CLA	CHD-C4C-C3C	-5.31	117.04	124.84
14	cB	830	CLA	C2C-C1C-NC	5.31	114.94	109.97
14	cA	808	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
14	cA	815	CLA	C2C-C1C-NC	5.30	114.94	109.97
14	bA	831	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
14	A	852	CLA	CHD-C1D-ND	-5.30	119.58	124.45
14	B	829	CLA	O2D-CGD-CBD	5.30	120.68	111.27
14	B	823	CLA	C2C-C1C-NC	5.30	114.94	109.97
14	cB	824	CLA	C2C-C1C-NC	5.29	114.93	109.97
14	bB	829	CLA	O2D-CGD-CBD	5.29	120.67	111.27
14	B	808	CLA	C2C-C1C-NC	5.29	114.93	109.97
14	cB	835	CLA	C2C-C1C-NC	5.29	114.93	109.97
14	bB	816	CLA	C4A-NA-C1A	-5.29	104.33	106.71
14	bB	823	CLA	C2C-C1C-NC	5.28	114.92	109.97
14	B	816	CLA	C4A-NA-C1A	-5.28	104.33	106.71
14	cA	831	CLA	CHD-C4C-C3C	-5.28	117.08	124.84
14	bA	815	CLA	C2C-C1C-NC	5.28	114.92	109.97
14	cL	202	CLA	CHD-C4C-C3C	-5.28	117.08	124.84
14	bA	852	CLA	C2B-C1B-NB	5.27	113.77	110.23
14	cB	809	CLA	C2C-C1C-NC	5.27	114.91	109.97
14	bB	834	CLA	C2C-C1C-NC	5.27	114.91	109.97
14	bB	836	CLA	CHD-C4C-C3C	-5.27	117.10	124.84
14	bB	809	CLA	CHD-C1D-ND	-5.27	119.61	124.45
14	bA	842	CLA	C2C-C1C-NC	5.26	114.90	109.97
14	bA	852	CLA	CHD-C1D-ND	-5.26	119.62	124.45
14	B	836	CLA	CHD-C4C-C3C	-5.26	117.10	124.84
14	cA	814	CLA	CHD-C4C-C3C	-5.26	117.11	124.84
14	cA	852	CLA	CHD-C1D-ND	-5.26	119.62	124.45
14	bA	814	CLA	CHD-C4C-C3C	-5.26	117.11	124.84
14	B	834	CLA	C2C-C1C-NC	5.26	114.90	109.97
14	cB	837	CLA	CHD-C4C-C3C	-5.26	117.11	124.84
14	bA	817	CLA	CHD-C4C-C3C	-5.25	117.12	124.84
14	bL	201	CLA	CHD-C4C-C3C	-5.25	117.12	124.84
14	cA	817	CLA	CHD-C4C-C3C	-5.25	117.12	124.84
14	cA	842	CLA	C2C-C1C-NC	5.25	114.89	109.97
14	bX	201	CLA	CHD-C4C-C3C	-5.25	117.12	124.84
14	A	842	CLA	C2C-C1C-NC	5.25	114.89	109.97
14	A	814	CLA	CHD-C4C-C3C	-5.25	117.13	124.84
14	B	808	CLA	CHD-C4C-C3C	-5.25	117.13	124.84
14	A	817	CLA	CHD-C4C-C3C	-5.24	117.13	124.84
14	X	201	CLA	CHD-C4C-C3C	-5.24	117.13	124.84
14	cB	803	CLA	CHD-C4C-C3C	-5.24	117.13	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cJ	102	CLA	CHD-C4C-C3C	-5.24	117.13	124.84
14	L	201	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
14	A	815	CLA	C2C-C1C-NC	5.24	114.88	109.97
14	bA	809	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
14	bA	842	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
14	cX	201	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
14	B	802	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
14	bJ	102	CLA	CHD-C4C-C3C	-5.23	117.15	124.84
14	L	204	CLA	O2D-CGD-CBD	5.23	120.56	111.27
13	cA	801	CL0	CHD-C4C-C3C	-5.23	117.15	124.84
14	bB	802	CLA	CHD-C4C-C3C	-5.23	117.15	124.84
14	cL	205	CLA	O2D-CGD-CBD	5.23	120.56	111.27
14	A	842	CLA	CHD-C4C-C3C	-5.23	117.15	124.84
14	cA	828	CLA	C2C-C1C-NC	5.23	114.87	109.97
14	J	102	CLA	CHD-C4C-C3C	-5.23	117.16	124.84
13	A	801	CL0	CHD-C4C-C3C	-5.23	117.16	124.84
14	bA	838	CLA	CHD-C4C-C3C	-5.23	117.16	124.84
14	cA	809	CLA	CHD-C4C-C3C	-5.23	117.16	124.84
14	bB	808	CLA	CHD-C4C-C3C	-5.23	117.16	124.84
14	B	809	CLA	CHD-C1D-ND	-5.23	119.65	124.45
14	cB	809	CLA	CHD-C4C-C3C	-5.22	117.16	124.84
14	cB	825	CLA	CHD-C4C-C3C	-5.22	117.16	124.84
14	A	809	CLA	CHD-C4C-C3C	-5.22	117.16	124.84
14	cA	838	CLA	CHD-C4C-C3C	-5.22	117.16	124.84
13	bA	801	CL0	CHD-C4C-C3C	-5.22	117.17	124.84
14	A	838	CLA	CHD-C4C-C3C	-5.22	117.17	124.84
14	bL	203	CLA	O2D-CGD-CBD	5.22	120.54	111.27
14	cB	810	CLA	CHD-C1D-ND	-5.22	119.66	124.45
14	bL	204	CLA	O2D-CGD-CBD	5.22	120.54	111.27
14	bB	809	CLA	CHD-C4C-C3C	-5.22	117.17	124.84
14	bA	804	CLA	C3B-C2B-C1B	-5.21	100.87	107.16
14	cB	810	CLA	CHD-C4C-C3C	-5.21	117.18	124.84
14	cA	842	CLA	CHD-C4C-C3C	-5.21	117.18	124.84
14	cL	204	CLA	O2D-CGD-CBD	5.21	120.53	111.27
14	B	826	CLA	CHD-C4C-C3C	-5.21	117.18	124.84
14	L	203	CLA	C2C-C1C-NC	5.21	114.85	109.97
14	B	809	CLA	CHD-C4C-C3C	-5.21	117.19	124.84
14	bB	826	CLA	CHD-C4C-C3C	-5.21	117.19	124.84
14	cA	804	CLA	C3B-C2B-C1B	-5.20	100.88	107.16
14	B	821	CLA	C2C-C1C-NC	5.20	114.85	109.97
14	bB	824	CLA	CHD-C4C-C3C	-5.20	117.19	124.84
14	cA	839	CLA	CHD-C4C-C3C	-5.20	117.19	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bB	824	CLA	C3B-C2B-C1B	-5.20	100.88	107.16
14	B	824	CLA	CHD-C4C-C3C	-5.20	117.20	124.84
14	L	203	CLA	O2D-CGD-CBD	5.20	120.51	111.27
14	cB	822	CLA	C2C-C1C-NC	5.20	114.84	109.97
14	bB	833	CLA	CHD-C4C-C3C	-5.20	117.20	124.84
14	A	804	CLA	CHD-C4C-C3C	-5.20	117.20	124.84
14	bB	837	CLA	C2C-C1C-NC	5.20	114.84	109.97
14	bA	815	CLA	CHD-C4C-C3C	-5.20	117.20	124.84
14	cA	810	CLA	CHD-C4C-C3C	-5.19	117.20	124.84
14	bA	810	CLA	CHD-C4C-C3C	-5.19	117.20	124.84
14	cB	827	CLA	CHD-C4C-C3C	-5.19	117.20	124.84
14	A	839	CLA	CHD-C4C-C3C	-5.19	117.21	124.84
14	cB	825	CLA	C3B-C2B-C1B	-5.19	100.89	107.16
14	bA	828	CLA	C2C-C1C-NC	5.19	114.84	109.97
14	B	833	CLA	CHD-C4C-C3C	-5.19	117.21	124.84
14	bA	839	CLA	CHD-C4C-C3C	-5.19	117.21	124.84
14	B	824	CLA	C3B-C2B-C1B	-5.19	100.90	107.16
14	A	804	CLA	C3B-C2B-C1B	-5.19	100.90	107.16
14	bA	804	CLA	CHD-C4C-C3C	-5.19	117.22	124.84
14	A	828	CLA	C2C-C1C-NC	5.19	114.83	109.97
14	bB	821	CLA	C2C-C1C-NC	5.19	114.83	109.97
14	bL	203	CLA	C2C-C1C-NC	5.19	114.83	109.97
14	cB	814	CLA	C2C-C1C-NC	5.19	114.83	109.97
14	cA	804	CLA	CHD-C4C-C3C	-5.19	117.22	124.84
14	bB	813	CLA	C2C-C1C-NC	5.18	114.83	109.97
14	A	810	CLA	CHD-C4C-C3C	-5.18	117.22	124.84
14	bA	821	CLA	C2C-C1C-NC	5.18	114.83	109.97
14	bA	841	CLA	CHD-C1D-ND	-5.18	119.69	124.45
14	B	837	CLA	C2C-C1C-NC	5.18	114.82	109.97
14	cB	838	CLA	C2C-C1C-NC	5.18	114.82	109.97
14	A	815	CLA	CHD-C4C-C3C	-5.18	117.23	124.84
14	cA	815	CLA	CHD-C4C-C3C	-5.18	117.23	124.84
14	bB	801	CLA	CMD-C2D-C1D	5.18	133.84	124.71
14	B	813	CLA	C2C-C1C-NC	5.18	114.82	109.97
14	B	801	CLA	CMD-C2D-C1D	5.17	133.83	124.71
14	cL	204	CLA	C2C-C1C-NC	5.17	114.82	109.97
14	bA	840	CLA	CHD-C4C-C3C	-5.17	117.24	124.84
14	B	803	CLA	CHD-C1D-ND	-5.17	119.70	124.45
14	bL	201	CLA	C3D-C2D-C1D	-5.17	98.77	105.83
14	cB	834	CLA	CHD-C4C-C3C	-5.17	117.24	124.84
14	L	201	CLA	C3D-C2D-C1D	-5.17	98.78	105.83
14	B	835	CLA	CHD-C4C-C3C	-5.17	117.24	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bA	824	CLA	C2C-C1C-NC	5.17	114.81	109.97
14	A	840	CLA	CHD-C4C-C3C	-5.16	117.25	124.84
14	cL	202	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
14	cB	802	CLA	CMD-C2D-C1D	5.16	133.81	124.71
14	cB	836	CLA	CHD-C4C-C3C	-5.16	117.26	124.84
14	A	821	CLA	CHD-C4C-C3C	-5.16	117.26	124.84
14	cA	821	CLA	C2C-C1C-NC	5.16	114.80	109.97
14	bB	835	CLA	CHD-C4C-C3C	-5.16	117.26	124.84
14	bB	812	CLA	CHD-C4C-C3C	-5.16	117.26	124.84
14	cB	813	CLA	CHD-C4C-C3C	-5.16	117.26	124.84
14	cA	840	CLA	CHD-C4C-C3C	-5.16	117.26	124.84
14	cA	836	CLA	C2C-C1C-NC	5.15	114.80	109.97
14	B	812	CLA	CHD-C4C-C3C	-5.15	117.27	124.84
14	A	821	CLA	C2C-C1C-NC	5.15	114.80	109.97
14	A	841	CLA	CHD-C1D-ND	-5.15	119.72	124.45
14	A	834	CLA	C2C-C1C-NC	5.15	114.79	109.97
14	cA	822	CLA	C2C-C1C-NC	5.14	114.79	109.97
14	B	819	CLA	O2D-CGD-CBD	5.14	120.41	111.27
14	bA	822	CLA	C2C-C1C-NC	5.14	114.79	109.97
14	cB	820	CLA	O2D-CGD-CBD	5.14	120.41	111.27
14	A	822	CLA	C2C-C1C-NC	5.14	114.79	109.97
14	bA	836	CLA	C2C-C1C-NC	5.14	114.79	109.97
14	bA	839	CLA	C2C-C1C-NC	5.14	114.79	109.97
14	bB	819	CLA	O2D-CGD-CBD	5.14	120.40	111.27
14	bB	831	CLA	CHD-C4C-C3C	-5.14	117.29	124.84
14	bA	829	CLA	C2C-C1C-NC	5.14	114.78	109.97
14	bB	811	CLA	C2C-C1C-NC	5.14	114.78	109.97
14	cA	839	CLA	C2C-C1C-NC	5.14	114.78	109.97
14	A	836	CLA	C2C-C1C-NC	5.14	114.78	109.97
14	A	812	CLA	O2D-CGD-CBD	5.14	120.39	111.27
14	cA	812	CLA	O2D-CGD-CBD	5.14	120.39	111.27
14	B	808	CLA	CHD-C1D-ND	-5.14	119.73	124.45
14	cA	821	CLA	CHD-C4C-C3C	-5.14	117.29	124.84
14	bA	812	CLA	O2D-CGD-CBD	5.13	120.39	111.27
14	bA	821	CLA	CHD-C4C-C3C	-5.13	117.29	124.84
14	cA	835	CLA	C2C-C1C-NC	5.13	114.78	109.97
14	B	817	CLA	C3B-C2B-C1B	-5.13	100.97	107.16
14	cA	827	CLA	CHD-C4C-C3C	-5.13	117.30	124.84
14	bB	817	CLA	C3B-C2B-C1B	-5.13	100.97	107.16
14	cB	811	CLA	C2C-C1C-NC	5.13	114.78	109.97
14	A	839	CLA	C2C-C1C-NC	5.13	114.78	109.97
14	bA	827	CLA	CHD-C4C-C3C	-5.13	117.30	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	828	CLA	C3B-C2B-C1B	-5.13	100.97	107.16
14	bA	835	CLA	C2C-C1C-NC	5.12	114.77	109.97
14	cA	834	CLA	C2C-C1C-NC	5.12	114.77	109.97
14	cA	828	CLA	C3B-C2B-C1B	-5.12	100.97	107.16
14	cB	809	CLA	CHD-C1D-ND	-5.12	119.75	124.45
14	B	811	CLA	C2C-C1C-NC	5.12	114.77	109.97
14	cB	818	CLA	C3B-C2B-C1B	-5.12	100.98	107.16
14	J	101	CLA	CHD-C4C-C3C	-5.12	117.31	124.84
14	bA	829	CLA	CHD-C4C-C3C	-5.12	117.31	124.84
14	bB	807	CLA	CHD-C4C-C3C	-5.12	117.31	124.84
14	B	831	CLA	CHD-C4C-C3C	-5.12	117.31	124.84
14	cA	824	CLA	C2C-C1C-NC	5.12	114.77	109.97
14	bB	803	CLA	CHD-C1D-ND	-5.12	119.75	124.45
14	bJ	101	CLA	CHD-C4C-C3C	-5.12	117.31	124.84
14	cB	808	CLA	CHD-C4C-C3C	-5.12	117.31	124.84
14	cB	832	CLA	CHD-C4C-C3C	-5.12	117.31	124.84
14	cB	812	CLA	C2C-C1C-NC	5.12	114.77	109.97
14	bA	834	CLA	C2C-C1C-NC	5.12	114.77	109.97
14	A	827	CLA	CHD-C4C-C3C	-5.12	117.32	124.84
14	cJ	101	CLA	CHD-C4C-C3C	-5.12	117.32	124.84
14	A	824	CLA	C2C-C1C-NC	5.12	114.77	109.97
14	cB	836	CLA	C2C-C1C-NC	5.12	114.77	109.97
14	B	807	CLA	CHD-C4C-C3C	-5.11	117.32	124.84
14	bB	818	CLA	CHD-C4C-C3C	-5.11	117.32	124.84
14	cA	841	CLA	CHD-C1D-ND	-5.11	119.76	124.45
14	cA	829	CLA	CHD-C4C-C3C	-5.11	117.33	124.84
14	cB	804	CLA	CHD-C1D-ND	-5.11	119.76	124.45
14	A	835	CLA	C2C-C1C-NC	5.11	114.76	109.97
14	B	810	CLA	C2C-C1C-NC	5.11	114.76	109.97
14	bA	807	CLA	C2C-C1C-NC	5.11	114.76	109.97
14	A	829	CLA	CHD-C4C-C3C	-5.11	117.33	124.84
14	B	818	CLA	CHD-C4C-C3C	-5.10	117.34	124.84
14	B	835	CLA	C2C-C1C-NC	5.10	114.75	109.97
14	bB	810	CLA	C2C-C1C-NC	5.10	114.75	109.97
14	bA	828	CLA	C3B-C2B-C1B	-5.10	101.01	107.16
14	bA	835	CLA	CHD-C4C-C3C	-5.10	117.35	124.84
14	bB	835	CLA	C2C-C1C-NC	5.10	114.75	109.97
14	bB	811	CLA	CHD-C4C-C3C	-5.10	117.35	124.84
14	bB	808	CLA	CHD-C1D-ND	-5.10	119.77	124.45
14	cA	807	CLA	C2C-C1C-NC	5.09	114.75	109.97
14	A	825	CLA	C3D-C2D-C1D	-5.09	98.88	105.83
14	B	811	CLA	CHD-C4C-C3C	-5.09	117.35	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	835	CLA	CHD-C4C-C3C	-5.09	117.36	124.84
14	cA	835	CLA	CHD-C4C-C3C	-5.09	117.36	124.84
14	cB	819	CLA	CHD-C4C-C3C	-5.09	117.36	124.84
14	bA	814	CLA	C2C-C1C-NC	5.09	114.74	109.97
14	A	807	CLA	C2C-C1C-NC	5.08	114.73	109.97
14	cB	812	CLA	CHD-C4C-C3C	-5.08	117.37	124.84
14	A	829	CLA	C2C-C1C-NC	5.08	114.73	109.97
14	bA	825	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
14	A	805	CLA	O2D-CGD-CBD	5.08	120.29	111.27
14	cA	825	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
14	bA	805	CLA	O2D-CGD-CBD	5.08	120.29	111.27
14	A	837	CLA	C2C-C1C-NC	5.08	114.73	109.97
14	bA	837	CLA	C2C-C1C-NC	5.08	114.73	109.97
14	cA	805	CLA	O2D-CGD-CBD	5.08	120.29	111.27
14	cL	203	CLA	CHD-C4C-C3C	-5.08	117.38	124.84
14	cA	837	CLA	C2C-C1C-NC	5.07	114.73	109.97
14	L	202	CLA	CHD-C4C-C3C	-5.07	117.38	124.84
14	cA	829	CLA	C2C-C1C-NC	5.07	114.72	109.97
14	B	849	CLA	C2C-C1C-NC	5.07	114.72	109.97
14	B	837	CLA	CHD-C4C-C3C	-5.07	117.39	124.84
14	cA	814	CLA	C2C-C1C-NC	5.07	114.72	109.97
14	A	814	CLA	C2C-C1C-NC	5.07	114.72	109.97
14	cB	838	CLA	CHD-C4C-C3C	-5.06	117.40	124.84
14	B	802	CLA	CHD-C1D-ND	-5.06	119.80	124.45
14	A	832	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
14	bB	849	CLA	C2C-C1C-NC	5.06	114.71	109.97
14	bB	837	CLA	CHD-C4C-C3C	-5.06	117.41	124.84
14	bL	202	CLA	CHD-C4C-C3C	-5.06	117.41	124.84
14	B	851	CLA	O2D-CGD-CBD	5.05	120.25	111.27
14	cB	801	CLA	O2D-CGD-CBD	5.05	120.24	111.27
14	bJ	102	CLA	C2C-C1C-NC	5.05	114.70	109.97
14	cB	806	CLA	C2C-C1C-NC	5.05	114.70	109.97
14	cJ	102	CLA	C2C-C1C-NC	5.05	114.70	109.97
14	bA	832	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
14	bB	803	CLA	C3B-C2B-C1B	-5.05	101.07	107.16
14	bB	802	CLA	CHD-C1D-ND	-5.04	119.82	124.45
14	cA	832	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
14	cA	813	CLA	CHD-C4C-C3C	-5.04	117.43	124.84
14	bB	851	CLA	O2D-CGD-CBD	5.04	120.22	111.27
14	cB	804	CLA	C3B-C2B-C1B	-5.04	101.08	107.16
14	J	102	CLA	C2C-C1C-NC	5.04	114.69	109.97
14	A	813	CLA	CHD-C4C-C3C	-5.04	117.44	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	803	CLA	C3B-C2B-C1B	-5.04	101.08	107.16
14	bA	813	CLA	CHD-C4C-C3C	-5.04	117.44	124.84
14	cB	850	CLA	C2C-C1C-NC	5.04	114.69	109.97
14	B	837	CLA	C3B-C2B-C1B	-5.03	101.08	107.16
14	bA	822	CLA	C4A-NA-C1A	-5.03	104.44	106.71
13	cA	801	CL0	CHD-C1D-ND	-5.03	119.83	124.45
14	B	804	CLA	C3B-C2B-C1B	-5.03	101.09	107.16
14	bB	837	CLA	C3B-C2B-C1B	-5.03	101.09	107.16
14	A	825	CLA	C3B-C2B-C1B	-5.03	101.09	107.16
14	cA	825	CLA	C3B-C2B-C1B	-5.03	101.09	107.16
14	cB	803	CLA	CHD-C1D-ND	-5.03	119.84	124.45
14	bA	842	CLA	O2D-CGD-CBD	5.02	120.19	111.27
14	bA	825	CLA	C3B-C2B-C1B	-5.02	101.10	107.16
14	A	819	CLA	C2C-C1C-NC	5.02	114.67	109.97
14	cA	820	CLA	C3D-C4D-ND	5.02	118.35	110.24
14	bA	820	CLA	C3D-C4D-ND	5.02	118.35	110.24
14	A	842	CLA	O2D-CGD-CBD	5.02	120.18	111.27
14	bB	839	CLA	C3D-C2D-C1D	-5.02	98.99	105.83
14	A	820	CLA	C3D-C4D-ND	5.02	118.35	110.24
14	bB	805	CLA	C2C-C1C-NC	5.01	114.67	109.97
14	B	823	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
14	bB	823	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
14	cB	805	CLA	C3B-C2B-C1B	-5.01	101.11	107.16
14	bA	806	CLA	C2C-C1C-NC	5.01	114.67	109.97
14	cB	819	CLA	C2C-C1C-NC	5.01	114.67	109.97
14	cB	850	CLA	CHD-C4C-C3C	-5.01	117.48	124.84
14	cA	842	CLA	O2D-CGD-CBD	5.01	120.17	111.27
14	B	805	CLA	C2C-C1C-NC	5.01	114.66	109.97
14	cB	838	CLA	C3B-C2B-C1B	-5.01	101.12	107.16
14	B	839	CLA	C3D-C2D-C1D	-5.01	99.00	105.83
14	cA	819	CLA	C2C-C1C-NC	5.00	114.66	109.97
14	bB	804	CLA	C3B-C2B-C1B	-5.00	101.12	107.16
14	A	806	CLA	C2C-C1C-NC	5.00	114.66	109.97
14	bA	819	CLA	C2C-C1C-NC	5.00	114.66	109.97
14	cL	205	CLA	CHD-C4C-C3C	-5.00	117.49	124.84
14	cB	840	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
14	cB	821	CLA	C2C-C1C-NC	5.00	114.66	109.97
14	A	825	CLA	C2C-C1C-NC	5.00	114.66	109.97
14	B	849	CLA	CHD-C4C-C3C	-5.00	117.49	124.84
14	cA	836	CLA	C3B-C2B-C1B	-5.00	101.13	107.16
14	bB	849	CLA	CHD-C4C-C3C	-5.00	117.50	124.84
14	bL	204	CLA	CHD-C4C-C3C	-5.00	117.50	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bA	825	CLA	C2C-C1C-NC	4.99	114.65	109.97
14	cB	824	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
14	cA	822	CLA	C4A-NA-C1A	-4.99	104.46	106.71
14	L	204	CLA	CHD-C4C-C3C	-4.99	117.50	124.84
14	A	809	CLA	C2C-C1C-NC	4.99	114.65	109.97
14	cA	806	CLA	C2C-C1C-NC	4.99	114.65	109.97
14	bA	836	CLA	C3B-C2B-C1B	-4.99	101.14	107.16
13	bA	801	CL0	CHD-C1D-ND	-4.99	119.87	124.45
14	bB	820	CLA	C2C-C1C-NC	4.99	114.64	109.97
14	cA	841	CLA	CHD-C4C-C3C	-4.99	117.51	124.84
14	A	818	CLA	CHD-C4C-C3C	-4.99	117.51	124.84
14	bA	811	CLA	CHD-C4C-C3C	-4.99	117.51	124.84
14	cA	818	CLA	CHD-C4C-C3C	-4.99	117.51	124.84
13	A	801	CL0	CHD-C1D-ND	-4.99	119.87	124.45
14	A	836	CLA	C3B-C2B-C1B	-4.98	101.14	107.16
14	bA	841	CLA	CHD-C4C-C3C	-4.98	117.51	124.84
14	cA	825	CLA	C2C-C1C-NC	4.98	114.64	109.97
14	A	811	CLA	CHD-C4C-C3C	-4.98	117.52	124.84
14	A	841	CLA	CHD-C4C-C3C	-4.98	117.52	124.84
14	cA	838	CLA	C2C-C1C-NC	4.98	114.64	109.97
14	cA	827	CLA	C3B-C2B-C1B	-4.98	101.15	107.16
14	A	838	CLA	C2C-C1C-NC	4.98	114.64	109.97
14	bA	819	CLA	O2D-CGD-CBD	4.98	120.11	111.27
14	A	819	CLA	O2D-CGD-CBD	4.98	120.11	111.27
14	bA	809	CLA	C2C-C1C-NC	4.98	114.63	109.97
14	bA	818	CLA	CHD-C4C-C3C	-4.97	117.53	124.84
14	bA	827	CLA	C3B-C2B-C1B	-4.97	101.16	107.16
14	cA	819	CLA	O2D-CGD-CBD	4.97	120.10	111.27
14	A	822	CLA	C4A-NA-C1A	-4.97	104.47	106.71
14	cA	811	CLA	CHD-C4C-C3C	-4.97	117.54	124.84
14	bA	803	CLA	C2C-C1C-NC	4.97	114.62	109.97
14	bB	818	CLA	C2C-C1C-NC	4.97	114.62	109.97
14	cB	810	CLA	CMD-C2D-C1D	4.97	133.47	124.71
14	cB	817	CLA	CHD-C4C-C3C	-4.97	117.54	124.84
14	L	201	CLA	O2D-CGD-CBD	4.97	120.09	111.27
14	bB	809	CLA	CMD-C2D-C1D	4.96	133.46	124.71
14	A	827	CLA	C3B-C2B-C1B	-4.96	101.17	107.16
14	bB	816	CLA	CHD-C4C-C3C	-4.96	117.55	124.84
14	B	809	CLA	CMD-C2D-C1D	4.96	133.46	124.71
14	A	803	CLA	C2C-C1C-NC	4.96	114.62	109.97
14	cA	803	CLA	C2C-C1C-NC	4.96	114.62	109.97
14	B	816	CLA	CHD-C4C-C3C	-4.96	117.55	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	803	CLA	CHD-C4C-C3C	-4.95	117.56	124.84
14	B	818	CLA	C2C-C1C-NC	4.95	114.61	109.97
14	bA	803	CLA	CHD-C4C-C3C	-4.95	117.56	124.84
14	B	820	CLA	C2C-C1C-NC	4.95	114.61	109.97
14	bA	838	CLA	C2C-C1C-NC	4.95	114.61	109.97
14	cA	809	CLA	C2C-C1C-NC	4.95	114.61	109.97
14	bA	813	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
14	bB	809	CLA	O2D-CGD-CBD	4.95	120.06	111.27
14	cA	802	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
14	B	812	CLA	O2D-CGD-CBD	4.94	120.06	111.27
14	bA	830	CLA	CHD-C4C-C3C	-4.94	117.57	124.84
14	cL	202	CLA	O2D-CGD-CBD	4.94	120.05	111.27
14	bA	802	CLA	C3D-C2D-C1D	-4.94	99.08	105.83
14	A	807	CLA	CAC-C3C-C4C	4.94	131.22	124.81
14	cB	810	CLA	O2D-CGD-CBD	4.94	120.05	111.27
14	A	813	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
14	cA	813	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
14	B	809	CLA	O2D-CGD-CBD	4.94	120.05	111.27
14	bL	201	CLA	O2D-CGD-CBD	4.94	120.05	111.27
14	cA	803	CLA	CHD-C4C-C3C	-4.94	117.58	124.84
14	A	802	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
14	cB	813	CLA	O2D-CGD-CBD	4.94	120.04	111.27
14	cA	833	CLA	C3B-C2B-C1B	-4.94	101.20	107.16
14	bB	822	CLA	C3B-C2B-C1B	-4.94	101.20	107.16
14	A	840	CLA	O2D-CGD-CBD	4.94	120.04	111.27
14	bA	840	CLA	O2D-CGD-CBD	4.93	120.03	111.27
14	bB	812	CLA	O2D-CGD-CBD	4.93	120.03	111.27
14	L	202	CLA	O2D-CGD-CBD	4.93	120.03	111.27
14	A	830	CLA	CHD-C4C-C3C	-4.93	117.59	124.84
14	B	822	CLA	C3B-C2B-C1B	-4.93	101.21	107.16
14	L	203	CLA	C3B-C2B-C1B	-4.93	101.21	107.16
14	cA	807	CLA	CAC-C3C-C4C	4.93	131.21	124.81
14	cA	830	CLA	CHD-C4C-C3C	-4.93	117.60	124.84
14	bA	833	CLA	C3B-C2B-C1B	-4.93	101.22	107.16
14	cB	823	CLA	C3B-C2B-C1B	-4.93	101.22	107.16
14	B	818	CLA	C4A-NA-C1A	-4.92	104.49	106.71
14	bA	807	CLA	CAC-C3C-C4C	4.92	131.20	124.81
14	cB	835	CLA	O2D-CGD-CBD	4.92	120.02	111.27
14	cA	806	CLA	C3D-C2D-C1D	-4.92	99.11	105.83
14	bB	804	CLA	CHD-C4C-C3C	-4.92	117.61	124.84
14	B	806	CLA	C2C-C1C-NC	4.92	114.58	109.97
14	A	833	CLA	C3B-C2B-C1B	-4.92	101.22	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	818	CLA	C4A-NA-C1A	-4.92	104.50	106.71
14	cL	204	CLA	C3B-C2B-C1B	-4.92	101.22	107.16
14	bL	202	CLA	O2D-CGD-CBD	4.92	120.01	111.27
14	bB	826	CLA	C3D-C2D-C1D	-4.92	99.12	105.83
14	cL	203	CLA	O2D-CGD-CBD	4.92	120.00	111.27
14	B	817	CLA	C2C-C1C-NC	4.91	114.58	109.97
14	cA	840	CLA	O2D-CGD-CBD	4.91	120.00	111.27
14	B	826	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
14	bB	834	CLA	O2D-CGD-CBD	4.91	120.00	111.27
14	bA	806	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
14	A	813	CLA	CAC-C3C-C4C	4.91	131.18	124.81
14	bB	806	CLA	C2C-C1C-NC	4.91	114.57	109.97
14	bB	812	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
14	cB	813	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
14	cB	831	CLA	C2C-C1C-NC	4.91	114.57	109.97
14	B	814	CLA	C3B-C2B-C1B	-4.91	101.23	107.16
14	B	834	CLA	O2D-CGD-CBD	4.91	119.99	111.27
14	cB	805	CLA	CHD-C4C-C3C	-4.91	117.63	124.84
14	B	830	CLA	C2C-C1C-NC	4.91	114.57	109.97
14	bJ	101	CLA	C2C-C1C-NC	4.91	114.57	109.97
14	cB	818	CLA	C2C-C1C-NC	4.91	114.57	109.97
14	bB	822	CLA	C2C-C1C-NC	4.91	114.57	109.97
14	cB	815	CLA	C3B-C2B-C1B	-4.90	101.24	107.16
14	cB	827	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
14	B	804	CLA	CHD-C4C-C3C	-4.90	117.63	124.84
14	B	829	CLA	C3B-C2B-C1B	-4.90	101.24	107.16
14	bL	203	CLA	C3B-C2B-C1B	-4.90	101.25	107.16
14	B	812	CLA	C3D-C2D-C1D	-4.90	99.15	105.83
14	A	806	CLA	C3D-C2D-C1D	-4.90	99.15	105.83
14	B	825	CLA	C3D-C2D-C1D	-4.90	99.15	105.83
14	X	201	CLA	C2C-C1C-NC	4.90	114.56	109.97
14	cA	818	CLA	C4A-NA-C1A	-4.90	104.50	106.71
14	cA	813	CLA	CAC-C3C-C4C	4.89	131.16	124.81
14	A	816	CLA	C3B-C2B-C1B	-4.89	101.25	107.16
14	cB	830	CLA	C3B-C2B-C1B	-4.89	101.25	107.16
14	bB	825	CLA	C3D-C2D-C1D	-4.89	99.15	105.83
14	bA	826	CLA	C3D-C2D-C1D	-4.89	99.15	105.83
14	bL	201	CLA	CHD-C1D-ND	-4.89	119.96	124.45
14	bA	820	CLA	C2C-C1C-NC	4.89	114.56	109.97
14	bB	825	CLA	O2D-CGD-CBD	4.89	119.96	111.27
14	B	825	CLA	O2D-CGD-CBD	4.89	119.96	111.27
14	bA	816	CLA	C3B-C2B-C1B	-4.89	101.26	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bB	812	CLA	CAC-C3C-C4C	4.89	131.15	124.81
14	bB	814	CLA	C3B-C2B-C1B	-4.89	101.26	107.16
14	bA	813	CLA	CAC-C3C-C4C	4.89	131.15	124.81
14	cA	826	CLA	C3B-C2B-C1B	-4.89	101.26	107.16
14	bB	810	CLA	CHD-C4C-C3C	-4.88	117.66	124.84
14	cB	826	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
14	bB	829	CLA	C3B-C2B-C1B	-4.88	101.27	107.16
14	cB	819	CLA	O2D-CGD-CBD	4.88	119.94	111.27
14	A	826	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
14	cA	821	CLA	C3B-C2B-C1B	-4.88	101.27	107.16
14	cX	201	CLA	C2C-C1C-NC	4.88	114.54	109.97
14	cB	819	CLA	C4A-NA-C1A	-4.88	104.51	106.71
14	bB	817	CLA	C2C-C1C-NC	4.88	114.54	109.97
14	cB	826	CLA	O2D-CGD-CBD	4.88	119.94	111.27
14	A	820	CLA	C2C-C1C-NC	4.88	114.54	109.97
14	J	101	CLA	C2C-C1C-NC	4.88	114.54	109.97
14	bX	201	CLA	C2C-C1C-NC	4.88	114.54	109.97
14	bA	826	CLA	C3B-C2B-C1B	-4.88	101.27	107.16
14	cL	202	CLA	CHD-C1D-ND	-4.88	119.97	124.45
14	bA	834	CLA	C4A-NA-C1A	-4.88	104.51	106.71
14	bB	818	CLA	C4A-NA-C1A	-4.88	104.51	106.71
14	cB	834	CLA	C2C-C1C-NC	4.88	114.54	109.97
14	bB	830	CLA	C2C-C1C-NC	4.87	114.54	109.97
14	bA	814	CLA	C3B-C2B-C1B	-4.87	101.28	107.16
14	bB	818	CLA	O2D-CGD-CBD	4.87	119.93	111.27
14	B	818	CLA	O2D-CGD-CBD	4.87	119.93	111.27
14	cB	813	CLA	CAC-C3C-C4C	4.87	131.13	124.81
14	bA	818	CLA	C4A-NA-C1A	-4.87	104.52	106.71
14	A	821	CLA	C3B-C2B-C1B	-4.87	101.28	107.16
14	cB	836	CLA	O2D-CGD-CBD	4.87	119.92	111.27
14	B	828	CLA	C3D-C4D-ND	4.87	118.11	110.24
14	cB	811	CLA	CHD-C4C-C3C	-4.87	117.69	124.84
14	B	822	CLA	C2C-C1C-NC	4.87	114.53	109.97
14	cB	807	CLA	C2C-C1C-NC	4.87	114.53	109.97
14	bB	828	CLA	C3D-C4D-ND	4.87	118.11	110.24
14	cA	816	CLA	C3B-C2B-C1B	-4.87	101.29	107.16
14	B	812	CLA	CAC-C3C-C4C	4.87	131.12	124.81
14	cB	829	CLA	C3D-C4D-ND	4.87	118.11	110.24
14	B	810	CLA	CHD-C4C-C3C	-4.87	117.69	124.84
14	L	203	CLA	C3D-C4D-ND	4.87	118.11	110.24
14	B	835	CLA	O2D-CGD-CBD	4.86	119.91	111.27
14	cB	823	CLA	C2C-C1C-NC	4.86	114.53	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	L	201	CLA	CHD-C1D-ND	-4.86	119.99	124.45
14	bA	821	CLA	C3B-C2B-C1B	-4.86	101.30	107.16
14	cB	828	CLA	C2C-C1C-NC	4.86	114.52	109.97
14	cA	826	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
14	B	839	CLA	CHD-C4C-C3C	-4.86	117.70	124.84
14	cB	840	CLA	CHD-C4C-C3C	-4.86	117.70	124.84
17	J	103	BCR	C15-C16-C17	4.86	133.42	123.47
14	A	839	CLA	C3B-C2B-C1B	-4.86	101.30	107.16
14	bB	827	CLA	C3B-C2B-C1B	-4.86	101.30	107.16
14	cA	814	CLA	C3B-C2B-C1B	-4.86	101.30	107.16
14	B	805	CLA	CHD-C4C-C3C	-4.85	117.70	124.84
14	bB	839	CLA	CHD-C4C-C3C	-4.85	117.70	124.84
14	cA	822	CLA	O2D-CGD-CBD	4.85	119.89	111.27
14	bL	203	CLA	C3D-C4D-ND	4.85	118.09	110.24
14	cJ	101	CLA	C2C-C1C-NC	4.85	114.52	109.97
14	cA	820	CLA	C2C-C1C-NC	4.85	114.52	109.97
14	A	826	CLA	C3B-C2B-C1B	-4.85	101.31	107.16
17	bJ	103	BCR	C15-C16-C17	4.85	133.41	123.47
14	bB	835	CLA	O2D-CGD-CBD	4.85	119.89	111.27
14	A	814	CLA	C3B-C2B-C1B	-4.85	101.31	107.16
14	cL	204	CLA	C3D-C4D-ND	4.85	118.08	110.24
14	A	822	CLA	CHD-C4C-C3C	-4.85	117.71	124.84
14	cB	814	CLA	C3D-C4D-ND	4.85	118.08	110.24
17	cJ	103	BCR	C15-C16-C17	4.84	133.40	123.47
14	cA	820	CLA	CHD-C4C-C3C	-4.84	117.72	124.84
14	A	822	CLA	O2D-CGD-CBD	4.84	119.87	111.27
14	bB	832	CLA	C2C-C1C-NC	4.84	114.51	109.97
14	cB	802	CLA	C3B-C2B-C1B	-4.84	101.32	107.16
14	cB	828	CLA	C3B-C2B-C1B	-4.84	101.32	107.16
14	bA	822	CLA	O2D-CGD-CBD	4.84	119.87	111.27
14	B	827	CLA	C3B-C2B-C1B	-4.84	101.32	107.16
14	bB	801	CLA	C3B-C2B-C1B	-4.84	101.32	107.16
14	cA	822	CLA	CHD-C4C-C3C	-4.84	117.73	124.84
14	bA	823	CLA	C2C-C1C-NC	4.84	114.50	109.97
14	bA	822	CLA	CHD-C4C-C3C	-4.84	117.73	124.84
14	B	813	CLA	C3D-C4D-ND	4.84	118.06	110.24
14	cA	839	CLA	C3B-C2B-C1B	-4.84	101.32	107.16
14	B	831	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
14	bB	813	CLA	C3D-C4D-ND	4.84	118.06	110.24
14	B	827	CLA	C2C-C1C-NC	4.83	114.50	109.97
14	bB	805	CLA	CHD-C4C-C3C	-4.83	117.74	124.84
14	cA	823	CLA	CHD-C4C-C3C	-4.83	117.74	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	833	CLA	C2C-C1C-NC	4.83	114.50	109.97
14	cB	815	CLA	C2C-C1C-NC	4.83	114.50	109.97
14	bB	827	CLA	C2C-C1C-NC	4.83	114.50	109.97
14	bA	839	CLA	C3B-C2B-C1B	-4.83	101.33	107.16
14	B	801	CLA	C3B-C2B-C1B	-4.83	101.33	107.16
14	A	820	CLA	CHD-C4C-C3C	-4.83	117.75	124.84
14	cB	806	CLA	CHD-C4C-C3C	-4.83	117.75	124.84
14	B	814	CLA	C2C-C1C-NC	4.83	114.49	109.97
14	cB	833	CLA	C2C-C1C-NC	4.83	114.49	109.97
14	bB	814	CLA	C2C-C1C-NC	4.82	114.49	109.97
14	bA	823	CLA	CHD-C4C-C3C	-4.82	117.75	124.84
14	bB	831	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
14	cB	832	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
14	cA	812	CLA	CHD-C4C-C3C	-4.82	117.75	124.84
14	J	101	CLA	O2D-CGD-CBD	4.82	119.83	111.27
14	bF	201	CLA	C2C-C1C-NC	4.82	114.49	109.97
14	bA	820	CLA	CHD-C4C-C3C	-4.82	117.76	124.84
14	B	832	CLA	C2C-C1C-NC	4.82	114.49	109.97
14	A	834	CLA	C4A-NA-C1A	-4.82	104.54	106.71
14	B	823	CLA	C3B-C2B-C1B	-4.82	101.35	107.16
14	cA	823	CLA	C2C-C1C-NC	4.82	114.48	109.97
14	bL	203	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
14	L	203	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
14	cL	204	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
14	bA	805	CLA	C2C-C1C-NC	4.82	114.48	109.97
14	bA	812	CLA	CHD-C4C-C3C	-4.81	117.76	124.84
14	cA	838	CLA	C3D-C4D-ND	4.81	118.03	110.24
14	B	851	CLA	C2C-C1C-NC	4.81	114.48	109.97
14	cJ	101	CLA	O2D-CGD-CBD	4.81	119.82	111.27
14	A	812	CLA	CHD-C4C-C3C	-4.81	117.77	124.84
14	bA	838	CLA	C3D-C4D-ND	4.81	118.02	110.24
14	A	823	CLA	CHD-C4C-C3C	-4.81	117.77	124.84
14	F	201	CLA	C2C-C1C-NC	4.81	114.48	109.97
14	bB	838	CLA	CHD-C1D-ND	-4.81	120.03	124.45
14	A	813	CLA	C4A-NA-C1A	-4.80	104.55	106.71
14	cB	839	CLA	CHD-C1D-ND	-4.80	120.04	124.45
14	bB	803	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
14	A	838	CLA	C3D-C4D-ND	4.80	118.00	110.24
14	A	805	CLA	CHD-C4C-C3C	-4.80	117.78	124.84
14	cB	801	CLA	C2C-C1C-NC	4.80	114.47	109.97
14	A	805	CLA	C2C-C1C-NC	4.80	114.47	109.97
14	cA	805	CLA	CHD-C4C-C3C	-4.80	117.79	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	823	CLA	C2C-C1C-NC	4.80	114.47	109.97
14	bA	805	CLA	CHD-C4C-C3C	-4.79	117.79	124.84
14	cB	807	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
14	bB	821	CLA	CAC-C3C-C4C	4.79	131.03	124.81
14	bJ	101	CLA	O2D-CGD-CBD	4.79	119.79	111.27
14	bB	816	CLA	C2C-C1C-NC	4.79	114.46	109.97
14	cB	824	CLA	C3B-C2B-C1B	-4.79	101.38	107.16
14	cB	801	CLA	C4A-NA-C1A	-4.79	104.55	106.71
14	bB	817	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
14	B	804	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
14	B	813	CLA	C3B-C2B-C1B	-4.79	101.38	107.16
14	cA	812	CLA	C3B-C2B-C1B	-4.79	101.38	107.16
14	cA	813	CLA	C4A-NA-C1A	-4.79	104.55	106.71
14	bB	851	CLA	C2C-C1C-NC	4.79	114.46	109.97
14	bB	806	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
14	B	817	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
14	B	803	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
14	cB	805	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
14	cA	805	CLA	C2C-C1C-NC	4.79	114.45	109.97
14	cB	831	CLA	C3B-C2B-C1B	-4.79	101.39	107.16
14	bB	823	CLA	C3B-C2B-C1B	-4.78	101.39	107.16
14	cF	201	CLA	C2C-C1C-NC	4.78	114.45	109.97
14	cB	804	CLA	C3D-C2D-C1D	-4.78	99.30	105.83
14	B	820	CLA	C3D-C4D-ND	4.78	117.97	110.24
14	bB	820	CLA	C3D-C4D-ND	4.78	117.97	110.24
14	B	806	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
14	cA	824	CLA	O2D-CGD-CBD	4.78	119.76	111.27
14	bB	813	CLA	C3B-C2B-C1B	-4.78	101.39	107.16
14	B	824	CLA	C2C-C1C-NC	4.78	114.45	109.97
14	bB	819	CLA	C2C-C1C-NC	4.78	114.45	109.97
14	cB	814	CLA	C3B-C2B-C1B	-4.78	101.39	107.16
14	cB	817	CLA	C2C-C1C-NC	4.78	114.45	109.97
14	A	824	CLA	O2D-CGD-CBD	4.78	119.76	111.27
14	bB	804	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
14	B	830	CLA	C3B-C2B-C1B	-4.77	101.40	107.16
14	cB	821	CLA	C3D-C4D-ND	4.77	117.96	110.24
14	cB	840	CLA	O2D-CGD-CBD	4.77	119.75	111.27
14	B	838	CLA	CHD-C1D-ND	-4.77	120.07	124.45
14	A	823	CLA	O2D-CGD-CBD	4.77	119.75	111.27
14	cA	840	CLA	C4A-NA-C1A	-4.77	104.56	106.71
14	cA	830	CLA	C3B-C2B-C1B	-4.77	101.40	107.16
14	B	831	CLA	C3D-C4D-ND	4.77	117.95	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	816	CLA	C2C-C1C-NC	4.77	114.44	109.97
14	cB	803	CLA	C3B-C2B-C1B	-4.77	101.40	107.16
14	bA	823	CLA	O2D-CGD-CBD	4.77	119.74	111.27
14	bB	830	CLA	C3B-C2B-C1B	-4.77	101.40	107.16
14	bB	833	CLA	C2C-C1C-NC	4.77	114.44	109.97
14	bB	802	CLA	C3B-C2B-C1B	-4.77	101.41	107.16
14	B	839	CLA	O2D-CGD-CBD	4.77	119.74	111.27
14	bB	839	CLA	O2D-CGD-CBD	4.77	119.74	111.27
14	bB	831	CLA	C3D-C4D-ND	4.77	117.95	110.24
14	cB	818	CLA	C3D-C2D-C1D	-4.77	99.33	105.83
14	bA	824	CLA	O2D-CGD-CBD	4.77	119.74	111.27
14	bL	204	CLA	C3B-C2B-C1B	-4.77	101.41	107.16
14	bA	813	CLA	C4A-NA-C1A	-4.76	104.56	106.71
14	L	204	CLA	C3B-C2B-C1B	-4.76	101.41	107.16
14	B	821	CLA	CAC-C3C-C4C	4.76	130.99	124.81
14	cB	822	CLA	CAC-C3C-C4C	4.76	130.99	124.81
14	bA	818	CLA	C3D-C4D-ND	4.76	117.94	110.24
14	cA	834	CLA	C4A-NA-C1A	-4.76	104.56	106.71
14	bB	821	CLA	O2D-CGD-CBD	4.76	119.73	111.27
14	cA	823	CLA	O2D-CGD-CBD	4.76	119.73	111.27
14	cA	852	CLA	C2C-C1C-NC	4.76	114.43	109.97
14	bA	812	CLA	C3B-C2B-C1B	-4.76	101.42	107.16
14	bA	852	CLA	C2C-C1C-NC	4.76	114.43	109.97
14	bA	830	CLA	C3B-C2B-C1B	-4.76	101.42	107.16
14	A	827	CLA	C3D-C2D-C1D	-4.76	99.34	105.83
14	B	802	CLA	C3B-C2B-C1B	-4.76	101.42	107.16
17	bI	102	BCR	C37-C22-C21	-4.76	116.26	122.92
14	A	814	CLA	O2D-CGD-CBD	4.75	119.72	111.27
14	bA	819	CLA	CHD-C4C-C3C	-4.75	117.85	124.84
14	cB	832	CLA	C3D-C4D-ND	4.75	117.93	110.24
14	cA	827	CLA	C3D-C2D-C1D	-4.75	99.34	105.83
14	cL	205	CLA	C3B-C2B-C1B	-4.75	101.42	107.16
14	cA	814	CLA	O2D-CGD-CBD	4.75	119.71	111.27
14	cA	819	CLA	CHD-C4C-C3C	-4.75	117.86	124.84
14	B	821	CLA	O2D-CGD-CBD	4.75	119.71	111.27
14	B	836	CLA	C3B-C2B-C1B	-4.75	101.43	107.16
17	I	102	BCR	C37-C22-C21	-4.75	116.27	122.92
14	bA	827	CLA	CAC-C3C-C4C	4.75	130.97	124.81
14	cA	827	CLA	CAC-C3C-C4C	4.75	130.97	124.81
14	cB	825	CLA	C2C-C1C-NC	4.75	114.42	109.97
14	A	812	CLA	C3B-C2B-C1B	-4.75	101.43	107.16
17	cI	102	BCR	C37-C22-C21	-4.75	116.27	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	818	CLA	C3D-C4D-ND	4.75	117.92	110.24
14	B	819	CLA	C2C-C1C-NC	4.75	114.42	109.97
14	cB	801	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
14	cA	837	CLA	O2D-CGD-CBD	4.75	119.70	111.27
14	cB	822	CLA	O2D-CGD-CBD	4.75	119.70	111.27
14	bA	827	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
14	bB	824	CLA	C2C-C1C-NC	4.75	114.42	109.97
14	A	817	CLA	C3B-C2B-C1B	-4.75	101.43	107.16
14	cA	813	CLA	O2D-CGD-CBD	4.75	119.70	111.27
14	bB	851	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
14	bB	820	CLA	CHD-C4C-C3C	-4.74	117.87	124.84
14	cA	818	CLA	C3D-C4D-ND	4.74	117.91	110.24
14	A	852	CLA	C2C-C1C-NC	4.74	114.41	109.97
14	A	830	CLA	C3B-C2B-C1B	-4.74	101.44	107.16
14	bA	813	CLA	O2D-CGD-CBD	4.74	119.69	111.27
14	cA	840	CLA	C2C-C1C-NC	4.74	114.41	109.97
14	B	851	CLA	C4A-NA-C1A	-4.74	104.58	106.71
14	bA	817	CLA	C3B-C2B-C1B	-4.74	101.44	107.16
14	cA	817	CLA	C3B-C2B-C1B	-4.74	101.44	107.16
14	bA	814	CLA	O2D-CGD-CBD	4.73	119.68	111.27
14	cA	823	CLA	C3D-C2D-C1D	-4.73	99.37	105.83
14	bB	836	CLA	C3B-C2B-C1B	-4.73	101.45	107.16
14	A	824	CLA	C4A-NA-C1A	-4.73	104.58	106.71
14	B	807	CLA	CMC-C2C-C1C	4.73	132.25	125.04
14	A	827	CLA	CAC-C3C-C4C	4.73	130.95	124.81
14	bB	851	CLA	C4A-NA-C1A	-4.73	104.58	106.71
14	A	837	CLA	O2D-CGD-CBD	4.73	119.67	111.27
14	bB	834	CLA	CHD-C4C-C3C	-4.73	117.89	124.84
14	B	851	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
14	A	819	CLA	CHD-C4C-C3C	-4.73	117.89	124.84
14	cB	835	CLA	CHD-C4C-C3C	-4.73	117.89	124.84
14	cB	821	CLA	CHD-C4C-C3C	-4.73	117.89	124.84
14	B	834	CLA	C4A-NA-C1A	-4.73	104.58	106.71
14	A	840	CLA	C2C-C1C-NC	4.73	114.40	109.97
14	cA	815	CLA	C3B-C2B-C1B	-4.73	101.46	107.16
14	bB	807	CLA	CMC-C2C-C1C	4.73	132.24	125.04
14	A	813	CLA	O2D-CGD-CBD	4.72	119.66	111.27
14	cB	820	CLA	C2C-C1C-NC	4.72	114.40	109.97
14	bB	834	CLA	C4A-NA-C1A	-4.72	104.58	106.71
14	B	834	CLA	CHD-C4C-C3C	-4.72	117.90	124.84
14	bA	837	CLA	O2D-CGD-CBD	4.72	119.66	111.27
14	bA	823	CLA	C3D-C2D-C1D	-4.72	99.39	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cB	837	CLA	C3B-C2B-C1B	-4.72	101.46	107.16
14	cB	805	CLA	C4A-NA-C1A	-4.72	104.58	106.71
14	A	823	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
14	cA	821	CLA	O2D-CGD-CBD	4.72	119.65	111.27
14	A	821	CLA	O2D-CGD-CBD	4.72	119.65	111.27
14	bA	821	CLA	O2D-CGD-CBD	4.72	119.65	111.27
14	B	815	CLA	C3D-C4D-ND	4.72	117.87	110.24
14	bA	840	CLA	C2C-C1C-NC	4.72	114.39	109.97
14	cB	808	CLA	CMC-C2C-C1C	4.71	132.22	125.04
14	A	840	CLA	C4A-NA-C1A	-4.71	104.59	106.71
14	bB	815	CLA	C3D-C4D-ND	4.71	117.86	110.24
14	A	811	CLA	C2C-C1C-NC	4.71	114.39	109.97
14	bB	804	CLA	C4A-NA-C1A	-4.71	104.59	106.71
14	B	820	CLA	CHD-C4C-C3C	-4.71	117.92	124.84
14	bB	818	CLA	C3D-C4D-ND	4.70	117.85	110.24
14	A	815	CLA	C3B-C2B-C1B	-4.70	101.48	107.16
14	cA	809	CLA	C3B-C2B-C1B	-4.70	101.48	107.16
14	cA	811	CLA	C2C-C1C-NC	4.70	114.38	109.97
14	B	814	CLA	CHD-C4C-C3C	-4.70	117.93	124.84
14	bA	811	CLA	C2C-C1C-NC	4.70	114.37	109.97
14	cB	815	CLA	CHD-C4C-C3C	-4.70	117.94	124.84
14	cB	819	CLA	C3D-C4D-ND	4.70	117.83	110.24
14	A	835	CLA	O2D-CGD-CBD	4.70	119.61	111.27
14	cB	816	CLA	C3D-C4D-ND	4.70	117.83	110.24
14	bA	804	CLA	C3D-C4D-ND	4.70	117.83	110.24
14	bA	835	CLA	O2D-CGD-CBD	4.69	119.61	111.27
14	cA	835	CLA	O2D-CGD-CBD	4.69	119.61	111.27
14	cB	838	CLA	C3D-C4D-ND	4.69	117.83	110.24
14	bB	807	CLA	C3D-C2D-C1D	-4.69	99.42	105.83
14	bB	830	CLA	C4A-NA-C1A	-4.69	104.60	106.71
14	bA	838	CLA	C4A-NA-C1A	-4.69	104.60	106.71
14	cA	824	CLA	C4A-NA-C1A	-4.69	104.60	106.71
14	bB	814	CLA	CHD-C4C-C3C	-4.69	117.95	124.84
14	A	809	CLA	C3B-C2B-C1B	-4.69	101.50	107.16
14	bB	812	CLA	C3B-C2B-C1B	-4.69	101.50	107.16
14	cA	804	CLA	C3D-C4D-ND	4.69	117.82	110.24
14	cB	837	CLA	O2D-CGD-CBD	4.69	119.60	111.27
14	bA	815	CLA	C3B-C2B-C1B	-4.69	101.50	107.16
14	bB	810	CLA	C3D-C4D-ND	4.69	117.82	110.24
14	cB	813	CLA	C3B-C2B-C1B	-4.68	101.51	107.16
14	bA	809	CLA	C3B-C2B-C1B	-4.68	101.51	107.16
14	bB	804	CLA	C2C-C1C-NC	4.68	114.36	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	807	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
14	B	812	CLA	C3B-C2B-C1B	-4.68	101.51	107.16
14	B	818	CLA	C3D-C4D-ND	4.68	117.81	110.24
14	cB	808	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
14	A	804	CLA	C3D-C4D-ND	4.68	117.81	110.24
14	bA	824	CLA	C4A-NA-C1A	-4.68	104.60	106.71
14	cA	808	CLA	C2C-C1C-NC	4.68	114.35	109.97
14	B	804	CLA	C4A-NA-C1A	-4.68	104.60	106.71
14	bA	840	CLA	C4A-NA-C1A	-4.68	104.60	106.71
14	B	804	CLA	C2C-C1C-NC	4.68	114.35	109.97
14	bB	822	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
14	cA	811	CLA	C3D-C4D-ND	4.67	117.80	110.24
14	cA	834	CLA	C3D-C4D-ND	4.67	117.80	110.24
14	bA	808	CLA	C2C-C1C-NC	4.67	114.35	109.97
14	B	822	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
14	cB	811	CLA	C3D-C4D-ND	4.67	117.80	110.24
14	B	835	CLA	C3B-C2B-C1B	-4.67	101.52	107.16
14	bB	835	CLA	C3B-C2B-C1B	-4.67	101.52	107.16
14	cB	836	CLA	C3B-C2B-C1B	-4.67	101.52	107.16
14	B	837	CLA	C3D-C4D-ND	4.67	117.80	110.24
14	bB	836	CLA	O2D-CGD-CBD	4.67	119.57	111.27
14	bB	821	CLA	C3B-C2B-C1B	-4.67	101.52	107.16
14	bB	820	CLA	C3B-C2B-C1B	-4.67	101.52	107.16
14	A	811	CLA	C3D-C4D-ND	4.67	117.79	110.24
14	cA	812	CLA	C3D-C4D-ND	4.67	117.79	110.24
14	B	830	CLA	C4A-NA-C1A	-4.67	104.61	106.71
14	cB	823	CLA	O2D-CGD-CBD	4.67	119.56	111.27
14	B	820	CLA	C3B-C2B-C1B	-4.67	101.53	107.16
14	bB	822	CLA	O2D-CGD-CBD	4.66	119.56	111.27
14	B	810	CLA	C3D-C4D-ND	4.66	117.78	110.24
14	bA	811	CLA	C3D-C4D-ND	4.66	117.78	110.24
14	cB	823	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
14	A	805	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
14	cB	840	CLA	CAC-C3C-C4C	4.66	130.86	124.81
14	B	822	CLA	O2D-CGD-CBD	4.66	119.55	111.27
14	bA	821	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
14	bB	835	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
14	bA	837	CLA	C3D-C4D-ND	4.66	117.78	110.24
14	cB	805	CLA	C2C-C1C-NC	4.66	114.34	109.97
14	A	837	CLA	C3D-C4D-ND	4.66	117.78	110.24
14	bB	839	CLA	CAC-C3C-C4C	4.66	130.85	124.81
14	B	836	CLA	O2D-CGD-CBD	4.66	119.55	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	838	CLA	C4A-NA-C1A	-4.66	104.61	106.71
14	cB	831	CLA	C4A-NA-C1A	-4.66	104.61	106.71
14	cB	835	CLA	C4A-NA-C1A	-4.66	104.61	106.71
14	B	839	CLA	CAC-C3C-C4C	4.66	130.85	124.81
14	cB	836	CLA	C3D-C2D-C1D	-4.66	99.48	105.83
14	A	821	CLA	C3D-C2D-C1D	-4.66	99.48	105.83
14	cB	821	CLA	C3B-C2B-C1B	-4.66	101.54	107.16
14	B	835	CLA	C3D-C2D-C1D	-4.66	99.48	105.83
14	cA	838	CLA	C4A-NA-C1A	-4.66	104.61	106.71
14	B	802	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
14	B	811	CLA	C3D-C4D-ND	4.65	117.77	110.24
14	cA	840	CLA	C3D-C4D-ND	4.65	117.77	110.24
14	cA	810	CLA	C3D-C4D-ND	4.65	117.77	110.24
14	bB	811	CLA	C3D-C4D-ND	4.65	117.76	110.24
14	cB	820	CLA	C3D-C4D-ND	4.65	117.76	110.24
14	bB	802	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
14	B	837	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
14	cA	803	CLA	C3B-C2B-C1B	-4.65	101.55	107.16
14	bA	805	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
14	bA	803	CLA	C3B-C2B-C1B	-4.65	101.55	107.16
14	A	803	CLA	C3B-C2B-C1B	-4.65	101.55	107.16
14	cB	822	CLA	C3B-C2B-C1B	-4.65	101.55	107.16
14	B	815	CLA	C2C-C1C-NC	4.65	114.33	109.97
14	cA	805	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
14	A	840	CLA	C3D-C4D-ND	4.65	117.76	110.24
14	bA	810	CLA	C3D-C4D-ND	4.65	117.76	110.24
14	cA	837	CLA	C3D-C4D-ND	4.65	117.76	110.24
14	A	810	CLA	C3D-C4D-ND	4.65	117.76	110.24
14	L	202	CLA	C3D-C4D-ND	4.65	117.76	110.24
14	A	834	CLA	C3D-C4D-ND	4.65	117.76	110.24
14	B	807	CLA	C3B-C2B-C1B	-4.65	101.55	107.16
14	B	830	CLA	C3D-C4D-ND	4.65	117.76	110.24
14	cA	821	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
14	B	821	CLA	C3B-C2B-C1B	-4.65	101.55	107.16
14	bA	812	CLA	C3D-C4D-ND	4.65	117.75	110.24
14	bB	830	CLA	C3D-C4D-ND	4.64	117.75	110.24
14	A	808	CLA	C2C-C1C-NC	4.64	114.32	109.97
14	bL	202	CLA	C3D-C4D-ND	4.64	117.75	110.24
14	cB	831	CLA	C3D-C4D-ND	4.64	117.75	110.24
14	bB	815	CLA	C2C-C1C-NC	4.64	114.32	109.97
14	cB	822	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
14	cA	828	CLA	C3D-C2D-C1D	-4.64	99.50	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cB	808	CLA	C3B-C2B-C1B	-4.64	101.56	107.16
14	B	821	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
14	bB	837	CLA	C3D-C4D-ND	4.64	117.75	110.24
14	cA	831	CLA	C3D-C4D-ND	4.64	117.75	110.24
14	A	831	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
14	cB	837	CLA	C2C-C1C-NC	4.64	114.32	109.97
14	bB	829	CLA	CHD-C4C-C3C	-4.64	118.02	124.84
14	B	836	CLA	C2C-C1C-NC	4.64	114.32	109.97
14	bB	819	CLA	C3D-C4D-ND	4.64	117.74	110.24
14	bA	840	CLA	C3D-C4D-ND	4.64	117.74	110.24
14	cB	812	CLA	C3D-C4D-ND	4.64	117.74	110.24
14	cB	838	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
14	bA	831	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
14	bA	831	CLA	C3D-C4D-ND	4.64	117.74	110.24
14	cA	813	CLA	C2C-C1C-NC	4.64	114.31	109.97
14	bB	821	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
14	A	831	CLA	C3D-C4D-ND	4.64	117.74	110.24
14	bB	805	CLA	C3D-C4D-ND	4.64	117.74	110.24
14	bA	813	CLA	C2C-C1C-NC	4.63	114.31	109.97
14	cB	837	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
14	A	812	CLA	C3D-C4D-ND	4.63	117.73	110.24
14	cB	815	CLA	CAC-C3C-C4C	4.63	130.82	124.81
14	cB	803	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
14	A	823	CLA	C3D-C4D-ND	4.63	117.73	110.24
14	bA	816	CLA	C3D-C4D-ND	4.63	117.73	110.24
14	bA	834	CLA	C3D-C4D-ND	4.63	117.73	110.24
14	cL	203	CLA	C3D-C4D-ND	4.63	117.73	110.24
14	A	813	CLA	C2C-C1C-NC	4.63	114.31	109.97
14	B	836	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
14	B	814	CLA	CAC-C3C-C4C	4.63	130.82	124.81
14	bB	836	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
14	bB	807	CLA	C3B-C2B-C1B	-4.63	101.57	107.16
14	cB	816	CLA	C2C-C1C-NC	4.63	114.31	109.97
14	B	829	CLA	CHD-C4C-C3C	-4.63	118.03	124.84
14	bB	837	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
14	B	819	CLA	C3D-C4D-ND	4.63	117.73	110.24
14	bB	814	CLA	CAC-C3C-C4C	4.63	130.82	124.81
14	bA	823	CLA	C3D-C4D-ND	4.63	117.73	110.24
14	A	820	CLA	O2D-CGD-CBD	4.63	119.49	111.27
14	bB	832	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
14	B	805	CLA	C3D-C4D-ND	4.63	117.72	110.24
14	A	822	CLA	C3D-C2D-C1D	-4.63	99.52	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	828	CLA	C3D-C2D-C1D	-4.63	99.52	105.83
14	bB	836	CLA	C3D-C4D-ND	4.62	117.72	110.24
14	cB	814	CLA	CAC-C3C-C4C	4.62	130.81	124.81
14	cA	807	CLA	CHD-C4C-C3C	-4.62	118.05	124.84
14	bB	836	CLA	C2C-C1C-NC	4.62	114.30	109.97
14	bJ	101	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
14	A	816	CLA	C3D-C4D-ND	4.62	117.71	110.24
14	B	813	CLA	CAC-C3C-C4C	4.62	130.81	124.81
14	bA	828	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
14	B	826	CLA	C3B-C2B-C1B	-4.62	101.58	107.16
14	bA	836	CLA	C4A-NA-C1A	-4.62	104.63	106.71
14	cA	828	CLA	CMD-C2D-C1D	4.62	132.85	124.71
14	cB	833	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
14	bX	201	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
14	cB	806	CLA	C3D-C4D-ND	4.62	117.71	110.24
14	bB	813	CLA	CAC-C3C-C4C	4.62	130.80	124.81
14	cX	201	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
14	cB	830	CLA	CHD-C4C-C3C	-4.62	118.06	124.84
14	J	101	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
14	bA	805	CLA	C3B-C2B-C1B	-4.62	101.59	107.16
14	B	836	CLA	C3D-C4D-ND	4.62	117.70	110.24
14	cB	837	CLA	C3D-C4D-ND	4.62	117.70	110.24
14	cJ	101	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
14	X	201	CLA	C3D-C2D-C1D	-4.61	99.53	105.83
14	cA	831	CLA	C3D-C2D-C1D	-4.61	99.53	105.83
14	B	812	CLA	C3D-C4D-ND	4.61	117.70	110.24
14	bA	820	CLA	O2D-CGD-CBD	4.61	119.47	111.27
14	cA	816	CLA	C3D-C4D-ND	4.61	117.70	110.24
14	cA	823	CLA	C3D-C4D-ND	4.61	117.70	110.24
14	bA	809	CLA	C4A-NA-C1A	-4.61	104.63	106.71
14	cB	827	CLA	C3B-C2B-C1B	-4.61	101.59	107.16
14	A	807	CLA	CHD-C4C-C3C	-4.61	118.06	124.84
14	cA	812	CLA	CAC-C3C-C4C	4.61	130.79	124.81
14	B	832	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
14	A	828	CLA	C4A-NA-C1A	-4.61	104.63	106.71
14	bA	828	CLA	C4A-NA-C1A	-4.61	104.63	106.71
14	bA	828	CLA	CMD-C2D-C1D	4.61	132.84	124.71
14	cA	820	CLA	O2D-CGD-CBD	4.61	119.46	111.27
14	cB	813	CLA	C3D-C4D-ND	4.61	117.69	110.24
14	A	828	CLA	CMD-C2D-C1D	4.61	132.83	124.71
14	bA	807	CLA	CHD-C4C-C3C	-4.61	118.07	124.84
14	bB	812	CLA	C3D-C4D-ND	4.61	117.69	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cB	820	CLA	C4A-NA-C1A	-4.61	104.64	106.71
14	cB	814	CLA	CHD-C4C-C3C	-4.61	118.07	124.84
14	cA	805	CLA	C3B-C2B-C1B	-4.61	101.60	107.16
14	bA	812	CLA	CAC-C3C-C4C	4.61	130.78	124.81
14	bL	202	CLA	C2C-C1C-NC	4.60	114.29	109.97
14	cA	822	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
14	A	836	CLA	C4A-NA-C1A	-4.60	104.64	106.71
14	A	842	CLA	C3D-C4D-ND	4.60	117.69	110.24
14	cB	828	CLA	C3D-C4D-ND	4.60	117.68	110.24
14	bB	802	CLA	O2D-CGD-CBD	4.60	119.45	111.27
14	B	826	CLA	O2D-CGD-CBD	4.60	119.44	111.27
14	B	827	CLA	C3D-C4D-ND	4.60	117.68	110.24
14	bA	809	CLA	C3D-C4D-ND	4.60	117.68	110.24
14	cB	803	CLA	O2D-CGD-CBD	4.60	119.44	111.27
14	bB	816	CLA	C3B-C2B-C1B	-4.60	101.61	107.16
14	cA	836	CLA	C4A-NA-C1A	-4.60	104.64	106.71
14	A	808	CLA	C3D-C4D-ND	4.60	117.67	110.24
14	J	102	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
14	B	813	CLA	CHD-C4C-C3C	-4.60	118.08	124.84
14	B	829	CLA	C3D-C4D-ND	4.60	117.67	110.24
14	bB	826	CLA	C3B-C2B-C1B	-4.60	101.61	107.16
14	B	802	CLA	O2D-CGD-CBD	4.60	119.44	111.27
14	cB	817	CLA	C3B-C2B-C1B	-4.60	101.61	107.16
14	bB	813	CLA	CHD-C4C-C3C	-4.59	118.09	124.84
14	bA	839	CLA	C3D-C4D-ND	4.59	117.67	110.24
14	A	812	CLA	CAC-C3C-C4C	4.59	130.77	124.81
14	bB	816	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
14	B	816	CLA	C3B-C2B-C1B	-4.59	101.62	107.16
14	bB	815	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
14	bA	822	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
14	bB	833	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
14	A	805	CLA	C3B-C2B-C1B	-4.59	101.62	107.16
14	bA	808	CLA	C3D-C4D-ND	4.59	117.67	110.24
14	cB	816	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
14	bA	842	CLA	C3D-C4D-ND	4.59	117.67	110.24
14	cB	830	CLA	C3D-C4D-ND	4.59	117.67	110.24
14	cB	827	CLA	O2D-CGD-CBD	4.59	119.42	111.27
14	bB	816	CLA	C3D-C4D-ND	4.59	117.66	110.24
14	bB	826	CLA	O2D-CGD-CBD	4.59	119.42	111.27
14	B	816	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
14	A	807	CLA	C3D-C4D-ND	4.59	117.66	110.24
14	cB	817	CLA	C3D-C4D-ND	4.59	117.66	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	815	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
14	A	809	CLA	C3D-C4D-ND	4.59	117.66	110.24
14	bA	807	CLA	C3D-C4D-ND	4.59	117.66	110.24
14	B	833	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
14	cL	203	CLA	C2C-C1C-NC	4.59	114.27	109.97
14	cA	807	CLA	C3D-C4D-ND	4.58	117.66	110.24
14	cA	809	CLA	C3D-C4D-ND	4.58	117.66	110.24
14	bJ	102	CLA	C3D-C2D-C1D	-4.58	99.57	105.83
14	B	816	CLA	C3D-C4D-ND	4.58	117.65	110.24
14	bA	838	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
14	cA	808	CLA	C3D-C4D-ND	4.58	117.65	110.24
14	bA	810	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
14	cA	839	CLA	C3D-C4D-ND	4.58	117.65	110.24
14	A	839	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
14	bA	803	CLA	C3D-C4D-ND	4.58	117.65	110.24
14	A	839	CLA	C3D-C4D-ND	4.58	117.65	110.24
14	cB	810	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
14	cA	828	CLA	C4A-NA-C1A	-4.58	104.65	106.71
14	bB	827	CLA	C3D-C4D-ND	4.58	117.65	110.24
14	cA	842	CLA	C3D-C4D-ND	4.58	117.65	110.24
14	cB	834	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
14	bA	815	CLA	C3D-C4D-ND	4.58	117.64	110.24
14	cJ	102	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
14	bB	809	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
14	B	809	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
14	L	202	CLA	C2C-C1C-NC	4.58	114.26	109.97
14	A	815	CLA	C3D-C4D-ND	4.58	117.64	110.24
14	cB	817	CLA	C3D-C2D-C1D	-4.58	99.59	105.83
14	cA	812	CLA	C3D-C2D-C1D	-4.58	99.59	105.83
14	bA	805	CLA	C4A-NA-C1A	-4.58	104.65	106.71
14	cA	810	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
14	cA	803	CLA	C3D-C4D-ND	4.57	117.64	110.24
14	A	812	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
14	A	852	CLA	C3B-C2B-C1B	-4.57	101.64	107.16
14	bB	829	CLA	C3D-C4D-ND	4.57	117.64	110.24
14	A	838	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
14	cA	852	CLA	C3B-C2B-C1B	-4.57	101.64	107.16
14	A	810	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
14	B	814	CLA	C3D-C4D-ND	4.57	117.63	110.24
14	cA	838	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
14	A	803	CLA	C3D-C4D-ND	4.57	117.63	110.24
14	bA	805	CLA	C3D-C4D-ND	4.57	117.63	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	811	CLA	C4A-NA-C1A	-4.57	104.65	106.71
14	B	849	CLA	C4A-NA-C1A	-4.57	104.65	106.71
14	cA	819	CLA	C3D-C4D-ND	4.57	117.63	110.24
14	cB	815	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
14	A	852	CLA	CMD-C2D-C1D	4.57	132.76	124.71
14	cA	816	CLA	C2C-C1C-NC	4.57	114.25	109.97
14	cA	852	CLA	CMD-C2D-C1D	4.56	132.76	124.71
14	bA	841	CLA	C3D-C2D-C1D	-4.56	99.60	105.83
14	bB	811	CLA	C4A-NA-C1A	-4.56	104.65	106.71
14	bB	814	CLA	C3D-C4D-ND	4.56	117.62	110.24
14	cA	839	CLA	C3D-C2D-C1D	-4.56	99.60	105.83
14	A	810	CLA	C4A-NA-C1A	-4.56	104.66	106.71
14	A	810	CLA	O2D-CGD-CBD	4.56	119.37	111.27
14	bA	819	CLA	C3D-C4D-ND	4.56	117.62	110.24
14	A	831	CLA	C3B-C2B-C1B	-4.56	101.66	107.16
14	B	808	CLA	CAC-C3C-C4C	4.56	130.73	124.81
14	B	825	CLA	C2C-C1C-NC	4.56	114.24	109.97
14	bA	839	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
14	A	805	CLA	C3D-C4D-ND	4.56	117.61	110.24
14	bB	814	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
14	bB	824	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
14	B	819	CLA	C4A-NA-C1A	-4.56	104.66	106.71
14	cB	804	CLA	C3C-C4C-NC	4.56	115.68	110.57
14	cB	826	CLA	C2C-C1C-NC	4.56	114.24	109.97
14	A	841	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
14	cA	805	CLA	C3D-C4D-ND	4.56	117.61	110.24
14	A	822	CLA	C3D-C4D-ND	4.56	117.61	110.24
14	B	824	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
14	cA	841	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
14	cA	815	CLA	C3D-C4D-ND	4.56	117.61	110.24
14	cB	809	CLA	CAC-C3C-C4C	4.55	130.72	124.81
14	B	814	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
14	bA	814	CLA	C3D-C4D-ND	4.55	117.60	110.24
14	cB	815	CLA	C3D-C4D-ND	4.55	117.60	110.24
14	B	810	CLA	C3B-C2B-C1B	-4.55	101.67	107.16
14	bA	852	CLA	C3B-C2B-C1B	-4.55	101.67	107.16
14	bB	808	CLA	CAC-C3C-C4C	4.55	130.72	124.81
14	bB	812	CLA	CMC-C2C-C1C	4.55	131.97	125.04
14	B	830	CLA	O2D-CGD-CBD	4.55	119.35	111.27
14	cA	810	CLA	O2D-CGD-CBD	4.55	119.35	111.27
14	B	830	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
14	A	832	CLA	C4A-NA-C1A	-4.55	104.66	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	805	CLA	C4A-NA-C1A	-4.55	104.66	106.71
14	cL	203	CLA	C3B-C2B-C1B	-4.55	101.67	107.16
14	cF	201	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
14	L	202	CLA	C3B-C2B-C1B	-4.55	101.67	107.16
14	bB	830	CLA	C3D-C2D-C1D	-4.55	99.63	105.83
14	bB	830	CLA	O2D-CGD-CBD	4.55	119.35	111.27
14	bF	201	CLA	C3D-C2D-C1D	-4.55	99.63	105.83
14	cA	834	CLA	CHD-C4C-C3C	-4.55	118.16	124.84
14	bA	852	CLA	CMD-C2D-C1D	4.54	132.72	124.71
14	cA	831	CLA	C3B-C2B-C1B	-4.54	101.67	107.16
14	F	201	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
14	bA	832	CLA	C4A-NA-C1A	-4.54	104.66	106.71
14	bA	810	CLA	O2D-CGD-CBD	4.54	119.34	111.27
14	cB	825	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
14	bA	812	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
14	B	812	CLA	CMC-C2C-C1C	4.54	131.96	125.04
14	bA	804	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
14	bA	816	CLA	C2C-C1C-NC	4.54	114.23	109.97
14	A	819	CLA	C3D-C4D-ND	4.54	117.58	110.24
14	B	803	CLA	C3C-C4C-NC	4.54	115.66	110.57
14	B	821	CLA	C3D-C4D-ND	4.54	117.58	110.24
14	cB	831	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
14	B	833	CLA	O2D-CGD-CBD	4.54	119.33	111.27
14	cA	830	CLA	CMC-C2C-C1C	4.54	131.95	125.04
14	A	805	CLA	C4A-NA-C1A	-4.54	104.67	106.71
14	bA	816	CLA	O2D-CGD-CBD	4.54	119.33	111.27
14	A	814	CLA	C3D-C4D-ND	4.54	117.58	110.24
14	A	837	CLA	CMC-C2C-C1C	4.54	131.95	125.04
14	cB	813	CLA	CMC-C2C-C1C	4.54	131.95	125.04
14	bB	819	CLA	C4A-NA-C1A	-4.54	104.67	106.71
14	bB	833	CLA	O2D-CGD-CBD	4.54	119.33	111.27
14	cB	834	CLA	O2D-CGD-CBD	4.54	119.33	111.27
14	bA	831	CLA	C3B-C2B-C1B	-4.53	101.69	107.16
14	bB	825	CLA	C2C-C1C-NC	4.53	114.22	109.97
14	bA	822	CLA	C3D-C4D-ND	4.53	117.57	110.24
14	A	836	CLA	C3D-C2D-C1D	-4.53	99.64	105.83
14	cA	822	CLA	C3D-C4D-ND	4.53	117.57	110.24
14	bA	834	CLA	CHD-C4C-C3C	-4.53	118.18	124.84
14	A	807	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
14	cB	811	CLA	C3B-C2B-C1B	-4.53	101.69	107.16
14	cB	831	CLA	O2D-CGD-CBD	4.53	119.32	111.27
14	cA	836	CLA	C3D-C2D-C1D	-4.53	99.65	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	823	CLA	CAC-C3C-C4C	4.53	130.69	124.81
14	bA	807	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
14	bL	202	CLA	C3B-C2B-C1B	-4.53	101.69	107.16
14	bA	837	CLA	CMC-C2C-C1C	4.53	131.94	125.04
14	bB	821	CLA	C3D-C4D-ND	4.53	117.56	110.24
14	cA	809	CLA	C4A-NA-C1A	-4.53	104.67	106.71
14	cB	822	CLA	C3D-C4D-ND	4.53	117.56	110.24
14	bB	803	CLA	C3C-C4C-NC	4.53	115.65	110.57
14	bA	830	CLA	CMC-C2C-C1C	4.53	131.93	125.04
14	cA	837	CLA	CMC-C2C-C1C	4.53	131.93	125.04
14	bA	810	CLA	C4A-NA-C1A	-4.53	104.67	106.71
14	bB	815	CLA	O2D-CGD-CBD	4.53	119.31	111.27
14	A	816	CLA	O2D-CGD-CBD	4.53	119.31	111.27
14	cJ	101	CLA	C3D-C4D-ND	4.53	117.56	110.24
14	cA	817	CLA	C3D-C4D-ND	4.52	117.56	110.24
14	A	834	CLA	CHD-C4C-C3C	-4.52	118.19	124.84
14	cB	821	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
14	cA	816	CLA	O2D-CGD-CBD	4.52	119.31	111.27
14	A	809	CLA	C4A-NA-C1A	-4.52	104.67	106.71
14	bB	822	CLA	C3D-C4D-ND	4.52	117.55	110.24
14	A	816	CLA	C2C-C1C-NC	4.52	114.21	109.97
14	bA	823	CLA	CAC-C3C-C4C	4.52	130.68	124.81
14	cA	832	CLA	C4A-NA-C1A	-4.52	104.67	106.71
14	A	804	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
14	bJ	101	CLA	C3D-C4D-ND	4.52	117.55	110.24
14	bA	836	CLA	C3D-C2D-C1D	-4.52	99.67	105.83
14	B	849	CLA	C3D-C4D-ND	4.52	117.55	110.24
14	A	821	CLA	C3D-C4D-ND	4.52	117.55	110.24
14	cA	829	CLA	C3D-C4D-ND	4.52	117.55	110.24
14	bA	832	CLA	O2D-CGD-CBD	4.52	119.29	111.27
14	bB	810	CLA	C3B-C2B-C1B	-4.52	101.71	107.16
14	cA	814	CLA	C3D-C4D-ND	4.52	117.54	110.24
14	cL	205	CLA	C3D-C2D-C1D	-4.52	99.67	105.83
14	cB	850	CLA	C4A-NA-C1A	-4.52	104.68	106.71
14	A	817	CLA	C3D-C4D-ND	4.52	117.54	110.24
14	bA	821	CLA	C3D-C4D-ND	4.52	117.54	110.24
14	bA	814	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
14	cB	823	CLA	C3D-C4D-ND	4.51	117.54	110.24
14	B	815	CLA	O2D-CGD-CBD	4.51	119.29	111.27
14	A	814	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
14	A	835	CLA	C3D-C4D-ND	4.51	117.54	110.24
14	cA	804	CLA	C3D-C2D-C1D	-4.51	99.67	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	832	CLA	O2D-CGD-CBD	4.51	119.29	111.27
14	B	834	CLA	C3D-C4D-ND	4.51	117.54	110.24
14	J	101	CLA	C3D-C4D-ND	4.51	117.54	110.24
14	bA	829	CLA	C3D-C4D-ND	4.51	117.54	110.24
14	A	830	CLA	CMC-C2C-C1C	4.51	131.91	125.04
14	cA	807	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
14	cA	810	CLA	C4A-NA-C1A	-4.51	104.68	106.71
14	bB	834	CLA	C3D-C4D-ND	4.51	117.53	110.24
14	bB	804	CLA	CAC-C3C-C4C	4.51	130.66	124.81
14	A	829	CLA	C3D-C4D-ND	4.51	117.53	110.24
14	bA	817	CLA	C3D-C4D-ND	4.51	117.53	110.24
14	L	204	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
14	bL	204	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
14	cB	850	CLA	C3D-C4D-ND	4.51	117.53	110.24
14	cB	812	CLA	C4A-NA-C1A	-4.51	104.68	106.71
14	cB	816	CLA	O2D-CGD-CBD	4.51	119.28	111.27
14	cA	812	CLA	C2C-C1C-NC	4.51	114.19	109.97
14	A	832	CLA	O2D-CGD-CBD	4.50	119.27	111.27
14	bB	816	CLA	O2D-CGD-CBD	4.50	119.27	111.27
14	cB	850	CLA	C3D-C2D-C1D	-4.50	99.68	105.83
14	cB	805	CLA	CAC-C3C-C4C	4.50	130.65	124.81
14	B	801	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
14	cA	821	CLA	C3D-C4D-ND	4.50	117.52	110.24
14	A	827	CLA	C4A-NA-C1A	-4.50	104.68	106.71
14	B	822	CLA	C3D-C4D-ND	4.50	117.52	110.24
14	B	804	CLA	CAC-C3C-C4C	4.50	130.65	124.81
14	cB	835	CLA	C3D-C4D-ND	4.50	117.52	110.24
14	bB	801	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
14	bA	835	CLA	C3D-C4D-ND	4.50	117.52	110.24
14	bF	201	CLA	C4A-NA-C1A	-4.50	104.68	106.71
14	bB	820	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
14	A	827	CLA	O2D-CGD-CBD	4.50	119.26	111.27
14	B	828	CLA	C3D-C2D-C1D	-4.50	99.70	105.83
14	A	812	CLA	C2C-C1C-NC	4.49	114.18	109.97
14	B	820	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
14	cA	814	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
14	bA	817	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
14	B	805	CLA	C3B-C2B-C1B	-4.49	101.74	107.16
14	bB	849	CLA	C3D-C4D-ND	4.49	117.50	110.24
14	cA	835	CLA	C3D-C4D-ND	4.49	117.50	110.24
14	B	826	CLA	CAC-C3C-C4C	4.49	130.64	124.81
14	B	816	CLA	O2D-CGD-CBD	4.49	119.25	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bB	826	CLA	CAC-C3C-C4C	4.49	130.63	124.81
14	bA	829	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
14	bB	849	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
14	A	823	CLA	CAC-C3C-C4C	4.49	130.63	124.81
14	B	834	CLA	CAC-C3C-C4C	4.49	130.63	124.81
14	bB	835	CLA	C3D-C4D-ND	4.49	117.50	110.24
14	bB	851	CLA	C3D-C4D-ND	4.49	117.50	110.24
14	B	810	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
14	bA	827	CLA	C4A-NA-C1A	-4.48	104.69	106.71
14	bA	827	CLA	O2D-CGD-CBD	4.48	119.24	111.27
14	cB	802	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
14	A	829	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
14	cA	829	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
14	A	817	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
14	bB	810	CLA	O2D-CGD-CBD	4.48	119.23	111.27
14	B	849	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
14	bB	805	CLA	C3B-C2B-C1B	-4.48	101.75	107.16
14	cB	806	CLA	C3B-C2B-C1B	-4.48	101.75	107.16
14	bB	834	CLA	CAC-C3C-C4C	4.48	130.62	124.81
14	cB	835	CLA	CAC-C3C-C4C	4.48	130.62	124.81
14	B	851	CLA	C3D-C4D-ND	4.48	117.48	110.24
14	cA	827	CLA	O2D-CGD-CBD	4.48	119.22	111.27
14	cB	811	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
14	cX	201	CLA	C3D-C4D-ND	4.47	117.48	110.24
14	cB	817	CLA	O2D-CGD-CBD	4.47	119.22	111.27
14	B	835	CLA	C3D-C4D-ND	4.47	117.48	110.24
14	cA	815	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
14	bA	835	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
14	cB	811	CLA	O2D-CGD-CBD	4.47	119.22	111.27
14	cA	817	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
14	X	201	CLA	C3D-C4D-ND	4.47	117.47	110.24
14	cJ	102	CLA	C3D-C4D-ND	4.47	117.47	110.24
14	bA	818	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
14	A	816	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
14	cA	816	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
14	bX	201	CLA	C3D-C4D-ND	4.47	117.47	110.24
14	bA	836	CLA	CMC-C2C-C1C	4.47	131.85	125.04
14	cA	834	CLA	C3B-C2B-C1B	-4.47	101.77	107.16
14	bB	834	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
14	bB	821	CLA	CHD-C4C-C3C	-4.47	118.27	124.84
14	A	835	CLA	C4A-NA-C1A	-4.47	104.70	106.71
14	bA	812	CLA	C2C-C1C-NC	4.47	114.16	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	826	CLA	C2C-C1C-NC	4.47	114.16	109.97
14	bL	204	CLA	C3D-C4D-ND	4.47	117.47	110.24
14	bB	810	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
14	cB	829	CLA	C3D-C2D-C1D	-4.47	99.74	105.83
14	cA	817	CLA	C4A-NA-C1A	-4.47	104.70	106.71
14	cA	827	CLA	C4A-NA-C1A	-4.47	104.70	106.71
14	A	815	CLA	C3D-C2D-C1D	-4.47	99.74	105.83
14	cA	836	CLA	CMC-C2C-C1C	4.47	131.84	125.04
14	cB	801	CLA	C3D-C4D-ND	4.47	117.46	110.24
14	L	204	CLA	C3D-C4D-ND	4.46	117.46	110.24
13	cA	801	CL0	C3D-C2D-C1D	-4.46	99.74	105.83
14	bB	838	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
14	J	102	CLA	C3D-C4D-ND	4.46	117.46	110.24
14	A	836	CLA	CMC-C2C-C1C	4.46	131.84	125.04
14	bB	828	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
14	A	826	CLA	C2C-C1C-NC	4.46	114.15	109.97
14	B	810	CLA	O2D-CGD-CBD	4.46	119.20	111.27
14	bB	838	CLA	C3C-C4C-NC	4.46	115.58	110.57
14	cL	202	CLA	C3C-C4C-NC	4.46	115.57	110.57
14	cB	822	CLA	CHD-C4C-C3C	-4.46	118.28	124.84
14	bB	813	CLA	C4A-NA-C1A	-4.46	104.70	106.71
14	cB	836	CLA	C3D-C4D-ND	4.46	117.45	110.24
14	B	838	CLA	C3C-C4C-NC	4.46	115.57	110.57
14	bA	816	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
14	cA	818	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
14	bA	815	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
14	A	818	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
13	A	801	CL0	C3D-C2D-C1D	-4.45	99.75	105.83
14	cB	827	CLA	CAC-C3C-C4C	4.45	130.59	124.81
14	A	834	CLA	C3B-C2B-C1B	-4.45	101.78	107.16
14	A	835	CLA	C3D-C2D-C1D	-4.45	99.75	105.83
14	bB	808	CLA	C3D-C2D-C1D	-4.45	99.75	105.83
14	cL	205	CLA	C3D-C4D-ND	4.45	117.44	110.24
14	cA	835	CLA	C4A-NA-C1A	-4.45	104.70	106.71
14	cB	814	CLA	C4A-NA-C1A	-4.45	104.70	106.71
14	bA	826	CLA	C2C-C1C-NC	4.45	114.14	109.97
14	B	821	CLA	CHD-C4C-C3C	-4.45	118.30	124.84
14	cB	839	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
14	bJ	102	CLA	C3D-C4D-ND	4.45	117.44	110.24
14	bL	201	CLA	C3C-C4C-NC	4.45	115.56	110.57
14	F	201	CLA	C4A-NA-C1A	-4.45	104.71	106.71
14	cF	201	CLA	C4A-NA-C1A	-4.45	104.71	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	827	CLA	C2C-C1C-NC	4.45	114.14	109.97
14	bA	827	CLA	C2C-C1C-NC	4.45	114.14	109.97
14	bB	818	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
14	bA	834	CLA	C3B-C2B-C1B	-4.45	101.79	107.16
14	cB	806	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
14	A	817	CLA	C4A-NA-C1A	-4.45	104.71	106.71
14	cA	808	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
14	cA	830	CLA	C3D-C4D-ND	4.45	117.43	110.24
14	B	808	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
14	cA	835	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
13	bA	801	CL0	C3D-C2D-C1D	-4.44	99.77	105.83
14	cB	835	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
14	A	838	CLA	C3B-C2B-C1B	-4.44	101.80	107.16
14	A	808	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
14	bB	805	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
14	B	838	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
14	cA	811	CLA	O2D-CGD-CBD	4.44	119.16	111.27
14	bB	849	CLA	C4A-NA-C1A	-4.44	104.71	106.71
14	A	804	CLA	C2C-C1C-NC	4.44	114.13	109.97
14	bA	804	CLA	C2C-C1C-NC	4.44	114.13	109.97
14	B	804	CLA	C3D-C4D-ND	4.44	117.42	110.24
14	bA	837	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
14	B	818	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
14	cA	819	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
14	cA	837	CLA	C3D-C2D-C1D	-4.44	99.78	105.83
14	bA	830	CLA	C3D-C4D-ND	4.44	117.42	110.24
14	cB	805	CLA	C3D-C4D-ND	4.44	117.42	110.24
14	bA	838	CLA	C3B-C2B-C1B	-4.44	101.81	107.16
14	A	830	CLA	C3D-C4D-ND	4.44	117.41	110.24
14	cA	852	CLA	C3D-C2D-C1D	-4.44	99.78	105.83
14	cB	819	CLA	C3D-C2D-C1D	-4.44	99.78	105.83
14	bB	804	CLA	C3D-C4D-ND	4.43	117.41	110.24
14	cA	827	CLA	C2C-C1C-NC	4.43	114.13	109.97
14	cA	804	CLA	C2C-C1C-NC	4.43	114.12	109.97
14	B	834	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
14	bA	824	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
14	cB	809	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
14	A	811	CLA	O2D-CGD-CBD	4.43	119.14	111.27
14	A	837	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
14	bA	819	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
14	bA	811	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
14	bA	808	CLA	C3D-C2D-C1D	-4.43	99.79	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bA	835	CLA	C4A-NA-C1A	-4.43	104.72	106.71
14	B	805	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
14	A	852	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
14	A	842	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
14	bA	817	CLA	C4A-NA-C1A	-4.43	104.72	106.71
14	L	201	CLA	C3C-C4C-NC	4.42	115.53	110.57
14	cA	838	CLA	C3B-C2B-C1B	-4.42	101.82	107.16
14	A	819	CLA	C3D-C2D-C1D	-4.42	99.79	105.83
14	bA	805	CLA	CMC-C2C-C1C	4.42	131.78	125.04
14	bB	828	CLA	C3B-C2B-C1B	-4.42	101.82	107.16
14	bA	811	CLA	O2D-CGD-CBD	4.42	119.13	111.27
14	cB	839	CLA	C3C-C4C-NC	4.42	115.53	110.57
14	bA	833	CLA	CHD-C4C-C3C	-4.42	118.34	124.84
14	cB	825	CLA	C4A-NA-C1A	-4.42	104.72	106.71
14	A	824	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
14	cA	809	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
14	bA	827	CLA	C3D-C4D-ND	4.42	117.38	110.24
14	bA	808	CLA	CMC-C2C-C1C	4.41	131.76	125.04
14	A	811	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
14	cA	827	CLA	C3D-C4D-ND	4.41	117.38	110.24
14	cA	833	CLA	CHD-C4C-C3C	-4.41	118.36	124.84
14	bA	809	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
14	A	827	CLA	C3D-C4D-ND	4.41	117.37	110.24
14	cA	842	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
14	bA	852	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
14	A	809	CLA	C3D-C2D-C1D	-4.41	99.82	105.83
14	B	801	CLA	C3D-C4D-ND	4.41	117.37	110.24
14	cA	824	CLA	C3D-C2D-C1D	-4.41	99.82	105.83
14	A	803	CLA	C4A-NA-C1A	-4.41	104.72	106.71
14	cA	808	CLA	CMC-C2C-C1C	4.41	131.75	125.04
14	B	839	CLA	C3D-C4D-ND	4.40	117.36	110.24
14	cA	838	CLA	CAC-C3C-C4C	4.40	130.52	124.81
14	cB	829	CLA	C3B-C2B-C1B	-4.40	101.85	107.16
14	bA	828	CLA	C3D-C4D-ND	4.40	117.36	110.24
14	B	811	CLA	C3D-C2D-C1D	-4.40	99.82	105.83
14	A	805	CLA	CMC-C2C-C1C	4.40	131.74	125.04
14	cB	811	CLA	C4A-NA-C1A	-4.40	104.73	106.71
14	A	838	CLA	CAC-C3C-C4C	4.40	130.52	124.81
14	bA	838	CLA	CAC-C3C-C4C	4.40	130.52	124.81
14	cB	812	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
14	bB	839	CLA	C3D-C4D-ND	4.40	117.35	110.24
14	bA	842	CLA	C3D-C2D-C1D	-4.40	99.83	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	817	CLA	O2D-CGD-CBD	4.40	119.08	111.27
14	cA	803	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
17	bB	842	BCR	C16-C15-C14	4.40	132.48	123.47
14	A	828	CLA	C3D-C4D-ND	4.40	117.35	110.24
14	cA	805	CLA	CMC-C2C-C1C	4.40	131.73	125.04
14	cA	811	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
14	A	803	CLA	C3D-C2D-C1D	-4.39	99.83	105.83
14	cA	828	CLA	C3D-C4D-ND	4.39	117.34	110.24
14	cB	840	CLA	C3D-C4D-ND	4.39	117.34	110.24
14	A	808	CLA	CMC-C2C-C1C	4.39	131.73	125.04
14	bA	803	CLA	C3D-C2D-C1D	-4.39	99.84	105.83
14	cB	818	CLA	O2D-CGD-CBD	4.39	119.07	111.27
14	F	201	CLA	C3D-C4D-ND	4.39	117.34	110.24
14	bA	836	CLA	O2D-CGD-CBD	4.39	119.07	111.27
14	bB	817	CLA	O2D-CGD-CBD	4.39	119.07	111.27
14	cB	802	CLA	C3D-C4D-ND	4.39	117.34	110.24
14	B	813	CLA	C4A-NA-C1A	-4.39	104.73	106.71
17	cB	843	BCR	C16-C15-C14	4.39	132.46	123.47
14	A	833	CLA	CHD-C4C-C3C	-4.39	118.39	124.84
14	B	828	CLA	C2C-C1C-NC	4.39	114.08	109.97
14	bB	828	CLA	C2C-C1C-NC	4.39	114.08	109.97
17	B	842	BCR	C16-C15-C14	4.39	132.46	123.47
14	A	806	CLA	C4A-NA-C1A	-4.38	104.73	106.71
14	bX	201	CLA	C4A-NA-C1A	-4.38	104.73	106.71
14	cB	818	CLA	C3D-C4D-ND	4.38	117.33	110.24
14	bB	801	CLA	C3D-C4D-ND	4.38	117.33	110.24
14	bB	811	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
14	A	836	CLA	O2D-CGD-CBD	4.38	119.05	111.27
14	B	828	CLA	C3B-C2B-C1B	-4.38	101.88	107.16
14	cA	836	CLA	O2D-CGD-CBD	4.38	119.05	111.27
14	cL	203	CLA	C3D-C2D-C1D	-4.38	99.86	105.83
14	bL	202	CLA	C3D-C2D-C1D	-4.38	99.86	105.83
14	cB	806	CLA	CMC-C2C-C1C	4.38	131.71	125.04
14	cB	807	CLA	C3D-C4D-ND	4.38	117.32	110.24
14	B	817	CLA	C3D-C4D-ND	4.37	117.31	110.24
14	B	806	CLA	C3D-C4D-ND	4.37	117.31	110.24
17	bA	846	BCR	C37-C22-C21	-4.37	116.80	122.92
14	B	807	CLA	C3D-C4D-ND	4.37	117.31	110.24
14	cA	806	CLA	C4A-NA-C1A	-4.37	104.74	106.71
14	bA	836	CLA	C3D-C4D-ND	4.37	117.31	110.24
14	bA	819	CLA	CAC-C3C-C4C	4.37	130.48	124.81
14	bA	806	CLA	C3D-C4D-ND	4.37	117.31	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bB	807	CLA	C3D-C4D-ND	4.37	117.31	110.24
14	L	202	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
14	bB	805	CLA	CMC-C2C-C1C	4.37	131.69	125.04
14	A	806	CLA	C3D-C4D-ND	4.37	117.31	110.24
14	cF	201	CLA	C3D-C4D-ND	4.37	117.31	110.24
14	bA	806	CLA	C4A-NA-C1A	-4.37	104.74	106.71
14	cA	819	CLA	CAC-C3C-C4C	4.37	130.48	124.81
17	cA	846	BCR	C37-C22-C21	-4.37	116.81	122.92
14	cB	829	CLA	C2C-C1C-NC	4.37	114.06	109.97
14	bB	803	CLA	CMD-C2D-C1D	4.37	132.41	124.71
14	B	805	CLA	CMC-C2C-C1C	4.36	131.69	125.04
14	bA	825	CLA	O2D-CGD-CBD	4.36	119.02	111.27
14	A	836	CLA	C3D-C4D-ND	4.36	117.30	110.24
14	bB	809	CLA	C3C-C4C-NC	4.36	115.46	110.57
14	bB	806	CLA	C3D-C4D-ND	4.36	117.29	110.24
14	cA	825	CLA	O2D-CGD-CBD	4.36	119.02	111.27
14	bB	849	CLA	O2D-CGD-CBD	4.36	119.01	111.27
14	bA	830	CLA	CAC-C3C-C4C	4.36	130.46	124.81
14	bF	201	CLA	C3D-C4D-ND	4.36	117.29	110.24
14	bB	817	CLA	C3D-C4D-ND	4.36	117.29	110.24
14	cA	830	CLA	CAC-C3C-C4C	4.36	130.46	124.81
14	cA	836	CLA	C3D-C4D-ND	4.36	117.28	110.24
14	A	833	CLA	C3D-C4D-ND	4.36	117.28	110.24
17	A	846	BCR	C37-C22-C21	-4.35	116.82	122.92
14	B	849	CLA	O2D-CGD-CBD	4.35	119.00	111.27
14	cB	850	CLA	O2D-CGD-CBD	4.35	119.00	111.27
14	A	819	CLA	CAC-C3C-C4C	4.35	130.46	124.81
14	cB	808	CLA	C3D-C4D-ND	4.35	117.28	110.24
14	A	830	CLA	CAC-C3C-C4C	4.35	130.46	124.81
14	A	825	CLA	O2D-CGD-CBD	4.35	119.00	111.27
14	bB	829	CLA	C3D-C2D-C1D	-4.35	99.90	105.83
14	cA	806	CLA	C3D-C4D-ND	4.35	117.27	110.24
14	bA	807	CLA	O2D-CGD-CBD	4.35	118.99	111.27
14	B	809	CLA	C3C-C4C-NC	4.35	115.45	110.57
14	cJ	101	CLA	C4A-NA-C1A	-4.35	104.75	106.71
14	cB	830	CLA	C3D-C2D-C1D	-4.34	99.90	105.83
14	bA	833	CLA	C3D-C4D-ND	4.34	117.27	110.24
14	cA	803	CLA	C4A-NA-C1A	-4.34	104.75	106.71
14	cB	820	CLA	C3D-C2D-C1D	-4.34	99.90	105.83
14	cA	822	CLA	C3B-C2B-C1B	-4.34	101.92	107.16
14	B	833	CLA	C3D-C4D-ND	4.34	117.26	110.24
14	B	803	CLA	CMD-C2D-C1D	4.34	132.36	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	810	CLA	C4A-NA-C1A	-4.34	104.75	106.71
14	cB	810	CLA	C3C-C4C-NC	4.34	115.44	110.57
14	A	822	CLA	C3B-C2B-C1B	-4.34	101.92	107.16
14	bF	201	CLA	CMC-C2C-C1C	4.34	131.65	125.04
14	cA	807	CLA	O2D-CGD-CBD	4.34	118.97	111.27
14	B	824	CLA	C4A-NA-C1A	-4.34	104.76	106.71
14	F	201	CLA	CMC-C2C-C1C	4.33	131.64	125.04
14	bA	822	CLA	C3B-C2B-C1B	-4.33	101.93	107.16
14	bB	810	CLA	C4A-NA-C1A	-4.33	104.76	106.71
14	bB	824	CLA	C4A-NA-C1A	-4.33	104.76	106.71
14	cA	802	CLA	C3C-C4C-NC	4.33	115.43	110.57
14	A	818	CLA	C2C-C1C-NC	4.33	114.03	109.97
14	A	832	CLA	CMC-C2C-C1C	4.33	131.63	125.04
14	bA	842	CLA	C3B-C2B-C1B	-4.33	101.93	107.16
14	cA	842	CLA	C3B-C2B-C1B	-4.33	101.93	107.16
14	bB	833	CLA	C3D-C4D-ND	4.33	117.24	110.24
14	bA	802	CLA	C3C-C4C-NC	4.33	115.43	110.57
14	cX	201	CLA	C4A-NA-C1A	-4.33	104.76	106.71
14	cB	804	CLA	CMD-C2D-C1D	4.33	132.34	124.71
14	cA	832	CLA	CMC-C2C-C1C	4.33	131.63	125.04
14	A	852	CLA	C3C-C4C-NC	4.33	115.42	110.57
14	A	807	CLA	O2D-CGD-CBD	4.33	118.96	111.27
14	J	101	CLA	C4A-NA-C1A	-4.33	104.76	106.71
14	bB	819	CLA	C3D-C2D-C1D	-4.33	99.93	105.83
14	bA	852	CLA	C3C-C4C-NC	4.32	115.42	110.57
14	X	201	CLA	C4A-NA-C1A	-4.32	104.76	106.71
14	A	830	CLA	C3D-C2D-C1D	-4.32	99.93	105.83
14	cA	833	CLA	C3D-C4D-ND	4.32	117.23	110.24
14	bA	820	CLA	C3D-C2D-C1D	-4.32	99.94	105.83
14	cB	834	CLA	C3D-C4D-ND	4.32	117.22	110.24
14	cF	201	CLA	CMC-C2C-C1C	4.32	131.61	125.04
14	cA	820	CLA	C3D-C2D-C1D	-4.32	99.94	105.83
14	bA	832	CLA	CMC-C2C-C1C	4.32	131.61	125.04
14	cJ	102	CLA	CMC-C2C-C1C	4.31	131.61	125.04
14	B	819	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
14	bA	830	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
14	A	842	CLA	C3B-C2B-C1B	-4.31	101.96	107.16
14	bA	831	CLA	O2D-CGD-CBD	4.31	118.93	111.27
14	bA	837	CLA	CAC-C3C-C4C	4.31	130.40	124.81
14	cA	837	CLA	CAC-C3C-C4C	4.31	130.40	124.81
14	A	837	CLA	CAC-C3C-C4C	4.31	130.40	124.81
14	A	802	CLA	C3C-C4C-NC	4.31	115.40	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	831	CLA	O2D-CGD-CBD	4.31	118.92	111.27
14	bA	803	CLA	C4A-NA-C1A	-4.31	104.77	106.71
14	bA	818	CLA	C2C-C1C-NC	4.31	114.01	109.97
14	B	829	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
14	cA	852	CLA	C3C-C4C-NC	4.31	115.40	110.57
14	A	841	CLA	C2B-C1B-NB	4.30	113.12	110.23
14	bA	840	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
14	cB	833	CLA	C3B-C2B-C1B	-4.30	101.97	107.16
14	A	820	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
14	bA	841	CLA	C2B-C1B-NB	4.30	113.11	110.23
14	bJ	102	CLA	CMC-C2C-C1C	4.30	131.58	125.04
14	bJ	101	CLA	C4A-NA-C1A	-4.30	104.78	106.71
14	cA	818	CLA	C2C-C1C-NC	4.29	113.99	109.97
14	cA	830	CLA	C3D-C2D-C1D	-4.29	99.98	105.83
14	bB	825	CLA	C4A-NA-C1A	-4.29	104.78	106.71
14	A	831	CLA	O2D-CGD-CBD	4.29	118.89	111.27
14	B	832	CLA	C3D-C4D-ND	4.29	117.18	110.24
14	A	840	CLA	C3D-C2D-C1D	-4.29	99.98	105.83
14	cA	834	CLA	CAC-C3C-C4C	4.29	130.37	124.81
14	bA	802	CLA	C3B-C2B-C1B	-4.29	101.99	107.16
14	bJ	101	CLA	CMC-C2C-C1C	4.28	131.56	125.04
14	B	832	CLA	C3B-C2B-C1B	-4.28	101.99	107.16
14	J	102	CLA	CMC-C2C-C1C	4.28	131.56	125.04
14	cA	840	CLA	C3D-C2D-C1D	-4.28	99.99	105.83
14	bB	833	CLA	C4A-NA-C1A	-4.28	104.78	106.71
14	bB	824	CLA	C3D-C4D-ND	4.28	117.16	110.24
14	bL	201	CLA	O2A-CGA-CBA	4.28	125.33	111.91
14	bB	832	CLA	C3B-C2B-C1B	-4.28	102.00	107.16
14	A	832	CLA	C1C-C2C-C3C	-4.27	102.46	106.96
14	B	825	CLA	C4A-NA-C1A	-4.27	104.78	106.71
14	L	201	CLA	O2A-CGA-CBA	4.27	125.32	111.91
14	A	834	CLA	CAC-C3C-C4C	4.27	130.35	124.81
14	cB	839	CLA	C3D-C4D-ND	4.27	117.15	110.24
14	bB	832	CLA	C3D-C4D-ND	4.27	117.15	110.24
14	cA	824	CLA	C3D-C4D-ND	4.27	117.14	110.24
14	cA	832	CLA	C1C-C2C-C3C	-4.27	102.47	106.96
14	B	824	CLA	C3D-C4D-ND	4.27	117.14	110.24
14	bA	829	CLA	C4A-NA-C1A	-4.27	104.79	106.71
14	J	101	CLA	CMC-C2C-C1C	4.27	131.54	125.04
14	bA	826	CLA	C3D-C4D-ND	4.27	117.14	110.24
14	bB	838	CLA	C3D-C4D-ND	4.27	117.14	110.24
14	cL	202	CLA	O2A-CGA-CBA	4.26	125.29	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bA	834	CLA	CAC-C3C-C4C	4.26	130.34	124.81
14	A	824	CLA	C3D-C4D-ND	4.26	117.13	110.24
14	bA	824	CLA	C3D-C4D-ND	4.26	117.13	110.24
14	B	801	CLA	CMC-C2C-C1C	4.26	131.52	125.04
14	A	802	CLA	C3B-C2B-C1B	-4.26	102.02	107.16
14	A	826	CLA	C3D-C4D-ND	4.26	117.12	110.24
14	cA	807	CLA	C4A-NA-C1A	-4.26	104.79	106.71
14	bA	832	CLA	C1C-C2C-C3C	-4.26	102.48	106.96
14	B	838	CLA	C3D-C4D-ND	4.26	117.12	110.24
14	A	841	CLA	C3D-C4D-ND	4.26	117.12	110.24
14	A	829	CLA	C4A-NA-C1A	-4.26	104.79	106.71
14	cA	826	CLA	C3D-C4D-ND	4.25	117.12	110.24
14	bA	841	CLA	C1C-C2C-C3C	-4.25	102.48	106.96
14	A	803	CLA	CAC-C3C-C4C	4.25	130.33	124.81
14	cA	802	CLA	C3B-C2B-C1B	-4.25	102.03	107.16
14	cB	833	CLA	C3D-C4D-ND	4.25	117.12	110.24
14	cA	841	CLA	C3D-C4D-ND	4.25	117.11	110.24
14	A	841	CLA	C1C-C2C-C3C	-4.25	102.49	106.96
17	B	846	BCR	C15-C16-C17	4.25	132.18	123.47
14	cB	802	CLA	CMC-C2C-C1C	4.25	131.51	125.04
14	cA	829	CLA	C4A-NA-C1A	-4.25	104.80	106.71
14	bA	841	CLA	C3D-C4D-ND	4.25	117.11	110.24
14	bA	803	CLA	CAC-C3C-C4C	4.25	130.32	124.81
14	cA	802	CLA	C3D-C4D-ND	4.25	117.11	110.24
14	cB	825	CLA	C3D-C4D-ND	4.25	117.11	110.24
14	bB	801	CLA	CMC-C2C-C1C	4.25	131.50	125.04
17	bB	846	BCR	C15-C16-C17	4.25	132.17	123.47
14	cA	803	CLA	CMC-C2C-C1C	4.24	131.50	125.04
17	cB	847	BCR	C15-C16-C17	4.24	132.17	123.47
14	bA	825	CLA	C3D-C4D-ND	4.24	117.10	110.24
14	cA	803	CLA	CAC-C3C-C4C	4.24	130.32	124.81
14	cA	841	CLA	C2B-C1B-NB	4.24	113.08	110.23
14	L	204	CLA	C4A-NA-C1A	-4.24	104.80	106.71
14	A	825	CLA	C3D-C4D-ND	4.24	117.10	110.24
14	cJ	102	CLA	O2D-CGD-CBD	4.24	118.80	111.27
14	cA	825	CLA	C3D-C4D-ND	4.24	117.10	110.24
14	A	802	CLA	C3D-C4D-ND	4.24	117.09	110.24
14	bB	831	CLA	C2C-C1C-NC	4.24	113.94	109.97
14	A	803	CLA	CMC-C2C-C1C	4.24	131.49	125.04
14	bA	803	CLA	CMC-C2C-C1C	4.24	131.49	125.04
14	bL	204	CLA	C4A-NA-C1A	-4.24	104.80	106.71
14	cA	828	CLA	C3C-C4C-NC	4.24	115.32	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	J	102	CLA	O2D-CGD-CBD	4.24	118.80	111.27
14	cJ	101	CLA	CMC-C2C-C1C	4.23	131.49	125.04
14	A	828	CLA	C3C-C4C-NC	4.23	115.32	110.57
14	cB	802	CLA	C2C-C1C-NC	4.23	113.94	109.97
17	I	101	BCR	C37-C22-C21	-4.23	117.00	122.92
14	B	833	CLA	C4A-NA-C1A	-4.23	104.81	106.71
14	cB	832	CLA	C2C-C1C-NC	4.23	113.93	109.97
14	B	801	CLA	C2C-C1C-NC	4.23	113.93	109.97
14	bA	802	CLA	C3D-C4D-ND	4.23	117.07	110.24
14	cB	826	CLA	C4A-NA-C1A	-4.22	104.81	106.71
14	bA	828	CLA	C3C-C4C-NC	4.22	115.31	110.57
14	cA	841	CLA	C1C-C2C-C3C	-4.22	102.52	106.96
14	bJ	102	CLA	O2D-CGD-CBD	4.22	118.77	111.27
17	bI	101	BCR	C37-C22-C21	-4.22	117.01	122.92
17	bA	849	BCR	C15-C16-C17	4.22	132.12	123.47
17	cA	849	BCR	C15-C16-C17	4.22	132.12	123.47
14	A	818	CLA	C3B-C2B-C1B	-4.22	102.07	107.16
14	bB	801	CLA	C2C-C1C-NC	4.22	113.92	109.97
17	A	849	BCR	C15-C16-C17	4.21	132.11	123.47
14	cA	813	CLA	C3B-C2B-C1B	-4.21	102.08	107.16
14	A	813	CLA	C3D-C4D-ND	4.21	117.05	110.24
14	bA	807	CLA	C4A-NA-C1A	-4.21	104.81	106.71
14	bA	819	CLA	C4A-NA-C1A	-4.21	104.81	106.71
14	cB	810	CLA	CAC-C3C-C4C	4.21	130.28	124.81
14	A	813	CLA	C3B-C2B-C1B	-4.21	102.08	107.16
14	bB	827	CLA	C3D-C2D-C1D	-4.21	100.08	105.83
14	cA	804	CLA	C4A-NA-C1A	-4.21	104.81	106.71
14	bA	814	CLA	CMC-C2C-C1C	4.21	131.45	125.04
14	B	827	CLA	C3D-C2D-C1D	-4.21	100.09	105.83
14	bA	811	CLA	C3B-C2B-C1B	-4.21	102.08	107.16
14	bA	813	CLA	C3B-C2B-C1B	-4.21	102.08	107.16
14	cA	813	CLA	C3D-C4D-ND	4.21	117.05	110.24
14	A	814	CLA	CMC-C2C-C1C	4.21	131.45	125.04
14	bA	834	CLA	C3D-C2D-C1D	-4.21	100.09	105.83
14	cA	811	CLA	C3B-C2B-C1B	-4.21	102.08	107.16
14	cA	818	CLA	C3B-C2B-C1B	-4.21	102.08	107.16
17	cI	101	BCR	C37-C22-C21	-4.21	117.03	122.92
14	cA	828	CLA	O2D-CGD-CBD	4.20	118.74	111.27
14	cL	205	CLA	C4A-NA-C1A	-4.20	104.82	106.71
14	cA	814	CLA	CMC-C2C-C1C	4.20	131.44	125.04
14	bB	809	CLA	CAC-C3C-C4C	4.20	130.26	124.81
14	bA	813	CLA	C3D-C4D-ND	4.20	117.03	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	804	CLA	C4A-NA-C1A	-4.20	104.82	106.71
14	A	807	CLA	C4A-NA-C1A	-4.20	104.82	106.71
14	A	828	CLA	O2D-CGD-CBD	4.20	118.73	111.27
14	bB	808	CLA	C3D-C4D-ND	4.20	117.03	110.24
14	cA	834	CLA	C3D-C2D-C1D	-4.20	100.10	105.83
14	A	811	CLA	C3B-C2B-C1B	-4.20	102.09	107.16
14	bA	818	CLA	C3B-C2B-C1B	-4.20	102.09	107.16
14	bA	828	CLA	O2D-CGD-CBD	4.20	118.73	111.27
14	bB	833	CLA	C3B-C2B-C1B	-4.20	102.10	107.16
14	bA	832	CLA	C3C-C4C-NC	4.19	115.28	110.57
14	B	831	CLA	C2C-C1C-NC	4.19	113.90	109.97
14	cB	828	CLA	C3D-C2D-C1D	-4.19	100.11	105.83
14	A	834	CLA	C3D-C2D-C1D	-4.19	100.11	105.83
14	bB	809	CLA	C3D-C4D-ND	4.19	117.02	110.24
17	cB	844	BCR	C37-C22-C21	-4.19	117.06	122.92
14	B	808	CLA	C3D-C4D-ND	4.19	117.01	110.24
14	B	809	CLA	CAC-C3C-C4C	4.19	130.24	124.81
14	cA	832	CLA	C3C-C4C-NC	4.19	115.27	110.57
17	bB	843	BCR	C37-C22-C21	-4.19	117.06	122.92
17	B	843	BCR	C37-C22-C21	-4.19	117.06	122.92
14	bB	808	CLA	CMB-C2B-C1B	4.18	131.74	125.37
14	B	809	CLA	C3D-C4D-ND	4.18	117.01	110.24
14	bB	831	CLA	C3B-C2B-C1B	-4.18	102.11	107.16
14	cB	809	CLA	C3D-C4D-ND	4.18	117.00	110.24
14	B	831	CLA	C3B-C2B-C1B	-4.18	102.11	107.16
14	B	833	CLA	C3B-C2B-C1B	-4.18	102.11	107.16
14	cB	834	CLA	C3B-C2B-C1B	-4.18	102.11	107.16
14	A	832	CLA	C3C-C4C-NC	4.18	115.26	110.57
17	cA	849	BCR	C34-C9-C10	-4.18	117.07	122.92
17	bA	849	BCR	C34-C9-C10	-4.18	117.07	122.92
14	bL	203	CLA	C3C-C4C-NC	4.17	115.25	110.57
14	L	203	CLA	C3C-C4C-NC	4.17	115.25	110.57
14	cB	832	CLA	C3B-C2B-C1B	-4.17	102.13	107.16
14	cB	810	CLA	C3D-C4D-ND	4.17	116.98	110.24
14	bA	832	CLA	C3B-C2B-C1B	-4.17	102.13	107.16
14	cL	204	CLA	C3C-C4C-NC	4.17	115.25	110.57
14	bB	815	CLA	C4A-NA-C1A	-4.17	104.83	106.71
14	B	823	CLA	C3C-C4C-NC	4.17	115.24	110.57
14	cB	834	CLA	C4A-NA-C1A	-4.16	104.83	106.71
17	bF	202	BCR	C37-C22-C21	-4.16	117.09	122.92
14	cB	824	CLA	C3C-C4C-NC	4.16	115.24	110.57
14	cA	832	CLA	C3B-C2B-C1B	-4.16	102.14	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	811	CLA	C4A-NA-C1A	-4.16	104.84	106.71
14	A	832	CLA	C3B-C2B-C1B	-4.16	102.14	107.16
14	bL	201	CLA	C3B-C2B-C1B	-4.16	102.14	107.16
14	B	808	CLA	CMB-C2B-C1B	4.16	131.70	125.37
14	A	819	CLA	C4A-NA-C1A	-4.15	104.84	106.71
14	cA	818	CLA	CAC-C3C-C4C	4.15	130.20	124.81
14	bB	823	CLA	C3C-C4C-NC	4.15	115.23	110.57
14	cJ	102	CLA	C3B-C2B-C1B	-4.15	102.15	107.16
14	cL	202	CLA	C3B-C2B-C1B	-4.15	102.15	107.16
17	A	849	BCR	C34-C9-C10	-4.15	117.11	122.92
17	F	202	BCR	C37-C22-C21	-4.15	117.11	122.92
14	cB	816	CLA	C4A-NA-C1A	-4.15	104.84	106.71
14	A	833	CLA	C3D-C2D-C1D	-4.15	100.17	105.83
14	A	818	CLA	CAC-C3C-C4C	4.15	130.19	124.81
14	cA	826	CLA	C4A-NA-C1A	-4.15	104.84	106.71
14	F	201	CLA	C3B-C2B-C1B	-4.14	102.16	107.16
14	cF	201	CLA	C3B-C2B-C1B	-4.14	102.16	107.16
14	bB	825	CLA	C3D-C4D-ND	4.14	116.94	110.24
14	B	815	CLA	C4A-NA-C1A	-4.14	104.84	106.71
14	bA	818	CLA	CAC-C3C-C4C	4.14	130.18	124.81
14	L	201	CLA	C3B-C2B-C1B	-4.14	102.17	107.16
14	bA	804	CLA	C4A-NA-C1A	-4.14	104.85	106.71
14	bF	201	CLA	C3B-C2B-C1B	-4.14	102.17	107.16
14	cB	809	CLA	CMB-C2B-C1B	4.13	131.67	125.37
14	bA	833	CLA	C3D-C2D-C1D	-4.13	100.19	105.83
17	B	842	BCR	C34-C9-C10	-4.13	117.13	122.92
14	A	826	CLA	C4A-NA-C1A	-4.13	104.85	106.71
17	cF	202	BCR	C37-C22-C21	-4.13	117.13	122.92
17	bB	842	BCR	C34-C9-C10	-4.13	117.14	122.92
14	B	808	CLA	C3C-C4C-NC	4.13	115.20	110.57
14	J	102	CLA	C3B-C2B-C1B	-4.13	102.17	107.16
14	bB	808	CLA	C3C-C4C-NC	4.13	115.20	110.57
14	B	815	CLA	C3B-C2B-C1B	-4.13	102.18	107.16
14	B	825	CLA	C3D-C4D-ND	4.13	116.92	110.24
14	cA	833	CLA	C3D-C2D-C1D	-4.13	100.20	105.83
17	cB	843	BCR	C34-C9-C10	-4.13	117.14	122.92
14	cB	826	CLA	C3D-C4D-ND	4.13	116.91	110.24
14	cB	836	CLA	CMC-C2C-C1C	4.13	131.32	125.04
17	L	206	BCR	C37-C22-C21	-4.12	117.14	122.92
17	bL	206	BCR	C37-C22-C21	-4.12	117.14	122.92
14	J	101	CLA	C3B-C2B-C1B	-4.12	102.18	107.16
14	bJ	101	CLA	C3B-C2B-C1B	-4.12	102.18	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bJ	102	CLA	C3B-C2B-C1B	-4.12	102.18	107.16
13	bA	801	CL0	C3D-C4D-ND	4.12	116.91	110.24
14	bA	826	CLA	C4A-NA-C1A	-4.12	104.85	106.71
14	B	835	CLA	CMC-C2C-C1C	4.12	131.31	125.04
13	cA	801	CL0	C3D-C4D-ND	4.12	116.90	110.24
13	A	801	CL0	C3D-C4D-ND	4.12	116.90	110.24
14	cA	819	CLA	C4A-NA-C1A	-4.12	104.85	106.71
14	B	802	CLA	C1C-C2C-C3C	-4.12	102.63	106.96
14	bB	815	CLA	C3B-C2B-C1B	-4.12	102.19	107.16
14	bB	835	CLA	CMC-C2C-C1C	4.11	131.31	125.04
14	cB	836	CLA	CAC-C3C-C4C	4.11	130.15	124.81
14	bA	832	CLA	C3D-C4D-ND	4.11	116.89	110.24
14	cB	809	CLA	C3C-C4C-NC	4.11	115.18	110.57
14	bB	802	CLA	C1C-C2C-C3C	-4.11	102.64	106.96
14	J	102	CLA	C4A-NA-C1A	-4.11	104.86	106.71
14	bA	817	CLA	O2D-CGD-CBD	4.11	118.57	111.27
14	cA	832	CLA	C3D-C4D-ND	4.11	116.88	110.24
14	cL	202	CLA	C3D-C4D-ND	4.11	116.88	110.24
14	cB	826	CLA	C3B-C2B-C1B	-4.11	102.20	107.16
14	B	825	CLA	C3B-C2B-C1B	-4.10	102.21	107.16
14	B	835	CLA	CAC-C3C-C4C	4.10	130.13	124.81
14	A	806	CLA	C3B-C2B-C1B	-4.10	102.21	107.16
14	cB	816	CLA	C3B-C2B-C1B	-4.10	102.21	107.16
14	A	806	CLA	CMC-C2C-C1C	4.10	131.29	125.04
14	bA	806	CLA	CMC-C2C-C1C	4.10	131.29	125.04
14	cA	802	CLA	C1C-C2C-C3C	-4.10	102.64	106.96
14	bA	819	CLA	C3B-C2B-C1B	-4.10	102.21	107.16
14	bB	813	CLA	C3D-C2D-C1D	-4.10	100.23	105.83
13	cA	801	CL0	C1C-C2C-C3C	-4.10	102.64	106.96
14	cB	807	CLA	C3B-C2B-C1B	-4.10	102.21	107.16
14	cB	820	CLA	C3B-C2B-C1B	-4.10	102.21	107.16
14	cJ	101	CLA	C3B-C2B-C1B	-4.10	102.21	107.16
14	L	201	CLA	C3D-C4D-ND	4.10	116.87	110.24
14	cB	814	CLA	C3D-C2D-C1D	-4.10	100.24	105.83
14	cA	806	CLA	CMC-C2C-C1C	4.10	131.28	125.04
14	cA	806	CLA	C3B-C2B-C1B	-4.10	102.22	107.16
14	A	817	CLA	O2D-CGD-CBD	4.10	118.55	111.27
14	B	813	CLA	C3D-C2D-C1D	-4.10	100.24	105.83
13	cA	801	CL0	C3C-C4C-NC	4.09	115.16	110.57
17	cL	207	BCR	C37-C22-C21	-4.09	117.19	122.92
14	bA	802	CLA	C1C-C2C-C3C	-4.09	102.65	106.96
14	cB	803	CLA	C3C-C4C-NC	4.09	115.16	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	819	CLA	C3B-C2B-C1B	-4.09	102.22	107.16
14	cB	803	CLA	C1C-C2C-C3C	-4.09	102.66	106.96
13	A	801	CL0	C1C-C2C-C3C	-4.09	102.66	106.96
14	bL	201	CLA	C3D-C4D-ND	4.09	116.85	110.24
14	A	832	CLA	C3D-C4D-ND	4.09	116.85	110.24
14	bB	806	CLA	C3B-C2B-C1B	-4.09	102.23	107.16
14	A	811	CLA	C4A-NA-C1A	-4.09	104.87	106.71
14	cF	201	CLA	O2D-CGD-CBD	4.08	118.53	111.27
14	A	819	CLA	C3B-C2B-C1B	-4.08	102.23	107.16
14	B	819	CLA	C3B-C2B-C1B	-4.08	102.23	107.16
14	bB	835	CLA	CAC-C3C-C4C	4.08	130.11	124.81
14	B	851	CLA	C3B-C2B-C1B	-4.08	102.23	107.16
14	F	201	CLA	O2D-CGD-CBD	4.08	118.52	111.27
14	bB	819	CLA	C3B-C2B-C1B	-4.08	102.23	107.16
14	bB	825	CLA	C3B-C2B-C1B	-4.08	102.24	107.16
14	A	802	CLA	C1C-C2C-C3C	-4.08	102.67	106.96
14	cB	812	CLA	C3B-C2B-C1B	-4.08	102.24	107.16
14	bB	851	CLA	C3B-C2B-C1B	-4.08	102.24	107.16
14	B	802	CLA	C3C-C4C-NC	4.08	115.14	110.57
14	B	826	CLA	C3C-C4C-NC	4.08	115.14	110.57
13	bA	801	CL0	C3C-C4C-NC	4.08	115.14	110.57
14	B	811	CLA	O2D-CGD-CBD	4.07	118.51	111.27
14	cB	801	CLA	C3B-C2B-C1B	-4.07	102.25	107.16
14	B	837	CLA	C4A-NA-C1A	-4.07	104.88	106.71
14	B	806	CLA	C3B-C2B-C1B	-4.07	102.25	107.16
14	bB	832	CLA	C3C-C4C-NC	4.07	115.14	110.57
14	bA	811	CLA	C4A-NA-C1A	-4.07	104.88	106.71
17	bB	843	BCR	C16-C15-C14	4.07	131.81	123.47
13	bA	801	CL0	C1C-C2C-C3C	-4.07	102.68	106.96
14	bJ	102	CLA	C4A-NA-C1A	-4.07	104.88	106.71
17	cB	844	BCR	C16-C15-C14	4.07	131.81	123.47
14	bF	201	CLA	O2D-CGD-CBD	4.07	118.50	111.27
14	bA	806	CLA	C3B-C2B-C1B	-4.07	102.25	107.16
13	A	801	CL0	C3C-C4C-NC	4.07	115.13	110.57
14	B	832	CLA	C3C-C4C-NC	4.07	115.13	110.57
17	B	843	BCR	C16-C15-C14	4.06	131.80	123.47
14	bB	811	CLA	O2D-CGD-CBD	4.06	118.49	111.27
17	cB	851	BCR	C37-C22-C21	-4.06	117.24	122.92
14	bA	815	CLA	C4A-NA-C1A	-4.06	104.88	106.71
14	B	811	CLA	C3B-C2B-C1B	-4.06	102.26	107.16
14	cB	808	CLA	CAC-C3C-C4C	4.06	130.08	124.81
14	B	849	CLA	CAC-C3C-C4C	4.06	130.07	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bB	837	CLA	C4A-NA-C1A	-4.06	104.88	106.71
14	bB	811	CLA	C3B-C2B-C1B	-4.06	102.26	107.16
14	cA	817	CLA	O2D-CGD-CBD	4.06	118.48	111.27
14	bA	833	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
14	bB	807	CLA	CAC-C3C-C4C	4.06	130.07	124.81
14	bB	849	CLA	C3B-C2B-C1B	-4.05	102.27	107.16
17	bA	849	BCR	C37-C22-C21	-4.05	117.25	122.92
14	bB	803	CLA	C4A-NA-C1A	-4.05	104.88	106.71
14	cB	850	CLA	CAC-C3C-C4C	4.05	130.07	124.81
14	A	833	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
17	B	850	BCR	C37-C22-C21	-4.05	117.25	122.92
14	cB	833	CLA	C3C-C4C-NC	4.05	115.11	110.57
14	cB	812	CLA	O2D-CGD-CBD	4.05	118.46	111.27
17	A	849	BCR	C37-C22-C21	-4.05	117.25	122.92
14	A	815	CLA	C4A-NA-C1A	-4.05	104.89	106.71
14	cJ	102	CLA	C4A-NA-C1A	-4.05	104.89	106.71
14	cB	850	CLA	C3B-C2B-C1B	-4.05	102.28	107.16
14	cX	201	CLA	C3B-C2B-C1B	-4.05	102.28	107.16
14	cL	203	CLA	C4A-NA-C1A	-4.05	104.89	106.71
14	bB	826	CLA	C3C-C4C-NC	4.05	115.11	110.57
17	A	848	BCR	C30-C25-C26	-4.04	116.92	122.61
17	cA	849	BCR	C37-C22-C21	-4.04	117.26	122.92
14	B	849	CLA	C3B-C2B-C1B	-4.04	102.28	107.16
17	bA	846	BCR	C34-C9-C10	-4.04	117.26	122.92
14	cB	827	CLA	C3C-C4C-NC	4.04	115.10	110.57
14	cL	202	CLA	C1D-CHD-C4C	-4.04	117.34	126.06
14	bL	202	CLA	C4A-NA-C1A	-4.04	104.89	106.71
14	cA	833	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
14	A	838	CLA	CMC-C2C-C1C	4.04	131.19	125.04
14	bB	802	CLA	C3C-C4C-NC	4.04	115.10	110.57
14	bB	849	CLA	CAC-C3C-C4C	4.04	130.05	124.81
14	A	839	CLA	O2D-CGD-CBD	4.04	118.45	111.27
14	X	201	CLA	C3B-C2B-C1B	-4.04	102.28	107.16
14	L	202	CLA	C4A-NA-C1A	-4.04	104.89	106.71
17	cA	848	BCR	C30-C25-C26	-4.04	116.93	122.61
17	bB	850	BCR	C37-C22-C21	-4.04	117.27	122.92
14	B	807	CLA	CAC-C3C-C4C	4.04	130.05	124.81
14	L	201	CLA	C1D-CHD-C4C	-4.04	117.35	126.06
14	bX	201	CLA	C3B-C2B-C1B	-4.03	102.29	107.16
14	bL	201	CLA	C1D-CHD-C4C	-4.03	117.36	126.06
17	A	846	BCR	C34-C9-C10	-4.03	117.28	122.92
14	bA	839	CLA	O2D-CGD-CBD	4.03	118.43	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cB	838	CLA	C4A-NA-C1A	-4.03	104.89	106.71
14	cB	804	CLA	C3D-C4D-ND	4.03	116.76	110.24
14	A	823	CLA	C3B-C2B-C1B	-4.03	102.30	107.16
17	bA	848	BCR	C30-C25-C26	-4.03	116.94	122.61
14	cA	815	CLA	C4A-NA-C1A	-4.03	104.89	106.71
14	L	201	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
14	cA	823	CLA	C3B-C2B-C1B	-4.03	102.30	107.16
17	cA	846	BCR	C34-C9-C10	-4.02	117.28	122.92
14	bB	803	CLA	C3D-C4D-ND	4.02	116.75	110.24
14	B	807	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
14	cA	839	CLA	O2D-CGD-CBD	4.02	118.42	111.27
14	B	814	CLA	C4A-NA-C1A	-4.02	104.90	106.71
14	cL	202	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
14	bA	838	CLA	CMC-C2C-C1C	4.02	131.16	125.04
14	cA	838	CLA	CMC-C2C-C1C	4.02	131.16	125.04
14	bB	839	CLA	C3C-C4C-NC	4.02	115.08	110.57
14	A	837	CLA	C4A-NA-C1A	-4.02	104.90	106.71
14	A	825	CLA	C3C-C4C-NC	4.02	115.08	110.57
14	bL	201	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
14	bA	823	CLA	C3B-C2B-C1B	-4.02	102.31	107.16
14	bA	825	CLA	C3C-C4C-NC	4.02	115.08	110.57
14	cA	807	CLA	C3B-C2B-C1B	-4.02	102.31	107.16
14	B	803	CLA	C3D-C4D-ND	4.02	116.73	110.24
14	cB	804	CLA	C4A-NA-C1A	-4.01	104.90	106.71
14	bB	807	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
14	cB	808	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
14	B	839	CLA	C3C-C4C-NC	4.01	115.07	110.57
14	cA	837	CLA	C4A-NA-C1A	-4.01	104.90	106.71
14	cB	840	CLA	C3C-C4C-NC	4.01	115.07	110.57
14	cA	805	CLA	CAC-C3C-C4C	4.01	130.01	124.81
14	A	805	CLA	CAC-C3C-C4C	4.01	130.01	124.81
14	cA	824	CLA	C3B-C2B-C1B	-4.01	102.32	107.16
14	bA	809	CLA	CMC-C2C-C1C	4.01	131.14	125.04
14	B	826	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
14	bA	852	CLA	CMC-C2C-C1C	4.01	131.14	125.04
14	bL	204	CLA	C3C-C4C-NC	4.00	115.06	110.57
14	bA	805	CLA	CAC-C3C-C4C	4.00	130.00	124.81
14	cA	825	CLA	C3C-C4C-NC	4.00	115.06	110.57
14	B	827	CLA	C4A-NA-C1A	-4.00	104.91	106.71
17	J	103	BCR	C19-C18-C17	4.00	125.08	118.94
14	cB	827	CLA	C3D-C4D-ND	4.00	116.71	110.24
14	bB	827	CLA	C4A-NA-C1A	-4.00	104.91	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bA	806	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
14	bA	824	CLA	C3B-C2B-C1B	-4.00	102.33	107.16
14	A	809	CLA	CMC-C2C-C1C	4.00	131.13	125.04
17	bB	845	BCR	C37-C22-C21	-4.00	117.32	122.92
14	cA	852	CLA	CMC-C2C-C1C	4.00	131.13	125.04
14	A	806	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
14	cB	828	CLA	C4A-NA-C1A	-4.00	104.91	106.71
17	bJ	103	BCR	C19-C18-C17	4.00	125.07	118.94
14	A	822	CLA	CAC-C3C-C4C	4.00	129.99	124.81
14	A	852	CLA	CMC-C2C-C1C	4.00	131.12	125.04
14	A	807	CLA	C3B-C2B-C1B	-3.99	102.34	107.16
14	cA	822	CLA	CAC-C3C-C4C	3.99	129.99	124.81
14	cA	809	CLA	CMC-C2C-C1C	3.99	131.12	125.04
14	cB	803	CLA	C3D-C4D-ND	3.99	116.70	110.24
14	A	834	CLA	O2D-CGD-CBD	3.99	118.36	111.27
14	cA	806	CLA	C1C-C2C-C3C	-3.99	102.76	106.96
17	cB	846	BCR	C37-C22-C21	-3.99	117.33	122.92
14	bB	809	CLA	C3B-C4B-NB	3.99	114.22	110.52
14	cB	827	CLA	C1C-C2C-C3C	-3.99	102.76	106.96
14	cL	205	CLA	C3C-C4C-NC	3.99	115.05	110.57
14	bA	807	CLA	C3B-C2B-C1B	-3.99	102.35	107.16
17	cJ	103	BCR	C19-C18-C17	3.99	125.06	118.94
14	B	826	CLA	C3D-C4D-ND	3.99	116.69	110.24
17	B	845	BCR	C37-C22-C21	-3.99	117.34	122.92
14	B	802	CLA	C3D-C4D-ND	3.99	116.69	110.24
14	bA	822	CLA	CAC-C3C-C4C	3.98	129.98	124.81
14	A	840	CLA	C3B-C2B-C1B	-3.98	102.35	107.16
14	L	204	CLA	C3C-C4C-NC	3.98	115.04	110.57
14	B	829	CLA	C4A-NA-C1A	-3.98	104.92	106.71
14	bB	826	CLA	C3D-C4D-ND	3.98	116.68	110.24
14	bB	802	CLA	C3D-C4D-ND	3.98	116.68	110.24
14	J	101	CLA	CAC-C3C-C4C	3.98	129.98	124.81
14	cB	802	CLA	C3C-C4C-NC	3.98	115.04	110.57
14	cA	808	CLA	C3B-C2B-C1B	-3.98	102.36	107.16
14	B	820	CLA	C4A-NA-C1A	-3.98	104.92	106.71
13	cA	801	CL0	CMB-C2B-C1B	3.98	131.43	125.37
14	cA	834	CLA	O2D-CGD-CBD	3.98	118.34	111.27
14	A	813	CLA	C3C-C4C-NC	3.98	115.03	110.57
14	bA	841	CLA	C3C-C4C-NC	3.98	115.03	110.57
14	A	824	CLA	C3B-C2B-C1B	-3.98	102.36	107.16
14	bA	834	CLA	O2D-CGD-CBD	3.98	118.34	111.27
14	B	801	CLA	C3C-C4C-NC	3.98	115.03	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	bA	801	CL0	CMB-C2B-C1B	3.98	131.42	125.37
17	B	845	BCR	C16-C15-C14	3.98	131.62	123.47
14	B	803	CLA	C4A-NA-C1A	-3.97	104.92	106.71
14	X	201	CLA	CMC-C2C-C1C	3.97	131.09	125.04
14	bB	801	CLA	C3C-C4C-NC	3.97	115.03	110.57
14	bJ	101	CLA	CAC-C3C-C4C	3.97	129.97	124.81
14	bB	808	CLA	C3B-C2B-C1B	-3.97	102.37	107.16
13	A	801	CL0	CMB-C2B-C1B	3.97	131.42	125.37
14	bB	826	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
14	A	808	CLA	C3B-C2B-C1B	-3.97	102.37	107.16
14	bB	820	CLA	C4A-NA-C1A	-3.97	104.92	106.71
17	bB	845	BCR	C16-C15-C14	3.97	131.61	123.47
14	cJ	101	CLA	CAC-C3C-C4C	3.97	129.96	124.81
14	bB	835	CLA	C4A-NA-C1A	-3.97	104.92	106.71
14	cB	810	CLA	C3B-C4B-NB	3.97	114.20	110.52
14	cA	829	CLA	C3B-C2B-C1B	-3.97	102.37	107.16
17	cB	846	BCR	C16-C15-C14	3.97	131.60	123.47
14	cA	841	CLA	C3C-C4C-NC	3.97	115.02	110.57
14	cX	201	CLA	CMC-C2C-C1C	3.96	131.08	125.04
14	A	818	CLA	CMC-C2C-C1C	3.96	131.08	125.04
14	bX	201	CLA	CMC-C2C-C1C	3.96	131.08	125.04
14	cB	826	CLA	C3C-C4C-NC	3.96	115.02	110.57
14	bB	831	CLA	CMC-C2C-C1C	3.96	131.07	125.04
14	cA	840	CLA	C3B-C2B-C1B	-3.96	102.38	107.16
14	cB	832	CLA	CMC-C2C-C1C	3.96	131.07	125.04
14	B	838	CLA	C3B-C2B-C1B	-3.96	102.38	107.16
14	bA	829	CLA	C3B-C2B-C1B	-3.96	102.38	107.16
14	bA	852	CLA	C3D-C4D-ND	3.96	116.64	110.24
14	bB	814	CLA	C4A-NA-C1A	-3.96	104.93	106.71
14	bB	817	CLA	C4A-NA-C1A	-3.96	104.93	106.71
14	bB	825	CLA	C3C-C4C-NC	3.96	115.01	110.57
14	bB	822	CLA	C4A-NA-C1A	-3.96	104.93	106.71
14	bA	818	CLA	CMC-C2C-C1C	3.96	131.06	125.04
14	bB	829	CLA	C4A-NA-C1A	-3.95	104.93	106.71
14	A	829	CLA	C3B-C2B-C1B	-3.95	102.39	107.16
14	B	831	CLA	CMC-C2C-C1C	3.95	131.06	125.04
14	cB	839	CLA	C3B-C2B-C1B	-3.95	102.39	107.16
14	A	841	CLA	C3C-C4C-NC	3.95	115.00	110.57
14	bA	817	CLA	C3C-C4C-NC	3.95	115.00	110.57
14	bA	840	CLA	C3B-C2B-C1B	-3.95	102.39	107.16
14	B	825	CLA	C3C-C4C-NC	3.95	115.00	110.57
14	cB	819	CLA	C3B-C2B-C1B	-3.95	102.39	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	835	CLA	C4A-NA-C1A	-3.95	104.93	106.71
14	cB	815	CLA	C4A-NA-C1A	-3.95	104.93	106.71
14	A	852	CLA	C3D-C4D-ND	3.95	116.62	110.24
14	bB	818	CLA	C3B-C2B-C1B	-3.95	102.40	107.16
14	cA	813	CLA	C3C-C4C-NC	3.95	115.00	110.57
14	cA	852	CLA	C3D-C4D-ND	3.95	116.62	110.24
14	bB	838	CLA	C3B-C2B-C1B	-3.95	102.40	107.16
14	bA	813	CLA	C3C-C4C-NC	3.95	115.00	110.57
14	bA	811	CLA	CMC-C2C-C1C	3.95	131.05	125.04
14	A	811	CLA	CMC-C2C-C1C	3.95	131.05	125.04
14	cA	818	CLA	CMC-C2C-C1C	3.95	131.05	125.04
14	B	818	CLA	C3B-C2B-C1B	-3.94	102.40	107.16
14	cB	840	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
14	A	826	CLA	CMC-C2C-C1C	3.94	131.04	125.04
14	cB	810	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
17	B	842	BCR	C37-C22-C21	-3.94	117.40	122.92
14	cB	806	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
14	B	808	CLA	C3B-C2B-C1B	-3.94	102.40	107.16
14	bL	201	CLA	C4A-NA-C1A	-3.94	104.93	106.71
14	cB	818	CLA	C4A-NA-C1A	-3.94	104.93	106.71
14	cA	811	CLA	CMC-C2C-C1C	3.94	131.04	125.04
14	B	839	CLA	C1C-C2C-C3C	-3.94	102.82	106.96
17	bA	846	BCR	C15-C16-C17	3.94	131.54	123.47
17	cA	846	BCR	C15-C16-C17	3.94	131.54	123.47
14	bA	805	CLA	C1C-C2C-C3C	-3.94	102.82	106.96
14	bB	839	CLA	C3B-C2B-C1B	-3.94	102.41	107.16
17	A	846	BCR	C15-C16-C17	3.94	131.54	123.47
14	B	809	CLA	C3B-C4B-NB	3.94	114.17	110.52
14	cA	826	CLA	CMC-C2C-C1C	3.94	131.03	125.04
14	B	817	CLA	C4A-NA-C1A	-3.93	104.94	106.71
14	bA	808	CLA	C3B-C2B-C1B	-3.93	102.41	107.16
14	bB	839	CLA	C1C-C2C-C3C	-3.93	102.82	106.96
14	B	839	CLA	C3B-C2B-C1B	-3.93	102.41	107.16
14	L	201	CLA	C4A-NA-C1A	-3.93	104.94	106.71
14	cB	823	CLA	C4A-NA-C1A	-3.93	104.94	106.71
14	cL	202	CLA	C4A-NA-C1A	-3.93	104.94	106.71
14	A	831	CLA	C3C-C4C-NC	3.93	114.98	110.57
14	cA	841	CLA	CMC-C2C-C1C	3.93	131.02	125.04
17	bB	842	BCR	C37-C22-C21	-3.93	117.42	122.92
14	cB	840	CLA	C3B-C2B-C1B	-3.93	102.42	107.16
14	bB	805	CLA	C1C-C2C-C3C	-3.92	102.83	106.96
14	bA	841	CLA	CMC-C2C-C1C	3.92	131.02	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cB	809	CLA	C3B-C2B-C1B	-3.92	102.42	107.16
14	cA	823	CLA	C4A-NA-C1A	-3.92	104.94	106.71
17	cB	843	BCR	C37-C22-C21	-3.92	117.43	122.92
14	B	805	CLA	C1C-C2C-C3C	-3.92	102.83	106.96
14	bB	803	CLA	C1D-CHD-C4C	-3.92	117.60	126.06
14	bB	805	CLA	C3B-C4B-NB	3.92	114.15	110.52
14	cA	817	CLA	C3C-C4C-NC	3.92	114.97	110.57
14	A	841	CLA	CMC-C2C-C1C	3.92	131.01	125.04
14	bA	836	CLA	C1C-C2C-C3C	-3.92	102.84	106.96
14	cA	805	CLA	C1C-C2C-C3C	-3.92	102.84	106.96
14	bA	837	CLA	C4A-NA-C1A	-3.92	104.94	106.71
14	cB	830	CLA	C4A-NA-C1A	-3.92	104.94	106.71
14	bA	826	CLA	CMC-C2C-C1C	3.92	131.00	125.04
17	bA	846	BCR	C12-C13-C14	3.92	124.95	118.94
14	A	817	CLA	C3C-C4C-NC	3.92	114.96	110.57
17	A	846	BCR	C12-C13-C14	3.92	124.95	118.94
14	cB	804	CLA	C1D-CHD-C4C	-3.92	117.61	126.06
14	A	809	CLA	O2D-CGD-CBD	3.92	118.22	111.27
14	bB	820	CLA	CAC-C3C-C4C	3.91	129.89	124.81
14	cA	830	CLA	C1C-C2C-C3C	-3.91	102.84	106.96
17	cA	846	BCR	C12-C13-C14	3.91	124.95	118.94
14	bA	821	CLA	C4A-NA-C1A	-3.91	104.95	106.71
14	B	827	CLA	O2D-CGD-CBD	3.91	118.22	111.27
14	B	809	CLA	C1C-C2C-C3C	-3.91	102.84	106.96
14	A	821	CLA	C4A-NA-C1A	-3.91	104.95	106.71
14	bA	812	CLA	C4A-NA-C1A	-3.91	104.95	106.71
17	B	843	BCR	C34-C9-C10	-3.91	117.45	122.92
14	A	805	CLA	C1C-C2C-C3C	-3.91	102.85	106.96
14	A	830	CLA	C1C-C2C-C3C	-3.91	102.85	106.96
17	bB	843	BCR	C34-C9-C10	-3.91	117.45	122.92
14	bA	831	CLA	C3C-C4C-NC	3.91	114.95	110.57
14	bA	830	CLA	C1C-C2C-C3C	-3.91	102.85	106.96
14	B	805	CLA	C3B-C4B-NB	3.91	114.14	110.52
14	cA	809	CLA	O2D-CGD-CBD	3.91	118.21	111.27
14	bB	809	CLA	C1C-C2C-C3C	-3.90	102.85	106.96
14	cA	836	CLA	C1C-C2C-C3C	-3.90	102.85	106.96
14	cB	821	CLA	C4A-NA-C1A	-3.90	104.95	106.71
17	M	101	BCR	C37-C22-C21	-3.90	117.45	122.92
14	cB	836	CLA	C4A-NA-C1A	-3.90	104.95	106.71
14	cB	828	CLA	O2D-CGD-CBD	3.90	118.20	111.27
17	cM	101	BCR	C37-C22-C21	-3.90	117.46	122.92
14	A	824	CLA	C3C-C4C-NC	3.90	114.94	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	831	CLA	C3C-C4C-NC	3.90	114.94	110.57
14	B	803	CLA	C1D-CHD-C4C	-3.90	117.65	126.06
17	bB	847	BCR	C37-C22-C21	-3.90	117.47	122.92
14	bA	827	CLA	CMC-C2C-C1C	3.90	130.97	125.04
14	cA	838	CLA	C3C-C4C-NC	3.89	114.94	110.57
14	cB	822	CLA	C4A-NA-C1A	-3.89	104.95	106.71
14	bB	827	CLA	O2D-CGD-CBD	3.89	118.19	111.27
14	cB	821	CLA	CAC-C3C-C4C	3.89	129.86	124.81
17	cA	847	BCR	C37-C22-C21	-3.89	117.47	122.92
14	cB	806	CLA	C3B-C4B-NB	3.89	114.13	110.52
14	bA	809	CLA	O2D-CGD-CBD	3.89	118.18	111.27
14	A	836	CLA	C1C-C2C-C3C	-3.89	102.86	106.96
17	bM	101	BCR	C37-C22-C21	-3.89	117.47	122.92
17	cB	848	BCR	C37-C22-C21	-3.89	117.47	122.92
14	bB	838	CLA	O2D-CGD-CBD	3.89	118.18	111.27
14	cB	839	CLA	O2D-CGD-CBD	3.89	118.18	111.27
14	A	823	CLA	C4A-NA-C1A	-3.89	104.96	106.71
14	A	827	CLA	CMC-C2C-C1C	3.89	130.96	125.04
14	bA	824	CLA	C3C-C4C-NC	3.89	114.93	110.57
14	bB	817	CLA	C3C-C4C-NC	3.89	114.93	110.57
14	cB	836	CLA	C3C-C4C-NC	3.89	114.93	110.57
14	bB	821	CLA	C4A-NA-C1A	-3.89	104.96	106.71
17	B	847	BCR	C37-C22-C21	-3.88	117.48	122.92
14	cA	827	CLA	CMC-C2C-C1C	3.88	130.95	125.04
14	F	201	CLA	C3C-C4C-NC	3.88	114.93	110.57
17	cB	844	BCR	C34-C9-C10	-3.88	117.49	122.92
14	A	838	CLA	C3C-C4C-NC	3.88	114.92	110.57
14	bA	809	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
14	cA	809	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
14	bB	827	CLA	C3C-C4C-NC	3.88	114.92	110.57
14	B	838	CLA	O2D-CGD-CBD	3.88	118.16	111.27
17	bA	847	BCR	C37-C22-C21	-3.88	117.49	122.92
14	B	822	CLA	C4A-NA-C1A	-3.88	104.96	106.71
14	B	808	CLA	C1D-CHD-C4C	-3.88	117.69	126.06
14	B	820	CLA	CAC-C3C-C4C	3.88	129.84	124.81
17	A	847	BCR	C37-C22-C21	-3.88	117.49	122.92
14	bB	808	CLA	C1D-CHD-C4C	-3.88	117.70	126.06
14	cA	835	CLA	C3B-C2B-C1B	-3.87	102.48	107.16
14	A	816	CLA	C4A-NA-C1A	-3.87	104.96	106.71
17	B	846	BCR	C37-C22-C21	-3.87	117.50	122.92
14	A	809	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
14	A	812	CLA	C4A-NA-C1A	-3.87	104.97	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bA	816	CLA	C4A-NA-C1A	-3.87	104.97	106.71
14	bA	838	CLA	C3C-C4C-NC	3.87	114.91	110.57
14	cB	809	CLA	C1D-CHD-C4C	-3.87	117.71	126.06
14	B	817	CLA	C3C-C4C-NC	3.87	114.91	110.57
14	cB	828	CLA	C3C-C4C-NC	3.87	114.91	110.57
14	cB	802	CLA	C4A-NA-C1A	-3.87	104.97	106.71
14	cA	824	CLA	C3C-C4C-NC	3.87	114.91	110.57
14	B	827	CLA	C3C-C4C-NC	3.87	114.91	110.57
14	bA	823	CLA	C4A-NA-C1A	-3.87	104.97	106.71
14	cA	821	CLA	C4A-NA-C1A	-3.87	104.97	106.71
14	bF	201	CLA	C3C-C4C-NC	3.86	114.90	110.57
14	cB	823	CLA	C3C-C4C-NC	3.86	114.90	110.57
17	bB	846	BCR	C37-C22-C21	-3.86	117.51	122.92
17	cB	847	BCR	C37-C22-C21	-3.86	117.51	122.92
14	A	826	CLA	C3C-C4C-NC	3.86	114.90	110.57
14	bB	801	CLA	C4A-NA-C1A	-3.86	104.97	106.71
14	cB	818	CLA	C3C-C4C-NC	3.86	114.90	110.57
14	bA	835	CLA	C3B-C2B-C1B	-3.86	102.50	107.16
14	B	822	CLA	C3C-C4C-NC	3.86	114.90	110.57
14	bB	835	CLA	C3C-C4C-NC	3.86	114.90	110.57
14	cB	811	CLA	CMC-C2C-C1C	3.86	130.91	125.04
14	B	835	CLA	C3C-C4C-NC	3.85	114.89	110.57
14	A	835	CLA	C3B-C2B-C1B	-3.85	102.51	107.16
14	B	821	CLA	C4A-NA-C1A	-3.85	104.97	106.71
14	cA	840	CLA	C3C-C4C-NC	3.85	114.89	110.57
14	cA	810	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
14	cB	810	CLA	CMC-C2C-C1C	3.85	130.90	125.04
14	cA	826	CLA	C3C-C4C-NC	3.85	114.89	110.57
14	bA	831	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
14	bA	810	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
14	bB	822	CLA	C3C-C4C-NC	3.84	114.88	110.57
14	cA	816	CLA	C4A-NA-C1A	-3.84	104.98	106.71
14	bA	807	CLA	CMB-C2B-C1B	3.84	131.22	125.37
14	cA	841	CLA	O2D-CGD-CBD	3.84	118.09	111.27
14	bB	809	CLA	CMC-C2C-C1C	3.84	130.89	125.04
14	B	801	CLA	C4A-NA-C1A	-3.84	104.98	106.71
14	A	807	CLA	CMB-C2B-C1B	3.84	131.22	125.37
14	A	841	CLA	O2D-CGD-CBD	3.84	118.09	111.27
14	B	810	CLA	CMC-C2C-C1C	3.84	130.88	125.04
14	bA	826	CLA	C3C-C4C-NC	3.84	114.87	110.57
14	cB	803	CLA	CAC-C3C-C4C	3.84	129.79	124.81
14	bA	841	CLA	O2D-CGD-CBD	3.83	118.08	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bB	810	CLA	CMC-C2C-C1C	3.83	130.88	125.04
14	cA	812	CLA	C4A-NA-C1A	-3.83	104.98	106.71
14	cA	807	CLA	CMB-C2B-C1B	3.83	131.21	125.37
14	A	840	CLA	C3C-C4C-NC	3.83	114.87	110.57
14	cF	201	CLA	C3C-C4C-NC	3.83	114.87	110.57
14	bA	840	CLA	C3C-C4C-NC	3.83	114.87	110.57
14	B	809	CLA	CMC-C2C-C1C	3.83	130.87	125.04
14	B	802	CLA	CAC-C3C-C4C	3.83	129.78	124.81
14	A	831	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
14	bB	839	CLA	CMB-C2B-C1B	3.83	131.20	125.37
14	B	826	CLA	C4A-NA-C1A	-3.82	104.99	106.71
14	A	842	CLA	C4A-NA-C1A	-3.82	104.99	106.71
14	bB	807	CLA	C4A-NA-C1A	-3.82	104.99	106.71
14	B	839	CLA	CMB-C2B-C1B	3.82	131.19	125.37
14	A	816	CLA	C3C-C4C-NC	3.82	114.86	110.57
14	bB	811	CLA	C3C-C4C-NC	3.82	114.86	110.57
14	bB	838	CLA	C4A-NA-C1A	-3.82	104.99	106.71
14	A	810	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
14	cA	815	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
14	A	818	CLA	O2A-CGA-CBA	3.82	123.89	111.91
14	B	811	CLA	C3C-C4C-NC	3.82	114.85	110.57
14	cB	812	CLA	C3C-C4C-NC	3.82	114.85	110.57
14	cA	831	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
14	cA	816	CLA	C3C-C4C-NC	3.81	114.85	110.57
14	B	805	CLA	CAC-C3C-C4C	3.81	129.76	124.81
14	cB	840	CLA	CMB-C2B-C1B	3.81	131.18	125.37
14	cA	818	CLA	O2A-CGA-CBA	3.81	123.87	111.91
14	bA	816	CLA	C3C-C4C-NC	3.81	114.84	110.57
17	J	103	BCR	C36-C18-C17	-3.81	117.58	122.92
14	B	838	CLA	C4A-NA-C1A	-3.81	104.99	106.71
14	bB	806	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
14	bA	818	CLA	O2A-CGA-CBA	3.81	123.86	111.91
17	cB	842	BCR	C15-C16-C17	3.81	131.27	123.47
14	B	807	CLA	C4A-NA-C1A	-3.81	105.00	106.71
17	bB	841	BCR	C15-C16-C17	3.80	131.27	123.47
14	cB	808	CLA	C4A-NA-C1A	-3.80	105.00	106.71
14	B	806	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
14	cA	842	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
14	cB	824	CLA	C3D-C4D-ND	3.80	116.39	110.24
14	cB	801	CLA	C3C-C4C-NC	3.80	114.83	110.57
17	M	101	BCR	C15-C16-C17	3.80	131.26	123.47
14	bB	802	CLA	CAC-C3C-C4C	3.80	129.74	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bB	815	CLA	C3C-C4C-NC	3.80	114.83	110.57
14	cA	842	CLA	C4A-NA-C1A	-3.80	105.00	106.71
17	bM	101	BCR	C15-C16-C17	3.80	131.25	123.47
17	bJ	103	BCR	C36-C18-C17	-3.80	117.60	122.92
14	cA	837	CLA	C3C-C4C-NC	3.80	114.83	110.57
14	cB	816	CLA	C3C-C4C-NC	3.80	114.83	110.57
17	bA	845	BCR	C16-C15-C14	3.80	131.25	123.47
14	cA	836	CLA	C1D-CHD-C4C	-3.80	117.87	126.06
14	bA	842	CLA	C1C-C2C-C3C	-3.80	102.97	106.96
17	B	841	BCR	C15-C16-C17	3.80	131.25	123.47
14	bB	826	CLA	C1D-CHD-C4C	-3.80	117.87	126.06
14	B	838	CLA	C1C-C2C-C3C	-3.80	102.97	106.96
14	A	836	CLA	C1D-CHD-C4C	-3.79	117.87	126.06
14	bA	836	CLA	C1D-CHD-C4C	-3.79	117.87	126.06
17	cA	845	BCR	C16-C15-C14	3.79	131.25	123.47
14	B	819	CLA	C3C-C4C-NC	3.79	114.83	110.57
14	B	826	CLA	C1D-CHD-C4C	-3.79	117.88	126.06
14	A	836	CLA	C3C-C4C-NC	3.79	114.83	110.57
14	cB	839	CLA	CMB-C2B-C1B	3.79	131.15	125.37
17	bB	844	BCR	C37-C22-C21	-3.79	117.61	122.92
17	A	845	BCR	C16-C15-C14	3.79	131.24	123.47
14	bB	819	CLA	C3C-C4C-NC	3.79	114.82	110.57
17	B	844	BCR	C37-C22-C21	-3.79	117.61	122.92
14	bB	823	CLA	C3D-C4D-ND	3.79	116.37	110.24
14	B	838	CLA	CMB-C2B-C1B	3.79	131.14	125.37
14	cA	820	CLA	C3B-C2B-C1B	-3.79	102.58	107.16
13	A	801	CL0	C3B-C2B-C1B	-3.79	102.59	107.16
14	cB	839	CLA	C4A-NA-C1A	-3.79	105.00	106.71
14	bB	826	CLA	C3B-C4B-NB	3.79	114.03	110.52
14	cB	820	CLA	C3C-C4C-NC	3.79	114.82	110.57
14	bA	820	CLA	C3B-C2B-C1B	-3.79	102.59	107.16
14	bA	837	CLA	C3C-C4C-NC	3.79	114.82	110.57
14	cA	836	CLA	C3C-C4C-NC	3.79	114.82	110.57
14	cB	827	CLA	C1D-CHD-C4C	-3.79	117.89	126.06
17	cM	101	BCR	C15-C16-C17	3.79	131.23	123.47
14	bB	838	CLA	CMB-C2B-C1B	3.79	131.14	125.37
14	B	823	CLA	C3D-C4D-ND	3.79	116.36	110.24
14	cB	827	CLA	C4A-NA-C1A	-3.79	105.00	106.71
14	bA	836	CLA	C3C-C4C-NC	3.79	114.82	110.57
14	bB	805	CLA	CAC-C3C-C4C	3.79	129.72	124.81
14	A	842	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
14	B	826	CLA	C3B-C4B-NB	3.78	114.03	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bB	830	CLA	C3C-C4C-NC	3.78	114.81	110.57
14	A	815	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
14	cB	839	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
14	bA	811	CLA	CAC-C3C-C4C	3.78	129.71	124.81
14	bA	815	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
14	cB	807	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
14	A	802	CLA	C4A-NA-C1A	-3.78	105.01	106.71
14	bB	826	CLA	C4A-NA-C1A	-3.78	105.01	106.71
14	A	820	CLA	C3B-C2B-C1B	-3.78	102.60	107.16
17	cJ	103	BCR	C36-C18-C17	-3.78	117.63	122.92
14	bA	842	CLA	C4A-NA-C1A	-3.78	105.01	106.71
14	A	837	CLA	C3C-C4C-NC	3.78	114.81	110.57
14	cL	205	CLA	C1C-C2C-C3C	-3.78	102.99	106.96
14	B	815	CLA	C3C-C4C-NC	3.78	114.81	110.57
14	bB	838	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
14	cB	827	CLA	C3B-C4B-NB	3.77	114.02	110.52
14	bB	804	CLA	C3C-C4C-NC	3.77	114.80	110.57
14	A	811	CLA	CAC-C3C-C4C	3.77	129.71	124.81
14	cB	831	CLA	C3C-C4C-NC	3.77	114.80	110.57
13	cA	801	CL0	C3B-C2B-C1B	-3.77	102.61	107.16
17	cB	845	BCR	C34-C9-C8	3.77	124.02	118.08
14	bL	204	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
14	B	804	CLA	C3C-C4C-NC	3.77	114.80	110.57
14	cB	805	CLA	C3C-C4C-NC	3.77	114.80	110.57
17	cB	845	BCR	C37-C22-C21	-3.77	117.64	122.92
14	bB	851	CLA	C3C-C4C-NC	3.77	114.80	110.57
14	L	204	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
14	bA	829	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
17	cA	848	BCR	C37-C22-C21	-3.77	117.64	122.92
14	cB	811	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
14	bB	837	CLA	CAC-C3C-C4C	3.77	129.70	124.81
14	B	837	CLA	CAC-C3C-C4C	3.77	129.70	124.81
13	bA	801	CL0	C3B-C2B-C1B	-3.77	102.61	107.16
14	cB	838	CLA	CAC-C3C-C4C	3.77	129.70	124.81
17	bA	848	BCR	C37-C22-C21	-3.77	117.65	122.92
14	B	830	CLA	C3C-C4C-NC	3.77	114.79	110.57
14	cA	811	CLA	CAC-C3C-C4C	3.76	129.69	124.81
17	B	844	BCR	C34-C9-C8	3.76	124.01	118.08
14	cB	806	CLA	CAC-C3C-C4C	3.76	129.69	124.81
14	B	851	CLA	C3C-C4C-NC	3.76	114.79	110.57
17	A	848	BCR	C37-C22-C21	-3.76	117.66	122.92
14	bB	812	CLA	C2C-C1C-NC	3.76	113.49	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cJ	102	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
17	bB	844	BCR	C34-C9-C8	3.76	124.00	118.08
14	cB	813	CLA	C3C-C4C-NC	3.75	114.78	110.57
14	B	810	CLA	C1C-C2C-C3C	-3.75	103.01	106.96
17	bB	844	BCR	C16-C15-C14	3.75	131.16	123.47
14	B	821	CLA	C3B-C4B-NB	3.75	114.00	110.52
14	cB	808	CLA	C3C-C4C-NC	3.75	114.78	110.57
14	B	812	CLA	C2C-C1C-NC	3.75	113.49	109.97
14	A	829	CLA	C1C-C2C-C3C	-3.75	103.01	106.96
14	cA	804	CLA	CAC-C3C-C4C	3.75	129.68	124.81
14	B	806	CLA	C4A-NA-C1A	-3.75	105.02	106.71
14	bA	802	CLA	C4A-NA-C1A	-3.75	105.02	106.71
14	bB	807	CLA	C3C-C4C-NC	3.75	114.78	110.57
14	J	102	CLA	C1C-C2C-C3C	-3.75	103.02	106.96
14	cA	814	CLA	C1C-C2C-C3C	-3.75	103.02	106.96
14	cA	802	CLA	C4A-NA-C1A	-3.75	105.02	106.71
14	cB	813	CLA	C2C-C1C-NC	3.75	113.48	109.97
14	B	812	CLA	C3C-C4C-NC	3.75	114.77	110.57
17	B	841	BCR	C37-C22-C21	-3.75	117.67	122.92
14	cB	822	CLA	C3B-C4B-NB	3.75	113.99	110.52
17	A	845	BCR	C37-C22-C21	-3.75	117.68	122.92
14	A	804	CLA	CAC-C3C-C4C	3.74	129.67	124.81
17	cF	202	BCR	C16-C15-C14	3.74	131.15	123.47
14	bB	821	CLA	C3B-C4B-NB	3.74	113.99	110.52
17	cB	842	BCR	C37-C22-C21	-3.74	117.68	122.92
17	cB	845	BCR	C16-C15-C14	3.74	131.14	123.47
14	bB	824	CLA	C3C-C4C-NC	3.74	114.77	110.57
17	bB	841	BCR	C37-C22-C21	-3.74	117.68	122.92
17	cA	845	BCR	C37-C22-C21	-3.74	117.68	122.92
17	F	202	BCR	C16-C15-C14	3.74	131.14	123.47
14	bB	810	CLA	C1C-C2C-C3C	-3.74	103.02	106.96
14	bA	814	CLA	C1C-C2C-C3C	-3.74	103.02	106.96
14	cA	829	CLA	C1C-C2C-C3C	-3.74	103.02	106.96
14	bA	841	CLA	CED-O2D-CGD	3.74	124.40	115.94
17	bF	202	BCR	C16-C15-C14	3.74	131.14	123.47
14	cA	802	CLA	CMC-C2C-C1C	3.74	130.73	125.04
17	B	844	BCR	C16-C15-C14	3.74	131.13	123.47
14	bB	812	CLA	CMB-C2B-C1B	3.74	131.06	125.37
14	bB	828	CLA	C3C-C4C-NC	3.74	114.76	110.57
14	cB	813	CLA	CMB-C2B-C1B	3.74	131.06	125.37
14	A	841	CLA	CED-O2D-CGD	3.74	124.39	115.94
14	bJ	102	CLA	C1C-C2C-C3C	-3.74	103.03	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	841	CLA	CED-O2D-CGD	3.73	124.38	115.94
14	bB	812	CLA	C3C-C4C-NC	3.73	114.76	110.57
14	cB	825	CLA	C3C-C4C-NC	3.73	114.76	110.57
14	F	201	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
14	bA	804	CLA	CAC-C3C-C4C	3.73	129.65	124.81
14	bA	802	CLA	CMC-C2C-C1C	3.73	130.72	125.04
14	bA	814	CLA	C4A-NA-C1A	-3.73	105.03	106.71
14	B	824	CLA	C3C-C4C-NC	3.73	114.76	110.57
14	A	814	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
14	cJ	102	CLA	C3C-C4C-NC	3.73	114.75	110.57
14	B	812	CLA	CMB-C2B-C1B	3.73	131.05	125.37
14	J	102	CLA	C3C-C4C-NC	3.73	114.75	110.57
14	cA	808	CLA	CAC-C3C-C4C	3.73	129.65	124.81
14	A	802	CLA	CMC-C2C-C1C	3.73	130.72	125.04
14	bA	835	CLA	C1C-C2C-C3C	-3.73	103.04	106.96
14	B	807	CLA	C3C-C4C-NC	3.72	114.75	110.57
14	A	835	CLA	C1C-C2C-C3C	-3.72	103.04	106.96
14	B	836	CLA	C4A-NA-C1A	-3.72	105.03	106.71
14	A	808	CLA	CAC-C3C-C4C	3.72	129.64	124.81
14	X	201	CLA	C3C-C4C-NC	3.72	114.74	110.57
14	bJ	102	CLA	C3C-C4C-NC	3.72	114.74	110.57
14	cA	835	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
14	bA	820	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
14	A	820	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
14	bF	201	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
14	B	828	CLA	C3C-C4C-NC	3.72	114.74	110.57
14	cB	829	CLA	C3C-C4C-NC	3.72	114.74	110.57
14	A	825	CLA	C1D-CHD-C4C	-3.72	118.04	126.06
14	cB	833	CLA	CMB-C2B-C1B	3.72	131.03	125.37
14	bA	808	CLA	CAC-C3C-C4C	3.72	129.63	124.81
14	bA	814	CLA	C3C-C4C-NC	3.72	114.74	110.57
14	bA	825	CLA	C1D-CHD-C4C	-3.71	118.04	126.06
14	A	814	CLA	C3C-C4C-NC	3.71	114.74	110.57
17	bA	845	BCR	C37-C22-C21	-3.71	117.73	122.92
14	bB	831	CLA	CAC-C3C-C4C	3.71	129.62	124.81
14	cA	820	CLA	C1C-C2C-C3C	-3.70	103.06	106.96
14	cF	201	CLA	C1C-C2C-C3C	-3.70	103.06	106.96
14	cA	825	CLA	C1D-CHD-C4C	-3.70	118.08	126.06
14	bB	832	CLA	CMB-C2B-C1B	3.70	131.00	125.37
14	cA	814	CLA	C3C-C4C-NC	3.70	114.72	110.57
14	cB	837	CLA	C4A-NA-C1A	-3.70	105.04	106.71
14	B	823	CLA	C1C-C2C-C3C	-3.70	103.07	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	816	CLA	CAC-C3C-C4C	3.70	129.61	124.81
14	bX	201	CLA	C3C-C4C-NC	3.70	114.72	110.57
14	cA	814	CLA	CAC-C3C-C4C	3.70	129.61	124.81
14	bB	823	CLA	C1C-C2C-C3C	-3.69	103.07	106.96
14	B	832	CLA	CMB-C2B-C1B	3.69	131.00	125.37
14	B	831	CLA	CAC-C3C-C4C	3.69	129.60	124.81
14	cA	816	CLA	CAC-C3C-C4C	3.69	129.60	124.81
14	cB	824	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
14	cB	832	CLA	CAC-C3C-C4C	3.69	129.60	124.81
14	cX	201	CLA	C3C-C4C-NC	3.69	114.71	110.57
14	B	809	CLA	C4-C3-C5	3.69	121.47	115.27
14	B	805	CLA	C4A-NA-C1A	-3.69	105.05	106.71
14	bB	836	CLA	C4A-NA-C1A	-3.69	105.05	106.71
14	bA	814	CLA	CAC-C3C-C4C	3.68	129.59	124.81
14	A	817	CLA	C1C-C2C-C3C	-3.68	103.08	106.96
14	cA	803	CLA	C1C-C2C-C3C	-3.68	103.08	106.96
14	bB	838	CLA	CAC-C3C-C4C	3.68	129.59	124.81
14	bA	815	CLA	C3C-C4C-NC	3.68	114.70	110.57
14	A	814	CLA	CAC-C3C-C4C	3.68	129.58	124.81
14	bB	806	CLA	C4A-NA-C1A	-3.68	105.05	106.71
14	bA	816	CLA	CAC-C3C-C4C	3.68	129.58	124.81
14	bB	809	CLA	C4-C3-C5	3.68	121.46	115.27
14	B	829	CLA	C3C-C4C-NC	3.68	114.69	110.57
14	bB	829	CLA	C3C-C4C-NC	3.68	114.69	110.57
14	A	825	CLA	CMC-C2C-C1C	3.68	130.64	125.04
14	cA	825	CLA	CMC-C2C-C1C	3.68	130.64	125.04
14	bA	803	CLA	C1C-C2C-C3C	-3.67	103.09	106.96
14	bA	839	CLA	C1C-C2C-C3C	-3.67	103.09	106.96
14	cB	834	CLA	C1C-C2C-C3C	-3.67	103.09	106.96
14	cB	807	CLA	C4A-NA-C1A	-3.67	105.05	106.71
14	bA	829	CLA	C3C-C4C-NC	3.67	114.69	110.57
14	bB	833	CLA	C3C-C4C-NC	3.67	114.69	110.57
14	bB	837	CLA	C3C-C4C-NC	3.67	114.69	110.57
14	cB	806	CLA	C4A-NA-C1A	-3.67	105.06	106.71
14	bA	817	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
14	B	837	CLA	C3C-C4C-NC	3.67	114.69	110.57
14	cL	203	CLA	CAC-C3C-C4C	3.67	129.57	124.81
14	B	838	CLA	CAC-C3C-C4C	3.67	129.57	124.81
14	bA	825	CLA	CMC-C2C-C1C	3.67	130.62	125.04
14	cA	808	CLA	C4A-NA-C1A	-3.67	105.06	106.71
14	bA	810	CLA	C3C-C4C-NC	3.66	114.68	110.57
14	cA	817	CLA	C1C-C2C-C3C	-3.66	103.10	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	839	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
14	cA	829	CLA	C3C-C4C-NC	3.66	114.68	110.57
14	L	204	CLA	CAC-C3C-C4C	3.66	129.56	124.81
14	bL	204	CLA	CAC-C3C-C4C	3.66	129.56	124.81
14	cA	815	CLA	C3C-C4C-NC	3.66	114.68	110.57
14	cB	810	CLA	C4-C3-C5	3.66	121.43	115.27
14	A	829	CLA	C3C-C4C-NC	3.66	114.67	110.57
14	L	202	CLA	CAC-C3C-C4C	3.66	129.56	124.81
14	bL	202	CLA	CAC-C3C-C4C	3.66	129.56	124.81
14	cB	839	CLA	CAC-C3C-C4C	3.66	129.56	124.81
14	bA	827	CLA	C3C-C4C-NC	3.65	114.67	110.57
14	cL	205	CLA	CAC-C3C-C4C	3.65	129.55	124.81
14	bA	822	CLA	CMC-C2C-C1C	3.65	130.60	125.04
14	A	815	CLA	C3C-C4C-NC	3.65	114.67	110.57
14	cB	834	CLA	C3C-C4C-NC	3.65	114.67	110.57
14	cJ	102	CLA	CAC-C3C-C4C	3.65	129.55	124.81
14	cB	838	CLA	C3C-C4C-NC	3.65	114.67	110.57
14	cA	810	CLA	C3C-C4C-NC	3.65	114.67	110.57
14	A	840	CLA	CAC-C3C-C4C	3.65	129.54	124.81
14	A	839	CLA	C3C-C4C-NC	3.65	114.66	110.57
14	bB	805	CLA	C4A-NA-C1A	-3.65	105.07	106.71
14	B	833	CLA	C3C-C4C-NC	3.65	114.66	110.57
14	bA	833	CLA	CAC-C3C-C4C	3.65	129.54	124.81
14	bA	840	CLA	CAC-C3C-C4C	3.65	129.54	124.81
14	cA	833	CLA	CAC-C3C-C4C	3.65	129.54	124.81
14	A	803	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
14	cB	830	CLA	C3C-C4C-NC	3.65	114.66	110.57
14	cA	810	CLA	C3B-C2B-C1B	-3.65	102.76	107.16
14	A	811	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
14	cA	827	CLA	C3C-C4C-NC	3.65	114.66	110.57
14	A	805	CLA	C3B-C4B-NB	3.64	113.90	110.52
17	bB	847	BCR	C37-C22-C23	3.64	123.82	118.08
14	A	839	CLA	C1C-C2C-C3C	-3.64	103.12	106.96
14	bB	831	CLA	C3C-C4C-NC	3.64	114.66	110.57
14	cB	826	CLA	C1D-CHD-C4C	-3.64	118.20	126.06
14	A	808	CLA	C4A-NA-C1A	-3.64	105.07	106.71
14	A	830	CLA	C4A-NA-C1A	-3.64	105.07	106.71
14	bA	806	CLA	C3C-C4C-NC	3.64	114.66	110.57
14	bA	821	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
14	cA	822	CLA	CMC-C2C-C1C	3.64	130.59	125.04
14	J	102	CLA	CAC-C3C-C4C	3.64	129.54	124.81
14	bJ	102	CLA	CAC-C3C-C4C	3.64	129.54	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	837	CLA	C3B-C2B-C1B	-3.64	102.77	107.16
14	cA	840	CLA	CAC-C3C-C4C	3.64	129.53	124.81
14	cA	839	CLA	C3C-C4C-NC	3.64	114.66	110.57
14	bA	822	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
14	J	101	CLA	C3C-C4C-NC	3.64	114.65	110.57
14	bA	811	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
14	A	810	CLA	C3C-C4C-NC	3.64	114.65	110.57
14	cA	814	CLA	C4A-NA-C1A	-3.64	105.07	106.71
14	A	833	CLA	CAC-C3C-C4C	3.64	129.53	124.81
14	B	818	CLA	C3C-C4C-NC	3.64	114.65	110.57
14	A	822	CLA	CMC-C2C-C1C	3.64	130.58	125.04
14	cA	805	CLA	C3B-C4B-NB	3.64	113.89	110.52
14	bA	837	CLA	C3B-C2B-C1B	-3.64	102.77	107.16
14	B	825	CLA	C1D-CHD-C4C	-3.64	118.22	126.06
14	cA	828	CLA	C1D-CHD-C4C	-3.64	118.22	126.06
14	bB	810	CLA	CAC-C3C-C4C	3.63	129.53	124.81
14	A	822	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
14	cA	808	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
14	cA	811	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
14	bB	818	CLA	C3C-C4C-NC	3.63	114.64	110.57
14	B	833	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
14	cA	822	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
14	bA	805	CLA	C3B-C4B-NB	3.63	113.88	110.52
14	A	821	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
14	A	821	CLA	C3C-C4C-NC	3.63	114.64	110.57
14	bJ	101	CLA	C3C-C4C-NC	3.63	114.64	110.57
14	B	815	CLA	CMB-C2B-C1B	3.63	130.90	125.37
14	B	831	CLA	C3C-C4C-NC	3.63	114.64	110.57
14	bA	828	CLA	C1D-CHD-C4C	-3.63	118.23	126.06
14	cA	821	CLA	C3C-C4C-NC	3.63	114.64	110.57
14	cB	832	CLA	C3C-C4C-NC	3.63	114.64	110.57
14	A	814	CLA	C4A-NA-C1A	-3.63	105.08	106.71
14	bB	815	CLA	CMB-C2B-C1B	3.63	130.89	125.37
14	bB	825	CLA	C1D-CHD-C4C	-3.63	118.23	126.06
14	cA	806	CLA	C3C-C4C-NC	3.63	114.64	110.57
17	cB	848	BCR	C37-C22-C23	3.63	123.79	118.08
14	bB	828	CLA	C1D-CHD-C4C	-3.63	118.23	126.06
17	B	847	BCR	C37-C22-C23	3.63	123.79	118.08
14	bA	808	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
14	cJ	101	CLA	C3C-C4C-NC	3.62	114.64	110.57
14	cA	812	CLA	C3B-C4B-NB	3.62	113.88	110.52
14	cB	816	CLA	CMB-C2B-C1B	3.62	130.89	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bA	838	CLA	C1D-CHD-C4C	-3.62	118.24	126.06
14	B	828	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
14	A	808	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
14	cB	828	CLA	CMC-C2C-C1C	3.62	130.55	125.04
14	A	828	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
14	A	827	CLA	C3C-C4C-NC	3.62	114.63	110.57
14	bA	810	CLA	C3B-C2B-C1B	-3.62	102.79	107.16
14	A	838	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
14	bA	841	CLA	CAC-C3C-C4C	3.62	129.50	124.81
14	cA	841	CLA	CAC-C3C-C4C	3.62	129.50	124.81
14	cB	850	CLA	C3C-C4C-NC	3.62	114.63	110.57
14	A	837	CLA	C3B-C2B-C1B	-3.62	102.80	107.16
14	cA	821	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
14	B	849	CLA	C3C-C4C-NC	3.62	114.63	110.57
14	B	810	CLA	CAC-C3C-C4C	3.61	129.50	124.81
14	cA	825	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
14	cA	838	CLA	C1D-CHD-C4C	-3.61	118.27	126.06
14	bA	807	CLA	C3C-C4C-NC	3.61	114.62	110.57
14	cB	819	CLA	C3C-C4C-NC	3.61	114.62	110.57
14	bB	813	CLA	C3B-C4B-NB	3.61	113.87	110.52
14	cB	811	CLA	CAC-C3C-C4C	3.61	129.50	124.81
14	bA	839	CLA	C3C-C4C-NC	3.61	114.62	110.57
14	bA	825	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
14	cB	829	CLA	C1D-CHD-C4C	-3.61	118.27	126.06
14	cA	812	CLA	C3C-C4C-NC	3.61	114.62	110.57
14	cB	814	CLA	C3B-C4B-NB	3.61	113.86	110.52
14	A	807	CLA	C3C-C4C-NC	3.61	114.62	110.57
14	bA	821	CLA	C3C-C4C-NC	3.61	114.62	110.57
14	bA	842	CLA	C3C-C4C-NC	3.61	114.62	110.57
14	bB	833	CLA	C1C-C2C-C3C	-3.61	103.17	106.96
14	A	806	CLA	C3C-C4C-NC	3.61	114.61	110.57
14	bA	812	CLA	C3C-C4C-NC	3.61	114.61	110.57
14	A	812	CLA	C3C-C4C-NC	3.60	114.61	110.57
14	A	810	CLA	C3B-C2B-C1B	-3.60	102.81	107.16
17	cJ	103	BCR	C34-C9-C10	-3.60	117.88	122.92
17	cL	206	BCR	C37-C22-C21	-3.60	117.88	122.92
14	A	825	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
14	bA	824	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
14	cA	807	CLA	C3C-C4C-NC	3.60	114.61	110.57
17	bJ	103	BCR	C34-C9-C10	-3.60	117.88	122.92
14	B	823	CLA	CMC-C2C-C1C	3.60	130.52	125.04
17	J	103	BCR	C34-C9-C10	-3.60	117.88	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	842	CLA	C3C-C4C-NC	3.60	114.61	110.57
14	bB	810	CLA	C3B-C4B-NB	3.60	113.86	110.52
14	bA	830	CLA	C4A-NA-C1A	-3.60	105.09	106.71
14	L	203	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
14	B	813	CLA	C3B-C4B-NB	3.60	113.86	110.52
14	B	827	CLA	CMC-C2C-C1C	3.60	130.52	125.04
14	bB	827	CLA	CMC-C2C-C1C	3.60	130.52	125.04
14	A	834	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
14	bA	812	CLA	C3B-C4B-NB	3.60	113.85	110.52
14	bB	849	CLA	C1C-C2C-C3C	-3.60	103.18	106.96
14	bA	808	CLA	C4A-NA-C1A	-3.59	105.09	106.71
14	B	802	CLA	CMC-C2C-C1C	3.59	130.51	125.04
17	bL	205	BCR	C37-C22-C21	-3.59	117.89	122.92
14	bJ	101	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
14	bL	203	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
14	A	812	CLA	C3B-C4B-NB	3.59	113.85	110.52
14	bB	823	CLA	CMC-C2C-C1C	3.59	130.51	125.04
14	bB	820	CLA	C3C-C4C-NC	3.59	114.60	110.57
14	B	810	CLA	C3B-C4B-NB	3.59	113.85	110.52
14	cB	824	CLA	CMC-C2C-C1C	3.59	130.51	125.04
14	A	841	CLA	CAC-C3C-C4C	3.59	129.47	124.81
14	cB	802	CLA	C1D-CHD-C4C	-3.59	118.31	126.06
14	X	201	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
14	B	801	CLA	C1D-CHD-C4C	-3.59	118.32	126.06
17	bA	846	BCR	C35-C13-C14	-3.59	117.90	122.92
14	cF	201	CLA	C1D-CHD-C4C	-3.59	118.32	126.06
17	L	205	BCR	C37-C22-C21	-3.59	117.90	122.92
14	bB	849	CLA	CMC-C2C-C1C	3.59	130.50	125.04
14	bB	802	CLA	CMC-C2C-C1C	3.59	130.50	125.04
14	F	201	CLA	C1D-CHD-C4C	-3.59	118.32	126.06
14	cB	836	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
14	cA	830	CLA	C4A-NA-C1A	-3.58	105.09	106.71
14	bB	801	CLA	C1D-CHD-C4C	-3.58	118.33	126.06
14	bB	849	CLA	C3C-C4C-NC	3.58	114.59	110.57
14	B	849	CLA	CMC-C2C-C1C	3.58	130.50	125.04
14	A	831	CLA	C3B-C4B-NB	3.58	113.84	110.52
14	cB	811	CLA	C3B-C4B-NB	3.58	113.84	110.52
14	bA	830	CLA	C1D-CHD-C4C	-3.58	118.33	126.06
14	cA	824	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
14	X	201	CLA	CAC-C3C-C4C	3.58	129.45	124.81
14	bX	201	CLA	CAC-C3C-C4C	3.58	129.45	124.81
14	cA	804	CLA	C3C-C4C-NC	3.58	114.58	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	842	CLA	C3C-C4C-NC	3.58	114.58	110.57
14	cA	830	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
14	A	830	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
14	B	806	CLA	O2D-CGD-CBD	3.57	117.62	111.27
14	cB	817	CLA	CAC-C3C-C4C	3.57	129.45	124.81
14	cB	833	CLA	C1D-CHD-C4C	-3.57	118.35	126.06
14	cL	204	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
14	bB	816	CLA	CAC-C3C-C4C	3.57	129.44	124.81
14	J	101	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
14	cB	803	CLA	CMC-C2C-C1C	3.57	130.48	125.04
14	B	816	CLA	CAC-C3C-C4C	3.57	129.44	124.81
14	A	804	CLA	C3C-C4C-NC	3.57	114.58	110.57
14	cB	824	CLA	C1D-CHD-C4C	-3.57	118.36	126.06
14	cJ	101	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
14	A	822	CLA	C3C-C4C-NC	3.57	114.57	110.57
14	cA	822	CLA	C3C-C4C-NC	3.57	114.57	110.57
14	B	823	CLA	C1D-CHD-C4C	-3.57	118.36	126.06
14	bB	823	CLA	C1D-CHD-C4C	-3.57	118.36	126.06
14	bB	832	CLA	C1D-CHD-C4C	-3.57	118.36	126.06
14	A	824	CLA	C1C-C2C-C3C	-3.57	103.21	106.96
14	bB	836	CLA	C1C-C2C-C3C	-3.57	103.21	106.96
14	B	832	CLA	C1D-CHD-C4C	-3.57	118.36	126.06
14	bF	201	CLA	C1D-CHD-C4C	-3.57	118.36	126.06
17	A	846	BCR	C35-C13-C14	-3.57	117.93	122.92
14	bA	835	CLA	C3C-C4C-NC	3.57	114.57	110.57
14	bA	831	CLA	C3B-C4B-NB	3.57	113.82	110.52
14	cB	814	CLA	C1C-C2C-C3C	-3.57	103.21	106.96
14	cB	807	CLA	O2D-CGD-CBD	3.57	117.60	111.27
14	B	849	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
14	cB	835	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
14	bB	806	CLA	O2D-CGD-CBD	3.56	117.60	111.27
14	bA	804	CLA	C3C-C4C-NC	3.56	114.57	110.57
14	cA	835	CLA	C3C-C4C-NC	3.56	114.57	110.57
14	bA	834	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
14	bX	201	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
14	cB	830	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
14	A	842	CLA	C3B-C4B-NB	3.56	113.82	110.52
14	cB	821	CLA	C3C-C4C-NC	3.56	114.56	110.57
14	cB	850	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
14	bA	842	CLA	C3B-C4B-NB	3.56	113.82	110.52
14	B	835	CLA	C1C-C2C-C3C	-3.56	103.22	106.96
14	cA	831	CLA	C3B-C4B-NB	3.56	113.82	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	842	CLA	C3B-C4B-NB	3.56	113.81	110.52
14	B	834	CLA	C1C-C2C-C3C	-3.56	103.22	106.96
14	cB	828	CLA	C1C-C2C-C3C	-3.56	103.22	106.96
14	B	820	CLA	C3C-C4C-NC	3.56	114.56	110.57
14	cB	837	CLA	C1C-C2C-C3C	-3.56	103.22	106.96
14	cA	808	CLA	CMB-C2B-C1B	3.55	130.78	125.37
14	cB	850	CLA	CMC-C2C-C1C	3.55	130.45	125.04
14	A	837	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
14	cX	201	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
14	B	829	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
17	bL	205	BCR	C34-C9-C10	-3.55	117.95	122.92
14	cX	201	CLA	CAC-C3C-C4C	3.55	129.41	124.81
14	B	813	CLA	C1C-C2C-C3C	-3.55	103.23	106.96
17	L	205	BCR	C34-C9-C10	-3.55	117.95	122.92
14	bA	837	CLA	C1C-C2C-C3C	-3.55	103.23	106.96
14	bB	813	CLA	C1C-C2C-C3C	-3.55	103.23	106.96
14	cA	837	CLA	C1C-C2C-C3C	-3.55	103.23	106.96
17	cL	206	BCR	C34-C9-C10	-3.54	117.96	122.92
14	B	806	CLA	CMC-C2C-C1C	3.54	130.43	125.04
14	cA	834	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
14	B	832	CLA	C4A-NA-C1A	-3.54	105.11	106.71
14	A	808	CLA	CMB-C2B-C1B	3.54	130.76	125.37
14	B	827	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
14	bB	806	CLA	CMC-C2C-C1C	3.54	130.43	125.04
14	B	836	CLA	C1C-C2C-C3C	-3.54	103.24	106.96
14	bB	829	CLA	C1C-C2C-C3C	-3.54	103.24	106.96
14	B	802	CLA	C3B-C4B-NB	3.54	113.80	110.52
14	bF	201	CLA	CMB-C2B-C1B	3.54	130.75	125.37
14	bA	822	CLA	C3C-C4C-NC	3.54	114.54	110.57
14	bB	835	CLA	C1C-C2C-C3C	-3.53	103.24	106.96
14	bB	827	CLA	C1C-C2C-C3C	-3.53	103.24	106.96
14	cB	822	CLA	C1C-C2C-C3C	-3.53	103.24	106.96
17	cA	846	BCR	C35-C13-C14	-3.53	117.97	122.92
14	cA	808	CLA	C3C-C4C-NC	3.53	114.53	110.57
14	cB	803	CLA	C3B-C4B-NB	3.53	113.79	110.52
14	F	201	CLA	CMB-C2B-C1B	3.53	130.75	125.37
14	A	835	CLA	C3C-C4C-NC	3.53	114.53	110.57
14	bB	817	CLA	C1D-CHD-C4C	-3.53	118.44	126.06
14	bB	837	CLA	O2D-CGD-O1D	-3.53	116.94	123.84
14	cB	838	CLA	O2D-CGD-O1D	-3.53	116.94	123.84
14	B	809	CLA	C4A-NA-C1A	-3.53	105.12	106.71
14	cA	809	CLA	C3C-C4C-NC	3.53	114.53	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	837	CLA	O2D-CGD-O1D	-3.53	116.94	123.84
14	cA	803	CLA	C3B-C4B-NB	3.53	113.79	110.52
14	bA	809	CLA	C3C-C4C-NC	3.53	114.53	110.57
14	bB	809	CLA	C4A-NA-C1A	-3.53	105.12	106.71
14	B	811	CLA	CAC-C3C-C4C	3.52	129.38	124.81
14	B	821	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
14	B	807	CLA	C3B-C4B-NB	3.52	113.78	110.52
14	bB	802	CLA	C3B-C4B-NB	3.52	113.78	110.52
14	bB	811	CLA	CAC-C3C-C4C	3.52	129.38	124.81
14	bA	808	CLA	C3C-C4C-NC	3.52	114.52	110.57
14	cB	818	CLA	C1D-CHD-C4C	-3.52	118.46	126.06
14	cA	821	CLA	C3B-C4B-NB	3.52	113.78	110.52
14	cB	835	CLA	C3B-C2B-C1B	-3.52	102.91	107.16
14	bB	834	CLA	C1C-C2C-C3C	-3.52	103.26	106.96
14	bB	821	CLA	C1C-C2C-C3C	-3.52	103.26	106.96
14	B	817	CLA	C1D-CHD-C4C	-3.52	118.47	126.06
14	bA	803	CLA	C3B-C4B-NB	3.52	113.78	110.52
14	cF	201	CLA	CMB-C2B-C1B	3.52	130.72	125.37
17	cB	843	BCR	C8-C9-C10	3.52	124.34	118.94
14	A	815	CLA	C3B-C4B-NB	3.51	113.78	110.52
14	cB	810	CLA	CED-O2D-CGD	3.51	123.89	115.94
14	A	838	CLA	CMB-C2B-C1B	3.51	130.72	125.37
14	bB	838	CLA	C1D-CHD-C4C	-3.51	118.48	126.06
14	bB	823	CLA	C3B-C4B-NB	3.51	113.77	110.52
14	bA	808	CLA	CMB-C2B-C1B	3.51	130.72	125.37
14	B	809	CLA	CED-O2D-CGD	3.51	123.88	115.94
14	bB	839	CLA	C4-C3-C5	3.51	121.18	115.27
14	B	834	CLA	C3B-C2B-C1B	-3.51	102.92	107.16
14	A	803	CLA	C3B-C4B-NB	3.51	113.77	110.52
14	cB	812	CLA	CAC-C3C-C4C	3.51	129.37	124.81
14	cB	824	CLA	C3B-C4B-NB	3.51	113.77	110.52
14	cB	840	CLA	C4-C3-C5	3.51	121.18	115.27
14	L	201	CLA	CAA-CBA-CGA	3.51	123.51	113.25
14	cB	807	CLA	CMC-C2C-C1C	3.51	130.38	125.04
14	B	838	CLA	C1D-CHD-C4C	-3.51	118.49	126.06
14	bB	832	CLA	C4A-NA-C1A	-3.51	105.13	106.71
14	cA	829	CLA	C3B-C4B-NB	3.51	113.77	110.52
14	bB	809	CLA	CED-O2D-CGD	3.51	123.87	115.94
14	bB	834	CLA	C3B-C2B-C1B	-3.51	102.93	107.16
14	A	808	CLA	C3C-C4C-NC	3.51	114.50	110.57
14	cL	202	CLA	CAA-CBA-CGA	3.51	123.50	113.25
14	bA	838	CLA	CMB-C2B-C1B	3.51	130.71	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	803	CLA	C1C-C2C-C3C	-3.51	103.27	106.96
14	B	824	CLA	C1C-C2C-C3C	-3.50	103.27	106.96
14	cB	825	CLA	C1C-C2C-C3C	-3.50	103.27	106.96
14	A	809	CLA	C3C-C4C-NC	3.50	114.50	110.57
14	cA	830	CLA	C3C-C4C-NC	3.50	114.50	110.57
14	A	828	CLA	CAC-C3C-C4C	3.50	129.35	124.81
14	B	837	CLA	C1D-CHD-C4C	-3.50	118.50	126.06
17	B	842	BCR	C8-C9-C10	3.50	124.31	118.94
17	bB	842	BCR	C8-C9-C10	3.50	124.31	118.94
14	bA	828	CLA	CAC-C3C-C4C	3.50	129.35	124.81
14	cB	838	CLA	C1D-CHD-C4C	-3.50	118.51	126.06
14	bB	824	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
14	B	839	CLA	C4-C3-C5	3.50	121.16	115.27
14	cA	813	CLA	CMB-C2B-C1B	3.50	130.70	125.37
14	cA	828	CLA	CAC-C3C-C4C	3.50	129.35	124.81
14	A	821	CLA	CAC-C3C-C4C	3.50	129.35	124.81
14	cA	821	CLA	CAC-C3C-C4C	3.50	129.35	124.81
14	cB	839	CLA	C1D-CHD-C4C	-3.50	118.52	126.06
14	cB	838	CLA	C1C-C2C-C3C	-3.49	103.28	106.96
13	A	801	CL0	CAC-C3C-C4C	3.49	129.34	124.81
14	bA	821	CLA	CAC-C3C-C4C	3.49	129.34	124.81
14	B	823	CLA	C3B-C4B-NB	3.49	113.75	110.52
14	bL	201	CLA	CAA-CBA-CGA	3.49	123.46	113.25
14	bB	814	CLA	C3C-C4C-NC	3.49	114.49	110.57
14	bB	807	CLA	C3B-C4B-NB	3.49	113.75	110.52
14	A	829	CLA	C3B-C4B-NB	3.49	113.75	110.52
14	A	830	CLA	C3C-C4C-NC	3.49	114.48	110.57
14	B	819	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
14	cA	838	CLA	CMB-C2B-C1B	3.49	130.68	125.37
14	bB	803	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
14	bB	837	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
14	A	803	CLA	C3C-C4C-NC	3.49	114.48	110.57
14	bA	830	CLA	C3C-C4C-NC	3.49	114.48	110.57
17	F	202	BCR	C34-C9-C10	-3.49	118.04	122.92
17	bF	202	BCR	C34-C9-C10	-3.49	118.04	122.92
14	cA	837	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
14	bA	808	CLA	C1D-CHD-C4C	-3.49	118.54	126.06
14	bB	837	CLA	C1D-CHD-C4C	-3.49	118.54	126.06
14	bA	819	CLA	C3C-C4C-NC	3.48	114.48	110.57
14	bA	838	CLA	C1C-C2C-C3C	-3.48	103.29	106.96
14	A	837	CLA	C1D-CHD-C4C	-3.48	118.54	126.06
14	cB	820	CLA	C1D-CHD-C4C	-3.48	118.54	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cB	815	CLA	C3C-C4C-NC	3.48	114.48	110.57
14	B	851	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
14	cB	804	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
14	cB	819	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
13	cA	801	CL0	CAC-C3C-C4C	3.48	129.33	124.81
14	bB	806	CLA	C3C-C4C-NC	3.48	114.48	110.57
14	cB	807	CLA	C3C-C4C-NC	3.48	114.48	110.57
14	bA	837	CLA	C1D-CHD-C4C	-3.48	118.55	126.06
14	cB	807	CLA	C1D-CHD-C4C	-3.48	118.55	126.06
14	A	838	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
14	B	837	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
14	B	825	CLA	CMC-C2C-C1C	3.48	130.34	125.04
14	bA	829	CLA	C3B-C4B-NB	3.48	113.74	110.52
14	A	806	CLA	C1D-CHD-C4C	-3.48	118.55	126.06
14	B	814	CLA	C3C-C4C-NC	3.48	114.47	110.57
14	bA	813	CLA	CMB-C2B-C1B	3.48	130.67	125.37
14	bB	816	CLA	C3C-C4C-NC	3.48	114.47	110.57
14	cA	819	CLA	C3C-C4C-NC	3.48	114.47	110.57
14	B	806	CLA	C1D-CHD-C4C	-3.48	118.55	126.06
14	bA	806	CLA	C1D-CHD-C4C	-3.48	118.55	126.06
14	bB	819	CLA	C1D-CHD-C4C	-3.48	118.56	126.06
14	cB	817	CLA	C3C-C4C-NC	3.48	114.47	110.57
14	B	830	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
14	cB	833	CLA	C4A-NA-C1A	-3.48	105.14	106.71
14	cB	808	CLA	C3B-C4B-NB	3.48	113.74	110.52
14	cB	826	CLA	CMC-C2C-C1C	3.48	130.33	125.04
14	cA	806	CLA	C1D-CHD-C4C	-3.48	118.56	126.06
14	B	851	CLA	C1D-CHD-C4C	-3.48	118.56	126.06
14	bB	818	CLA	C1C-C2C-C3C	-3.47	103.30	106.96
14	B	829	CLA	CAC-C3C-C4C	3.47	129.32	124.81
14	bA	824	CLA	C1D-CHD-C4C	-3.47	118.56	126.06
14	bB	806	CLA	C1D-CHD-C4C	-3.47	118.56	126.06
14	bA	815	CLA	C3B-C4B-NB	3.47	113.74	110.52
14	B	816	CLA	C3C-C4C-NC	3.47	114.47	110.57
17	cB	847	BCR	C36-C18-C17	-3.47	118.06	122.92
14	cB	801	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
14	bB	825	CLA	CMC-C2C-C1C	3.47	130.33	125.04
14	A	813	CLA	CMB-C2B-C1B	3.47	130.66	125.37
14	A	808	CLA	C1D-CHD-C4C	-3.47	118.57	126.06
14	A	824	CLA	C1D-CHD-C4C	-3.47	118.57	126.06
14	bA	814	CLA	C1D-CHD-C4C	-3.47	118.57	126.06
14	cA	808	CLA	C1D-CHD-C4C	-3.47	118.57	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	824	CLA	C1D-CHD-C4C	-3.47	118.57	126.06
14	cA	815	CLA	C3B-C4B-NB	3.47	113.73	110.52
14	B	822	CLA	C1D-CHD-C4C	-3.47	118.57	126.06
14	cA	838	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
14	A	821	CLA	C3B-C4B-NB	3.47	113.73	110.52
14	cL	202	CLA	CAC-C3C-C4C	3.47	129.31	124.81
14	cA	814	CLA	C1D-CHD-C4C	-3.47	118.57	126.06
14	bB	851	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
14	cB	801	CLA	C1D-CHD-C4C	-3.47	118.57	126.06
14	cB	823	CLA	C1D-CHD-C4C	-3.47	118.57	126.06
14	bA	833	CLA	C3C-C4C-NC	3.47	114.46	110.57
14	cA	803	CLA	C3C-C4C-NC	3.47	114.46	110.57
13	bA	801	CL0	CAC-C3C-C4C	3.47	129.31	124.81
14	cB	831	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
17	cF	202	BCR	C34-C9-C10	-3.47	118.07	122.92
14	bB	822	CLA	C1D-CHD-C4C	-3.47	118.58	126.06
14	B	820	CLA	C3B-C4B-NB	3.47	113.73	110.52
14	bB	820	CLA	C3B-C4B-NB	3.47	113.73	110.52
14	A	819	CLA	C3C-C4C-NC	3.47	114.46	110.57
17	B	846	BCR	C36-C18-C17	-3.47	118.07	122.92
14	bB	851	CLA	C1D-CHD-C4C	-3.46	118.58	126.06
14	B	806	CLA	C3C-C4C-NC	3.46	114.45	110.57
14	A	821	CLA	C1D-CHD-C4C	-3.46	118.59	126.06
17	bF	202	BCR	C35-C13-C14	-3.46	118.07	122.92
14	bA	813	CLA	CMC-C2C-C1C	3.46	130.31	125.04
14	cB	834	CLA	CMC-C2C-C1C	3.46	130.31	125.04
14	bB	816	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
14	cA	813	CLA	CMC-C2C-C1C	3.46	130.31	125.04
14	B	818	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
14	A	813	CLA	CMC-C2C-C1C	3.46	130.31	125.04
14	B	833	CLA	CMC-C2C-C1C	3.46	130.31	125.04
14	bB	830	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
14	A	852	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
14	bA	821	CLA	C3B-C4B-NB	3.45	113.72	110.52
14	A	814	CLA	C1D-CHD-C4C	-3.45	118.61	126.06
17	bB	846	BCR	C36-C18-C17	-3.45	118.08	122.92
14	cB	810	CLA	C4A-NA-C1A	-3.45	105.15	106.71
14	bA	852	CLA	CAC-C3C-C4C	3.45	129.29	124.81
14	cB	817	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
14	A	852	CLA	CAC-C3C-C4C	3.45	129.29	124.81
14	bA	839	CLA	C1D-CHD-C4C	-3.45	118.61	126.06
14	bA	823	CLA	C3C-C4C-NC	3.45	114.44	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bB	829	CLA	CAC-C3C-C4C	3.45	129.29	124.81
14	bB	836	CLA	C1D-CHD-C4C	-3.45	118.61	126.06
14	cB	821	CLA	C3B-C4B-NB	3.45	113.72	110.52
14	cA	839	CLA	C1D-CHD-C4C	-3.45	118.62	126.06
14	cA	852	CLA	CAC-C3C-C4C	3.45	129.28	124.81
14	B	811	CLA	C1D-CHD-C4C	-3.45	118.62	126.06
14	cA	823	CLA	C3C-C4C-NC	3.45	114.44	110.57
14	cA	833	CLA	C3C-C4C-NC	3.45	114.44	110.57
14	cB	837	CLA	C3C-C4C-NC	3.45	114.44	110.57
14	B	816	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
14	bB	818	CLA	C1D-CHD-C4C	-3.45	118.62	126.06
14	B	836	CLA	C3C-C4C-NC	3.45	114.44	110.57
14	bA	803	CLA	C3C-C4C-NC	3.45	114.44	110.57
14	cA	821	CLA	C1D-CHD-C4C	-3.45	118.62	126.06
14	cA	852	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
14	bL	201	CLA	CAC-C3C-C4C	3.45	129.28	124.81
14	B	818	CLA	C1D-CHD-C4C	-3.44	118.63	126.06
14	cB	830	CLA	CAC-C3C-C4C	3.44	129.28	124.81
14	B	836	CLA	C1D-CHD-C4C	-3.44	118.63	126.06
14	bB	811	CLA	C1D-CHD-C4C	-3.44	118.63	126.06
14	A	839	CLA	C1D-CHD-C4C	-3.44	118.63	126.06
14	cA	826	CLA	C1D-CHD-C4C	-3.44	118.63	126.06
14	bA	821	CLA	C1D-CHD-C4C	-3.44	118.64	126.06
13	cA	801	CL0	CMC-C2C-C1C	3.44	130.28	125.04
17	bA	845	BCR	C36-C18-C17	-3.44	118.11	122.92
14	A	833	CLA	C3C-C4C-NC	3.44	114.43	110.57
14	bA	852	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
14	bB	836	CLA	C3C-C4C-NC	3.44	114.42	110.57
14	bB	833	CLA	CMC-C2C-C1C	3.44	130.27	125.04
14	A	827	CLA	C1D-CHD-C4C	-3.44	118.65	126.06
17	cF	202	BCR	C35-C13-C14	-3.44	118.11	122.92
14	cB	837	CLA	C1D-CHD-C4C	-3.43	118.65	126.06
14	cB	802	CLA	C1-O2A-CGA	3.43	125.45	116.44
17	cA	845	BCR	C36-C18-C17	-3.43	118.11	122.92
17	cA	849	BCR	C36-C18-C17	-3.43	118.11	122.92
13	A	801	CL0	CMC-C2C-C1C	3.43	130.27	125.04
14	bA	826	CLA	C1D-CHD-C4C	-3.43	118.65	126.06
14	A	840	CLA	CMB-C2B-C1B	3.43	130.60	125.37
14	bL	202	CLA	CMC-C2C-C1C	3.43	130.27	125.04
14	cL	203	CLA	C3C-C4C-NC	3.43	114.42	110.57
14	bB	801	CLA	C1-O2A-CGA	3.43	125.45	116.44
17	B	841	BCR	C34-C9-C10	-3.43	118.12	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	845	BCR	C34-C9-C10	-3.43	118.12	122.92
14	A	816	CLA	C1D-CHD-C4C	-3.43	118.66	126.06
14	bA	835	CLA	C1D-CHD-C4C	-3.43	118.66	126.06
14	cA	827	CLA	C1D-CHD-C4C	-3.43	118.66	126.06
14	cA	809	CLA	C1D-CHD-C4C	-3.43	118.66	126.06
14	A	826	CLA	C1D-CHD-C4C	-3.43	118.66	126.06
17	bA	849	BCR	C36-C18-C17	-3.43	118.12	122.92
14	A	809	CLA	C1D-CHD-C4C	-3.43	118.66	126.06
14	cA	816	CLA	C1D-CHD-C4C	-3.43	118.66	126.06
14	cB	819	CLA	C1D-CHD-C4C	-3.43	118.66	126.06
17	F	202	BCR	C35-C13-C14	-3.43	118.12	122.92
17	cB	846	BCR	C34-C9-C10	-3.43	118.12	122.92
14	bA	827	CLA	C1D-CHD-C4C	-3.43	118.66	126.06
14	bA	816	CLA	C1D-CHD-C4C	-3.43	118.67	126.06
14	cB	812	CLA	C1D-CHD-C4C	-3.43	118.67	126.06
14	A	802	CLA	C1D-CHD-C4C	-3.43	118.67	126.06
17	cB	842	BCR	C34-C9-C10	-3.43	118.12	122.92
14	B	801	CLA	C1-O2A-CGA	3.43	125.43	116.44
14	cA	804	CLA	CMC-C2C-C1C	3.43	130.25	125.04
14	L	201	CLA	CAC-C3C-C4C	3.42	129.25	124.81
14	bA	829	CLA	CMC-C2C-C1C	3.42	130.25	125.04
14	bL	202	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
14	bA	802	CLA	C1D-CHD-C4C	-3.42	118.67	126.06
14	cL	203	CLA	CMC-C2C-C1C	3.42	130.25	125.04
14	bA	809	CLA	C1D-CHD-C4C	-3.42	118.68	126.06
17	bB	845	BCR	C34-C9-C10	-3.42	118.13	122.92
14	A	835	CLA	C1D-CHD-C4C	-3.42	118.68	126.06
13	bA	801	CL0	CMC-C2C-C1C	3.42	130.25	125.04
17	A	845	BCR	C36-C18-C17	-3.42	118.13	122.92
14	bA	804	CLA	CMC-C2C-C1C	3.42	130.25	125.04
14	cB	835	CLA	C1D-CHD-C4C	-3.42	118.68	126.06
14	bA	813	CLA	C1D-CHD-C4C	-3.42	118.69	126.06
14	cA	802	CLA	C1D-CHD-C4C	-3.42	118.69	126.06
14	cA	813	CLA	C1D-CHD-C4C	-3.42	118.69	126.06
14	bL	202	CLA	C3C-C4C-NC	3.42	114.40	110.57
14	cJ	102	CLA	C1D-CHD-C4C	-3.41	118.69	126.06
14	A	813	CLA	C1D-CHD-C4C	-3.41	118.70	126.06
17	A	849	BCR	C36-C18-C17	-3.41	118.14	122.92
14	bA	840	CLA	C1D-CHD-C4C	-3.41	118.70	126.06
14	cB	836	CLA	C3B-C4B-NB	3.41	113.68	110.52
14	bB	819	CLA	CMC-C2C-C1C	3.41	130.23	125.04
14	cA	840	CLA	CMB-C2B-C1B	3.41	130.56	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bA	836	CLA	CAC-C3C-C4C	3.41	129.23	124.81
14	bB	834	CLA	C1D-CHD-C4C	-3.41	118.70	126.06
14	bJ	102	CLA	C1D-CHD-C4C	-3.41	118.70	126.06
14	cL	203	CLA	C1C-C2C-C3C	-3.41	103.37	106.96
14	A	804	CLA	CMC-C2C-C1C	3.41	130.23	125.04
14	L	202	CLA	CMC-C2C-C1C	3.41	130.23	125.04
14	J	102	CLA	C1D-CHD-C4C	-3.41	118.71	126.06
14	B	823	CLA	C4A-NA-C1A	-3.41	105.17	106.71
14	B	835	CLA	C3B-C4B-NB	3.41	113.68	110.52
14	B	834	CLA	C1D-CHD-C4C	-3.41	118.71	126.06
14	bA	842	CLA	C1D-CHD-C4C	-3.41	118.71	126.06
17	bB	841	BCR	C34-C9-C10	-3.41	118.15	122.92
14	cA	828	CLA	C1C-C2C-C3C	-3.41	103.38	106.96
14	L	202	CLA	C3C-C4C-NC	3.41	114.39	110.57
14	L	202	CLA	C1C-C2C-C3C	-3.41	103.38	106.96
14	cA	829	CLA	CMC-C2C-C1C	3.41	130.22	125.04
14	A	823	CLA	C3C-C4C-NC	3.41	114.39	110.57
17	bM	101	BCR	C34-C9-C10	-3.41	118.15	122.92
14	A	842	CLA	C1D-CHD-C4C	-3.41	118.71	126.06
14	cA	842	CLA	C1D-CHD-C4C	-3.40	118.71	126.06
14	bB	835	CLA	C3B-C4B-NB	3.40	113.67	110.52
14	cA	835	CLA	C1D-CHD-C4C	-3.40	118.72	126.06
14	A	828	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
14	A	840	CLA	C1D-CHD-C4C	-3.40	118.72	126.06
14	cA	802	CLA	C3B-C4B-NB	3.40	113.67	110.52
14	A	810	CLA	C1D-CHD-C4C	-3.40	118.72	126.06
14	cA	810	CLA	C1D-CHD-C4C	-3.40	118.72	126.06
17	cA	848	BCR	C34-C9-C10	-3.40	118.16	122.92
14	bA	828	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
14	bA	839	CLA	C3B-C4B-NB	3.40	113.67	110.52
14	cA	840	CLA	C1D-CHD-C4C	-3.40	118.73	126.06
14	bX	201	CLA	C1D-CHD-C4C	-3.40	118.73	126.06
14	bB	828	CLA	CMC-C2C-C1C	3.40	130.21	125.04
14	A	818	CLA	C3C-C4C-NC	3.40	114.38	110.57
14	A	802	CLA	C3B-C4B-NB	3.40	113.67	110.52
14	bA	809	CLA	C3B-C4B-NB	3.40	113.67	110.52
14	bA	840	CLA	CMB-C2B-C1B	3.40	130.54	125.37
14	cA	818	CLA	C3C-C4C-NC	3.39	114.38	110.57
14	cX	201	CLA	C1D-CHD-C4C	-3.39	118.73	126.06
14	X	201	CLA	C1D-CHD-C4C	-3.39	118.74	126.06
14	bA	810	CLA	C1D-CHD-C4C	-3.39	118.74	126.06
14	A	809	CLA	C3B-C4B-NB	3.39	113.66	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	cA	847	BCR	C16-C15-C14	3.39	130.42	123.47
14	cB	810	CLA	C1D-CHD-C4C	-3.39	118.74	126.06
14	A	836	CLA	CAC-C3C-C4C	3.39	129.21	124.81
14	cA	836	CLA	CAC-C3C-C4C	3.39	129.21	124.81
14	bA	823	CLA	C1D-CHD-C4C	-3.39	118.74	126.06
14	bA	814	CLA	C3B-C4B-NB	3.39	113.66	110.52
14	cA	809	CLA	C3B-C4B-NB	3.39	113.66	110.52
14	A	829	CLA	CMC-C2C-C1C	3.39	130.20	125.04
14	B	819	CLA	CMC-C2C-C1C	3.39	130.20	125.04
14	B	819	CLA	CAC-C3C-C4C	3.39	129.21	124.81
14	A	839	CLA	C3B-C4B-NB	3.39	113.66	110.52
14	bB	819	CLA	CAC-C3C-C4C	3.39	129.21	124.81
17	cM	101	BCR	C34-C9-C10	-3.39	118.18	122.92
14	cA	817	CLA	C1D-CHD-C4C	-3.39	118.75	126.06
14	bB	819	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
14	B	812	CLA	CED-O2D-CGD	3.39	123.60	115.94
14	cB	820	CLA	CMC-C2C-C1C	3.39	130.20	125.04
14	B	809	CLA	C1D-CHD-C4C	-3.39	118.75	126.06
17	M	101	BCR	C34-C9-C10	-3.39	118.18	122.92
14	cB	820	CLA	CAC-C3C-C4C	3.39	129.21	124.81
14	bB	812	CLA	CED-O2D-CGD	3.39	123.60	115.94
14	cA	823	CLA	C1D-CHD-C4C	-3.39	118.75	126.06
17	A	848	BCR	C34-C9-C10	-3.39	118.18	122.92
14	cB	813	CLA	CED-O2D-CGD	3.39	123.59	115.94
14	bA	811	CLA	C3C-C4C-NC	3.39	114.37	110.57
17	cA	846	BCR	C36-C18-C17	-3.39	118.18	122.92
14	bL	204	CLA	CMC-C2C-C1C	3.39	130.19	125.04
14	cA	816	CLA	CMC-C2C-C1C	3.39	130.19	125.04
14	bB	834	CLA	C3C-C4C-NC	3.38	114.37	110.57
14	bB	809	CLA	C1D-CHD-C4C	-3.38	118.76	126.06
14	X	201	CLA	CMB-C2B-C1B	3.38	130.52	125.37
14	A	817	CLA	C1D-CHD-C4C	-3.38	118.76	126.06
14	A	811	CLA	C3C-C4C-NC	3.38	114.36	110.57
14	bX	201	CLA	CMB-C2B-C1B	3.38	130.52	125.37
14	B	819	CLA	C1C-C2C-C3C	-3.38	103.40	106.96
14	bB	811	CLA	C1C-C2C-C3C	-3.38	103.40	106.96
14	B	828	CLA	CMC-C2C-C1C	3.38	130.19	125.04
17	bA	846	BCR	C36-C18-C17	-3.38	118.19	122.92
14	cB	820	CLA	C1C-C2C-C3C	-3.38	103.40	106.96
14	bB	822	CLA	C1C-C2C-C3C	-3.38	103.40	106.96
14	cB	803	CLA	C1D-CHD-C4C	-3.38	118.77	126.06
13	cA	801	CL0	CAA-C2A-C3A	-3.38	103.52	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bA	818	CLA	C3C-C4C-NC	3.38	114.36	110.57
14	bB	815	CLA	C1D-CHD-C4C	-3.38	118.77	126.06
17	A	847	BCR	C16-C15-C14	3.38	130.40	123.47
14	bB	821	CLA	C3C-C4C-NC	3.38	114.36	110.57
14	cB	815	CLA	CMC-C2C-C1C	3.38	130.18	125.04
13	A	801	CL0	CAA-C2A-C3A	-3.38	103.53	112.78
14	cA	814	CLA	C3B-C4B-NB	3.38	113.65	110.52
17	bA	848	BCR	C34-C9-C10	-3.38	118.19	122.92
14	cB	812	CLA	C1C-C2C-C3C	-3.38	103.41	106.96
14	cJ	102	CLA	CMB-C2B-C1B	3.38	130.51	125.37
14	bA	817	CLA	C1D-CHD-C4C	-3.38	118.77	126.06
17	A	846	BCR	C36-C18-C17	-3.38	118.19	122.92
14	B	802	CLA	C1D-CHD-C4C	-3.38	118.78	126.06
14	A	819	CLA	C1C-C2C-C3C	-3.38	103.41	106.96
14	J	102	CLA	CMB-C2B-C1B	3.37	130.51	125.37
14	bB	823	CLA	C4A-NA-C1A	-3.37	105.19	106.71
14	bJ	102	CLA	CMB-C2B-C1B	3.37	130.51	125.37
14	cB	822	CLA	C3C-C4C-NC	3.37	114.36	110.57
14	bA	802	CLA	C3B-C4B-NB	3.37	113.64	110.52
14	A	823	CLA	C1D-CHD-C4C	-3.37	118.78	126.06
13	bA	801	CL0	CAA-C2A-C3A	-3.37	103.54	112.78
14	L	204	CLA	CMC-C2C-C1C	3.37	130.18	125.04
14	bB	814	CLA	CMC-C2C-C1C	3.37	130.18	125.04
14	B	822	CLA	C1C-C2C-C3C	-3.37	103.41	106.96
14	bB	802	CLA	C1D-CHD-C4C	-3.37	118.78	126.06
14	bJ	101	CLA	C1D-CHD-C4C	-3.37	118.78	126.06
14	bA	804	CLA	C1D-CHD-C4C	-3.37	118.78	126.06
14	cL	205	CLA	CMC-C2C-C1C	3.37	130.17	125.04
14	cA	839	CLA	C3B-C4B-NB	3.37	113.64	110.52
14	B	834	CLA	C3C-C4C-NC	3.37	114.35	110.57
14	B	830	CLA	C1D-CHD-C4C	-3.37	118.78	126.06
14	B	815	CLA	C1D-CHD-C4C	-3.37	118.79	126.06
14	cB	816	CLA	C1D-CHD-C4C	-3.37	118.79	126.06
14	cX	201	CLA	CMB-C2B-C1B	3.37	130.50	125.37
14	bB	833	CLA	C1D-CHD-C4C	-3.37	118.79	126.06
14	cB	835	CLA	C3C-C4C-NC	3.37	114.35	110.57
17	bA	847	BCR	C16-C15-C14	3.37	130.38	123.47
14	cA	852	CLA	C1D-CHD-C4C	-3.37	118.79	126.06
14	B	814	CLA	CMC-C2C-C1C	3.37	130.17	125.04
14	B	833	CLA	C1D-CHD-C4C	-3.37	118.79	126.06
17	cI	102	BCR	C16-C15-C14	3.37	130.37	123.47
14	bA	819	CLA	C1C-C2C-C3C	-3.37	103.42	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	J	101	CLA	C1D-CHD-C4C	-3.37	118.80	126.06
14	B	811	CLA	C1C-C2C-C3C	-3.37	103.42	106.96
14	bB	815	CLA	CAC-C3C-C4C	3.37	129.18	124.81
14	cA	816	CLA	C3B-C4B-NB	3.37	113.64	110.52
14	cB	814	CLA	C1D-CHD-C4C	-3.37	118.80	126.06
14	cJ	101	CLA	C1D-CHD-C4C	-3.37	118.80	126.06
14	bB	820	CLA	C1C-C2C-C3C	-3.37	103.42	106.96
14	A	816	CLA	C3B-C4B-NB	3.37	113.64	110.52
14	A	804	CLA	C1D-CHD-C4C	-3.37	118.80	126.06
14	cB	834	CLA	C1D-CHD-C4C	-3.36	118.80	126.06
14	bB	830	CLA	C1D-CHD-C4C	-3.36	118.80	126.06
14	bB	832	CLA	C1C-C2C-C3C	-3.36	103.42	106.96
17	I	102	BCR	C16-C15-C14	3.36	130.36	123.47
14	cB	816	CLA	CAC-C3C-C4C	3.36	129.17	124.81
14	A	816	CLA	CMC-C2C-C1C	3.36	130.16	125.04
14	B	815	CLA	C1C-C2C-C3C	-3.36	103.42	106.96
14	cA	819	CLA	C1D-CHD-C4C	-3.36	118.81	126.06
14	cA	819	CLA	C1C-C2C-C3C	-3.36	103.42	106.96
17	bI	102	BCR	C16-C15-C14	3.36	130.36	123.47
14	cA	825	CLA	CED-O2D-CGD	3.36	123.54	115.94
14	B	830	CLA	C3B-C4B-NB	3.36	113.63	110.52
14	cB	823	CLA	C1C-C2C-C3C	-3.36	103.42	106.96
14	bA	852	CLA	C1D-CHD-C4C	-3.36	118.81	126.06
14	A	814	CLA	C3B-C4B-NB	3.36	113.63	110.52
14	bA	816	CLA	C3B-C4B-NB	3.36	113.63	110.52
14	bB	813	CLA	C1D-CHD-C4C	-3.36	118.81	126.06
14	bB	815	CLA	C1C-C2C-C3C	-3.36	103.43	106.96
14	A	852	CLA	C1D-CHD-C4C	-3.36	118.82	126.06
14	B	813	CLA	C1D-CHD-C4C	-3.36	118.82	126.06
14	B	849	CLA	C1D-CHD-C4C	-3.36	118.82	126.06
14	cB	850	CLA	C1D-CHD-C4C	-3.36	118.82	126.06
14	cA	811	CLA	C3C-C4C-NC	3.36	114.33	110.57
14	bA	816	CLA	CMC-C2C-C1C	3.36	130.15	125.04
14	bA	825	CLA	CED-O2D-CGD	3.36	123.53	115.94
14	cB	816	CLA	C1C-C2C-C3C	-3.36	103.43	106.96
14	cB	831	CLA	C1D-CHD-C4C	-3.35	118.82	126.06
17	bA	848	BCR	C37-C22-C23	3.35	123.36	118.08
14	cA	804	CLA	C1D-CHD-C4C	-3.35	118.82	126.06
14	bB	830	CLA	C3B-C4B-NB	3.35	113.63	110.52
14	bB	849	CLA	C1D-CHD-C4C	-3.35	118.82	126.06
14	B	821	CLA	C3C-C4C-NC	3.35	114.33	110.57
14	B	813	CLA	C3C-C4C-NC	3.35	114.33	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bB	827	CLA	C1D-CHD-C4C	-3.35	118.83	126.06
14	cB	824	CLA	C4A-NA-C1A	-3.35	105.20	106.71
14	bB	813	CLA	C3C-C4C-NC	3.35	114.33	110.57
14	bA	803	CLA	C1D-CHD-C4C	-3.35	118.83	126.06
14	bA	815	CLA	C1D-CHD-C4C	-3.35	118.83	126.06
14	cB	821	CLA	C1C-C2C-C3C	-3.35	103.44	106.96
14	B	827	CLA	C1D-CHD-C4C	-3.35	118.83	126.06
17	A	848	BCR	C37-C22-C23	3.35	123.35	118.08
14	bA	819	CLA	C1D-CHD-C4C	-3.35	118.84	126.06
14	cB	833	CLA	C1C-C2C-C3C	-3.35	103.44	106.96
14	B	815	CLA	CAC-C3C-C4C	3.35	129.15	124.81
14	cA	803	CLA	C1D-CHD-C4C	-3.35	118.84	126.06
14	A	825	CLA	CED-O2D-CGD	3.35	123.50	115.94
14	bA	809	CLA	CAC-C3C-C4C	3.34	129.15	124.81
14	A	819	CLA	C1D-CHD-C4C	-3.34	118.84	126.06
14	bB	817	CLA	C3B-C4B-NB	3.34	113.62	110.52
14	bA	825	CLA	CAC-C3C-C4C	3.34	129.15	124.81
14	cB	828	CLA	C1D-CHD-C4C	-3.34	118.85	126.06
14	B	820	CLA	C1C-C2C-C3C	-3.34	103.44	106.96
17	cA	848	BCR	C37-C22-C23	3.34	123.34	118.08
14	A	803	CLA	C1D-CHD-C4C	-3.34	118.85	126.06
14	A	815	CLA	C1D-CHD-C4C	-3.34	118.85	126.06
14	B	801	CLA	O2D-CGD-CBD	3.34	117.20	111.27
14	B	832	CLA	C1C-C2C-C3C	-3.34	103.44	106.96
14	cB	829	CLA	CMC-C2C-C1C	3.34	130.12	125.04
14	cA	815	CLA	C1D-CHD-C4C	-3.34	118.86	126.06
14	cA	842	CLA	CMC-C2C-C1C	3.34	130.12	125.04
14	cB	831	CLA	C3B-C4B-NB	3.34	113.61	110.52
14	A	825	CLA	CAC-C3C-C4C	3.34	129.14	124.81
14	cB	804	CLA	C4C-C3C-C2C	-3.34	102.04	106.90
14	bA	823	CLA	C1C-C2C-C3C	-3.33	103.45	106.96
14	A	842	CLA	CMC-C2C-C1C	3.33	130.12	125.04
17	B	846	BCR	C34-C9-C10	-3.33	118.26	122.92
14	cB	808	CLA	C1D-CHD-C4C	-3.33	118.87	126.06
14	cB	823	CLA	CAC-C3C-C4C	3.33	129.13	124.81
14	bA	832	CLA	C1D-CHD-C4C	-3.33	118.88	126.06
17	bB	846	BCR	C34-C9-C10	-3.33	118.26	122.92
17	cB	847	BCR	C34-C9-C10	-3.33	118.26	122.92
14	B	822	CLA	CAC-C3C-C4C	3.33	129.13	124.81
14	cA	805	CLA	C1D-CHD-C4C	-3.33	118.88	126.06
14	bA	842	CLA	CMC-C2C-C1C	3.33	130.11	125.04
14	bB	801	CLA	O2D-CGD-CBD	3.33	117.18	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cB	802	CLA	O2D-CGD-CBD	3.33	117.18	111.27
14	cA	825	CLA	CAC-C3C-C4C	3.33	129.12	124.81
14	bA	805	CLA	C1D-CHD-C4C	-3.33	118.88	126.06
14	bB	807	CLA	C1D-CHD-C4C	-3.33	118.88	126.06
14	bB	808	CLA	C4A-NA-C1A	-3.33	105.21	106.71
14	B	807	CLA	C1D-CHD-C4C	-3.32	118.89	126.06
14	B	826	CLA	CHC-C1C-C2C	-3.32	117.50	126.73
14	cB	814	CLA	C3C-C4C-NC	3.32	114.30	110.57
14	B	809	CLA	C5-C3-C2	-3.32	114.39	121.12
14	cB	818	CLA	C3B-C4B-NB	3.32	113.60	110.52
14	cA	809	CLA	CAC-C3C-C4C	3.32	129.12	124.81
14	A	841	CLA	O2A-CGA-CBA	3.32	122.33	111.91
14	cA	820	CLA	C3C-C4C-NC	3.32	114.30	110.57
14	A	812	CLA	C1D-CHD-C4C	-3.32	118.89	126.06
14	A	824	CLA	CAC-C3C-C4C	3.32	129.12	124.81
14	bB	816	CLA	C1D-CHD-C4C	-3.32	118.90	126.06
14	cA	832	CLA	C1D-CHD-C4C	-3.32	118.90	126.06
14	bB	809	CLA	C5-C3-C2	-3.32	114.40	121.12
14	A	805	CLA	C1D-CHD-C4C	-3.32	118.90	126.06
14	cB	822	CLA	CMC-C2C-C1C	3.32	130.09	125.04
14	B	816	CLA	C1D-CHD-C4C	-3.32	118.90	126.06
14	bA	841	CLA	O2A-CGA-CBA	3.32	122.32	111.91
14	bB	836	CLA	CAC-C3C-C4C	3.32	129.11	124.81
14	bA	831	CLA	CMC-C2C-C1C	3.32	130.09	125.04
14	bA	812	CLA	C1D-CHD-C4C	-3.32	118.90	126.06
14	cB	827	CLA	CHC-C1C-C2C	-3.32	117.52	126.73
14	cB	817	CLA	C1D-CHD-C4C	-3.32	118.91	126.06
14	bB	822	CLA	CAC-C3C-C4C	3.31	129.11	124.81
14	bA	817	CLA	CED-O2D-CGD	3.31	123.43	115.94
14	bB	803	CLA	C4C-C3C-C2C	-3.31	102.07	106.90
14	cB	809	CLA	C4A-NA-C1A	-3.31	105.22	106.71
14	cA	841	CLA	O2A-CGA-CBA	3.31	122.31	111.91
14	cB	802	CLA	C1C-C2C-C3C	-3.31	103.47	106.96
14	cB	825	CLA	C1D-CHD-C4C	-3.31	118.91	126.06
14	bB	826	CLA	CHC-C1C-C2C	-3.31	117.53	126.73
14	B	817	CLA	C3B-C4B-NB	3.31	113.59	110.52
17	I	101	BCR	C37-C22-C23	3.31	123.29	118.08
14	A	817	CLA	CED-O2D-CGD	3.31	123.43	115.94
14	cA	812	CLA	C1D-CHD-C4C	-3.31	118.92	126.06
14	A	809	CLA	CAC-C3C-C4C	3.31	129.11	124.81
14	B	821	CLA	CMC-C2C-C1C	3.31	130.08	125.04
14	cB	815	CLA	C3B-C4B-NB	3.31	113.59	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	832	CLA	C1D-CHD-C4C	-3.31	118.92	126.06
14	B	803	CLA	C4C-C3C-C2C	-3.31	102.07	106.90
14	cB	837	CLA	CAC-C3C-C4C	3.31	129.10	124.81
14	A	813	CLA	C4C-C3C-C2C	-3.31	102.08	106.90
17	bB	850	BCR	C16-C15-C14	3.31	130.25	123.47
14	B	801	CLA	C1C-C2C-C3C	-3.31	103.48	106.96
17	cB	851	BCR	C16-C15-C14	3.31	130.25	123.47
14	B	836	CLA	CAC-C3C-C4C	3.31	129.10	124.81
14	cA	813	CLA	C4C-C3C-C2C	-3.30	102.08	106.90
14	cB	810	CLA	C5-C3-C2	-3.30	114.43	121.12
14	cA	817	CLA	CED-O2D-CGD	3.30	123.40	115.94
14	bA	813	CLA	C4C-C3C-C2C	-3.30	102.09	106.90
14	bA	824	CLA	CAC-C3C-C4C	3.30	129.09	124.81
17	B	850	BCR	C16-C15-C14	3.30	130.23	123.47
14	cA	823	CLA	C1C-C2C-C3C	-3.30	103.49	106.96
17	cI	101	BCR	C37-C22-C23	3.30	123.27	118.08
14	B	824	CLA	C1D-CHD-C4C	-3.30	118.94	126.06
14	bB	821	CLA	CMC-C2C-C1C	3.30	130.06	125.04
17	bB	843	BCR	C23-C22-C21	3.30	124.00	118.94
14	B	817	CLA	C1C-C2C-C3C	-3.30	103.49	106.96
14	bB	801	CLA	C1C-C2C-C3C	-3.30	103.49	106.96
17	bI	101	BCR	C34-C9-C10	-3.30	118.31	122.92
14	F	201	CLA	CAC-C3C-C4C	3.30	129.09	124.81
14	bB	825	CLA	CAC-C3C-C4C	3.29	129.09	124.81
14	bB	824	CLA	C1D-CHD-C4C	-3.29	118.95	126.06
14	A	820	CLA	C3C-C4C-NC	3.29	114.27	110.57
14	bA	820	CLA	C3C-C4C-NC	3.29	114.27	110.57
17	bI	101	BCR	C37-C22-C23	3.29	123.27	118.08
14	A	831	CLA	CMC-C2C-C1C	3.29	130.06	125.04
14	A	823	CLA	C1C-C2C-C3C	-3.29	103.49	106.96
14	B	814	CLA	C3B-C4B-NB	3.29	113.57	110.52
14	bA	836	CLA	C3B-C4B-NB	3.29	113.57	110.52
14	bB	810	CLA	C3C-C4C-NC	3.29	114.26	110.57
14	B	815	CLA	CMC-C2C-C1C	3.29	130.05	125.04
14	B	808	CLA	C4A-NA-C1A	-3.29	105.23	106.71
14	A	818	CLA	C1D-CHD-C4C	-3.29	118.96	126.06
14	cA	818	CLA	C1D-CHD-C4C	-3.29	118.96	126.06
14	A	807	CLA	C1C-C2C-C3C	-3.29	103.50	106.96
17	B	843	BCR	C23-C22-C21	3.29	123.99	118.94
17	I	101	BCR	C34-C9-C10	-3.29	118.32	122.92
14	A	836	CLA	C3B-C4B-NB	3.29	113.56	110.52
14	bA	829	CLA	C1D-CHD-C4C	-3.29	118.97	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bB	816	CLA	CMC-C2C-C1C	3.29	130.04	125.04
14	A	829	CLA	C1D-CHD-C4C	-3.29	118.97	126.06
14	bA	807	CLA	C1C-C2C-C3C	-3.29	103.50	106.96
14	cA	807	CLA	C1C-C2C-C3C	-3.28	103.50	106.96
14	bB	822	CLA	C3B-C4B-NB	3.28	113.56	110.52
14	cB	823	CLA	C3B-C4B-NB	3.28	113.56	110.52
14	cB	826	CLA	CAC-C3C-C4C	3.28	129.07	124.81
14	cA	829	CLA	C1D-CHD-C4C	-3.28	118.97	126.06
14	bA	817	CLA	CAC-C3C-C4C	3.28	129.07	124.81
14	cA	824	CLA	CAC-C3C-C4C	3.28	129.07	124.81
14	bA	811	CLA	C1D-CHD-C4C	-3.28	118.97	126.06
14	bB	802	CLA	CMB-C2B-C1B	3.28	130.37	125.37
14	bB	808	CLA	C1C-C2C-C3C	-3.28	103.50	106.96
17	cB	844	BCR	C23-C22-C21	3.28	123.98	118.94
14	cB	811	CLA	C3C-C4C-NC	3.28	114.25	110.57
14	B	808	CLA	C4C-C3C-C2C	-3.28	102.11	106.90
14	cA	812	CLA	C4C-C3C-C2C	-3.28	102.11	106.90
14	bB	813	CLA	CMC-C2C-C1C	3.28	130.04	125.04
14	bA	812	CLA	C4C-C3C-C2C	-3.28	102.12	106.90
14	cA	831	CLA	C4-C3-C5	3.28	120.79	115.27
14	bA	818	CLA	C1D-CHD-C4C	-3.28	118.98	126.06
14	B	802	CLA	CMB-C2B-C1B	3.28	130.36	125.37
14	A	831	CLA	C1D-CHD-C4C	-3.28	118.99	126.06
14	B	828	CLA	C1C-C2C-C3C	-3.28	103.51	106.96
14	B	816	CLA	CMC-C2C-C1C	3.28	130.03	125.04
14	bB	815	CLA	CMC-C2C-C1C	3.28	130.03	125.04
14	cB	817	CLA	CMC-C2C-C1C	3.28	130.03	125.04
14	bA	831	CLA	C1D-CHD-C4C	-3.28	118.99	126.06
14	bB	828	CLA	C1C-C2C-C3C	-3.28	103.51	106.96
14	B	813	CLA	CMC-C2C-C1C	3.27	130.03	125.04
14	B	803	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
14	A	812	CLA	C4C-C3C-C2C	-3.27	102.13	106.90
14	cB	816	CLA	CMC-C2C-C1C	3.27	130.02	125.04
14	cB	818	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
17	cA	846	BCR	C16-C15-C14	3.27	130.18	123.47
14	A	834	CLA	CED-O2D-CGD	3.27	123.34	115.94
14	A	817	CLA	CAC-C3C-C4C	3.27	129.06	124.81
17	cI	101	BCR	C34-C9-C10	-3.27	118.34	122.92
14	cB	829	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
14	bB	808	CLA	C4C-C3C-C2C	-3.27	102.13	106.90
14	bA	834	CLA	CED-O2D-CGD	3.27	123.34	115.94
14	A	811	CLA	C1D-CHD-C4C	-3.27	119.00	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	836	CLA	C3B-C4B-NB	3.27	113.55	110.52
14	B	839	CLA	CMC-C2C-C1C	3.27	130.02	125.04
14	cB	814	CLA	CMC-C2C-C1C	3.27	130.02	125.04
14	bB	803	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
14	cB	803	CLA	CMB-C2B-C1B	3.27	130.35	125.37
14	B	825	CLA	CAC-C3C-C4C	3.27	129.05	124.81
14	B	810	CLA	C3C-C4C-NC	3.27	114.24	110.57
14	bB	814	CLA	C3B-C4B-NB	3.27	113.55	110.52
14	bA	806	CLA	O2A-CGA-CBA	3.27	122.17	111.91
14	cA	817	CLA	CAC-C3C-C4C	3.27	129.05	124.81
14	cB	809	CLA	C4C-C3C-C2C	-3.27	102.13	106.90
14	bB	817	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
14	cB	840	CLA	CMC-C2C-C1C	3.27	130.01	125.04
14	A	806	CLA	O2A-CGA-CBA	3.27	122.16	111.91
14	bF	201	CLA	CAC-C3C-C4C	3.27	129.05	124.81
17	A	846	BCR	C16-C15-C14	3.27	130.16	123.47
14	cB	835	CLA	CHC-C1C-C2C	-3.27	117.66	126.73
14	cB	804	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
14	cB	809	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
14	bB	839	CLA	CMC-C2C-C1C	3.27	130.01	125.04
14	cA	806	CLA	O2A-CGA-CBA	3.27	122.16	111.91
17	bA	846	BCR	C16-C15-C14	3.26	130.16	123.47
17	I	102	BCR	C37-C22-C23	3.26	123.22	118.08
17	cI	102	BCR	C37-C22-C23	3.26	123.22	118.08
14	A	831	CLA	C4-C3-C5	3.26	120.76	115.27
14	bA	831	CLA	C4-C3-C5	3.26	120.76	115.27
14	cB	810	CLA	C3B-C2B-C1B	-3.26	103.22	107.16
14	cA	811	CLA	C1D-CHD-C4C	-3.26	119.02	126.06
14	A	840	CLA	C1C-C2C-C3C	-3.26	103.53	106.96
14	cA	834	CLA	C3C-C4C-NC	3.26	114.23	110.57
14	cA	831	CLA	CMC-C2C-C1C	3.26	130.00	125.04
14	cA	826	CLA	C1C-C2C-C3C	-3.26	103.53	106.96
14	cA	831	CLA	C1D-CHD-C4C	-3.26	119.03	126.06
14	B	822	CLA	C3B-C4B-NB	3.26	113.54	110.52
14	cA	834	CLA	CED-O2D-CGD	3.26	123.31	115.94
14	B	834	CLA	CHC-C1C-C2C	-3.26	117.68	126.73
14	B	814	CLA	C1D-CHD-C4C	-3.26	119.03	126.06
14	bB	805	CLA	C1D-CHD-C4C	-3.26	119.03	126.06
14	bA	834	CLA	C1D-CHD-C4C	-3.26	119.03	126.06
14	cA	834	CLA	C1D-CHD-C4C	-3.26	119.03	126.06
17	bI	102	BCR	C37-C22-C23	3.26	123.21	118.08
14	bB	809	CLA	C3B-C2B-C1B	-3.26	103.23	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cF	201	CLA	CAC-C3C-C4C	3.25	129.03	124.81
14	A	826	CLA	C1C-C2C-C3C	-3.25	103.53	106.96
14	bB	834	CLA	CHC-C1C-C2C	-3.25	117.69	126.73
14	A	834	CLA	C1D-CHD-C4C	-3.25	119.04	126.06
14	B	808	CLA	C1C-C2C-C3C	-3.25	103.54	106.96
14	bB	822	CLA	CMC-C2C-C1C	3.25	129.99	125.04
14	B	805	CLA	C1D-CHD-C4C	-3.25	119.04	126.06
14	bA	840	CLA	C1C-C2C-C3C	-3.25	103.54	106.96
14	bA	834	CLA	C3C-C4C-NC	3.25	114.22	110.57
14	B	809	CLA	C3B-C2B-C1B	-3.25	103.24	107.16
17	bB	847	BCR	C15-C16-C17	3.25	130.13	123.47
14	bB	814	CLA	C1D-CHD-C4C	-3.25	119.05	126.06
14	cB	815	CLA	C1D-CHD-C4C	-3.25	119.05	126.06
14	A	831	CLA	CAC-C3C-C4C	3.25	129.02	124.81
17	cB	848	BCR	C11-C10-C9	3.25	131.94	127.31
14	cB	806	CLA	C1D-CHD-C4C	-3.25	119.05	126.06
14	A	834	CLA	C3C-C4C-NC	3.25	114.21	110.57
17	B	847	BCR	C15-C16-C17	3.25	130.12	123.47
14	cA	839	CLA	CAC-C3C-C4C	3.24	129.02	124.81
17	cB	848	BCR	C15-C16-C17	3.24	130.12	123.47
14	bA	826	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
14	cA	802	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
14	A	839	CLA	C4A-NA-C1A	-3.24	105.25	106.71
14	cA	820	CLA	C1D-CHD-C4C	-3.24	119.06	126.06
14	cA	835	CLA	CAC-C3C-C4C	3.24	129.02	124.81
13	A	801	CL0	C1D-CHD-C4C	-3.24	119.06	126.06
17	bB	847	BCR	C11-C10-C9	3.24	131.94	127.31
13	bA	801	CL0	C1D-CHD-C4C	-3.24	119.07	126.06
14	L	203	CLA	C1D-CHD-C4C	-3.24	119.07	126.06
14	bA	833	CLA	C3B-C4B-NB	3.24	113.52	110.52
14	B	822	CLA	CMC-C2C-C1C	3.24	129.97	125.04
17	B	847	BCR	C11-C10-C9	3.24	131.93	127.31
14	cB	826	CLA	CMB-C2B-C1B	3.24	130.30	125.37
14	bB	804	CLA	C1D-CHD-C4C	-3.24	119.08	126.06
14	bA	802	CLA	O2D-CGD-O1D	-3.23	117.51	123.84
13	cA	801	CL0	C1D-CHD-C4C	-3.23	119.08	126.06
14	bA	813	CLA	CED-O2D-CGD	3.23	123.25	115.94
14	cA	833	CLA	C3B-C4B-NB	3.23	113.51	110.52
14	cL	204	CLA	C1D-CHD-C4C	-3.23	119.08	126.06
14	cB	823	CLA	CMC-C2C-C1C	3.23	129.96	125.04
14	bL	203	CLA	C1D-CHD-C4C	-3.23	119.08	126.06
14	cA	840	CLA	C1C-C2C-C3C	-3.23	103.56	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bB	851	CLA	CMC-C2C-C1C	3.23	129.96	125.04
14	bB	825	CLA	CMB-C2B-C1B	3.23	130.29	125.37
14	cB	805	CLA	C1D-CHD-C4C	-3.23	119.09	126.06
14	B	825	CLA	CMB-C2B-C1B	3.23	130.29	125.37
14	bA	820	CLA	C1D-CHD-C4C	-3.23	119.09	126.06
14	cA	813	CLA	CED-O2D-CGD	3.23	123.24	115.94
14	A	820	CLA	C1D-CHD-C4C	-3.23	119.09	126.06
14	A	833	CLA	C3B-C4B-NB	3.23	113.51	110.52
14	B	810	CLA	C1D-CHD-C4C	-3.23	119.10	126.06
14	cB	835	CLA	CMC-C2C-C1C	3.23	129.95	125.04
14	A	835	CLA	CAC-C3C-C4C	3.23	129.00	124.81
14	bA	835	CLA	CAC-C3C-C4C	3.22	128.99	124.81
14	bB	827	CLA	CAC-C3C-C4C	3.22	128.99	124.81
14	B	804	CLA	C1D-CHD-C4C	-3.22	119.10	126.06
14	B	851	CLA	CMC-C2C-C1C	3.22	129.95	125.04
14	bB	810	CLA	C1D-CHD-C4C	-3.22	119.10	126.06
14	bA	839	CLA	C4A-NA-C1A	-3.22	105.26	106.71
14	B	835	CLA	C1D-CHD-C4C	-3.22	119.11	126.06
14	A	802	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
14	bA	831	CLA	CAC-C3C-C4C	3.22	128.99	124.81
14	cB	811	CLA	C1D-CHD-C4C	-3.22	119.11	126.06
14	cB	801	CLA	CMC-C2C-C1C	3.22	129.94	125.04
14	A	813	CLA	CED-O2D-CGD	3.22	123.22	115.94
14	bB	835	CLA	C1D-CHD-C4C	-3.22	119.11	126.06
14	cB	839	CLA	CMC-C2C-C1C	3.22	129.94	125.04
14	cB	836	CLA	C1D-CHD-C4C	-3.22	119.12	126.06
14	A	839	CLA	CAC-C3C-C4C	3.21	128.98	124.81
14	A	842	CLA	CAC-C3C-C4C	3.21	128.98	124.81
14	bA	839	CLA	CAC-C3C-C4C	3.21	128.98	124.81
14	bA	842	CLA	CAC-C3C-C4C	3.21	128.98	124.81
14	cA	831	CLA	CAC-C3C-C4C	3.21	128.98	124.81
14	bB	829	CLA	C1D-CHD-C4C	-3.21	119.13	126.06
14	B	838	CLA	CMC-C2C-C1C	3.21	129.93	125.04
14	bA	821	CLA	CMC-C2C-C1C	3.21	129.93	125.04
14	B	827	CLA	CAC-C3C-C4C	3.21	128.97	124.81
14	B	839	CLA	CHC-C1C-C2C	-3.21	117.82	126.73
14	bA	852	CLA	O2D-CGD-CBD	3.21	116.97	111.27
14	cB	840	CLA	C4A-NA-C1A	-3.21	105.26	106.71
14	cB	840	CLA	CHC-C1C-C2C	-3.21	117.82	126.73
14	bB	839	CLA	CHC-C1C-C2C	-3.21	117.83	126.73
14	B	834	CLA	CMC-C2C-C1C	3.21	129.92	125.04
14	bA	829	CLA	CAC-C3C-C4C	3.21	128.97	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bB	829	CLA	C3B-C4B-NB	3.20	113.49	110.52
14	B	825	CLA	CED-O2D-CGD	3.20	123.18	115.94
14	cB	826	CLA	CED-O2D-CGD	3.20	123.18	115.94
14	cB	828	CLA	CAC-C3C-C4C	3.20	128.97	124.81
14	cA	839	CLA	C4A-NA-C1A	-3.20	105.27	106.71
14	bB	834	CLA	CMC-C2C-C1C	3.20	129.92	125.04
13	cA	801	CL0	CHB-C4A-NA	3.20	128.94	124.51
17	L	206	BCR	C34-C9-C10	-3.20	118.44	122.92
14	bB	838	CLA	CMC-C2C-C1C	3.20	129.91	125.04
14	cL	203	CLA	C1D-CHD-C4C	-3.20	119.15	126.06
14	bB	827	CLA	C3B-C4B-NB	3.20	113.48	110.52
17	cB	845	BCR	C34-C9-C10	-3.20	118.44	122.92
14	cA	810	CLA	CMB-C2B-C1B	3.20	130.24	125.37
14	B	805	CLA	C3C-C4C-NC	3.20	114.16	110.57
14	cA	852	CLA	O2D-CGD-CBD	3.20	116.95	111.27
14	bB	825	CLA	CED-O2D-CGD	3.20	123.17	115.94
14	B	815	CLA	C4-C3-C5	3.20	120.65	115.27
14	bL	202	CLA	C1D-CHD-C4C	-3.20	119.16	126.06
14	cA	807	CLA	C1D-CHD-C4C	-3.20	119.16	126.06
14	bA	824	CLA	CMC-C2C-C1C	3.20	129.91	125.04
14	A	806	CLA	O2D-CGD-CBD	3.20	116.95	111.27
13	bA	801	CL0	CHB-C4A-NA	3.20	128.93	124.51
14	bA	818	CLA	C1C-C2C-C3C	-3.20	103.60	106.96
14	L	202	CLA	C1D-CHD-C4C	-3.20	119.17	126.06
14	A	810	CLA	CMB-C2B-C1B	3.19	130.24	125.37
17	cL	207	BCR	C34-C9-C10	-3.19	118.45	122.92
14	B	839	CLA	C4A-NA-C1A	-3.19	105.27	106.71
14	A	826	CLA	CAC-C3C-C4C	3.19	128.95	124.81
14	cA	829	CLA	CAC-C3C-C4C	3.19	128.95	124.81
14	cA	821	CLA	CMC-C2C-C1C	3.19	129.90	125.04
17	cJ	103	BCR	C37-C22-C21	-3.19	118.45	122.92
14	A	818	CLA	C1C-C2C-C3C	-3.19	103.60	106.96
14	bA	804	CLA	C1C-C2C-C3C	-3.19	103.60	106.96
14	cB	830	CLA	C1D-CHD-C4C	-3.19	119.17	126.06
14	A	839	CLA	CMC-C2C-C1C	3.19	129.90	125.04
14	bB	808	CLA	CHC-C1C-C2C	-3.19	117.87	126.73
17	B	844	BCR	C34-C9-C10	-3.19	118.45	122.92
14	B	829	CLA	C1D-CHD-C4C	-3.19	119.18	126.06
14	bA	826	CLA	CAC-C3C-C4C	3.19	128.95	124.81
14	cA	842	CLA	CAC-C3C-C4C	3.19	128.95	124.81
14	cB	828	CLA	C3B-C4B-NB	3.19	113.47	110.52
14	bA	807	CLA	C1D-CHD-C4C	-3.19	119.18	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	801	CL0	CHB-C4A-NA	3.19	128.92	124.51
14	cB	816	CLA	C4-C3-C5	3.19	120.63	115.27
14	A	852	CLA	O2D-CGD-CBD	3.19	116.93	111.27
14	B	829	CLA	C3B-C4B-NB	3.19	113.47	110.52
14	A	819	CLA	CHC-C1C-C2C	-3.19	117.88	126.73
14	cA	819	CLA	CHC-C1C-C2C	-3.19	117.88	126.73
14	bA	819	CLA	CHC-C1C-C2C	-3.19	117.88	126.73
14	B	827	CLA	C3B-C4B-NB	3.19	113.47	110.52
14	B	836	CLA	CMC-C2C-C1C	3.19	129.89	125.04
14	A	804	CLA	C1C-C2C-C3C	-3.19	103.61	106.96
14	cB	809	CLA	CHC-C1C-C2C	-3.19	117.88	126.73
14	B	812	CLA	C1D-CHD-C4C	-3.19	119.19	126.06
14	A	829	CLA	CAC-C3C-C4C	3.18	128.94	124.81
14	cA	810	CLA	CMC-C2C-C1C	3.18	129.89	125.04
14	cA	839	CLA	CMC-C2C-C1C	3.18	129.89	125.04
14	bB	815	CLA	C4-C3-C5	3.18	120.63	115.27
17	J	103	BCR	C37-C22-C21	-3.18	118.46	122.92
14	cL	204	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
14	bB	812	CLA	C1D-CHD-C4C	-3.18	119.19	126.06
14	cB	837	CLA	CMC-C2C-C1C	3.18	129.89	125.04
17	cL	206	BCR	C16-C15-C14	3.18	129.99	123.47
17	bL	206	BCR	C34-C9-C10	-3.18	118.47	122.92
14	A	807	CLA	C1D-CHD-C4C	-3.18	119.19	126.06
14	cB	813	CLA	C1D-CHD-C4C	-3.18	119.19	126.06
14	bB	836	CLA	CMC-C2C-C1C	3.18	129.88	125.04
14	bL	203	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
17	bL	205	BCR	C16-C15-C14	3.18	129.99	123.47
17	bJ	103	BCR	C37-C22-C21	-3.18	118.47	122.92
14	cA	818	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
14	A	834	CLA	CHC-C1C-C2C	-3.18	117.90	126.73
14	cA	826	CLA	CAC-C3C-C4C	3.18	128.94	124.81
14	cA	804	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
17	L	205	BCR	C16-C15-C14	3.18	129.99	123.47
17	bA	845	BCR	C19-C18-C17	3.18	123.82	118.94
14	cA	806	CLA	O2D-CGD-CBD	3.18	116.92	111.27
14	bB	806	CLA	CAC-C3C-C4C	3.18	128.93	124.81
14	bA	810	CLA	CMB-C2B-C1B	3.18	130.21	125.37
14	bB	805	CLA	C3C-C4C-NC	3.18	114.13	110.57
14	L	203	CLA	C4C-C3C-C2C	-3.18	102.27	106.90
14	bA	834	CLA	CHC-C1C-C2C	-3.18	117.91	126.73
14	bA	806	CLA	O2D-CGD-CBD	3.18	116.91	111.27
14	bA	839	CLA	CMC-C2C-C1C	3.18	129.88	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	bB	844	BCR	C34-C9-C10	-3.18	118.47	122.92
14	cA	834	CLA	CHC-C1C-C2C	-3.17	117.91	126.73
14	B	808	CLA	CHC-C1C-C2C	-3.17	117.91	126.73
14	bA	827	CLA	C1C-C2C-C3C	-3.17	103.62	106.96
14	bB	839	CLA	C4A-NA-C1A	-3.17	105.28	106.71
14	cA	824	CLA	CMC-C2C-C1C	3.17	129.87	125.04
14	A	821	CLA	CMC-C2C-C1C	3.17	129.87	125.04
14	cB	821	CLA	C1D-CHD-C4C	-3.17	119.22	126.06
14	cA	838	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
14	bB	820	CLA	C1D-CHD-C4C	-3.17	119.22	126.06
14	bA	832	CLA	CAC-C3C-C4C	3.17	128.92	124.81
14	cB	816	CLA	O2A-CGA-CBA	3.16	121.84	111.91
14	bA	810	CLA	CMC-C2C-C1C	3.16	129.86	125.04
14	B	806	CLA	CAC-C3C-C4C	3.16	128.91	124.81
14	L	201	CLA	C4-C3-C2	-3.16	115.56	123.68
14	A	824	CLA	CMC-C2C-C1C	3.16	129.85	125.04
14	bB	815	CLA	O2A-CGA-CBA	3.16	121.83	111.91
14	bB	828	CLA	CAC-C3C-C4C	3.16	128.91	124.81
14	cB	837	CLA	C3B-C4B-NB	3.16	113.45	110.52
14	cB	807	CLA	CAC-C3C-C4C	3.16	128.91	124.81
14	bL	201	CLA	C4-C3-C2	-3.16	115.57	123.68
14	cB	838	CLA	C3B-C4B-NB	3.16	113.45	110.52
17	bB	850	BCR	C15-C16-C17	3.16	129.94	123.47
17	A	845	BCR	C19-C18-C17	3.16	123.79	118.94
14	A	827	CLA	C1C-C2C-C3C	-3.16	103.64	106.96
14	cB	830	CLA	C3B-C4B-NB	3.16	113.44	110.52
14	B	815	CLA	O2A-CGA-CBA	3.16	121.81	111.91
14	cA	832	CLA	CAC-C3C-C4C	3.16	128.91	124.81
14	cB	822	CLA	CHC-C1C-C2C	-3.16	117.96	126.73
17	B	850	BCR	C15-C16-C17	3.16	129.94	123.47
14	cL	202	CLA	C4-C3-C2	-3.16	115.58	123.68
14	cB	807	CLA	C4-C3-C5	3.16	120.58	115.27
14	bB	806	CLA	C4-C3-C5	3.15	120.58	115.27
17	cA	845	BCR	C19-C18-C17	3.15	123.78	118.94
14	bA	806	CLA	CMB-C2B-C1B	3.15	130.17	125.37
14	B	820	CLA	C1D-CHD-C4C	-3.15	119.25	126.06
14	A	810	CLA	CMC-C2C-C1C	3.15	129.84	125.04
14	B	828	CLA	CAC-C3C-C4C	3.15	128.90	124.81
14	cB	829	CLA	CAC-C3C-C4C	3.15	128.90	124.81
17	cB	851	BCR	C15-C16-C17	3.15	129.93	123.47
14	cA	827	CLA	C1C-C2C-C3C	-3.15	103.64	106.96
14	B	821	CLA	CHC-C1C-C2C	-3.15	117.97	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	810	CLA	CAC-C3C-C4C	3.15	128.90	124.81
14	A	838	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
17	bA	846	BCR	C1-C6-C5	-3.15	118.18	122.61
14	A	806	CLA	CMB-C2B-C1B	3.15	130.17	125.37
14	bB	802	CLA	C4A-NA-C1A	-3.15	105.29	106.71
14	A	832	CLA	CAC-C3C-C4C	3.15	128.90	124.81
14	bB	821	CLA	CHC-C1C-C2C	-3.15	117.99	126.73
14	bA	838	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
17	A	846	BCR	C1-C6-C5	-3.15	118.18	122.61
17	bB	845	BCR	C37-C22-C23	3.14	123.03	118.08
14	cB	806	CLA	C3C-C4C-NC	3.14	114.10	110.57
14	bA	807	CLA	CHC-C1C-C2C	-3.14	118.00	126.73
17	cA	846	BCR	C1-C6-C5	-3.14	118.19	122.61
14	A	818	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
14	cA	816	CLA	C1C-C2C-C3C	-3.14	103.66	106.96
14	B	837	CLA	C3B-C4B-NB	3.14	113.43	110.52
14	cA	807	CLA	CHC-C1C-C2C	-3.14	118.01	126.73
14	A	807	CLA	CHC-C1C-C2C	-3.14	118.01	126.73
14	bB	831	CLA	C1D-CHD-C4C	-3.14	119.29	126.06
14	B	831	CLA	C1D-CHD-C4C	-3.14	119.29	126.06
14	bA	817	CLA	C3B-C4B-NB	3.14	113.43	110.52
14	B	814	CLA	C1C-C2C-C3C	-3.14	103.66	106.96
14	cB	832	CLA	C1D-CHD-C4C	-3.14	119.29	126.06
14	bA	823	CLA	CHC-C1C-C2C	-3.14	118.02	126.73
14	bA	810	CLA	CAC-C3C-C4C	3.14	128.88	124.81
14	cA	806	CLA	CMB-C2B-C1B	3.14	130.15	125.37
14	B	804	CLA	C1C-C2C-C3C	-3.14	103.66	106.96
14	B	825	CLA	C1C-C2C-C3C	-3.14	103.66	106.96
14	A	822	CLA	C1D-CHD-C4C	-3.14	119.29	126.06
14	bA	832	CLA	CMB-C2B-C1B	3.14	130.14	125.37
14	B	806	CLA	C4-C3-C5	3.14	120.55	115.27
14	bA	822	CLA	C1D-CHD-C4C	-3.13	119.30	126.06
14	cA	817	CLA	C3B-C4B-NB	3.13	113.42	110.52
14	bB	804	CLA	C1C-C2C-C3C	-3.13	103.66	106.96
14	bA	818	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
14	bB	837	CLA	C3B-C4B-NB	3.13	113.42	110.52
14	cB	832	CLA	C1C-C2C-C3C	-3.13	103.66	106.96
14	cA	823	CLA	CHC-C1C-C2C	-3.13	118.03	126.73
14	cB	826	CLA	C1C-C2C-C3C	-3.13	103.67	106.96
14	bB	828	CLA	C2A-C1A-CHA	-3.13	118.39	123.86
14	bA	816	CLA	C1C-C2C-C3C	-3.13	103.67	106.96
14	cA	822	CLA	C1D-CHD-C4C	-3.13	119.31	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	823	CLA	CHC-C1C-C2C	-3.13	118.04	126.73
17	cB	846	BCR	C37-C22-C23	3.13	123.00	118.08
14	cA	828	CLA	C4C-C3C-C2C	-3.13	102.34	106.90
14	cA	818	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
14	bB	836	CLA	C3B-C4B-NB	3.13	113.42	110.52
14	cB	813	CLA	C4C-C3C-C2C	-3.13	102.34	106.90
14	B	828	CLA	C2A-C1A-CHA	-3.12	118.40	123.86
14	A	828	CLA	C4C-C3C-C2C	-3.12	102.34	106.90
14	A	832	CLA	CMB-C2B-C1B	3.12	130.13	125.37
14	bB	838	CLA	C4C-C3C-C2C	-3.12	102.34	106.90
17	I	102	BCR	C36-C18-C17	-3.12	118.55	122.92
14	bA	828	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
17	cF	202	BCR	C15-C16-C17	3.12	129.87	123.47
14	cB	805	CLA	C1C-C2C-C3C	-3.12	103.67	106.96
14	bB	825	CLA	C1C-C2C-C3C	-3.12	103.68	106.96
14	bB	831	CLA	C1C-C2C-C3C	-3.12	103.68	106.96
14	B	812	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
14	A	810	CLA	CAC-C3C-C4C	3.12	128.86	124.81
14	A	816	CLA	C1C-C2C-C3C	-3.12	103.68	106.96
17	B	845	BCR	C37-C22-C23	3.12	122.99	118.08
13	A	801	CL0	C4A-NA-C1A	-3.12	105.30	106.71
14	B	802	CLA	C4A-NA-C1A	-3.12	105.30	106.71
14	bB	828	CLA	C3B-C4B-NB	3.12	113.41	110.52
14	bB	812	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
14	B	836	CLA	C3B-C4B-NB	3.12	113.41	110.52
14	B	831	CLA	C1C-C2C-C3C	-3.12	103.68	106.96
14	cB	829	CLA	C2A-C1A-CHA	-3.12	118.41	123.86
14	cA	810	CLA	CHC-C1C-C2C	-3.11	118.08	126.73
17	bI	102	BCR	C36-C18-C17	-3.11	118.56	122.92
14	A	840	CLA	CMC-C2C-C1C	3.11	129.78	125.04
17	bF	202	BCR	C15-C16-C17	3.11	129.85	123.47
14	bA	810	CLA	CHC-C1C-C2C	-3.11	118.09	126.73
14	cB	815	CLA	C1C-C2C-C3C	-3.11	103.69	106.96
17	F	202	BCR	C15-C16-C17	3.11	129.85	123.47
14	cA	832	CLA	CMB-C2B-C1B	3.11	130.11	125.37
14	A	817	CLA	C3B-C4B-NB	3.11	113.40	110.52
14	bA	835	CLA	CHC-C1C-C2C	-3.11	118.09	126.73
14	cA	840	CLA	CMC-C2C-C1C	3.11	129.78	125.04
17	bI	102	BCR	C34-C9-C10	-3.11	118.57	122.92
14	B	826	CLA	CMC-C2C-C1C	3.11	129.78	125.04
14	cB	829	CLA	C3B-C4B-NB	3.11	113.40	110.52
14	cA	835	CLA	CHC-C1C-C2C	-3.11	118.10	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	cB	842	BCR	C36-C18-C17	-3.11	118.57	122.92
14	bA	840	CLA	CMC-C2C-C1C	3.11	129.77	125.04
14	bB	817	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
14	bB	833	CLA	CAC-C3C-C4C	3.11	128.84	124.81
14	A	835	CLA	CHC-C1C-C2C	-3.11	118.10	126.73
14	cA	820	CLA	C2A-C1A-CHA	-3.11	118.43	123.86
14	cB	803	CLA	C4A-NA-C1A	-3.11	105.31	106.71
14	bB	814	CLA	C1C-C2C-C3C	-3.10	103.69	106.96
17	bB	841	BCR	C36-C18-C17	-3.10	118.57	122.92
14	B	828	CLA	C3B-C4B-NB	3.10	113.39	110.52
14	B	838	CLA	CED-O2D-CGD	3.10	122.96	115.94
14	cB	822	CLA	C1D-CHD-C4C	-3.10	119.36	126.06
14	cL	203	CLA	C3B-C4B-NB	3.10	113.39	110.52
14	A	810	CLA	CHC-C1C-C2C	-3.10	118.11	126.73
14	L	201	CLA	C1-O2A-CGA	3.10	124.59	116.44
17	cI	102	BCR	C34-C9-C10	-3.10	118.58	122.92
14	cB	808	CLA	CMB-C2B-C1B	3.10	130.09	125.37
14	bA	828	CLA	C3B-C4B-NB	3.10	113.39	110.52
14	A	820	CLA	C2A-C1A-CHA	-3.10	118.44	123.86
14	bB	838	CLA	CED-O2D-CGD	3.10	122.95	115.94
14	B	838	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
14	cB	818	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
14	bL	201	CLA	C1-O2A-CGA	3.10	124.58	116.44
14	bA	823	CLA	CMC-C2C-C1C	3.10	129.76	125.04
17	cI	102	BCR	C36-C18-C17	-3.10	118.58	122.92
14	B	817	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
14	cB	839	CLA	CED-O2D-CGD	3.10	122.95	115.94
14	cB	839	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
17	I	102	BCR	C34-C9-C10	-3.10	118.58	122.92
13	bA	801	CL0	C4A-NA-C1A	-3.10	105.31	106.71
14	cB	827	CLA	CMC-C2C-C1C	3.10	129.76	125.04
17	B	841	BCR	C36-C18-C17	-3.10	118.58	122.92
14	cA	828	CLA	CMC-C2C-C1C	3.10	129.75	125.04
14	cL	202	CLA	C1-O2A-CGA	3.09	124.56	116.44
14	B	821	CLA	C1D-CHD-C4C	-3.09	119.38	126.06
13	cA	801	CL0	C4A-NA-C1A	-3.09	105.31	106.71
14	A	835	CLA	CMC-C2C-C1C	3.09	129.75	125.04
14	B	833	CLA	CAC-C3C-C4C	3.09	128.82	124.81
14	L	203	CLA	C3B-C4B-NB	3.09	113.38	110.52
14	bB	811	CLA	CHC-C1C-C2C	-3.09	118.14	126.73
17	M	101	BCR	C37-C22-C23	3.09	122.95	118.08
14	B	811	CLA	CED-O2D-CGD	3.09	122.93	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	L	202	CLA	C3B-C4B-NB	3.09	113.38	110.52
14	bL	202	CLA	C3B-C4B-NB	3.09	113.38	110.52
14	cB	840	CLA	C3B-C4B-NB	3.09	113.38	110.52
14	bB	808	CLA	CMC-C2C-C1C	3.09	129.75	125.04
14	cA	823	CLA	CMC-C2C-C1C	3.09	129.75	125.04
14	bB	821	CLA	C1D-CHD-C4C	-3.09	119.39	126.06
17	B	842	BCR	C36-C18-C17	-3.09	118.60	122.92
14	cA	815	CLA	CMC-C2C-C1C	3.09	129.74	125.04
14	bB	811	CLA	CED-O2D-CGD	3.09	122.92	115.94
14	cB	812	CLA	CHC-C1C-C2C	-3.09	118.15	126.73
14	B	807	CLA	CMB-C2B-C1B	3.09	130.07	125.37
14	B	811	CLA	CHC-C1C-C2C	-3.09	118.15	126.73
14	cB	810	CLA	CHC-C1C-C2C	-3.09	118.15	126.73
14	B	811	CLA	C4C-C3C-C2C	-3.09	102.40	106.90
14	A	833	CLA	CMC-C2C-C1C	3.09	129.74	125.04
14	bB	826	CLA	CMC-C2C-C1C	3.09	129.74	125.04
14	bB	811	CLA	C4C-C3C-C2C	-3.09	102.40	106.90
14	cA	835	CLA	CMC-C2C-C1C	3.09	129.74	125.04
14	bA	835	CLA	CMC-C2C-C1C	3.08	129.74	125.04
14	bA	820	CLA	C2A-C1A-CHA	-3.08	118.47	123.86
14	A	815	CLA	CMC-C2C-C1C	3.08	129.73	125.04
14	bA	815	CLA	CMC-C2C-C1C	3.08	129.73	125.04
14	bA	828	CLA	CMC-C2C-C1C	3.08	129.73	125.04
14	A	828	CLA	CMC-C2C-C1C	3.08	129.73	125.04
14	bA	852	CLA	CHB-C4A-NA	3.08	128.77	124.51
17	bM	101	BCR	C37-C22-C23	3.08	122.93	118.08
14	bB	804	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
14	cB	805	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
14	L	201	CLA	CMC-C2C-C1C	3.08	129.73	125.04
14	bA	833	CLA	CMC-C2C-C1C	3.08	129.73	125.04
17	cM	101	BCR	C37-C22-C23	3.08	122.93	118.08
14	B	808	CLA	CMC-C2C-C1C	3.08	129.73	125.04
14	bB	802	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
14	bB	809	CLA	CHC-C1C-C2C	-3.08	118.18	126.73
14	cB	812	CLA	CED-O2D-CGD	3.08	122.90	115.94
14	cB	812	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
14	cB	840	CLA	C1D-CHD-C4C	-3.08	119.42	126.06
14	B	804	CLA	C4C-C3C-C2C	-3.08	102.42	106.90
14	cL	204	CLA	C3B-C4B-NB	3.08	113.37	110.52
14	B	839	CLA	C1D-CHD-C4C	-3.08	119.42	126.06
14	bB	807	CLA	CMB-C2B-C1B	3.07	130.05	125.37
14	bB	839	CLA	C1D-CHD-C4C	-3.07	119.43	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bB	819	CLA	O2A-CGA-CBA	3.07	121.56	111.91
14	B	809	CLA	CHC-C1C-C2C	-3.07	118.19	126.73
14	cL	202	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
14	cA	828	CLA	C3B-C4B-NB	3.07	113.37	110.52
14	A	823	CLA	CMC-C2C-C1C	3.07	129.72	125.04
14	cJ	102	CLA	CED-O2D-CGD	3.07	122.89	115.94
14	A	812	CLA	CHC-C1C-C2C	-3.07	118.20	126.73
14	cB	834	CLA	CAC-C3C-C4C	3.07	128.79	124.81
14	B	839	CLA	C3B-C4B-NB	3.07	113.36	110.52
14	B	813	CLA	CHC-C1C-C2C	-3.07	118.20	126.73
14	bA	812	CLA	CHC-C1C-C2C	-3.07	118.20	126.73
14	cA	812	CLA	CHC-C1C-C2C	-3.07	118.20	126.73
14	A	828	CLA	C3B-C4B-NB	3.07	113.36	110.52
17	bB	843	BCR	C12-C13-C14	3.07	123.65	118.94
14	cB	809	CLA	CMC-C2C-C1C	3.07	129.71	125.04
14	bB	813	CLA	CHC-C1C-C2C	-3.07	118.21	126.73
17	bB	842	BCR	C36-C18-C17	-3.07	118.62	122.92
14	B	819	CLA	O2A-CGA-CBA	3.07	121.53	111.91
14	cL	202	CLA	CMC-C2C-C1C	3.07	129.71	125.04
14	cB	820	CLA	O2A-CGA-CBA	3.07	121.53	111.91
14	cB	814	CLA	CHC-C1C-C2C	-3.07	118.21	126.73
14	B	817	CLA	CHC-C1C-C2C	-3.07	118.21	126.73
14	cA	833	CLA	CMC-C2C-C1C	3.07	129.71	125.04
14	J	102	CLA	CED-O2D-CGD	3.07	122.87	115.94
14	bB	825	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
14	bL	203	CLA	C3B-C4B-NB	3.06	113.36	110.52
14	cB	826	CLA	C4C-C3C-C2C	-3.06	102.43	106.90
14	cB	803	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
14	bL	201	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
14	bB	839	CLA	C3B-C4B-NB	3.06	113.35	110.52
14	bL	201	CLA	CMC-C2C-C1C	3.06	129.70	125.04
14	B	826	CLA	O2A-CGA-CBA	3.06	121.51	111.91
14	cL	205	CLA	C3B-C4B-NB	3.06	113.35	110.52
14	B	832	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
14	bB	817	CLA	CHC-C1C-C2C	-3.06	118.24	126.73
14	B	802	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
14	bJ	102	CLA	CED-O2D-CGD	3.06	122.85	115.94
14	bA	841	CLA	CHC-C1C-C2C	-3.06	118.24	126.73
14	cB	818	CLA	CHC-C1C-C2C	-3.06	118.24	126.73
14	B	825	CLA	C4C-C3C-C2C	-3.05	102.44	106.90
14	A	841	CLA	CHC-C1C-C2C	-3.05	118.25	126.73
14	bB	818	CLA	CHC-C1C-C2C	-3.05	118.25	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cB	819	CLA	CHC-C1C-C2C	-3.05	118.25	126.73
17	cB	843	BCR	C36-C18-C17	-3.05	118.64	122.92
17	cB	844	BCR	C12-C13-C14	3.05	123.63	118.94
14	cB	827	CLA	O2A-CGA-CBA	3.05	121.49	111.91
14	bB	826	CLA	O2A-CGA-CBA	3.05	121.49	111.91
17	B	843	BCR	C12-C13-C14	3.05	123.63	118.94
14	L	203	CLA	CMC-C2C-C1C	3.05	129.69	125.04
14	bL	204	CLA	C3B-C4B-NB	3.05	113.34	110.52
14	cA	841	CLA	CHC-C1C-C2C	-3.05	118.26	126.73
14	L	201	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
14	A	852	CLA	CHB-C4A-NA	3.05	128.73	124.51
14	cB	839	CLA	CHC-C1C-C2C	-3.05	118.26	126.73
14	L	204	CLA	C3B-C4B-NB	3.05	113.34	110.52
14	B	838	CLA	CHC-C1C-C2C	-3.05	118.26	126.73
14	cL	204	CLA	CMC-C2C-C1C	3.05	129.68	125.04
17	cL	207	BCR	C16-C15-C14	3.04	129.71	123.47
14	cA	852	CLA	CHB-C4A-NA	3.04	128.72	124.51
14	B	818	CLA	CHC-C1C-C2C	-3.04	118.28	126.73
17	L	206	BCR	C16-C15-C14	3.04	129.71	123.47
14	bL	203	CLA	CMC-C2C-C1C	3.04	129.67	125.04
14	A	837	CLA	CED-O2D-CGD	3.04	122.82	115.94
14	cA	820	CLA	CAC-C3C-C4C	3.04	128.76	124.81
14	cA	840	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
14	cB	833	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
14	bB	832	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
14	bB	838	CLA	CHC-C1C-C2C	-3.04	118.29	126.73
14	cA	837	CLA	CED-O2D-CGD	3.04	122.81	115.94
14	bB	826	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
14	B	826	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
14	cA	822	CLA	CHC-C1C-C2C	-3.03	118.30	126.73
14	bA	840	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
17	bL	205	BCR	C37-C22-C23	3.03	122.85	118.08
17	cL	206	BCR	C37-C22-C23	3.03	122.85	118.08
14	bA	837	CLA	CED-O2D-CGD	3.03	122.79	115.94
14	bA	822	CLA	CHC-C1C-C2C	-3.03	118.32	126.73
14	cB	827	CLA	C4C-C3C-C2C	-3.03	102.49	106.90
14	cB	807	CLA	CMB-C2B-C1B	3.02	129.98	125.37
14	bB	806	CLA	CMB-C2B-C1B	3.02	129.97	125.37
14	A	822	CLA	CHC-C1C-C2C	-3.02	118.33	126.73
14	A	840	CLA	C4C-C3C-C2C	-3.02	102.49	106.90
14	cA	806	CLA	CAC-C3C-C4C	3.02	128.73	124.81
14	B	849	CLA	CHC-C1C-C2C	-3.02	118.34	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	L	205	BCR	C37-C22-C23	3.02	122.84	118.08
14	A	820	CLA	CAC-C3C-C4C	3.02	128.73	124.81
17	cA	845	BCR	C34-C9-C10	-3.02	118.69	122.92
14	bA	824	CLA	CHC-C1C-C2C	-3.02	118.34	126.73
14	B	832	CLA	CMC-C2C-C1C	3.02	129.64	125.04
17	bL	206	BCR	C16-C15-C14	3.02	129.66	123.47
14	bA	820	CLA	CAC-C3C-C4C	3.02	128.72	124.81
14	bB	849	CLA	CHC-C1C-C2C	-3.02	118.35	126.73
14	bL	204	CLA	C1D-CHD-C4C	-3.02	119.55	126.06
14	bB	839	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
14	B	839	CLA	C4C-C3C-C2C	-3.01	102.50	106.90
14	bA	826	CLA	C3B-C4B-NB	3.01	113.31	110.52
14	cA	824	CLA	CHC-C1C-C2C	-3.01	118.36	126.73
14	cA	826	CLA	C3B-C4B-NB	3.01	113.31	110.52
14	bA	833	CLA	C1D-CHD-C4C	-3.01	119.56	126.06
14	A	834	CLA	CMC-C2C-C1C	3.01	129.63	125.04
14	bA	833	CLA	CHC-C1C-C2C	-3.01	118.36	126.73
14	B	806	CLA	CMB-C2B-C1B	3.01	129.96	125.37
14	cA	807	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
14	A	833	CLA	CHC-C1C-C2C	-3.01	118.36	126.73
14	bA	806	CLA	CAC-C3C-C4C	3.01	128.72	124.81
14	cB	801	CLA	CAC-C3C-C4C	3.01	128.72	124.81
14	cB	833	CLA	CMC-C2C-C1C	3.01	129.62	125.04
14	cA	833	CLA	CHC-C1C-C2C	-3.01	118.37	126.73
14	cB	840	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
14	cB	850	CLA	CHC-C1C-C2C	-3.01	118.37	126.73
14	A	820	CLA	CHC-C1C-C2C	-3.01	118.37	126.73
14	bA	807	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
14	B	809	CLA	O2A-CGA-CBA	3.01	121.35	111.91
14	cL	202	CLA	CMB-C2B-C1B	3.01	129.95	125.37
14	bA	820	CLA	CHC-C1C-C2C	-3.01	118.38	126.73
14	B	837	CLA	CHC-C1C-C2C	-3.01	118.38	126.73
14	A	824	CLA	CHC-C1C-C2C	-3.01	118.38	126.73
14	A	842	CLA	CHC-C1C-C2C	-3.01	118.38	126.73
14	bB	820	CLA	C4C-C3C-C2C	-3.01	102.52	106.90
14	B	801	CLA	CAC-C3C-C4C	3.01	128.71	124.81
14	L	204	CLA	C1D-CHD-C4C	-3.01	119.57	126.06
14	A	807	CLA	C4C-C3C-C2C	-3.01	102.52	106.90
14	bA	833	CLA	O1D-CGD-CBD	-3.01	118.33	124.48
14	cL	205	CLA	C1D-CHD-C4C	-3.01	119.58	126.06
13	cA	801	CL0	CHC-C1C-C2C	-3.01	118.38	126.73
14	bB	837	CLA	CHC-C1C-C2C	-3.00	118.39	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	833	CLA	C1D-CHD-C4C	-3.00	119.58	126.06
14	bB	832	CLA	CAC-C3C-C4C	3.00	128.71	124.81
14	cA	820	CLA	CHC-C1C-C2C	-3.00	118.39	126.73
14	bL	201	CLA	CMB-C2B-C1B	3.00	129.94	125.37
14	cB	803	CLA	CHB-C4A-NA	3.00	128.66	124.51
17	cL	206	BCR	C15-C16-C17	3.00	129.62	123.47
14	cB	810	CLA	O2A-CGA-CBA	3.00	121.33	111.91
14	cB	829	CLA	CAA-C2A-C1A	-3.00	102.14	111.97
17	bL	205	BCR	C15-C16-C17	3.00	129.62	123.47
14	cB	838	CLA	CHC-C1C-C2C	-3.00	118.39	126.73
14	A	833	CLA	C1D-CHD-C4C	-3.00	119.59	126.06
13	A	801	CL0	CHC-C1C-C2C	-3.00	118.40	126.73
14	B	802	CLA	CHB-C4A-NA	3.00	128.66	124.51
14	cA	842	CLA	CHC-C1C-C2C	-3.00	118.40	126.73
14	bB	832	CLA	CMC-C2C-C1C	3.00	129.61	125.04
14	cB	802	CLA	CAC-C3C-C4C	3.00	128.70	124.81
13	bA	801	CL0	CHC-C1C-C2C	-3.00	118.40	126.73
14	cA	833	CLA	O1D-CGD-CBD	-3.00	118.35	124.48
17	L	205	BCR	C15-C16-C17	3.00	129.62	123.47
14	bA	842	CLA	CHC-C1C-C2C	-3.00	118.40	126.73
14	cB	821	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
14	A	815	CLA	CHC-C1C-C2C	-3.00	118.40	126.73
14	cA	815	CLA	CHC-C1C-C2C	-3.00	118.40	126.73
14	A	806	CLA	CAC-C3C-C4C	3.00	128.70	124.81
14	bB	828	CLA	CAA-C2A-C1A	-3.00	102.15	111.97
14	cB	830	CLA	CHC-C1C-C2C	-3.00	118.41	126.73
14	B	829	CLA	CHC-C1C-C2C	-3.00	118.41	126.73
14	B	828	CLA	CAA-C2A-C1A	-3.00	102.16	111.97
14	bB	809	CLA	O2A-CGA-CBA	3.00	121.31	111.91
14	L	201	CLA	CMB-C2B-C1B	2.99	129.93	125.37
14	B	832	CLA	CAC-C3C-C4C	2.99	128.69	124.81
14	B	851	CLA	CAC-C3C-C4C	2.99	128.69	124.81
17	bA	845	BCR	C34-C9-C10	-2.99	118.73	122.92
14	A	833	CLA	O1D-CGD-CBD	-2.99	118.36	124.48
14	bA	807	CLA	CMC-C2C-C1C	2.99	129.60	125.04
14	bB	801	CLA	CAC-C3C-C4C	2.99	128.69	124.81
14	bB	851	CLA	CAC-C3C-C4C	2.99	128.69	124.81
17	A	845	BCR	C34-C9-C10	-2.99	118.73	122.92
14	cA	834	CLA	CMC-C2C-C1C	2.99	129.59	125.04
14	A	816	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
14	bA	821	CLA	CHC-C1C-C2C	-2.99	118.42	126.73
14	bA	834	CLA	CMC-C2C-C1C	2.99	129.59	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bB	829	CLA	CHC-C1C-C2C	-2.99	118.42	126.73
14	B	823	CLA	CAC-C3C-C4C	2.99	128.69	124.81
14	cA	816	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
14	A	821	CLA	CHC-C1C-C2C	-2.99	118.43	126.73
14	bB	802	CLA	O2A-CGA-CBA	2.99	121.28	111.91
14	bB	802	CLA	CHB-C4A-NA	2.99	128.64	124.51
14	A	826	CLA	C3B-C4B-NB	2.99	113.28	110.52
14	cB	803	CLA	O2A-CGA-CBA	2.98	121.28	111.91
14	cA	821	CLA	CHC-C1C-C2C	-2.98	118.44	126.73
14	B	802	CLA	O2A-CGA-CBA	2.98	121.27	111.91
14	B	829	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
14	cA	807	CLA	CMC-C2C-C1C	2.98	129.58	125.04
14	bA	815	CLA	CHC-C1C-C2C	-2.98	118.44	126.73
17	bF	202	BCR	C12-C13-C14	2.98	123.52	118.94
17	cB	844	BCR	C15-C16-C17	2.98	129.58	123.47
17	J	103	BCR	C23-C22-C21	2.98	123.52	118.94
14	bB	817	CLA	CAC-C3C-C4C	2.98	128.68	124.81
14	bB	829	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
17	cA	846	BCR	C19-C18-C17	2.98	123.51	118.94
14	B	837	CLA	CMC-C2C-C1C	2.98	129.57	125.04
14	cB	833	CLA	CAC-C3C-C4C	2.98	128.67	124.81
14	bB	820	CLA	CMC-C2C-C1C	2.98	129.57	125.04
14	bA	816	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
17	bB	843	BCR	C15-C16-C17	2.98	129.57	123.47
14	cB	824	CLA	CAC-C3C-C4C	2.98	128.67	124.81
14	bA	831	CLA	CHC-C1C-C2C	-2.98	118.46	126.73
17	bA	846	BCR	C19-C18-C17	2.98	123.51	118.94
14	bA	852	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
14	B	820	CLA	C4C-C3C-C2C	-2.97	102.56	106.90
14	cB	811	CLA	CHC-C1C-C2C	-2.97	118.47	126.73
14	bB	837	CLA	CMC-C2C-C1C	2.97	129.57	125.04
17	bM	101	BCR	C36-C18-C17	-2.97	118.76	122.92
14	A	831	CLA	CHC-C1C-C2C	-2.97	118.47	126.73
14	cB	835	CLA	C3B-C4B-NB	2.97	113.27	110.52
17	cF	202	BCR	C12-C13-C14	2.97	123.50	118.94
17	B	843	BCR	C15-C16-C17	2.97	129.56	123.47
14	cB	838	CLA	CMC-C2C-C1C	2.97	129.56	125.04
14	A	805	CLA	C3C-C4C-NC	2.97	113.90	110.57
17	F	202	BCR	C12-C13-C14	2.97	123.50	118.94
14	B	817	CLA	CAC-C3C-C4C	2.97	128.66	124.81
14	A	807	CLA	CMC-C2C-C1C	2.97	129.56	125.04
17	A	846	BCR	C19-C18-C17	2.97	123.50	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bB	831	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
14	cB	815	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
14	bB	823	CLA	CAC-C3C-C4C	2.97	128.66	124.81
14	B	810	CLA	CHC-C1C-C2C	-2.97	118.49	126.73
14	bB	810	CLA	CHC-C1C-C2C	-2.97	118.49	126.73
14	bA	805	CLA	C3C-C4C-NC	2.97	113.90	110.57
14	cB	824	CLA	CHC-C1C-C2C	-2.97	118.49	126.73
14	B	822	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
14	bB	814	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
14	cA	805	CLA	C3C-C4C-NC	2.96	113.90	110.57
14	B	806	CLA	CHC-C1C-C2C	-2.96	118.50	126.73
14	bB	834	CLA	C3B-C4B-NB	2.96	113.27	110.52
14	bB	806	CLA	CHC-C1C-C2C	-2.96	118.50	126.73
14	cB	818	CLA	CAC-C3C-C4C	2.96	128.66	124.81
14	A	825	CLA	C3B-C4B-NB	2.96	113.26	110.52
14	B	823	CLA	CHC-C1C-C2C	-2.96	118.50	126.73
14	cA	831	CLA	CHC-C1C-C2C	-2.96	118.50	126.73
14	bB	823	CLA	CHC-C1C-C2C	-2.96	118.50	126.73
17	bJ	103	BCR	C23-C22-C21	2.96	123.48	118.94
17	M	101	BCR	C36-C18-C17	-2.96	118.78	122.92
14	cB	821	CLA	CMC-C2C-C1C	2.96	129.55	125.04
14	bA	841	CLA	C4A-NA-C1A	-2.96	105.38	106.71
14	cB	823	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
14	cA	837	CLA	CMB-C2B-C1B	2.96	129.88	125.37
14	bB	830	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
17	cJ	103	BCR	C23-C22-C21	2.96	123.48	118.94
17	cM	101	BCR	C36-C18-C17	-2.96	118.78	122.92
14	bB	822	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
14	cB	830	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
14	cB	807	CLA	CHC-C1C-C2C	-2.96	118.52	126.73
14	cB	825	CLA	CMC-C2C-C1C	2.95	129.54	125.04
14	cA	825	CLA	C3B-C4B-NB	2.95	113.25	110.52
14	cA	830	CLA	C3B-C4B-NB	2.95	113.25	110.52
17	bA	846	BCR	C37-C22-C23	2.95	122.73	118.08
14	cB	831	CLA	C4C-C3C-C2C	-2.95	102.59	106.90
14	bB	802	CLA	CHC-C1C-C2C	-2.95	118.53	126.73
14	bA	837	CLA	CMB-C2B-C1B	2.95	129.87	125.37
14	A	852	CLA	C4C-C3C-C2C	-2.95	102.59	106.90
14	B	814	CLA	CHC-C1C-C2C	-2.95	118.53	126.73
17	cA	846	BCR	C37-C22-C23	2.95	122.73	118.08
14	bA	815	CLA	CAC-C3C-C4C	2.95	128.64	124.81
14	bB	814	CLA	CHC-C1C-C2C	-2.95	118.54	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bA	819	CLA	CMB-C2B-C1B	2.95	129.86	125.37
14	A	817	CLA	CHC-C1C-C2C	-2.95	118.54	126.73
14	cA	852	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
14	cB	832	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
14	A	817	CLA	CMC-C2C-C1C	2.95	129.53	125.04
14	B	824	CLA	CMC-C2C-C1C	2.95	129.53	125.04
14	bA	817	CLA	CHC-C1C-C2C	-2.95	118.54	126.73
14	B	831	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
14	cA	819	CLA	CMB-C2B-C1B	2.95	129.86	125.37
14	bB	828	CLA	C4A-NA-C1A	-2.95	105.38	106.71
14	B	802	CLA	CHC-C1C-C2C	-2.95	118.54	126.73
14	B	814	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
14	A	828	CLA	CHC-C1C-C2C	-2.95	118.55	126.73
14	A	819	CLA	CMB-C2B-C1B	2.95	129.86	125.37
14	cA	828	CLA	CHC-C1C-C2C	-2.95	118.55	126.73
14	B	830	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
14	L	203	CLA	C4A-NA-C1A	-2.94	105.38	106.71
14	B	834	CLA	C3B-C4B-NB	2.94	113.25	110.52
14	cB	806	CLA	CHC-C1C-C2C	-2.94	118.56	126.73
17	A	846	BCR	C37-C22-C23	2.94	122.71	118.08
14	cB	815	CLA	CHC-C1C-C2C	-2.94	118.56	126.73
17	bI	101	BCR	C34-C9-C8	2.94	122.71	118.08
14	bA	828	CLA	CHC-C1C-C2C	-2.94	118.56	126.73
14	bA	825	CLA	C3B-C4B-NB	2.94	113.24	110.52
14	cA	815	CLA	CAC-C3C-C4C	2.94	128.62	124.81
14	L	201	CLA	C5-C3-C2	2.94	127.07	121.12
14	A	815	CLA	CAC-C3C-C4C	2.94	128.62	124.81
14	cA	817	CLA	CHC-C1C-C2C	-2.94	118.57	126.73
17	bB	850	BCR	C36-C18-C17	-2.94	118.81	122.92
14	B	828	CLA	C4A-NA-C1A	-2.94	105.39	106.71
14	bB	824	CLA	CMC-C2C-C1C	2.94	129.51	125.04
17	I	101	BCR	C34-C9-C8	2.94	122.70	118.08
14	bL	203	CLA	C4A-NA-C1A	-2.94	105.39	106.71
14	cA	838	CLA	C4C-C3C-C2C	-2.94	102.62	106.90
14	B	805	CLA	CHC-C1C-C2C	-2.94	118.58	126.73
14	B	820	CLA	CMC-C2C-C1C	2.94	129.51	125.04
14	bB	820	CLA	CHC-C1C-C2C	-2.94	118.58	126.73
14	cB	803	CLA	CHC-C1C-C2C	-2.93	118.58	126.73
14	bL	201	CLA	C5-C3-C2	2.93	127.05	121.12
14	cL	202	CLA	C5-C3-C2	2.93	127.05	121.12
14	bA	829	CLA	CHC-C1C-C2C	-2.93	118.58	126.73
14	bB	805	CLA	CHC-C1C-C2C	-2.93	118.58	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	cA	848	BCR	C16-C15-C14	2.93	129.48	123.47
14	bB	809	CLA	C4C-C3C-C2C	-2.93	102.62	106.90
14	bA	817	CLA	CMC-C2C-C1C	2.93	129.51	125.04
14	bB	819	CLA	C4C-C3C-C2C	-2.93	102.62	106.90
14	A	837	CLA	CMB-C2B-C1B	2.93	129.84	125.37
14	cA	817	CLA	CMC-C2C-C1C	2.93	129.50	125.04
17	cB	851	BCR	C36-C18-C17	-2.93	118.82	122.92
14	B	819	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
14	B	823	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
14	cB	821	CLA	CHC-C1C-C2C	-2.93	118.59	126.73
14	bB	807	CLA	CHC-C1C-C2C	-2.93	118.60	126.73
14	A	830	CLA	C3B-C4B-NB	2.93	113.23	110.52
14	A	839	CLA	CHC-C1C-C2C	-2.93	118.60	126.73
14	bA	806	CLA	CHC-C1C-C2C	-2.93	118.60	126.73
14	cA	829	CLA	CHC-C1C-C2C	-2.93	118.60	126.73
17	bB	843	BCR	C36-C18-C17	-2.93	118.82	122.92
14	B	831	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
14	cB	824	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
14	cA	841	CLA	C1D-CHD-C4C	-2.93	119.75	126.06
14	B	807	CLA	CHC-C1C-C2C	-2.93	118.60	126.73
14	cB	820	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
14	bA	827	CLA	C3B-C4B-NB	2.93	113.23	110.52
14	A	841	CLA	C4A-NA-C1A	-2.92	105.39	106.71
14	bB	831	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
14	A	827	CLA	C3B-C4B-NB	2.92	113.23	110.52
14	bA	830	CLA	C3B-C4B-NB	2.92	113.23	110.52
14	bA	817	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
14	A	829	CLA	CHC-C1C-C2C	-2.92	118.61	126.73
14	B	820	CLA	CHC-C1C-C2C	-2.92	118.61	126.73
17	bA	848	BCR	C16-C15-C14	2.92	129.46	123.47
14	B	803	CLA	CHC-C1C-C2C	-2.92	118.61	126.73
14	cB	804	CLA	CHC-C1C-C2C	-2.92	118.61	126.73
14	A	838	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
14	A	804	CLA	C3B-C4B-NB	2.92	113.23	110.52
17	A	846	BCR	C8-C9-C10	2.92	123.42	118.94
17	B	850	BCR	C36-C18-C17	-2.92	118.83	122.92
14	A	841	CLA	C3B-C4B-NB	2.92	113.22	110.52
14	A	806	CLA	CHC-C1C-C2C	-2.92	118.62	126.73
14	cB	808	CLA	CHC-C1C-C2C	-2.92	118.62	126.73
14	A	841	CLA	C1D-CHD-C4C	-2.92	119.76	126.06
14	cB	834	CLA	CHC-C1C-C2C	-2.92	118.62	126.73
14	bA	838	CLA	C4C-C3C-C2C	-2.92	102.64	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	804	CLA	CMC-C2C-C1C	2.92	129.49	125.04
14	cB	820	CLA	CMB-C2B-C1B	2.92	129.82	125.37
14	bB	803	CLA	CHC-C1C-C2C	-2.92	118.62	126.73
14	B	809	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
14	bB	823	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
14	bA	839	CLA	CHC-C1C-C2C	-2.92	118.62	126.73
14	cA	806	CLA	CHC-C1C-C2C	-2.92	118.62	126.73
14	bA	841	CLA	C3B-C4B-NB	2.92	113.22	110.52
17	cI	101	BCR	C34-C9-C8	2.92	122.67	118.08
14	bB	828	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
14	cB	835	CLA	CMB-C2B-C1B	2.92	129.81	125.37
17	A	848	BCR	C16-C15-C14	2.92	129.45	123.47
14	cA	827	CLA	C3B-C4B-NB	2.92	113.22	110.52
14	B	830	CLA	CHC-C1C-C2C	-2.92	118.63	126.73
14	cA	817	CLA	C4C-C3C-C2C	-2.92	102.65	106.90
14	cB	810	CLA	C4C-C3C-C2C	-2.92	102.65	106.90
14	cA	837	CLA	C2A-C1A-CHA	-2.91	118.76	123.86
14	bB	818	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
14	cB	818	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
14	cB	832	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
14	B	819	CLA	CMB-C2B-C1B	2.91	129.81	125.37
14	cB	831	CLA	CHC-C1C-C2C	-2.91	118.64	126.73
14	B	818	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
14	bA	830	CLA	CHC-C1C-C2C	-2.91	118.64	126.73
14	cL	204	CLA	C4A-NA-C1A	-2.91	105.40	106.71
14	cA	839	CLA	CHC-C1C-C2C	-2.91	118.64	126.73
14	bB	819	CLA	CMB-C2B-C1B	2.91	129.80	125.37
14	bB	830	CLA	CHC-C1C-C2C	-2.91	118.65	126.73
17	B	843	BCR	C36-C18-C17	-2.91	118.85	122.92
14	cA	841	CLA	C4A-NA-C1A	-2.91	105.40	106.71
14	bB	834	CLA	CMB-C2B-C1B	2.91	129.80	125.37
14	B	833	CLA	CHC-C1C-C2C	-2.91	118.65	126.73
14	bB	817	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
17	cB	844	BCR	C36-C18-C17	-2.91	118.85	122.92
17	cA	846	BCR	C8-C9-C10	2.91	123.40	118.94
14	cB	804	CLA	CAC-C3C-C4C	2.91	128.58	124.81
14	cA	830	CLA	CHC-C1C-C2C	-2.91	118.66	126.73
14	A	817	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
14	bB	804	CLA	CMC-C2C-C1C	2.91	129.47	125.04
14	bA	841	CLA	C1D-CHD-C4C	-2.91	119.79	126.06
17	bA	846	BCR	C8-C9-C10	2.90	123.40	118.94
14	A	830	CLA	CHC-C1C-C2C	-2.90	118.66	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	817	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
14	bA	809	CLA	CHC-C1C-C2C	-2.90	118.67	126.73
14	bL	204	CLA	CHC-C1C-C2C	-2.90	118.67	126.73
14	cB	819	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
14	A	832	CLA	CHC-C1C-C2C	-2.90	118.67	126.73
14	cL	205	CLA	CHC-C1C-C2C	-2.90	118.67	126.73
17	B	842	BCR	C1-C6-C5	-2.90	118.53	122.61
14	A	806	CLA	CHD-C4C-NC	2.90	128.78	124.20
14	B	828	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
14	cA	832	CLA	CHC-C1C-C2C	-2.90	118.67	126.73
14	bA	837	CLA	C2A-C1A-CHA	-2.90	118.79	123.86
14	L	204	CLA	CHC-C1C-C2C	-2.90	118.68	126.73
14	bA	832	CLA	CHC-C1C-C2C	-2.90	118.68	126.73
14	bB	833	CLA	CHC-C1C-C2C	-2.90	118.68	126.73
14	bA	805	CLA	CHC-C1C-C2C	-2.90	118.68	126.73
14	B	831	CLA	CMB-C2B-C1B	2.90	129.78	125.37
14	bB	816	CLA	CHC-C1C-C2C	-2.90	118.68	126.73
14	cA	804	CLA	C3B-C4B-NB	2.90	113.20	110.52
14	bB	831	CLA	CMB-C2B-C1B	2.90	129.78	125.37
14	A	837	CLA	C2A-C1A-CHA	-2.90	118.79	123.86
14	bB	815	CLA	C4C-C3C-C2C	-2.90	102.68	106.90
14	cA	806	CLA	CHD-C4C-NC	2.89	128.76	124.20
14	cB	832	CLA	CMB-C2B-C1B	2.89	129.78	125.37
14	B	804	CLA	C3B-C4B-NB	2.89	113.20	110.52
14	bA	804	CLA	C3B-C4B-NB	2.89	113.20	110.52
14	B	834	CLA	CMB-C2B-C1B	2.89	129.78	125.37
14	cB	805	CLA	CMC-C2C-C1C	2.89	129.44	125.04
14	bB	836	CLA	CHC-C1C-C2C	-2.89	118.69	126.73
14	bB	831	CLA	C2A-C1A-CHA	-2.89	118.80	123.86
17	A	847	BCR	C36-C18-C17	-2.89	118.87	122.92
14	cB	816	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
14	cA	813	CLA	CHC-C1C-C2C	-2.89	118.70	126.73
14	cA	809	CLA	CHC-C1C-C2C	-2.89	118.70	126.73
14	cB	837	CLA	CHC-C1C-C2C	-2.89	118.70	126.73
14	bA	806	CLA	CHD-C4C-NC	2.89	128.76	124.20
17	cF	202	BCR	C36-C18-C17	-2.89	118.88	122.92
14	cB	829	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
14	bA	813	CLA	CHC-C1C-C2C	-2.89	118.71	126.73
14	A	809	CLA	CHC-C1C-C2C	-2.89	118.71	126.73
14	B	851	CLA	CHC-C1C-C2C	-2.89	118.71	126.73
14	bB	807	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
14	A	813	CLA	CHC-C1C-C2C	-2.89	118.71	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	816	CLA	CHC-C1C-C2C	-2.89	118.71	126.73
14	cB	817	CLA	CHC-C1C-C2C	-2.89	118.71	126.73
14	cA	805	CLA	CHC-C1C-C2C	-2.89	118.71	126.73
14	B	836	CLA	CHC-C1C-C2C	-2.89	118.71	126.73
14	bB	851	CLA	CHC-C1C-C2C	-2.89	118.71	126.73
14	cB	832	CLA	C2A-C1A-CHA	-2.89	118.81	123.86
14	cB	804	CLA	C3B-C4B-NB	2.89	113.19	110.52
14	B	837	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
14	A	805	CLA	CHC-C1C-C2C	-2.89	118.72	126.73
14	cB	829	CLA	C4A-NA-C1A	-2.88	105.41	106.71
17	bA	847	BCR	C36-C18-C17	-2.88	118.88	122.92
17	bF	202	BCR	C36-C18-C17	-2.88	118.88	122.92
14	B	829	CLA	CMC-C2C-C1C	2.88	129.43	125.04
14	cA	819	CLA	C4C-C3C-C2C	-2.88	102.69	106.90
14	cB	805	CLA	C3B-C4B-NB	2.88	113.19	110.52
14	bA	811	CLA	CHC-C1C-C2C	-2.88	118.72	126.73
14	A	838	CLA	CHC-C1C-C2C	-2.88	118.72	126.73
14	bB	801	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
14	cB	808	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
14	cB	801	CLA	CHC-C1C-C2C	-2.88	118.73	126.73
17	bB	842	BCR	C1-C6-C5	-2.88	118.56	122.61
14	A	811	CLA	CHC-C1C-C2C	-2.88	118.73	126.73
14	B	815	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
14	bL	204	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
14	B	807	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
17	F	202	BCR	C36-C18-C17	-2.88	118.89	122.92
14	cA	811	CLA	CHC-C1C-C2C	-2.88	118.73	126.73
14	B	831	CLA	C2A-C1A-CHA	-2.88	118.82	123.86
14	B	801	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
14	bB	837	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
14	cB	801	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
14	L	201	CLA	CHC-C1C-C2C	-2.88	118.73	126.73
14	cB	804	CLA	CMC-C2C-C1C	2.88	129.42	125.04
17	A	845	BCR	C15-C16-C17	2.88	129.37	123.47
14	cL	202	CLA	CHC-C1C-C2C	-2.88	118.73	126.73
14	B	803	CLA	CAC-C3C-C4C	2.88	128.54	124.81
14	L	204	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
14	bA	819	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
14	cB	833	CLA	CHC-C1C-C2C	-2.88	118.73	126.73
17	bA	845	BCR	C15-C16-C17	2.88	129.37	123.47
14	cL	205	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
14	B	832	CLA	CHC-C1C-C2C	-2.88	118.74	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bB	819	CLA	CHC-C1C-C2C	-2.88	118.74	126.73
14	bB	803	CLA	CAC-C3C-C4C	2.88	128.54	124.81
14	bL	201	CLA	CHC-C1C-C2C	-2.88	118.74	126.73
14	B	815	CLA	CHC-C1C-C2C	-2.88	118.74	126.73
14	cB	825	CLA	C3B-C4B-NB	2.88	113.18	110.52
14	bA	838	CLA	CHC-C1C-C2C	-2.88	118.74	126.73
14	B	803	CLA	C3B-C4B-NB	2.87	113.18	110.52
14	cA	841	CLA	C3B-C4B-NB	2.87	113.18	110.52
14	B	819	CLA	CHC-C1C-C2C	-2.87	118.75	126.73
14	bB	815	CLA	CHC-C1C-C2C	-2.87	118.75	126.73
14	cA	823	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
14	cB	802	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
14	bB	829	CLA	CMC-C2C-C1C	2.87	129.42	125.04
14	cB	830	CLA	CMC-C2C-C1C	2.87	129.42	125.04
14	bB	830	CLA	CAC-C3C-C4C	2.87	128.54	124.81
14	bB	832	CLA	CHC-C1C-C2C	-2.87	118.75	126.73
14	cB	820	CLA	CHC-C1C-C2C	-2.87	118.75	126.73
14	cB	816	CLA	CHC-C1C-C2C	-2.87	118.75	126.73
14	B	803	CLA	CMC-C2C-C1C	2.87	129.41	125.04
14	cA	838	CLA	CHC-C1C-C2C	-2.87	118.75	126.73
14	bB	804	CLA	C3B-C4B-NB	2.87	113.18	110.52
14	bB	851	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
17	cA	845	BCR	C15-C16-C17	2.87	129.36	123.47
17	cB	843	BCR	C1-C6-C5	-2.87	118.57	122.61
14	cB	838	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
14	cJ	102	CLA	CHC-C1C-C2C	-2.87	118.76	126.73
14	bB	803	CLA	CMC-C2C-C1C	2.87	129.41	125.04
14	bA	825	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
14	cA	804	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
17	cA	847	BCR	C36-C18-C17	-2.87	118.90	122.92
14	A	825	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
14	bB	824	CLA	CAC-C3C-C4C	2.86	128.53	124.81
14	cB	825	CLA	CAC-C3C-C4C	2.86	128.53	124.81
14	bB	824	CLA	C4C-C3C-C2C	-2.86	102.72	106.90
14	cA	809	CLA	CED-O2D-CGD	2.86	122.42	115.94
14	A	819	CLA	C4C-C3C-C2C	-2.86	102.72	106.90
14	cB	825	CLA	C4C-C3C-C2C	-2.86	102.72	106.90
14	bB	803	CLA	C3B-C4B-NB	2.86	113.17	110.52
14	A	804	CLA	C4C-C3C-C2C	-2.86	102.72	106.90
14	B	851	CLA	C4C-C3C-C2C	-2.86	102.72	106.90
14	B	818	CLA	CAC-C3C-C4C	2.86	128.52	124.81
14	cA	819	CLA	CMC-C2C-C1C	2.86	129.40	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	809	CLA	CED-O2D-CGD	2.86	122.41	115.94
14	bJ	102	CLA	CHC-C1C-C2C	-2.86	118.78	126.73
14	B	822	CLA	CHC-C1C-C2C	-2.86	118.78	126.73
14	cB	831	CLA	CAC-C3C-C4C	2.86	128.52	124.81
14	A	819	CLA	CMC-C2C-C1C	2.86	129.39	125.04
14	bB	822	CLA	CHC-C1C-C2C	-2.86	118.79	126.73
14	B	824	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
14	bB	824	CLA	C3B-C4B-NB	2.86	113.17	110.52
14	cL	203	CLA	CMD-C2D-C3D	-2.86	121.04	127.61
14	A	806	CLA	C1-O2A-CGA	2.86	123.94	116.44
14	J	102	CLA	CHC-C1C-C2C	-2.86	118.79	126.73
14	cA	806	CLA	C1-O2A-CGA	2.86	123.94	116.44
14	B	824	CLA	CAC-C3C-C4C	2.86	128.52	124.81
14	cA	823	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
14	bB	818	CLA	CAC-C3C-C4C	2.85	128.51	124.81
14	cA	837	CLA	CHC-C1C-C2C	-2.85	118.80	126.73
14	bB	835	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
14	cA	825	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
14	A	837	CLA	CHC-C1C-C2C	-2.85	118.80	126.73
14	A	823	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
14	A	840	CLA	CHC-C1C-C2C	-2.85	118.80	126.73
14	L	202	CLA	CMD-C2D-C3D	-2.85	121.05	127.61
14	B	830	CLA	CAC-C3C-C4C	2.85	128.51	124.81
14	cB	823	CLA	CHC-C1C-C2C	-2.85	118.81	126.73
14	bL	202	CLA	CMD-C2D-C3D	-2.85	121.05	127.61
14	cB	819	CLA	CAC-C3C-C4C	2.85	128.51	124.81
14	bA	837	CLA	CHC-C1C-C2C	-2.85	118.81	126.73
14	bA	806	CLA	C1-O2A-CGA	2.85	123.92	116.44
14	bA	804	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
14	bA	823	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
14	bA	823	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
14	cA	827	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
14	bA	802	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
14	bA	840	CLA	CHC-C1C-C2C	-2.85	118.82	126.73
14	bA	809	CLA	CED-O2D-CGD	2.85	122.38	115.94
14	B	835	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
14	cA	812	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
14	A	823	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
14	bA	819	CLA	CMC-C2C-C1C	2.84	129.37	125.04
14	cA	840	CLA	CHC-C1C-C2C	-2.84	118.83	126.73
14	bA	802	CLA	CAC-C3C-C4C	2.84	128.50	124.81
14	A	802	CLA	C4C-C3C-C2C	-2.84	102.75	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bA	803	CLA	CHC-C1C-C2C	-2.84	118.83	126.73
14	bA	827	CLA	C4C-C3C-C2C	-2.84	102.75	106.90
14	cA	802	CLA	C4C-C3C-C2C	-2.84	102.75	106.90
14	cA	803	CLA	CHC-C1C-C2C	-2.84	118.84	126.73
14	cA	825	CLA	CHC-C1C-C2C	-2.84	118.84	126.73
14	X	201	CLA	CHC-C1C-C2C	-2.84	118.84	126.73
17	cL	207	BCR	C37-C22-C23	2.84	122.55	118.08
14	A	825	CLA	CHC-C1C-C2C	-2.84	118.84	126.73
14	A	826	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
14	bJ	101	CLA	CHC-C1C-C2C	-2.84	118.84	126.73
14	cA	802	CLA	CAC-C3C-C4C	2.84	128.49	124.81
17	L	206	BCR	C37-C22-C23	2.84	122.55	118.08
14	A	827	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
14	cB	836	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
17	A	847	BCR	C34-C9-C10	-2.84	118.95	122.92
14	bA	825	CLA	CHC-C1C-C2C	-2.84	118.85	126.73
14	bA	824	CLA	CMB-C2B-C1B	2.84	129.69	125.37
17	bB	847	BCR	C15-C14-C13	2.84	131.36	127.31
14	cA	839	CLA	CED-O2D-CGD	2.84	122.35	115.94
14	A	812	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
14	bA	812	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
14	cB	806	CLA	O2A-CGA-CBA	2.83	120.80	111.91
14	A	802	CLA	CAC-C3C-C4C	2.83	128.49	124.81
14	bA	814	CLA	CHC-C1C-C2C	-2.83	118.86	126.73
14	A	831	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
17	cA	847	BCR	C15-C16-C17	2.83	129.27	123.47
14	bB	805	CLA	O2A-CGA-CBA	2.83	120.79	111.91
14	bB	827	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
14	A	803	CLA	CHC-C1C-C2C	-2.83	118.87	126.73
14	cX	201	CLA	CHC-C1C-C2C	-2.83	118.87	126.73
17	cB	848	BCR	C15-C14-C13	2.83	131.35	127.31
14	B	824	CLA	C3B-C4B-NB	2.83	113.14	110.52
14	A	824	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
14	cA	826	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
14	J	101	CLA	CHC-C1C-C2C	-2.83	118.88	126.73
14	A	814	CLA	CHC-C1C-C2C	-2.83	118.88	126.73
14	bB	824	CLA	CHC-C1C-C2C	-2.83	118.88	126.73
14	bA	839	CLA	CED-O2D-CGD	2.83	122.33	115.94
14	cA	814	CLA	CHC-C1C-C2C	-2.83	118.88	126.73
14	cJ	101	CLA	CHC-C1C-C2C	-2.83	118.88	126.73
17	bL	206	BCR	C37-C22-C23	2.82	122.53	118.08
14	bX	201	CLA	CHC-C1C-C2C	-2.82	118.89	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	824	CLA	CHC-C1C-C2C	-2.82	118.89	126.73
14	A	839	CLA	CED-O2D-CGD	2.82	122.32	115.94
14	bA	826	CLA	C4C-C3C-C2C	-2.82	102.78	106.90
14	A	827	CLA	CED-O2D-CGD	2.82	122.32	115.94
17	A	847	BCR	C15-C16-C17	2.82	129.26	123.47
14	B	805	CLA	O2A-CGA-CBA	2.82	120.77	111.91
14	cB	825	CLA	CHC-C1C-C2C	-2.82	118.89	126.73
14	bA	831	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
14	cA	824	CLA	CMB-C2B-C1B	2.82	129.66	125.37
17	bA	847	BCR	C34-C9-C10	-2.82	118.97	122.92
14	bA	824	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
14	B	804	CLA	O2A-CGA-CBA	2.82	120.75	111.91
14	bA	824	CLA	CED-O2D-CGD	2.82	122.31	115.94
14	bA	827	CLA	CED-O2D-CGD	2.82	122.31	115.94
17	bA	847	BCR	C15-C16-C17	2.82	129.24	123.47
14	cA	835	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
14	A	824	CLA	CMB-C2B-C1B	2.82	129.66	125.37
14	cA	824	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
14	B	827	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
17	cA	847	BCR	C34-C9-C10	-2.81	118.98	122.92
14	cB	828	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
14	B	804	CLA	CHC-C1C-C2C	-2.81	118.92	126.73
17	B	847	BCR	C15-C14-C13	2.81	131.32	127.31
14	bA	835	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
14	cB	814	CLA	C2A-C1A-CHA	-2.81	118.94	123.86
14	cB	805	CLA	O2A-CGA-CBA	2.81	120.73	111.91
14	bL	202	CLA	CHC-C1C-C2C	-2.81	118.92	126.73
14	cL	203	CLA	CHC-C1C-C2C	-2.81	118.92	126.73
14	cA	824	CLA	CED-O2D-CGD	2.81	122.29	115.94
14	B	805	CLA	C2A-C1A-CHA	-2.81	118.95	123.86
14	A	804	CLA	O2A-CGA-CBA	2.81	120.72	111.91
14	A	835	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
14	bB	804	CLA	CHC-C1C-C2C	-2.81	118.93	126.73
14	cB	805	CLA	CHC-C1C-C2C	-2.81	118.93	126.73
14	bB	804	CLA	O2A-CGA-CBA	2.81	120.72	111.91
17	bA	849	BCR	C37-C22-C23	2.81	122.50	118.08
14	cA	836	CLA	CED-O2D-CGD	2.81	122.28	115.94
14	cA	808	CLA	CHC-C1C-C2C	-2.81	118.94	126.73
14	A	836	CLA	CED-O2D-CGD	2.81	122.28	115.94
14	L	202	CLA	CHC-C1C-C2C	-2.80	118.94	126.73
14	bA	840	CLA	C1-O2A-CGA	2.80	123.80	116.44
14	A	822	CLA	CMB-C2B-C1B	2.80	129.64	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	804	CLA	O2A-CGA-CBA	2.80	120.71	111.91
14	A	818	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
14	cA	821	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
14	cA	831	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
14	cA	834	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
14	A	824	CLA	CED-O2D-CGD	2.80	122.28	115.94
14	bB	815	CLA	C2A-C1A-CHA	-2.80	118.96	123.86
14	bA	804	CLA	O2A-CGA-CBA	2.80	120.70	111.91
14	bJ	101	CLA	CMB-C2B-C1B	2.80	129.64	125.37
14	bB	816	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
14	A	840	CLA	C1-O2A-CGA	2.80	123.79	116.44
14	cA	827	CLA	CED-O2D-CGD	2.80	122.27	115.94
14	J	101	CLA	CMB-C2B-C1B	2.80	129.63	125.37
14	B	816	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
14	bB	813	CLA	C2A-C1A-CHA	-2.80	118.96	123.86
14	bA	836	CLA	CED-O2D-CGD	2.80	122.27	115.94
17	cM	101	BCR	C34-C9-C8	2.80	122.49	118.08
14	cB	817	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
14	cA	822	CLA	CMB-C2B-C1B	2.80	129.63	125.37
14	A	821	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
14	cB	830	CLA	C2A-C1A-CHA	-2.80	118.97	123.86
14	bB	815	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
14	bA	822	CLA	CMB-C2B-C1B	2.80	129.63	125.37
14	A	808	CLA	CHC-C1C-C2C	-2.80	118.97	126.73
14	B	813	CLA	C2A-C1A-CHA	-2.79	118.97	123.86
14	A	839	CLA	C4C-C3C-C2C	-2.79	102.82	106.90
14	cA	818	CLA	C4C-C3C-C2C	-2.79	102.82	106.90
14	cA	840	CLA	C1-O2A-CGA	2.79	123.78	116.44
14	bB	829	CLA	C2A-C1A-CHA	-2.79	118.97	123.86
14	bA	808	CLA	CHC-C1C-C2C	-2.79	118.97	126.73
17	bM	101	BCR	C34-C9-C8	2.79	122.48	118.08
14	cA	808	CLA	C3B-C4B-NB	2.79	113.11	110.52
14	bA	818	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
14	B	829	CLA	C2A-C1A-CHA	-2.79	118.98	123.86
14	bA	821	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
14	cB	806	CLA	C2A-C1A-CHA	-2.79	118.98	123.86
14	cB	828	CLA	CHC-C1C-C2C	-2.79	118.98	126.73
14	B	815	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
14	bB	805	CLA	C2A-C1A-CHA	-2.79	118.98	123.86
14	cB	816	CLA	C2A-C1A-CHA	-2.79	118.98	123.86
17	cA	849	BCR	C37-C22-C23	2.79	122.47	118.08
14	cB	836	CLA	CHC-C1C-C2C	-2.79	118.99	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cB	816	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
14	B	827	CLA	CHC-C1C-C2C	-2.78	119.00	126.73
17	A	849	BCR	C37-C22-C23	2.78	122.46	118.08
14	cA	804	CLA	CHC-C1C-C2C	-2.78	119.00	126.73
14	bB	849	CLA	CMB-C2B-C1B	2.78	129.61	125.37
14	B	835	CLA	CHC-C1C-C2C	-2.78	119.00	126.73
13	bA	801	CL0	O2D-CGD-O1D	-2.78	118.40	123.84
14	bB	827	CLA	CHC-C1C-C2C	-2.78	119.00	126.73
14	cA	839	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
14	bA	804	CLA	CHC-C1C-C2C	-2.78	119.00	126.73
14	B	830	CLA	CMC-C2C-C1C	2.78	129.27	125.04
17	cB	846	BCR	C35-C13-C14	-2.78	119.03	122.92
14	cJ	101	CLA	CMB-C2B-C1B	2.78	129.60	125.37
14	B	808	CLA	CED-O2D-CGD	2.78	122.22	115.94
14	bA	813	CLA	C1C-C2C-C3C	-2.78	104.04	106.96
14	cA	813	CLA	C1C-C2C-C3C	-2.78	104.04	106.96
14	B	805	CLA	CHB-C4A-NA	2.78	128.35	124.51
14	cA	816	CLA	CHC-C1C-C2C	-2.78	119.02	126.73
17	B	843	BCR	C35-C13-C14	-2.78	119.03	122.92
14	cB	850	CLA	CMB-C2B-C1B	2.78	129.60	125.37
14	B	815	CLA	C2A-C1A-CHA	-2.78	119.00	123.86
14	B	825	CLA	CHC-C1C-C2C	-2.78	119.02	126.73
14	cA	826	CLA	CHD-C4C-NC	2.78	128.58	124.20
14	cB	803	CLA	C4C-C3C-C2C	-2.78	102.85	106.90
14	B	849	CLA	CMB-C2B-C1B	2.78	129.60	125.37
14	bA	819	CLA	C3B-C4B-NB	2.78	113.09	110.52
17	bB	843	BCR	C35-C13-C14	-2.78	119.03	122.92
17	bB	845	BCR	C35-C13-C14	-2.78	119.03	122.92
14	A	802	CLA	CAA-C2A-C3A	-2.77	105.18	112.78
14	bA	802	CLA	CAA-C2A-C3A	-2.77	105.18	112.78
14	A	804	CLA	CHC-C1C-C2C	-2.77	119.02	126.73
14	B	837	CLA	C2A-C1A-CHA	-2.77	119.01	123.86
14	bL	203	CLA	C2A-C1A-CHA	-2.77	119.01	123.86
14	bA	834	CLA	C4C-C3C-C2C	-2.77	102.85	106.90
14	B	827	CLA	C1-O2A-CGA	2.77	123.72	116.44
14	cB	826	CLA	CHC-C1C-C2C	-2.77	119.02	126.73
17	bB	847	BCR	C34-C9-C10	-2.77	119.04	122.92
17	cB	844	BCR	C35-C13-C14	-2.77	119.04	122.92
17	cI	101	BCR	C16-C15-C14	2.77	129.16	123.47
14	cA	802	CLA	CAA-C2A-C3A	-2.77	105.18	112.78
14	A	813	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
14	bB	837	CLA	C2A-C1A-CHA	-2.77	119.01	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bB	835	CLA	CHC-C1C-C2C	-2.77	119.03	126.73
14	bA	826	CLA	CHD-C4C-NC	2.77	128.57	124.20
14	cB	831	CLA	CMC-C2C-C1C	2.77	129.26	125.04
14	bB	827	CLA	C1-O2A-CGA	2.77	123.72	116.44
14	bA	802	CLA	CHC-C1C-C2C	-2.77	119.03	126.73
14	bB	825	CLA	CHC-C1C-C2C	-2.77	119.03	126.73
14	bA	836	CLA	CHD-C4C-NC	2.77	128.57	124.20
14	cA	802	CLA	CHC-C1C-C2C	-2.77	119.03	126.73
14	bB	834	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
17	B	845	BCR	C35-C13-C14	-2.77	119.04	122.92
17	B	847	BCR	C34-C9-C10	-2.77	119.04	122.92
17	cB	848	BCR	C34-C9-C10	-2.77	119.04	122.92
14	bA	836	CLA	O2A-CGA-CBA	2.77	120.60	111.91
17	M	101	BCR	C34-C9-C8	2.77	122.44	118.08
14	bA	816	CLA	CHC-C1C-C2C	-2.77	119.03	126.73
14	bA	837	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
14	A	816	CLA	CHC-C1C-C2C	-2.77	119.04	126.73
17	cL	207	BCR	C15-C16-C17	2.77	129.15	123.47
14	A	818	CLA	CHC-C1C-C2C	-2.77	119.04	126.73
14	bA	831	CLA	C4A-NA-C1A	-2.77	105.46	106.71
14	cB	806	CLA	CHB-C4A-NA	2.77	128.34	124.51
14	bA	818	CLA	CHC-C1C-C2C	-2.77	119.04	126.73
14	bB	805	CLA	CHB-C4A-NA	2.77	128.34	124.51
14	cA	836	CLA	CHD-C4C-NC	2.77	128.56	124.20
14	bB	830	CLA	CMC-C2C-C1C	2.77	129.25	125.04
14	A	802	CLA	CHC-C1C-C2C	-2.77	119.04	126.73
17	I	101	BCR	C16-C15-C14	2.77	129.14	123.47
14	cL	204	CLA	C2A-C1A-CHA	-2.77	119.02	123.86
14	bB	808	CLA	CED-O2D-CGD	2.77	122.19	115.94
14	A	818	CLA	C1-C2-C3	-2.77	121.26	126.04
14	A	834	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
17	L	206	BCR	C15-C16-C17	2.77	129.14	123.47
14	cA	818	CLA	C1-C2-C3	-2.77	121.26	126.04
14	cA	837	CLA	C4C-C3C-C2C	-2.77	102.87	106.90
14	A	826	CLA	CHD-C4C-NC	2.76	128.56	124.20
14	cB	838	CLA	C2A-C1A-CHA	-2.76	119.03	123.86
14	cB	828	CLA	C1-O2A-CGA	2.76	123.70	116.44
14	B	802	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
13	cA	801	CL0	O2D-CGD-O1D	-2.76	118.44	123.84
13	A	801	CL0	O2D-CGD-O1D	-2.76	118.44	123.84
14	cA	818	CLA	CHC-C1C-C2C	-2.76	119.06	126.73
14	cA	831	CLA	O2A-CGA-CBA	2.76	120.58	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	836	CLA	CHD-C4C-NC	2.76	128.56	124.20
17	bI	101	BCR	C16-C15-C14	2.76	129.13	123.47
14	B	808	CLA	O2A-CGA-CBA	2.76	120.57	111.91
14	A	802	CLA	CMB-C2B-C1B	2.76	129.57	125.37
14	bA	852	CLA	O2A-CGA-CBA	2.76	120.57	111.91
14	bA	839	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
14	A	832	CLA	C1-C2-C3	-2.76	121.27	126.04
14	B	832	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
14	A	836	CLA	O2A-CGA-CBA	2.76	120.57	111.91
14	bA	832	CLA	C1-C2-C3	-2.76	121.27	126.04
14	bB	802	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
14	cA	832	CLA	C1-C2-C3	-2.76	121.27	126.04
14	bB	828	CLA	CHC-C1C-C2C	-2.76	119.07	126.73
14	cB	840	CLA	C1-O2A-CGA	2.76	123.68	116.44
14	cB	809	CLA	CED-O2D-CGD	2.76	122.17	115.94
14	bB	832	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
14	cB	835	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
14	cA	836	CLA	O2A-CGA-CBA	2.76	120.56	111.91
13	bA	801	CL0	C4C-C3C-C2C	-2.76	102.88	106.90
13	cA	801	CL0	C4C-C3C-C2C	-2.76	102.88	106.90
14	B	828	CLA	CHC-C1C-C2C	-2.76	119.07	126.73
14	cA	833	CLA	C1-O2A-CGA	2.76	123.68	116.44
14	bA	802	CLA	CMB-C2B-C1B	2.76	129.57	125.37
14	A	837	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
14	B	813	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
14	cA	852	CLA	O2A-CGA-CBA	2.76	120.56	111.91
14	cB	809	CLA	O2A-CGA-CBA	2.76	120.56	111.91
14	bA	821	CLA	CED-O2D-CGD	2.75	122.17	115.94
14	L	203	CLA	C2A-C1A-CHA	-2.75	119.04	123.86
14	B	806	CLA	CHD-C4C-NC	2.75	128.54	124.20
14	bA	818	CLA	C1-C2-C3	-2.75	121.28	126.04
14	B	820	CLA	C2A-C1A-CHA	-2.75	119.04	123.86
14	bA	831	CLA	O2A-CGA-CBA	2.75	120.55	111.91
13	A	801	CL0	C4C-C3C-C2C	-2.75	102.88	106.90
17	bB	842	BCR	C35-C13-C14	-2.75	119.06	122.92
14	cA	821	CLA	CED-O2D-CGD	2.75	122.17	115.94
17	bL	206	BCR	C15-C16-C17	2.75	129.12	123.47
14	bB	820	CLA	C2A-C1A-CHA	-2.75	119.04	123.86
14	A	831	CLA	O2A-CGA-CBA	2.75	120.55	111.91
14	A	852	CLA	O2A-CGA-CBA	2.75	120.55	111.91
14	bA	808	CLA	C3B-C4B-NB	2.75	113.07	110.52
14	bB	808	CLA	O2A-CGA-CBA	2.75	120.55	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bB	813	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
14	A	821	CLA	CED-O2D-CGD	2.75	122.16	115.94
14	bB	806	CLA	CHD-C4C-NC	2.75	128.54	124.20
14	bA	837	CLA	C3B-C4B-NB	2.75	113.07	110.52
14	L	202	CLA	C2A-C1A-CHA	-2.75	119.05	123.86
17	B	842	BCR	C35-C13-C14	-2.75	119.07	122.92
14	bA	825	CLA	CHD-C4C-NC	2.75	128.54	124.20
14	cA	802	CLA	CMB-C2B-C1B	2.75	129.56	125.37
14	cB	833	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
14	B	849	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
14	cB	821	CLA	C2A-C1A-CHA	-2.75	119.05	123.86
14	cB	829	CLA	CHC-C1C-C2C	-2.75	119.10	126.73
14	bA	833	CLA	C1-O2A-CGA	2.75	123.65	116.44
14	bB	839	CLA	C1-O2A-CGA	2.75	123.65	116.44
14	A	822	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
14	bB	833	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
14	A	819	CLA	C3B-C4B-NB	2.75	113.06	110.52
14	A	833	CLA	C1-O2A-CGA	2.75	123.65	116.44
14	B	833	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
14	cA	822	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
17	B	841	BCR	C16-C15-C14	2.74	129.10	123.47
17	bB	841	BCR	C16-C15-C14	2.74	129.10	123.47
14	B	834	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
14	cB	850	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
14	cL	203	CLA	C2A-C1A-CHA	-2.74	119.06	123.86
14	bA	836	CLA	CHC-C1C-C2C	-2.74	119.11	126.73
14	bA	820	CLA	CMC-C2C-C1C	2.74	129.22	125.04
14	cX	201	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
17	B	850	BCR	C34-C9-C10	-2.74	119.08	122.92
14	bB	812	CLA	O2A-CGA-CBA	2.74	120.51	111.91
14	cA	819	CLA	C3B-C4B-NB	2.74	113.06	110.52
14	cB	807	CLA	CHD-C4C-NC	2.74	128.52	124.20
14	cA	837	CLA	C3B-C4B-NB	2.74	113.06	110.52
14	B	812	CLA	O2A-CGA-CBA	2.74	120.50	111.91
14	B	839	CLA	C1-O2A-CGA	2.74	123.63	116.44
14	A	825	CLA	CHD-C4C-NC	2.74	128.52	124.20
14	bX	201	CLA	C4C-C3C-C2C	-2.74	102.91	106.90
14	A	808	CLA	C3B-C4B-NB	2.74	113.05	110.52
14	cB	813	CLA	O2A-CGA-CBA	2.74	120.50	111.91
14	cB	814	CLA	C4C-C3C-C2C	-2.74	102.91	106.90
14	cB	811	CLA	C2A-C1A-CHA	-2.74	119.08	123.86
14	bL	202	CLA	C2A-C1A-CHA	-2.73	119.08	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	cB	842	BCR	C16-C15-C14	2.73	129.07	123.47
14	cA	825	CLA	CHD-C4C-NC	2.73	128.51	124.20
14	cA	836	CLA	CHC-C1C-C2C	-2.73	119.14	126.73
14	A	836	CLA	CHC-C1C-C2C	-2.73	119.14	126.73
14	X	201	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
14	J	102	CLA	C3B-C4B-NB	2.73	113.05	110.52
14	bB	810	CLA	C2A-C1A-CHA	-2.73	119.08	123.86
17	cB	843	BCR	C35-C13-C14	-2.73	119.10	122.92
14	B	810	CLA	C2A-C1A-CHA	-2.73	119.08	123.86
14	bA	822	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
14	bA	819	CLA	CED-O2D-CGD	2.73	122.11	115.94
17	cB	851	BCR	C34-C9-C10	-2.73	119.10	122.92
14	B	801	CLA	CHD-C4C-NC	2.73	128.50	124.20
14	cB	802	CLA	CHD-C4C-NC	2.73	128.50	124.20
14	bB	801	CLA	CHD-C4C-NC	2.73	128.50	124.20
14	A	837	CLA	C3B-C4B-NB	2.72	113.04	110.52
14	bB	849	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
14	cA	819	CLA	CED-O2D-CGD	2.72	122.10	115.94
17	bB	850	BCR	C34-C9-C10	-2.72	119.11	122.92
14	bB	821	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
14	bJ	102	CLA	C3B-C4B-NB	2.72	113.04	110.52
17	bB	846	BCR	C34-C9-C8	2.72	122.37	118.08
14	L	203	CLA	CHC-C1C-C2C	-2.72	119.17	126.73
14	A	819	CLA	CED-O2D-CGD	2.72	122.09	115.94
14	B	806	CLA	CED-O2D-CGD	2.72	122.09	115.94
14	cB	807	CLA	CED-O2D-CGD	2.72	122.09	115.94
14	A	820	CLA	CMC-C2C-C1C	2.72	129.18	125.04
14	bB	806	CLA	CED-O2D-CGD	2.72	122.09	115.94
14	cB	822	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
14	bA	840	CLA	C2A-C1A-CHA	-2.72	119.10	123.86
14	cA	828	CLA	CED-O2D-CGD	2.72	122.09	115.94
14	cA	822	CLA	C3B-C4B-NB	2.72	113.04	110.52
17	bA	845	BCR	C35-C13-C14	-2.72	119.12	122.92
14	bA	832	CLA	C4C-C3C-C2C	-2.72	102.94	106.90
14	bL	203	CLA	CHC-C1C-C2C	-2.72	119.18	126.73
14	B	827	CLA	CED-O2D-CGD	2.72	122.08	115.94
14	A	840	CLA	C2A-C1A-CHA	-2.72	119.11	123.86
14	cL	203	CLA	C4C-C3C-C2C	-2.72	102.94	106.90
14	B	829	CLA	CMB-C2B-C1B	2.72	129.50	125.37
14	bA	815	CLA	C4C-C3C-C2C	-2.71	102.94	106.90
14	cA	820	CLA	CMC-C2C-C1C	2.71	129.17	125.04
14	cB	830	CLA	CMB-C2B-C1B	2.71	129.50	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	831	CLA	C4A-NA-C1A	-2.71	105.49	106.71
17	A	845	BCR	C37-C22-C23	2.71	122.35	118.08
14	A	814	CLA	CED-O2D-CGD	2.71	122.07	115.94
14	B	821	CLA	C4C-C3C-C2C	-2.71	102.94	106.90
14	A	822	CLA	C3B-C4B-NB	2.71	113.03	110.52
14	bB	849	CLA	C3B-C4B-NB	2.71	113.03	110.52
14	L	202	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
14	cB	834	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
14	bB	836	CLA	CHD-C4C-NC	2.71	128.47	124.20
14	A	812	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
17	cA	845	BCR	C35-C13-C14	-2.71	119.13	122.92
14	bB	802	CLA	CAA-C2A-C3A	-2.71	105.36	112.78
14	cA	812	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
14	cB	828	CLA	CED-O2D-CGD	2.71	122.06	115.94
14	cA	840	CLA	C2A-C1A-CHA	-2.71	119.12	123.86
14	cL	204	CLA	CHC-C1C-C2C	-2.71	119.21	126.73
14	cB	850	CLA	C3B-C4B-NB	2.71	113.03	110.52
17	cA	845	BCR	C37-C22-C23	2.71	122.34	118.08
14	bB	827	CLA	CED-O2D-CGD	2.71	122.06	115.94
14	cA	830	CLA	CMB-C2B-C1B	2.71	129.49	125.37
14	bL	202	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
14	bA	812	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
14	A	828	CLA	CED-O2D-CGD	2.70	122.06	115.94
14	B	849	CLA	C3B-C4B-NB	2.70	113.02	110.52
14	B	802	CLA	CAA-C2A-C3A	-2.70	105.37	112.78
17	bA	845	BCR	C37-C22-C23	2.70	122.34	118.08
14	bF	201	CLA	CHC-C1C-C2C	-2.70	119.22	126.73
17	A	845	BCR	C35-C13-C14	-2.70	119.14	122.92
17	L	205	BCR	C36-C18-C17	-2.70	119.14	122.92
14	A	815	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
14	bA	829	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
14	cA	814	CLA	CED-O2D-CGD	2.70	122.05	115.94
14	F	201	CLA	CHC-C1C-C2C	-2.70	119.22	126.73
14	cA	822	CLA	C2A-C1A-CHA	-2.70	119.13	123.86
14	cA	832	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
14	cB	803	CLA	CAA-C2A-C3A	-2.70	105.38	112.78
14	bA	828	CLA	CED-O2D-CGD	2.70	122.05	115.94
14	A	808	CLA	CHD-C4C-NC	2.70	128.46	124.20
14	bB	829	CLA	CMB-C2B-C1B	2.70	129.48	125.37
14	A	831	CLA	C4A-NA-C1A	-2.70	105.49	106.71
14	B	836	CLA	CHD-C4C-NC	2.70	128.46	124.20
14	J	101	CLA	C4C-C3C-C2C	-2.70	102.96	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	829	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
14	bA	811	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
14	bA	814	CLA	CED-O2D-CGD	2.70	122.04	115.94
14	bA	808	CLA	CHD-C4C-NC	2.70	128.45	124.20
14	cB	820	CLA	CED-O2D-CGD	2.70	122.03	115.94
14	cB	812	CLA	C3B-C4B-NB	2.70	113.02	110.52
14	cB	833	CLA	O1D-CGD-CBD	-2.70	118.97	124.48
14	bB	819	CLA	CED-O2D-CGD	2.70	122.03	115.94
14	A	832	CLA	C4C-C3C-C2C	-2.70	102.97	106.90
14	cB	837	CLA	CHD-C4C-NC	2.69	128.45	124.20
14	bA	822	CLA	C3B-C4B-NB	2.69	113.02	110.52
14	bB	828	CLA	CHD-C4C-NC	2.69	128.45	124.20
14	B	819	CLA	CED-O2D-CGD	2.69	122.03	115.94
17	A	847	BCR	C35-C13-C14	-2.69	119.15	122.92
14	A	811	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
14	cF	201	CLA	CHC-C1C-C2C	-2.69	119.25	126.73
14	cA	815	CLA	C4C-C3C-C2C	-2.69	102.97	106.90
14	cA	833	CLA	C4C-C3C-C2C	-2.69	102.97	106.90
14	bJ	101	CLA	C4C-C3C-C2C	-2.69	102.97	106.90
14	B	828	CLA	CHD-C4C-NC	2.69	128.45	124.20
14	cA	811	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
17	cA	847	BCR	C35-C13-C14	-2.69	119.15	122.92
17	cL	206	BCR	C36-C18-C17	-2.69	119.15	122.92
14	A	822	CLA	C2A-C1A-CHA	-2.69	119.15	123.86
14	B	817	CLA	CHD-C4C-NC	2.69	128.44	124.20
14	A	829	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
14	bA	830	CLA	CMB-C2B-C1B	2.69	129.47	125.37
14	bA	833	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
14	bB	806	CLA	C1-O2A-CGA	2.69	123.50	116.44
14	cB	818	CLA	CHD-C4C-NC	2.69	128.44	124.20
17	B	846	BCR	C34-C9-C8	2.69	122.31	118.08
14	cA	835	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
17	cB	847	BCR	C34-C9-C8	2.69	122.31	118.08
14	bA	822	CLA	C2A-C1A-CHA	-2.69	119.16	123.86
14	bA	835	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
14	bJ	102	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
14	cJ	101	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
14	cB	829	CLA	CHD-C4C-NC	2.69	128.44	124.20
14	bA	840	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
17	bA	847	BCR	C35-C13-C14	-2.68	119.16	122.92
14	A	827	CLA	CHC-C1C-C2C	-2.68	119.28	126.73
14	cA	830	CLA	C1-C2-C3	-2.68	122.41	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cB	807	CLA	C1-O2A-CGA	2.68	123.48	116.44
14	B	806	CLA	C1-O2A-CGA	2.68	123.48	116.44
14	bB	817	CLA	CHD-C4C-NC	2.68	128.43	124.20
14	bB	811	CLA	C3B-C4B-NB	2.68	113.00	110.52
14	cA	810	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
17	bL	205	BCR	C36-C18-C17	-2.68	119.17	122.92
17	cA	848	BCR	C34-C9-C8	2.68	122.30	118.08
14	A	833	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
14	B	832	CLA	O1D-CGD-CBD	-2.68	119.00	124.48
14	bA	827	CLA	CHC-C1C-C2C	-2.68	119.29	126.73
14	cJ	102	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
14	B	811	CLA	C3B-C4B-NB	2.68	113.00	110.52
14	A	835	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
14	B	803	CLA	CHB-C4A-NA	2.68	128.22	124.51
14	cA	820	CLA	C4C-C3C-C2C	-2.68	103.00	106.90
14	bA	805	CLA	C1-O2A-CGA	2.68	123.47	116.44
14	A	810	CLA	C2A-C1A-CHA	-2.68	119.18	123.86
14	cA	808	CLA	CHD-C4C-NC	2.68	128.42	124.20
14	cB	804	CLA	CHB-C4A-NA	2.67	128.21	124.51
14	A	810	CLA	C3B-C4B-NB	2.67	113.00	110.52
14	A	830	CLA	CMB-C2B-C1B	2.67	129.44	125.37
14	bB	811	CLA	CMC-C2C-C1C	2.67	129.11	125.04
14	A	810	CLA	C4C-C3C-C2C	-2.67	103.00	106.90
14	bA	830	CLA	C1-C2-C3	-2.67	122.43	126.75
14	bB	832	CLA	O1D-CGD-CBD	-2.67	119.02	124.48
14	cA	827	CLA	CHC-C1C-C2C	-2.67	119.31	126.73
17	bA	848	BCR	C34-C9-C8	2.67	122.29	118.08
14	cA	810	CLA	C2A-C1A-CHA	-2.67	119.19	123.86
14	bB	811	CLA	C2A-C1A-CHA	-2.67	119.19	123.86
17	A	848	BCR	C34-C9-C8	2.67	122.28	118.08
14	J	102	CLA	C4C-C3C-C2C	-2.67	103.01	106.90
14	cA	805	CLA	C1-O2A-CGA	2.67	123.45	116.44
14	bA	810	CLA	C4C-C3C-C2C	-2.67	103.01	106.90
14	cJ	101	CLA	C3B-C4B-NB	2.67	112.99	110.52
14	A	823	CLA	CMB-C2B-C1B	2.67	129.43	125.37
14	cB	826	CLA	CHD-C4C-NC	2.67	128.41	124.20
14	bA	829	CLA	O1D-CGD-CBD	-2.67	119.03	124.48
14	bX	201	CLA	C3B-C4B-NB	2.67	112.99	110.52
14	bA	833	CLA	C2A-C1A-CHA	-2.67	119.20	123.86
14	B	811	CLA	C2A-C1A-CHA	-2.67	119.20	123.86
14	cA	840	CLA	O2D-CGD-O1D	-2.67	118.63	123.84
14	bA	823	CLA	CMB-C2B-C1B	2.67	129.43	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cB	812	CLA	C2A-C1A-CHA	-2.67	119.20	123.86
14	A	840	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
14	A	805	CLA	C1-O2A-CGA	2.66	123.44	116.44
14	A	820	CLA	C4C-C3C-C2C	-2.66	103.01	106.90
14	bB	803	CLA	CHB-C4A-NA	2.66	128.20	124.51
14	bA	825	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
14	bB	825	CLA	CHD-C4C-NC	2.66	128.40	124.20
14	cA	825	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
14	cA	823	CLA	C2A-C1A-CHA	-2.66	119.20	123.86
14	A	835	CLA	CMB-C2B-C1B	2.66	129.42	125.37
14	bA	835	CLA	CMB-C2B-C1B	2.66	129.42	125.37
14	bA	810	CLA	C2A-C1A-CHA	-2.66	119.21	123.86
14	bA	820	CLA	C4C-C3C-C2C	-2.66	103.02	106.90
14	B	825	CLA	CHD-C4C-NC	2.66	128.40	124.20
17	bI	102	BCR	C11-C10-C9	2.66	131.11	127.31
14	X	201	CLA	C3B-C4B-NB	2.66	112.98	110.52
14	cJ	102	CLA	C3B-C4B-NB	2.66	112.98	110.52
14	cF	201	CLA	CHD-C4C-NC	2.66	128.39	124.20
14	A	830	CLA	C1-C2-C3	-2.66	122.45	126.75
17	cL	207	BCR	C36-C18-C17	-2.66	119.20	122.92
14	cA	811	CLA	C3B-C4B-NB	2.66	112.98	110.52
14	cB	812	CLA	CMC-C2C-C1C	2.65	129.08	125.04
14	cA	833	CLA	C2A-C1A-CHA	-2.65	119.22	123.86
14	cA	841	CLA	C4C-C3C-C2C	-2.65	103.03	106.90
14	A	825	CLA	C4A-NA-C1A	-2.65	105.51	106.71
14	B	811	CLA	CMC-C2C-C1C	2.65	129.08	125.04
14	cA	829	CLA	O1D-CGD-CBD	-2.65	119.06	124.48
14	bA	810	CLA	C3B-C4B-NB	2.65	112.98	110.52
14	cA	823	CLA	CMB-C2B-C1B	2.65	129.41	125.37
13	A	801	CL0	CGD-CBD-CAD	-2.65	102.14	110.73
14	F	201	CLA	CHD-C4C-NC	2.65	128.38	124.20
14	A	825	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
14	A	833	CLA	C2A-C1A-CHA	-2.65	119.22	123.86
14	cA	837	CLA	C4-C3-C5	2.65	119.73	115.27
14	B	813	CLA	CMB-C2B-C1B	2.65	129.41	125.37
14	F	201	CLA	C4C-C3C-C2C	-2.65	103.03	106.90
14	bA	837	CLA	C4-C3-C5	2.65	119.73	115.27
14	B	837	CLA	CMB-C2B-C1B	2.65	129.40	125.37
17	bL	206	BCR	C36-C18-C17	-2.65	119.21	122.92
14	bF	201	CLA	C4C-C3C-C2C	-2.65	103.04	106.90
14	bB	828	CLA	CBC-CAC-C3C	-2.65	105.13	112.43
14	cL	205	CLA	O2D-CGD-O1D	-2.65	118.66	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	L	206	BCR	C36-C18-C17	-2.65	119.21	122.92
14	bB	837	CLA	CMB-C2B-C1B	2.65	129.40	125.37
14	L	204	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
14	bA	823	CLA	C2A-C1A-CHA	-2.65	119.23	123.86
14	cA	825	CLA	C1-O2A-CGA	2.65	123.39	116.44
14	cA	835	CLA	CMB-C2B-C1B	2.65	129.40	125.37
17	I	102	BCR	C11-C10-C9	2.65	131.09	127.31
14	cB	814	CLA	CMB-C2B-C1B	2.65	129.40	125.37
14	B	801	CLA	CHB-C4A-NA	2.65	128.17	124.51
14	bA	825	CLA	C1-O2A-CGA	2.65	123.38	116.44
14	B	828	CLA	CBC-CAC-C3C	-2.65	105.14	112.43
14	J	101	CLA	C3B-C4B-NB	2.64	112.97	110.52
14	bA	835	CLA	C3B-C4B-NB	2.64	112.97	110.52
14	cA	841	CLA	CBA-CAA-C2A	2.64	121.67	113.86
14	bB	813	CLA	CMB-C2B-C1B	2.64	129.40	125.37
14	A	829	CLA	O1D-CGD-CBD	-2.64	119.07	124.48
13	bA	801	CL0	CGD-CBD-CAD	-2.64	102.17	110.73
14	A	823	CLA	C2A-C1A-CHA	-2.64	119.24	123.86
14	bL	204	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
17	cI	102	BCR	C11-C10-C9	2.64	131.08	127.31
14	A	835	CLA	C3B-C4B-NB	2.64	112.97	110.52
14	bA	811	CLA	C3B-C4B-NB	2.64	112.97	110.52
13	cA	801	CL0	CGD-CBD-CAD	-2.64	102.18	110.73
14	cB	829	CLA	CBC-CAC-C3C	-2.64	105.15	112.43
14	A	837	CLA	C4-C3-C5	2.64	119.71	115.27
14	cA	808	CLA	C2A-C1A-CHA	-2.64	119.24	123.86
14	cA	810	CLA	C3B-C4B-NB	2.64	112.96	110.52
14	cF	201	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
14	cB	802	CLA	CHB-C4A-NA	2.64	128.16	124.51
14	A	823	CLA	C3B-C4B-NB	2.64	112.96	110.52
14	bB	830	CLA	C2A-C1A-CHA	-2.64	119.25	123.86
14	bA	831	CLA	C2A-C1A-CHA	-2.64	119.25	123.86
14	cB	831	CLA	C2A-C1A-CHA	-2.64	119.25	123.86
14	A	825	CLA	C1-O2A-CGA	2.64	123.36	116.44
14	bA	841	CLA	CBA-CAA-C2A	2.64	121.64	113.86
14	bA	841	CLA	C4C-C3C-C2C	-2.64	103.06	106.90
14	A	842	CLA	C4C-C3C-C2C	-2.64	103.06	106.90
14	bB	801	CLA	CHB-C4A-NA	2.64	128.16	124.51
14	B	808	CLA	O1D-CGD-CBD	-2.63	119.09	124.48
14	bB	816	CLA	CED-O2D-CGD	2.63	121.89	115.94
14	cB	823	CLA	CED-O2D-CGD	2.63	121.89	115.94
14	cA	831	CLA	C2A-C1A-CHA	-2.63	119.25	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	816	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
14	B	830	CLA	C2A-C1A-CHA	-2.63	119.25	123.86
14	cB	809	CLA	O1D-CGD-CBD	-2.63	119.10	124.48
14	bB	823	CLA	CHD-C4C-NC	2.63	128.35	124.20
14	A	841	CLA	CBA-CAA-C2A	2.63	121.63	113.86
14	bA	816	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
14	B	823	CLA	CHD-C4C-NC	2.63	128.35	124.20
14	bF	201	CLA	C4-C3-C5	2.63	118.99	115.98
14	B	828	CLA	O1D-CGD-CBD	-2.63	119.10	124.48
14	A	808	CLA	C2A-C1A-CHA	-2.63	119.26	123.86
14	bB	812	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
14	A	829	CLA	C2A-C1A-CHA	-2.63	119.26	123.86
14	bA	823	CLA	C3B-C4B-NB	2.63	112.95	110.52
14	bF	201	CLA	CHD-C4C-NC	2.63	128.35	124.20
14	cB	824	CLA	CHD-C4C-NC	2.63	128.35	124.20
14	bA	829	CLA	C2A-C1A-CHA	-2.63	119.26	123.86
14	cX	201	CLA	C3B-C4B-NB	2.63	112.95	110.52
14	A	816	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
14	A	841	CLA	C4C-C3C-C2C	-2.63	103.07	106.90
14	A	831	CLA	C2A-C1A-CHA	-2.63	119.26	123.86
14	A	826	CLA	CHC-C1C-C2C	-2.63	119.43	126.73
14	bA	842	CLA	C4C-C3C-C2C	-2.63	103.07	106.90
17	cJ	103	BCR	C15-C14-C13	2.63	131.06	127.31
14	cL	204	CLA	O2A-CGA-CBA	2.63	120.15	111.91
14	A	842	CLA	C2A-C1A-CHA	-2.63	119.27	123.86
17	bJ	103	BCR	C15-C14-C13	2.63	131.06	127.31
14	L	203	CLA	O2A-CGA-CBA	2.63	120.15	111.91
14	bA	811	CLA	C2A-C1A-CHA	-2.63	119.27	123.86
14	bB	808	CLA	O1D-CGD-CBD	-2.63	119.11	124.48
14	cA	826	CLA	CHC-C1C-C2C	-2.63	119.44	126.73
14	A	811	CLA	C3B-C4B-NB	2.63	112.95	110.52
14	cB	838	CLA	CMB-C2B-C1B	2.63	129.37	125.37
14	B	816	CLA	CED-O2D-CGD	2.63	121.88	115.94
14	bA	808	CLA	C2A-C1A-CHA	-2.62	119.27	123.86
14	A	814	CLA	C4C-C3C-C2C	-2.62	103.07	106.90
14	A	825	CLA	CHB-C4A-NA	2.62	128.14	124.51
14	cB	828	CLA	C2A-C1A-CHA	-2.62	119.27	123.86
14	B	827	CLA	C2A-C1A-CHA	-2.62	119.27	123.86
14	cA	811	CLA	C2A-C1A-CHA	-2.62	119.27	123.86
14	bB	831	CLA	C1-O2A-CGA	2.62	123.33	116.44
14	A	809	CLA	CHD-C4C-NC	2.62	128.34	124.20
14	bA	809	CLA	CHD-C4C-NC	2.62	128.34	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bB	828	CLA	O1D-CGD-CBD	-2.62	119.12	124.48
14	bJ	101	CLA	C3B-C4B-NB	2.62	112.95	110.52
14	A	805	CLA	CHB-C4A-NA	2.62	128.14	124.51
14	F	201	CLA	C4-C3-C5	2.62	118.98	115.98
14	bA	814	CLA	C4C-C3C-C2C	-2.62	103.08	106.90
14	cA	842	CLA	C2A-C1A-CHA	-2.62	119.28	123.86
14	cB	817	CLA	CED-O2D-CGD	2.62	121.86	115.94
14	bA	842	CLA	C2A-C1A-CHA	-2.62	119.28	123.86
14	bB	827	CLA	C2A-C1A-CHA	-2.62	119.28	123.86
14	cA	835	CLA	C3B-C4B-NB	2.62	112.94	110.52
14	bA	826	CLA	CHC-C1C-C2C	-2.62	119.45	126.73
14	cB	814	CLA	O2A-CGA-CBA	2.62	120.13	111.91
14	A	811	CLA	C2A-C1A-CHA	-2.62	119.28	123.86
14	B	831	CLA	C1-O2A-CGA	2.62	123.31	116.44
14	bA	825	CLA	C4A-NA-C1A	-2.62	105.53	106.71
14	bL	203	CLA	O2A-CGA-CBA	2.62	120.12	111.91
14	cA	829	CLA	C2A-C1A-CHA	-2.62	119.28	123.86
14	B	812	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
14	B	836	CLA	C4C-C3C-C2C	-2.62	103.08	106.90
14	cB	832	CLA	C1-O2A-CGA	2.62	123.31	116.44
14	B	822	CLA	CED-O2D-CGD	2.62	121.85	115.94
17	J	103	BCR	C15-C14-C13	2.61	131.04	127.31
14	cA	823	CLA	C3B-C4B-NB	2.61	112.94	110.52
14	bB	828	CLA	O2A-CGA-CBA	2.61	120.11	111.91
14	bB	813	CLA	O2A-CGA-CBA	2.61	120.11	111.91
14	cA	805	CLA	CHB-C4A-NA	2.61	128.12	124.51
14	cA	814	CLA	C4C-C3C-C2C	-2.61	103.09	106.90
14	cA	825	CLA	CHB-C4A-NA	2.61	128.12	124.51
14	A	842	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
14	bA	805	CLA	CHB-C4A-NA	2.61	128.12	124.51
14	bA	817	CLA	C2A-C1A-CHA	-2.61	119.30	123.86
14	cA	809	CLA	CHD-C4C-NC	2.61	128.31	124.20
14	bA	842	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
14	cA	802	CLA	O2A-CGA-O1A	-2.61	117.01	123.59
14	cA	834	CLA	C3B-C4B-NB	2.61	112.93	110.52
14	cB	829	CLA	O1D-CGD-CBD	-2.61	119.15	124.48
14	bA	825	CLA	CHB-C4A-NA	2.61	128.12	124.51
14	cB	813	CLA	C1C-C2C-C3C	-2.61	104.22	106.96
14	cA	842	CLA	C4C-C3C-C2C	-2.61	103.10	106.90
14	cA	817	CLA	C2A-C1A-CHA	-2.60	119.30	123.86
14	bB	801	CLA	C3B-C4B-NB	2.60	112.93	110.52
14	B	813	CLA	O2A-CGA-CBA	2.60	120.08	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cF	201	CLA	C4-C3-C5	2.60	118.96	115.98
14	bA	834	CLA	C3B-C4B-NB	2.60	112.93	110.52
14	B	828	CLA	O2A-CGA-CBA	2.60	120.08	111.91
14	cB	829	CLA	O2A-CGA-CBA	2.60	120.08	111.91
14	cB	838	CLA	O2A-CGA-CBA	2.60	120.08	111.91
14	cA	842	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
14	bA	811	CLA	C4C-C3C-C2C	-2.60	103.11	106.90
14	bB	822	CLA	CED-O2D-CGD	2.60	121.82	115.94
14	bB	824	CLA	CHB-C4A-NA	2.60	128.11	124.51
14	A	811	CLA	CMB-C2B-C1B	2.60	129.33	125.37
14	bB	837	CLA	O2A-CGA-CBA	2.60	120.07	111.91
14	cA	825	CLA	C4A-NA-C1A	-2.60	105.54	106.71
14	B	837	CLA	O2A-CGA-CBA	2.60	120.07	111.91
14	bA	807	CLA	C3B-C4B-NB	2.60	112.93	110.52
14	cA	805	CLA	CHD-C4C-NC	2.60	128.30	124.20
14	A	805	CLA	CHD-C4C-NC	2.60	128.30	124.20
14	A	810	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
14	bA	807	CLA	CED-O2D-CGD	2.60	121.81	115.94
14	bA	805	CLA	CHD-C4C-NC	2.60	128.30	124.20
14	cB	837	CLA	C4C-C3C-C2C	-2.60	103.11	106.90
14	cA	810	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
14	bB	810	CLA	CED-O2D-CGD	2.60	121.81	115.94
14	bB	836	CLA	C4C-C3C-C2C	-2.59	103.11	106.90
14	bA	810	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
14	A	802	CLA	CBC-CAC-C3C	-2.59	105.28	112.43
14	cA	807	CLA	C3B-C4B-NB	2.59	112.92	110.52
14	bA	839	CLA	O2A-CGA-CBA	2.59	120.05	111.91
14	bB	804	CLA	CMB-C2B-C1B	2.59	129.32	125.37
14	A	818	CLA	CHB-C1B-C2B	-2.59	119.91	127.24
14	bA	818	CLA	CHB-C1B-C2B	-2.59	119.91	127.24
14	A	838	CLA	C2A-C1A-CHA	-2.59	119.32	123.86
14	A	817	CLA	C2A-C1A-CHA	-2.59	119.32	123.86
14	B	819	CLA	C3B-C4B-NB	2.59	112.92	110.52
14	cA	802	CLA	CBC-CAC-C3C	-2.59	105.28	112.43
14	B	804	CLA	CMB-C2B-C1B	2.59	129.32	125.37
14	cA	811	CLA	CMB-C2B-C1B	2.59	129.32	125.37
14	B	805	CLA	C4-C3-C5	2.59	119.63	115.27
14	bA	802	CLA	CBC-CAC-C3C	-2.59	105.28	112.43
14	A	811	CLA	C4C-C3C-C2C	-2.59	103.12	106.90
14	cA	839	CLA	O2A-CGA-CBA	2.59	120.04	111.91
14	A	803	CLA	C4C-C3C-C2C	-2.59	103.12	106.90
14	A	836	CLA	C4C-C3C-C2C	-2.59	103.12	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	810	CLA	CED-O2D-CGD	2.59	121.80	115.94
14	B	851	CLA	CHD-C4C-NC	2.59	128.29	124.20
14	cA	818	CLA	CHB-C1B-C2B	-2.59	119.92	127.24
14	B	803	CLA	O2A-CGA-CBA	2.59	120.04	111.91
14	A	839	CLA	O2A-CGA-CBA	2.59	120.03	111.91
14	bA	838	CLA	C2A-C1A-CHA	-2.59	119.33	123.86
14	bB	819	CLA	C3B-C4B-NB	2.59	112.92	110.52
14	A	802	CLA	O2A-CGA-O1A	-2.59	117.06	123.59
14	cA	807	CLA	CED-O2D-CGD	2.59	121.79	115.94
14	bB	851	CLA	CHD-C4C-NC	2.59	128.28	124.20
14	bA	841	CLA	O2A-CGA-O1A	-2.59	117.06	123.59
14	A	828	CLA	O2A-CGA-CBA	2.59	120.03	111.91
14	B	833	CLA	C3B-C4B-NB	2.59	112.92	110.52
14	bA	811	CLA	CMB-C2B-C1B	2.59	129.31	125.37
14	B	824	CLA	CHB-C4A-NA	2.59	128.09	124.51
14	bB	803	CLA	O2A-CGA-CBA	2.59	120.03	111.91
14	cB	811	CLA	CED-O2D-CGD	2.59	121.79	115.94
14	cB	805	CLA	CMB-C2B-C1B	2.59	129.31	125.37
14	bA	802	CLA	O2A-CGA-O1A	-2.59	117.06	123.59
14	cA	836	CLA	C4C-C3C-C2C	-2.59	103.13	106.90
14	cA	828	CLA	O2A-CGA-CBA	2.59	120.02	111.91
14	cB	804	CLA	O2A-CGA-CBA	2.59	120.02	111.91
14	A	807	CLA	C3B-C4B-NB	2.59	112.91	110.52
14	A	834	CLA	C3B-C4B-NB	2.59	112.91	110.52
14	bA	828	CLA	O2A-CGA-CBA	2.59	120.02	111.91
14	B	802	CLA	CED-O2D-CGD	2.58	121.78	115.94
14	cA	811	CLA	C4C-C3C-C2C	-2.58	103.13	106.90
14	bB	802	CLA	CED-O2D-CGD	2.58	121.78	115.94
14	B	801	CLA	C3B-C4B-NB	2.58	112.91	110.52
14	cA	838	CLA	C2A-C1A-CHA	-2.58	119.34	123.86
14	bA	836	CLA	C4C-C3C-C2C	-2.58	103.14	106.90
17	B	844	BCR	C37-C22-C23	2.58	122.14	118.08
14	cB	820	CLA	C3B-C4B-NB	2.58	112.91	110.52
14	cB	806	CLA	C4-C3-C5	2.58	119.61	115.27
13	bA	801	CL0	CMA-C3A-C2A	-2.58	103.42	113.83
13	cA	801	CL0	CMA-C3A-C2A	-2.58	103.42	113.83
17	I	101	BCR	C36-C18-C17	-2.58	119.31	122.92
14	cB	839	CLA	C2A-C1A-CHA	-2.58	119.35	123.86
17	bB	844	BCR	C37-C22-C23	2.58	122.14	118.08
13	A	801	CL0	CMA-C3A-C2A	-2.58	103.43	113.83
14	A	806	CLA	C2A-C1A-CHA	-2.58	119.35	123.86
14	bA	806	CLA	C2A-C1A-CHA	-2.58	119.35	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cB	801	CLA	CHD-C4C-NC	2.58	128.26	124.20
14	A	841	CLA	O2A-CGA-O1A	-2.58	117.09	123.59
14	bA	803	CLA	C4C-C3C-C2C	-2.58	103.14	106.90
14	bB	805	CLA	C4-C3-C5	2.57	119.60	115.27
14	bB	810	CLA	CMB-C2B-C1B	2.57	129.29	125.37
17	cM	101	BCR	C15-C14-C13	2.57	130.98	127.31
14	A	807	CLA	CED-O2D-CGD	2.57	121.76	115.94
14	cB	803	CLA	CED-O2D-CGD	2.57	121.76	115.94
14	L	201	CLA	CAA-C2A-C1A	2.57	120.40	111.97
14	cB	802	CLA	C3B-C4B-NB	2.57	112.90	110.52
14	cA	803	CLA	C4C-C3C-C2C	-2.57	103.15	106.90
14	bL	201	CLA	CAA-C2A-C1A	2.57	120.40	111.97
14	cB	850	CLA	CED-O2D-CGD	2.57	121.75	115.94
14	B	838	CLA	C2A-C1A-CHA	-2.57	119.37	123.86
14	cL	202	CLA	CAA-C2A-C1A	2.57	120.39	111.97
14	B	810	CLA	CMB-C2B-C1B	2.57	129.28	125.37
14	cA	827	CLA	O2A-CGA-CBA	2.57	119.97	111.91
14	bB	834	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
14	cB	832	CLA	CHC-C1C-C2C	-2.57	119.59	126.73
14	A	803	CLA	C2A-C1A-CHA	-2.57	119.37	123.86
14	bA	803	CLA	C2A-C1A-CHA	-2.57	119.37	123.86
14	cA	806	CLA	C2A-C1A-CHA	-2.57	119.37	123.86
14	cB	805	CLA	C4-C3-C5	2.57	118.92	115.98
14	cJ	101	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
14	B	831	CLA	CHC-C1C-C2C	-2.57	119.60	126.73
14	B	849	CLA	CED-O2D-CGD	2.57	121.74	115.94
14	A	827	CLA	O2A-CGA-CBA	2.57	119.96	111.91
14	J	101	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
14	bB	838	CLA	C2A-C1A-CHA	-2.57	119.37	123.86
14	bA	827	CLA	O2A-CGA-CBA	2.57	119.96	111.91
14	cB	835	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
14	bB	831	CLA	CHC-C1C-C2C	-2.56	119.61	126.73
14	bB	849	CLA	CED-O2D-CGD	2.56	121.74	115.94
17	cB	845	BCR	C37-C22-C23	2.56	122.12	118.08
17	bB	847	BCR	C16-C15-C14	2.56	128.72	123.47
17	bI	101	BCR	C36-C18-C17	-2.56	119.33	122.92
14	B	834	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
14	B	804	CLA	C4-C3-C5	2.56	118.91	115.98
14	bA	842	CLA	CHD-C4C-NC	2.56	128.24	124.20
14	cB	825	CLA	CHB-C4A-NA	2.56	128.05	124.51
14	cA	825	CLA	CMB-C2B-C1B	2.56	129.27	125.37
14	cB	811	CLA	CMB-C2B-C1B	2.56	129.27	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bA	852	CLA	CED-O2D-CGD	2.56	121.73	115.94
14	bB	804	CLA	C4-C3-C5	2.56	118.91	115.98
14	A	825	CLA	CMB-C2B-C1B	2.56	129.27	125.37
17	cI	101	BCR	C36-C18-C17	-2.56	119.34	122.92
14	cB	809	CLA	CAA-C2A-C3A	-2.56	105.77	112.78
14	cA	842	CLA	CHD-C4C-NC	2.56	128.24	124.20
14	bJ	101	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
14	B	808	CLA	CAA-C2A-C3A	-2.56	105.77	112.78
14	cA	841	CLA	O2A-CGA-O1A	-2.56	117.14	123.59
14	cA	852	CLA	CED-O2D-CGD	2.56	121.72	115.94
14	A	842	CLA	CHD-C4C-NC	2.56	128.23	124.20
14	A	841	CLA	C3B-C2B-C1B	-2.56	104.08	107.16
14	bA	825	CLA	CMB-C2B-C1B	2.56	129.26	125.37
17	cB	848	BCR	C16-C15-C14	2.56	128.71	123.47
14	bB	808	CLA	CAA-C2A-C3A	-2.55	105.78	112.78
14	cA	812	CLA	C2A-C1A-CHA	-2.55	119.39	123.86
14	bB	822	CLA	CHD-C4C-NC	2.55	128.23	124.20
14	A	852	CLA	CED-O2D-CGD	2.55	121.71	115.94
14	B	822	CLA	CHD-C4C-NC	2.55	128.23	124.20
14	L	202	CLA	CHD-C4C-NC	2.55	128.22	124.20
17	cB	848	BCR	C24-C23-C22	2.55	130.09	126.23
14	bA	812	CLA	C2A-C1A-CHA	-2.55	119.40	123.86
14	bA	811	CLA	CED-O2D-CGD	2.55	121.70	115.94
17	B	847	BCR	C24-C23-C22	2.55	130.09	126.23
17	cB	846	BCR	C36-C18-C17	-2.55	119.35	122.92
14	cA	804	CLA	O1D-CGD-CBD	-2.55	119.27	124.48
17	bM	101	BCR	C15-C14-C13	2.55	130.95	127.31
14	A	836	CLA	C2A-C1A-CHA	-2.55	119.40	123.86
14	A	804	CLA	CHD-C4C-NC	2.55	128.22	124.20
14	cB	824	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
17	B	847	BCR	C16-C15-C14	2.55	128.69	123.47
14	bB	802	CLA	CHB-C1B-NB	-2.55	121.56	124.26
14	cA	803	CLA	C2A-C1A-CHA	-2.55	119.41	123.86
14	bB	808	CLA	C2A-C3A-C4A	-2.55	97.76	101.87
14	A	811	CLA	CED-O2D-CGD	2.55	121.69	115.94
14	cB	803	CLA	CHB-C1B-NB	-2.54	121.56	124.26
14	B	805	CLA	O2D-CGD-O1D	-2.54	118.86	123.84
14	A	839	CLA	CMB-C2B-C1B	2.54	129.24	125.37
14	cB	801	CLA	C2A-C1A-CHA	-2.54	119.41	123.86
14	bB	812	CLA	CHC-C1C-C2C	-2.54	119.66	126.73
17	bA	846	BCR	C1-C6-C7	2.54	122.97	115.78
17	bB	844	BCR	C35-C13-C14	-2.54	119.36	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	812	CLA	C2A-C1A-CHA	-2.54	119.41	123.86
14	bA	804	CLA	CHD-C4C-NC	2.54	128.21	124.20
17	cA	846	BCR	C1-C6-C7	2.54	122.97	115.78
14	cB	806	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
17	A	846	BCR	C1-C6-C7	2.54	122.97	115.78
14	B	851	CLA	C2A-C1A-CHA	-2.54	119.41	123.86
14	cB	823	CLA	CHD-C4C-NC	2.54	128.21	124.20
14	B	802	CLA	CHB-C1B-NB	-2.54	121.57	124.26
14	cB	834	CLA	C3B-C4B-NB	2.54	112.87	110.52
17	B	844	BCR	C35-C13-C14	-2.54	119.36	122.92
14	bF	201	CLA	O2A-CGA-CBA	2.54	119.88	111.91
14	bB	815	CLA	CHD-C4C-NC	2.54	128.21	124.20
14	bB	805	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
14	B	808	CLA	C3B-C4B-NB	2.54	112.87	110.52
17	M	101	BCR	C15-C14-C13	2.54	130.94	127.31
14	cB	810	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
14	B	812	CLA	CHC-C1C-C2C	-2.54	119.68	126.73
14	B	815	CLA	CHD-C4C-NC	2.54	128.20	124.20
14	bB	823	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
14	cB	819	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
14	cB	819	CLA	CMB-C2B-C1B	2.54	129.24	125.37
14	B	818	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
14	cB	813	CLA	CHC-C1C-C2C	-2.54	119.68	126.73
17	cB	845	BCR	C35-C13-C14	-2.54	119.37	122.92
14	A	816	CLA	C2A-C1A-CHA	-2.54	119.42	123.86
14	bA	836	CLA	C2A-C1A-CHA	-2.54	119.42	123.86
17	bB	847	BCR	C24-C23-C22	2.54	130.07	126.23
14	bB	833	CLA	C3B-C4B-NB	2.54	112.87	110.52
14	cL	203	CLA	CHD-C4C-NC	2.54	128.20	124.20
14	bB	818	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
14	cA	811	CLA	CED-O2D-CGD	2.54	121.67	115.94
17	B	845	BCR	C36-C18-C17	-2.53	119.37	122.92
14	B	823	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
14	bB	818	CLA	CMB-C2B-C1B	2.53	129.23	125.37
14	B	801	CLA	CHC-C1C-C2C	-2.53	119.69	126.73
14	cB	822	CLA	CMB-C2B-C1B	2.53	129.23	125.37
14	cB	819	CLA	CMC-C2C-C1C	2.53	128.90	125.04
14	bB	851	CLA	C2A-C1A-CHA	-2.53	119.43	123.86
14	cA	804	CLA	CHD-C4C-NC	2.53	128.19	124.20
14	cB	816	CLA	CHD-C4C-NC	2.53	128.19	124.20
14	bA	816	CLA	C2A-C1A-CHA	-2.53	119.43	123.86
14	bL	202	CLA	CHD-C4C-NC	2.53	128.19	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	804	CLA	O1D-CGD-CBD	-2.53	119.31	124.48
14	cA	816	CLA	C2A-C1A-CHA	-2.53	119.43	123.86
14	A	832	CLA	C4-C3-C5	2.53	119.53	115.27
14	bA	841	CLA	C3B-C2B-C1B	-2.53	104.11	107.16
14	F	201	CLA	O2A-CGA-CBA	2.53	119.85	111.91
14	bA	839	CLA	CMB-C2B-C1B	2.53	129.22	125.37
14	bB	804	CLA	O1D-CGD-CBD	-2.53	119.31	124.48
14	cA	841	CLA	C3B-C2B-C1B	-2.53	104.11	107.16
14	cB	802	CLA	CHC-C1C-C2C	-2.53	119.70	126.73
14	B	809	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
14	bB	821	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
14	B	818	CLA	CMB-C2B-C1B	2.53	129.22	125.37
14	bA	804	CLA	O1D-CGD-CBD	-2.53	119.31	124.48
14	cB	817	CLA	C2A-C1A-CHA	-2.53	119.44	123.86
14	A	817	CLA	O2A-CGA-CBA	2.53	119.84	111.91
14	cA	836	CLA	C2A-C1A-CHA	-2.53	119.44	123.86
14	cB	825	CLA	O1D-CGD-CBD	-2.53	119.31	124.48
14	cF	201	CLA	O2A-CGA-CBA	2.53	119.84	111.91
14	cB	809	CLA	C3B-C4B-NB	2.53	112.86	110.52
14	bA	830	CLA	CHB-C4A-NA	2.53	128.01	124.51
14	B	824	CLA	O1D-CGD-CBD	-2.53	119.31	124.48
14	bB	801	CLA	CHC-C1C-C2C	-2.53	119.71	126.73
14	bB	821	CLA	CMB-C2B-C1B	2.53	129.22	125.37
14	bL	204	CLA	CMB-C2B-C1B	2.53	129.22	125.37
14	cA	827	CLA	C2A-C1A-CHA	-2.53	119.44	123.86
14	A	804	CLA	O1D-CGD-CBD	-2.53	119.32	124.48
14	cA	817	CLA	O2A-CGA-CBA	2.53	119.83	111.91
14	bA	817	CLA	O2A-CGA-CBA	2.52	119.83	111.91
14	bA	809	CLA	C4C-C3C-C2C	-2.52	103.22	106.90
14	bB	807	CLA	C4C-C3C-C2C	-2.52	103.22	106.90
14	B	803	CLA	O2A-CGA-O1A	-2.52	117.22	123.59
14	bB	802	CLA	CMA-C3A-C4A	-2.52	104.99	111.77
14	bB	806	CLA	C4C-C3C-C2C	-2.52	103.22	106.90
14	cA	832	CLA	C4-C3-C5	2.52	119.52	115.27
17	bB	845	BCR	C36-C18-C17	-2.52	119.39	122.92
14	B	821	CLA	CMB-C2B-C1B	2.52	129.21	125.37
14	B	806	CLA	C4C-C3C-C2C	-2.52	103.22	106.90
14	bB	808	CLA	C3B-C4B-NB	2.52	112.85	110.52
14	bA	826	CLA	O1D-CGD-CBD	-2.52	119.33	124.48
14	A	827	CLA	C2A-C1A-CHA	-2.52	119.45	123.86
14	bB	830	CLA	CHD-C4C-NC	2.52	128.17	124.20
14	cB	807	CLA	C4C-C3C-C2C	-2.52	103.22	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cB	803	CLA	CMA-C3A-C4A	-2.52	105.00	111.77
14	B	821	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
14	B	808	CLA	C2A-C3A-C4A	-2.52	97.80	101.87
14	cA	830	CLA	CHB-C4A-NA	2.52	127.99	124.51
14	cA	814	CLA	CHD-C4C-NC	2.52	128.17	124.20
14	bA	830	CLA	C4C-C3C-C2C	-2.52	103.23	106.90
14	B	830	CLA	CHD-C4C-NC	2.52	128.17	124.20
14	cB	831	CLA	CHD-C4C-NC	2.52	128.17	124.20
14	A	833	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
14	bB	809	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
14	A	820	CLA	CED-O2D-CGD	2.52	121.63	115.94
17	bB	841	BCR	C35-C13-C14	-2.52	119.40	122.92
14	bA	832	CLA	C4-C3-C5	2.52	119.50	115.27
14	cA	818	CLA	CMB-C2B-C1B	2.51	129.20	125.37
14	cA	839	CLA	CMB-C2B-C1B	2.51	129.20	125.37
14	B	825	CLA	C1-O2A-CGA	2.51	123.04	116.44
14	bA	806	CLA	C4C-C3C-C2C	-2.51	103.23	106.90
14	bB	810	CLA	C4C-C3C-C2C	-2.51	103.23	106.90
14	cA	833	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
14	bA	852	CLA	CHC-C1C-C2C	-2.51	119.75	126.73
14	bA	827	CLA	C2A-C1A-CHA	-2.51	119.46	123.86
14	B	819	CLA	CHD-C4C-NC	2.51	128.16	124.20
14	bB	803	CLA	CMB-C2B-C1B	2.51	129.20	125.37
14	cA	832	CLA	C3B-C4B-NB	2.51	112.85	110.52
14	cL	205	CLA	CMB-C2B-C1B	2.51	129.19	125.37
14	cA	808	CLA	C4C-C3C-C2C	-2.51	103.24	106.90
14	cA	826	CLA	O1D-CGD-CBD	-2.51	119.35	124.48
14	cB	804	CLA	O2A-CGA-O1A	-2.51	117.25	123.59
14	bA	839	CLA	CHD-C4C-NC	2.51	128.16	124.20
14	bX	201	CLA	CHD-C4C-NC	2.51	128.16	124.20
14	A	830	CLA	CHB-C4A-NA	2.51	127.98	124.51
14	B	816	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
17	A	848	BCR	C36-C18-C17	-2.51	119.41	122.92
14	bA	808	CLA	C4C-C3C-C2C	-2.51	103.24	106.90
14	cB	822	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
14	L	204	CLA	O2A-CGA-CBA	2.51	119.78	111.91
14	cA	830	CLA	C4C-C3C-C2C	-2.51	103.24	106.90
17	cL	206	BCR	C34-C9-C8	2.51	122.03	118.08
14	L	204	CLA	CMB-C2B-C1B	2.51	129.19	125.37
14	cB	805	CLA	O1D-CGD-CBD	-2.51	119.35	124.48
14	cB	808	CLA	C4C-C3C-C2C	-2.51	103.24	106.90
14	cB	820	CLA	CHD-C4C-NC	2.51	128.16	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	802	CLA	CMA-C3A-C4A	-2.51	105.03	111.77
17	bA	848	BCR	C36-C18-C17	-2.51	119.41	122.92
17	cA	848	BCR	C36-C18-C17	-2.51	119.41	122.92
14	bA	833	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
14	bB	803	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
14	cB	826	CLA	C1-O2A-CGA	2.51	123.02	116.44
14	B	807	CLA	C4C-C3C-C2C	-2.51	103.24	106.90
14	bB	819	CLA	CHD-C4C-NC	2.51	128.15	124.20
14	bA	820	CLA	CED-O2D-CGD	2.51	121.61	115.94
17	L	205	BCR	C34-C9-C8	2.51	122.03	118.08
17	bL	205	BCR	C34-C9-C8	2.51	122.03	118.08
14	cA	820	CLA	CED-O2D-CGD	2.51	121.61	115.94
17	B	841	BCR	C35-C13-C14	-2.51	119.41	122.92
14	bB	825	CLA	C1-O2A-CGA	2.51	123.02	116.44
14	bB	824	CLA	O1D-CGD-CBD	-2.51	119.36	124.48
14	cA	852	CLA	CHC-C1C-C2C	-2.51	119.77	126.73
14	bA	814	CLA	CHD-C4C-NC	2.51	128.15	124.20
14	B	803	CLA	CMB-C2B-C1B	2.50	129.18	125.37
14	bL	204	CLA	O2A-CGA-CBA	2.50	119.77	111.91
14	cL	205	CLA	O2A-CGA-CBA	2.50	119.77	111.91
14	A	808	CLA	O1D-CGD-CBD	-2.50	119.36	124.48
14	cX	201	CLA	CHD-C4C-NC	2.50	128.15	124.20
14	bB	816	CLA	C2A-C1A-CHA	-2.50	119.48	123.86
14	cX	201	CLA	CED-O2D-CGD	2.50	121.60	115.94
14	cA	806	CLA	C4C-C3C-C2C	-2.50	103.25	106.90
14	cB	811	CLA	C4C-C3C-C2C	-2.50	103.25	106.90
14	bB	826	CLA	CHB-C4A-NA	2.50	127.97	124.51
14	A	852	CLA	CHC-C1C-C2C	-2.50	119.78	126.73
14	bA	818	CLA	CMB-C2B-C1B	2.50	129.18	125.37
14	A	837	CLA	CHD-C4C-NC	2.50	128.15	124.20
14	cB	806	CLA	CHD-C4C-NC	2.50	128.15	124.20
17	bA	849	BCR	C8-C9-C10	2.50	122.78	118.94
14	bA	837	CLA	CHD-C4C-NC	2.50	128.15	124.20
14	A	808	CLA	C4C-C3C-C2C	-2.50	103.25	106.90
14	A	809	CLA	C4C-C3C-C2C	-2.50	103.25	106.90
14	bB	818	CLA	CMC-C2C-C1C	2.50	128.85	125.04
14	B	810	CLA	C4C-C3C-C2C	-2.50	103.25	106.90
14	B	839	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
14	cA	829	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
14	bX	201	CLA	CED-O2D-CGD	2.50	121.59	115.94
14	bB	825	CLA	C3B-C4B-NB	2.50	112.83	110.52
14	bB	823	CLA	O2A-CGA-CBA	2.50	119.75	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	839	CLA	CHD-C4C-NC	2.50	128.14	124.20
14	A	818	CLA	CMB-C2B-C1B	2.50	129.18	125.37
14	cA	815	CLA	CMB-C2B-C1B	2.50	129.18	125.37
14	A	830	CLA	C4C-C3C-C2C	-2.50	103.25	106.90
14	cA	809	CLA	C4C-C3C-C2C	-2.50	103.25	106.90
14	cB	818	CLA	O2A-CGA-CBA	2.50	119.75	111.91
14	cB	804	CLA	CMB-C2B-C1B	2.50	129.17	125.37
14	A	829	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
14	cA	852	CLA	C3B-C4B-NB	2.50	112.83	110.52
14	bB	814	CLA	C2A-C1A-CHA	-2.50	119.49	123.86
14	cB	840	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
14	cB	827	CLA	CHB-C4A-NA	2.50	127.96	124.51
14	B	817	CLA	O2A-CGA-CBA	2.50	119.74	111.91
14	A	814	CLA	CHD-C4C-NC	2.49	128.13	124.20
14	B	818	CLA	CMC-C2C-C1C	2.49	128.84	125.04
14	bB	839	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
17	cB	842	BCR	C35-C13-C14	-2.49	119.43	122.92
14	cB	809	CLA	C2A-C3A-C4A	-2.49	97.84	101.87
14	A	826	CLA	O1D-CGD-CBD	-2.49	119.38	124.48
14	cA	810	CLA	CHD-C4C-NC	2.49	128.13	124.20
14	bB	817	CLA	O2A-CGA-CBA	2.49	119.73	111.91
14	B	802	CLA	CMA-C3A-C2A	-2.49	103.78	113.83
17	bI	102	BCR	C34-C9-C8	2.49	122.00	118.08
14	A	806	CLA	C4C-C3C-C2C	-2.49	103.27	106.90
14	A	852	CLA	C3B-C4B-NB	2.49	112.83	110.52
14	B	806	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
14	cB	815	CLA	C2A-C1A-CHA	-2.49	119.50	123.86
14	A	810	CLA	CHD-C4C-NC	2.49	128.13	124.20
14	B	805	CLA	CHD-C4C-NC	2.49	128.13	124.20
14	bA	829	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
14	A	841	CLA	CHB-C4A-NA	2.49	127.95	124.51
14	B	814	CLA	C2A-C1A-CHA	-2.49	119.51	123.86
14	cA	837	CLA	CHD-C4C-NC	2.49	128.13	124.20
14	A	821	CLA	CMB-C2B-C1B	2.49	129.16	125.37
14	B	823	CLA	O2A-CGA-CBA	2.49	119.72	111.91
14	A	841	CLA	CBC-CAC-C3C	-2.49	105.57	112.43
14	cA	834	CLA	CMB-C2B-C1B	2.49	129.16	125.37
14	A	820	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
14	A	839	CLA	CHD-C4C-NC	2.49	128.12	124.20
14	X	201	CLA	CED-O2D-CGD	2.49	121.56	115.94
14	bB	806	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
14	cB	824	CLA	O2A-CGA-CBA	2.49	119.71	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	X	201	CLA	CHD-C4C-NC	2.49	128.12	124.20
14	bB	802	CLA	CMA-C3A-C2A	-2.49	103.80	113.83
13	bA	801	CL0	C3B-C4B-NB	2.49	112.82	110.52
14	bB	805	CLA	CHD-C4C-NC	2.49	128.12	124.20
17	cI	102	BCR	C34-C9-C8	2.49	122.00	118.08
14	L	202	CLA	CMB-C2B-C1B	2.49	129.16	125.37
17	I	102	BCR	C34-C9-C8	2.49	121.99	118.08
14	B	825	CLA	C3B-C4B-NB	2.49	112.82	110.52
14	bA	841	CLA	CBC-CAC-C3C	-2.49	105.58	112.43
14	B	833	CLA	CHD-C4C-NC	2.49	128.12	124.20
14	cB	807	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
14	B	826	CLA	CHB-C4A-NA	2.48	127.95	124.51
14	B	816	CLA	CHB-C1B-C2B	-2.48	120.22	127.24
14	cB	837	CLA	CED-O2D-CGD	2.48	121.56	115.94
14	B	827	CLA	O2A-CGA-CBA	2.48	119.70	111.91
14	bB	827	CLA	O2A-CGA-CBA	2.48	119.70	111.91
14	B	851	CLA	C3B-C4B-NB	2.48	112.82	110.52
14	bA	808	CLA	O1D-CGD-CBD	-2.48	119.41	124.48
13	bA	801	CL0	O2A-CGA-CBA	2.48	119.70	111.91
14	A	803	CLA	O1D-CGD-CBD	-2.48	119.41	124.48
14	cA	816	CLA	CHD-C4C-NC	2.48	128.11	124.20
14	bB	839	CLA	C5-C3-C2	-2.48	116.10	121.12
14	bA	810	CLA	CHD-C4C-NC	2.48	128.11	124.20
14	bA	816	CLA	CHD-C4C-NC	2.48	128.11	124.20
13	cA	801	CL0	O2A-CGA-CBA	2.48	119.69	111.91
14	A	812	CLA	CMC-C2C-C1C	2.48	128.82	125.04
14	bB	824	CLA	CED-O2D-CGD	2.48	121.55	115.94
14	cB	805	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
14	cA	804	CLA	CMB-C2B-C1B	2.48	129.15	125.37
14	cB	803	CLA	CMA-C3A-C2A	-2.48	103.82	113.83
14	cA	841	CLA	CHB-C4A-NA	2.48	127.94	124.51
17	A	849	BCR	C8-C9-C10	2.48	122.75	118.94
14	cA	824	CLA	O2A-CGA-CBA	2.48	119.69	111.91
14	A	816	CLA	CHD-C4C-NC	2.48	128.11	124.20
14	cJ	102	CLA	CHD-C4C-NC	2.48	128.11	124.20
14	bB	816	CLA	CHB-C1B-C2B	-2.48	120.23	127.24
14	cA	821	CLA	CMB-C2B-C1B	2.48	129.15	125.37
14	cA	841	CLA	CBC-CAC-C3C	-2.48	105.60	112.43
14	bJ	102	CLA	CHD-C4C-NC	2.48	128.11	124.20
14	A	824	CLA	C4-C3-C5	2.48	119.44	115.27
14	cB	817	CLA	CHB-C1B-C2B	-2.48	120.24	127.24
14	B	824	CLA	CED-O2D-CGD	2.48	121.54	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	836	CLA	CED-O2D-CGD	2.48	121.54	115.94
14	A	835	CLA	CHD-C4C-NC	2.48	128.11	124.20
14	bA	820	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
14	cA	820	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
14	cB	828	CLA	O2A-CGA-CBA	2.48	119.68	111.91
14	B	818	CLA	CED-O2D-CGD	2.48	121.54	115.94
14	cB	819	CLA	CED-O2D-CGD	2.48	121.54	115.94
14	bA	804	CLA	CMB-C2B-C1B	2.48	129.14	125.37
14	bA	824	CLA	C4-C3-C5	2.48	119.44	115.27
14	A	837	CLA	O2A-CGA-CBA	2.48	119.68	111.91
14	bA	821	CLA	CMB-C2B-C1B	2.48	129.14	125.37
14	bB	833	CLA	CHD-C4C-NC	2.48	128.11	124.20
14	bB	818	CLA	CED-O2D-CGD	2.48	121.54	115.94
14	cA	803	CLA	O1D-CGD-CBD	-2.47	119.42	124.48
14	bA	812	CLA	CMC-C2C-C1C	2.47	128.81	125.04
13	A	801	CL0	O2A-CGA-CBA	2.47	119.67	111.91
14	B	827	CLA	CHD-C4C-NC	2.47	128.10	124.20
14	A	804	CLA	CHB-C4A-NA	2.47	127.93	124.51
14	cA	837	CLA	O2A-CGA-CBA	2.47	119.67	111.91
14	A	833	CLA	C4-C3-C5	2.47	119.43	115.27
14	bB	851	CLA	C3B-C4B-NB	2.47	112.81	110.52
14	A	824	CLA	O2A-CGA-CBA	2.47	119.67	111.91
14	bB	836	CLA	CED-O2D-CGD	2.47	121.53	115.94
14	bA	803	CLA	O1D-CGD-CBD	-2.47	119.42	124.48
14	bA	832	CLA	C3B-C4B-NB	2.47	112.81	110.52
14	cB	826	CLA	C3B-C4B-NB	2.47	112.81	110.52
14	A	815	CLA	CMB-C2B-C1B	2.47	129.13	125.37
14	bB	827	CLA	CHD-C4C-NC	2.47	128.10	124.20
14	B	804	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
14	B	839	CLA	C5-C3-C2	-2.47	116.11	121.12
14	cA	812	CLA	CMC-C2C-C1C	2.47	128.80	125.04
14	bA	824	CLA	O2A-CGA-CBA	2.47	119.67	111.91
14	bA	837	CLA	O2A-CGA-CBA	2.47	119.67	111.91
14	A	815	CLA	CHD-C4C-NC	2.47	128.10	124.20
14	cA	818	CLA	CHD-C4C-NC	2.47	128.10	124.20
17	bB	842	BCR	C15-C16-C17	2.47	128.54	123.47
14	A	821	CLA	CHD-C4C-NC	2.47	128.10	124.20
14	bA	815	CLA	CHD-C4C-NC	2.47	128.10	124.20
14	bA	818	CLA	CHD-C4C-NC	2.47	128.10	124.20
14	bA	815	CLA	CMB-C2B-C1B	2.47	129.13	125.37
14	cA	808	CLA	O1D-CGD-CBD	-2.47	119.43	124.48
14	bL	202	CLA	CMB-C2B-C1B	2.47	129.13	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	822	CLA	CHB-C4A-NA	2.47	127.93	124.51
14	A	818	CLA	CHD-C4C-NC	2.47	128.10	124.20
14	cB	840	CLA	C5-C3-C2	-2.47	116.12	121.12
14	bB	827	CLA	CHB-C4A-NA	2.47	127.93	124.51
13	A	801	CL0	C3B-C4B-NB	2.47	112.81	110.52
14	cB	825	CLA	CED-O2D-CGD	2.47	121.52	115.94
13	cA	801	CL0	C3B-C4B-NB	2.47	112.81	110.52
14	cB	801	CLA	C3B-C4B-NB	2.47	112.81	110.52
14	J	102	CLA	CHD-C4C-NC	2.47	128.09	124.20
14	bA	833	CLA	C4-C3-C5	2.47	119.42	115.27
14	bA	834	CLA	CMB-C2B-C1B	2.47	129.13	125.37
14	bA	852	CLA	C3B-C4B-NB	2.47	112.80	110.52
17	B	845	BCR	C15-C16-C17	2.47	128.53	123.47
14	A	805	CLA	CED-O2D-CGD	2.47	121.52	115.94
17	cA	849	BCR	C8-C9-C10	2.47	122.73	118.94
14	bA	821	CLA	CHD-C4C-NC	2.47	128.09	124.20
14	cA	815	CLA	CHD-C4C-NC	2.47	128.09	124.20
14	bB	804	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
14	cB	828	CLA	CHD-C4C-NC	2.47	128.09	124.20
17	cB	843	BCR	C15-C16-C17	2.47	128.52	123.47
14	cB	823	CLA	CHB-C4A-NA	2.47	127.92	124.51
14	cL	203	CLA	CMB-C2B-C1B	2.46	129.12	125.37
14	bA	841	CLA	CHB-C4A-NA	2.46	127.92	124.51
14	cF	201	CLA	C2A-C1A-CHA	-2.46	119.55	123.86
14	cA	824	CLA	C4-C3-C5	2.46	119.41	115.27
14	cB	834	CLA	CHD-C4C-NC	2.46	128.08	124.20
14	A	832	CLA	CHB-C4A-NA	2.46	127.92	124.51
14	B	833	CLA	CMB-C2B-C1B	2.46	129.12	125.37
14	cA	805	CLA	CED-O2D-CGD	2.46	121.51	115.94
14	cA	811	CLA	CHD-C4C-NC	2.46	128.08	124.20
14	cA	833	CLA	C4-C3-C5	2.46	119.41	115.27
14	bA	835	CLA	CHD-C4C-NC	2.46	128.08	124.20
14	A	804	CLA	CMB-C2B-C1B	2.46	129.12	125.37
17	cB	846	BCR	C15-C16-C17	2.46	128.51	123.47
14	cA	813	CLA	O1D-CGD-CBD	-2.46	119.45	124.48
14	B	827	CLA	CHB-C4A-NA	2.46	127.91	124.51
14	cB	828	CLA	CHB-C4A-NA	2.46	127.91	124.51
14	bA	811	CLA	CHD-C4C-NC	2.46	128.08	124.20
14	B	827	CLA	CMB-C2B-C1B	2.46	129.11	125.37
14	B	832	CLA	CHD-C4C-NC	2.46	128.08	124.20
14	B	833	CLA	CED-O2D-CGD	2.46	121.50	115.94
14	cB	825	CLA	CHD-C4C-NC	2.46	128.08	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	836	CLA	C4-C3-C5	2.46	118.79	115.98
14	A	811	CLA	CHD-C4C-NC	2.46	128.08	124.20
14	cB	833	CLA	CHD-C4C-NC	2.46	128.08	124.20
14	B	807	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
17	B	842	BCR	C15-C16-C17	2.46	128.51	123.47
14	bB	833	CLA	CED-O2D-CGD	2.46	121.49	115.94
14	A	818	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
14	bA	832	CLA	CHB-C4A-NA	2.46	127.91	124.51
14	bB	827	CLA	CMB-C2B-C1B	2.46	129.11	125.37
14	cA	828	CLA	CMB-C2B-C1B	2.46	129.11	125.37
14	cB	812	CLA	CMB-C2B-C1B	2.46	129.11	125.37
14	cA	802	CLA	CHB-C4A-NA	2.46	127.91	124.51
14	bA	818	CLA	C2A-C1A-CHA	-2.46	119.57	123.86
14	cA	832	CLA	CHB-C4A-NA	2.46	127.91	124.51
14	cA	839	CLA	C1-C2-C3	-2.46	121.80	126.04
14	B	811	CLA	CMB-C2B-C1B	2.46	129.11	125.37
14	cA	835	CLA	CHD-C4C-NC	2.45	128.07	124.20
14	bA	839	CLA	C1-C2-C3	-2.45	121.80	126.04
14	bB	822	CLA	CHB-C4A-NA	2.45	127.91	124.51
14	bA	836	CLA	C4-C3-C5	2.45	118.79	115.98
14	bA	832	CLA	CED-O2D-CGD	2.45	121.49	115.94
14	bB	810	CLA	CHD-C4C-NC	2.45	128.07	124.20
14	cB	828	CLA	CMB-C2B-C1B	2.45	129.10	125.37
14	cA	804	CLA	CHB-C4A-NA	2.45	127.90	124.51
14	bA	830	CLA	O1D-CGD-CBD	-2.45	119.47	124.48
14	B	810	CLA	CHD-C4C-NC	2.45	128.07	124.20
14	cB	834	CLA	CMB-C2B-C1B	2.45	129.10	125.37
14	F	201	CLA	C2A-C1A-CHA	-2.45	119.57	123.86
14	bB	832	CLA	CHD-C4C-NC	2.45	128.07	124.20
14	bA	805	CLA	CED-O2D-CGD	2.45	121.48	115.94
14	bA	804	CLA	CHB-C4A-NA	2.45	127.90	124.51
14	cA	821	CLA	CHD-C4C-NC	2.45	128.07	124.20
17	bB	845	BCR	C15-C16-C17	2.45	128.50	123.47
14	A	828	CLA	CMB-C2B-C1B	2.45	129.10	125.37
14	bB	822	CLA	CMB-C2B-C1B	2.45	129.10	125.37
14	bB	811	CLA	CMB-C2B-C1B	2.45	129.10	125.37
14	A	832	CLA	C3B-C4B-NB	2.45	112.79	110.52
14	cB	808	CLA	C2A-C1A-CHA	-2.45	119.58	123.86
14	bB	833	CLA	CMB-C2B-C1B	2.45	129.10	125.37
14	cA	824	CLA	CHD-C4C-NC	2.45	128.06	124.20
14	cA	836	CLA	C4-C3-C5	2.45	118.78	115.98
14	A	834	CLA	CMB-C2B-C1B	2.45	129.10	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cB	834	CLA	CED-O2D-CGD	2.45	121.48	115.94
14	A	839	CLA	C1-C2-C3	-2.45	121.81	126.04
14	A	802	CLA	CHB-C4A-NA	2.45	127.90	124.51
14	cB	815	CLA	O1D-CGD-CBD	-2.45	119.47	124.48
17	cJ	103	BCR	C21-C20-C19	2.45	130.86	123.22
14	cB	823	CLA	CMB-C2B-C1B	2.45	129.10	125.37
14	cA	832	CLA	CED-O2D-CGD	2.45	121.47	115.94
14	B	830	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
14	cB	811	CLA	CHD-C4C-NC	2.45	128.06	124.20
14	cA	818	CLA	C2A-C1A-CHA	-2.45	119.58	123.86
14	A	826	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
17	B	850	BCR	C37-C22-C23	2.44	121.93	118.08
14	A	832	CLA	CED-O2D-CGD	2.44	121.47	115.94
14	B	823	CLA	CED-O2D-CGD	2.44	121.47	115.94
14	A	834	CLA	C2A-C1A-CHA	-2.44	119.58	123.86
14	cA	830	CLA	O1D-CGD-CBD	-2.44	119.48	124.48
14	bF	201	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
14	B	822	CLA	CMB-C2B-C1B	2.44	129.09	125.37
14	bB	826	CLA	CMB-C2B-C1B	2.44	129.09	125.37
17	bB	850	BCR	C35-C13-C14	-2.44	119.50	122.92
14	cB	824	CLA	CED-O2D-CGD	2.44	121.46	115.94
17	B	850	BCR	C35-C13-C14	-2.44	119.50	122.92
14	A	852	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
14	cA	834	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
17	bJ	103	BCR	C21-C20-C19	2.44	130.84	123.22
14	bA	852	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
14	A	813	CLA	O1D-CGD-CBD	-2.44	119.49	124.48
14	bA	802	CLA	CHB-C4A-NA	2.44	127.89	124.51
14	bA	828	CLA	CMB-C2B-C1B	2.44	129.09	125.37
14	B	819	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
14	bB	807	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
14	A	824	CLA	CHD-C4C-NC	2.44	128.05	124.20
14	cJ	101	CLA	CHD-C4C-NC	2.44	128.05	124.20
14	B	814	CLA	O1D-CGD-CBD	-2.44	119.50	124.48
14	bB	830	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
14	B	824	CLA	CHD-C4C-NC	2.44	128.04	124.20
14	bB	831	CLA	CHD-C4C-NC	2.44	128.04	124.20
14	cB	813	CLA	C2A-C1A-CHA	-2.44	119.60	123.86
14	bA	813	CLA	O1D-CGD-CBD	-2.44	119.50	124.48
14	bB	814	CLA	O1D-CGD-CBD	-2.44	119.50	124.48
14	bJ	101	CLA	CHD-C4C-NC	2.44	128.04	124.20
14	bB	823	CLA	CED-O2D-CGD	2.44	121.44	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	J	103	BCR	C21-C20-C19	2.43	130.81	123.22
14	B	808	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
14	J	101	CLA	CHD-C4C-NC	2.43	128.04	124.20
14	cB	831	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
14	cB	820	CLA	C2A-C1A-CHA	-2.43	119.60	123.86
14	cB	827	CLA	CMB-C2B-C1B	2.43	129.07	125.37
14	B	831	CLA	CHD-C4C-NC	2.43	128.03	124.20
14	bA	824	CLA	CHD-C4C-NC	2.43	128.03	124.20
14	bB	824	CLA	CHD-C4C-NC	2.43	128.03	124.20
14	bB	819	CLA	C2A-C1A-CHA	-2.43	119.61	123.86
14	bB	818	CLA	CHD-C4C-NC	2.43	128.03	124.20
14	cB	832	CLA	CHD-C4C-NC	2.43	128.03	124.20
14	bA	834	CLA	C2A-C1A-CHA	-2.43	119.61	123.86
14	cA	802	CLA	C1-O2A-CGA	2.43	122.82	116.44
17	cB	851	BCR	C37-C22-C23	2.43	121.90	118.08
14	cB	801	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
14	bB	808	CLA	O2A-CGA-O1A	-2.43	117.47	123.59
14	bF	201	CLA	CED-O2D-CGD	2.43	121.43	115.94
17	cI	101	BCR	C15-C16-C17	2.43	128.45	123.47
14	cA	852	CLA	C2A-C1A-CHA	-2.43	119.61	123.86
14	A	830	CLA	O1D-CGD-CBD	-2.43	119.52	124.48
14	cB	809	CLA	O2A-CGA-O1A	-2.43	117.47	123.59
14	cA	826	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
14	A	802	CLA	CHD-C4C-NC	2.43	128.03	124.20
14	cA	816	CLA	CMB-C2B-C1B	2.43	129.06	125.37
14	F	201	CLA	CED-O2D-CGD	2.43	121.42	115.94
14	cF	201	CLA	CED-O2D-CGD	2.43	121.42	115.94
14	B	821	CLA	CHB-C4A-NA	2.43	127.87	124.51
17	cB	851	BCR	C35-C13-C14	-2.43	119.53	122.92
14	B	812	CLA	C2A-C1A-CHA	-2.42	119.62	123.86
17	bB	850	BCR	C37-C22-C23	2.42	121.90	118.08
14	A	816	CLA	CMB-C2B-C1B	2.42	129.06	125.37
14	A	827	CLA	CHD-C4C-NC	2.42	128.02	124.20
14	bA	802	CLA	C1-O2A-CGA	2.42	122.80	116.44
17	cA	848	BCR	C15-C16-C17	2.42	128.44	123.47
14	cB	822	CLA	CHB-C4A-NA	2.42	127.86	124.51
14	B	826	CLA	CMB-C2B-C1B	2.42	129.06	125.37
17	bA	848	BCR	C15-C16-C17	2.42	128.43	123.47
14	bA	826	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
14	cB	823	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
14	A	818	CLA	O2A-CGA-O1A	-2.42	117.48	123.59
14	bA	826	CLA	CHB-C4A-NA	2.42	127.86	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	806	CLA	CED-O2D-CGD	2.42	121.41	115.94
14	bL	203	CLA	CAC-C3C-C4C	2.42	127.95	124.81
14	cB	819	CLA	CHD-C4C-NC	2.42	128.02	124.20
14	cB	821	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
14	cA	826	CLA	CHB-C4A-NA	2.42	127.86	124.51
17	J	103	BCR	C20-C21-C22	2.42	130.76	127.31
14	bB	851	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
14	cL	204	CLA	CAC-C3C-C4C	2.42	127.95	124.81
14	A	802	CLA	C1-O2A-CGA	2.42	122.79	116.44
14	A	836	CLA	CMB-C2B-C1B	2.42	129.05	125.37
14	B	820	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
14	bA	802	CLA	CHD-C4C-NC	2.42	128.01	124.20
17	A	848	BCR	C15-C16-C17	2.42	128.43	123.47
14	cA	827	CLA	CHD-C4C-NC	2.42	128.01	124.20
14	B	822	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
14	bA	818	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
14	cA	818	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
14	bB	833	CLA	CHB-C4A-NA	2.42	127.85	124.51
14	B	818	CLA	CHD-C4C-NC	2.42	128.01	124.20
14	bA	830	CLA	CED-O2D-CGD	2.42	121.40	115.94
14	bA	816	CLA	CMB-C2B-C1B	2.41	129.05	125.37
14	cA	814	CLA	C2A-C1A-CHA	-2.41	119.64	123.86
14	A	803	CLA	CMB-C2B-C1B	2.41	129.05	125.37
14	cA	836	CLA	CMB-C2B-C1B	2.41	129.05	125.37
14	cA	806	CLA	CED-O2D-CGD	2.41	121.40	115.94
14	cB	834	CLA	CHB-C4A-NA	2.41	127.85	124.51
14	B	851	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
14	bB	836	CLA	C2A-C1A-CHA	-2.41	119.64	123.86
14	cA	815	CLA	C2A-C1A-CHA	-2.41	119.64	123.86
14	cA	812	CLA	CHB-C4A-NA	2.41	127.85	124.51
14	bB	820	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
14	bB	822	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
17	bI	101	BCR	C15-C16-C17	2.41	128.42	123.47
17	bA	849	BCR	C15-C14-C13	2.41	130.75	127.31
14	A	826	CLA	CHB-C4A-NA	2.41	127.85	124.51
14	bA	814	CLA	C2A-C1A-CHA	-2.41	119.64	123.86
14	bB	821	CLA	CHB-C4A-NA	2.41	127.85	124.51
17	I	101	BCR	C15-C16-C17	2.41	128.41	123.47
17	cM	101	BCR	C16-C15-C14	2.41	128.41	123.47
14	A	812	CLA	CHB-C4A-NA	2.41	127.85	124.51
14	bA	812	CLA	CHB-C4A-NA	2.41	127.85	124.51
14	cL	204	CLA	O2D-CGD-O1D	-2.41	119.13	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cB	801	CLA	CHB-C1B-C2B	-2.41	120.43	127.24
14	bA	806	CLA	CED-O2D-CGD	2.41	121.39	115.94
14	bB	812	CLA	C2A-C1A-CHA	-2.41	119.64	123.86
14	cA	802	CLA	CHD-C4C-NC	2.41	128.00	124.20
14	bB	826	CLA	CED-O2D-CGD	2.41	121.39	115.94
14	cB	827	CLA	CED-O2D-CGD	2.41	121.39	115.94
14	B	826	CLA	CED-O2D-CGD	2.41	121.39	115.94
14	bA	827	CLA	CHD-C4C-NC	2.41	128.00	124.20
14	bB	812	CLA	CHB-C1B-C2B	-2.41	120.43	127.24
14	bA	803	CLA	CHD-C4C-NC	2.41	128.00	124.20
14	cB	813	CLA	CHB-C1B-C2B	-2.41	120.44	127.24
14	bA	831	CLA	CHD-C4C-NC	2.41	128.00	124.20
14	B	817	CLA	CMC-C2C-C1C	2.41	128.71	125.04
14	B	836	CLA	C2A-C1A-CHA	-2.41	119.65	123.86
14	bA	803	CLA	CMB-C2B-C1B	2.41	129.03	125.37
14	cA	830	CLA	CED-O2D-CGD	2.41	121.38	115.94
14	cB	837	CLA	C2A-C1A-CHA	-2.41	119.65	123.86
14	bB	851	CLA	CHB-C1B-C2B	-2.41	120.44	127.24
14	cA	803	CLA	CMB-C2B-C1B	2.41	129.03	125.37
14	B	812	CLA	CHB-C1B-C2B	-2.41	120.44	127.24
17	cB	848	BCR	C36-C18-C17	-2.41	119.55	122.92
14	bB	836	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
14	bA	826	CLA	CMB-C2B-C1B	2.40	129.03	125.37
14	bA	836	CLA	CMB-C2B-C1B	2.40	129.03	125.37
14	A	831	CLA	CHD-C4C-NC	2.40	127.99	124.20
14	B	851	CLA	CHB-C1B-C2B	-2.40	120.45	127.24
14	bL	203	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
14	cB	832	CLA	O2A-CGA-CBA	2.40	119.45	111.91
14	A	820	CLA	CHD-C4C-NC	2.40	127.99	124.20
14	cB	817	CLA	CHD-C4C-NC	2.40	127.99	124.20
14	cB	837	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
14	A	815	CLA	C2A-C1A-CHA	-2.40	119.66	123.86
14	B	833	CLA	CHB-C4A-NA	2.40	127.83	124.51
17	bM	101	BCR	C16-C15-C14	2.40	128.39	123.47
14	A	830	CLA	CED-O2D-CGD	2.40	121.37	115.94
17	cA	849	BCR	C15-C14-C13	2.40	130.74	127.31
14	bA	829	CLA	CHD-C4C-NC	2.40	127.98	124.20
14	B	831	CLA	O2A-CGA-CBA	2.40	119.44	111.91
14	bB	831	CLA	O2A-CGA-CBA	2.40	119.44	111.91
14	cA	826	CLA	CMB-C2B-C1B	2.40	129.02	125.37
17	A	849	BCR	C15-C14-C13	2.40	130.73	127.31
14	cA	820	CLA	CHD-C4C-NC	2.40	127.98	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	831	CLA	CHD-C4C-NC	2.40	127.98	124.20
14	bA	804	CLA	C2A-C1A-CHA	-2.40	119.67	123.86
14	cX	201	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
14	B	836	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
14	bB	816	CLA	CHD-C4C-NC	2.40	127.98	124.20
14	B	816	CLA	CHD-C4C-NC	2.40	127.98	124.20
14	bB	812	CLA	CHD-C4C-NC	2.40	127.98	124.20
14	cA	829	CLA	CHD-C4C-NC	2.40	127.98	124.20
17	bB	847	BCR	C36-C18-C17	-2.40	119.57	122.92
14	cA	804	CLA	C2A-C1A-CHA	-2.40	119.67	123.86
14	bA	820	CLA	CHD-C4C-NC	2.40	127.98	124.20
14	B	817	CLA	CHB-C4A-NA	2.40	127.82	124.51
17	cJ	103	BCR	C20-C21-C22	2.39	130.73	127.31
14	L	203	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
14	L	203	CLA	CHD-C4C-NC	2.39	127.98	124.20
14	cL	204	CLA	CHD-C4C-NC	2.39	127.98	124.20
14	L	203	CLA	CAC-C3C-C4C	2.39	127.92	124.81
14	bA	815	CLA	C2A-C1A-CHA	-2.39	119.67	123.86
17	bJ	103	BCR	C20-C21-C22	2.39	130.73	127.31
14	cA	831	CLA	C1-O2A-CGA	2.39	122.72	116.44
14	A	826	CLA	CMB-C2B-C1B	2.39	129.01	125.37
17	B	847	BCR	C36-C18-C17	-2.39	119.57	122.92
14	A	829	CLA	CHD-C4C-NC	2.39	127.97	124.20
17	M	101	BCR	C16-C15-C14	2.39	128.38	123.47
14	A	804	CLA	C2A-C1A-CHA	-2.39	119.68	123.86
14	A	814	CLA	C2A-C1A-CHA	-2.39	119.68	123.86
14	cB	818	CLA	CMC-C2C-C1C	2.39	128.68	125.04
14	bL	203	CLA	CHD-C4C-NC	2.39	127.97	124.20
14	cA	816	CLA	CED-O2D-CGD	2.39	121.35	115.94
14	bA	814	CLA	CMB-C2B-C1B	2.39	129.01	125.37
14	A	831	CLA	C1-O2A-CGA	2.39	122.72	116.44
14	bA	831	CLA	C1-O2A-CGA	2.39	122.72	116.44
14	bB	806	CLA	C2A-C1A-CHA	-2.39	119.68	123.86
14	X	201	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
14	bB	817	CLA	CHB-C4A-NA	2.39	127.81	124.51
14	cB	819	CLA	C3B-C4B-NB	2.39	112.73	110.52
14	cB	818	CLA	CHB-C4A-NA	2.38	127.81	124.51
14	bF	201	CLA	C3B-C4B-NB	2.38	112.73	110.52
14	bB	817	CLA	CMC-C2C-C1C	2.38	128.67	125.04
14	cA	836	CLA	CHB-C4A-NA	2.38	127.81	124.51
14	B	812	CLA	CHD-C4C-NC	2.38	127.96	124.20
14	cA	803	CLA	CHD-C4C-NC	2.38	127.96	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	833	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
17	B	845	BCR	C16-C17-C18	2.38	130.71	127.31
14	A	803	CLA	CHD-C4C-NC	2.38	127.96	124.20
14	cB	813	CLA	CHD-C4C-NC	2.38	127.96	124.20
14	bX	201	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
14	A	832	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
14	B	806	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
14	B	818	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
17	bB	844	BCR	C36-C18-C17	-2.38	119.59	122.92
14	A	816	CLA	CED-O2D-CGD	2.38	121.32	115.94
14	cB	829	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
17	cB	845	BCR	C36-C18-C17	-2.38	119.59	122.92
14	cB	807	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
14	cB	834	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
14	bA	830	CLA	CHD-C4C-NC	2.37	127.95	124.20
14	A	831	CLA	CMB-C2B-C1B	2.37	128.99	125.37
14	A	815	CLA	O2D-CGD-O1D	-2.37	119.19	123.84
17	cB	846	BCR	C16-C17-C18	2.37	130.70	127.31
14	bA	832	CLA	C2A-C1A-CHA	-2.37	119.71	123.86
14	bB	828	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
14	bB	813	CLA	CED-O2D-CGD	2.37	121.30	115.94
14	bB	833	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
14	bA	820	CLA	CHB-C1B-C2B	-2.37	120.54	127.24
14	bA	816	CLA	CED-O2D-CGD	2.37	121.30	115.94
14	bA	831	CLA	CMB-C2B-C1B	2.37	128.98	125.37
14	cA	814	CLA	O1D-CGD-CBD	-2.37	119.63	124.48
14	B	828	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
14	cA	831	CLA	CMB-C2B-C1B	2.37	128.98	125.37
17	B	844	BCR	C36-C18-C17	-2.37	119.60	122.92
14	cB	819	CLA	C2A-C1A-CHA	-2.37	119.72	123.86
14	bB	832	CLA	C3B-C4B-NB	2.37	112.71	110.52
14	cA	832	CLA	C2A-C1A-CHA	-2.37	119.72	123.86
14	B	820	CLA	CMB-C2B-C1B	2.37	128.98	125.37
14	cB	814	CLA	CED-O2D-CGD	2.37	121.29	115.94
14	bB	820	CLA	CMB-C2B-C1B	2.37	128.97	125.37
14	B	832	CLA	C3B-C4B-NB	2.37	112.71	110.52
14	bB	825	CLA	O1D-CGD-CBD	-2.37	119.64	124.48
14	cB	838	CLA	CHD-C4C-NC	2.37	127.93	124.20
14	A	814	CLA	CMB-C2B-C1B	2.37	128.97	125.37
14	A	820	CLA	CHB-C1B-C2B	-2.37	120.55	127.24
14	bB	818	CLA	C2A-C1A-CHA	-2.36	119.72	123.86
14	cB	826	CLA	O1D-CGD-CBD	-2.36	119.65	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bA	808	CLA	CHB-C4A-NA	2.36	127.78	124.51
14	A	839	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
14	bA	833	CLA	CMB-C2B-C1B	2.36	128.97	125.37
14	cB	814	CLA	O1D-CGD-CBD	-2.36	119.65	124.48
14	F	201	CLA	C3B-C4B-NB	2.36	112.71	110.52
14	bA	839	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
14	cB	833	CLA	C3B-C4B-NB	2.36	112.70	110.52
14	B	827	CLA	CBA-CAA-C2A	2.36	120.83	113.86
14	bB	824	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
14	cA	839	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
14	cB	828	CLA	CBA-CAA-C2A	2.36	120.83	113.86
14	cB	821	CLA	CMB-C2B-C1B	2.36	128.96	125.37
14	A	830	CLA	CHD-C4C-NC	2.36	127.92	124.20
14	B	837	CLA	CHD-C4C-NC	2.36	127.92	124.20
14	bA	838	CLA	CHD-C4C-NC	2.36	127.92	124.20
14	cA	815	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
17	bB	845	BCR	C16-C17-C18	2.36	130.68	127.31
14	B	813	CLA	CED-O2D-CGD	2.36	121.27	115.94
14	bA	828	CLA	CHD-C4C-NC	2.36	127.92	124.20
14	cA	820	CLA	CHB-C1B-C2B	-2.36	120.58	127.24
14	bB	810	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
14	B	807	CLA	CHD-C4C-NC	2.36	127.92	124.20
14	L	204	CLA	C2A-C1A-CHA	-2.36	119.74	123.86
14	A	828	CLA	CHD-C4C-NC	2.36	127.92	124.20
14	B	825	CLA	O1D-CGD-CBD	-2.36	119.67	124.48
14	bA	814	CLA	O1D-CGD-CBD	-2.36	119.67	124.48
14	A	807	CLA	C2A-C1A-CHA	-2.36	119.74	123.86
14	bB	849	CLA	CHD-C4C-NC	2.35	127.91	124.20
14	A	808	CLA	CHB-C4A-NA	2.35	127.77	124.51
14	cA	808	CLA	CHB-C4A-NA	2.35	127.77	124.51
14	bA	807	CLA	C2A-C1A-CHA	-2.35	119.74	123.86
14	A	814	CLA	O1D-CGD-CBD	-2.35	119.67	124.48
14	B	818	CLA	C3B-C4B-NB	2.35	112.70	110.52
14	A	836	CLA	CHB-C4A-NA	2.35	127.77	124.51
17	bI	101	BCR	C11-C10-C9	2.35	130.67	127.31
14	cA	817	CLA	CHD-C4C-NC	2.35	127.91	124.20
14	cA	833	CLA	CMB-C2B-C1B	2.35	128.95	125.37
14	bB	835	CLA	CED-O2D-CGD	2.35	121.26	115.94
14	cL	205	CLA	C2A-C1A-CHA	-2.35	119.75	123.86
14	cA	828	CLA	CHD-C4C-NC	2.35	127.91	124.20
14	bA	815	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
14	L	204	CLA	CHB-C4A-NA	2.35	127.76	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	813	CLA	O1D-CGD-CBD	-2.35	119.67	124.48
14	bB	837	CLA	CHD-C4C-NC	2.35	127.91	124.20
17	I	101	BCR	C11-C10-C9	2.35	130.66	127.31
14	bB	827	CLA	CBA-CAA-C2A	2.35	120.80	113.86
14	A	817	CLA	CHD-C4C-NC	2.35	127.91	124.20
14	cA	807	CLA	C2A-C1A-CHA	-2.35	119.75	123.86
14	A	833	CLA	CMB-C2B-C1B	2.35	128.95	125.37
14	cB	818	CLA	CMB-C2B-C1B	2.35	128.95	125.37
14	B	835	CLA	CED-O2D-CGD	2.35	121.25	115.94
14	cA	830	CLA	CHD-C4C-NC	2.35	127.90	124.20
14	cA	822	CLA	CED-O2D-CGD	2.35	121.25	115.94
14	bL	204	CLA	CHB-C4A-NA	2.35	127.76	124.51
14	B	817	CLA	CMB-C2B-C1B	2.35	128.94	125.37
14	cF	201	CLA	C3B-C4B-NB	2.35	112.69	110.52
14	bA	818	CLA	CBA-CAA-C2A	2.35	120.79	113.86
17	L	205	BCR	C35-C13-C14	-2.35	119.64	122.92
14	cB	814	CLA	C1-O2A-CGA	2.35	122.60	116.44
14	cL	205	CLA	CHB-C4A-NA	2.35	127.76	124.51
14	cB	811	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
14	A	838	CLA	CHD-C4C-NC	2.35	127.90	124.20
14	cA	808	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
14	bB	818	CLA	C3B-C4B-NB	2.35	112.69	110.52
14	cB	819	CLA	CHB-C1B-C2B	-2.35	120.61	127.24
14	bB	807	CLA	CHD-C4C-NC	2.35	127.90	124.20
14	B	810	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
17	bB	844	BCR	C15-C16-C17	2.34	128.28	123.47
14	cB	836	CLA	CED-O2D-CGD	2.34	121.24	115.94
14	bA	808	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
17	bA	849	BCR	C16-C15-C14	2.34	128.27	123.47
14	cB	850	CLA	CHD-C4C-NC	2.34	127.89	124.20
14	bB	813	CLA	O1D-CGD-CBD	-2.34	119.69	124.48
14	bB	839	CLA	O2A-CGA-CBA	2.34	119.26	111.91
14	cA	814	CLA	CMB-C2B-C1B	2.34	128.94	125.37
13	bA	801	CL0	C1-O2A-CGA	2.34	122.59	116.44
14	B	807	CLA	CBC-CAC-C3C	-2.34	105.98	112.43
17	cB	845	BCR	C16-C17-C18	2.34	130.65	127.31
14	bB	813	CLA	C1-O2A-CGA	2.34	122.58	116.44
17	B	844	BCR	C15-C16-C17	2.34	128.27	123.47
14	cB	808	CLA	CHD-C4C-NC	2.34	127.89	124.20
14	cB	840	CLA	O2A-CGA-CBA	2.34	119.25	111.91
14	cA	803	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
14	bB	817	CLA	CMB-C2B-C1B	2.34	128.93	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	818	CLA	CBA-CAA-C2A	2.34	120.77	113.86
14	bB	818	CLA	CHB-C1B-C2B	-2.34	120.63	127.24
14	A	818	CLA	CBA-CAA-C2A	2.34	120.77	113.86
17	B	842	BCR	C12-C13-C14	2.34	122.53	118.94
17	bB	844	BCR	C16-C17-C18	2.34	130.65	127.31
14	cL	204	CLA	C4-C3-C5	2.34	119.20	115.27
14	B	824	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
17	cB	845	BCR	C15-C16-C17	2.34	128.26	123.47
14	cA	838	CLA	CHD-C4C-NC	2.34	127.89	124.20
17	cI	101	BCR	C11-C10-C9	2.34	130.65	127.31
14	bB	806	CLA	CBC-CAC-C3C	-2.34	105.99	112.43
17	cA	849	BCR	C16-C15-C14	2.34	128.26	123.47
14	bA	836	CLA	CHB-C4A-NA	2.34	127.74	124.51
14	bB	820	CLA	O1D-CGD-CBD	-2.34	119.70	124.48
14	bB	807	CLA	CBC-CAC-C3C	-2.34	105.99	112.43
14	bL	204	CLA	C2A-C1A-CHA	-2.34	119.78	123.86
14	bB	831	CLA	CHB-C1B-C2B	-2.33	120.64	127.24
14	B	816	CLA	O2A-CGA-CBA	2.33	121.53	114.03
14	cA	824	CLA	O1D-CGD-CBD	-2.33	119.71	124.48
14	B	818	CLA	CHB-C1B-C2B	-2.33	120.64	127.24
17	A	849	BCR	C16-C15-C14	2.33	128.26	123.47
14	bB	832	CLA	CHB-C4A-NA	2.33	127.74	124.51
14	cB	833	CLA	CHB-C4A-NA	2.33	127.74	124.51
14	B	851	CLA	CHC-C4B-NB	-2.33	121.79	124.26
14	cA	834	CLA	CHB-C1B-C2B	-2.33	120.64	127.24
14	bB	816	CLA	O2A-CGA-CBA	2.33	121.53	114.03
14	B	849	CLA	CHD-C4C-NC	2.33	127.88	124.20
14	A	822	CLA	CED-O2D-CGD	2.33	121.22	115.94
14	cB	825	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
14	L	203	CLA	C4-C3-C5	2.33	119.20	115.27
14	bA	817	CLA	CHD-C4C-NC	2.33	127.88	124.20
13	cA	801	CL0	C1-O2A-CGA	2.33	122.56	116.44
14	B	806	CLA	CBC-CAC-C3C	-2.33	106.00	112.43
17	B	844	BCR	C16-C17-C18	2.33	130.64	127.31
17	cL	206	BCR	C35-C13-C14	-2.33	119.66	122.92
14	bA	840	CLA	CHD-C4C-NC	2.33	127.88	124.20
14	bA	803	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
14	B	839	CLA	O2A-CGA-CBA	2.33	119.22	111.91
14	A	824	CLA	O1D-CGD-CBD	-2.33	119.71	124.48
14	B	831	CLA	CHB-C1B-C2B	-2.33	120.65	127.24
14	cB	808	CLA	CBC-CAC-C3C	-2.33	106.00	112.43
17	cB	848	BCR	C20-C21-C22	2.33	130.64	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	814	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
14	cB	807	CLA	CBC-CAC-C3C	-2.33	106.01	112.43
13	A	801	CL0	C1-O2A-CGA	2.33	122.56	116.44
14	cB	817	CLA	O2A-CGA-CBA	2.33	121.51	114.03
17	J	103	BCR	C35-C13-C14	-2.33	119.66	122.92
14	cB	821	CLA	O1D-CGD-CBD	-2.33	119.72	124.48
14	bA	807	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
13	cA	801	CL0	CMA-C3A-C4A	-2.33	105.52	111.77
14	A	808	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
17	cF	202	BCR	C37-C22-C23	2.33	121.75	118.08
14	bA	820	CLA	CMB-C2B-C1B	2.33	128.91	125.37
14	B	813	CLA	C1-O2A-CGA	2.33	122.55	116.44
14	cB	832	CLA	CHB-C1B-C2B	-2.33	120.67	127.24
14	B	805	CLA	C4C-C3C-C2C	-2.33	103.51	106.90
17	bL	205	BCR	C35-C13-C14	-2.33	119.66	122.92
17	bB	842	BCR	C12-C13-C14	2.33	122.51	118.94
14	bA	822	CLA	CED-O2D-CGD	2.33	121.20	115.94
14	A	834	CLA	CHB-C1B-C2B	-2.33	120.67	127.24
14	cA	842	CLA	CMB-C2B-C1B	2.33	128.91	125.37
14	bB	819	CLA	O1D-CGD-CBD	-2.32	119.73	124.48
14	bA	834	CLA	CHB-C1B-C2B	-2.32	120.67	127.24
14	B	820	CLA	O1D-CGD-CBD	-2.32	119.73	124.48
14	bA	824	CLA	O1D-CGD-CBD	-2.32	119.73	124.48
17	cB	843	BCR	C12-C13-C14	2.32	122.50	118.94
17	bF	202	BCR	C37-C22-C23	2.32	121.74	118.08
14	A	820	CLA	CMB-C2B-C1B	2.32	128.91	125.37
14	A	840	CLA	CHD-C4C-NC	2.32	127.86	124.20
14	bL	202	CLA	C4-C3-C5	2.32	119.18	115.27
14	A	803	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
14	B	835	CLA	CHD-C4C-NC	2.32	127.86	124.20
14	bA	832	CLA	CHD-C4C-NC	2.32	127.86	124.20
14	L	202	CLA	C4-C3-C5	2.32	119.17	115.27
17	bB	847	BCR	C20-C21-C22	2.32	130.62	127.31
14	bL	203	CLA	C4-C3-C5	2.32	119.17	115.27
17	bJ	103	BCR	C35-C13-C14	-2.32	119.67	122.92
13	A	801	CL0	CMA-C3A-C4A	-2.32	105.54	111.77
14	cL	203	CLA	C4-C3-C5	2.32	119.17	115.27
13	bA	801	CL0	CMA-C3A-C4A	-2.32	105.54	111.77
14	cB	820	CLA	O1D-CGD-CBD	-2.32	119.74	124.48
14	bB	804	CLA	O2A-C1-C2	2.32	114.73	108.64
17	cI	102	BCR	C15-C16-C17	2.32	128.22	123.47
14	bB	814	CLA	O2D-CGD-O1D	-2.32	119.31	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	F	202	BCR	C37-C22-C23	2.32	121.73	118.08
17	A	847	BCR	C11-C10-C9	2.32	130.62	127.31
14	B	819	CLA	O1D-CGD-CBD	-2.32	119.74	124.48
17	bI	102	BCR	C15-C16-C17	2.32	128.22	123.47
14	A	842	CLA	CMB-C2B-C1B	2.32	128.90	125.37
14	bB	803	CLA	CHD-C4C-NC	2.32	127.85	124.20
14	B	823	CLA	CMB-C2B-C3B	2.32	132.19	126.59
14	A	807	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
14	cB	805	CLA	O2A-C1-C2	2.31	114.72	108.64
17	I	102	BCR	C15-C16-C17	2.31	128.21	123.47
14	cA	807	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
14	B	804	CLA	O2A-C1-C2	2.31	114.71	108.64
14	B	832	CLA	CHB-C4A-NA	2.31	127.71	124.51
17	bA	846	BCR	C10-C11-C12	2.31	130.43	123.22
14	bB	806	CLA	CHB-C4A-NA	2.31	127.71	124.51
17	cA	846	BCR	C10-C11-C12	2.31	130.43	123.22
14	bA	842	CLA	CMB-C2B-C1B	2.31	128.89	125.37
14	L	201	CLA	CED-O2D-CGD	2.31	121.16	115.94
17	B	846	BCR	C37-C22-C23	2.31	121.72	118.08
14	bB	835	CLA	CHD-C4C-NC	2.31	127.84	124.20
14	cB	804	CLA	CHD-C4C-NC	2.31	127.84	124.20
14	bB	824	CLA	CMB-C2B-C1B	2.31	128.89	125.37
14	A	819	CLA	CHB-C4A-NA	2.31	127.71	124.51
14	cA	832	CLA	CHD-C4C-NC	2.31	127.84	124.20
14	cB	825	CLA	CMB-C2B-C1B	2.31	128.89	125.37
14	bA	821	CLA	O1D-CGD-CBD	-2.31	119.76	124.48
14	bB	805	CLA	C4C-C3C-C2C	-2.31	103.53	106.90
14	cA	820	CLA	CMB-C2B-C1B	2.31	128.88	125.37
14	cA	821	CLA	O1D-CGD-CBD	-2.31	119.76	124.48
17	A	846	BCR	C10-C11-C12	2.31	130.41	123.22
14	bB	830	CLA	CED-O2D-CGD	2.31	121.15	115.94
14	B	807	CLA	O2A-CGA-CBA	2.31	119.14	111.91
17	cJ	103	BCR	C35-C13-C14	-2.31	119.69	122.92
17	B	847	BCR	C20-C21-C22	2.31	130.60	127.31
14	cB	815	CLA	O2D-CGD-O1D	-2.30	119.33	123.84
14	A	823	CLA	CHD-C4C-NC	2.30	127.83	124.20
17	cA	847	BCR	C11-C10-C9	2.30	130.60	127.31
14	bB	807	CLA	O2A-CGA-CBA	2.30	119.14	111.91
14	B	834	CLA	C2A-C1A-CHA	-2.30	119.83	123.86
14	cA	809	CLA	C2A-C1A-CHA	-2.30	119.83	123.86
14	cB	807	CLA	CHB-C4A-NA	2.30	127.69	124.51
14	A	821	CLA	O1D-CGD-CBD	-2.30	119.78	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	824	CLA	CMB-C2B-C1B	2.30	128.87	125.37
17	B	842	BCR	C37-C22-C23	2.30	121.70	118.08
14	cA	840	CLA	CHD-C4C-NC	2.30	127.83	124.20
14	cB	806	CLA	C4C-C3C-C2C	-2.30	103.54	106.90
14	bB	834	CLA	C2A-C1A-CHA	-2.30	119.84	123.86
14	A	832	CLA	CHD-C4C-NC	2.30	127.83	124.20
14	bB	851	CLA	CHC-C4B-NB	-2.30	121.82	124.26
14	cB	802	CLA	CBC-CAC-C3C	-2.30	106.09	112.43
14	cB	801	CLA	CHC-C4B-NB	-2.30	121.82	124.26
14	cL	202	CLA	CED-O2D-CGD	2.30	121.14	115.94
14	bB	804	CLA	C2A-C1A-CHA	-2.30	119.84	123.86
14	bB	823	CLA	CMB-C2B-C3B	2.30	132.15	126.59
14	bB	801	CLA	CBC-CAC-C3C	-2.30	106.10	112.43
17	bA	847	BCR	C37-C22-C23	2.30	121.70	118.08
14	cL	203	CLA	C1-O2A-CGA	2.30	122.47	116.44
14	bB	803	CLA	C4-C3-C5	2.30	119.13	115.27
14	B	830	CLA	CED-O2D-CGD	2.30	121.13	115.94
17	cB	847	BCR	C37-C22-C23	2.30	121.69	118.08
14	B	803	CLA	CHD-C4C-NC	2.30	127.82	124.20
14	cB	824	CLA	CMB-C2B-C3B	2.30	132.15	126.59
14	bL	203	CLA	CED-O2D-CGD	2.30	121.13	115.94
17	bA	847	BCR	C11-C10-C9	2.30	130.59	127.31
14	B	803	CLA	C4-C3-C5	2.30	119.13	115.27
14	cA	819	CLA	O1D-CGD-CBD	-2.30	119.79	124.48
17	cA	847	BCR	C37-C22-C23	2.29	121.69	118.08
14	cB	831	CLA	CED-O2D-CGD	2.29	121.13	115.94
14	A	809	CLA	C2A-C1A-CHA	-2.29	119.85	123.86
14	bA	837	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
14	cB	804	CLA	C4-C3-C5	2.29	119.13	115.27
14	bL	201	CLA	CED-O2D-CGD	2.29	121.12	115.94
14	cA	823	CLA	CHD-C4C-NC	2.29	127.82	124.20
14	cA	837	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
14	bA	825	CLA	CAA-C2A-C3A	-2.29	106.50	112.78
14	cB	804	CLA	CAA-C2A-C3A	-2.29	106.50	112.78
14	bA	839	CLA	CHB-C4A-NA	2.29	127.68	124.51
17	bA	848	BCR	C30-C25-C24	2.29	122.26	115.78
17	bB	846	BCR	C37-C22-C23	2.29	121.69	118.08
14	cB	836	CLA	CHD-C4C-NC	2.29	127.81	124.20
14	bA	819	CLA	O1D-CGD-CBD	-2.29	119.80	124.48
14	A	819	CLA	O1D-CGD-CBD	-2.29	119.80	124.48
14	cB	808	CLA	O2A-CGA-CBA	2.29	119.09	111.91
14	cB	830	CLA	O2D-CGD-O1D	-2.29	119.36	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bB	803	CLA	CAA-C2A-C3A	-2.29	106.51	112.78
14	cL	204	CLA	CED-O2D-CGD	2.29	121.11	115.94
14	B	806	CLA	CHB-C4A-NA	2.29	127.68	124.51
14	bL	202	CLA	C1-O2A-CGA	2.29	122.45	116.44
14	B	801	CLA	CBC-CAC-C3C	-2.29	106.12	112.43
14	L	203	CLA	CED-O2D-CGD	2.29	121.11	115.94
14	bA	805	CLA	C2A-C1A-CHA	-2.29	119.86	123.86
14	bA	819	CLA	CHB-C4A-NA	2.29	127.68	124.51
14	L	202	CLA	C1-O2A-CGA	2.29	122.45	116.44
14	cA	815	CLA	CED-O2D-CGD	2.29	121.11	115.94
17	B	846	BCR	C15-C14-C13	2.29	130.57	127.31
17	cB	847	BCR	C15-C14-C13	2.29	130.57	127.31
14	B	804	CLA	C2A-C1A-CHA	-2.29	119.86	123.86
14	cB	827	CLA	C1-O2A-CGA	2.29	122.44	116.44
14	cA	819	CLA	CHB-C4A-NA	2.29	127.67	124.51
14	cA	805	CLA	C2A-C1A-CHA	-2.29	119.86	123.86
14	B	803	CLA	CAA-C2A-C3A	-2.28	106.52	112.78
14	bB	849	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
17	cB	843	BCR	C37-C22-C23	2.28	121.68	118.08
14	B	826	CLA	C1-O2A-CGA	2.28	122.44	116.44
14	L	201	CLA	C3B-C4B-NB	2.28	112.63	110.52
14	cA	840	CLA	C3B-C4B-NB	2.28	112.63	110.52
14	bA	823	CLA	CHD-C4C-NC	2.28	127.80	124.20
14	A	837	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
14	A	815	CLA	CED-O2D-CGD	2.28	121.10	115.94
17	cA	848	BCR	C30-C25-C24	2.28	122.23	115.78
14	bB	826	CLA	C1-O2A-CGA	2.28	122.43	116.44
14	bB	801	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
17	A	848	BCR	C30-C25-C24	2.28	122.23	115.78
14	cB	805	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
14	cB	835	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
14	cA	825	CLA	CAA-C2A-C3A	-2.28	106.53	112.78
14	bB	829	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
17	A	847	BCR	C37-C22-C23	2.28	121.67	118.08
14	A	825	CLA	CAA-C2A-C3A	-2.28	106.53	112.78
14	A	839	CLA	CHB-C4A-NA	2.28	127.67	124.51
14	bA	840	CLA	C3B-C4B-NB	2.28	112.63	110.52
14	B	849	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
17	bB	842	BCR	C37-C22-C23	2.28	121.67	118.08
14	B	811	CLA	CHD-C4C-NC	2.28	127.79	124.20
14	cA	839	CLA	CHB-C4A-NA	2.28	127.66	124.51
14	bB	811	CLA	CHD-C4C-NC	2.28	127.79	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	837	CLA	C1-O2A-CGA	2.28	122.42	116.44
14	bL	201	CLA	C3B-C4B-NB	2.28	112.63	110.52
14	bA	815	CLA	CED-O2D-CGD	2.28	121.09	115.94
14	A	806	CLA	C3B-C4B-NB	2.28	112.63	110.52
14	B	829	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
14	cA	829	CLA	CMB-C2B-C1B	2.28	128.84	125.37
14	A	837	CLA	C1-O2A-CGA	2.28	122.42	116.44
14	bA	809	CLA	C2A-C1A-CHA	-2.28	119.88	123.86
14	bA	837	CLA	C1-O2A-CGA	2.28	122.42	116.44
14	bA	819	CLA	C2A-C1A-CHA	-2.28	119.88	123.86
14	bB	828	CLA	CMB-C2B-C1B	2.28	128.83	125.37
14	bL	203	CLA	CHB-C4A-NA	2.28	127.66	124.51
14	bB	819	CLA	CMD-C2D-C3D	-2.27	122.38	127.61
14	bB	805	CLA	CMB-C2B-C1B	2.27	128.83	125.37
17	bA	849	BCR	C35-C13-C14	-2.27	119.74	122.92
14	L	204	CLA	C1-C2-C3	-2.27	122.11	126.04
14	A	829	CLA	CMB-C2B-C1B	2.27	128.83	125.37
17	I	102	BCR	C15-C14-C13	2.27	130.55	127.31
17	bB	846	BCR	C15-C14-C13	2.27	130.55	127.31
14	B	806	CLA	C3B-C4B-NB	2.27	112.62	110.52
17	cL	207	BCR	C15-C14-C13	2.27	130.55	127.31
14	cB	850	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
14	bA	829	CLA	CMB-C2B-C1B	2.27	128.83	125.37
14	B	819	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
14	cA	819	CLA	C2A-C1A-CHA	-2.27	119.89	123.86
17	bI	102	BCR	C15-C14-C13	2.27	130.55	127.31
14	cL	204	CLA	CHB-C4A-NA	2.27	127.65	124.51
14	cB	829	CLA	CMB-C2B-C1B	2.27	128.83	125.37
14	A	805	CLA	C2A-C1A-CHA	-2.27	119.89	123.86
14	A	819	CLA	C2A-C1A-CHA	-2.27	119.89	123.86
14	cB	812	CLA	CHD-C4C-NC	2.27	127.78	124.20
17	cI	102	BCR	C15-C14-C13	2.27	130.55	127.31
14	cB	806	CLA	CMB-C2B-C1B	2.27	128.82	125.37
14	cB	820	CLA	CMD-C2D-C3D	-2.27	122.40	127.61
14	B	813	CLA	O2D-CGD-O1D	-2.27	119.41	123.84
14	cA	809	CLA	CMB-C2B-C1B	2.27	128.82	125.37
14	bL	204	CLA	C1-C2-C3	-2.27	122.12	126.04
14	L	203	CLA	CHB-C4A-NA	2.26	127.64	124.51
14	L	202	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
17	A	849	BCR	C35-C13-C14	-2.26	119.75	122.92
14	B	801	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
14	cB	802	CLA	O2D-CGD-O1D	-2.26	119.41	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cB	830	CLA	CED-O2D-CGD	2.26	121.06	115.94
14	bA	805	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
14	cL	203	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
14	cB	839	CLA	C4-C3-C5	2.26	119.08	115.27
14	cA	815	CLA	O1D-CGD-CBD	-2.26	119.85	124.48
14	B	805	CLA	CMB-C2B-C1B	2.26	128.81	125.37
14	bB	822	CLA	C2A-C1A-CHA	-2.26	119.90	123.86
14	bB	835	CLA	C2A-C1A-CHA	-2.26	119.90	123.86
14	bB	813	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
14	A	815	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
14	bB	803	CLA	CHA-C1A-NA	-2.26	121.22	126.40
14	cA	835	CLA	CHB-C1B-C2B	-2.26	120.85	127.24
14	L	203	CLA	CMB-C2B-C1B	2.26	128.81	125.37
14	B	849	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
14	cL	204	CLA	CMB-C2B-C1B	2.26	128.81	125.37
14	bA	835	CLA	CHB-C1B-C2B	-2.26	120.85	127.24
14	cB	815	CLA	CMB-C2B-C1B	2.26	128.81	125.37
14	cL	202	CLA	C3B-C4B-NB	2.26	112.61	110.52
14	A	835	CLA	CHB-C1B-C2B	-2.26	120.86	127.24
14	bA	815	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
14	cA	805	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
14	cL	205	CLA	C1-C2-C3	-2.26	122.14	126.04
14	bB	806	CLA	C3B-C4B-NB	2.26	112.61	110.52
14	cA	822	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
14	B	825	CLA	O2A-CGA-CBA	2.26	118.99	111.91
14	cB	810	CLA	CHB-C4A-NA	2.26	127.63	124.51
14	B	828	CLA	CMB-C2B-C1B	2.26	128.81	125.37
14	bA	809	CLA	CMB-C2B-C1B	2.26	128.81	125.37
14	bB	838	CLA	C4-C3-C5	2.26	119.07	115.27
14	bB	834	CLA	CED-O2D-CGD	2.26	121.04	115.94
14	A	822	CLA	O2D-CGD-O1D	-2.26	119.43	123.84
14	cB	804	CLA	CHA-C1A-NA	-2.26	121.23	126.40
14	cA	806	CLA	C3B-C4B-NB	2.26	112.61	110.52
14	bL	202	CLA	O2D-CGD-O1D	-2.25	119.43	123.84
14	A	805	CLA	O2D-CGD-O1D	-2.25	119.43	123.84
14	B	838	CLA	C4-C3-C5	2.25	119.06	115.27
14	cB	835	CLA	CHD-C4C-NC	2.25	127.75	124.20
14	cB	823	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
14	B	803	CLA	CHA-C1A-NA	-2.25	121.24	126.40
14	A	840	CLA	C3B-C4B-NB	2.25	112.60	110.52
14	bB	821	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
14	bA	806	CLA	C3B-C4B-NB	2.25	112.60	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bA	813	CLA	C3B-C4B-NB	2.25	112.60	110.52
14	cA	813	CLA	C3B-C4B-NB	2.25	112.60	110.52
14	B	814	CLA	CMB-C2B-C1B	2.25	128.79	125.37
17	cA	849	BCR	C35-C13-C14	-2.25	119.77	122.92
14	B	835	CLA	C2A-C1A-CHA	-2.25	119.93	123.86
14	bA	822	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
14	bA	830	CLA	C2A-C1A-CHA	-2.25	119.93	123.86
14	bA	803	CLA	CED-O2D-CGD	2.25	121.02	115.94
14	A	824	CLA	C3B-C4B-NB	2.25	112.60	110.52
14	cB	807	CLA	C3B-C4B-NB	2.25	112.60	110.52
14	cB	826	CLA	O2A-CGA-CBA	2.25	118.96	111.91
14	A	809	CLA	CMB-C2B-C1B	2.25	128.79	125.37
14	cB	814	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
14	bB	829	CLA	CED-O2D-CGD	2.25	121.02	115.94
14	bB	825	CLA	O2A-CGA-CBA	2.25	118.96	111.91
14	A	830	CLA	C2A-C1A-CHA	-2.25	119.93	123.86
14	B	822	CLA	C2A-C1A-CHA	-2.25	119.93	123.86
14	cA	830	CLA	C2A-C1A-CHA	-2.25	119.93	123.86
14	bA	812	CLA	CHC-C1C-NC	2.25	127.61	124.20
14	cA	803	CLA	CED-O2D-CGD	2.25	121.02	115.94
14	B	834	CLA	CHD-C4C-NC	2.25	127.74	124.20
14	bA	824	CLA	C3B-C4B-NB	2.25	112.60	110.52
14	B	834	CLA	CED-O2D-CGD	2.24	121.01	115.94
14	bA	832	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
14	cB	850	CLA	C2A-C1A-CHA	-2.24	119.94	123.86
14	B	835	CLA	CMB-C2B-C1B	2.24	128.78	125.37
14	cB	831	CLA	CMB-C2B-C1B	2.24	128.78	125.37
14	cB	835	CLA	CED-O2D-CGD	2.24	121.01	115.94
14	bB	834	CLA	CHD-C4C-NC	2.24	127.74	124.20
14	cA	832	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
14	cB	836	CLA	CMB-C2B-C1B	2.24	128.78	125.37
14	A	813	CLA	C3B-C4B-NB	2.24	112.59	110.52
14	A	803	CLA	CED-O2D-CGD	2.24	121.01	115.94
14	cB	839	CLA	C3B-C4B-NB	2.24	112.59	110.52
14	cB	836	CLA	C2A-C1A-CHA	-2.24	119.94	123.86
14	A	829	CLA	CED-O2D-CGD	2.24	121.00	115.94
14	cA	824	CLA	C3B-C4B-NB	2.24	112.59	110.52
14	cA	829	CLA	CED-O2D-CGD	2.24	121.00	115.94
14	bB	814	CLA	CMB-C2B-C1B	2.24	128.78	125.37
14	bB	830	CLA	CMB-C2B-C1B	2.24	128.78	125.37
14	cB	840	CLA	CHB-C4A-NA	2.24	127.61	124.51
14	bB	838	CLA	C3B-C4B-NB	2.24	112.59	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	L	206	BCR	C15-C14-C13	2.24	130.50	127.31
14	cA	802	CLA	O2A-CGA-CBA	2.24	118.93	111.91
14	bA	822	CLA	CHD-C4C-NC	2.24	127.73	124.20
14	B	829	CLA	CED-O2D-CGD	2.24	121.00	115.94
14	B	830	CLA	CMB-C2B-C1B	2.24	128.78	125.37
14	A	832	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
14	A	822	CLA	CHB-C1B-C2B	-2.24	120.92	127.24
17	cB	846	BCR	C12-C13-C14	2.24	122.37	118.94
14	bB	820	CLA	CED-O2D-CGD	2.24	121.00	115.94
14	bA	839	CLA	C4-C3-C5	2.24	119.03	115.27
14	A	804	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
14	bB	849	CLA	C2A-C1A-CHA	-2.24	119.95	123.86
14	bA	829	CLA	CED-O2D-CGD	2.24	120.99	115.94
17	M	101	BCR	C11-C10-C9	2.24	130.50	127.31
14	bA	803	CLA	CHB-C4A-NA	2.23	127.60	124.51
14	A	802	CLA	O2A-CGA-CBA	2.23	118.92	111.91
14	cB	822	CLA	C2A-C1A-CHA	-2.23	119.95	123.86
14	B	821	CLA	C2A-C1A-CHA	-2.23	119.95	123.86
14	bB	835	CLA	CMB-C2B-C1B	2.23	128.77	125.37
14	J	101	CLA	CED-O2D-CGD	2.23	120.99	115.94
17	bL	206	BCR	C15-C14-C13	2.23	130.50	127.31
14	bX	201	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
14	cA	822	CLA	CHB-C1B-C2B	-2.23	120.93	127.24
14	A	812	CLA	CHC-C1C-NC	2.23	127.59	124.20
14	bA	802	CLA	O2A-CGA-CBA	2.23	118.91	111.91
17	B	843	BCR	C10-C11-C12	2.23	130.18	123.22
17	bM	101	BCR	C11-C10-C9	2.23	130.49	127.31
14	B	809	CLA	CHB-C4A-NA	2.23	127.59	124.51
17	cB	844	BCR	C10-C11-C12	2.23	130.17	123.22
14	cB	816	CLA	C1-O2A-CGA	2.23	122.29	116.44
14	A	839	CLA	C4-C3-C5	2.23	119.02	115.27
14	B	815	CLA	C1-O2A-CGA	2.23	122.29	116.44
14	bA	822	CLA	CHB-C1B-C2B	-2.23	120.94	127.24
14	cB	830	CLA	O1D-CGD-CBD	-2.23	119.93	124.48
14	B	829	CLA	O1D-CGD-CBD	-2.23	119.93	124.48
14	bB	809	CLA	CHB-C4A-NA	2.23	127.59	124.51
14	bA	804	CLA	O2D-CGD-O1D	-2.23	119.49	123.84
14	B	820	CLA	CED-O2D-CGD	2.23	120.97	115.94
14	cB	821	CLA	CED-O2D-CGD	2.23	120.97	115.94
17	B	845	BCR	C12-C13-C14	2.23	122.36	118.94
14	bF	201	CLA	O2D-CGD-O1D	-2.23	119.49	123.84
14	cX	201	CLA	O1D-CGD-CBD	-2.22	119.93	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	824	CLA	C1-O2A-CGA	2.22	122.28	116.44
13	A	801	CL0	CHD-C4C-NC	2.22	127.71	124.20
14	A	822	CLA	CHD-C4C-NC	2.22	127.71	124.20
14	cA	839	CLA	C4-C3-C5	2.22	119.01	115.27
14	bL	203	CLA	CMB-C2B-C1B	2.22	128.75	125.37
14	bB	823	CLA	C1-O2A-CGA	2.22	122.28	116.44
14	cA	812	CLA	CHC-C1C-NC	2.22	127.58	124.20
14	bA	824	CLA	C1-O2A-CGA	2.22	122.28	116.44
14	cA	810	CLA	CED-O2D-CGD	2.22	120.96	115.94
14	cB	816	CLA	C3B-C4B-NB	2.22	112.58	110.52
17	bB	843	BCR	C10-C11-C12	2.22	130.15	123.22
14	B	823	CLA	C1-O2A-CGA	2.22	122.27	116.44
14	bA	810	CLA	CED-O2D-CGD	2.22	120.96	115.94
14	bB	802	CLA	CHD-C4C-NC	2.22	127.70	124.20
17	cA	848	BCR	C15-C14-C13	2.22	130.48	127.31
14	bJ	101	CLA	CED-O2D-CGD	2.22	120.95	115.94
14	A	804	CLA	CED-O2D-CGD	2.22	120.95	115.94
14	X	201	CLA	CHB-C4A-NA	2.22	127.58	124.51
14	B	802	CLA	C2A-C1A-CHA	-2.22	119.98	123.86
17	bB	845	BCR	C12-C13-C14	2.22	122.34	118.94
14	cA	821	CLA	O2A-CGA-CBA	2.22	121.15	114.03
14	A	824	CLA	C1-O2A-CGA	2.22	122.26	116.44
14	cA	803	CLA	CHB-C4A-NA	2.22	127.58	124.51
14	cA	804	CLA	O2D-CGD-O1D	-2.22	119.51	123.84
14	cA	822	CLA	CHD-C4C-NC	2.22	127.69	124.20
14	A	810	CLA	CED-O2D-CGD	2.22	120.95	115.94
14	bB	829	CLA	O1D-CGD-CBD	-2.22	119.95	124.48
14	bB	815	CLA	C1-O2A-CGA	2.22	122.26	116.44
14	cB	803	CLA	C2A-C1A-CHA	-2.21	119.99	123.86
14	X	201	CLA	O1D-CGD-CBD	-2.21	119.95	124.48
14	B	839	CLA	CHB-C4A-NA	2.21	127.57	124.51
14	B	838	CLA	C3B-C4B-NB	2.21	112.57	110.52
14	A	821	CLA	C2A-C1A-CHA	-2.21	119.99	123.86
14	cA	818	CLA	CHC-C4B-NB	-2.21	121.92	124.26
14	bB	802	CLA	C2A-C1A-CHA	-2.21	119.99	123.86
14	bB	809	CLA	C2A-C1A-CHA	-2.21	119.99	123.86
14	bB	826	CLA	CHD-C4C-NC	2.21	127.69	124.20
14	F	201	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
13	bA	801	CL0	CHD-C4C-NC	2.21	127.69	124.20
17	B	844	BCR	C7-C8-C9	2.21	129.57	126.23
14	A	821	CLA	O2A-CGA-CBA	2.21	121.13	114.03
14	cJ	101	CLA	CED-O2D-CGD	2.21	120.93	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	cM	101	BCR	C11-C10-C9	2.21	130.46	127.31
14	bB	839	CLA	CHB-C4A-NA	2.21	127.56	124.51
13	cA	801	CL0	CHD-C4C-NC	2.21	127.68	124.20
14	cX	201	CLA	CHB-C4A-NA	2.21	127.56	124.51
14	cA	809	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
14	cB	824	CLA	C1-O2A-CGA	2.21	122.23	116.44
14	B	817	CLA	CBA-CAA-C2A	2.21	120.38	113.86
14	bA	821	CLA	O2A-CGA-CBA	2.21	121.12	114.03
14	bB	817	CLA	CBA-CAA-C2A	2.21	120.37	113.86
14	cF	201	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
14	cB	827	CLA	CHD-C4C-NC	2.20	127.68	124.20
17	B	841	BCR	C37-C22-C23	2.20	121.55	118.08
14	J	101	CLA	CHB-C4A-NA	2.20	127.56	124.51
17	bB	844	BCR	C7-C8-C9	2.20	129.56	126.23
14	cB	813	CLA	CHC-C4B-NB	-2.20	121.92	124.26
14	bB	849	CLA	CHB-C4A-NA	2.20	127.56	124.51
14	bJ	101	CLA	CHB-C4A-NA	2.20	127.56	124.51
14	cA	815	CLA	CHB-C4A-NA	2.20	127.56	124.51
14	cB	850	CLA	CHB-C4A-NA	2.20	127.56	124.51
14	bA	815	CLA	CHB-C4A-NA	2.20	127.56	124.51
14	cB	818	CLA	CBA-CAA-C2A	2.20	120.36	113.86
14	bA	804	CLA	CED-O2D-CGD	2.20	120.92	115.94
14	cA	832	CLA	O2A-CGA-CBA	2.20	118.82	111.91
17	cB	845	BCR	C7-C8-C9	2.20	129.56	126.23
14	cA	819	CLA	CHD-C4C-NC	2.20	127.67	124.20
17	bA	848	BCR	C15-C14-C13	2.20	130.45	127.31
14	A	841	CLA	C4-C3-C5	2.20	118.97	115.27
14	bA	841	CLA	C4-C3-C5	2.20	118.97	115.27
14	B	816	CLA	CMB-C2B-C1B	2.20	128.72	125.37
14	cB	817	CLA	CMB-C2B-C1B	2.20	128.72	125.37
17	bA	849	BCR	C19-C18-C17	2.20	122.32	118.94
17	cA	849	BCR	C19-C18-C17	2.20	122.32	118.94
14	bB	815	CLA	C3B-C4B-NB	2.20	112.56	110.52
14	bA	819	CLA	CHD-C4C-NC	2.20	127.67	124.20
14	A	815	CLA	CHB-C4A-NA	2.20	127.55	124.51
14	cA	804	CLA	CED-O2D-CGD	2.20	120.91	115.94
14	B	812	CLA	CHC-C4B-NB	-2.20	121.93	124.26
14	B	802	CLA	CHD-C4C-NC	2.20	127.67	124.20
17	A	849	BCR	C19-C18-C17	2.20	122.31	118.94
14	bA	818	CLA	CHC-C4B-NB	-2.20	121.93	124.26
14	A	809	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
14	cA	841	CLA	C4-C3-C5	2.20	118.97	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bA	832	CLA	O2A-CGA-CBA	2.20	118.80	111.91
14	cB	803	CLA	CHD-C4C-NC	2.20	127.67	124.20
14	bX	201	CLA	CHB-C4A-NA	2.20	127.55	124.51
14	A	805	CLA	C4C-C3C-C2C	-2.20	103.70	106.90
17	L	205	BCR	C11-C10-C9	2.20	130.44	127.31
14	A	818	CLA	CHC-C4B-NB	-2.20	121.93	124.26
14	cJ	101	CLA	CHB-C4A-NA	2.19	127.55	124.51
17	A	848	BCR	C15-C14-C13	2.19	130.44	127.31
17	M	101	BCR	C19-C18-C17	2.19	122.31	118.94
14	B	809	CLA	C2A-C1A-CHA	-2.19	120.02	123.86
14	bA	833	CLA	CHB-C1B-C2B	-2.19	121.04	127.24
14	A	832	CLA	O2A-CGA-CBA	2.19	118.79	111.91
14	bF	201	CLA	C1-O2A-CGA	2.19	122.20	116.44
14	bB	816	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
14	B	826	CLA	CHD-C4C-NC	2.19	127.66	124.20
14	A	803	CLA	CHB-C4A-NA	2.19	127.54	124.51
14	bJ	102	CLA	CHB-C4A-NA	2.19	127.54	124.51
14	bA	821	CLA	C2A-C1A-CHA	-2.19	120.03	123.86
14	bB	812	CLA	CHC-C4B-NB	-2.19	121.94	124.26
14	B	833	CLA	CHB-C1B-C2B	-2.19	121.05	127.24
17	cB	842	BCR	C37-C22-C23	2.19	121.53	118.08
14	bA	805	CLA	C4C-C3C-C2C	-2.19	103.71	106.90
14	B	815	CLA	C3B-C4B-NB	2.19	112.55	110.52
14	cA	833	CLA	CHB-C1B-C2B	-2.19	121.05	127.24
17	bB	841	BCR	C37-C22-C23	2.19	121.53	118.08
14	A	819	CLA	CHD-C4C-NC	2.19	127.65	124.20
14	cB	818	CLA	C1-O2A-CGA	2.19	122.19	116.44
17	cM	101	BCR	C19-C18-C17	2.19	122.30	118.94
14	bA	838	CLA	CHB-C4A-NA	2.19	127.54	124.51
14	A	833	CLA	CHB-C1B-C2B	-2.19	121.06	127.24
17	bM	101	BCR	C19-C18-C17	2.19	122.30	118.94
14	cA	821	CLA	C2A-C1A-CHA	-2.19	120.04	123.86
14	A	838	CLA	CHB-C4A-NA	2.19	127.53	124.51
14	cF	201	CLA	C1-O2A-CGA	2.19	122.18	116.44
14	X	201	CLA	C2A-C1A-CHA	-2.19	120.04	123.86
14	cB	810	CLA	C2A-C1A-CHA	-2.18	120.04	123.86
14	cA	805	CLA	C4C-C3C-C2C	-2.18	103.71	106.90
14	bB	816	CLA	CMB-C2B-C1B	2.18	128.70	125.37
14	A	811	CLA	CHB-C1B-C2B	-2.18	121.07	127.24
17	bB	846	BCR	C19-C18-C17	2.18	122.29	118.94
14	bX	201	CLA	C2A-C1A-CHA	-2.18	120.04	123.86
14	cJ	101	CLA	C2A-C1A-CHA	-2.18	120.04	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bB	825	CLA	CHB-C4A-NA	2.18	127.53	124.51
14	cB	826	CLA	CHB-C4A-NA	2.18	127.53	124.51
14	bB	825	CLA	CHC-C4B-NB	-2.18	121.95	124.26
14	cA	820	CLA	C3B-C4B-NB	2.18	112.54	110.52
14	cA	811	CLA	CHB-C1B-C2B	-2.18	121.07	127.24
17	cL	206	BCR	C11-C10-C9	2.18	130.43	127.31
14	B	849	CLA	CHB-C4A-NA	2.18	127.53	124.51
14	bA	830	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
14	A	830	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
14	A	842	CLA	CBC-CAC-C3C	-2.18	106.42	112.43
17	bL	205	BCR	C11-C10-C9	2.18	130.42	127.31
14	bA	811	CLA	O2A-CGA-O1A	-2.18	117.86	123.30
14	bA	809	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
14	J	102	CLA	CHB-C4A-NA	2.18	127.53	124.51
14	cA	838	CLA	CHB-C4A-NA	2.18	127.53	124.51
14	B	816	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
14	B	808	CLA	CHD-C4C-NC	2.18	127.64	124.20
14	bA	820	CLA	C3B-C4B-NB	2.18	112.54	110.52
14	cB	812	CLA	CHC-C4B-NB	-2.18	121.95	124.26
14	cF	201	CLA	C1-C2-C3	-2.18	122.28	126.04
14	A	809	CLA	CHB-C4A-NA	2.18	127.52	124.51
14	cA	830	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
14	bB	833	CLA	CHB-C1B-C2B	-2.18	121.09	127.24
14	bA	842	CLA	CBC-CAC-C3C	-2.18	106.43	112.43
14	B	825	CLA	CHB-C4A-NA	2.18	127.52	124.51
14	bB	805	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
14	cB	814	CLA	CHD-C4C-NC	2.17	127.63	124.20
14	bA	811	CLA	CHB-C1B-C2B	-2.17	121.09	127.24
14	B	805	CLA	O1D-CGD-CBD	-2.17	120.03	124.48
14	cB	817	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
14	cB	834	CLA	CHB-C1B-C2B	-2.17	121.10	127.24
14	cB	809	CLA	CHD-C4C-NC	2.17	127.63	124.20
14	bB	826	CLA	C4-C3-C5	2.17	118.93	115.27
14	A	820	CLA	C3B-C4B-NB	2.17	112.53	110.52
14	cA	842	CLA	CBC-CAC-C3C	-2.17	106.44	112.43
17	cB	847	BCR	C19-C18-C17	2.17	122.28	118.94
14	B	836	CLA	CMB-C2B-C1B	2.17	128.68	125.37
14	A	805	CLA	O2A-CGA-CBA	2.17	118.72	111.91
14	bA	805	CLA	O2A-CGA-CBA	2.17	118.72	111.91
14	bA	835	CLA	CHB-C4A-NA	2.17	127.52	124.51
14	B	817	CLA	C1-O2A-CGA	2.17	122.14	116.44
14	B	833	CLA	CHC-C4B-NB	-2.17	121.96	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bJ	101	CLA	C2A-C1A-CHA	-2.17	120.06	123.86
14	cA	823	CLA	CED-O2D-CGD	2.17	120.85	115.94
14	cA	812	CLA	CHD-C4C-NC	2.17	127.62	124.20
14	bB	819	CLA	CHB-C4A-NA	2.17	127.51	124.51
14	B	825	CLA	CHC-C4B-NB	-2.17	121.96	124.26
14	cA	809	CLA	CHB-C4A-NA	2.17	127.51	124.51
14	B	815	CLA	C4-C3-C2	-2.17	118.11	123.68
14	cJ	102	CLA	CHB-C4A-NA	2.17	127.51	124.51
14	J	101	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
14	A	823	CLA	CHC-C1C-NC	2.17	127.49	124.20
14	bL	201	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
17	cA	848	BCR	C35-C13-C14	-2.17	119.89	122.92
14	B	819	CLA	CHB-C4A-NA	2.17	127.51	124.51
14	bA	812	CLA	CHD-C4C-NC	2.17	127.62	124.20
14	B	826	CLA	C4-C3-C5	2.17	118.92	115.27
14	F	201	CLA	C1-O2A-CGA	2.17	122.13	116.44
14	cL	202	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
17	B	846	BCR	C19-C18-C17	2.17	122.27	118.94
14	A	812	CLA	CHD-C4C-NC	2.17	127.62	124.20
14	bA	809	CLA	CHB-C4A-NA	2.17	127.51	124.51
14	F	201	CLA	C1-C2-C3	-2.17	122.30	126.04
14	bB	836	CLA	CHB-C4A-NA	2.17	127.51	124.51
14	cB	816	CLA	C4-C3-C2	-2.17	118.12	123.68
14	cB	806	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
14	cA	811	CLA	O2A-CGA-O1A	-2.16	117.90	123.30
14	cA	805	CLA	O2A-CGA-CBA	2.16	118.70	111.91
14	cX	201	CLA	C2A-C1A-CHA	-2.16	120.08	123.86
14	cA	823	CLA	CHC-C1C-NC	2.16	127.49	124.20
14	bB	817	CLA	C1-O2A-CGA	2.16	122.12	116.44
14	A	811	CLA	O2A-CGA-O1A	-2.16	117.91	123.30
14	cB	827	CLA	C4-C3-C5	2.16	118.91	115.27
14	L	201	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
14	bB	808	CLA	CHB-C1B-C2B	-2.16	121.13	127.24
14	bB	839	CLA	C2A-C1A-CHA	-2.16	120.08	123.86
14	bA	823	CLA	CED-O2D-CGD	2.16	120.83	115.94
14	bB	808	CLA	CHD-C4C-NC	2.16	127.61	124.20
14	cA	834	CLA	CHD-C4C-NC	2.16	127.61	124.20
14	bB	811	CLA	CHC-C4B-NB	-2.16	121.97	124.26
14	cA	820	CLA	CHC-C4B-NB	-2.16	121.97	124.26
14	B	836	CLA	CHB-C4A-NA	2.16	127.50	124.51
14	A	823	CLA	CED-O2D-CGD	2.16	120.82	115.94
14	bA	820	CLA	CHC-C4B-NB	-2.16	121.97	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bB	815	CLA	C4-C3-C2	-2.16	118.14	123.68
14	bA	823	CLA	CHC-C1C-NC	2.16	127.48	124.20
14	B	811	CLA	CHB-C1B-C2B	-2.16	121.14	127.24
14	bA	834	CLA	CHD-C4C-NC	2.16	127.60	124.20
14	bB	804	CLA	CHB-C4A-NA	2.16	127.49	124.51
14	cB	820	CLA	CHB-C4A-NA	2.16	127.49	124.51
14	cB	812	CLA	CHB-C1B-C2B	-2.16	121.15	127.24
14	A	802	CLA	CHA-C1A-NA	-2.16	121.46	126.40
14	bB	836	CLA	CMB-C2B-C1B	2.16	128.65	125.37
14	B	839	CLA	C2A-C1A-CHA	-2.15	120.09	123.86
14	A	832	CLA	CAA-C2A-C3A	-2.15	106.88	112.78
14	B	808	CLA	CHB-C1B-C2B	-2.15	121.16	127.24
14	cB	837	CLA	CMB-C2B-C1B	2.15	128.65	125.37
14	B	814	CLA	CHD-C4C-NC	2.15	127.59	124.20
14	cA	835	CLA	CHB-C4A-NA	2.15	127.49	124.51
17	cJ	103	BCR	C16-C15-C14	2.15	127.88	123.47
17	cB	847	BCR	C35-C13-C14	-2.15	119.91	122.92
14	bA	832	CLA	CAA-C2A-C3A	-2.15	106.89	112.78
14	B	811	CLA	CHC-C4B-NB	-2.15	121.98	124.26
14	bF	201	CLA	C1-C2-C3	-2.15	122.33	126.04
14	cA	802	CLA	CHA-C1A-NA	-2.15	121.47	126.40
14	A	834	CLA	CHD-C4C-NC	2.15	127.59	124.20
14	bA	831	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
14	J	102	CLA	C2A-C1A-CHA	-2.15	120.10	123.86
14	bJ	102	CLA	C2A-C1A-CHA	-2.15	120.10	123.86
14	cA	832	CLA	CAA-C2A-C3A	-2.15	106.89	112.78
17	bA	848	BCR	C35-C13-C14	-2.15	119.91	122.92
14	bA	819	CLA	CHC-C1C-NC	2.15	127.46	124.20
14	cA	819	CLA	CHC-C1C-NC	2.15	127.46	124.20
14	B	802	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
14	bB	802	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
14	bB	811	CLA	CHB-C1B-C2B	-2.15	121.17	127.24
14	bA	808	CLA	CED-O2D-CGD	2.15	120.80	115.94
14	bJ	101	CLA	CHB-C1B-C2B	-2.15	121.17	127.24
14	bB	813	CLA	CHD-C4C-NC	2.15	127.59	124.20
17	J	103	BCR	C16-C15-C14	2.15	127.87	123.47
14	cA	808	CLA	CED-O2D-CGD	2.15	120.79	115.94
14	A	823	CLA	CHB-C1B-C2B	-2.15	121.17	127.24
14	B	813	CLA	CHD-C4C-NC	2.15	127.59	124.20
14	cB	815	CLA	CHB-C4A-NA	2.15	127.48	124.51
14	cB	809	CLA	CHB-C1B-C2B	-2.15	121.17	127.24
14	bA	836	CLA	C1-O2A-CGA	2.15	122.08	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	836	CLA	C1-O2A-CGA	2.15	122.08	116.44
14	cB	826	CLA	CHC-C4B-NB	-2.15	121.98	124.26
14	A	838	CLA	CHB-C1B-C2B	-2.15	121.18	127.24
14	A	836	CLA	C1-O2A-CGA	2.15	122.07	116.44
14	cB	815	CLA	CHD-C4C-NC	2.15	127.58	124.20
14	cB	805	CLA	CHB-C4A-NA	2.15	127.48	124.51
14	bA	802	CLA	CHA-C1A-NA	-2.15	121.48	126.40
17	A	848	BCR	C35-C13-C14	-2.15	119.92	122.92
14	cB	803	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
14	J	101	CLA	CHB-C1B-C2B	-2.14	121.18	127.24
14	bB	833	CLA	CHC-C4B-NB	-2.14	121.99	124.26
14	cB	837	CLA	CHB-C4A-NA	2.14	127.48	124.51
14	cB	840	CLA	C2A-C1A-CHA	-2.14	120.11	123.86
14	B	851	CLA	CED-O2D-CGD	2.14	120.79	115.94
14	bA	831	CLA	CED-O2D-CGD	2.14	120.79	115.94
17	bB	846	BCR	C35-C13-C14	-2.14	119.92	122.92
17	bJ	103	BCR	C16-C15-C14	2.14	127.86	123.47
14	cA	831	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
14	bB	829	CLA	CHB-C4A-NA	2.14	127.47	124.51
14	cF	201	CLA	CHB-C4A-NA	2.14	127.47	124.51
14	bA	817	CLA	CMB-C2B-C1B	2.14	128.63	125.37
14	cA	817	CLA	CMB-C2B-C1B	2.14	128.63	125.37
14	bA	813	CLA	CHB-C4A-NA	2.14	127.47	124.51
14	bA	823	CLA	CHB-C1B-C2B	-2.14	121.19	127.24
14	A	833	CLA	CHB-C4A-NA	2.14	127.47	124.51
14	B	801	CLA	CMB-C2B-C1B	2.14	128.63	125.37
14	A	820	CLA	CHC-C4B-NB	-2.14	121.99	124.26
14	A	819	CLA	CHC-C1C-NC	2.14	127.45	124.20
14	cA	831	CLA	CED-O2D-CGD	2.14	120.78	115.94
14	A	817	CLA	CMB-C2B-C1B	2.14	128.63	125.37
14	A	835	CLA	CHB-C4A-NA	2.14	127.47	124.51
14	B	804	CLA	CHB-C4A-NA	2.14	127.47	124.51
14	bB	851	CLA	CED-O2D-CGD	2.14	120.78	115.94
14	cB	810	CLA	CAA-C2A-C3A	-2.14	106.92	112.78
14	bB	816	CLA	CHB-C4A-NA	2.14	127.47	124.51
14	cA	813	CLA	CHB-C4A-NA	2.14	127.47	124.51
14	cJ	102	CLA	C2A-C1A-CHA	-2.14	120.12	123.86
14	bA	838	CLA	CHB-C1B-C2B	-2.14	121.20	127.24
14	A	831	CLA	CED-O2D-CGD	2.14	120.77	115.94
14	B	826	CLA	CHB-C1B-NB	-2.14	121.99	124.26
17	B	845	BCR	C24-C23-C22	2.14	129.47	126.23
14	B	813	CLA	CBC-CAC-C3C	-2.14	106.54	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cB	839	CLA	C1-O2A-CGA	2.14	122.05	116.44
14	bA	824	CLA	CHB-C1B-C2B	-2.14	121.20	127.24
14	cA	824	CLA	CHB-C1B-C2B	-2.14	121.20	127.24
14	cA	813	CLA	CHD-C4C-NC	2.14	127.57	124.20
14	bB	809	CLA	CAA-C2A-C3A	-2.14	106.93	112.78
14	cB	802	CLA	CMB-C2B-C1B	2.14	128.62	125.37
14	A	831	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
14	A	808	CLA	CED-O2D-CGD	2.14	120.77	115.94
14	cB	801	CLA	CED-O2D-CGD	2.14	120.77	115.94
17	I	101	BCR	C15-C14-C13	2.14	130.36	127.31
17	cB	844	BCR	C16-C17-C18	2.14	130.36	127.31
17	cB	846	BCR	C24-C23-C22	2.14	129.46	126.23
14	bA	816	CLA	CHB-C4A-NA	2.14	127.47	124.51
14	cA	833	CLA	CHB-C4A-NA	2.14	127.47	124.51
14	A	829	CLA	C1-C2-C3	-2.14	122.35	126.04
14	B	838	CLA	C1-O2A-CGA	2.14	122.05	116.44
14	F	201	CLA	CHB-C4A-NA	2.13	127.46	124.51
14	B	809	CLA	CAA-C2A-C3A	-2.13	106.93	112.78
14	cA	823	CLA	CHB-C1B-C2B	-2.13	121.21	127.24
17	bA	845	BCR	C12-C13-C14	2.13	122.22	118.94
14	cA	838	CLA	CHB-C1B-C2B	-2.13	121.21	127.24
14	B	812	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
14	bA	813	CLA	CHD-C4C-NC	2.13	127.56	124.20
14	bB	814	CLA	CHD-C4C-NC	2.13	127.56	124.20
17	B	846	BCR	C35-C13-C14	-2.13	119.94	122.92
13	bA	801	CL0	CBC-CAC-C3C	-2.13	106.55	112.43
14	B	816	CLA	CHB-C4A-NA	2.13	127.46	124.51
14	bB	838	CLA	C1-O2A-CGA	2.13	122.04	116.44
14	cJ	101	CLA	CHB-C1B-C2B	-2.13	121.22	127.24
14	bA	832	CLA	CBC-CAC-C3C	-2.13	106.55	112.43
14	B	804	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
14	A	818	CLA	CHB-C4A-NA	2.13	127.46	124.51
14	bB	814	CLA	CHB-C4A-NA	2.13	127.46	124.51
14	bB	813	CLA	CBC-CAC-C3C	-2.13	106.56	112.43
14	bB	801	CLA	CMB-C2B-C1B	2.13	128.61	125.37
14	bA	833	CLA	CAA-C2A-C3A	-2.13	106.94	112.78
14	A	824	CLA	CHB-C1B-C2B	-2.13	121.22	127.24
14	bA	829	CLA	C1-C2-C3	-2.13	122.36	126.04
14	A	813	CLA	CHB-C4A-NA	2.13	127.46	124.51
14	A	833	CLA	CAA-C2A-C3A	-2.13	106.95	112.78
14	cB	830	CLA	CHB-C4A-NA	2.13	127.46	124.51
17	cB	844	BCR	C1-C6-C5	-2.13	119.61	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cB	814	CLA	CBC-CAC-C3C	-2.13	106.56	112.43
14	cB	834	CLA	CHC-C4B-NB	-2.13	122.00	124.26
14	cA	808	CLA	O2A-CGA-O1A	-2.13	118.00	123.30
14	cA	832	CLA	CBC-CAC-C3C	-2.13	106.56	112.43
14	cA	813	CLA	CHB-C1B-C2B	-2.13	121.23	127.24
13	A	801	CL0	CBC-CAC-C3C	-2.13	106.57	112.43
14	bA	808	CLA	O2A-CGA-O1A	-2.13	118.00	123.30
14	bB	804	CLA	CHD-C4C-NC	2.13	127.56	124.20
14	bA	813	CLA	CHB-C1B-C2B	-2.13	121.23	127.24
14	A	808	CLA	O2A-CGA-O1A	-2.13	118.00	123.30
17	cB	846	BCR	C34-C9-C8	2.13	121.43	118.08
17	B	842	BCR	C10-C11-C12	2.13	129.85	123.22
14	cB	813	CLA	C1-C2-C3	-2.13	122.37	126.04
14	cA	827	CLA	C4-C3-C5	2.13	118.85	115.27
14	cA	829	CLA	C1-C2-C3	-2.12	122.37	126.04
14	cA	852	CLA	CHD-C4C-NC	2.12	127.55	124.20
14	cB	817	CLA	CHB-C4A-NA	2.12	127.45	124.51
17	bB	842	BCR	C10-C11-C12	2.12	129.85	123.22
14	A	813	CLA	CHB-C1B-C2B	-2.12	121.24	127.24
14	cB	805	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
17	B	843	BCR	C1-C6-C5	-2.12	119.62	122.61
17	cA	845	BCR	C12-C13-C14	2.12	122.20	118.94
14	A	831	CLA	CBA-CAA-C2A	2.12	120.13	113.86
14	A	816	CLA	CHB-C4A-NA	2.12	127.45	124.51
14	cB	813	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
17	cI	101	BCR	C15-C14-C13	2.12	130.34	127.31
17	B	843	BCR	C16-C17-C18	2.12	130.34	127.31
14	A	826	CLA	C2A-C1A-CHA	-2.12	120.15	123.86
14	cA	833	CLA	CAA-C2A-C3A	-2.12	106.97	112.78
14	A	832	CLA	CBC-CAC-C3C	-2.12	106.58	112.43
17	bB	843	BCR	C16-C17-C18	2.12	130.34	127.31
14	bB	812	CLA	C1-C2-C3	-2.12	122.38	126.04
17	A	845	BCR	C12-C13-C14	2.12	122.19	118.94
14	B	834	CLA	CHC-C1C-NC	2.12	127.42	124.20
14	bA	833	CLA	CHB-C4A-NA	2.12	127.44	124.51
14	bF	201	CLA	CHB-C4A-NA	2.12	127.44	124.51
14	cA	842	CLA	CHB-C4A-NA	2.12	127.44	124.51
13	cA	801	CL0	CBC-CAC-C3C	-2.12	106.59	112.43
14	cA	831	CLA	CBA-CAA-C2A	2.12	120.12	113.86
17	cB	843	BCR	C10-C11-C12	2.12	129.83	123.22
14	cA	818	CLA	CHB-C4A-NA	2.12	127.44	124.51
14	A	805	CLA	CMB-C2B-C1B	2.12	128.60	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cB	821	CLA	CHD-C4C-NC	2.12	127.54	124.20
14	bA	826	CLA	C2A-C1A-CHA	-2.12	120.15	123.86
14	B	829	CLA	CHB-C4A-NA	2.12	127.44	124.51
14	cA	816	CLA	CHB-C4A-NA	2.12	127.44	124.51
14	bA	852	CLA	CHD-C4C-NC	2.12	127.54	124.20
14	B	815	CLA	CED-O2D-CGD	2.12	120.73	115.94
14	bA	818	CLA	CHB-C4A-NA	2.12	127.44	124.51
14	bA	842	CLA	CHB-C4A-NA	2.12	127.44	124.51
14	cB	805	CLA	CHD-C4C-NC	2.12	127.54	124.20
14	cA	826	CLA	C2A-C1A-CHA	-2.12	120.16	123.86
14	cA	852	CLA	C4-C3-C5	2.12	118.83	115.27
14	bB	804	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
17	bB	843	BCR	C1-C6-C5	-2.12	119.63	122.61
17	B	845	BCR	C34-C9-C8	2.12	121.41	118.08
14	B	814	CLA	CHB-C4A-NA	2.12	127.44	124.51
14	bA	819	CLA	CHC-C4B-NB	-2.12	122.02	124.26
17	bB	845	BCR	C24-C23-C22	2.12	129.43	126.23
14	B	812	CLA	C1-C2-C3	-2.12	122.38	126.04
14	A	836	CLA	CAA-C2A-C1A	2.12	118.91	111.97
14	cB	835	CLA	CHC-C1C-NC	2.12	127.41	124.20
14	cA	836	CLA	CAA-C2A-C1A	2.12	118.91	111.97
17	bI	101	BCR	C15-C14-C13	2.11	130.33	127.31
14	cA	805	CLA	CMB-C2B-C1B	2.11	128.59	125.37
14	bB	826	CLA	CHA-C1A-NA	-2.11	121.56	126.40
14	bA	831	CLA	CHB-C4A-NA	2.11	127.44	124.51
14	bB	826	CLA	C2A-C1A-CHA	-2.11	120.16	123.86
14	bA	811	CLA	CHC-C4B-NB	-2.11	122.02	124.26
14	bB	820	CLA	CHD-C4C-NC	2.11	127.53	124.20
14	A	852	CLA	C4-C3-C5	2.11	118.83	115.27
17	bB	841	BCR	C15-C14-C13	2.11	130.32	127.31
14	bA	806	CLA	CHB-C1B-C2B	-2.11	121.27	127.24
17	cA	848	BCR	C20-C21-C22	2.11	130.32	127.31
14	A	842	CLA	CHB-C4A-NA	2.11	127.43	124.51
14	bA	805	CLA	CMB-C2B-C1B	2.11	128.59	125.37
14	A	806	CLA	CHB-C1B-C2B	-2.11	121.27	127.24
14	B	804	CLA	CHD-C4C-NC	2.11	127.53	124.20
14	cB	827	CLA	CHA-C1A-NA	-2.11	121.56	126.40
14	A	813	CLA	CHD-C4C-NC	2.11	127.53	124.20
14	bA	836	CLA	CAA-C2A-C1A	2.11	118.89	111.97
14	B	826	CLA	CHA-C1A-NA	-2.11	121.57	126.40
14	A	852	CLA	CHD-C4C-NC	2.11	127.53	124.20
14	bA	852	CLA	C4-C3-C5	2.11	118.82	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	847	BCR	C16-C17-C18	2.11	130.32	127.31
14	bA	836	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
14	cB	826	CLA	CMD-C2D-C3D	-2.11	122.77	127.61
17	bB	847	BCR	C16-C17-C18	2.11	130.32	127.31
14	A	833	CLA	C1-C2-C3	-2.11	122.40	126.04
14	bB	812	CLA	O2D-CGD-O1D	-2.11	119.72	123.84
14	cA	806	CLA	CHB-C1B-C2B	-2.11	121.29	127.24
14	cA	831	CLA	CHB-C4A-NA	2.11	127.42	124.51
17	bB	845	BCR	C34-C9-C8	2.11	121.40	118.08
17	B	841	BCR	C15-C14-C13	2.11	130.32	127.31
14	bA	831	CLA	CBA-CAA-C2A	2.11	120.08	113.86
14	bB	838	CLA	CHD-C4C-NC	2.11	127.52	124.20
14	cB	850	CLA	CHB-C1B-C2B	-2.11	121.29	127.24
14	cA	818	CLA	C3B-C4B-NB	2.11	112.47	110.52
14	bA	827	CLA	C4-C3-C5	2.10	118.81	115.27
14	bB	834	CLA	CHC-C1C-NC	2.10	127.40	124.20
14	bB	815	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
14	bA	818	CLA	C3B-C4B-NB	2.10	112.47	110.52
14	cA	833	CLA	C1-C2-C3	-2.10	122.40	126.04
14	cA	808	CLA	CBC-CAC-C3C	-2.10	106.63	112.43
14	A	831	CLA	CHB-C4A-NA	2.10	127.42	124.51
14	bA	827	CLA	C1-C2-C3	-2.10	122.41	126.04
14	B	826	CLA	C2A-C1A-CHA	-2.10	120.18	123.86
14	bB	849	CLA	CHB-C1B-C2B	-2.10	121.30	127.24
14	cB	802	CLA	CHB-C1B-C2B	-2.10	121.30	127.24
14	B	820	CLA	CHD-C4C-NC	2.10	127.52	124.20
14	B	826	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
14	cA	825	CLA	CGD-CBD-CAD	-2.10	103.93	110.73
17	B	847	BCR	C34-C9-C8	2.10	121.39	118.08
14	bB	815	CLA	CED-O2D-CGD	2.10	120.69	115.94
17	bA	848	BCR	C16-C17-C18	2.10	130.31	127.31
14	B	825	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
14	bB	801	CLA	CHB-C1B-C2B	-2.10	121.30	127.24
14	bB	826	CLA	CHB-C1B-NB	-2.10	122.03	124.26
17	bA	848	BCR	C20-C21-C22	2.10	130.31	127.31
17	cB	848	BCR	C16-C17-C18	2.10	130.31	127.31
14	bB	825	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
14	B	849	CLA	CHB-C1B-C2B	-2.10	121.31	127.24
17	B	846	BCR	C11-C10-C9	2.10	130.31	127.31
14	bB	820	CLA	CHB-C4A-NA	2.10	127.41	124.51
14	A	825	CLA	CGD-CBD-CAD	-2.10	103.94	110.73
14	B	820	CLA	CHB-C4A-NA	2.10	127.41	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cB	827	CLA	C2A-C1A-CHA	-2.10	120.19	123.86
14	B	808	CLA	CHB-C4A-NA	2.10	127.41	124.51
14	B	819	CLA	CHC-C4B-NB	-2.10	122.04	124.26
14	bA	808	CLA	CBC-CAC-C3C	-2.10	106.65	112.43
14	cB	839	CLA	CHD-C4C-NC	2.10	127.51	124.20
14	cA	806	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
14	A	806	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
14	bL	201	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
14	bA	825	CLA	CGD-CBD-CAD	-2.10	103.94	110.73
14	cB	820	CLA	CHB-C1B-C2B	-2.10	121.32	127.24
14	bB	826	CLA	O2D-CGD-O1D	-2.10	119.74	123.84
14	A	836	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
17	cB	848	BCR	C34-C9-C8	2.10	121.38	118.08
14	cB	816	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
14	A	808	CLA	CBC-CAC-C3C	-2.09	106.66	112.43
14	cB	816	CLA	CED-O2D-CGD	2.09	120.67	115.94
14	cA	836	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
14	B	801	CLA	CHB-C1B-C2B	-2.09	121.32	127.24
14	L	201	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
14	bA	819	CLA	CHB-C1B-C2B	-2.09	121.32	127.24
14	bA	806	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
14	cB	836	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
17	A	848	BCR	C16-C17-C18	2.09	130.30	127.31
17	cA	848	BCR	C16-C17-C18	2.09	130.30	127.31
14	cB	821	CLA	CHB-C4A-NA	2.09	127.41	124.51
14	bB	835	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
17	bB	847	BCR	C34-C9-C8	2.09	121.37	118.08
14	L	203	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
14	bB	815	CLA	CHB-C1B-C2B	-2.09	121.33	127.24
14	cA	811	CLA	CHC-C4B-NB	-2.09	122.04	124.26
17	A	848	BCR	C20-C21-C22	2.09	130.30	127.31
14	A	827	CLA	C4-C3-C5	2.09	118.79	115.27
14	cB	827	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
14	B	819	CLA	CHB-C1B-C2B	-2.09	121.33	127.24
14	bA	833	CLA	C1-C2-C3	-2.09	122.43	126.04
14	bB	819	CLA	CHB-C1B-C2B	-2.09	121.33	127.24
14	A	818	CLA	C3B-C4B-NB	2.09	112.45	110.52
14	cB	826	CLA	OBD-CAD-C3D	-2.09	123.50	128.52
14	cL	202	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
14	A	819	CLA	CHC-C4B-NB	-2.09	122.05	124.26
14	A	819	CLA	CHB-C1B-C2B	-2.09	121.34	127.24
14	B	833	CLA	C2A-C1A-CHA	-2.09	120.21	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bA	823	CLA	CHC-C4B-NB	-2.09	122.05	124.26
14	bB	819	CLA	CHC-C4B-NB	-2.09	122.05	124.26
14	B	815	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
14	cL	204	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
14	B	805	CLA	CED-O2D-CGD	2.09	120.66	115.94
14	cA	835	CLA	C2A-C1A-CHA	-2.09	120.21	123.86
14	cA	827	CLA	C1-C2-C3	-2.09	122.44	126.04
14	B	815	CLA	CHB-C1B-C2B	-2.09	121.35	127.24
14	cA	819	CLA	CHB-C1B-C2B	-2.09	121.35	127.24
14	cB	809	CLA	CHB-C4A-NA	2.09	127.40	124.51
14	A	827	CLA	C1-C2-C3	-2.08	122.44	126.04
17	bB	846	BCR	C11-C10-C9	2.08	130.28	127.31
17	bB	845	BCR	C20-C21-C22	2.08	130.28	127.31
17	cB	846	BCR	C20-C21-C22	2.08	130.28	127.31
14	B	835	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
14	cB	816	CLA	CHB-C1B-C2B	-2.08	121.35	127.24
17	cB	847	BCR	C11-C10-C9	2.08	130.28	127.31
14	cB	807	CLA	O2A-CGA-CBA	2.08	118.44	111.91
14	bB	825	CLA	OBD-CAD-C3D	-2.08	123.51	128.52
17	cM	101	BCR	C35-C13-C14	-2.08	120.01	122.92
14	bB	806	CLA	O2A-CGA-CBA	2.08	118.43	111.91
14	B	838	CLA	CHD-C4C-NC	2.08	127.48	124.20
14	cA	828	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
14	cA	819	CLA	CHC-C4B-NB	-2.08	122.06	124.26
14	cB	827	CLA	CHB-C1B-NB	-2.08	122.06	124.26
14	cB	839	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
14	bA	830	CLA	O2A-CGA-CBA	2.08	118.43	111.91
13	cA	801	CL0	C2A-C1A-CHA	-2.08	120.23	123.86
17	cB	842	BCR	C15-C14-C13	2.08	130.27	127.31
14	A	841	CLA	C2A-C1A-CHA	-2.08	120.23	123.86
14	B	806	CLA	O2A-CGA-CBA	2.08	118.42	111.91
14	bB	805	CLA	CED-O2D-CGD	2.08	120.63	115.94
14	bB	833	CLA	C2A-C1A-CHA	-2.08	120.23	123.86
14	bA	820	CLA	CHB-C4A-NA	2.08	127.38	124.51
14	bB	808	CLA	CHB-C4A-NA	2.08	127.38	124.51
14	bA	835	CLA	C2A-C1A-CHA	-2.08	120.23	123.86
14	B	825	CLA	OBD-CAD-C3D	-2.08	123.53	128.52
14	cA	830	CLA	O2A-CGA-CBA	2.07	118.42	111.91
14	bB	825	CLA	C2A-C1A-CHA	-2.07	120.23	123.86
14	cB	802	CLA	C2A-C1A-CHA	-2.07	120.23	123.86
14	bL	203	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
14	bA	828	CLA	C2A-C1A-CHA	-2.07	120.23	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	835	CLA	CHC-C4B-NB	-2.07	122.06	124.26
14	cB	826	CLA	CHB-C1B-C2B	-2.07	121.38	127.24
14	A	828	CLA	C2A-C1A-CHA	-2.07	120.23	123.86
17	B	842	BCR	C16-C17-C18	2.07	130.27	127.31
14	A	836	CLA	C4-C3-C2	-2.07	118.36	123.68
14	bA	825	CLA	C2A-C1A-CHA	-2.07	120.24	123.86
14	cB	820	CLA	CHC-C4B-NB	-2.07	122.06	124.26
14	A	830	CLA	O2A-CGA-CBA	2.07	118.41	111.91
14	cB	834	CLA	C2A-C1A-CHA	-2.07	120.24	123.86
14	cA	840	CLA	O2A-CGA-CBA	2.07	118.41	111.91
14	A	811	CLA	CHC-C4B-NB	-2.07	122.06	124.26
14	bA	836	CLA	C4-C3-C2	-2.07	118.37	123.68
14	bB	812	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
14	B	825	CLA	C2A-C1A-CHA	-2.07	120.24	123.86
14	A	823	CLA	CHC-C4B-NB	-2.07	122.07	124.26
14	cB	833	CLA	CHB-C1B-C2B	-2.07	121.39	127.24
14	bA	840	CLA	O2A-CGA-CBA	2.07	118.40	111.91
14	B	825	CLA	CHB-C1B-C2B	-2.07	121.40	127.24
14	cA	802	CLA	CED-O2D-CGD	2.07	120.61	115.94
17	bB	842	BCR	C16-C17-C18	2.07	130.26	127.31
14	A	840	CLA	O2A-CGA-CBA	2.07	118.40	111.91
14	bB	825	CLA	CHB-C1B-C2B	-2.07	121.40	127.24
14	cL	205	CLA	CHD-C4C-NC	2.07	127.46	124.20
17	B	845	BCR	C20-C21-C22	2.07	130.26	127.31
14	cB	826	CLA	C2A-C1A-CHA	-2.07	120.25	123.86
14	cB	827	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
14	bB	817	CLA	CED-O2D-CGD	2.07	120.61	115.94
14	B	838	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
14	cB	806	CLA	CED-O2D-CGD	2.07	120.61	115.94
14	bA	802	CLA	CED-O2D-CGD	2.06	120.61	115.94
14	bA	829	CLA	CBC-CAC-C3C	-2.06	106.74	112.43
14	cB	818	CLA	C2A-C1A-CHA	-2.06	120.25	123.86
14	A	841	CLA	CHD-C4C-NC	2.06	127.46	124.20
17	bM	101	BCR	C30-C25-C26	-2.06	119.71	122.61
14	A	805	CLA	O1D-CGD-CBD	-2.06	120.26	124.48
14	cA	825	CLA	C2A-C1A-CHA	-2.06	120.25	123.86
14	L	204	CLA	CHD-C4C-NC	2.06	127.45	124.20
14	bB	838	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
14	A	835	CLA	CHC-C4B-NB	-2.06	122.07	124.26
14	cA	831	CLA	CHB-C1B-NB	-2.06	122.07	124.26
14	B	823	CLA	CHB-C1B-C2B	-2.06	121.41	127.24
14	cA	812	CLA	CMB-C2B-C3B	2.06	131.58	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	cA	823	CLA	CHC-C4B-NB	-2.06	122.08	124.26
14	B	817	CLA	C2A-C1A-CHA	-2.06	120.25	123.86
14	A	829	CLA	CBC-CAC-C3C	-2.06	106.75	112.43
14	cA	820	CLA	CHB-C4A-NA	2.06	127.36	124.51
14	bA	831	CLA	CHB-C1B-NB	-2.06	122.08	124.26
14	B	801	CLA	C2A-C1A-CHA	-2.06	120.26	123.86
14	bB	801	CLA	C2A-C1A-CHA	-2.06	120.26	123.86
14	bB	823	CLA	CHB-C1B-C2B	-2.06	121.42	127.24
14	cB	813	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
14	bA	834	CLA	CHC-C1C-NC	2.06	127.33	124.20
14	cB	818	CLA	CED-O2D-CGD	2.06	120.59	115.94
13	A	801	CL0	C2A-C1A-CHA	-2.06	120.26	123.86
14	A	825	CLA	C2A-C1A-CHA	-2.06	120.26	123.86
14	cA	841	CLA	CHD-C4C-NC	2.06	127.45	124.20
14	B	826	CLA	CMD-C2D-C3D	-2.06	122.88	127.61
14	L	201	CLA	O2D-CGD-O1D	-2.06	119.81	123.84
14	bB	826	CLA	CMD-C2D-C3D	-2.06	122.88	127.61
14	A	831	CLA	CHB-C1B-NB	-2.06	122.08	124.26
17	M	101	BCR	C35-C13-C14	-2.06	120.04	122.92
14	A	820	CLA	CHB-C4A-NA	2.06	127.36	124.51
14	cB	824	CLA	CHB-C1B-C2B	-2.06	121.42	127.24
14	bA	824	CLA	C2A-C1A-CHA	-2.06	120.26	123.86
14	B	823	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
14	B	832	CLA	CHB-C1B-C2B	-2.06	121.43	127.24
14	A	835	CLA	C2A-C1A-CHA	-2.06	120.26	123.86
14	bA	825	CLA	O2A-CGA-CBA	2.06	118.36	111.91
14	cA	829	CLA	CBC-CAC-C3C	-2.06	106.76	112.43
17	cA	845	BCR	C20-C21-C22	2.06	130.25	127.31
14	B	812	CLA	O1D-CGD-CBD	-2.06	120.28	124.48
14	bB	817	CLA	C2A-C1A-CHA	-2.06	120.26	123.86
14	bA	807	CLA	CHB-C4A-NA	2.06	127.36	124.51
14	cA	836	CLA	C4-C3-C2	-2.06	118.40	123.68
14	cA	805	CLA	O1D-CGD-CBD	-2.06	120.28	124.48
17	A	845	BCR	C20-C21-C22	2.05	130.24	127.31
14	bA	835	CLA	CHC-C4B-NB	-2.05	122.08	124.26
14	bB	832	CLA	CHB-C1B-C2B	-2.05	121.44	127.24
14	cA	804	CLA	CHB-C1B-C2B	-2.05	121.44	127.24
14	B	817	CLA	CED-O2D-CGD	2.05	120.58	115.94
14	bA	805	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
14	cA	841	CLA	CMA-C3A-C2A	-2.05	105.55	113.83
14	bA	841	CLA	C2A-C1A-CHA	-2.05	120.27	123.86
14	A	812	CLA	CMB-C2B-C3B	2.05	131.56	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bB	831	CLA	C4-C3-C5	2.05	118.72	115.27
14	cA	834	CLA	CHC-C1C-NC	2.05	127.31	124.20
17	cB	843	BCR	C16-C17-C18	2.05	130.24	127.31
14	cB	814	CLA	CHB-C4A-NA	2.05	127.35	124.51
14	bL	204	CLA	CHD-C4C-NC	2.05	127.44	124.20
14	A	802	CLA	CED-O2D-CGD	2.05	120.58	115.94
14	bA	812	CLA	CMB-C2B-C3B	2.05	131.55	126.59
14	cA	824	CLA	C2A-C1A-CHA	-2.05	120.27	123.86
14	B	821	CLA	CED-O2D-CGD	2.05	120.57	115.94
14	bA	804	CLA	CHB-C1B-C2B	-2.05	121.45	127.24
14	cB	824	CLA	O1D-CGD-CBD	-2.05	120.29	124.48
14	B	809	CLA	C7-C6-C5	-2.05	107.80	113.36
14	bA	826	CLA	O2A-CGA-CBA	2.05	120.33	112.23
14	bA	838	CLA	C3B-C4B-NB	2.05	112.42	110.52
14	B	816	CLA	CHC-C4B-NB	-2.05	122.09	124.26
14	bB	816	CLA	CHC-C4B-NB	-2.05	122.09	124.26
14	bB	809	CLA	C7-C6-C5	-2.05	107.80	113.36
14	A	834	CLA	CHC-C1C-NC	2.05	127.31	124.20
14	B	813	CLA	CHB-C4A-NA	2.05	127.34	124.51
14	bA	841	CLA	CHD-C4C-NC	2.05	127.43	124.20
14	bB	803	CLA	CHB-C1B-C2B	-2.05	121.46	127.24
17	cL	207	BCR	C35-C13-C14	-2.05	120.06	122.92
14	cB	807	CLA	C5-C3-C2	-2.05	116.98	121.12
14	cA	829	CLA	CHB-C4A-NA	2.05	127.34	124.51
17	bM	101	BCR	C35-C13-C14	-2.05	120.06	122.92
14	bB	821	CLA	CED-O2D-CGD	2.05	120.56	115.94
14	A	824	CLA	C2A-C1A-CHA	-2.05	120.28	123.86
14	A	807	CLA	CHB-C4A-NA	2.05	127.34	124.51
14	B	806	CLA	C5-C3-C2	-2.04	116.98	121.12
14	A	841	CLA	CMA-C3A-C2A	-2.04	105.58	113.83
14	bA	841	CLA	CMA-C3A-C2A	-2.04	105.58	113.83
14	A	804	CLA	CHB-C1B-C2B	-2.04	121.46	127.24
14	bB	813	CLA	CHB-C4A-NA	2.04	127.34	124.51
14	cA	825	CLA	O2A-CGA-CBA	2.04	118.32	111.91
14	B	803	CLA	CHB-C1B-C2B	-2.04	121.46	127.24
13	bA	801	CL0	C2A-C1A-CHA	-2.04	120.28	123.86
14	A	825	CLA	O2A-CGA-CBA	2.04	118.32	111.91
14	bB	828	CLA	CHB-C4A-NA	2.04	127.34	124.51
14	A	838	CLA	C3B-C4B-NB	2.04	112.41	110.52
14	bA	838	CLA	O2A-CGA-CBA	2.04	120.59	114.03
14	A	838	CLA	O2A-CGA-CBA	2.04	120.59	114.03
14	cA	826	CLA	O2A-CGA-CBA	2.04	120.30	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	bB	806	CLA	C5-C3-C2	-2.04	116.99	121.12
14	B	819	CLA	O2D-CGD-O1D	-2.04	119.85	123.84
14	cA	807	CLA	CHB-C4A-NA	2.04	127.33	124.51
14	A	852	CLA	CMB-C2B-C1B	2.04	128.48	125.37
14	cA	838	CLA	O2A-CGA-CBA	2.04	120.59	114.03
14	cA	852	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
14	bB	823	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
14	bA	829	CLA	CHB-C4A-NA	2.04	127.33	124.51
14	B	805	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
14	cA	852	CLA	CMB-C2B-C1B	2.04	128.47	125.37
14	A	829	CLA	CHB-C4A-NA	2.04	127.33	124.51
14	A	803	CLA	O2A-CGA-CBA	2.04	120.58	114.03
14	A	826	CLA	O2A-CGA-CBA	2.04	120.29	112.23
17	M	101	BCR	C30-C25-C26	-2.04	119.74	122.61
14	A	852	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
14	B	831	CLA	C4-C3-C5	2.04	118.70	115.27
14	cA	841	CLA	C2A-C1A-CHA	-2.04	120.30	123.86
14	cA	803	CLA	O2A-CGA-CBA	2.04	120.58	114.03
14	bA	852	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
14	cB	820	CLA	O2D-CGD-O1D	-2.04	119.86	123.84
14	bB	832	CLA	O2A-CGA-CBA	2.04	120.57	114.03
14	cB	804	CLA	CHB-C1B-C2B	-2.04	121.48	127.24
14	cA	808	CLA	CHC-C4B-NB	-2.04	122.10	124.26
14	bL	203	CLA	O1D-CGD-CBD	-2.04	120.32	124.48
14	cB	810	CLA	C7-C6-C5	-2.04	107.83	113.36
14	bB	805	CLA	CMD-C2D-C3D	-2.04	122.93	127.61
17	cB	848	BCR	C29-C30-C25	2.03	113.61	110.48
14	cB	815	CLA	O2A-CGA-CBA	2.03	120.56	114.03
14	cA	838	CLA	C3B-C4B-NB	2.03	112.40	110.52
17	bB	847	BCR	C29-C30-C25	2.03	113.61	110.48
14	cL	202	CLA	O2D-CGD-O1D	-2.03	119.86	123.84
14	B	828	CLA	CHB-C4A-NA	2.03	127.32	124.51
14	bB	819	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
14	cB	822	CLA	CED-O2D-CGD	2.03	120.53	115.94
14	A	808	CLA	CHC-C4B-NB	-2.03	122.11	124.26
14	B	819	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
17	I	101	BCR	C35-C13-C14	-2.03	120.08	122.92
14	bB	831	CLA	CHC-C4B-NB	-2.03	122.11	124.26
14	bA	803	CLA	O2A-CGA-CBA	2.03	120.55	114.03
14	cB	829	CLA	CHB-C4A-NA	2.03	127.32	124.51
14	bL	201	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
17	A	846	BCR	C24-C23-C22	2.03	129.30	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	cM	101	BCR	C30-C25-C26	-2.03	119.75	122.61
14	bB	814	CLA	O2A-CGA-CBA	2.03	120.55	114.03
17	bL	206	BCR	C35-C13-C14	-2.03	120.08	122.92
17	bA	846	BCR	C24-C23-C22	2.03	129.30	126.23
14	B	814	CLA	O2A-CGA-CBA	2.03	120.55	114.03
14	B	835	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
17	cI	101	BCR	C35-C13-C14	-2.03	120.08	122.92
14	bB	819	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
17	bA	845	BCR	C20-C21-C22	2.03	130.20	127.31
14	cB	832	CLA	C4-C3-C5	2.03	118.68	115.27
14	B	832	CLA	O2A-CGA-CBA	2.03	120.54	114.03
14	A	824	CLA	CMA-C3A-C4A	2.03	117.22	111.77
14	cB	833	CLA	O2A-CGA-CBA	2.03	120.54	114.03
14	L	203	CLA	O1D-CGD-CBD	-2.03	120.34	124.48
14	bA	814	CLA	O2A-CGA-O1A	-2.03	118.25	123.30
17	B	850	BCR	C11-C10-C9	2.03	130.20	127.31
14	cA	827	CLA	CHB-C4A-NA	2.03	127.31	124.51
14	cB	820	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
14	cB	806	CLA	CMD-C2D-C3D	-2.03	122.95	127.61
14	A	834	CLA	CHB-C4A-NA	2.03	127.31	124.51
14	X	201	CLA	CHB-C1B-C2B	-2.03	121.52	127.24
14	bF	201	CLA	CHB-C1B-C2B	-2.03	121.52	127.24
17	cA	846	BCR	C24-C23-C22	2.03	129.29	126.23
14	cB	836	CLA	O2D-CGD-O1D	-2.02	119.88	123.84
17	B	841	BCR	C34-C9-C8	2.02	121.27	118.08
14	bA	835	CLA	CED-O2D-CGD	2.02	120.51	115.94
14	bX	201	CLA	CHB-C1B-C2B	-2.02	121.52	127.24
14	cX	201	CLA	CHB-C1B-C2B	-2.02	121.52	127.24
14	A	814	CLA	O2A-CGA-O1A	-2.02	118.26	123.30
17	cB	851	BCR	C11-C10-C9	2.02	130.20	127.31
14	cL	204	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
14	cA	824	CLA	CMA-C3A-C4A	2.02	117.21	111.77
14	bB	831	CLA	C3B-C4B-NB	2.02	112.39	110.52
14	cA	807	CLA	CHB-C1B-C2B	-2.02	121.53	127.24
14	cB	817	CLA	CHC-C4B-NB	-2.02	122.12	124.26
17	bB	841	BCR	C34-C9-C8	2.02	121.26	118.08
17	B	847	BCR	C29-C30-C25	2.02	113.59	110.48
14	F	201	CLA	CHB-C1B-C2B	-2.02	121.54	127.24
14	cA	852	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
14	bA	824	CLA	CMA-C3A-C4A	2.02	117.20	111.77
14	bA	827	CLA	CHB-C4A-NA	2.02	127.30	124.51
17	cB	842	BCR	C34-C9-C8	2.02	121.25	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	817	CLA	CAA-C2A-C1A	2.02	118.58	111.97
14	bA	817	CLA	CAA-C2A-C1A	2.02	118.58	111.97
17	L	206	BCR	C35-C13-C14	-2.02	120.10	122.92
14	cA	835	CLA	CED-O2D-CGD	2.02	120.50	115.94
14	cB	810	CLA	CHD-C4C-NC	2.02	127.38	124.20
14	cA	834	CLA	CHB-C4A-NA	2.02	127.30	124.51
17	bI	101	BCR	C35-C13-C14	-2.02	120.10	122.92
14	B	807	CLA	CED-O2D-CGD	2.02	120.50	115.94
14	cA	817	CLA	CAA-C2A-C1A	2.02	118.58	111.97
14	J	102	CLA	CHB-C1B-C2B	-2.02	121.55	127.24
14	cB	817	CLA	CBA-CAA-C2A	2.02	119.81	113.86
14	B	834	CLA	CHB-C1B-C2B	-2.01	121.55	127.24
14	B	816	CLA	CBA-CAA-C2A	2.01	119.81	113.86
14	B	811	CLA	O2D-CGD-O1D	-2.01	119.90	123.84
14	bA	808	CLA	CHC-C4B-NB	-2.01	122.12	124.26
14	bB	834	CLA	CHB-C1B-C2B	-2.01	121.55	127.24
14	cA	814	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
14	A	827	CLA	O2D-CGD-O1D	-2.01	119.90	123.84
14	cB	808	CLA	CED-O2D-CGD	2.01	120.49	115.94
14	bB	807	CLA	CED-O2D-CGD	2.01	120.49	115.94
14	bB	816	CLA	C3B-C4B-NB	2.01	112.38	110.52
14	A	827	CLA	CHB-C1B-C2B	-2.01	121.55	127.24
14	cB	835	CLA	CHB-C1B-C2B	-2.01	121.55	127.24
14	bA	852	CLA	CMB-C2B-C1B	2.01	128.43	125.37
14	A	807	CLA	CHC-C1C-NC	2.01	127.25	124.20
14	bA	852	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
14	B	831	CLA	C3B-C4B-NB	2.01	112.38	110.52
17	bA	845	BCR	C21-C20-C19	2.01	129.49	123.22
14	cF	201	CLA	CHB-C1B-C2B	-2.01	121.56	127.24
14	B	821	CLA	CHD-C4C-NC	2.01	127.37	124.20
14	cB	818	CLA	CHB-C1B-C2B	-2.01	121.56	127.24
14	A	852	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
14	bJ	102	CLA	CHB-C1B-C2B	-2.01	121.56	127.24
14	B	831	CLA	CHC-C4B-NB	-2.01	122.13	124.26
14	A	807	CLA	CHB-C1B-C2B	-2.01	121.56	127.24
14	bB	835	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
14	bB	821	CLA	CHD-C4C-NC	2.01	127.37	124.20
14	bA	827	CLA	CHB-C1B-C2B	-2.01	121.57	127.24
14	cJ	102	CLA	CHB-C1B-C2B	-2.01	121.57	127.24
14	bB	816	CLA	CBA-CAA-C2A	2.01	119.79	113.86
17	bB	850	BCR	C11-C10-C9	2.01	130.17	127.31
14	B	817	CLA	CHB-C1B-C2B	-2.01	121.57	127.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	835	CLA	CED-O2D-CGD	2.01	120.47	115.94
14	bA	807	CLA	CHB-C1B-C2B	-2.01	121.57	127.24
14	A	827	CLA	CHB-C4A-NA	2.01	127.29	124.51
17	A	845	BCR	C21-C20-C19	2.01	129.48	123.22
17	cA	845	BCR	C21-C20-C19	2.01	129.48	123.22
14	bA	827	CLA	O2D-CGD-O1D	-2.01	119.92	123.84
14	cA	831	CLA	C5-C3-C2	-2.01	117.06	121.12
14	cA	807	CLA	CHC-C1C-NC	2.01	127.25	124.20
14	cA	827	CLA	CHB-C1B-C2B	-2.00	121.57	127.24
14	bB	817	CLA	CHB-C1B-C2B	-2.00	121.58	127.24
14	B	809	CLA	CHD-C4C-NC	2.00	127.36	124.20
14	cB	822	CLA	CHD-C4C-NC	2.00	127.36	124.20
14	bA	834	CLA	CHB-C4A-NA	2.00	127.28	124.51
14	bA	831	CLA	C5-C3-C2	-2.00	117.07	121.12
14	bB	809	CLA	CHD-C4C-NC	2.00	127.36	124.20
14	B	814	CLA	CMD-C2D-C3D	-2.00	123.01	127.61

There are no chirality outliers.

All (2531) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	803	CLA	C1A-C2A-CAA-CBA
14	A	806	CLA	C1A-C2A-CAA-CBA
14	A	808	CLA	C1A-C2A-CAA-CBA
14	A	808	CLA	C3A-C2A-CAA-CBA
14	A	812	CLA	CBD-CGD-O2D-CED
14	A	818	CLA	C3A-C2A-CAA-CBA
14	A	820	CLA	CBD-CGD-O2D-CED
14	A	821	CLA	C2A-CAA-CBA-CGA
14	A	823	CLA	CBD-CGD-O2D-CED
14	A	826	CLA	CBA-CGA-O2A-C1
14	A	831	CLA	C1A-C2A-CAA-CBA
14	A	831	CLA	C3A-C2A-CAA-CBA
14	A	831	CLA	C2-C3-C5-C6
14	A	831	CLA	C4-C3-C5-C6
14	A	835	CLA	CBD-CGD-O2D-CED
14	A	836	CLA	C2-C3-C5-C6
14	A	836	CLA	C4-C3-C5-C6
14	A	838	CLA	CHA-CBD-CGD-O1D
14	A	842	CLA	CHA-CBD-CGD-O1D
14	B	802	CLA	CHA-CBD-CGD-O1D
14	B	802	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	B	804	CLA	C2-C3-C5-C6
14	B	804	CLA	C4-C3-C5-C6
14	B	805	CLA	C3A-C2A-CAA-CBA
14	B	806	CLA	CBD-CGD-O2D-CED
14	B	806	CLA	C2-C3-C5-C6
14	B	808	CLA	CHA-CBD-CGD-O1D
14	B	808	CLA	CHA-CBD-CGD-O2D
14	B	809	CLA	C1A-C2A-CAA-CBA
14	B	809	CLA	C3A-C2A-CAA-CBA
14	B	814	CLA	C1A-C2A-CAA-CBA
14	B	815	CLA	O1A-CGA-O2A-C1
14	B	815	CLA	C2-C3-C5-C6
14	B	815	CLA	C4-C3-C5-C6
14	B	816	CLA	C1A-C2A-CAA-CBA
14	B	816	CLA	C3A-C2A-CAA-CBA
14	B	817	CLA	C1A-C2A-CAA-CBA
14	B	817	CLA	C3A-C2A-CAA-CBA
14	B	818	CLA	C2A-CAA-CBA-CGA
14	B	819	CLA	C1A-C2A-CAA-CBA
14	B	819	CLA	C3A-C2A-CAA-CBA
14	B	823	CLA	CHA-CBD-CGD-O1D
14	B	823	CLA	CHA-CBD-CGD-O2D
14	B	826	CLA	C1A-C2A-CAA-CBA
14	B	826	CLA	C3A-C2A-CAA-CBA
14	B	827	CLA	C3A-C2A-CAA-CBA
14	B	828	CLA	C1A-C2A-CAA-CBA
14	B	828	CLA	C3A-C2A-CAA-CBA
14	B	828	CLA	C11-C12-C13-C14
14	B	830	CLA	C1A-C2A-CAA-CBA
14	B	832	CLA	CHA-CBD-CGD-O1D
14	B	832	CLA	CHA-CBD-CGD-O2D
14	B	833	CLA	CBD-CGD-O2D-CED
14	B	839	CLA	C4-C3-C5-C6
14	bA	803	CLA	C1A-C2A-CAA-CBA
14	bA	806	CLA	C1A-C2A-CAA-CBA
14	bA	808	CLA	C1A-C2A-CAA-CBA
14	bA	808	CLA	C3A-C2A-CAA-CBA
14	bA	812	CLA	CBD-CGD-O2D-CED
14	bA	818	CLA	C3A-C2A-CAA-CBA
14	bA	820	CLA	CBD-CGD-O2D-CED
14	bA	821	CLA	C2A-CAA-CBA-CGA
14	bA	823	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	bA	826	CLA	CBA-CGA-O2A-C1
14	bA	831	CLA	C1A-C2A-CAA-CBA
14	bA	831	CLA	C3A-C2A-CAA-CBA
14	bA	831	CLA	C2-C3-C5-C6
14	bA	831	CLA	C4-C3-C5-C6
14	bA	835	CLA	CBD-CGD-O2D-CED
14	bA	836	CLA	C2-C3-C5-C6
14	bA	836	CLA	C4-C3-C5-C6
14	bA	838	CLA	CHA-CBD-CGD-O1D
14	bA	842	CLA	CHA-CBD-CGD-O1D
14	bB	802	CLA	CHA-CBD-CGD-O1D
14	bB	802	CLA	CHA-CBD-CGD-O2D
14	bB	804	CLA	C2-C3-C5-C6
14	bB	804	CLA	C4-C3-C5-C6
14	bB	805	CLA	C3A-C2A-CAA-CBA
14	bB	806	CLA	CBD-CGD-O2D-CED
14	bB	806	CLA	C2-C3-C5-C6
14	bB	806	CLA	C4-C3-C5-C6
14	bB	808	CLA	CHA-CBD-CGD-O1D
14	bB	808	CLA	CHA-CBD-CGD-O2D
14	bB	809	CLA	C1A-C2A-CAA-CBA
14	bB	809	CLA	C3A-C2A-CAA-CBA
14	bB	814	CLA	C1A-C2A-CAA-CBA
14	bB	815	CLA	O1A-CGA-O2A-C1
14	bB	815	CLA	C2-C3-C5-C6
14	bB	815	CLA	C4-C3-C5-C6
14	bB	816	CLA	C1A-C2A-CAA-CBA
14	bB	816	CLA	C3A-C2A-CAA-CBA
14	bB	817	CLA	C1A-C2A-CAA-CBA
14	bB	817	CLA	C3A-C2A-CAA-CBA
14	bB	818	CLA	C2A-CAA-CBA-CGA
14	bB	819	CLA	C1A-C2A-CAA-CBA
14	bB	819	CLA	C3A-C2A-CAA-CBA
14	bB	823	CLA	CHA-CBD-CGD-O1D
14	bB	823	CLA	CHA-CBD-CGD-O2D
14	bB	826	CLA	C1A-C2A-CAA-CBA
14	bB	826	CLA	C3A-C2A-CAA-CBA
14	bB	827	CLA	C3A-C2A-CAA-CBA
14	bB	828	CLA	C1A-C2A-CAA-CBA
14	bB	828	CLA	C3A-C2A-CAA-CBA
14	bB	828	CLA	C11-C12-C13-C14
14	bB	830	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	bB	832	CLA	CHA-CBD-CGD-O1D
14	bB	832	CLA	CHA-CBD-CGD-O2D
14	bB	833	CLA	CBD-CGD-O2D-CED
14	bB	839	CLA	C4-C3-C5-C6
14	cA	803	CLA	C1A-C2A-CAA-CBA
14	cA	806	CLA	C1A-C2A-CAA-CBA
14	cA	808	CLA	C1A-C2A-CAA-CBA
14	cA	808	CLA	C3A-C2A-CAA-CBA
14	cA	812	CLA	CBD-CGD-O2D-CED
14	cA	818	CLA	C3A-C2A-CAA-CBA
14	cA	820	CLA	CBD-CGD-O2D-CED
14	cA	821	CLA	C2A-CAA-CBA-CGA
14	cA	823	CLA	CBD-CGD-O2D-CED
14	cA	826	CLA	CBA-CGA-O2A-C1
14	cA	831	CLA	C1A-C2A-CAA-CBA
14	cA	831	CLA	C3A-C2A-CAA-CBA
14	cA	831	CLA	C2-C3-C5-C6
14	cA	831	CLA	C4-C3-C5-C6
14	cA	835	CLA	CBD-CGD-O2D-CED
14	cA	836	CLA	C2-C3-C5-C6
14	cA	836	CLA	C4-C3-C5-C6
14	cA	838	CLA	CHA-CBD-CGD-O1D
14	cA	842	CLA	CHA-CBD-CGD-O1D
14	cB	803	CLA	CHA-CBD-CGD-O1D
14	cB	803	CLA	CHA-CBD-CGD-O2D
14	cB	805	CLA	C2-C3-C5-C6
14	cB	805	CLA	C4-C3-C5-C6
14	cB	806	CLA	C3A-C2A-CAA-CBA
14	cB	807	CLA	CBD-CGD-O2D-CED
14	cB	807	CLA	C2-C3-C5-C6
14	cB	807	CLA	C4-C3-C5-C6
14	cB	809	CLA	CHA-CBD-CGD-O1D
14	cB	809	CLA	CHA-CBD-CGD-O2D
14	cB	810	CLA	C1A-C2A-CAA-CBA
14	cB	810	CLA	C3A-C2A-CAA-CBA
14	cB	815	CLA	C1A-C2A-CAA-CBA
14	cB	816	CLA	O1A-CGA-O2A-C1
14	cB	816	CLA	C2-C3-C5-C6
14	cB	816	CLA	C4-C3-C5-C6
14	cB	817	CLA	C1A-C2A-CAA-CBA
14	cB	817	CLA	C3A-C2A-CAA-CBA
14	cB	818	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	cB	818	CLA	C3A-C2A-CAA-CBA
14	cB	819	CLA	C2A-CAA-CBA-CGA
14	cB	820	CLA	C1A-C2A-CAA-CBA
14	cB	820	CLA	C3A-C2A-CAA-CBA
14	cB	824	CLA	CHA-CBD-CGD-O1D
14	cB	824	CLA	CHA-CBD-CGD-O2D
14	cB	827	CLA	C1A-C2A-CAA-CBA
14	cB	827	CLA	C3A-C2A-CAA-CBA
14	cB	828	CLA	C3A-C2A-CAA-CBA
14	cB	829	CLA	C1A-C2A-CAA-CBA
14	cB	829	CLA	C3A-C2A-CAA-CBA
14	cB	829	CLA	C11-C12-C13-C14
14	cB	831	CLA	C1A-C2A-CAA-CBA
14	cB	833	CLA	CHA-CBD-CGD-O1D
14	cB	833	CLA	CHA-CBD-CGD-O2D
14	cB	834	CLA	CBD-CGD-O2D-CED
14	cB	840	CLA	C4-C3-C5-C6
17	A	845	BCR	C6-C7-C8-C9
17	A	845	BCR	C7-C8-C9-C10
17	A	845	BCR	C7-C8-C9-C34
17	A	845	BCR	C19-C20-C21-C22
17	A	846	BCR	C7-C8-C9-C10
17	A	846	BCR	C7-C8-C9-C34
17	A	846	BCR	C11-C10-C9-C8
17	A	846	BCR	C11-C10-C9-C34
17	A	846	BCR	C10-C11-C12-C13
17	A	847	BCR	C22-C23-C24-C25
17	A	847	BCR	C23-C24-C25-C26
17	A	847	BCR	C23-C24-C25-C30
17	A	848	BCR	C22-C23-C24-C25
17	A	849	BCR	C22-C23-C24-C25
17	B	841	BCR	C6-C7-C8-C9
17	B	841	BCR	C21-C22-C23-C24
17	B	841	BCR	C37-C22-C23-C24
17	B	842	BCR	C11-C10-C9-C8
17	B	842	BCR	C11-C10-C9-C34
17	B	842	BCR	C37-C22-C23-C24
17	B	843	BCR	C7-C8-C9-C10
17	B	843	BCR	C7-C8-C9-C34
17	B	843	BCR	C11-C10-C9-C8
17	B	843	BCR	C11-C10-C9-C34
17	B	843	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
17	B	843	BCR	C11-C12-C13-C14
17	B	843	BCR	C11-C12-C13-C35
17	B	844	BCR	C11-C10-C9-C8
17	B	844	BCR	C11-C10-C9-C34
17	B	844	BCR	C11-C12-C13-C14
17	B	844	BCR	C11-C12-C13-C35
17	B	844	BCR	C21-C22-C23-C24
17	B	844	BCR	C37-C22-C23-C24
17	B	845	BCR	C6-C7-C8-C9
17	B	846	BCR	C6-C7-C8-C9
17	B	846	BCR	C35-C13-C14-C15
17	B	847	BCR	C7-C8-C9-C34
17	B	850	BCR	C1-C6-C7-C8
17	B	850	BCR	C5-C6-C7-C8
17	B	850	BCR	C6-C7-C8-C9
17	B	850	BCR	C7-C8-C9-C10
17	B	850	BCR	C7-C8-C9-C34
17	B	850	BCR	C22-C23-C24-C25
17	B	850	BCR	C23-C24-C25-C30
17	F	202	BCR	C22-C23-C24-C25
17	J	103	BCR	C6-C7-C8-C9
17	L	205	BCR	C21-C22-C23-C24
17	L	205	BCR	C37-C22-C23-C24
17	L	206	BCR	C22-C23-C24-C25
17	M	101	BCR	C1-C6-C7-C8
17	M	101	BCR	C5-C6-C7-C8
17	bA	845	BCR	C6-C7-C8-C9
17	bA	845	BCR	C7-C8-C9-C10
17	bA	845	BCR	C7-C8-C9-C34
17	bA	845	BCR	C19-C20-C21-C22
17	bA	846	BCR	C7-C8-C9-C10
17	bA	846	BCR	C7-C8-C9-C34
17	bA	846	BCR	C11-C10-C9-C8
17	bA	846	BCR	C11-C10-C9-C34
17	bA	846	BCR	C10-C11-C12-C13
17	bA	847	BCR	C22-C23-C24-C25
17	bA	847	BCR	C23-C24-C25-C26
17	bA	847	BCR	C23-C24-C25-C30
17	bA	848	BCR	C22-C23-C24-C25
17	bA	849	BCR	C22-C23-C24-C25
17	bB	841	BCR	C6-C7-C8-C9
17	bB	841	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
17	bB	841	BCR	C37-C22-C23-C24
17	bB	842	BCR	C11-C10-C9-C8
17	bB	842	BCR	C11-C10-C9-C34
17	bB	842	BCR	C37-C22-C23-C24
17	bB	843	BCR	C7-C8-C9-C10
17	bB	843	BCR	C7-C8-C9-C34
17	bB	843	BCR	C11-C10-C9-C8
17	bB	843	BCR	C11-C10-C9-C34
17	bB	843	BCR	C10-C11-C12-C13
17	bB	843	BCR	C11-C12-C13-C14
17	bB	843	BCR	C11-C12-C13-C35
17	bB	844	BCR	C11-C10-C9-C8
17	bB	844	BCR	C11-C10-C9-C34
17	bB	844	BCR	C11-C12-C13-C14
17	bB	844	BCR	C11-C12-C13-C35
17	bB	844	BCR	C21-C22-C23-C24
17	bB	844	BCR	C37-C22-C23-C24
17	bB	845	BCR	C6-C7-C8-C9
17	bB	846	BCR	C6-C7-C8-C9
17	bB	846	BCR	C35-C13-C14-C15
17	bB	847	BCR	C7-C8-C9-C34
17	bB	850	BCR	C1-C6-C7-C8
17	bB	850	BCR	C5-C6-C7-C8
17	bB	850	BCR	C6-C7-C8-C9
17	bB	850	BCR	C7-C8-C9-C10
17	bB	850	BCR	C7-C8-C9-C34
17	bB	850	BCR	C22-C23-C24-C25
17	bF	202	BCR	C22-C23-C24-C25
17	bJ	103	BCR	C6-C7-C8-C9
17	bL	205	BCR	C21-C22-C23-C24
17	bL	205	BCR	C37-C22-C23-C24
17	bL	206	BCR	C22-C23-C24-C25
17	bM	101	BCR	C1-C6-C7-C8
17	bM	101	BCR	C5-C6-C7-C8
17	cA	845	BCR	C6-C7-C8-C9
17	cA	845	BCR	C7-C8-C9-C10
17	cA	845	BCR	C7-C8-C9-C34
17	cA	845	BCR	C19-C20-C21-C22
17	cA	846	BCR	C7-C8-C9-C10
17	cA	846	BCR	C7-C8-C9-C34
17	cA	846	BCR	C11-C10-C9-C8
17	cA	846	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
17	cA	846	BCR	C10-C11-C12-C13
17	cA	847	BCR	C22-C23-C24-C25
17	cA	847	BCR	C23-C24-C25-C26
17	cA	847	BCR	C23-C24-C25-C30
17	cA	848	BCR	C22-C23-C24-C25
17	cA	849	BCR	C22-C23-C24-C25
17	cB	842	BCR	C6-C7-C8-C9
17	cB	842	BCR	C21-C22-C23-C24
17	cB	842	BCR	C37-C22-C23-C24
17	cB	843	BCR	C11-C10-C9-C8
17	cB	843	BCR	C11-C10-C9-C34
17	cB	843	BCR	C37-C22-C23-C24
17	cB	844	BCR	C7-C8-C9-C10
17	cB	844	BCR	C7-C8-C9-C34
17	cB	844	BCR	C11-C10-C9-C8
17	cB	844	BCR	C11-C10-C9-C34
17	cB	844	BCR	C10-C11-C12-C13
17	cB	844	BCR	C11-C12-C13-C14
17	cB	844	BCR	C11-C12-C13-C35
17	cB	845	BCR	C11-C10-C9-C8
17	cB	845	BCR	C11-C10-C9-C34
17	cB	845	BCR	C11-C12-C13-C14
17	cB	845	BCR	C11-C12-C13-C35
17	cB	845	BCR	C21-C22-C23-C24
17	cB	845	BCR	C37-C22-C23-C24
17	cB	846	BCR	C6-C7-C8-C9
17	cB	847	BCR	C6-C7-C8-C9
17	cB	847	BCR	C35-C13-C14-C15
17	cB	848	BCR	C7-C8-C9-C34
17	cB	851	BCR	C1-C6-C7-C8
17	cB	851	BCR	C5-C6-C7-C8
17	cB	851	BCR	C6-C7-C8-C9
17	cB	851	BCR	C7-C8-C9-C10
17	cB	851	BCR	C7-C8-C9-C34
17	cB	851	BCR	C22-C23-C24-C25
17	cB	851	BCR	C23-C24-C25-C30
17	cF	202	BCR	C22-C23-C24-C25
17	cJ	103	BCR	C6-C7-C8-C9
17	cL	206	BCR	C21-C22-C23-C24
17	cL	206	BCR	C37-C22-C23-C24
17	cL	207	BCR	C22-C23-C24-C25
17	cM	101	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
17	cM	101	BCR	C5-C6-C7-C8
18	A	851	LHG	C4-O6-P-O5
18	bA	851	LHG	C4-O6-P-O5
18	cA	851	LHG	C4-O6-P-O5
14	B	821	CLA	O1D-CGD-O2D-CED
14	B	834	CLA	O1D-CGD-O2D-CED
14	bB	821	CLA	O1D-CGD-O2D-CED
14	bB	834	CLA	O1D-CGD-O2D-CED
14	cB	822	CLA	O1D-CGD-O2D-CED
14	cB	835	CLA	O1D-CGD-O2D-CED
14	A	812	CLA	O1D-CGD-O2D-CED
14	B	801	CLA	O1D-CGD-O2D-CED
14	bA	812	CLA	O1D-CGD-O2D-CED
14	bB	801	CLA	O1D-CGD-O2D-CED
14	cA	812	CLA	O1D-CGD-O2D-CED
14	cB	802	CLA	O1D-CGD-O2D-CED
14	A	805	CLA	CBD-CGD-O2D-CED
14	A	810	CLA	CBD-CGD-O2D-CED
14	A	811	CLA	CBD-CGD-O2D-CED
14	A	815	CLA	CBD-CGD-O2D-CED
14	A	816	CLA	CBD-CGD-O2D-CED
14	A	818	CLA	CBD-CGD-O2D-CED
14	A	827	CLA	CBD-CGD-O2D-CED
14	A	842	CLA	CBD-CGD-O2D-CED
14	B	801	CLA	CBD-CGD-O2D-CED
14	B	802	CLA	CBD-CGD-O2D-CED
14	B	814	CLA	CBD-CGD-O2D-CED
14	B	815	CLA	CBD-CGD-O2D-CED
14	B	821	CLA	CBD-CGD-O2D-CED
14	B	822	CLA	CBD-CGD-O2D-CED
14	B	823	CLA	CBD-CGD-O2D-CED
14	B	831	CLA	CBD-CGD-O2D-CED
14	B	834	CLA	CBD-CGD-O2D-CED
14	B	835	CLA	CBD-CGD-O2D-CED
14	B	837	CLA	CBD-CGD-O2D-CED
14	B	839	CLA	CBD-CGD-O2D-CED
14	B	851	CLA	CBD-CGD-O2D-CED
14	F	201	CLA	CBD-CGD-O2D-CED
14	J	101	CLA	CBD-CGD-O2D-CED
14	L	204	CLA	CBD-CGD-O2D-CED
14	X	201	CLA	CBD-CGD-O2D-CED
14	bA	805	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	bA	810	CLA	CBD-CGD-O2D-CED
14	bA	811	CLA	CBD-CGD-O2D-CED
14	bA	815	CLA	CBD-CGD-O2D-CED
14	bA	816	CLA	CBD-CGD-O2D-CED
14	bA	818	CLA	CBD-CGD-O2D-CED
14	bA	827	CLA	CBD-CGD-O2D-CED
14	bA	842	CLA	CBD-CGD-O2D-CED
14	bB	801	CLA	CBD-CGD-O2D-CED
14	bB	802	CLA	CBD-CGD-O2D-CED
14	bB	814	CLA	CBD-CGD-O2D-CED
14	bB	815	CLA	CBD-CGD-O2D-CED
14	bB	821	CLA	CBD-CGD-O2D-CED
14	bB	822	CLA	CBD-CGD-O2D-CED
14	bB	823	CLA	CBD-CGD-O2D-CED
14	bB	831	CLA	CBD-CGD-O2D-CED
14	bB	834	CLA	CBD-CGD-O2D-CED
14	bB	835	CLA	CBD-CGD-O2D-CED
14	bB	837	CLA	CBD-CGD-O2D-CED
14	bB	839	CLA	CBD-CGD-O2D-CED
14	bB	851	CLA	CBD-CGD-O2D-CED
14	bF	201	CLA	CBD-CGD-O2D-CED
14	bJ	101	CLA	CBD-CGD-O2D-CED
14	bL	204	CLA	CBD-CGD-O2D-CED
14	bX	201	CLA	CBD-CGD-O2D-CED
14	cA	805	CLA	CBD-CGD-O2D-CED
14	cA	810	CLA	CBD-CGD-O2D-CED
14	cA	811	CLA	CBD-CGD-O2D-CED
14	cA	815	CLA	CBD-CGD-O2D-CED
14	cA	816	CLA	CBD-CGD-O2D-CED
14	cA	818	CLA	CBD-CGD-O2D-CED
14	cA	827	CLA	CBD-CGD-O2D-CED
14	cA	842	CLA	CBD-CGD-O2D-CED
14	cB	801	CLA	CBD-CGD-O2D-CED
14	cB	802	CLA	CBD-CGD-O2D-CED
14	cB	803	CLA	CBD-CGD-O2D-CED
14	cB	815	CLA	CBD-CGD-O2D-CED
14	cB	816	CLA	CBD-CGD-O2D-CED
14	cB	822	CLA	CBD-CGD-O2D-CED
14	cB	823	CLA	CBD-CGD-O2D-CED
14	cB	824	CLA	CBD-CGD-O2D-CED
14	cB	832	CLA	CBD-CGD-O2D-CED
14	cB	835	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	cB	836	CLA	CBD-CGD-O2D-CED
14	cB	838	CLA	CBD-CGD-O2D-CED
14	cB	840	CLA	CBD-CGD-O2D-CED
14	cF	201	CLA	CBD-CGD-O2D-CED
14	cJ	101	CLA	CBD-CGD-O2D-CED
14	cL	205	CLA	CBD-CGD-O2D-CED
14	cX	201	CLA	CBD-CGD-O2D-CED
14	A	806	CLA	O1A-CGA-O2A-C1
14	A	836	CLA	O1A-CGA-O2A-C1
14	L	202	CLA	O1A-CGA-O2A-C1
14	bA	806	CLA	O1A-CGA-O2A-C1
14	bA	836	CLA	O1A-CGA-O2A-C1
14	bL	202	CLA	O1A-CGA-O2A-C1
14	cA	806	CLA	O1A-CGA-O2A-C1
14	cA	836	CLA	O1A-CGA-O2A-C1
14	cL	203	CLA	O1A-CGA-O2A-C1
14	B	802	CLA	O1D-CGD-O2D-CED
14	B	806	CLA	O1D-CGD-O2D-CED
14	bB	802	CLA	O1D-CGD-O2D-CED
14	bB	806	CLA	O1D-CGD-O2D-CED
14	cB	803	CLA	O1D-CGD-O2D-CED
14	cB	807	CLA	O1D-CGD-O2D-CED
14	A	823	CLA	O1D-CGD-O2D-CED
14	A	835	CLA	O1D-CGD-O2D-CED
14	B	837	CLA	O1D-CGD-O2D-CED
14	B	851	CLA	O1D-CGD-O2D-CED
14	J	101	CLA	O1D-CGD-O2D-CED
14	bA	823	CLA	O1D-CGD-O2D-CED
14	bA	835	CLA	O1D-CGD-O2D-CED
14	bB	837	CLA	O1D-CGD-O2D-CED
14	bB	851	CLA	O1D-CGD-O2D-CED
14	bJ	101	CLA	O1D-CGD-O2D-CED
14	cA	823	CLA	O1D-CGD-O2D-CED
14	cA	835	CLA	O1D-CGD-O2D-CED
14	cB	801	CLA	O1D-CGD-O2D-CED
14	cB	838	CLA	O1D-CGD-O2D-CED
14	cJ	101	CLA	O1D-CGD-O2D-CED
14	A	808	CLA	CBD-CGD-O2D-CED
14	B	805	CLA	CBD-CGD-O2D-CED
14	B	818	CLA	CBD-CGD-O2D-CED
14	B	820	CLA	CBD-CGD-O2D-CED
14	B	829	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	B	830	CLA	CBD-CGD-O2D-CED
14	B	832	CLA	CBD-CGD-O2D-CED
14	B	836	CLA	CBD-CGD-O2D-CED
14	bA	808	CLA	CBD-CGD-O2D-CED
14	bB	805	CLA	CBD-CGD-O2D-CED
14	bB	818	CLA	CBD-CGD-O2D-CED
14	bB	820	CLA	CBD-CGD-O2D-CED
14	bB	829	CLA	CBD-CGD-O2D-CED
14	bB	830	CLA	CBD-CGD-O2D-CED
14	bB	832	CLA	CBD-CGD-O2D-CED
14	bB	836	CLA	CBD-CGD-O2D-CED
14	cA	808	CLA	CBD-CGD-O2D-CED
14	cB	806	CLA	CBD-CGD-O2D-CED
14	cB	819	CLA	CBD-CGD-O2D-CED
14	cB	821	CLA	CBD-CGD-O2D-CED
14	cB	830	CLA	CBD-CGD-O2D-CED
14	cB	831	CLA	CBD-CGD-O2D-CED
14	cB	833	CLA	CBD-CGD-O2D-CED
14	cB	837	CLA	CBD-CGD-O2D-CED
14	B	809	CLA	O1A-CGA-O2A-C1
14	L	203	CLA	O1A-CGA-O2A-C1
14	bB	809	CLA	O1A-CGA-O2A-C1
14	bL	203	CLA	O1A-CGA-O2A-C1
14	cB	810	CLA	O1A-CGA-O2A-C1
14	cL	204	CLA	O1A-CGA-O2A-C1
14	bB	829	CLA	C4C-C3C-CAC-CBC
14	cB	830	CLA	C4C-C3C-CAC-CBC
14	A	811	CLA	O1D-CGD-O2D-CED
14	A	820	CLA	O1D-CGD-O2D-CED
14	bA	811	CLA	O1D-CGD-O2D-CED
14	bA	820	CLA	O1D-CGD-O2D-CED
14	cA	811	CLA	O1D-CGD-O2D-CED
14	cA	820	CLA	O1D-CGD-O2D-CED
14	B	829	CLA	C4C-C3C-CAC-CBC
14	A	807	CLA	CBD-CGD-O2D-CED
14	A	833	CLA	CBD-CGD-O2D-CED
14	B	817	CLA	CBD-CGD-O2D-CED
14	bA	807	CLA	CBD-CGD-O2D-CED
14	bA	833	CLA	CBD-CGD-O2D-CED
14	bB	817	CLA	CBD-CGD-O2D-CED
14	cA	807	CLA	CBD-CGD-O2D-CED
14	cA	833	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	cB	818	CLA	CBD-CGD-O2D-CED
14	A	810	CLA	O1D-CGD-O2D-CED
14	B	833	CLA	O1D-CGD-O2D-CED
14	bA	810	CLA	O1D-CGD-O2D-CED
14	bB	833	CLA	O1D-CGD-O2D-CED
14	cA	810	CLA	O1D-CGD-O2D-CED
14	cB	834	CLA	O1D-CGD-O2D-CED
14	B	818	CLA	O1A-CGA-O2A-C1
14	bB	818	CLA	O1A-CGA-O2A-C1
14	cB	819	CLA	O1A-CGA-O2A-C1
14	A	805	CLA	C3-C5-C6-C7
14	A	832	CLA	C3-C5-C6-C7
14	bA	805	CLA	C3-C5-C6-C7
14	bA	832	CLA	C3-C5-C6-C7
14	cA	805	CLA	C3-C5-C6-C7
14	cA	832	CLA	C3-C5-C6-C7
14	A	806	CLA	CBA-CGA-O2A-C1
14	A	836	CLA	CBA-CGA-O2A-C1
14	B	805	CLA	CBA-CGA-O2A-C1
14	B	815	CLA	CBA-CGA-O2A-C1
14	L	203	CLA	CBA-CGA-O2A-C1
14	bA	806	CLA	CBA-CGA-O2A-C1
14	bA	836	CLA	CBA-CGA-O2A-C1
14	bB	805	CLA	CBA-CGA-O2A-C1
14	bB	815	CLA	CBA-CGA-O2A-C1
14	bL	203	CLA	CBA-CGA-O2A-C1
14	cA	806	CLA	CBA-CGA-O2A-C1
14	cA	836	CLA	CBA-CGA-O2A-C1
14	cB	806	CLA	CBA-CGA-O2A-C1
14	cB	816	CLA	CBA-CGA-O2A-C1
14	cL	204	CLA	CBA-CGA-O2A-C1
14	B	829	CLA	C2C-C3C-CAC-CBC
14	bB	829	CLA	C2C-C3C-CAC-CBC
14	cB	830	CLA	C2C-C3C-CAC-CBC
14	A	815	CLA	O1D-CGD-O2D-CED
14	F	201	CLA	O1D-CGD-O2D-CED
14	bA	815	CLA	O1D-CGD-O2D-CED
14	bB	822	CLA	O1D-CGD-O2D-CED
14	bF	201	CLA	O1D-CGD-O2D-CED
14	cA	815	CLA	O1D-CGD-O2D-CED
14	cF	201	CLA	O1D-CGD-O2D-CED
14	A	804	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	A	839	CLA	CBD-CGD-O2D-CED
14	A	840	CLA	CBD-CGD-O2D-CED
14	bA	804	CLA	CBD-CGD-O2D-CED
14	bA	839	CLA	CBD-CGD-O2D-CED
14	bA	840	CLA	CBD-CGD-O2D-CED
14	cA	804	CLA	CBD-CGD-O2D-CED
14	cA	839	CLA	CBD-CGD-O2D-CED
14	cA	840	CLA	CBD-CGD-O2D-CED
14	A	826	CLA	O1A-CGA-O2A-C1
14	bA	826	CLA	O1A-CGA-O2A-C1
14	cA	826	CLA	O1A-CGA-O2A-C1
14	B	822	CLA	O1D-CGD-O2D-CED
14	B	818	CLA	CBA-CGA-O2A-C1
14	bB	818	CLA	CBA-CGA-O2A-C1
14	cB	819	CLA	CBA-CGA-O2A-C1
14	B	806	CLA	C4-C3-C5-C6
14	B	839	CLA	C2-C3-C5-C6
14	bB	839	CLA	C2-C3-C5-C6
14	cB	840	CLA	C2-C3-C5-C6
14	A	828	CLA	CBD-CGD-O2D-CED
14	B	804	CLA	CBD-CGD-O2D-CED
14	bA	828	CLA	CBD-CGD-O2D-CED
14	bB	804	CLA	CBD-CGD-O2D-CED
14	cA	828	CLA	CBD-CGD-O2D-CED
14	cB	805	CLA	CBD-CGD-O2D-CED
14	A	807	CLA	C2A-CAA-CBA-CGA
14	A	830	CLA	C2A-CAA-CBA-CGA
14	A	835	CLA	C2A-CAA-CBA-CGA
14	B	821	CLA	C2A-CAA-CBA-CGA
14	B	822	CLA	C2A-CAA-CBA-CGA
14	B	838	CLA	C2A-CAA-CBA-CGA
14	X	201	CLA	C2A-CAA-CBA-CGA
14	bA	807	CLA	C2A-CAA-CBA-CGA
14	bA	830	CLA	C2A-CAA-CBA-CGA
14	bA	835	CLA	C2A-CAA-CBA-CGA
14	bB	821	CLA	C2A-CAA-CBA-CGA
14	bB	822	CLA	C2A-CAA-CBA-CGA
14	bB	838	CLA	C2A-CAA-CBA-CGA
14	bX	201	CLA	C2A-CAA-CBA-CGA
14	cA	807	CLA	C2A-CAA-CBA-CGA
14	cA	830	CLA	C2A-CAA-CBA-CGA
14	cA	835	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
14	cB	822	CLA	C2A-CAA-CBA-CGA
14	cB	823	CLA	C2A-CAA-CBA-CGA
14	cB	839	CLA	C2A-CAA-CBA-CGA
14	cX	201	CLA	C2A-CAA-CBA-CGA
14	cB	823	CLA	O1D-CGD-O2D-CED
14	B	802	CLA	CBA-CGA-O2A-C1
14	B	809	CLA	CBA-CGA-O2A-C1
14	B	828	CLA	CBA-CGA-O2A-C1
14	bB	802	CLA	CBA-CGA-O2A-C1
14	bB	809	CLA	CBA-CGA-O2A-C1
14	bB	828	CLA	CBA-CGA-O2A-C1
14	cB	803	CLA	CBA-CGA-O2A-C1
14	cB	810	CLA	CBA-CGA-O2A-C1
14	cB	829	CLA	CBA-CGA-O2A-C1
14	A	842	CLA	O1D-CGD-O2D-CED
14	X	201	CLA	O1D-CGD-O2D-CED
14	bA	842	CLA	O1D-CGD-O2D-CED
14	bX	201	CLA	O1D-CGD-O2D-CED
14	cA	842	CLA	O1D-CGD-O2D-CED
14	cX	201	CLA	O1D-CGD-O2D-CED
14	B	819	CLA	CBD-CGD-O2D-CED
14	B	849	CLA	CBD-CGD-O2D-CED
14	bB	819	CLA	CBD-CGD-O2D-CED
14	bB	849	CLA	CBD-CGD-O2D-CED
14	cB	820	CLA	CBD-CGD-O2D-CED
14	cB	850	CLA	CBD-CGD-O2D-CED
14	A	805	CLA	O1D-CGD-O2D-CED
14	B	831	CLA	O1D-CGD-O2D-CED
14	bA	805	CLA	O1D-CGD-O2D-CED
14	bB	831	CLA	O1D-CGD-O2D-CED
14	cA	805	CLA	O1D-CGD-O2D-CED
14	cB	832	CLA	O1D-CGD-O2D-CED
14	A	818	CLA	O1A-CGA-O2A-C1
14	B	805	CLA	O1A-CGA-O2A-C1
14	bA	818	CLA	O1A-CGA-O2A-C1
14	bB	805	CLA	O1A-CGA-O2A-C1
14	cA	818	CLA	O1A-CGA-O2A-C1
14	cB	806	CLA	O1A-CGA-O2A-C1
14	B	815	CLA	O1D-CGD-O2D-CED
14	L	204	CLA	O1D-CGD-O2D-CED
14	bB	815	CLA	O1D-CGD-O2D-CED
14	bL	204	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	cB	816	CLA	O1D-CGD-O2D-CED
14	cL	205	CLA	O1D-CGD-O2D-CED
17	J	103	BCR	C19-C20-C21-C22
17	bJ	103	BCR	C19-C20-C21-C22
17	cJ	103	BCR	C19-C20-C21-C22
14	A	829	CLA	CBD-CGD-O2D-CED
14	A	831	CLA	CBD-CGD-O2D-CED
14	B	812	CLA	CBD-CGD-O2D-CED
14	B	816	CLA	CBD-CGD-O2D-CED
14	bA	829	CLA	CBD-CGD-O2D-CED
14	bA	831	CLA	CBD-CGD-O2D-CED
14	bB	812	CLA	CBD-CGD-O2D-CED
14	bB	816	CLA	CBD-CGD-O2D-CED
14	cA	829	CLA	CBD-CGD-O2D-CED
14	cA	831	CLA	CBD-CGD-O2D-CED
14	cB	813	CLA	CBD-CGD-O2D-CED
14	cB	817	CLA	CBD-CGD-O2D-CED
14	A	818	CLA	O1D-CGD-O2D-CED
14	B	823	CLA	O1D-CGD-O2D-CED
14	B	835	CLA	O1D-CGD-O2D-CED
14	bA	818	CLA	O1D-CGD-O2D-CED
14	bB	823	CLA	O1D-CGD-O2D-CED
14	bB	835	CLA	O1D-CGD-O2D-CED
14	cA	818	CLA	O1D-CGD-O2D-CED
14	cB	824	CLA	O1D-CGD-O2D-CED
14	cB	836	CLA	O1D-CGD-O2D-CED
14	B	819	CLA	CBA-CGA-O2A-C1
14	bB	819	CLA	CBA-CGA-O2A-C1
14	cB	820	CLA	CBA-CGA-O2A-C1
14	B	814	CLA	O1D-CGD-O2D-CED
14	bB	814	CLA	O1D-CGD-O2D-CED
14	cB	815	CLA	O1D-CGD-O2D-CED
14	B	824	CLA	CBA-CGA-O2A-C1
14	bB	824	CLA	CBA-CGA-O2A-C1
14	cB	825	CLA	CBA-CGA-O2A-C1
14	A	836	CLA	CBD-CGD-O2D-CED
14	bA	836	CLA	CBD-CGD-O2D-CED
14	cA	836	CLA	CBD-CGD-O2D-CED
14	A	817	CLA	C3-C5-C6-C7
14	B	803	CLA	C3-C5-C6-C7
14	L	202	CLA	C3-C5-C6-C7
14	bA	817	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
14	bB	801	CLA	C3-C5-C6-C7
14	bB	803	CLA	C3-C5-C6-C7
14	bL	202	CLA	C3-C5-C6-C7
14	cA	817	CLA	C3-C5-C6-C7
14	cB	802	CLA	C3-C5-C6-C7
14	cB	804	CLA	C3-C5-C6-C7
14	cL	203	CLA	C3-C5-C6-C7
14	A	818	CLA	CBA-CGA-O2A-C1
14	bA	818	CLA	CBA-CGA-O2A-C1
14	cA	818	CLA	CBA-CGA-O2A-C1
14	A	816	CLA	O1D-CGD-O2D-CED
14	bA	816	CLA	O1D-CGD-O2D-CED
14	cA	816	CLA	O1D-CGD-O2D-CED
14	B	828	CLA	O1A-CGA-O2A-C1
14	bB	828	CLA	O1A-CGA-O2A-C1
14	cB	829	CLA	O1A-CGA-O2A-C1
14	B	809	CLA	C4-C3-C5-C6
14	bB	809	CLA	C4-C3-C5-C6
14	cB	810	CLA	C4-C3-C5-C6
14	B	809	CLA	C2-C3-C5-C6
14	bB	809	CLA	C2-C3-C5-C6
14	cB	810	CLA	C2-C3-C5-C6
14	A	819	CLA	CBD-CGD-O2D-CED
14	bA	819	CLA	CBD-CGD-O2D-CED
14	cA	819	CLA	CBD-CGD-O2D-CED
14	A	819	CLA	C2A-CAA-CBA-CGA
14	bA	819	CLA	C2A-CAA-CBA-CGA
14	cA	819	CLA	C2A-CAA-CBA-CGA
14	A	827	CLA	O1D-CGD-O2D-CED
14	bA	827	CLA	O1D-CGD-O2D-CED
14	cA	827	CLA	O1D-CGD-O2D-CED
14	B	802	CLA	O1A-CGA-O2A-C1
14	bB	802	CLA	O1A-CGA-O2A-C1
14	cB	803	CLA	O1A-CGA-O2A-C1
14	B	801	CLA	C3-C5-C6-C7
14	A	804	CLA	CBA-CGA-O2A-C1
14	bA	804	CLA	CBA-CGA-O2A-C1
14	cA	804	CLA	CBA-CGA-O2A-C1
14	B	839	CLA	O1D-CGD-O2D-CED
14	bB	839	CLA	O1D-CGD-O2D-CED
14	cB	840	CLA	O1D-CGD-O2D-CED
14	B	819	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	bB	819	CLA	O1A-CGA-O2A-C1
14	cB	820	CLA	O1A-CGA-O2A-C1
14	B	818	CLA	O1D-CGD-O2D-CED
14	B	830	CLA	O1D-CGD-O2D-CED
14	bB	818	CLA	O1D-CGD-O2D-CED
14	bB	830	CLA	O1D-CGD-O2D-CED
14	cB	819	CLA	O1D-CGD-O2D-CED
14	cB	831	CLA	O1D-CGD-O2D-CED
14	cB	837	CLA	O1D-CGD-O2D-CED
14	B	832	CLA	O1D-CGD-O2D-CED
14	B	836	CLA	O1D-CGD-O2D-CED
14	bB	832	CLA	O1D-CGD-O2D-CED
14	bB	836	CLA	O1D-CGD-O2D-CED
14	cB	833	CLA	O1D-CGD-O2D-CED
14	B	807	CLA	C3-C5-C6-C7
14	bB	807	CLA	C3-C5-C6-C7
14	cB	808	CLA	C3-C5-C6-C7
14	A	829	CLA	CBA-CGA-O2A-C1
14	B	817	CLA	CBA-CGA-O2A-C1
14	bA	829	CLA	CBA-CGA-O2A-C1
14	bB	817	CLA	CBA-CGA-O2A-C1
14	cA	829	CLA	CBA-CGA-O2A-C1
14	cB	818	CLA	CBA-CGA-O2A-C1
14	B	824	CLA	O1A-CGA-O2A-C1
14	bB	824	CLA	O1A-CGA-O2A-C1
14	cB	825	CLA	O1A-CGA-O2A-C1
14	B	807	CLA	C13-C15-C16-C17
14	bB	807	CLA	C13-C15-C16-C17
14	cB	808	CLA	C13-C15-C16-C17
14	B	808	CLA	C3-C5-C6-C7
14	bB	808	CLA	C3-C5-C6-C7
14	cB	809	CLA	C3-C5-C6-C7
14	L	203	CLA	C11-C10-C8-C9
14	L	204	CLA	C11-C10-C8-C9
14	bL	203	CLA	C11-C10-C8-C9
14	bL	204	CLA	C11-C10-C8-C9
14	cL	204	CLA	C11-C10-C8-C9
14	cL	205	CLA	C11-C10-C8-C9
14	A	808	CLA	O1D-CGD-O2D-CED
14	B	805	CLA	O1D-CGD-O2D-CED
14	B	829	CLA	O1D-CGD-O2D-CED
14	bA	808	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	bB	805	CLA	O1D-CGD-O2D-CED
14	bB	829	CLA	O1D-CGD-O2D-CED
14	cA	808	CLA	O1D-CGD-O2D-CED
14	cB	806	CLA	O1D-CGD-O2D-CED
14	cB	830	CLA	O1D-CGD-O2D-CED
14	A	803	CLA	CBD-CGD-O2D-CED
14	bA	803	CLA	CBD-CGD-O2D-CED
14	cA	803	CLA	CBD-CGD-O2D-CED
14	L	202	CLA	C13-C15-C16-C17
14	bL	202	CLA	C13-C15-C16-C17
14	cL	203	CLA	C13-C15-C16-C17
17	A	845	BCR	C36-C18-C19-C20
17	A	847	BCR	C37-C22-C23-C24
17	B	844	BCR	C36-C18-C19-C20
17	bA	845	BCR	C36-C18-C19-C20
17	bA	847	BCR	C37-C22-C23-C24
17	bB	844	BCR	C36-C18-C19-C20
17	cA	845	BCR	C36-C18-C19-C20
17	cA	847	BCR	C37-C22-C23-C24
17	cB	845	BCR	C36-C18-C19-C20
17	A	845	BCR	C17-C18-C19-C20
17	J	103	BCR	C17-C18-C19-C20
17	bA	845	BCR	C17-C18-C19-C20
17	bJ	103	BCR	C17-C18-C19-C20
17	cA	845	BCR	C17-C18-C19-C20
17	cJ	103	BCR	C17-C18-C19-C20
14	B	817	CLA	O1A-CGA-O2A-C1
14	bB	817	CLA	O1A-CGA-O2A-C1
14	cB	818	CLA	O1A-CGA-O2A-C1
14	bB	820	CLA	O1D-CGD-O2D-CED
14	A	828	CLA	C5-C6-C7-C8
14	bA	828	CLA	C5-C6-C7-C8
14	cA	828	CLA	C5-C6-C7-C8
14	B	820	CLA	O1D-CGD-O2D-CED
14	cB	821	CLA	O1D-CGD-O2D-CED
14	A	818	CLA	C8-C10-C11-C12
14	L	204	CLA	C5-C6-C7-C8
14	bA	818	CLA	C8-C10-C11-C12
14	bL	204	CLA	C5-C6-C7-C8
14	cA	818	CLA	C8-C10-C11-C12
14	cL	205	CLA	C5-C6-C7-C8
15	B	840	PQN	C18-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
15	bB	840	PQN	C18-C20-C21-C22
15	cB	841	PQN	C18-C20-C21-C22
14	B	839	CLA	C13-C15-C16-C17
14	bB	839	CLA	C13-C15-C16-C17
14	cB	840	CLA	C13-C15-C16-C17
14	B	801	CLA	C13-C15-C16-C17
14	bB	801	CLA	C13-C15-C16-C17
14	cB	802	CLA	C13-C15-C16-C17
14	L	202	CLA	CBD-CGD-O2D-CED
14	bL	202	CLA	CBD-CGD-O2D-CED
14	cL	203	CLA	CBD-CGD-O2D-CED
14	B	815	CLA	C3-C5-C6-C7
14	bB	815	CLA	C3-C5-C6-C7
14	cB	816	CLA	C3-C5-C6-C7
14	A	833	CLA	C5-C6-C7-C8
14	bA	833	CLA	C5-C6-C7-C8
14	cA	833	CLA	C5-C6-C7-C8
14	cB	818	CLA	O1D-CGD-O2D-CED
14	A	806	CLA	C3-C5-C6-C7
14	bA	806	CLA	C3-C5-C6-C7
14	cA	806	CLA	C3-C5-C6-C7
17	A	845	BCR	C9-C10-C11-C12
17	bA	845	BCR	C9-C10-C11-C12
17	cA	845	BCR	C9-C10-C11-C12
14	A	828	CLA	CBA-CGA-O2A-C1
14	bA	828	CLA	CBA-CGA-O2A-C1
14	cA	828	CLA	CBA-CGA-O2A-C1
14	B	819	CLA	C2A-CAA-CBA-CGA
14	L	201	CLA	C2A-CAA-CBA-CGA
14	bB	819	CLA	C2A-CAA-CBA-CGA
14	bL	201	CLA	C2A-CAA-CBA-CGA
14	cB	820	CLA	C2A-CAA-CBA-CGA
14	cL	202	CLA	C2A-CAA-CBA-CGA
14	B	817	CLA	O1D-CGD-O2D-CED
14	bB	817	CLA	O1D-CGD-O2D-CED
14	B	828	CLA	C15-C16-C17-C18
14	L	202	CLA	C8-C10-C11-C12
14	bB	828	CLA	C15-C16-C17-C18
14	bL	202	CLA	C8-C10-C11-C12
14	cB	829	CLA	C15-C16-C17-C18
14	cL	203	CLA	C8-C10-C11-C12
17	A	846	BCR	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
17	bA	846	BCR	C6-C7-C8-C9
17	cA	846	BCR	C6-C7-C8-C9
14	A	829	CLA	O1A-CGA-O2A-C1
14	bA	829	CLA	O1A-CGA-O2A-C1
14	cA	829	CLA	O1A-CGA-O2A-C1
14	A	804	CLA	O1D-CGD-O2D-CED
14	A	839	CLA	O1D-CGD-O2D-CED
14	bA	804	CLA	O1D-CGD-O2D-CED
14	cA	804	CLA	O1D-CGD-O2D-CED
17	A	845	BCR	C10-C11-C12-C13
17	B	841	BCR	C18-C19-C20-C21
17	bA	845	BCR	C10-C11-C12-C13
17	bB	841	BCR	C18-C19-C20-C21
17	cA	845	BCR	C10-C11-C12-C13
17	cB	842	BCR	C18-C19-C20-C21
14	bA	839	CLA	O1D-CGD-O2D-CED
14	cA	839	CLA	O1D-CGD-O2D-CED
14	B	828	CLA	C13-C15-C16-C17
14	bB	828	CLA	C13-C15-C16-C17
14	cB	829	CLA	C13-C15-C16-C17
14	A	804	CLA	O1A-CGA-O2A-C1
14	bA	804	CLA	O1A-CGA-O2A-C1
14	cA	804	CLA	O1A-CGA-O2A-C1
14	A	818	CLA	C5-C6-C7-C8
14	B	805	CLA	C15-C16-C17-C18
14	B	831	CLA	C15-C16-C17-C18
14	bA	818	CLA	C5-C6-C7-C8
14	bB	805	CLA	C15-C16-C17-C18
14	bB	831	CLA	C10-C11-C12-C13
14	bB	831	CLA	C15-C16-C17-C18
14	cA	818	CLA	C5-C6-C7-C8
14	cB	806	CLA	C15-C16-C17-C18
14	cB	832	CLA	C15-C16-C17-C18
15	A	843	PQN	C15-C16-C17-C18
15	bA	843	PQN	C15-C16-C17-C18
15	cA	843	PQN	C15-C16-C17-C18
14	A	807	CLA	O1D-CGD-O2D-CED
14	A	840	CLA	O1D-CGD-O2D-CED
14	bA	807	CLA	O1D-CGD-O2D-CED
14	bA	840	CLA	O1D-CGD-O2D-CED
14	cA	840	CLA	O1D-CGD-O2D-CED
14	cA	807	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	B	805	CLA	C13-C15-C16-C17
14	B	831	CLA	C10-C11-C12-C13
14	bB	805	CLA	C13-C15-C16-C17
14	cB	806	CLA	C13-C15-C16-C17
14	cB	832	CLA	C10-C11-C12-C13
15	B	840	PQN	C20-C21-C22-C23
15	bB	840	PQN	C20-C21-C22-C23
15	cB	841	PQN	C20-C21-C22-C23
18	A	851	LHG	C3-O3-P-O6
18	bA	851	LHG	C3-O3-P-O6
18	cA	851	LHG	C3-O3-P-O6
14	L	204	CLA	C3-C5-C6-C7
14	bL	204	CLA	C3-C5-C6-C7
14	cL	205	CLA	C3-C5-C6-C7
14	B	839	CLA	CBA-CGA-O2A-C1
14	bB	839	CLA	CBA-CGA-O2A-C1
14	cB	840	CLA	CBA-CGA-O2A-C1
14	bA	828	CLA	O1D-CGD-O2D-CED
14	cA	828	CLA	O1D-CGD-O2D-CED
14	A	828	CLA	O1D-CGD-O2D-CED
14	L	203	CLA	C4-C3-C5-C6
14	bL	203	CLA	C4-C3-C5-C6
14	cL	204	CLA	C4-C3-C5-C6
14	A	829	CLA	C13-C15-C16-C17
14	cA	829	CLA	C13-C15-C16-C17
14	B	815	CLA	C2A-CAA-CBA-CGA
14	B	829	CLA	C2A-CAA-CBA-CGA
14	bB	815	CLA	C2A-CAA-CBA-CGA
14	bB	829	CLA	C2A-CAA-CBA-CGA
14	cB	816	CLA	C2A-CAA-CBA-CGA
14	cB	830	CLA	C2A-CAA-CBA-CGA
14	A	831	CLA	CBA-CGA-O2A-C1
14	bA	831	CLA	CBA-CGA-O2A-C1
14	cA	831	CLA	CBA-CGA-O2A-C1
14	bA	829	CLA	C13-C15-C16-C17
14	A	833	CLA	O1D-CGD-O2D-CED
14	bA	833	CLA	O1D-CGD-O2D-CED
14	cA	833	CLA	O1D-CGD-O2D-CED
17	A	846	BCR	C16-C17-C18-C36
17	A	848	BCR	C11-C10-C9-C34
17	A	849	BCR	C11-C10-C9-C34
17	B	841	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
17	B	844	BCR	C35-C13-C14-C15
17	B	844	BCR	C20-C21-C22-C37
17	B	846	BCR	C11-C10-C9-C34
17	J	103	BCR	C11-C10-C9-C34
17	J	103	BCR	C16-C17-C18-C36
17	J	103	BCR	C20-C21-C22-C37
17	bA	846	BCR	C16-C17-C18-C36
17	bA	848	BCR	C11-C10-C9-C34
17	bA	849	BCR	C11-C10-C9-C34
17	bB	841	BCR	C20-C21-C22-C37
17	bB	844	BCR	C35-C13-C14-C15
17	bB	844	BCR	C20-C21-C22-C37
17	bB	846	BCR	C11-C10-C9-C34
17	bJ	103	BCR	C11-C10-C9-C34
17	bJ	103	BCR	C16-C17-C18-C36
17	bJ	103	BCR	C20-C21-C22-C37
17	cA	846	BCR	C16-C17-C18-C36
17	cA	848	BCR	C11-C10-C9-C34
17	cA	849	BCR	C11-C10-C9-C34
17	cB	842	BCR	C20-C21-C22-C37
17	cB	845	BCR	C35-C13-C14-C15
17	cB	845	BCR	C20-C21-C22-C37
17	cB	847	BCR	C11-C10-C9-C34
17	cJ	103	BCR	C11-C10-C9-C34
17	cJ	103	BCR	C16-C17-C18-C36
17	cJ	103	BCR	C20-C21-C22-C37
14	B	849	CLA	O1D-CGD-O2D-CED
14	bB	849	CLA	O1D-CGD-O2D-CED
14	cB	850	CLA	O1D-CGD-O2D-CED
14	B	819	CLA	O1D-CGD-O2D-CED
14	bB	819	CLA	O1D-CGD-O2D-CED
14	cB	820	CLA	O1D-CGD-O2D-CED
15	B	840	PQN	C15-C16-C17-C18
15	bB	840	PQN	C15-C16-C17-C18
15	cB	841	PQN	C15-C16-C17-C18
14	B	804	CLA	O1D-CGD-O2D-CED
14	bB	804	CLA	O1D-CGD-O2D-CED
14	cB	805	CLA	O1D-CGD-O2D-CED
14	B	807	CLA	C8-C10-C11-C12
14	bB	807	CLA	C8-C10-C11-C12
14	cB	808	CLA	C8-C10-C11-C12
14	B	825	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	A	846	BCR	C16-C17-C18-C19
17	A	848	BCR	C11-C10-C9-C8
17	A	849	BCR	C11-C10-C9-C8
17	B	844	BCR	C20-C21-C22-C23
17	B	846	BCR	C11-C10-C9-C8
17	B	846	BCR	C12-C13-C14-C15
17	J	103	BCR	C11-C10-C9-C8
17	J	103	BCR	C16-C17-C18-C19
17	J	103	BCR	C20-C21-C22-C23
17	bA	846	BCR	C16-C17-C18-C19
17	bA	848	BCR	C11-C10-C9-C8
17	bA	849	BCR	C11-C10-C9-C8
17	bB	844	BCR	C20-C21-C22-C23
17	bB	846	BCR	C11-C10-C9-C8
17	bB	846	BCR	C12-C13-C14-C15
17	bJ	103	BCR	C11-C10-C9-C8
17	bJ	103	BCR	C16-C17-C18-C19
17	bJ	103	BCR	C20-C21-C22-C23
17	cA	846	BCR	C16-C17-C18-C19
17	cA	848	BCR	C11-C10-C9-C8
17	cA	849	BCR	C11-C10-C9-C8
17	cB	845	BCR	C20-C21-C22-C23
17	cB	847	BCR	C11-C10-C9-C8
17	cB	847	BCR	C12-C13-C14-C15
17	cJ	103	BCR	C11-C10-C9-C8
17	cJ	103	BCR	C16-C17-C18-C19
17	cJ	103	BCR	C20-C21-C22-C23
14	A	852	CLA	C8-C10-C11-C12
14	bA	852	CLA	C8-C10-C11-C12
14	cA	852	CLA	C8-C10-C11-C12
14	A	831	CLA	O1A-CGA-O2A-C1
14	bA	831	CLA	O1A-CGA-O2A-C1
14	cA	831	CLA	O1A-CGA-O2A-C1
14	A	829	CLA	O1D-CGD-O2D-CED
14	bA	829	CLA	O1D-CGD-O2D-CED
14	cA	829	CLA	O1D-CGD-O2D-CED
14	B	816	CLA	O1D-CGD-O2D-CED
14	bB	816	CLA	O1D-CGD-O2D-CED
14	cB	817	CLA	O1D-CGD-O2D-CED
14	cB	826	CLA	CBD-CGD-O2D-CED
18	A	850	LHG	C27-C28-C29-C30
18	bA	850	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
18	cA	850	LHG	C27-C28-C29-C30
14	A	828	CLA	O1A-CGA-O2A-C1
14	bA	828	CLA	O1A-CGA-O2A-C1
14	cA	828	CLA	O1A-CGA-O2A-C1
17	B	846	BCR	C37-C22-C23-C24
17	bB	846	BCR	C37-C22-C23-C24
17	cB	847	BCR	C37-C22-C23-C24
15	B	840	PQN	C13-C15-C16-C17
15	bB	840	PQN	C13-C15-C16-C17
15	cB	841	PQN	C13-C15-C16-C17
14	bB	825	CLA	CBD-CGD-O2D-CED
14	A	852	CLA	C16-C17-C18-C19
14	bA	852	CLA	C16-C17-C18-C19
14	cA	852	CLA	C16-C17-C18-C19
15	A	843	PQN	C25-C26-C27-C28
15	bA	843	PQN	C25-C26-C27-C28
15	cA	843	PQN	C25-C26-C27-C28
14	B	807	CLA	C5-C6-C7-C8
14	bB	807	CLA	C5-C6-C7-C8
14	cB	808	CLA	C5-C6-C7-C8
14	B	839	CLA	O1A-CGA-O2A-C1
14	bB	839	CLA	O1A-CGA-O2A-C1
14	cB	840	CLA	O1A-CGA-O2A-C1
18	cA	850	LHG	C29-C30-C31-C32
14	B	812	CLA	O1D-CGD-O2D-CED
14	bB	812	CLA	O1D-CGD-O2D-CED
14	A	803	CLA	C3A-C2A-CAA-CBA
14	A	806	CLA	C3A-C2A-CAA-CBA
14	A	815	CLA	C3A-C2A-CAA-CBA
14	B	814	CLA	C3A-C2A-CAA-CBA
14	L	201	CLA	C3A-C2A-CAA-CBA
14	bA	803	CLA	C3A-C2A-CAA-CBA
14	bA	806	CLA	C3A-C2A-CAA-CBA
14	bA	815	CLA	C3A-C2A-CAA-CBA
14	bB	814	CLA	C3A-C2A-CAA-CBA
14	bL	201	CLA	C3A-C2A-CAA-CBA
14	cA	803	CLA	C3A-C2A-CAA-CBA
14	cA	806	CLA	C3A-C2A-CAA-CBA
14	cA	815	CLA	C3A-C2A-CAA-CBA
14	cB	815	CLA	C3A-C2A-CAA-CBA
14	cL	202	CLA	C3A-C2A-CAA-CBA
14	A	824	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
14	bA	824	CLA	C8-C10-C11-C12
14	cA	824	CLA	C8-C10-C11-C12
18	A	850	LHG	C29-C30-C31-C32
18	bA	850	LHG	C29-C30-C31-C32
14	cB	813	CLA	O1D-CGD-O2D-CED
20	B	848	LMG	C33-C34-C35-C36
20	bB	848	LMG	C33-C34-C35-C36
20	cB	849	LMG	C33-C34-C35-C36
14	B	810	CLA	CBD-CGD-O2D-CED
14	bB	810	CLA	CBD-CGD-O2D-CED
14	cB	811	CLA	CBD-CGD-O2D-CED
20	B	848	LMG	C35-C36-C37-C38
20	bB	848	LMG	C35-C36-C37-C38
20	cB	849	LMG	C35-C36-C37-C38
17	B	846	BCR	C14-C15-C16-C17
17	bB	846	BCR	C14-C15-C16-C17
17	cB	847	BCR	C14-C15-C16-C17
14	L	204	CLA	CBA-CGA-O2A-C1
14	bL	204	CLA	CBA-CGA-O2A-C1
14	cL	205	CLA	CBA-CGA-O2A-C1
18	A	850	LHG	C24-C23-O8-C6
18	bA	850	LHG	C24-C23-O8-C6
18	cA	850	LHG	C24-C23-O8-C6
14	L	201	CLA	C10-C11-C12-C13
14	cL	202	CLA	C10-C11-C12-C13
17	A	849	BCR	C23-C24-C25-C30
17	B	844	BCR	C1-C6-C7-C8
17	B	844	BCR	C5-C6-C7-C8
17	B	850	BCR	C23-C24-C25-C26
17	F	202	BCR	C23-C24-C25-C30
17	J	103	BCR	C23-C24-C25-C26
17	L	205	BCR	C23-C24-C25-C26
17	L	205	BCR	C23-C24-C25-C30
17	L	206	BCR	C23-C24-C25-C26
17	L	206	BCR	C23-C24-C25-C30
17	M	101	BCR	C23-C24-C25-C26
17	M	101	BCR	C23-C24-C25-C30
17	bA	849	BCR	C23-C24-C25-C30
17	bB	844	BCR	C1-C6-C7-C8
17	bB	844	BCR	C5-C6-C7-C8
17	bB	850	BCR	C23-C24-C25-C26
17	bB	850	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
17	bF	202	BCR	C23-C24-C25-C30
17	bJ	103	BCR	C23-C24-C25-C26
17	bL	205	BCR	C23-C24-C25-C26
17	bL	205	BCR	C23-C24-C25-C30
17	bL	206	BCR	C23-C24-C25-C26
17	bL	206	BCR	C23-C24-C25-C30
17	bM	101	BCR	C23-C24-C25-C26
17	bM	101	BCR	C23-C24-C25-C30
17	cA	849	BCR	C23-C24-C25-C30
17	cB	845	BCR	C1-C6-C7-C8
17	cB	845	BCR	C5-C6-C7-C8
17	cB	851	BCR	C23-C24-C25-C26
17	cF	202	BCR	C23-C24-C25-C30
17	cJ	103	BCR	C23-C24-C25-C26
17	cL	206	BCR	C23-C24-C25-C26
17	cL	206	BCR	C23-C24-C25-C30
17	cL	207	BCR	C23-C24-C25-C26
17	cL	207	BCR	C23-C24-C25-C30
17	cM	101	BCR	C23-C24-C25-C26
17	cM	101	BCR	C23-C24-C25-C30
14	F	201	CLA	CBA-CGA-O2A-C1
14	bF	201	CLA	CBA-CGA-O2A-C1
14	cF	201	CLA	CBA-CGA-O2A-C1
14	A	832	CLA	C5-C6-C7-C8
14	B	802	CLA	C15-C16-C17-C18
14	B	809	CLA	C15-C16-C17-C18
14	B	839	CLA	C5-C6-C7-C8
14	bA	832	CLA	C5-C6-C7-C8
14	bB	802	CLA	C15-C16-C17-C18
14	bB	809	CLA	C15-C16-C17-C18
14	bB	839	CLA	C5-C6-C7-C8
14	cA	832	CLA	C5-C6-C7-C8
14	cB	803	CLA	C15-C16-C17-C18
14	cB	810	CLA	C15-C16-C17-C18
14	cB	840	CLA	C5-C6-C7-C8
14	cA	831	CLA	O1D-CGD-O2D-CED
14	bL	201	CLA	C10-C11-C12-C13
14	A	831	CLA	O1D-CGD-O2D-CED
14	bA	831	CLA	O1D-CGD-O2D-CED
20	B	848	LMG	C29-C30-C31-C32
20	bB	848	LMG	C29-C30-C31-C32
20	cB	849	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
14	L	204	CLA	C4-C3-C5-C6
14	bL	204	CLA	C4-C3-C5-C6
14	cL	205	CLA	C4-C3-C5-C6
14	B	809	CLA	C6-C7-C8-C10
14	L	204	CLA	C2-C3-C5-C6
14	bA	840	CLA	C11-C10-C8-C7
14	bB	809	CLA	C6-C7-C8-C10
14	bL	204	CLA	C2-C3-C5-C6
14	cB	810	CLA	C6-C7-C8-C10
14	cL	205	CLA	C2-C3-C5-C6
14	A	831	CLA	C3-C5-C6-C7
14	bA	831	CLA	C3-C5-C6-C7
14	cA	831	CLA	C3-C5-C6-C7
14	F	201	CLA	O1A-CGA-O2A-C1
14	L	204	CLA	O1A-CGA-O2A-C1
14	bF	201	CLA	O1A-CGA-O2A-C1
14	bL	204	CLA	O1A-CGA-O2A-C1
14	cF	201	CLA	O1A-CGA-O2A-C1
14	cL	205	CLA	O1A-CGA-O2A-C1
17	B	844	BCR	C9-C10-C11-C12
17	bB	844	BCR	C9-C10-C11-C12
17	cB	845	BCR	C9-C10-C11-C12
14	A	816	CLA	C2A-CAA-CBA-CGA
14	bA	816	CLA	C2A-CAA-CBA-CGA
14	cA	816	CLA	C2A-CAA-CBA-CGA
14	B	839	CLA	C10-C11-C12-C13
14	bB	839	CLA	C10-C11-C12-C13
14	cB	840	CLA	C10-C11-C12-C13
18	bA	850	LHG	O10-C23-O8-C6
18	cA	850	LHG	O10-C23-O8-C6
14	A	819	CLA	O1D-CGD-O2D-CED
14	bA	819	CLA	O1D-CGD-O2D-CED
14	cA	819	CLA	O1D-CGD-O2D-CED
14	A	852	CLA	C3-C5-C6-C7
14	bA	852	CLA	C3-C5-C6-C7
14	cA	852	CLA	C3-C5-C6-C7
17	M	101	BCR	C22-C23-C24-C25
17	bM	101	BCR	C22-C23-C24-C25
17	cM	101	BCR	C22-C23-C24-C25
18	A	850	LHG	O10-C23-O8-C6
14	A	830	CLA	CBA-CGA-O2A-C1
14	bA	830	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	cA	830	CLA	CBA-CGA-O2A-C1
14	A	836	CLA	O1D-CGD-O2D-CED
14	bA	836	CLA	O1D-CGD-O2D-CED
14	cA	836	CLA	O1D-CGD-O2D-CED
14	A	809	CLA	CBD-CGD-O2D-CED
14	bA	809	CLA	CBD-CGD-O2D-CED
14	cA	809	CLA	CBD-CGD-O2D-CED
14	A	828	CLA	C10-C11-C12-C13
14	A	831	CLA	C5-C6-C7-C8
14	B	831	CLA	C13-C15-C16-C17
14	bA	828	CLA	C10-C11-C12-C13
14	bA	831	CLA	C5-C6-C7-C8
14	bB	831	CLA	C13-C15-C16-C17
14	cA	828	CLA	C10-C11-C12-C13
14	cA	831	CLA	C5-C6-C7-C8
14	cB	832	CLA	C13-C15-C16-C17
14	A	840	CLA	C6-C7-C8-C9
14	B	807	CLA	C14-C13-C15-C16
14	B	809	CLA	C6-C7-C8-C9
14	bA	840	CLA	C6-C7-C8-C9
14	bB	807	CLA	C14-C13-C15-C16
14	bB	809	CLA	C6-C7-C8-C9
14	cA	840	CLA	C6-C7-C8-C9
14	cB	808	CLA	C14-C13-C15-C16
14	cB	810	CLA	C6-C7-C8-C9
14	cB	827	CLA	C2C-C3C-CAC-CBC
14	A	840	CLA	C3-C5-C6-C7
14	bA	840	CLA	C3-C5-C6-C7
14	cA	840	CLA	C3-C5-C6-C7
14	A	828	CLA	C2A-CAA-CBA-CGA
14	bA	828	CLA	C2A-CAA-CBA-CGA
14	cA	828	CLA	C2A-CAA-CBA-CGA
14	B	826	CLA	C2C-C3C-CAC-CBC
14	bB	826	CLA	C2C-C3C-CAC-CBC
17	J	103	BCR	C36-C18-C19-C20
17	bJ	103	BCR	C36-C18-C19-C20
17	cJ	103	BCR	C36-C18-C19-C20
14	A	803	CLA	O1D-CGD-O2D-CED
14	bA	803	CLA	O1D-CGD-O2D-CED
14	cA	803	CLA	O1D-CGD-O2D-CED
14	A	807	CLA	C2C-C3C-CAC-CBC
14	B	831	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
14	bA	807	CLA	C2C-C3C-CAC-CBC
14	bB	831	CLA	C2C-C3C-CAC-CBC
14	cA	807	CLA	C2C-C3C-CAC-CBC
14	cB	832	CLA	C2C-C3C-CAC-CBC
14	A	815	CLA	C1A-C2A-CAA-CBA
14	A	817	CLA	C1A-C2A-CAA-CBA
14	A	818	CLA	C1A-C2A-CAA-CBA
14	A	829	CLA	C1A-C2A-CAA-CBA
14	B	805	CLA	C1A-C2A-CAA-CBA
14	B	810	CLA	C1A-C2A-CAA-CBA
14	B	827	CLA	C1A-C2A-CAA-CBA
14	B	837	CLA	C1A-C2A-CAA-CBA
14	L	201	CLA	C1A-C2A-CAA-CBA
14	L	202	CLA	C1A-C2A-CAA-CBA
14	bA	817	CLA	C1A-C2A-CAA-CBA
14	bA	818	CLA	C1A-C2A-CAA-CBA
14	bA	829	CLA	C1A-C2A-CAA-CBA
14	bB	805	CLA	C1A-C2A-CAA-CBA
14	bB	810	CLA	C1A-C2A-CAA-CBA
14	bB	827	CLA	C1A-C2A-CAA-CBA
14	bB	837	CLA	C1A-C2A-CAA-CBA
14	bL	201	CLA	C1A-C2A-CAA-CBA
14	bL	202	CLA	C1A-C2A-CAA-CBA
14	cA	817	CLA	C1A-C2A-CAA-CBA
14	cA	818	CLA	C1A-C2A-CAA-CBA
14	cA	829	CLA	C1A-C2A-CAA-CBA
14	cB	806	CLA	C1A-C2A-CAA-CBA
14	cB	811	CLA	C1A-C2A-CAA-CBA
14	cB	828	CLA	C1A-C2A-CAA-CBA
14	cB	838	CLA	C1A-C2A-CAA-CBA
14	cL	202	CLA	C1A-C2A-CAA-CBA
14	cL	203	CLA	C1A-C2A-CAA-CBA
14	A	806	CLA	C10-C11-C12-C13
14	bA	806	CLA	C10-C11-C12-C13
14	cA	806	CLA	C10-C11-C12-C13
14	B	828	CLA	C16-C17-C18-C20
14	bB	828	CLA	C16-C17-C18-C20
14	cB	829	CLA	C16-C17-C18-C20
14	A	806	CLA	C4-C3-C5-C6
14	bA	806	CLA	C4-C3-C5-C6
14	cA	806	CLA	C4-C3-C5-C6
14	L	202	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
14	bL	202	CLA	C15-C16-C17-C18
14	cL	203	CLA	C15-C16-C17-C18
18	A	850	LHG	C10-C11-C12-C13
18	bA	850	LHG	C10-C11-C12-C13
18	cA	850	LHG	C10-C11-C12-C13
14	bA	824	CLA	C10-C11-C12-C13
14	cA	824	CLA	C10-C11-C12-C13
14	A	824	CLA	C10-C11-C12-C13
14	B	826	CLA	C15-C16-C17-C18
14	bB	826	CLA	C15-C16-C17-C18
14	cB	827	CLA	C15-C16-C17-C18
14	B	824	CLA	CBD-CGD-O2D-CED
14	bB	824	CLA	CBD-CGD-O2D-CED
14	cB	825	CLA	CBD-CGD-O2D-CED
17	A	849	BCR	C16-C17-C18-C36
17	F	202	BCR	C35-C13-C14-C15
17	bA	849	BCR	C16-C17-C18-C36
17	bF	202	BCR	C35-C13-C14-C15
17	cA	849	BCR	C16-C17-C18-C36
17	cF	202	BCR	C35-C13-C14-C15
14	B	807	CLA	C4-C3-C5-C6
14	bB	807	CLA	C4-C3-C5-C6
14	cB	808	CLA	C4-C3-C5-C6
14	A	806	CLA	C2-C3-C5-C6
14	bA	806	CLA	C2-C3-C5-C6
14	cA	806	CLA	C2-C3-C5-C6
14	F	201	CLA	C2A-CAA-CBA-CGA
14	bF	201	CLA	C2A-CAA-CBA-CGA
14	cF	201	CLA	C2A-CAA-CBA-CGA
14	A	818	CLA	C2-C1-O2A-CGA
14	bA	818	CLA	C2-C1-O2A-CGA
14	cA	818	CLA	C2-C1-O2A-CGA
18	bA	850	LHG	C26-C27-C28-C29
18	cA	850	LHG	C26-C27-C28-C29
18	A	850	LHG	C26-C27-C28-C29
14	A	830	CLA	O1A-CGA-O2A-C1
14	bA	830	CLA	O1A-CGA-O2A-C1
14	cA	830	CLA	O1A-CGA-O2A-C1
17	B	841	BCR	C20-C21-C22-C23
17	B	844	BCR	C12-C13-C14-C15
17	bB	841	BCR	C20-C21-C22-C23
17	bB	844	BCR	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
17	cB	842	BCR	C20-C21-C22-C23
17	cB	845	BCR	C12-C13-C14-C15
14	A	840	CLA	C6-C7-C8-C10
14	A	840	CLA	C11-C10-C8-C7
14	B	807	CLA	C2-C3-C5-C6
14	B	807	CLA	C12-C13-C15-C16
14	B	831	CLA	C11-C10-C8-C7
14	L	203	CLA	C2-C3-C5-C6
14	bA	840	CLA	C6-C7-C8-C10
14	bB	807	CLA	C2-C3-C5-C6
14	bB	807	CLA	C12-C13-C15-C16
14	bB	831	CLA	C11-C10-C8-C7
14	cA	840	CLA	C6-C7-C8-C10
14	cA	840	CLA	C11-C10-C8-C7
14	cB	808	CLA	C2-C3-C5-C6
14	cB	808	CLA	C12-C13-C15-C16
14	cB	832	CLA	C11-C10-C8-C7
14	cL	204	CLA	C2-C3-C5-C6
18	A	850	LHG	C25-C26-C27-C28
18	bA	850	LHG	C25-C26-C27-C28
18	cA	850	LHG	C25-C26-C27-C28
14	A	829	CLA	C11-C10-C8-C9
14	A	832	CLA	C11-C10-C8-C9
14	A	837	CLA	C11-C10-C8-C9
14	A	840	CLA	C11-C10-C8-C9
14	B	805	CLA	C6-C7-C8-C9
14	B	831	CLA	C11-C10-C8-C9
14	L	203	CLA	C6-C7-C8-C9
14	bA	829	CLA	C11-C10-C8-C9
14	bA	832	CLA	C11-C10-C8-C9
14	bA	837	CLA	C11-C10-C8-C9
14	bA	840	CLA	C11-C10-C8-C9
14	bB	805	CLA	C6-C7-C8-C9
14	bB	831	CLA	C11-C10-C8-C9
14	bL	203	CLA	C6-C7-C8-C9
14	cA	829	CLA	C11-C10-C8-C9
14	cA	832	CLA	C11-C10-C8-C9
14	cA	837	CLA	C11-C10-C8-C9
14	cA	840	CLA	C11-C10-C8-C9
14	cB	806	CLA	C6-C7-C8-C9
14	cB	832	CLA	C11-C10-C8-C9
14	cL	204	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
14	B	825	CLA	O1D-CGD-O2D-CED
14	bB	825	CLA	O1D-CGD-O2D-CED
17	J	103	BCR	C21-C22-C23-C24
17	bJ	103	BCR	C21-C22-C23-C24
17	cJ	103	BCR	C21-C22-C23-C24
14	cB	826	CLA	O1D-CGD-O2D-CED
14	B	839	CLA	C15-C16-C17-C18
14	bB	839	CLA	C15-C16-C17-C18
14	cB	840	CLA	C15-C16-C17-C18
15	cA	843	PQN	C13-C15-C16-C17
18	A	851	LHG	C7-C8-C9-C10
18	bA	851	LHG	C7-C8-C9-C10
18	cA	851	LHG	C7-C8-C9-C10
14	bL	203	CLA	C2-C3-C5-C6
14	bA	809	CLA	O1D-CGD-O2D-CED
14	cA	840	CLA	C5-C6-C7-C8
14	A	809	CLA	O1D-CGD-O2D-CED
14	cA	809	CLA	O1D-CGD-O2D-CED
14	L	202	CLA	CBA-CGA-O2A-C1
14	bL	202	CLA	CBA-CGA-O2A-C1
18	A	851	LHG	C24-C23-O8-C6
18	bA	851	LHG	C24-C23-O8-C6
18	cA	851	LHG	C24-C23-O8-C6
14	bA	840	CLA	C5-C6-C7-C8
14	cB	811	CLA	O1D-CGD-O2D-CED
14	B	810	CLA	O1D-CGD-O2D-CED
14	bB	810	CLA	O1D-CGD-O2D-CED
15	A	843	PQN	C13-C15-C16-C17
15	bA	843	PQN	C13-C15-C16-C17
14	A	840	CLA	C5-C6-C7-C8
14	B	831	CLA	CBA-CGA-O2A-C1
14	bB	831	CLA	CBA-CGA-O2A-C1
14	cB	832	CLA	CBA-CGA-O2A-C1
14	cL	203	CLA	CBA-CGA-O2A-C1
14	B	806	CLA	C10-C11-C12-C13
14	bB	806	CLA	C10-C11-C12-C13
14	cB	807	CLA	C10-C11-C12-C13
18	A	851	LHG	C4-C5-C6-O8
18	bA	851	LHG	C4-C5-C6-O8
18	cA	851	LHG	C4-C5-C6-O8
14	cB	825	CLA	O1D-CGD-O2D-CED
14	bB	824	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	bL	202	CLA	O1D-CGD-O2D-CED
14	cL	203	CLA	O1D-CGD-O2D-CED
14	A	818	CLA	C10-C11-C12-C13
14	cA	818	CLA	C10-C11-C12-C13
14	B	824	CLA	O1D-CGD-O2D-CED
14	L	202	CLA	O1D-CGD-O2D-CED
14	bA	818	CLA	C10-C11-C12-C13
18	A	850	LHG	C13-C14-C15-C16
18	cA	850	LHG	C13-C14-C15-C16
18	bA	850	LHG	C13-C14-C15-C16
14	A	841	CLA	CBA-CGA-O2A-C1
14	bA	841	CLA	CBA-CGA-O2A-C1
14	cA	841	CLA	CBA-CGA-O2A-C1
18	A	851	LHG	O7-C5-C6-O8
18	bA	851	LHG	O7-C5-C6-O8
18	cA	851	LHG	O7-C5-C6-O8
14	L	201	CLA	C2-C1-O2A-CGA
14	bL	201	CLA	C2-C1-O2A-CGA
14	cL	202	CLA	C2-C1-O2A-CGA
14	L	202	CLA	C6-C7-C8-C9
14	L	202	CLA	C11-C10-C8-C9
14	bL	202	CLA	C6-C7-C8-C9
14	bL	202	CLA	C11-C10-C8-C9
14	cL	203	CLA	C6-C7-C8-C9
14	cL	203	CLA	C11-C10-C8-C9
14	B	803	CLA	C2A-CAA-CBA-CGA
14	bA	822	CLA	C2A-CAA-CBA-CGA
14	bB	803	CLA	C2A-CAA-CBA-CGA
14	cA	822	CLA	C2A-CAA-CBA-CGA
14	cB	804	CLA	C2A-CAA-CBA-CGA
17	A	849	BCR	C23-C24-C25-C26
17	B	845	BCR	C23-C24-C25-C26
17	B	845	BCR	C23-C24-C25-C30
17	F	202	BCR	C23-C24-C25-C26
17	bA	849	BCR	C23-C24-C25-C26
17	bB	845	BCR	C23-C24-C25-C26
17	bB	845	BCR	C23-C24-C25-C30
17	bF	202	BCR	C23-C24-C25-C26
17	cA	849	BCR	C23-C24-C25-C26
17	cB	846	BCR	C23-C24-C25-C26
17	cB	846	BCR	C23-C24-C25-C30
17	cF	202	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
14	B	827	CLA	C15-C16-C17-C18
17	B	842	BCR	C21-C22-C23-C24
17	B	847	BCR	C7-C8-C9-C10
17	bB	842	BCR	C21-C22-C23-C24
17	bB	847	BCR	C7-C8-C9-C10
17	cB	843	BCR	C21-C22-C23-C24
17	cB	848	BCR	C7-C8-C9-C10
14	bB	827	CLA	C15-C16-C17-C18
14	cB	828	CLA	C15-C16-C17-C18
18	A	850	LHG	C32-C33-C34-C35
18	bA	850	LHG	C32-C33-C34-C35
18	cA	850	LHG	C32-C33-C34-C35
14	A	852	CLA	C16-C17-C18-C20
14	bA	852	CLA	C16-C17-C18-C20
14	cA	852	CLA	C16-C17-C18-C20
14	A	841	CLA	O1A-CGA-O2A-C1
14	B	831	CLA	O1A-CGA-O2A-C1
14	bA	841	CLA	O1A-CGA-O2A-C1
14	bB	831	CLA	O1A-CGA-O2A-C1
14	cA	841	CLA	O1A-CGA-O2A-C1
14	cB	832	CLA	O1A-CGA-O2A-C1
14	A	832	CLA	C11-C10-C8-C7
14	A	833	CLA	C12-C13-C15-C16
14	A	837	CLA	C11-C10-C8-C7
14	A	839	CLA	C11-C10-C8-C7
14	A	852	CLA	C11-C10-C8-C7
14	B	828	CLA	C11-C12-C13-C15
14	L	202	CLA	C6-C7-C8-C10
14	L	203	CLA	C6-C7-C8-C10
14	bA	832	CLA	C11-C10-C8-C7
14	bA	833	CLA	C12-C13-C15-C16
14	bA	837	CLA	C11-C10-C8-C7
14	bA	839	CLA	C11-C10-C8-C7
14	bA	852	CLA	C11-C10-C8-C7
14	bB	828	CLA	C11-C12-C13-C15
14	bL	202	CLA	C6-C7-C8-C10
14	bL	203	CLA	C6-C7-C8-C10
14	cA	832	CLA	C11-C10-C8-C7
14	cA	833	CLA	C12-C13-C15-C16
14	cA	837	CLA	C11-C10-C8-C7
14	cA	839	CLA	C11-C10-C8-C7
14	cA	852	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
14	cB	829	CLA	C11-C12-C13-C15
14	cL	203	CLA	C6-C7-C8-C10
14	cL	204	CLA	C6-C7-C8-C10
14	B	807	CLA	C16-C17-C18-C20
14	bB	807	CLA	C16-C17-C18-C20
14	cA	832	CLA	CBA-CGA-O2A-C1
14	B	826	CLA	C10-C11-C12-C13
14	bB	826	CLA	C10-C11-C12-C13
14	cB	827	CLA	C10-C11-C12-C13
14	A	822	CLA	C2A-CAA-CBA-CGA
13	A	801	CL0	C5-C6-C7-C8
13	bA	801	CL0	C5-C6-C7-C8
13	cA	801	CL0	C5-C6-C7-C8
17	A	845	BCR	C20-C21-C22-C37
17	A	847	BCR	C35-C13-C14-C15
17	B	842	BCR	C35-C13-C14-C15
17	B	850	BCR	C20-C21-C22-C37
17	bA	845	BCR	C20-C21-C22-C37
17	bA	847	BCR	C35-C13-C14-C15
17	bB	842	BCR	C35-C13-C14-C15
17	bB	850	BCR	C20-C21-C22-C37
17	cA	845	BCR	C20-C21-C22-C37
17	cA	847	BCR	C35-C13-C14-C15
17	cB	843	BCR	C35-C13-C14-C15
17	cB	851	BCR	C20-C21-C22-C37
14	cB	808	CLA	C16-C17-C18-C20
14	A	832	CLA	CBA-CGA-O2A-C1
14	bA	832	CLA	CBA-CGA-O2A-C1
14	A	807	CLA	CAD-CBD-CGD-O2D
14	A	811	CLA	CAD-CBD-CGD-O2D
14	A	814	CLA	CAD-CBD-CGD-O2D
14	A	816	CLA	CAD-CBD-CGD-O2D
14	A	823	CLA	CAD-CBD-CGD-O2D
14	A	825	CLA	CAD-CBD-CGD-O2D
14	B	801	CLA	CAD-CBD-CGD-O2D
14	B	815	CLA	CAD-CBD-CGD-O2D
14	L	201	CLA	CAD-CBD-CGD-O2D
14	L	202	CLA	CAD-CBD-CGD-O2D
14	bA	807	CLA	CAD-CBD-CGD-O2D
14	bA	811	CLA	CAD-CBD-CGD-O2D
14	bA	814	CLA	CAD-CBD-CGD-O2D
14	bA	816	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	bA	823	CLA	CAD-CBD-CGD-O2D
14	bA	825	CLA	CAD-CBD-CGD-O2D
14	bB	801	CLA	CAD-CBD-CGD-O2D
14	bB	815	CLA	CAD-CBD-CGD-O2D
14	bL	201	CLA	CAD-CBD-CGD-O2D
14	bL	202	CLA	CAD-CBD-CGD-O2D
14	cA	807	CLA	CAD-CBD-CGD-O2D
14	cA	811	CLA	CAD-CBD-CGD-O2D
14	cA	814	CLA	CAD-CBD-CGD-O2D
14	cA	816	CLA	CAD-CBD-CGD-O2D
14	cA	823	CLA	CAD-CBD-CGD-O2D
14	cA	825	CLA	CAD-CBD-CGD-O2D
14	cB	802	CLA	CAD-CBD-CGD-O2D
14	cB	816	CLA	CAD-CBD-CGD-O2D
14	cL	202	CLA	CAD-CBD-CGD-O2D
14	cL	203	CLA	CAD-CBD-CGD-O2D
14	A	852	CLA	C15-C16-C17-C18
14	bA	852	CLA	C15-C16-C17-C18
14	cA	852	CLA	C15-C16-C17-C18
17	B	842	BCR	C6-C7-C8-C9
17	B	842	BCR	C22-C23-C24-C25
17	bB	842	BCR	C6-C7-C8-C9
17	bB	842	BCR	C22-C23-C24-C25
17	cB	843	BCR	C6-C7-C8-C9
17	cB	843	BCR	C22-C23-C24-C25
14	A	840	CLA	C8-C10-C11-C12
14	bA	840	CLA	C8-C10-C11-C12
14	cA	840	CLA	C8-C10-C11-C12
14	A	841	CLA	C15-C16-C17-C18
14	bA	841	CLA	C15-C16-C17-C18
14	cA	841	CLA	C15-C16-C17-C18
14	A	833	CLA	C2A-CAA-CBA-CGA
14	bA	833	CLA	C2A-CAA-CBA-CGA
14	cA	833	CLA	C2A-CAA-CBA-CGA
14	A	803	CLA	CHA-CBD-CGD-O1D
14	A	803	CLA	CHA-CBD-CGD-O2D
14	A	808	CLA	CHA-CBD-CGD-O1D
14	A	808	CLA	CHA-CBD-CGD-O2D
14	A	829	CLA	CHA-CBD-CGD-O1D
14	A	829	CLA	CHA-CBD-CGD-O2D
14	A	838	CLA	CHA-CBD-CGD-O2D
14	A	842	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	B	803	CLA	CHA-CBD-CGD-O1D
14	B	803	CLA	CHA-CBD-CGD-O2D
14	B	812	CLA	CHA-CBD-CGD-O1D
14	B	812	CLA	CHA-CBD-CGD-O2D
14	B	820	CLA	CHA-CBD-CGD-O1D
14	B	824	CLA	CHA-CBD-CGD-O1D
14	B	824	CLA	CHA-CBD-CGD-O2D
14	B	828	CLA	CHA-CBD-CGD-O1D
14	B	828	CLA	CHA-CBD-CGD-O2D
14	bA	803	CLA	CHA-CBD-CGD-O1D
14	bA	803	CLA	CHA-CBD-CGD-O2D
14	bA	808	CLA	CHA-CBD-CGD-O1D
14	bA	808	CLA	CHA-CBD-CGD-O2D
14	bA	829	CLA	CHA-CBD-CGD-O1D
14	bA	829	CLA	CHA-CBD-CGD-O2D
14	bA	838	CLA	CHA-CBD-CGD-O2D
14	bA	842	CLA	CHA-CBD-CGD-O2D
14	bB	803	CLA	CHA-CBD-CGD-O1D
14	bB	803	CLA	CHA-CBD-CGD-O2D
14	bB	812	CLA	CHA-CBD-CGD-O1D
14	bB	812	CLA	CHA-CBD-CGD-O2D
14	bB	820	CLA	CHA-CBD-CGD-O1D
14	bB	824	CLA	CHA-CBD-CGD-O1D
14	bB	824	CLA	CHA-CBD-CGD-O2D
14	bB	828	CLA	CHA-CBD-CGD-O1D
14	bB	828	CLA	CHA-CBD-CGD-O2D
14	cA	803	CLA	CHA-CBD-CGD-O1D
14	cA	803	CLA	CHA-CBD-CGD-O2D
14	cA	808	CLA	CHA-CBD-CGD-O1D
14	cA	808	CLA	CHA-CBD-CGD-O2D
14	cA	829	CLA	CHA-CBD-CGD-O1D
14	cA	829	CLA	CHA-CBD-CGD-O2D
14	cA	838	CLA	CHA-CBD-CGD-O2D
14	cA	842	CLA	CHA-CBD-CGD-O2D
14	cB	804	CLA	CHA-CBD-CGD-O1D
14	cB	804	CLA	CHA-CBD-CGD-O2D
14	cB	813	CLA	CHA-CBD-CGD-O1D
14	cB	813	CLA	CHA-CBD-CGD-O2D
14	cB	821	CLA	CHA-CBD-CGD-O1D
14	cB	825	CLA	CHA-CBD-CGD-O1D
14	cB	825	CLA	CHA-CBD-CGD-O2D
14	cB	829	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
14	cB	829	CLA	CHA-CBD-CGD-O2D
14	B	838	CLA	CBD-CGD-O2D-CED
14	bB	838	CLA	CBD-CGD-O2D-CED
14	cA	832	CLA	O1A-CGA-O2A-C1
18	A	851	LHG	O10-C23-O8-C6
18	bA	851	LHG	O10-C23-O8-C6
18	cA	851	LHG	O10-C23-O8-C6
17	I	102	BCR	C20-C21-C22-C23
17	bI	102	BCR	C20-C21-C22-C23
17	cI	102	BCR	C20-C21-C22-C23
14	L	204	CLA	C13-C15-C16-C17
14	bL	204	CLA	C13-C15-C16-C17
14	cL	205	CLA	C13-C15-C16-C17
14	cB	839	CLA	CBD-CGD-O2D-CED
14	A	832	CLA	O1A-CGA-O2A-C1
14	bA	832	CLA	O1A-CGA-O2A-C1
14	bA	807	CLA	C4C-C3C-CAC-CBC
14	cA	807	CLA	C4C-C3C-CAC-CBC
14	B	831	CLA	C4-C3-C5-C6
14	bB	831	CLA	C4-C3-C5-C6
14	cB	832	CLA	C4-C3-C5-C6
14	A	807	CLA	C4C-C3C-CAC-CBC
18	A	851	LHG	O9-C7-O7-C5
18	bA	851	LHG	O9-C7-O7-C5
18	cA	851	LHG	O9-C7-O7-C5
14	B	826	CLA	C13-C15-C16-C17
14	bB	826	CLA	C13-C15-C16-C17
14	cB	827	CLA	C13-C15-C16-C17
14	A	833	CLA	C14-C13-C15-C16
14	A	839	CLA	C11-C10-C8-C9
14	bA	833	CLA	C14-C13-C15-C16
14	bA	839	CLA	C11-C10-C8-C9
14	cA	833	CLA	C14-C13-C15-C16
14	cA	839	CLA	C11-C10-C8-C9
20	B	848	LMG	C38-C39-C40-C41
20	bB	848	LMG	C38-C39-C40-C41
14	A	811	CLA	C2A-CAA-CBA-CGA
14	bA	811	CLA	C2A-CAA-CBA-CGA
14	cA	811	CLA	C2A-CAA-CBA-CGA
20	cB	849	LMG	C38-C39-C40-C41
17	B	842	BCR	C7-C8-C9-C34
17	J	103	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
17	J	103	BCR	C37-C22-C23-C24
17	bB	842	BCR	C7-C8-C9-C34
17	bJ	103	BCR	C7-C8-C9-C34
17	bJ	103	BCR	C37-C22-C23-C24
17	cB	843	BCR	C7-C8-C9-C34
17	cJ	103	BCR	C7-C8-C9-C34
17	cJ	103	BCR	C37-C22-C23-C24
17	A	847	BCR	C21-C22-C23-C24
17	B	842	BCR	C7-C8-C9-C10
17	B	844	BCR	C17-C18-C19-C20
17	bA	847	BCR	C21-C22-C23-C24
17	bB	842	BCR	C7-C8-C9-C10
17	bB	844	BCR	C17-C18-C19-C20
17	cA	847	BCR	C21-C22-C23-C24
17	cB	843	BCR	C7-C8-C9-C10
17	cB	845	BCR	C17-C18-C19-C20
14	A	811	CLA	C1A-C2A-CAA-CBA
14	A	820	CLA	C1A-C2A-CAA-CBA
14	A	838	CLA	C1A-C2A-CAA-CBA
14	B	811	CLA	C1A-C2A-CAA-CBA
14	B	820	CLA	C1A-C2A-CAA-CBA
14	B	831	CLA	C1A-C2A-CAA-CBA
14	B	839	CLA	C1A-C2A-CAA-CBA
14	B	851	CLA	C1A-C2A-CAA-CBA
14	bA	811	CLA	C1A-C2A-CAA-CBA
14	bA	815	CLA	C1A-C2A-CAA-CBA
14	bA	820	CLA	C1A-C2A-CAA-CBA
14	bA	838	CLA	C1A-C2A-CAA-CBA
14	bB	811	CLA	C1A-C2A-CAA-CBA
14	bB	820	CLA	C1A-C2A-CAA-CBA
14	bB	831	CLA	C1A-C2A-CAA-CBA
14	bB	839	CLA	C1A-C2A-CAA-CBA
14	bB	851	CLA	C1A-C2A-CAA-CBA
14	cA	811	CLA	C1A-C2A-CAA-CBA
14	cA	815	CLA	C1A-C2A-CAA-CBA
14	cA	820	CLA	C1A-C2A-CAA-CBA
14	cA	838	CLA	C1A-C2A-CAA-CBA
14	cB	801	CLA	C1A-C2A-CAA-CBA
14	cB	812	CLA	C1A-C2A-CAA-CBA
14	cB	821	CLA	C1A-C2A-CAA-CBA
14	cB	832	CLA	C1A-C2A-CAA-CBA
14	cB	840	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	B	839	CLA	C16-C17-C18-C19
14	bB	839	CLA	C16-C17-C18-C19
14	cB	840	CLA	C16-C17-C18-C19
18	A	851	LHG	C3-O3-P-O5
18	bA	851	LHG	C3-O3-P-O5
18	cA	851	LHG	C3-O3-P-O5
14	B	821	CLA	C2C-C3C-CAC-CBC
14	bB	821	CLA	C2C-C3C-CAC-CBC
14	cB	822	CLA	C2C-C3C-CAC-CBC
14	B	803	CLA	CAD-CBD-CGD-O1D
14	B	812	CLA	CAD-CBD-CGD-O1D
14	B	828	CLA	CAD-CBD-CGD-O1D
14	bB	803	CLA	CAD-CBD-CGD-O1D
14	bB	812	CLA	CAD-CBD-CGD-O1D
14	bB	828	CLA	CAD-CBD-CGD-O1D
14	cB	804	CLA	CAD-CBD-CGD-O1D
14	cB	813	CLA	CAD-CBD-CGD-O1D
14	cB	829	CLA	CAD-CBD-CGD-O1D
14	bL	202	CLA	C10-C11-C12-C13
14	A	824	CLA	C4-C3-C5-C6
14	bA	824	CLA	C4-C3-C5-C6
14	cA	824	CLA	C4-C3-C5-C6
14	A	841	CLA	C11-C10-C8-C7
14	B	801	CLA	C12-C13-C15-C16
14	B	806	CLA	C12-C13-C15-C16
14	bA	841	CLA	C11-C10-C8-C7
14	bB	801	CLA	C12-C13-C15-C16
14	bB	806	CLA	C12-C13-C15-C16
14	cA	841	CLA	C11-C10-C8-C7
14	cB	802	CLA	C12-C13-C15-C16
14	cB	807	CLA	C12-C13-C15-C16
14	L	202	CLA	C10-C11-C12-C13
14	cL	203	CLA	C10-C11-C12-C13
14	A	839	CLA	C5-C6-C7-C8
14	B	806	CLA	C5-C6-C7-C8
14	bA	839	CLA	C5-C6-C7-C8
14	bB	806	CLA	C5-C6-C7-C8
14	cA	839	CLA	C5-C6-C7-C8
14	cB	807	CLA	C5-C6-C7-C8
14	cB	836	CLA	C2C-C3C-CAC-CBC
14	B	835	CLA	C2C-C3C-CAC-CBC
14	bB	835	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
14	B	831	CLA	C2-C3-C5-C6
14	bB	831	CLA	C2-C3-C5-C6
14	cB	832	CLA	C2-C3-C5-C6
18	A	851	LHG	C8-C7-O7-C5
18	bA	851	LHG	C8-C7-O7-C5
18	cA	851	LHG	C8-C7-O7-C5
14	A	837	CLA	C5-C6-C7-C8
14	bA	837	CLA	C5-C6-C7-C8
14	cA	837	CLA	C5-C6-C7-C8
14	A	837	CLA	C14-C13-C15-C16
14	A	852	CLA	C11-C10-C8-C9
14	bA	837	CLA	C14-C13-C15-C16
14	bA	852	CLA	C11-C10-C8-C9
14	cA	837	CLA	C14-C13-C15-C16
14	cA	852	CLA	C11-C10-C8-C9
17	A	849	BCR	C6-C7-C8-C9
17	cA	849	BCR	C6-C7-C8-C9
14	B	807	CLA	C16-C17-C18-C19
14	bB	807	CLA	C16-C17-C18-C19
14	bB	839	CLA	C16-C17-C18-C20
14	cB	808	CLA	C16-C17-C18-C19
14	cB	840	CLA	C16-C17-C18-C20
17	A	846	BCR	C11-C12-C13-C35
17	bA	846	BCR	C11-C12-C13-C35
17	cA	846	BCR	C11-C12-C13-C35
14	B	839	CLA	C16-C17-C18-C20
17	I	102	BCR	C20-C21-C22-C37
17	bI	102	BCR	C20-C21-C22-C37
17	cI	102	BCR	C20-C21-C22-C37
14	B	828	CLA	C10-C11-C12-C13
14	bB	828	CLA	C10-C11-C12-C13
14	cA	839	CLA	C8-C10-C11-C12
14	cB	829	CLA	C10-C11-C12-C13
14	A	839	CLA	C8-C10-C11-C12
14	bA	839	CLA	C8-C10-C11-C12
14	A	842	CLA	C2A-CAA-CBA-CGA
14	bA	842	CLA	C2A-CAA-CBA-CGA
14	cA	842	CLA	C2A-CAA-CBA-CGA
14	A	840	CLA	C2-C1-O2A-CGA
14	B	805	CLA	C2-C1-O2A-CGA
14	B	813	CLA	C2-C1-O2A-CGA
14	bA	840	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
14	bB	805	CLA	C2-C1-O2A-CGA
14	cA	840	CLA	C2-C1-O2A-CGA
14	cB	806	CLA	C2-C1-O2A-CGA
14	B	838	CLA	O1D-CGD-O2D-CED
14	bB	838	CLA	O1D-CGD-O2D-CED
14	cB	839	CLA	O1D-CGD-O2D-CED
14	cL	205	CLA	C8-C10-C11-C12
14	L	204	CLA	C8-C10-C11-C12
14	bL	204	CLA	C8-C10-C11-C12
17	A	845	BCR	C20-C21-C22-C23
17	A	849	BCR	C16-C17-C18-C19
17	F	202	BCR	C12-C13-C14-C15
17	bA	845	BCR	C20-C21-C22-C23
17	bA	849	BCR	C16-C17-C18-C19
17	bF	202	BCR	C12-C13-C14-C15
17	cA	845	BCR	C20-C21-C22-C23
17	cA	849	BCR	C16-C17-C18-C19
17	cF	202	BCR	C12-C13-C14-C15
18	A	850	LHG	C3-O3-P-O6
18	A	851	LHG	C4-O6-P-O3
18	bA	850	LHG	C3-O3-P-O6
18	bA	851	LHG	C4-O6-P-O3
18	cA	850	LHG	C3-O3-P-O6
18	cA	851	LHG	C4-O6-P-O3
14	A	832	CLA	C4-C3-C5-C6
14	bA	832	CLA	C4-C3-C5-C6
14	cA	832	CLA	C4-C3-C5-C6
14	A	829	CLA	C11-C10-C8-C7
14	L	204	CLA	C11-C10-C8-C7
14	bA	829	CLA	C11-C10-C8-C7
14	bL	204	CLA	C11-C10-C8-C7
14	cA	829	CLA	C11-C10-C8-C7
14	cL	205	CLA	C11-C10-C8-C7
14	bA	802	CLA	C10-C11-C12-C13
14	cB	828	CLA	C8-C10-C11-C12
13	A	801	CL0	C16-C17-C18-C20
13	bA	801	CL0	C16-C17-C18-C20
13	cA	801	CL0	C16-C17-C18-C20
14	A	802	CLA	C10-C11-C12-C13
14	bB	827	CLA	C8-C10-C11-C12
14	cA	802	CLA	C10-C11-C12-C13
14	B	827	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
14	A	839	CLA	O1A-CGA-O2A-C1
14	bA	839	CLA	O1A-CGA-O2A-C1
14	cA	839	CLA	O1A-CGA-O2A-C1
14	B	805	CLA	C4-C3-C5-C6
14	bB	805	CLA	C4-C3-C5-C6
14	cB	806	CLA	C4-C3-C5-C6
14	B	813	CLA	CBD-CGD-O2D-CED
14	bB	813	CLA	CBD-CGD-O2D-CED
14	A	815	CLA	CAA-CBA-CGA-O2A
14	bA	815	CLA	CAA-CBA-CGA-O2A
14	cA	815	CLA	CAA-CBA-CGA-O2A
14	B	802	CLA	C8-C10-C11-C12
14	bB	802	CLA	C8-C10-C11-C12
14	cB	803	CLA	C8-C10-C11-C12
17	bA	849	BCR	C6-C7-C8-C9
17	bF	202	BCR	C6-C7-C8-C9
17	cF	202	BCR	C6-C7-C8-C9
14	cB	814	CLA	CBD-CGD-O2D-CED
14	A	802	CLA	C2A-CAA-CBA-CGA
14	bA	802	CLA	C2A-CAA-CBA-CGA
14	cA	802	CLA	C2A-CAA-CBA-CGA
14	bA	841	CLA	C16-C17-C18-C20
14	cA	841	CLA	C16-C17-C18-C20
17	B	850	BCR	C9-C10-C11-C12
17	bB	850	BCR	C9-C10-C11-C12
17	cB	851	BCR	C9-C10-C11-C12
14	A	841	CLA	C16-C17-C18-C20
14	B	838	CLA	C3-C5-C6-C7
14	bB	838	CLA	C3-C5-C6-C7
14	cB	839	CLA	C3-C5-C6-C7
14	X	201	CLA	CAA-CBA-CGA-O1A
14	cX	201	CLA	CAA-CBA-CGA-O1A
14	bX	201	CLA	CAA-CBA-CGA-O1A
14	A	825	CLA	C2-C1-O2A-CGA
14	bA	825	CLA	C2-C1-O2A-CGA
14	bB	813	CLA	C2-C1-O2A-CGA
14	cA	825	CLA	C2-C1-O2A-CGA
14	cB	814	CLA	C2-C1-O2A-CGA
14	A	819	CLA	CAA-CBA-CGA-O1A
14	bA	819	CLA	CAA-CBA-CGA-O1A
14	cA	819	CLA	CAA-CBA-CGA-O1A
14	A	808	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
14	bA	808	CLA	C2A-CAA-CBA-CGA
14	cA	808	CLA	C2A-CAA-CBA-CGA
14	B	823	CLA	C3A-C2A-CAA-CBA
14	bB	823	CLA	C3A-C2A-CAA-CBA
14	cB	824	CLA	C3A-C2A-CAA-CBA
14	bA	821	CLA	CAA-CBA-CGA-O1A
14	cA	821	CLA	CAA-CBA-CGA-O1A
14	B	801	CLA	C16-C17-C18-C19
14	bB	801	CLA	C16-C17-C18-C19
14	cB	802	CLA	C16-C17-C18-C19
14	A	839	CLA	CBA-CGA-O2A-C1
14	bA	839	CLA	CBA-CGA-O2A-C1
14	bB	813	CLA	CBA-CGA-O2A-C1
14	cA	839	CLA	CBA-CGA-O2A-C1
14	A	821	CLA	CAA-CBA-CGA-O1A
14	B	811	CLA	CAA-CBA-CGA-O1A
14	A	829	CLA	C4-C3-C5-C6
14	bA	829	CLA	C4-C3-C5-C6
14	cA	829	CLA	C4-C3-C5-C6
14	bA	804	CLA	C5-C6-C7-C8
14	bL	203	CLA	C10-C11-C12-C13
14	cA	804	CLA	C5-C6-C7-C8
14	B	801	CLA	C14-C13-C15-C16
14	L	201	CLA	C11-C12-C13-C14
14	L	204	CLA	C11-C12-C13-C14
14	L	204	CLA	C14-C13-C15-C16
14	bB	801	CLA	C14-C13-C15-C16
14	bL	201	CLA	C11-C12-C13-C14
14	bL	204	CLA	C11-C12-C13-C14
14	bL	204	CLA	C14-C13-C15-C16
14	cB	802	CLA	C14-C13-C15-C16
14	cL	202	CLA	C11-C12-C13-C14
14	cL	205	CLA	C11-C12-C13-C14
14	cL	205	CLA	C14-C13-C15-C16
14	A	804	CLA	C5-C6-C7-C8
14	L	203	CLA	C10-C11-C12-C13
14	cL	204	CLA	C10-C11-C12-C13
14	A	842	CLA	CAA-CBA-CGA-O2A
14	bA	842	CLA	CAA-CBA-CGA-O2A
14	bB	811	CLA	CAA-CBA-CGA-O1A
14	cA	842	CLA	CAA-CBA-CGA-O2A
14	cB	812	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
14	B	813	CLA	CBA-CGA-O2A-C1
14	cB	814	CLA	CBA-CGA-O2A-C1
17	A	846	BCR	C35-C13-C14-C15
17	B	843	BCR	C20-C21-C22-C37
17	bA	846	BCR	C35-C13-C14-C15
17	bB	843	BCR	C20-C21-C22-C37
17	cA	846	BCR	C35-C13-C14-C15
17	cB	844	BCR	C20-C21-C22-C37
14	B	820	CLA	CAA-CBA-CGA-O1A
14	bB	820	CLA	CAA-CBA-CGA-O1A
14	cB	821	CLA	CAA-CBA-CGA-O1A
14	B	804	CLA	O2A-C1-C2-C3
14	bB	804	CLA	O2A-C1-C2-C3
14	cB	805	CLA	O2A-C1-C2-C3
18	bA	850	LHG	C9-C10-C11-C12
14	A	812	CLA	CAA-CBA-CGA-O1A
14	A	813	CLA	CAA-CBA-CGA-O1A
14	B	821	CLA	CAA-CBA-CGA-O1A
14	X	201	CLA	CAA-CBA-CGA-O2A
14	bA	812	CLA	CAA-CBA-CGA-O1A
14	bA	813	CLA	CAA-CBA-CGA-O1A
14	bX	201	CLA	CAA-CBA-CGA-O2A
14	cA	812	CLA	CAA-CBA-CGA-O1A
14	cA	813	CLA	CAA-CBA-CGA-O1A
14	cX	201	CLA	CAA-CBA-CGA-O2A
14	A	810	CLA	C1A-C2A-CAA-CBA
14	A	823	CLA	C1A-C2A-CAA-CBA
14	A	834	CLA	C1A-C2A-CAA-CBA
14	bA	810	CLA	C1A-C2A-CAA-CBA
14	bA	823	CLA	C1A-C2A-CAA-CBA
14	bA	834	CLA	C1A-C2A-CAA-CBA
14	cA	810	CLA	C1A-C2A-CAA-CBA
14	cA	823	CLA	C1A-C2A-CAA-CBA
14	cA	834	CLA	C1A-C2A-CAA-CBA
14	cB	822	CLA	C4C-C3C-CAC-CBC
18	A	850	LHG	C9-C10-C11-C12
18	cA	850	LHG	C9-C10-C11-C12
14	B	805	CLA	C6-C7-C8-C10
14	L	203	CLA	C11-C10-C8-C7
14	bB	805	CLA	C6-C7-C8-C10
14	bL	203	CLA	C11-C10-C8-C7
14	cB	806	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
14	cL	204	CLA	C11-C10-C8-C7
14	A	812	CLA	CAA-CBA-CGA-O2A
14	A	821	CLA	CAA-CBA-CGA-O2A
14	bA	812	CLA	CAA-CBA-CGA-O2A
14	bA	821	CLA	CAA-CBA-CGA-O2A
14	bB	821	CLA	CAA-CBA-CGA-O1A
14	cA	812	CLA	CAA-CBA-CGA-O2A
14	cA	821	CLA	CAA-CBA-CGA-O2A
14	cB	822	CLA	CAA-CBA-CGA-O1A
17	B	841	BCR	C19-C20-C21-C22
17	bB	841	BCR	C19-C20-C21-C22
17	cB	842	BCR	C19-C20-C21-C22
14	A	842	CLA	CAA-CBA-CGA-O1A
14	bA	842	CLA	CAA-CBA-CGA-O1A
14	cA	842	CLA	CAA-CBA-CGA-O1A
14	B	821	CLA	C4C-C3C-CAC-CBC
14	bB	821	CLA	C4C-C3C-CAC-CBC
14	A	812	CLA	C2A-CAA-CBA-CGA
14	bA	812	CLA	C2A-CAA-CBA-CGA
14	cA	812	CLA	C2A-CAA-CBA-CGA
14	A	813	CLA	CAA-CBA-CGA-O2A
14	A	819	CLA	CAA-CBA-CGA-O2A
14	B	811	CLA	CAA-CBA-CGA-O2A
14	B	821	CLA	CAA-CBA-CGA-O2A
14	J	101	CLA	CAA-CBA-CGA-O1A
14	bA	819	CLA	CAA-CBA-CGA-O2A
14	bB	811	CLA	CAA-CBA-CGA-O2A
14	bB	821	CLA	CAA-CBA-CGA-O2A
14	bJ	101	CLA	CAA-CBA-CGA-O1A
14	cA	813	CLA	CAA-CBA-CGA-O2A
14	cA	819	CLA	CAA-CBA-CGA-O2A
14	cB	812	CLA	CAA-CBA-CGA-O2A
14	cB	822	CLA	CAA-CBA-CGA-O2A
14	cJ	101	CLA	CAA-CBA-CGA-O1A
14	A	837	CLA	C16-C17-C18-C19
14	bA	837	CLA	C16-C17-C18-C19
14	cA	837	CLA	C16-C17-C18-C19
14	A	805	CLA	C4-C3-C5-C6
14	bA	805	CLA	C4-C3-C5-C6
14	cA	805	CLA	C4-C3-C5-C6
14	A	832	CLA	C2-C3-C5-C6
14	cA	832	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	A	815	CLA	CAA-CBA-CGA-O1A
14	bA	813	CLA	CAA-CBA-CGA-O2A
17	A	846	BCR	C12-C13-C14-C15
17	bA	846	BCR	C12-C13-C14-C15
17	cA	846	BCR	C12-C13-C14-C15
14	A	834	CLA	CAA-CBA-CGA-O2A
14	bA	815	CLA	CAA-CBA-CGA-O1A
14	bA	834	CLA	CAA-CBA-CGA-O2A
14	cA	815	CLA	CAA-CBA-CGA-O1A
14	cA	834	CLA	CAA-CBA-CGA-O2A
14	bA	840	CLA	C10-C11-C12-C13
14	J	102	CLA	CAA-CBA-CGA-O1A
14	cJ	102	CLA	CAA-CBA-CGA-O1A
17	F	202	BCR	C6-C7-C8-C9
17	J	103	BCR	C22-C23-C24-C25
17	bJ	103	BCR	C22-C23-C24-C25
17	cJ	103	BCR	C22-C23-C24-C25
14	A	840	CLA	C10-C11-C12-C13
14	A	827	CLA	C10-C11-C12-C13
14	bA	827	CLA	C10-C11-C12-C13
14	cA	827	CLA	C10-C11-C12-C13
14	cA	840	CLA	C10-C11-C12-C13
14	A	829	CLA	C2-C3-C5-C6
14	B	805	CLA	C2-C3-C5-C6
14	bA	829	CLA	C2-C3-C5-C6
14	bA	832	CLA	C2-C3-C5-C6
14	bB	805	CLA	C2-C3-C5-C6
14	cA	829	CLA	C2-C3-C5-C6
14	cB	806	CLA	C2-C3-C5-C6
14	bB	813	CLA	O1A-CGA-O2A-C1
14	A	807	CLA	CAA-CBA-CGA-O1A
14	bA	807	CLA	CAA-CBA-CGA-O1A
14	bJ	102	CLA	CAA-CBA-CGA-O1A
14	cA	807	CLA	CAA-CBA-CGA-O1A
14	cA	810	CLA	CAA-CBA-CGA-O2A
14	B	838	CLA	C6-C7-C8-C9
14	bB	838	CLA	C6-C7-C8-C9
14	cB	839	CLA	C6-C7-C8-C9
14	B	819	CLA	C2-C1-O2A-CGA
14	bB	819	CLA	C2-C1-O2A-CGA
14	cB	820	CLA	C2-C1-O2A-CGA
14	cB	821	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
15	bA	843	PQN	C20-C21-C22-C23
14	B	813	CLA	O1A-CGA-O2A-C1
14	cB	814	CLA	O1A-CGA-O2A-C1
14	B	820	CLA	C2C-C3C-CAC-CBC
14	A	807	CLA	CAA-CBA-CGA-O2A
14	A	810	CLA	CAA-CBA-CGA-O2A
14	bA	807	CLA	CAA-CBA-CGA-O2A
14	bA	810	CLA	CAA-CBA-CGA-O2A
14	cA	807	CLA	CAA-CBA-CGA-O2A
14	bB	820	CLA	C2C-C3C-CAC-CBC
15	A	843	PQN	C20-C21-C22-C23
15	cA	843	PQN	C20-C21-C22-C23
14	A	813	CLA	C2A-CAA-CBA-CGA
14	bA	813	CLA	C2A-CAA-CBA-CGA
14	cA	813	CLA	C2A-CAA-CBA-CGA
17	I	102	BCR	C23-C24-C25-C30
17	J	103	BCR	C23-C24-C25-C30
17	bI	102	BCR	C23-C24-C25-C30
17	bJ	103	BCR	C23-C24-C25-C30
17	cI	102	BCR	C23-C24-C25-C30
17	cJ	103	BCR	C23-C24-C25-C30
14	B	803	CLA	CBD-CGD-O2D-CED
14	L	201	CLA	C5-C6-C7-C8
14	bL	201	CLA	C5-C6-C7-C8
14	cL	202	CLA	C5-C6-C7-C8
14	A	824	CLA	C2-C3-C5-C6
14	bA	824	CLA	C2-C3-C5-C6
14	cA	824	CLA	C2-C3-C5-C6
14	bB	803	CLA	CBD-CGD-O2D-CED
14	J	101	CLA	CAA-CBA-CGA-O2A
14	J	102	CLA	CAA-CBA-CGA-O2A
14	bJ	101	CLA	CAA-CBA-CGA-O2A
14	cJ	101	CLA	CAA-CBA-CGA-O2A
14	cJ	102	CLA	CAA-CBA-CGA-O2A
18	A	850	LHG	C12-C13-C14-C15
18	bA	850	LHG	C12-C13-C14-C15
14	B	831	CLA	C4C-C3C-CAC-CBC
14	bB	831	CLA	C4C-C3C-CAC-CBC
14	cB	832	CLA	C4C-C3C-CAC-CBC
18	cA	850	LHG	C12-C13-C14-C15
14	A	835	CLA	CAA-CBA-CGA-O2A
14	B	829	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
14	bA	835	CLA	CAA-CBA-CGA-O2A
14	bB	829	CLA	CAA-CBA-CGA-O2A
14	bJ	102	CLA	CAA-CBA-CGA-O2A
14	cA	835	CLA	CAA-CBA-CGA-O2A
14	cB	830	CLA	CAA-CBA-CGA-O2A
14	cB	804	CLA	CBD-CGD-O2D-CED
14	bB	813	CLA	O1D-CGD-O2D-CED
14	cB	814	CLA	O1D-CGD-O2D-CED
14	B	829	CLA	CAA-CBA-CGA-O1A
14	bB	829	CLA	CAA-CBA-CGA-O1A
14	cB	830	CLA	CAA-CBA-CGA-O1A
14	A	831	CLA	C2A-CAA-CBA-CGA
14	bA	831	CLA	C2A-CAA-CBA-CGA
14	cA	831	CLA	C2A-CAA-CBA-CGA
14	B	802	CLA	CAA-CBA-CGA-O2A
14	bB	802	CLA	CAA-CBA-CGA-O2A
14	cB	803	CLA	CAA-CBA-CGA-O2A
14	B	813	CLA	O1D-CGD-O2D-CED
14	cB	828	CLA	O1D-CGD-O2D-CED
14	A	816	CLA	CAA-CBA-CGA-O2A
14	B	820	CLA	CAA-CBA-CGA-O2A
14	bA	816	CLA	CAA-CBA-CGA-O2A
14	bB	820	CLA	CAA-CBA-CGA-O2A
14	cA	816	CLA	CAA-CBA-CGA-O2A
14	cB	821	CLA	CAA-CBA-CGA-O2A
14	L	202	CLA	C4-C3-C5-C6
14	bL	202	CLA	C4-C3-C5-C6
14	cL	203	CLA	C4-C3-C5-C6
20	B	848	LMG	C15-C16-C17-C18
20	cB	849	LMG	C15-C16-C17-C18
14	B	807	CLA	C6-C7-C8-C10
14	L	201	CLA	C11-C12-C13-C15
14	bB	807	CLA	C6-C7-C8-C10
14	bL	201	CLA	C11-C12-C13-C15
14	cB	808	CLA	C6-C7-C8-C10
14	cL	202	CLA	C11-C12-C13-C15
20	bB	848	LMG	C15-C16-C17-C18
14	B	827	CLA	O1D-CGD-O2D-CED
18	A	851	LHG	O7-C7-C8-C9
18	bA	851	LHG	O7-C7-C8-C9
18	cA	851	LHG	O7-C7-C8-C9
14	A	817	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	bA	817	CLA	CBD-CGD-O2D-CED
14	cA	817	CLA	CBD-CGD-O2D-CED
14	bA	817	CLA	C6-C7-C8-C9
14	bB	827	CLA	O1D-CGD-O2D-CED
14	A	834	CLA	CAA-CBA-CGA-O1A
14	bA	834	CLA	CAA-CBA-CGA-O1A
14	cA	834	CLA	CAA-CBA-CGA-O1A
14	A	817	CLA	C6-C7-C8-C9
14	cA	817	CLA	C6-C7-C8-C9
14	A	835	CLA	CAA-CBA-CGA-O1A
14	B	849	CLA	CAA-CBA-CGA-O2A
14	bA	835	CLA	CAA-CBA-CGA-O1A
14	cA	835	CLA	CAA-CBA-CGA-O1A
17	B	843	BCR	C35-C13-C14-C15
17	B	850	BCR	C16-C17-C18-C36
17	M	101	BCR	C11-C10-C9-C34
17	bB	843	BCR	C35-C13-C14-C15
17	bB	850	BCR	C16-C17-C18-C36
17	cB	844	BCR	C35-C13-C14-C15
17	cB	851	BCR	C16-C17-C18-C36
17	cM	101	BCR	C11-C10-C9-C34
14	B	819	CLA	CAA-CBA-CGA-O2A
14	bB	819	CLA	CAA-CBA-CGA-O2A
14	cB	820	CLA	CAA-CBA-CGA-O2A
14	A	833	CLA	C4-C3-C5-C6
14	bA	833	CLA	C4-C3-C5-C6
14	cA	833	CLA	C4-C3-C5-C6
14	A	838	CLA	CAA-CBA-CGA-O2A
14	B	849	CLA	CAA-CBA-CGA-O1A
14	bA	838	CLA	CAA-CBA-CGA-O2A
14	bB	849	CLA	CAA-CBA-CGA-O1A
14	bB	849	CLA	CAA-CBA-CGA-O2A
14	cA	838	CLA	CAA-CBA-CGA-O2A
14	cB	850	CLA	CAA-CBA-CGA-O1A
14	cB	850	CLA	CAA-CBA-CGA-O2A
14	A	805	CLA	C2-C3-C5-C6
14	bA	805	CLA	C2-C3-C5-C6
14	cA	805	CLA	C2-C3-C5-C6
14	B	837	CLA	C2-C1-O2A-CGA
14	B	806	CLA	CAA-CBA-CGA-O2A
14	bB	806	CLA	CAA-CBA-CGA-O2A
14	A	806	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
14	A	837	CLA	C11-C12-C13-C14
14	A	841	CLA	C11-C10-C8-C9
14	B	806	CLA	C14-C13-C15-C16
14	bA	806	CLA	C6-C7-C8-C9
14	bA	841	CLA	C11-C10-C8-C9
14	bB	806	CLA	C14-C13-C15-C16
14	cA	806	CLA	C6-C7-C8-C9
14	cA	837	CLA	C11-C12-C13-C14
14	cA	841	CLA	C11-C10-C8-C9
14	cB	807	CLA	C14-C13-C15-C16
14	cB	838	CLA	C2-C1-O2A-CGA
14	A	822	CLA	CAA-CBA-CGA-O2A
14	B	814	CLA	CAA-CBA-CGA-O1A
14	B	836	CLA	CAA-CBA-CGA-O2A
14	bB	814	CLA	CAA-CBA-CGA-O1A
14	bB	836	CLA	CAA-CBA-CGA-O2A
14	cA	810	CLA	CAA-CBA-CGA-O1A
14	cB	815	CLA	CAA-CBA-CGA-O1A
14	bB	837	CLA	C2-C1-O2A-CGA
14	B	812	CLA	C3A-C2A-CAA-CBA
14	bB	812	CLA	C3A-C2A-CAA-CBA
14	cB	813	CLA	C3A-C2A-CAA-CBA
20	B	848	LMG	O10-C28-O8-C9
20	bB	848	LMG	O10-C28-O8-C9
20	cB	849	LMG	O10-C28-O8-C9
14	cB	807	CLA	CAA-CBA-CGA-O2A
14	A	810	CLA	CAA-CBA-CGA-O1A
14	A	816	CLA	CAA-CBA-CGA-O1A
14	A	820	CLA	CAA-CBA-CGA-O2A
14	B	851	CLA	CAA-CBA-CGA-O2A
14	bA	810	CLA	CAA-CBA-CGA-O1A
14	bA	816	CLA	CAA-CBA-CGA-O1A
14	bA	820	CLA	CAA-CBA-CGA-O2A
14	bA	822	CLA	CAA-CBA-CGA-O2A
14	bB	851	CLA	CAA-CBA-CGA-O2A
14	cA	820	CLA	CAA-CBA-CGA-O2A
14	cA	822	CLA	CAA-CBA-CGA-O2A
14	cB	801	CLA	CAA-CBA-CGA-O2A
14	cB	837	CLA	CAA-CBA-CGA-O2A
14	A	804	CLA	CAD-CBD-CGD-O2D
14	A	805	CLA	CAD-CBD-CGD-O2D
14	A	809	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	A	821	CLA	CAD-CBD-CGD-O2D
14	A	830	CLA	CAD-CBD-CGD-O2D
14	B	831	CLA	CAD-CBD-CGD-O2D
14	bA	804	CLA	CAD-CBD-CGD-O2D
14	bA	805	CLA	CAD-CBD-CGD-O2D
14	bA	809	CLA	CAD-CBD-CGD-O2D
14	bA	821	CLA	CAD-CBD-CGD-O2D
14	bA	830	CLA	CAD-CBD-CGD-O2D
14	bB	831	CLA	CAD-CBD-CGD-O2D
14	cA	804	CLA	CAD-CBD-CGD-O2D
14	cA	805	CLA	CAD-CBD-CGD-O2D
14	cA	809	CLA	CAD-CBD-CGD-O2D
14	cA	821	CLA	CAD-CBD-CGD-O2D
14	cA	830	CLA	CAD-CBD-CGD-O2D
14	cB	801	CLA	CAD-CBD-CGD-O2D
14	cB	832	CLA	CAD-CBD-CGD-O2D
14	A	841	CLA	C8-C10-C11-C12
14	bA	839	CLA	C15-C16-C17-C18
14	bA	841	CLA	C8-C10-C11-C12
14	cA	839	CLA	C15-C16-C17-C18
14	A	839	CLA	C15-C16-C17-C18
14	cA	841	CLA	C8-C10-C11-C12
14	cA	816	CLA	CAA-CBA-CGA-O1A
14	A	806	CLA	CAA-CBA-CGA-O2A
14	bA	806	CLA	CAA-CBA-CGA-O2A
14	cA	806	CLA	CAA-CBA-CGA-O2A
14	cB	816	CLA	CAA-CBA-CGA-O2A
14	B	803	CLA	O1D-CGD-O2D-CED
14	cB	804	CLA	O1D-CGD-O2D-CED
14	B	822	CLA	CAA-CBA-CGA-O2A
14	bB	822	CLA	CAA-CBA-CGA-O2A
14	cB	823	CLA	CAA-CBA-CGA-O2A
14	B	809	CLA	C13-C15-C16-C17
14	bB	815	CLA	CAA-CBA-CGA-O2A
18	bA	850	LHG	O8-C23-C24-C25
18	cA	850	LHG	O8-C23-C24-C25
20	B	848	LMG	O7-C10-C11-C12
17	B	846	BCR	C21-C22-C23-C24
17	J	103	BCR	C7-C8-C9-C10
17	bB	846	BCR	C21-C22-C23-C24
17	bJ	103	BCR	C7-C8-C9-C10
17	cB	847	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
17	cJ	103	BCR	C7-C8-C9-C10
14	cA	802	CLA	C3-C5-C6-C7
14	B	815	CLA	CAA-CBA-CGA-O2A
18	A	850	LHG	O8-C23-C24-C25
20	bB	848	LMG	O7-C10-C11-C12
20	cB	849	LMG	O7-C10-C11-C12
17	cB	847	BCR	C18-C19-C20-C21
14	A	824	CLA	O2A-C1-C2-C3
14	B	831	CLA	O2A-C1-C2-C3
14	bA	824	CLA	O2A-C1-C2-C3
14	bB	831	CLA	O2A-C1-C2-C3
14	cA	824	CLA	O2A-C1-C2-C3
14	cB	832	CLA	O2A-C1-C2-C3
14	B	802	CLA	C2A-CAA-CBA-CGA
14	bB	802	CLA	C2A-CAA-CBA-CGA
14	cB	803	CLA	C2A-CAA-CBA-CGA
14	A	802	CLA	C3-C5-C6-C7
14	bA	802	CLA	C3-C5-C6-C7
14	A	838	CLA	CAA-CBA-CGA-O1A
14	B	822	CLA	CAA-CBA-CGA-O1A
14	bA	838	CLA	CAA-CBA-CGA-O1A
14	bB	822	CLA	CAA-CBA-CGA-O1A
14	cA	838	CLA	CAA-CBA-CGA-O1A
14	cB	823	CLA	CAA-CBA-CGA-O1A
14	bB	803	CLA	O1D-CGD-O2D-CED
14	bB	809	CLA	C13-C15-C16-C17
14	cB	810	CLA	C13-C15-C16-C17
14	A	826	CLA	CHA-CBD-CGD-O1D
14	A	833	CLA	CHA-CBD-CGD-O1D
14	B	804	CLA	CHA-CBD-CGD-O2D
14	B	814	CLA	CHA-CBD-CGD-O1D
14	B	820	CLA	CHA-CBD-CGD-O2D
14	B	836	CLA	CHA-CBD-CGD-O1D
14	B	836	CLA	CHA-CBD-CGD-O2D
14	L	204	CLA	CHA-CBD-CGD-O1D
14	bA	826	CLA	CHA-CBD-CGD-O1D
14	bA	833	CLA	CHA-CBD-CGD-O1D
14	bB	804	CLA	CHA-CBD-CGD-O2D
14	bB	814	CLA	CHA-CBD-CGD-O1D
14	bB	820	CLA	CHA-CBD-CGD-O2D
14	bB	836	CLA	CHA-CBD-CGD-O1D
14	bB	836	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	bL	204	CLA	CHA-CBD-CGD-O1D
14	cA	826	CLA	CHA-CBD-CGD-O1D
14	cA	833	CLA	CHA-CBD-CGD-O1D
14	cB	805	CLA	CHA-CBD-CGD-O1D
14	cB	805	CLA	CHA-CBD-CGD-O2D
14	cB	815	CLA	CHA-CBD-CGD-O1D
14	cB	821	CLA	CHA-CBD-CGD-O2D
14	cB	837	CLA	CHA-CBD-CGD-O1D
14	cB	837	CLA	CHA-CBD-CGD-O2D
14	cL	205	CLA	CHA-CBD-CGD-O1D
14	A	822	CLA	CAA-CBA-CGA-O1A
14	B	836	CLA	CAA-CBA-CGA-O1A
14	B	851	CLA	CAA-CBA-CGA-O1A
14	bA	822	CLA	CAA-CBA-CGA-O1A
14	bB	836	CLA	CAA-CBA-CGA-O1A
14	bB	851	CLA	CAA-CBA-CGA-O1A
14	cB	801	CLA	CAA-CBA-CGA-O1A
14	cB	837	CLA	CAA-CBA-CGA-O1A
14	A	817	CLA	CAA-CBA-CGA-O2A
14	bA	817	CLA	CAA-CBA-CGA-O2A
14	cA	817	CLA	CAA-CBA-CGA-O2A
17	B	843	BCR	C20-C21-C22-C23
17	bB	843	BCR	C20-C21-C22-C23
17	cB	844	BCR	C20-C21-C22-C23
14	bA	820	CLA	CAA-CBA-CGA-O1A
14	cA	822	CLA	CAA-CBA-CGA-O1A
14	B	812	CLA	CAA-CBA-CGA-O2A
14	bB	812	CLA	CAA-CBA-CGA-O2A
14	cB	813	CLA	CAA-CBA-CGA-O2A
14	A	820	CLA	CAA-CBA-CGA-O1A
14	cA	820	CLA	CAA-CBA-CGA-O1A
14	A	824	CLA	CAA-CBA-CGA-O2A
14	bA	824	CLA	CAA-CBA-CGA-O2A
14	cA	824	CLA	CAA-CBA-CGA-O2A
14	bB	816	CLA	C2A-CAA-CBA-CGA
14	cB	817	CLA	C2A-CAA-CBA-CGA
14	B	810	CLA	CAA-CBA-CGA-O2A
14	B	814	CLA	CAA-CBA-CGA-O2A
14	bB	810	CLA	CAA-CBA-CGA-O2A
14	bB	814	CLA	CAA-CBA-CGA-O2A
14	cB	811	CLA	CAA-CBA-CGA-O2A
14	cB	815	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
20	B	848	LMG	C29-C28-O8-C9
20	bB	848	LMG	C29-C28-O8-C9
20	cB	849	LMG	C29-C28-O8-C9
14	B	825	CLA	C6-C7-C8-C9
14	bB	825	CLA	C6-C7-C8-C9
14	cB	826	CLA	C6-C7-C8-C9
14	bA	837	CLA	C11-C12-C13-C14
14	A	803	CLA	C2B-C3B-CAB-CBB
14	A	809	CLA	C2B-C3B-CAB-CBB
14	A	815	CLA	C2B-C3B-CAB-CBB
14	A	816	CLA	C2B-C3B-CAB-CBB
14	A	831	CLA	C2B-C3B-CAB-CBB
14	A	842	CLA	C2B-C3B-CAB-CBB
14	B	820	CLA	C2B-C3B-CAB-CBB
14	B	821	CLA	C2B-C3B-CAB-CBB
14	B	822	CLA	C2B-C3B-CAB-CBB
14	B	830	CLA	C2B-C3B-CAB-CBB
14	B	836	CLA	C2B-C3B-CAB-CBB
14	bA	803	CLA	C2B-C3B-CAB-CBB
14	bA	809	CLA	C2B-C3B-CAB-CBB
14	bA	815	CLA	C2B-C3B-CAB-CBB
14	bA	816	CLA	C2B-C3B-CAB-CBB
14	bA	831	CLA	C2B-C3B-CAB-CBB
14	bA	842	CLA	C2B-C3B-CAB-CBB
14	bB	820	CLA	C2B-C3B-CAB-CBB
14	bB	821	CLA	C2B-C3B-CAB-CBB
14	bB	822	CLA	C2B-C3B-CAB-CBB
14	bB	830	CLA	C2B-C3B-CAB-CBB
14	bB	836	CLA	C2B-C3B-CAB-CBB
14	cA	803	CLA	C2B-C3B-CAB-CBB
14	cA	809	CLA	C2B-C3B-CAB-CBB
14	cA	815	CLA	C2B-C3B-CAB-CBB
14	cA	816	CLA	C2B-C3B-CAB-CBB
14	cA	831	CLA	C2B-C3B-CAB-CBB
14	cA	842	CLA	C2B-C3B-CAB-CBB
14	cB	821	CLA	C2B-C3B-CAB-CBB
14	cB	822	CLA	C2B-C3B-CAB-CBB
14	cB	823	CLA	C2B-C3B-CAB-CBB
14	cB	831	CLA	C2B-C3B-CAB-CBB
14	cB	837	CLA	C2B-C3B-CAB-CBB
14	A	809	CLA	CAA-CBA-CGA-O2A
14	bA	809	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
14	cA	809	CLA	CAA-CBA-CGA-O2A
14	B	816	CLA	C2A-CAA-CBA-CGA
14	bA	817	CLA	O1D-CGD-O2D-CED
14	A	804	CLA	CAA-CBA-CGA-O2A
14	bA	804	CLA	CAA-CBA-CGA-O2A
14	cA	804	CLA	CAA-CBA-CGA-O2A
14	B	806	CLA	CAA-CBA-CGA-O1A
14	cB	807	CLA	CAA-CBA-CGA-O1A
20	B	848	LMG	O9-C10-C11-C12
20	bB	848	LMG	O9-C10-C11-C12
20	cB	849	LMG	O9-C10-C11-C12
17	B	846	BCR	C11-C12-C13-C14
17	B	850	BCR	C17-C18-C19-C20
17	bB	846	BCR	C11-C12-C13-C14
17	bB	850	BCR	C17-C18-C19-C20
17	cB	847	BCR	C11-C12-C13-C14
17	cB	851	BCR	C17-C18-C19-C20
14	A	817	CLA	O1D-CGD-O2D-CED
14	cA	817	CLA	O1D-CGD-O2D-CED
14	A	819	CLA	C1A-C2A-CAA-CBA
14	B	812	CLA	C1A-C2A-CAA-CBA
14	B	823	CLA	C1A-C2A-CAA-CBA
14	B	834	CLA	C1A-C2A-CAA-CBA
14	L	204	CLA	C1A-C2A-CAA-CBA
14	bA	819	CLA	C1A-C2A-CAA-CBA
14	bB	812	CLA	C1A-C2A-CAA-CBA
14	bB	823	CLA	C1A-C2A-CAA-CBA
14	bB	834	CLA	C1A-C2A-CAA-CBA
14	bL	204	CLA	C1A-C2A-CAA-CBA
14	cA	819	CLA	C1A-C2A-CAA-CBA
14	cB	813	CLA	C1A-C2A-CAA-CBA
14	cB	824	CLA	C1A-C2A-CAA-CBA
14	cB	835	CLA	C1A-C2A-CAA-CBA
14	cL	205	CLA	C1A-C2A-CAA-CBA
14	bB	806	CLA	CAA-CBA-CGA-O1A
14	L	201	CLA	C15-C16-C17-C18
14	bL	201	CLA	C15-C16-C17-C18
14	cL	202	CLA	C15-C16-C17-C18
14	B	812	CLA	CAA-CBA-CGA-O1A
14	B	819	CLA	CAA-CBA-CGA-O1A
14	bB	812	CLA	CAA-CBA-CGA-O1A
14	cB	813	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
18	A	850	LHG	O10-C23-C24-C25
18	bA	850	LHG	O10-C23-C24-C25
18	cA	850	LHG	O10-C23-C24-C25
14	bA	817	CLA	C5-C6-C7-C8
14	A	817	CLA	C5-C6-C7-C8
14	bB	819	CLA	CAA-CBA-CGA-O1A
14	cB	820	CLA	CAA-CBA-CGA-O1A
17	I	101	BCR	C6-C7-C8-C9
17	bI	101	BCR	C6-C7-C8-C9
17	cI	101	BCR	C6-C7-C8-C9
14	bA	803	CLA	CAA-CBA-CGA-O2A
14	cA	803	CLA	CAA-CBA-CGA-O2A
14	cA	817	CLA	C5-C6-C7-C8
14	B	819	CLA	C4B-C3B-CAB-CBB
14	B	825	CLA	C4B-C3B-CAB-CBB
14	bA	813	CLA	C4B-C3B-CAB-CBB
14	bB	819	CLA	C4B-C3B-CAB-CBB
14	cA	813	CLA	C4B-C3B-CAB-CBB
14	cB	820	CLA	C4B-C3B-CAB-CBB
18	A	850	LHG	C3-O3-P-O5
18	bA	850	LHG	C3-O3-P-O5
18	cA	850	LHG	C3-O3-P-O5
14	A	817	CLA	CAA-CBA-CGA-O1A
14	bA	817	CLA	CAA-CBA-CGA-O1A
14	cA	817	CLA	CAA-CBA-CGA-O1A
18	bA	851	LHG	O9-C7-C8-C9
14	A	803	CLA	CAA-CBA-CGA-O2A
17	A	846	BCR	C1-C6-C7-C8
17	A	846	BCR	C5-C6-C7-C8
17	bA	846	BCR	C1-C6-C7-C8
17	bA	846	BCR	C5-C6-C7-C8
17	cA	846	BCR	C1-C6-C7-C8
17	cA	846	BCR	C5-C6-C7-C8
14	cA	824	CLA	CAA-CBA-CGA-O1A
18	A	851	LHG	O9-C7-C8-C9
18	cA	851	LHG	O9-C7-C8-C9
14	A	823	CLA	CAA-CBA-CGA-O2A
14	bA	823	CLA	CAA-CBA-CGA-O2A
14	cA	823	CLA	CAA-CBA-CGA-O2A
14	A	837	CLA	C16-C17-C18-C20
14	B	801	CLA	C16-C17-C18-C20
14	bA	837	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
14	bB	801	CLA	C16-C17-C18-C20
14	cA	837	CLA	C16-C17-C18-C20
14	cB	802	CLA	C16-C17-C18-C20
17	B	846	BCR	C18-C19-C20-C21
17	bB	846	BCR	C18-C19-C20-C21
14	A	824	CLA	CAA-CBA-CGA-O1A
14	B	815	CLA	CAA-CBA-CGA-O1A
14	bA	824	CLA	CAA-CBA-CGA-O1A
14	bB	815	CLA	CAA-CBA-CGA-O1A
14	cB	816	CLA	CAA-CBA-CGA-O1A
14	B	810	CLA	CAA-CBA-CGA-O1A
14	bB	810	CLA	CAA-CBA-CGA-O1A
14	cB	811	CLA	CAA-CBA-CGA-O1A
14	A	831	CLA	CAA-CBA-CGA-O2A
14	A	806	CLA	CAA-CBA-CGA-O1A
14	bA	806	CLA	CAA-CBA-CGA-O1A
14	B	803	CLA	C4-C3-C5-C6
14	bB	803	CLA	C4-C3-C5-C6
14	cB	804	CLA	C4-C3-C5-C6
14	B	820	CLA	C4C-C3C-CAC-CBC
14	A	809	CLA	CAA-CBA-CGA-O1A
14	bA	809	CLA	CAA-CBA-CGA-O1A
14	cA	809	CLA	CAA-CBA-CGA-O1A
14	A	813	CLA	CAD-CBD-CGD-O1D
14	A	826	CLA	CAD-CBD-CGD-O1D
14	B	805	CLA	CAD-CBD-CGD-O1D
14	B	825	CLA	CAD-CBD-CGD-O1D
14	bA	813	CLA	CAD-CBD-CGD-O1D
14	bA	826	CLA	CAD-CBD-CGD-O1D
14	bB	805	CLA	CAD-CBD-CGD-O1D
14	bB	825	CLA	CAD-CBD-CGD-O1D
14	cA	813	CLA	CAD-CBD-CGD-O1D
14	cA	826	CLA	CAD-CBD-CGD-O1D
14	cB	806	CLA	CAD-CBD-CGD-O1D
14	cB	826	CLA	CAD-CBD-CGD-O1D
14	cA	806	CLA	CAA-CBA-CGA-O1A
14	A	841	CLA	CAA-CBA-CGA-O2A
14	bA	831	CLA	CAA-CBA-CGA-O2A
14	bA	841	CLA	CAA-CBA-CGA-O2A
14	cA	831	CLA	CAA-CBA-CGA-O2A
14	cA	841	CLA	CAA-CBA-CGA-O2A
14	bB	820	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
14	cB	821	CLA	C4C-C3C-CAC-CBC
14	A	840	CLA	CAA-CBA-CGA-O2A
14	B	807	CLA	CAA-CBA-CGA-O2A
14	bA	840	CLA	CAA-CBA-CGA-O2A
14	bB	807	CLA	CAA-CBA-CGA-O2A
14	cA	840	CLA	CAA-CBA-CGA-O2A
14	cB	808	CLA	CAA-CBA-CGA-O2A
14	A	837	CLA	C4-C3-C5-C6
14	bA	837	CLA	C4-C3-C5-C6
14	cA	837	CLA	C4-C3-C5-C6
13	A	801	CL0	C12-C13-C15-C16
13	bA	801	CL0	C12-C13-C15-C16
13	cA	801	CL0	C12-C13-C15-C16
14	A	837	CLA	C12-C13-C15-C16
14	A	841	CLA	C3A-C2A-CAA-CBA
14	A	841	CLA	C11-C12-C13-C15
14	B	802	CLA	C11-C12-C13-C15
14	L	204	CLA	C11-C12-C13-C15
14	bA	837	CLA	C12-C13-C15-C16
14	bA	841	CLA	C3A-C2A-CAA-CBA
14	bA	841	CLA	C11-C12-C13-C15
14	bB	802	CLA	C11-C12-C13-C15
14	bL	204	CLA	C11-C12-C13-C15
14	cA	837	CLA	C12-C13-C15-C16
14	cA	841	CLA	C3A-C2A-CAA-CBA
14	cA	841	CLA	C11-C12-C13-C15
14	cB	803	CLA	C11-C12-C13-C15
14	cL	205	CLA	C11-C12-C13-C15
14	A	823	CLA	CAA-CBA-CGA-O1A
14	bA	823	CLA	CAA-CBA-CGA-O1A
14	cA	823	CLA	CAA-CBA-CGA-O1A
13	A	801	CL0	CAA-CBA-CGA-O2A
13	bA	801	CL0	CAA-CBA-CGA-O2A
13	cA	801	CL0	CAA-CBA-CGA-O2A
14	B	837	CLA	CAA-CBA-CGA-O2A
14	bB	837	CLA	CAA-CBA-CGA-O2A
14	cB	806	CLA	CAA-CBA-CGA-O2A
14	cB	838	CLA	CAA-CBA-CGA-O2A
17	A	846	BCR	C11-C12-C13-C14
17	bA	846	BCR	C11-C12-C13-C14
17	cA	846	BCR	C11-C12-C13-C14
14	A	826	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
14	cA	804	CLA	CAA-CBA-CGA-O1A
17	A	846	BCR	C15-C16-C17-C18
17	bA	846	BCR	C15-C16-C17-C18
17	cA	846	BCR	C15-C16-C17-C18
14	A	826	CLA	CAA-CBA-CGA-O2A
14	B	805	CLA	CAA-CBA-CGA-O2A
14	bA	826	CLA	CAA-CBA-CGA-O2A
14	cA	826	CLA	CAA-CBA-CGA-O2A
14	A	804	CLA	CAA-CBA-CGA-O1A
14	bA	804	CLA	CAA-CBA-CGA-O1A
14	bA	826	CLA	CAA-CBA-CGA-O1A
14	cA	826	CLA	CAA-CBA-CGA-O1A
14	cJ	102	CLA	O1D-CGD-O2D-CED
18	A	851	LHG	O2-C2-C3-O3
18	cA	851	LHG	O2-C2-C3-O3
14	bB	805	CLA	CAA-CBA-CGA-O2A
14	bA	840	CLA	CAA-CBA-CGA-O1A
14	cA	840	CLA	CAA-CBA-CGA-O1A
14	B	804	CLA	C2A-CAA-CBA-CGA
14	B	809	CLA	C2A-CAA-CBA-CGA
14	bB	809	CLA	C2A-CAA-CBA-CGA
14	cB	805	CLA	C2A-CAA-CBA-CGA
14	cB	810	CLA	C2A-CAA-CBA-CGA
14	A	841	CLA	C16-C17-C18-C19
14	cA	841	CLA	C16-C17-C18-C19
14	A	840	CLA	CAA-CBA-CGA-O1A
14	B	837	CLA	CAA-CBA-CGA-O1A
14	bB	837	CLA	CAA-CBA-CGA-O1A
14	cB	838	CLA	CAA-CBA-CGA-O1A
14	bJ	102	CLA	O1D-CGD-O2D-CED
14	bB	816	CLA	CAA-CBA-CGA-O2A
14	cB	817	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

316 monomers are involved in 542 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	852	CLA	4	0
17	cL	206	BCR	2	0
14	bA	830	CLA	2	0
17	bB	850	BCR	2	0
14	cB	815	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	cA	806	CLA	2	0
14	X	201	CLA	3	0
14	cB	828	CLA	3	0
14	cA	811	CLA	1	0
14	B	821	CLA	1	0
14	J	102	CLA	1	0
14	A	826	CLA	2	0
14	bB	824	CLA	1	0
14	bA	838	CLA	3	0
13	bA	801	CL0	5	0
14	A	837	CLA	1	0
14	bA	818	CLA	1	0
14	B	813	CLA	3	0
17	cB	843	BCR	2	0
14	A	820	CLA	2	0
14	bA	816	CLA	1	0
14	cB	804	CLA	3	0
14	bA	828	CLA	1	0
14	cB	832	CLA	4	0
14	bA	839	CLA	1	0
14	bA	825	CLA	1	0
14	cA	829	CLA	4	0
14	bA	819	CLA	1	0
14	A	809	CLA	2	0
14	F	201	CLA	1	0
14	cB	827	CLA	3	0
17	B	847	BCR	1	0
14	A	827	CLA	4	0
14	cA	837	CLA	1	0
14	B	805	CLA	1	0
17	B	850	BCR	2	0
14	cA	839	CLA	1	0
14	A	822	CLA	1	0
14	bA	804	CLA	1	0
14	cA	810	CLA	2	0
17	bB	847	BCR	1	0
14	A	841	CLA	3	0
14	bB	837	CLA	2	0
14	bB	808	CLA	1	0
14	bA	807	CLA	2	0
17	bA	845	BCR	2	0
14	B	836	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	cB	826	CLA	3	0
14	bA	821	CLA	1	0
14	cA	826	CLA	2	0
14	B	804	CLA	1	0
14	bB	823	CLA	1	0
14	A	838	CLA	3	0
14	bA	831	CLA	5	0
14	cB	817	CLA	1	0
14	cX	201	CLA	3	0
14	B	851	CLA	1	0
14	bJ	102	CLA	1	0
14	cB	839	CLA	2	0
17	cA	849	BCR	2	0
14	B	837	CLA	2	0
14	cB	836	CLA	3	0
14	bB	834	CLA	1	0
14	cA	841	CLA	3	0
14	B	808	CLA	1	0
14	A	803	CLA	1	0
14	bB	806	CLA	2	0
14	cA	818	CLA	1	0
14	cB	812	CLA	1	0
14	B	802	CLA	4	0
14	A	836	CLA	1	0
14	A	832	CLA	2	0
14	A	810	CLA	2	0
14	L	201	CLA	4	0
14	cB	813	CLA	3	0
14	B	806	CLA	2	0
14	B	834	CLA	1	0
14	cB	835	CLA	1	0
14	bL	201	CLA	4	0
17	cB	846	BCR	2	0
17	cB	851	BCR	2	0
14	cB	808	CLA	1	0
14	bB	838	CLA	2	0
14	bL	204	CLA	8	0
14	bA	829	CLA	4	0
17	bJ	103	BCR	6	0
14	B	820	CLA	1	0
14	cB	824	CLA	1	0
14	cB	801	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	cB	806	CLA	1	0
13	cA	801	CL0	5	0
14	bB	816	CLA	1	0
14	bX	201	CLA	3	0
14	cA	836	CLA	1	0
14	B	824	CLA	1	0
14	bA	840	CLA	2	0
14	bA	813	CLA	3	0
14	A	815	CLA	2	0
14	cB	814	CLA	3	0
17	cB	847	BCR	3	0
17	A	847	BCR	1	0
14	cA	828	CLA	1	0
14	cA	834	CLA	1	0
14	cB	805	CLA	1	0
14	bB	821	CLA	1	0
14	cA	805	CLA	2	0
14	cB	820	CLA	2	0
14	cJ	102	CLA	1	0
14	bA	815	CLA	2	0
17	bB	843	BCR	2	0
17	B	844	BCR	2	0
14	cB	809	CLA	1	0
14	bA	817	CLA	1	0
14	bB	803	CLA	2	0
14	A	817	CLA	1	0
14	A	835	CLA	2	0
14	cA	823	CLA	1	0
17	bL	205	BCR	1	0
14	cA	803	CLA	1	0
14	cB	831	CLA	1	0
14	bA	814	CLA	1	0
17	B	843	BCR	2	0
14	bA	835	CLA	2	0
13	A	801	CL0	5	0
14	L	203	CLA	1	0
14	cL	204	CLA	1	0
14	bB	833	CLA	1	0
14	cA	802	CLA	5	0
14	cA	824	CLA	1	0
14	A	821	CLA	1	0
17	bA	849	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	bB	839	CLA	2	0
14	B	832	CLA	1	0
14	bB	825	CLA	2	0
14	bL	202	CLA	1	0
15	B	840	PQN	1	0
14	A	808	CLA	1	0
14	B	816	CLA	1	0
14	bA	852	CLA	5	0
14	A	807	CLA	2	0
17	A	845	BCR	2	0
14	bB	812	CLA	3	0
14	B	839	CLA	2	0
14	B	825	CLA	3	0
14	bB	818	CLA	1	0
14	B	833	CLA	1	0
14	bA	837	CLA	1	0
17	cB	848	BCR	1	0
14	cB	807	CLA	2	0
14	bA	812	CLA	1	0
14	bB	830	CLA	1	0
17	L	206	BCR	5	0
14	B	812	CLA	3	0
14	bA	832	CLA	2	0
14	cA	813	CLA	3	0
14	A	834	CLA	1	0
14	bA	805	CLA	3	0
14	bB	828	CLA	3	0
14	bA	820	CLA	2	0
14	B	817	CLA	1	0
14	B	835	CLA	3	0
14	cL	202	CLA	3	0
14	A	824	CLA	1	0
14	bA	808	CLA	1	0
14	J	101	CLA	2	0
14	bB	819	CLA	2	0
14	cB	811	CLA	1	0
17	B	846	BCR	2	0
17	I	102	BCR	2	0
14	bA	822	CLA	1	0
17	bB	845	BCR	2	0
14	bA	806	CLA	2	0
14	cA	821	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	bA	827	CLA	4	0
17	cB	844	BCR	2	0
17	bB	846	BCR	3	0
17	bB	842	BCR	2	0
17	J	103	BCR	6	0
14	A	829	CLA	4	0
14	cA	840	CLA	1	0
17	bA	847	BCR	1	0
17	B	845	BCR	2	0
14	bB	836	CLA	1	0
14	bA	826	CLA	2	0
14	cA	825	CLA	1	0
14	A	839	CLA	1	0
14	cA	830	CLA	2	0
14	cB	818	CLA	1	0
17	B	842	BCR	2	0
14	cF	201	CLA	1	0
14	cA	831	CLA	5	0
14	bB	849	CLA	1	0
14	B	823	CLA	1	0
14	A	812	CLA	1	0
14	cA	814	CLA	1	0
14	cA	816	CLA	1	0
14	bB	826	CLA	3	0
14	bL	203	CLA	2	0
14	cA	852	CLA	5	0
14	bB	815	CLA	1	0
17	A	849	BCR	2	0
14	cB	803	CLA	5	0
14	bA	810	CLA	2	0
17	cL	207	BCR	5	0
14	cB	802	CLA	2	0
14	A	811	CLA	1	0
14	A	818	CLA	1	0
14	A	802	CLA	5	0
14	bA	811	CLA	1	0
14	bB	801	CLA	2	0
17	cI	102	BCR	2	0
14	B	838	CLA	2	0
14	B	807	CLA	1	0
14	bA	803	CLA	1	0
14	cA	820	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	bB	804	CLA	1	0
14	cA	807	CLA	2	0
14	bB	813	CLA	3	0
14	bB	835	CLA	3	0
14	A	819	CLA	1	0
14	A	804	CLA	1	0
14	cA	809	CLA	2	0
14	bB	807	CLA	1	0
14	bB	822	CLA	2	0
14	cA	827	CLA	4	0
14	B	814	CLA	2	0
14	B	828	CLA	3	0
14	cB	837	CLA	1	0
14	A	828	CLA	1	0
14	A	825	CLA	1	0
14	bB	814	CLA	2	0
14	bB	805	CLA	1	0
14	B	830	CLA	1	0
14	cA	819	CLA	1	0
14	cB	823	CLA	2	0
14	cL	203	CLA	1	0
14	A	823	CLA	1	0
14	cB	821	CLA	1	0
14	bB	817	CLA	1	0
14	B	815	CLA	1	0
14	cA	838	CLA	3	0
15	cB	841	PQN	1	0
14	bB	831	CLA	4	0
14	bA	836	CLA	1	0
14	B	803	CLA	3	0
14	L	204	CLA	8	0
17	cM	101	BCR	2	0
14	bB	851	CLA	1	0
14	cB	822	CLA	1	0
14	B	822	CLA	2	0
14	B	831	CLA	3	0
14	bB	832	CLA	1	0
14	bA	834	CLA	1	0
14	bA	841	CLA	3	0
14	bB	810	CLA	1	0
14	cA	804	CLA	1	0
14	cL	205	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	818	CLA	1	0
17	M	101	BCR	2	0
14	cA	832	CLA	2	0
14	cB	838	CLA	2	0
14	B	801	CLA	2	0
14	bJ	101	CLA	2	0
14	cB	850	CLA	1	0
14	bA	802	CLA	5	0
14	bA	824	CLA	1	0
14	cB	834	CLA	1	0
14	bF	201	CLA	1	0
14	bB	811	CLA	1	0
14	bB	802	CLA	4	0
14	A	813	CLA	3	0
14	cA	822	CLA	1	0
14	cB	830	CLA	1	0
14	B	819	CLA	2	0
14	B	810	CLA	1	0
14	cB	833	CLA	1	0
14	bA	809	CLA	2	0
17	bL	206	BCR	5	0
14	bB	827	CLA	3	0
14	cA	815	CLA	2	0
17	cA	847	BCR	1	0
14	B	811	CLA	1	0
14	cB	829	CLA	3	0
14	bB	820	CLA	1	0
17	cJ	103	BCR	6	0
17	bI	102	BCR	2	0
14	A	842	CLA	1	0
14	L	202	CLA	1	0
14	cJ	101	CLA	2	0
14	A	805	CLA	2	0
14	cB	816	CLA	1	0
14	cB	840	CLA	2	0
14	cA	817	CLA	1	0
14	A	840	CLA	1	0
14	bA	842	CLA	1	0
17	cB	845	BCR	2	0
17	L	205	BCR	1	0
14	B	827	CLA	3	0
17	bB	844	BCR	2	0

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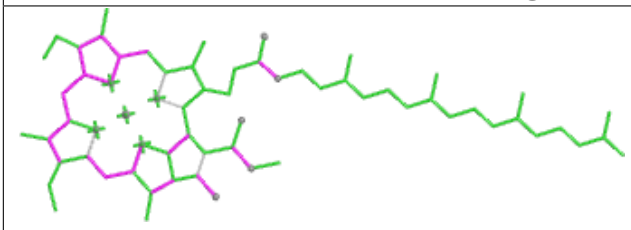
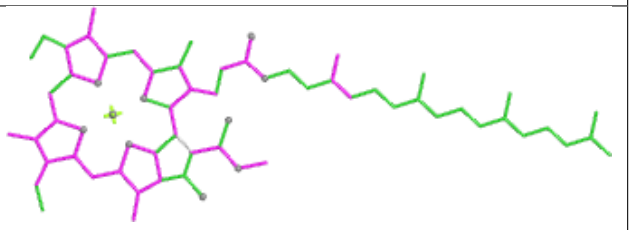
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	816	CLA	1	0
14	cB	825	CLA	1	0
14	A	830	CLA	2	0
14	A	831	CLA	5	0
14	cA	812	CLA	1	0
14	A	806	CLA	2	0
14	bA	823	CLA	1	0
17	bM	101	BCR	2	0
14	cA	842	CLA	1	0
14	B	849	CLA	1	0
14	B	826	CLA	3	0
14	A	814	CLA	1	0
17	cA	845	BCR	2	0
15	bB	840	PQN	1	0
14	cA	835	CLA	2	0
14	cB	819	CLA	1	0
14	cA	808	CLA	1	0

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

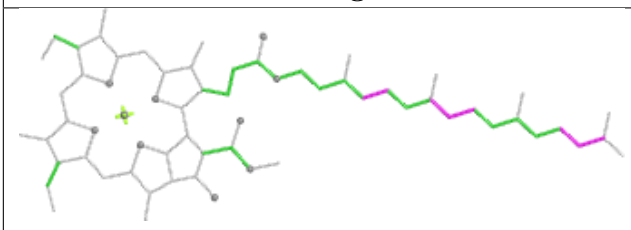
Ligand CLA A 852



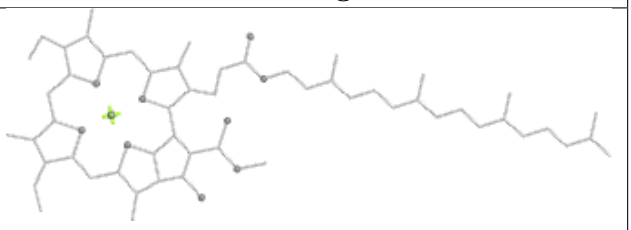
Bond lengths



Bond angles

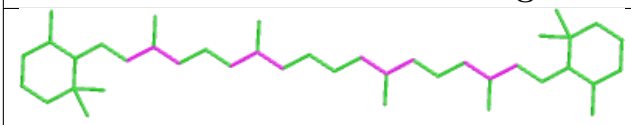


Torsions



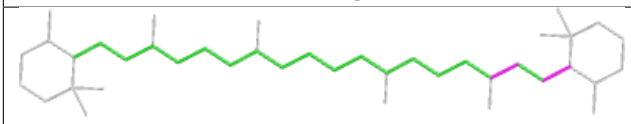
Rings

Ligand BCR cL 206



Bond lengths

Bond angles



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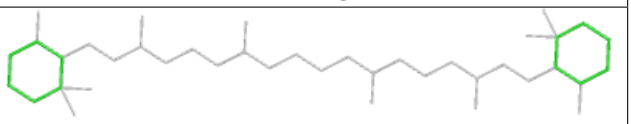
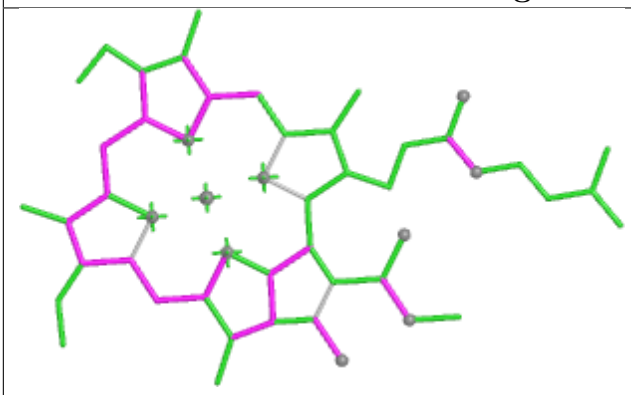


Rings

Ligand CLA bA 830



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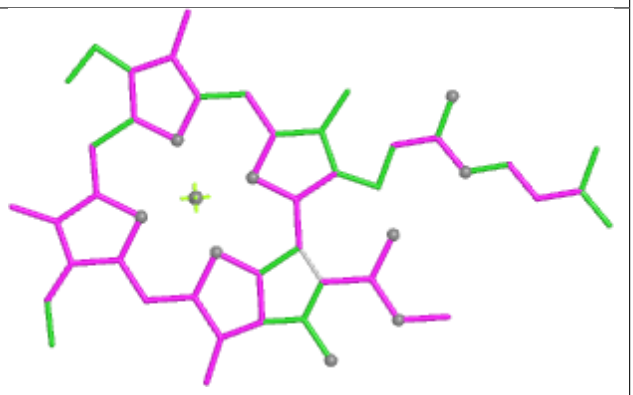

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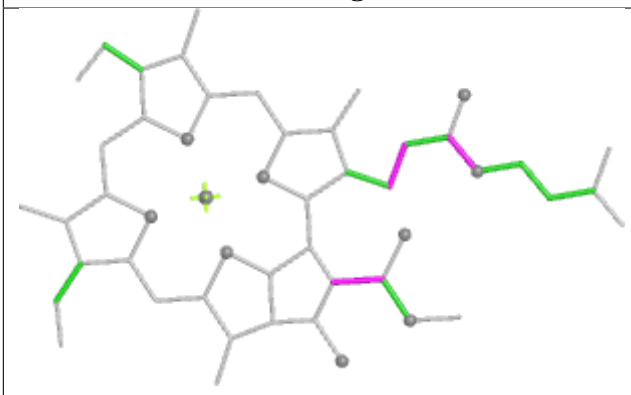

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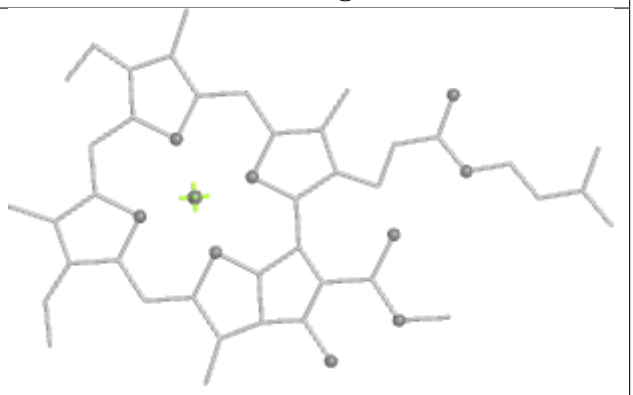
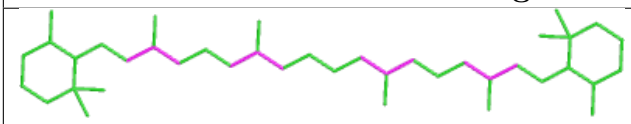


Rings

Ligand BCR bB 850



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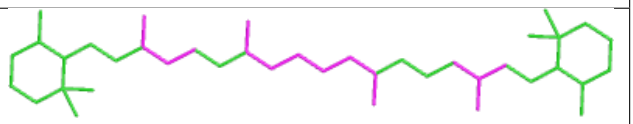
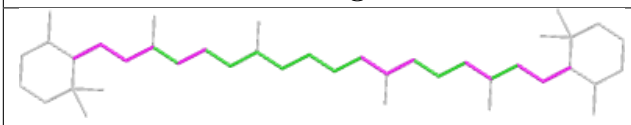


Bond angles



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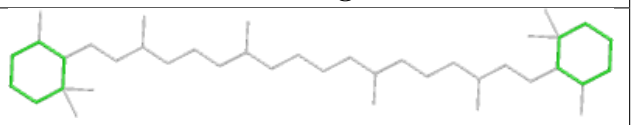
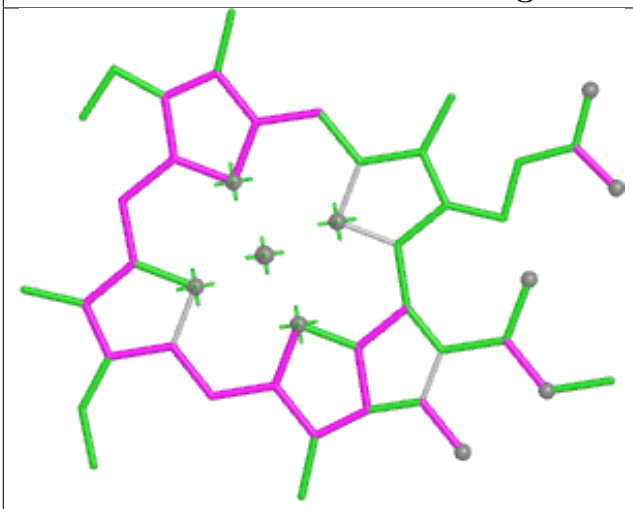


Rings

Ligand CLA cB 815



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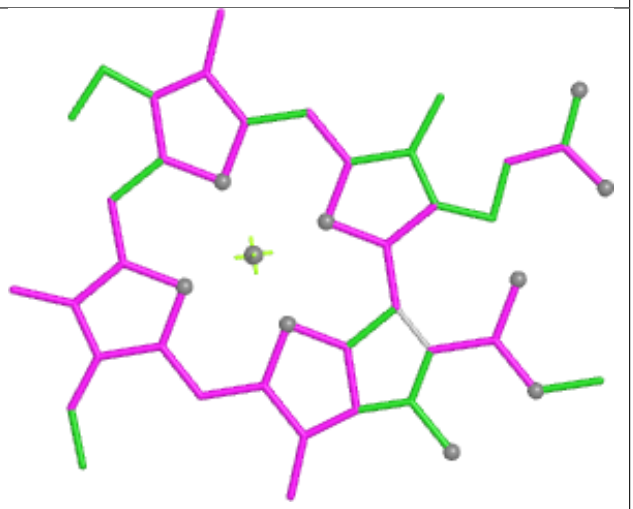
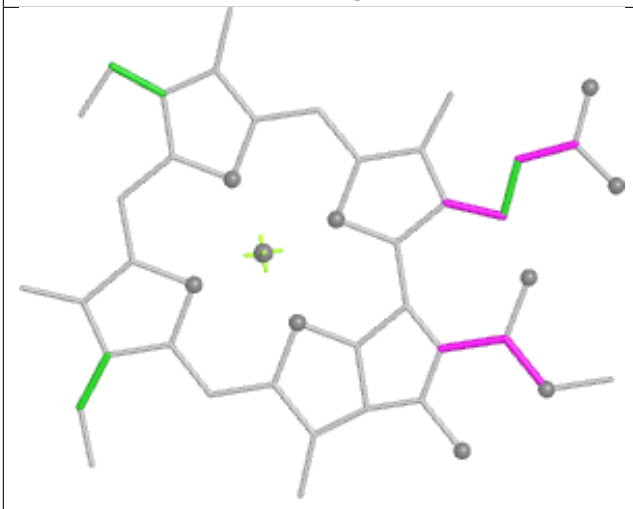


Bond angles



Torsions

Rings

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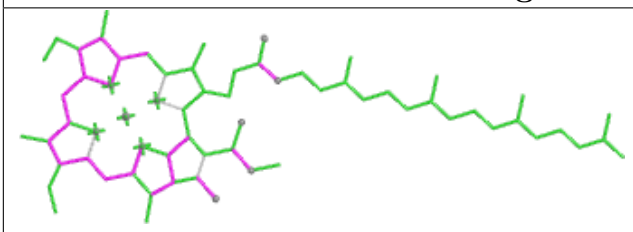

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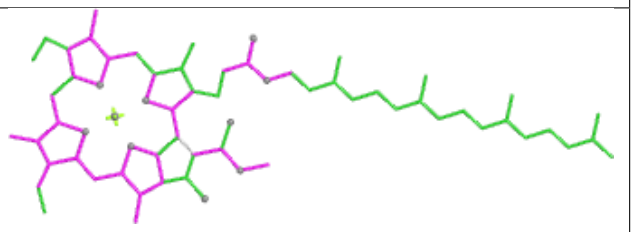
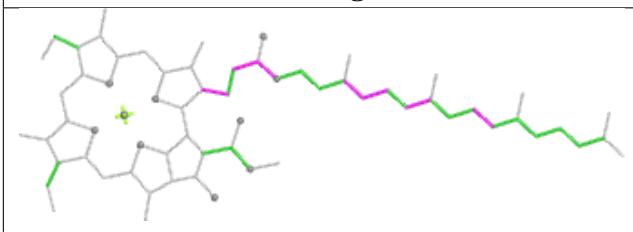


Bond angles



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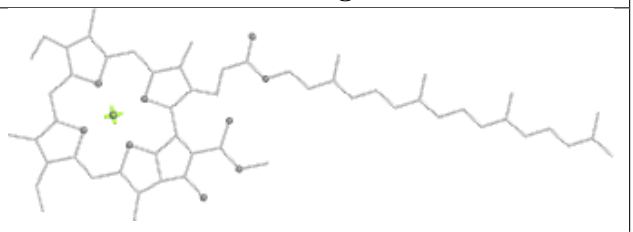
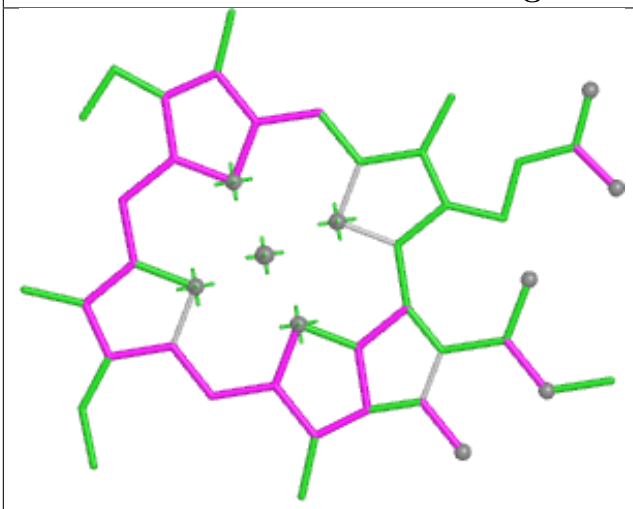


Rings

Ligand CLA X 201



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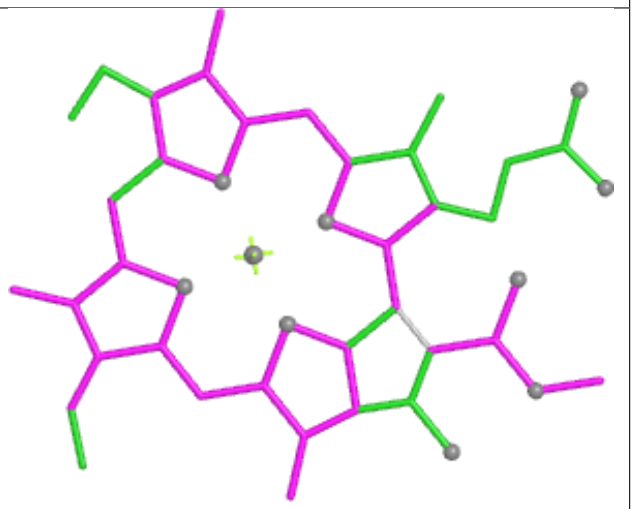
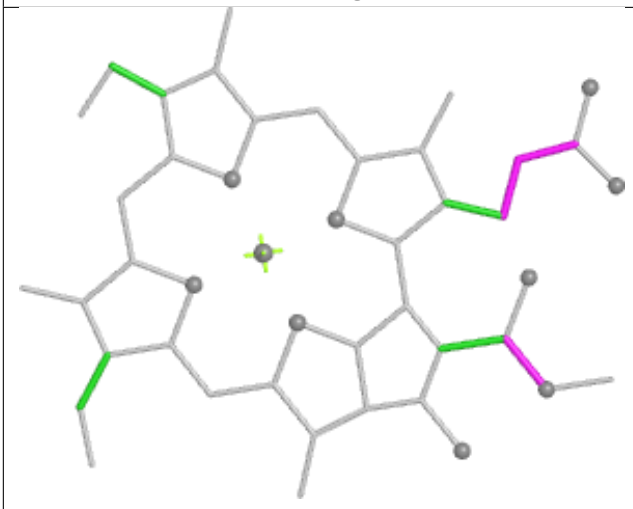


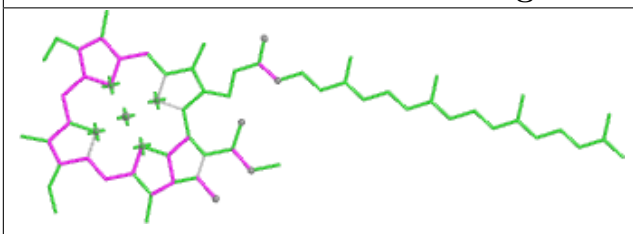
Bond angles



Torsions

Rings

Ligand CLA cB 828



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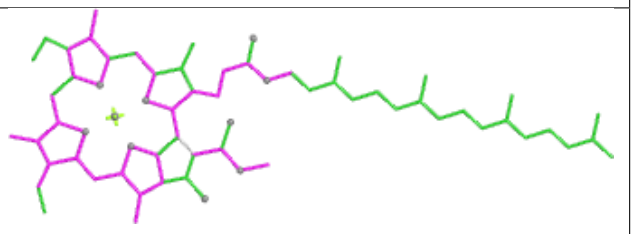

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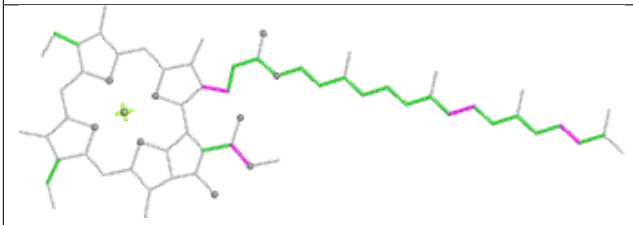

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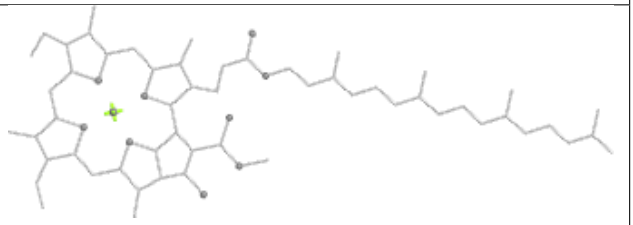
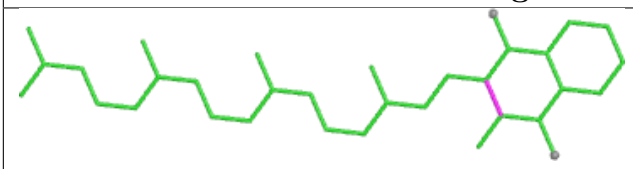


Rings

Ligand PQN bA 843



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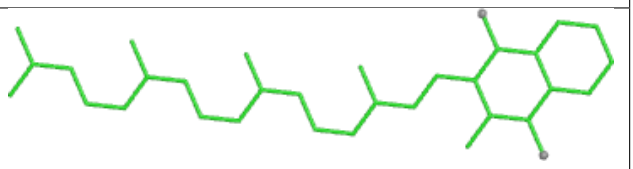

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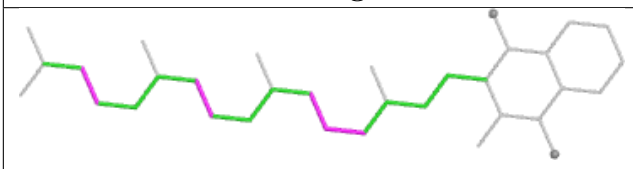

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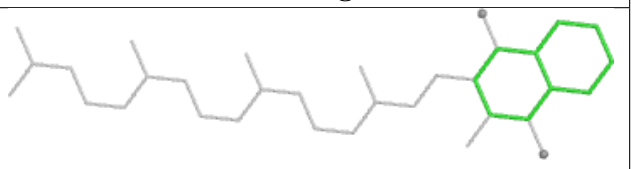
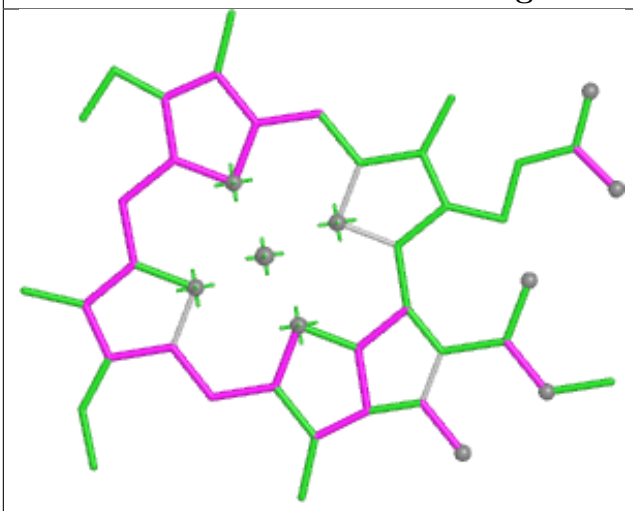


Rings

Ligand CLA cA 811



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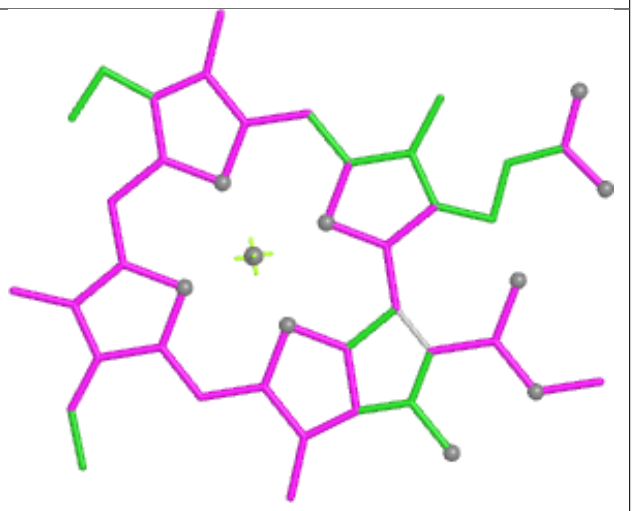

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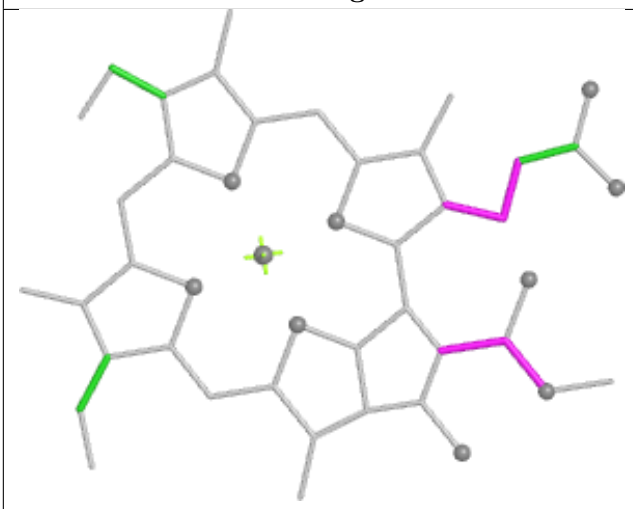
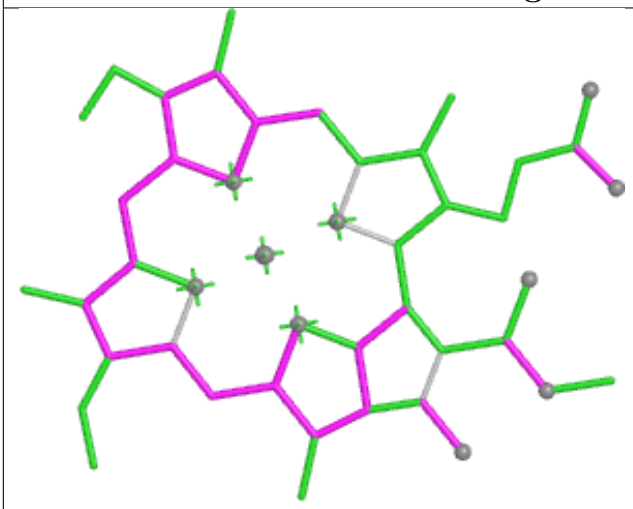


Torsions

Rings

Ligand CLA B 821



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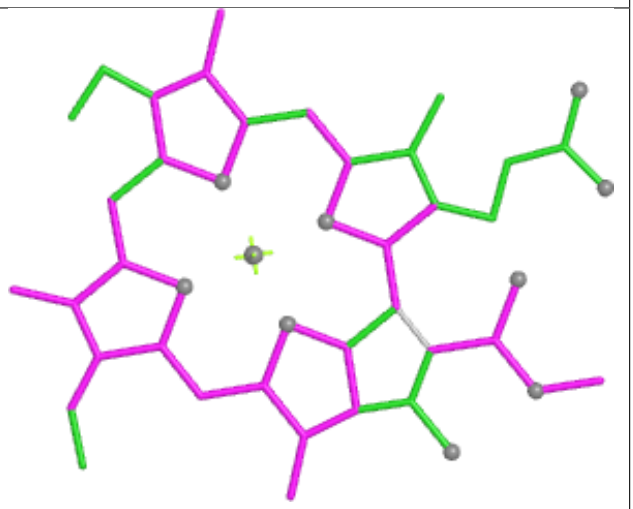

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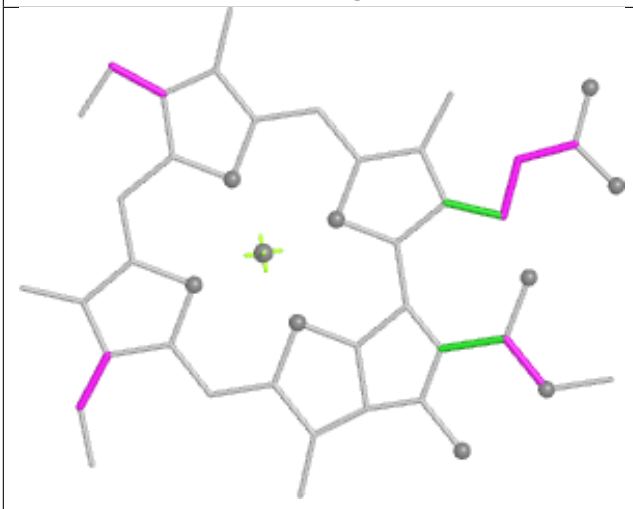
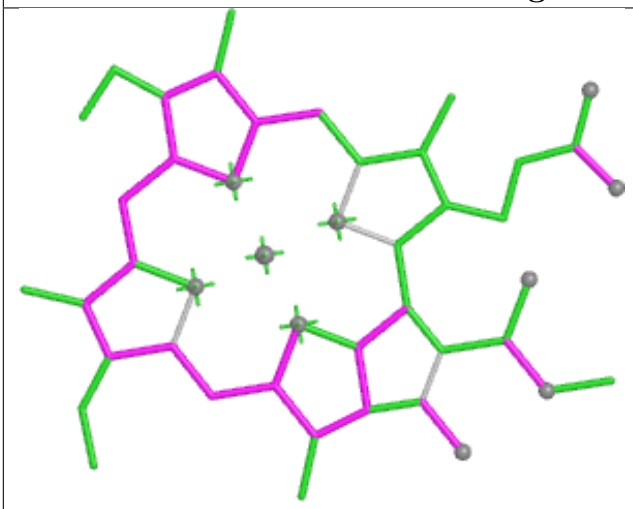


Torsions

Rings

Ligand CLA J 102



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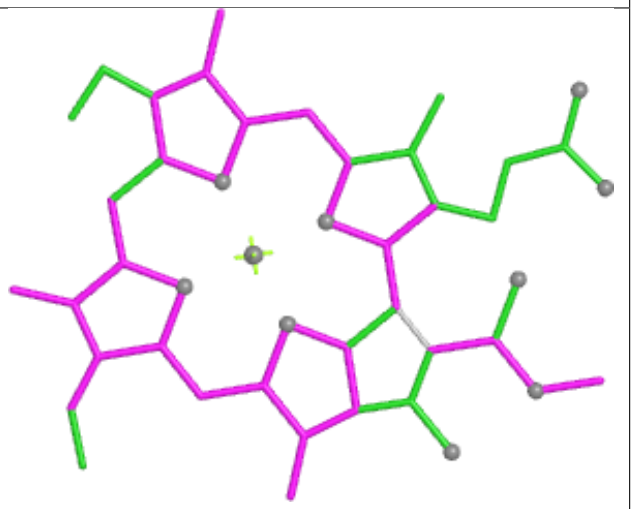
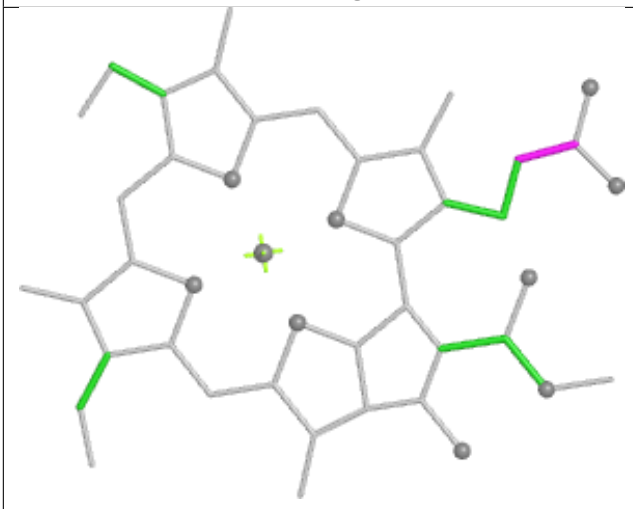


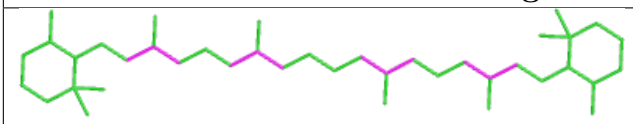
Bond angles



Torsions

Rings

Ligand BCR A 848



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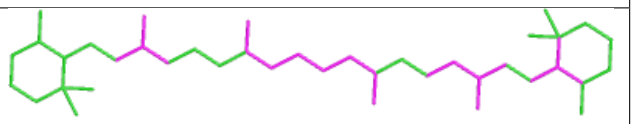

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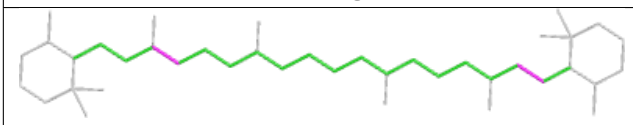

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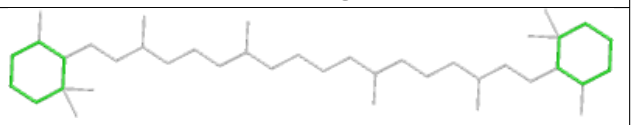
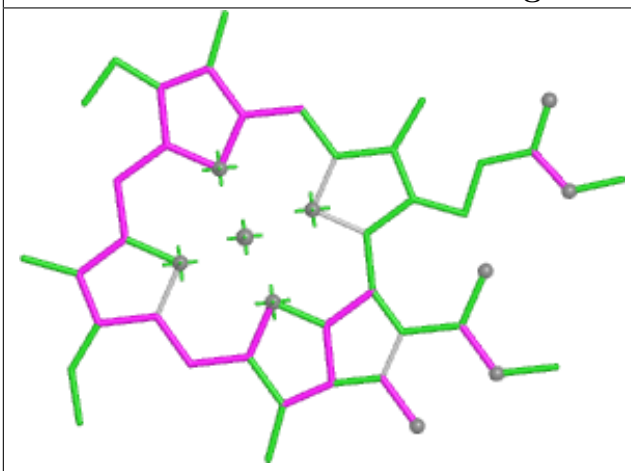
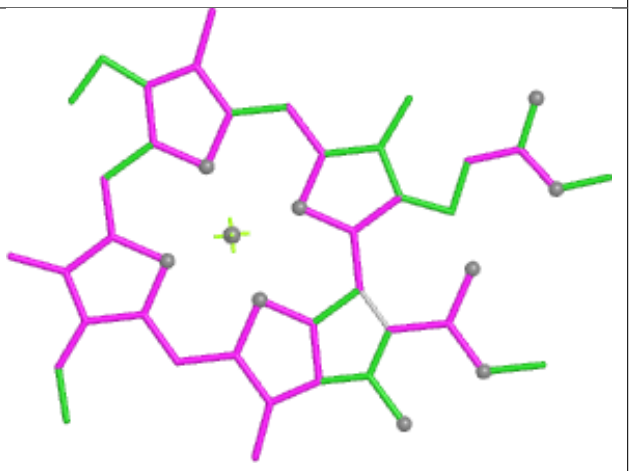
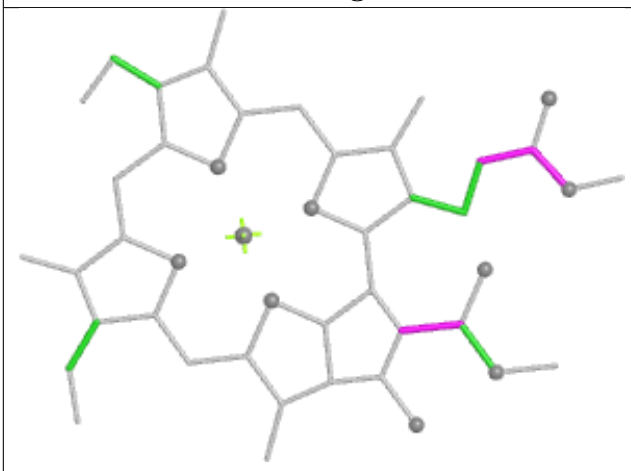
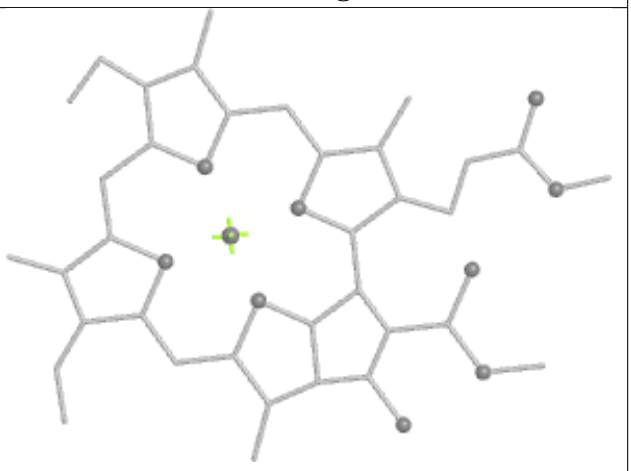
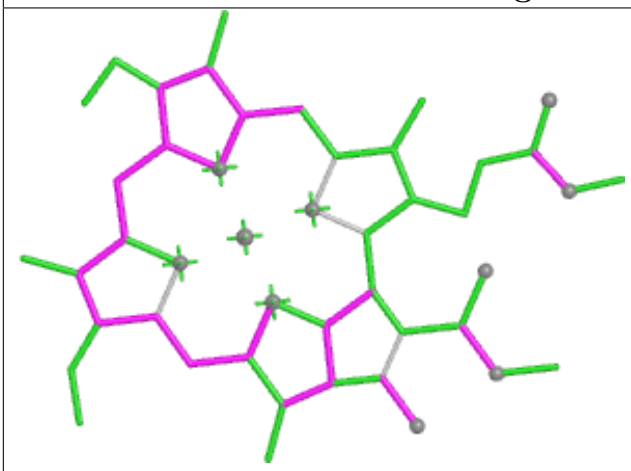


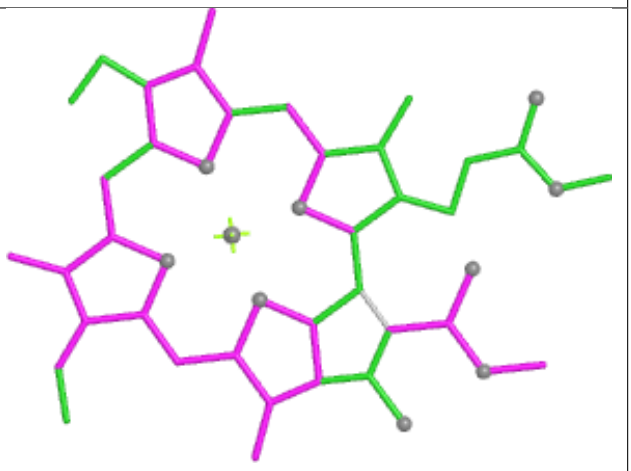
Rings

Ligand CLA A 826	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

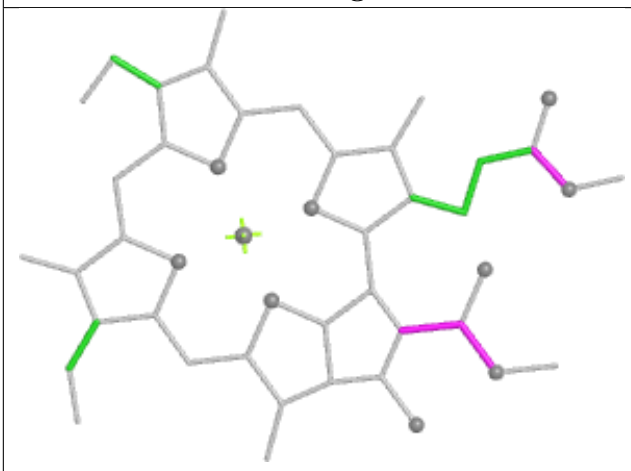
Ligand CLA bB 824



Bond lengths



Bond angles



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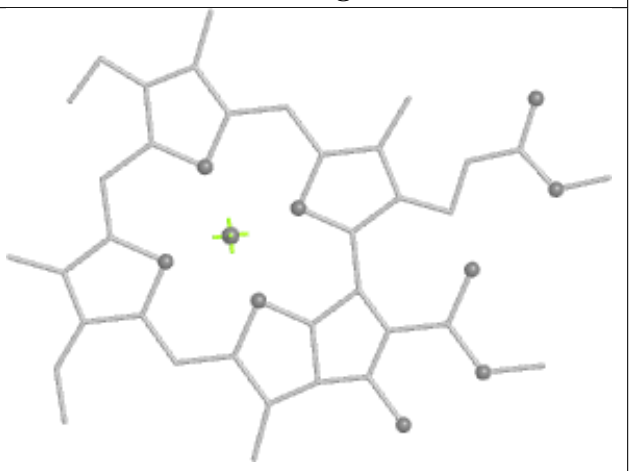
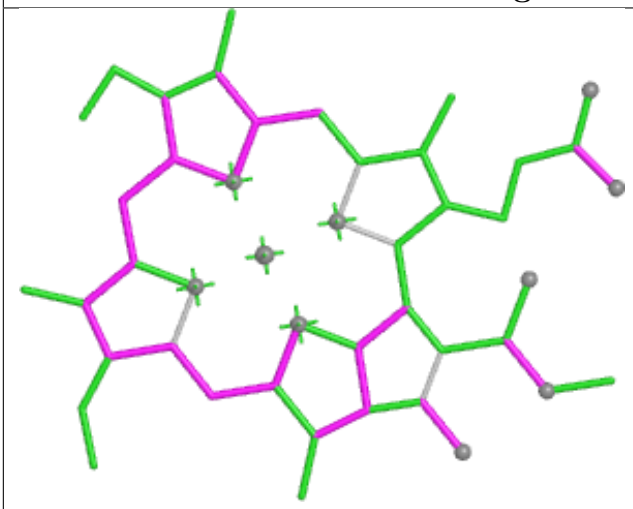
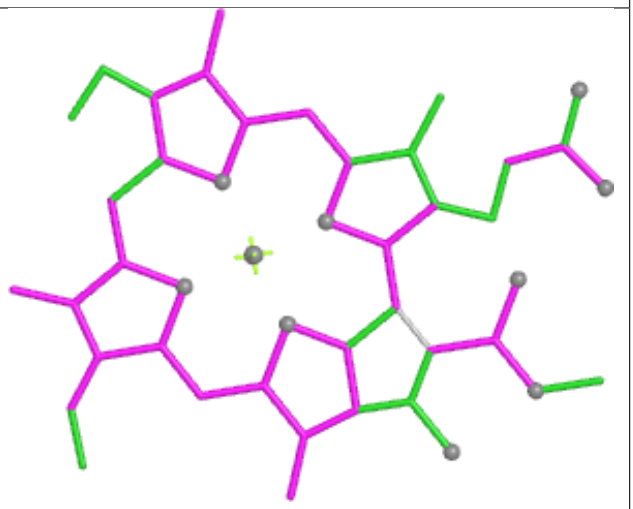


Rings

Ligand CLA bA 838



Bond lengths



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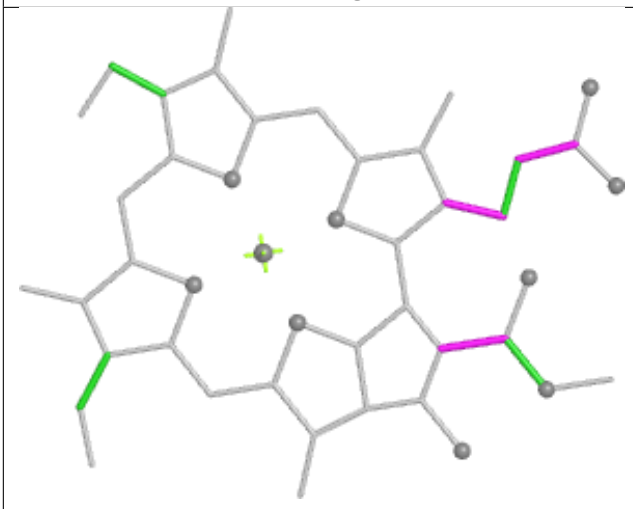
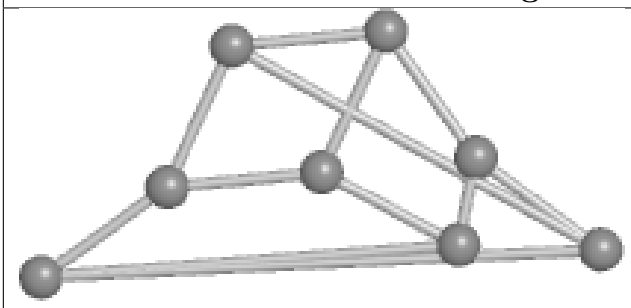


Torsions

Rings

Ligand SF4 bC 101



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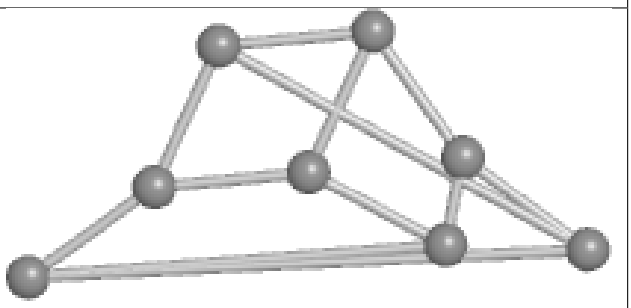
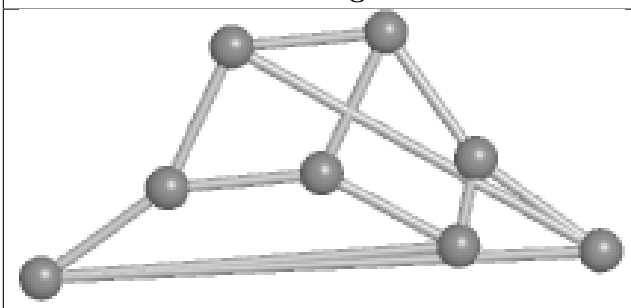


Bond angles



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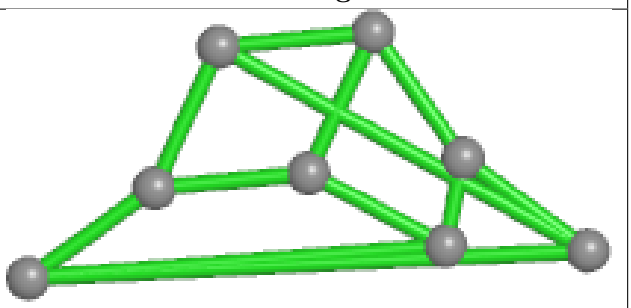
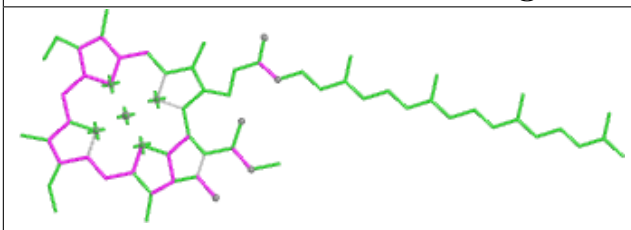


Rings

Ligand CL0 bA 801



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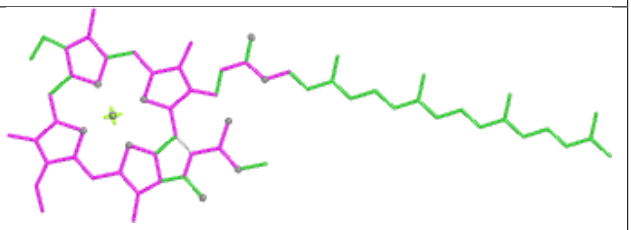
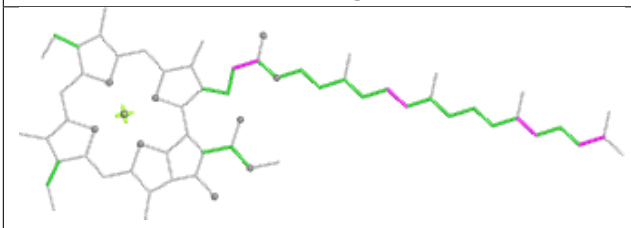


Bond angles



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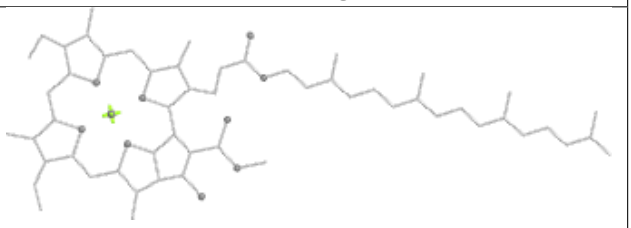
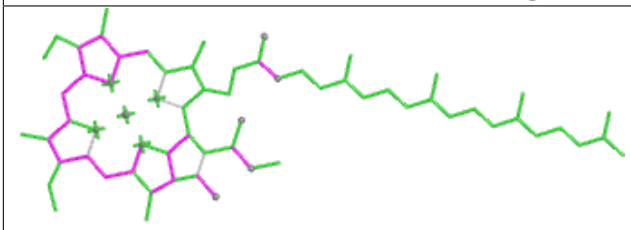
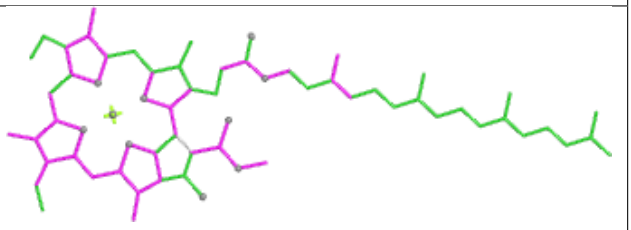
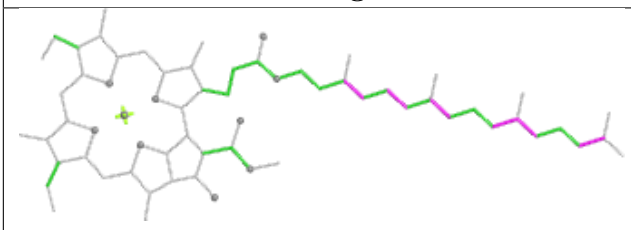
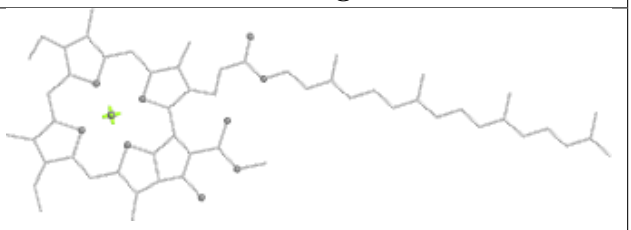
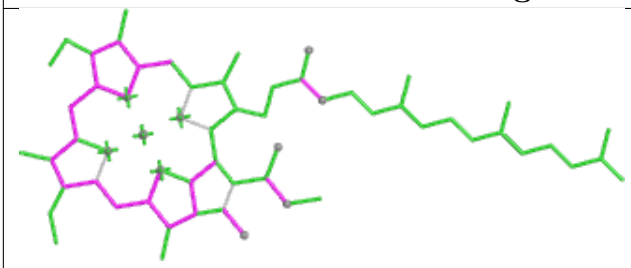
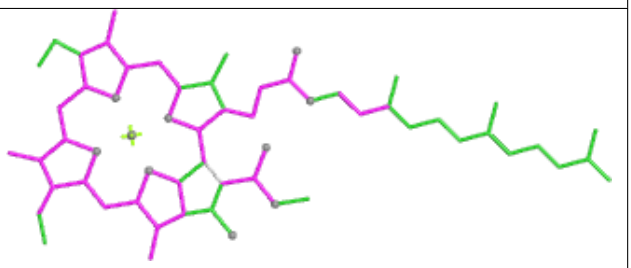
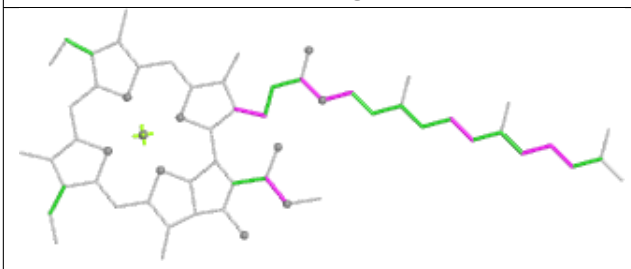
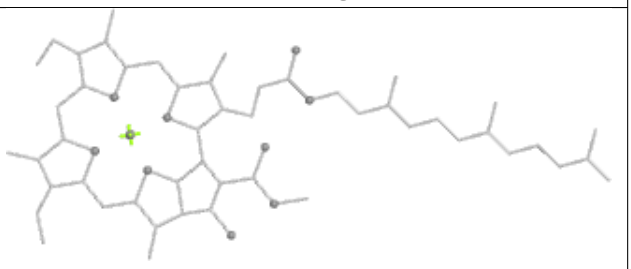
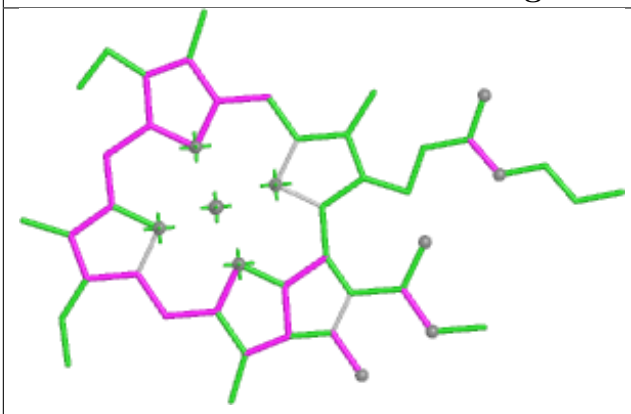


Rings

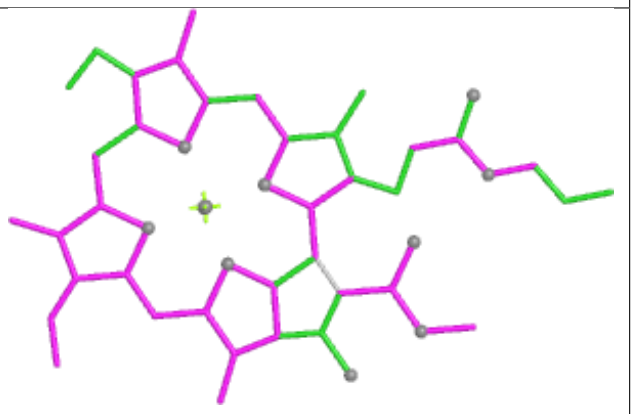
Ligand CLA A 837	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA bA 818	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 813



Bond lengths



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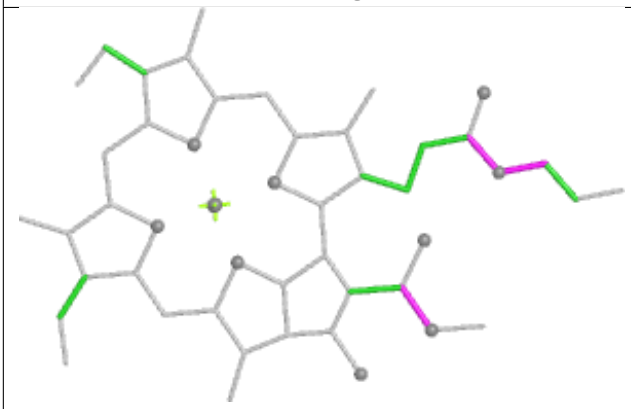
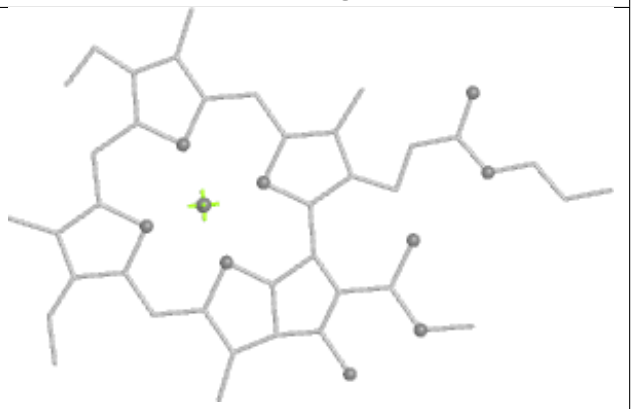
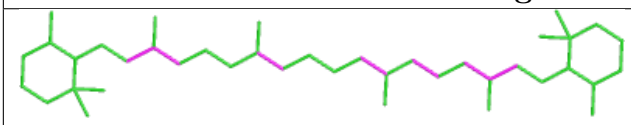


Torsions



Rings

Ligand BCR cB 843



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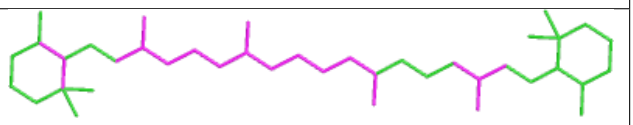
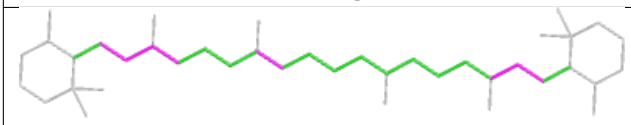


Bond angles



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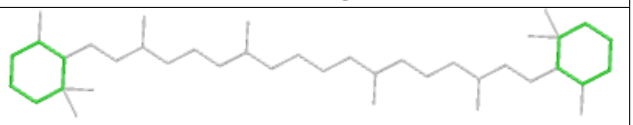
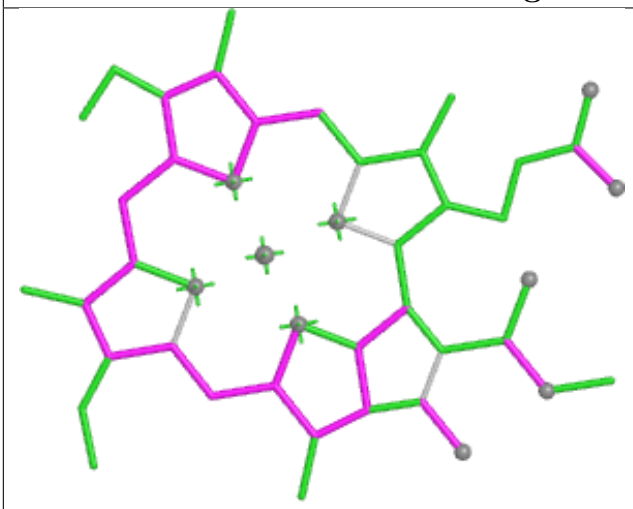


Rings

Ligand CLA A 820



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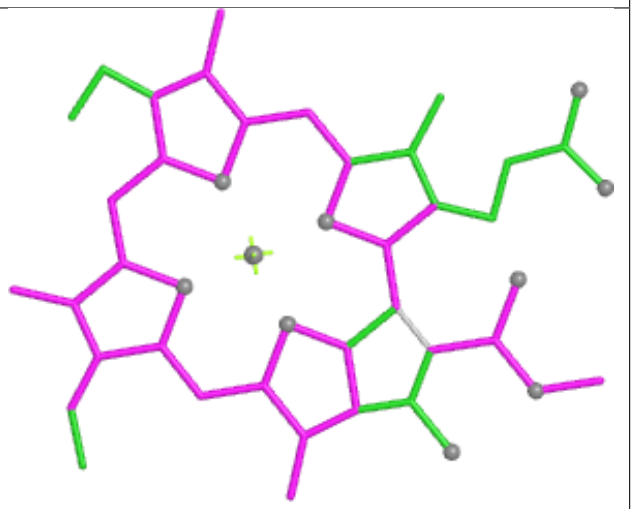
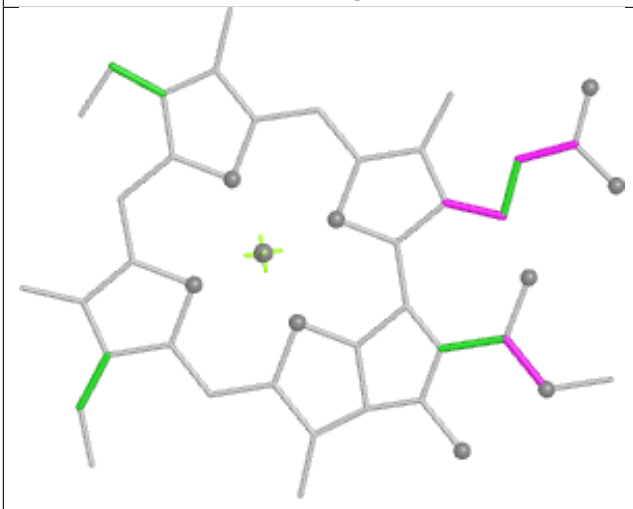


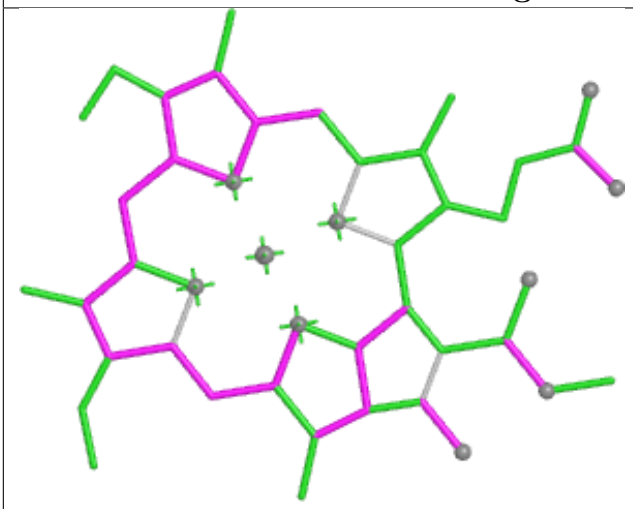
Bond angles



Torsions

Rings

Ligand CLA bA 816



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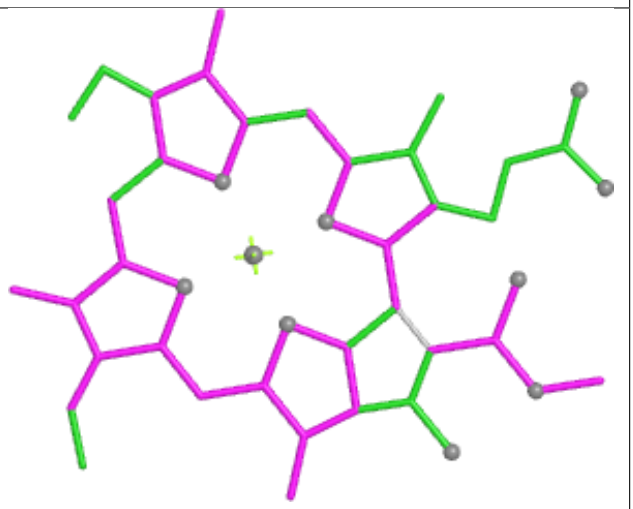
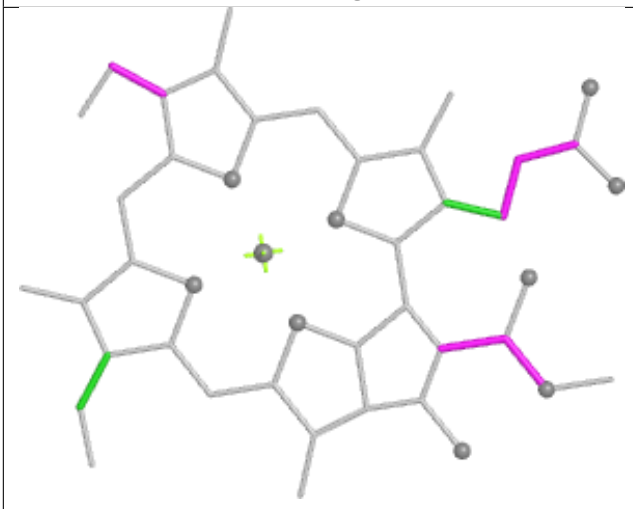
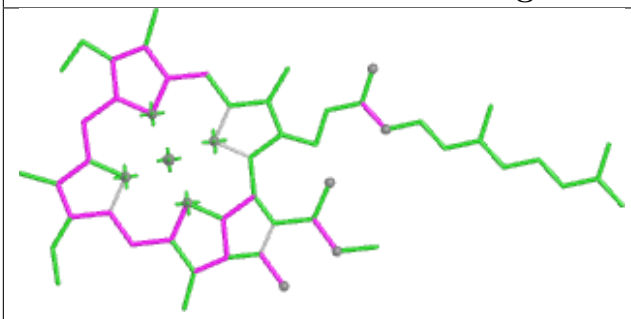
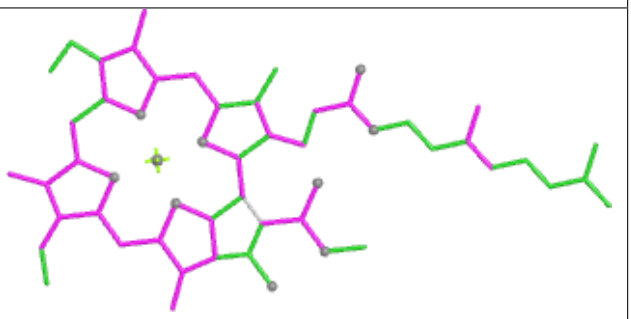
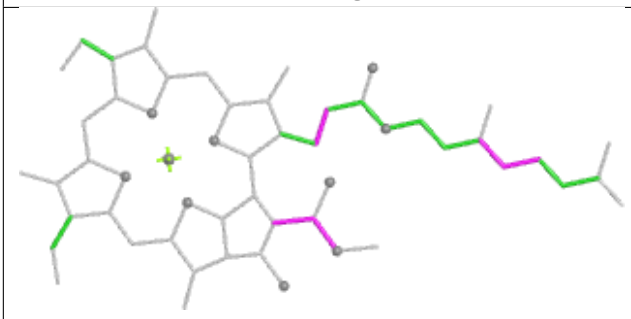
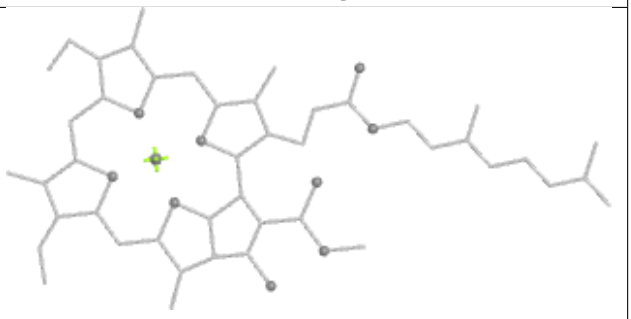


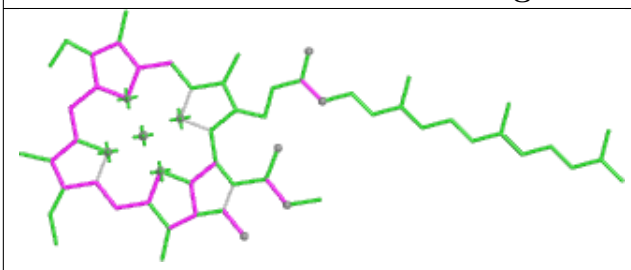
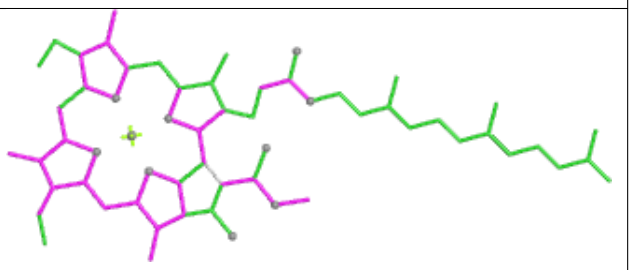
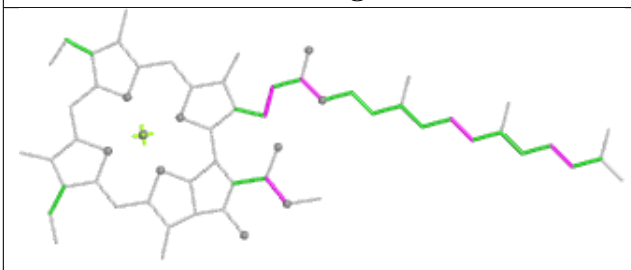
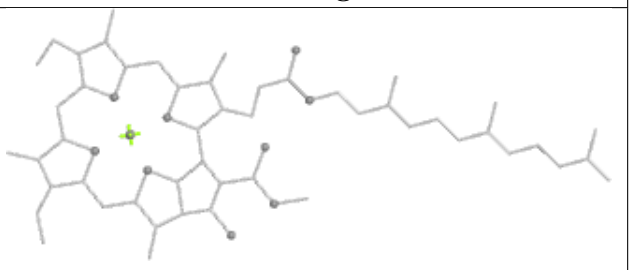
Bond angles



Torsions

Rings

Ligand CLA cB 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA bA 828	
 Bond lengths	 Bond angles
 Torsions	 Rings

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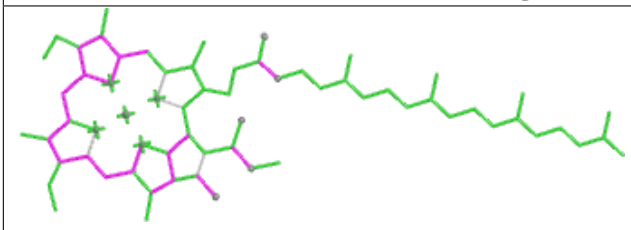
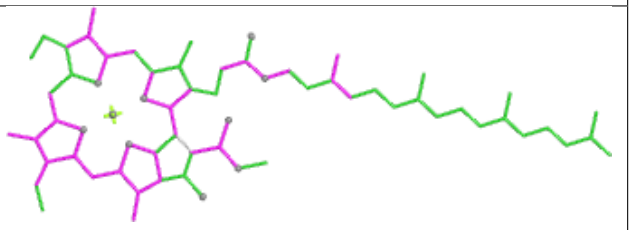
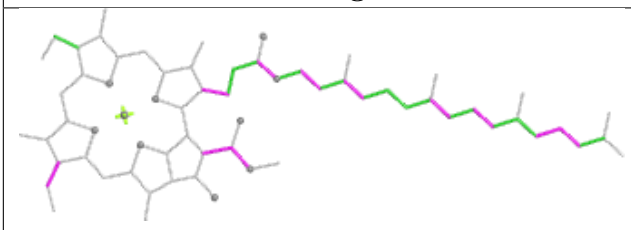
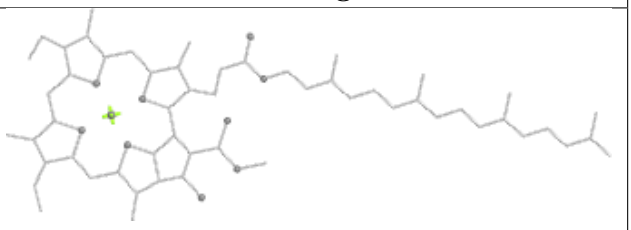
 Bond lengths	 Bond angles
 Torsions	 Rings

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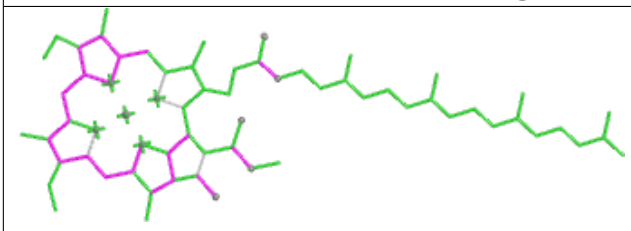
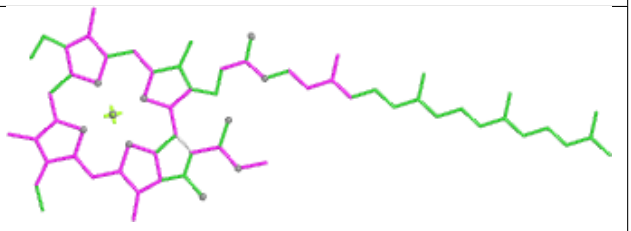
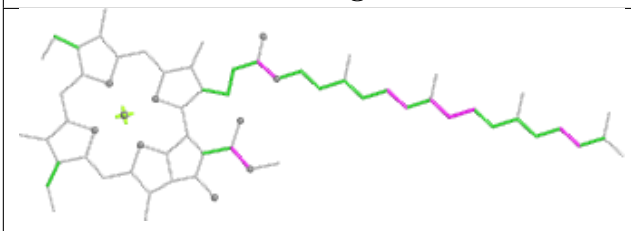
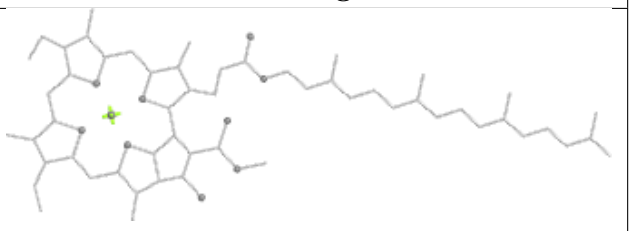
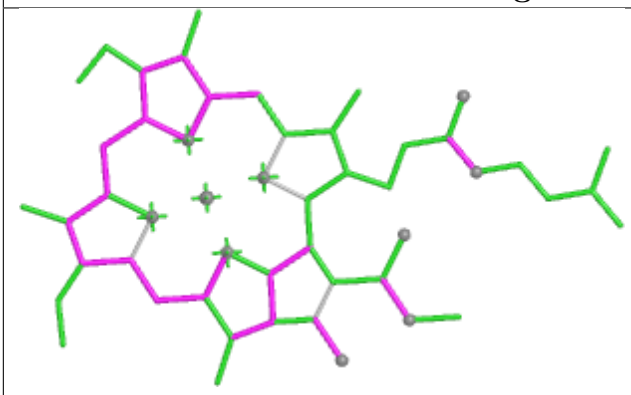
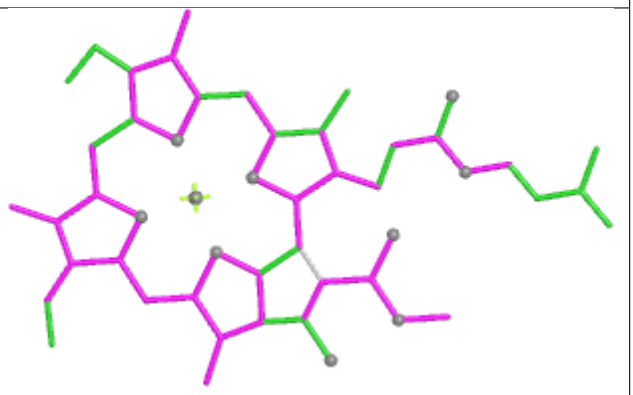
 Bond lengths	 Bond angles
 Torsions	 Rings

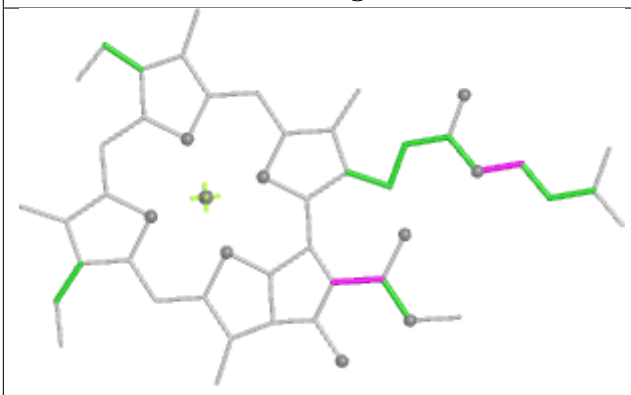
Ligand CLA bA 825



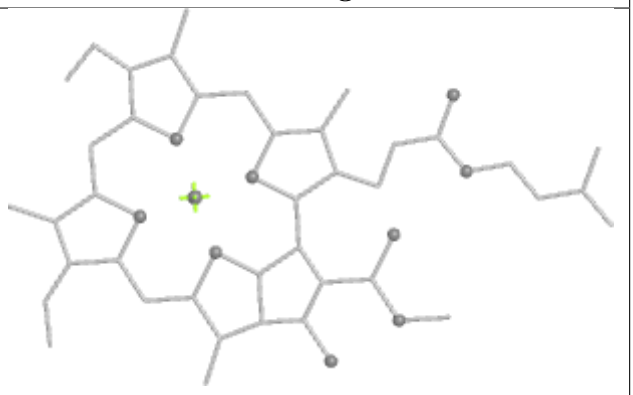
Bond lengths



Bond angles

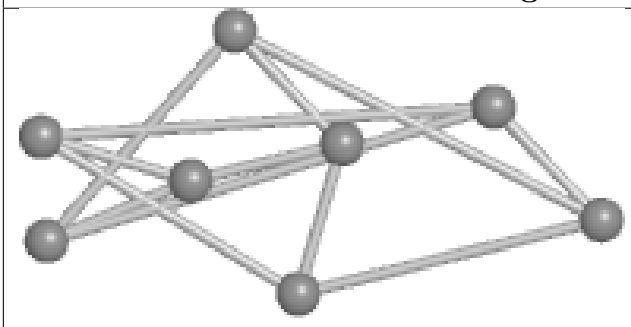


Torsions

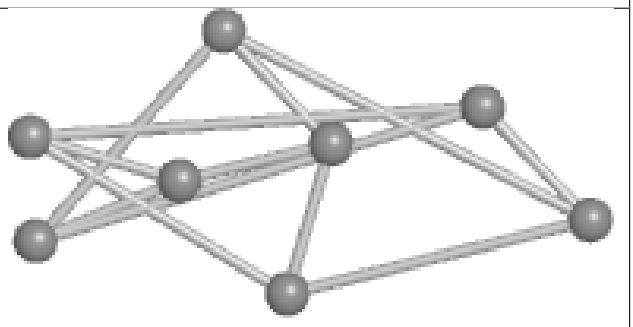


Rings

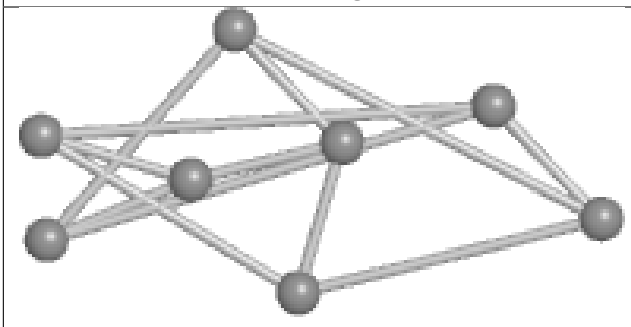
Ligand SF4 bA 844



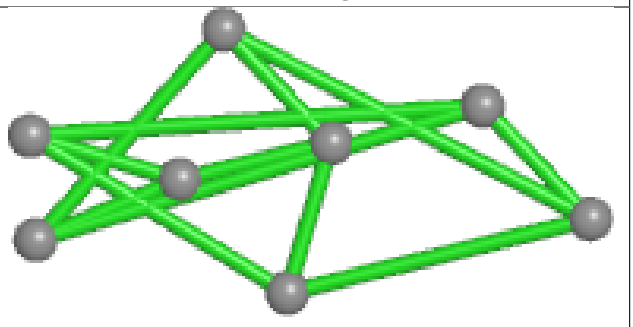
Bond lengths



Bond angles

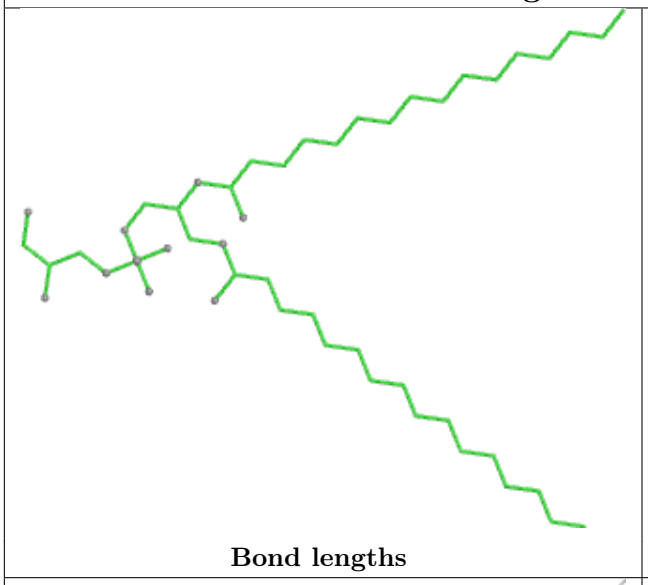


Torsions



Rings

Ligand LHG A 850



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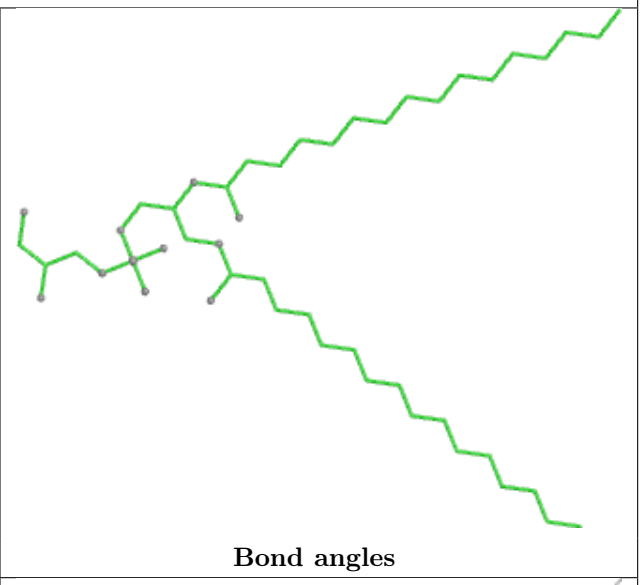
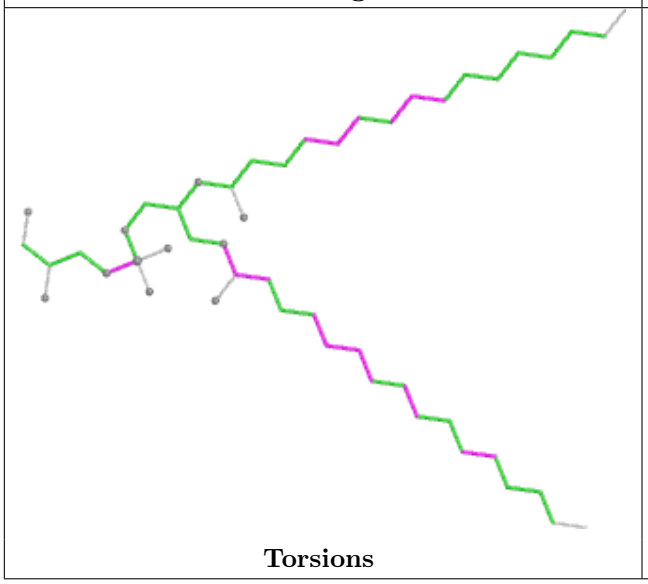


Bond angles



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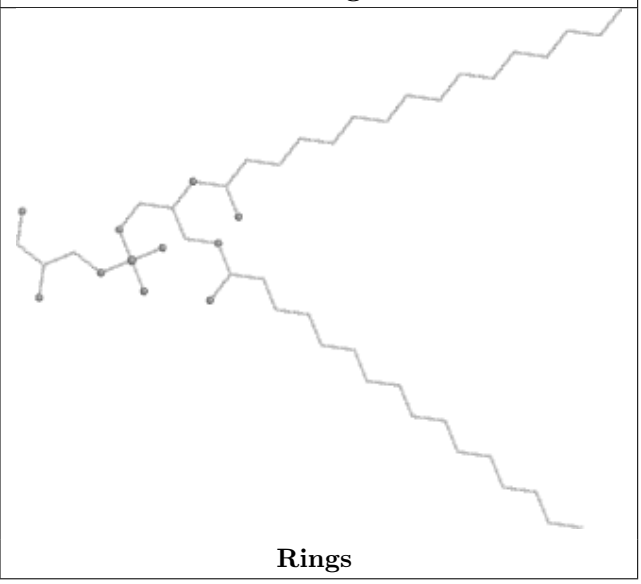
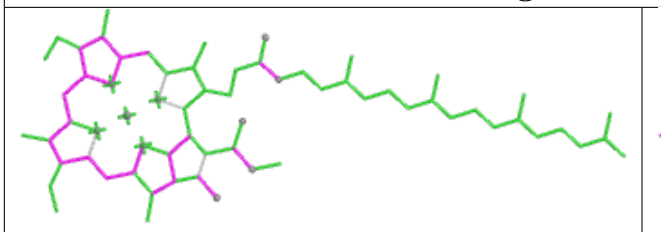


Rings

Ligand CLA cA 829



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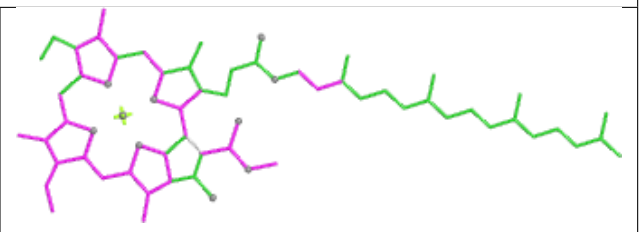

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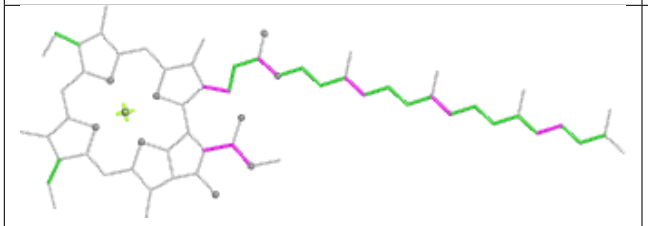

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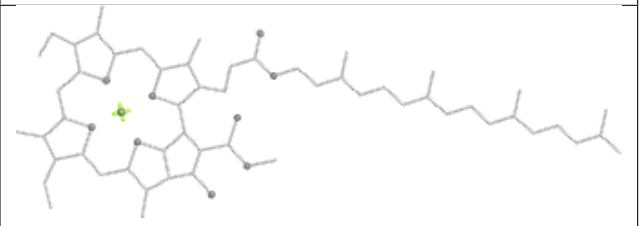
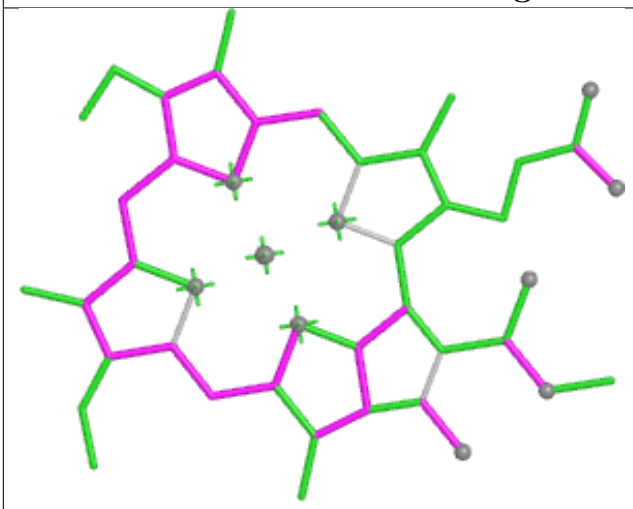


Rings

Ligand CLA bA 819



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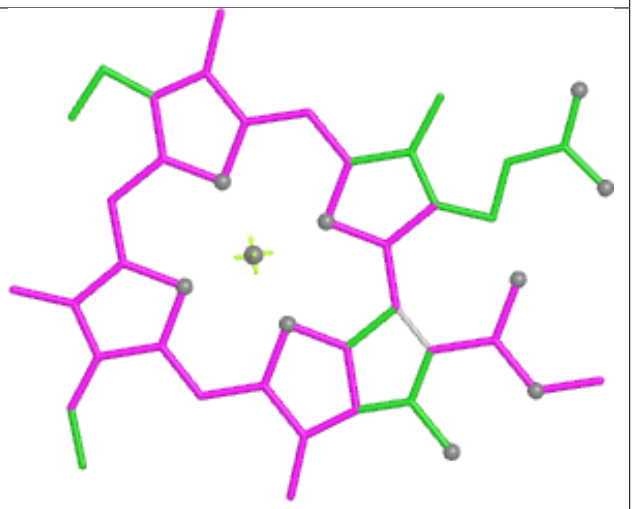
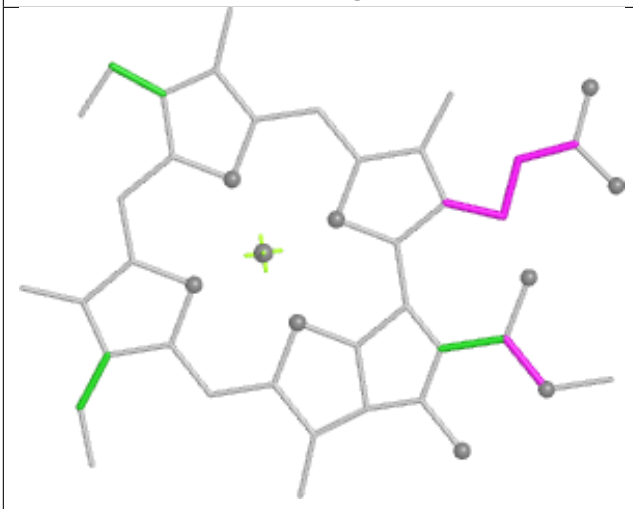


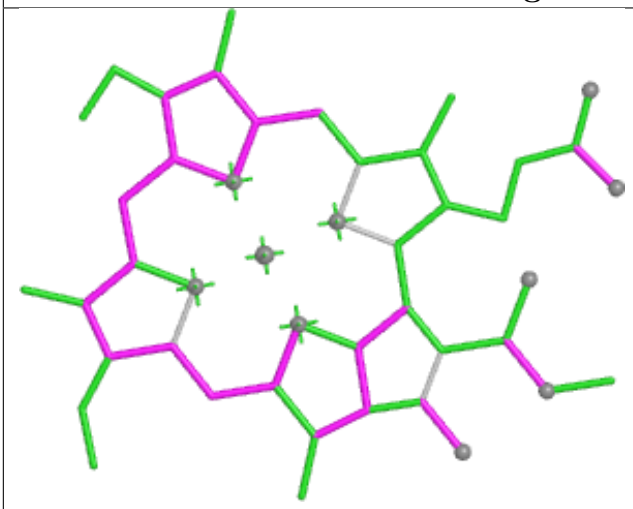
Bond angles



Torsions

Rings

Ligand CLA A 809



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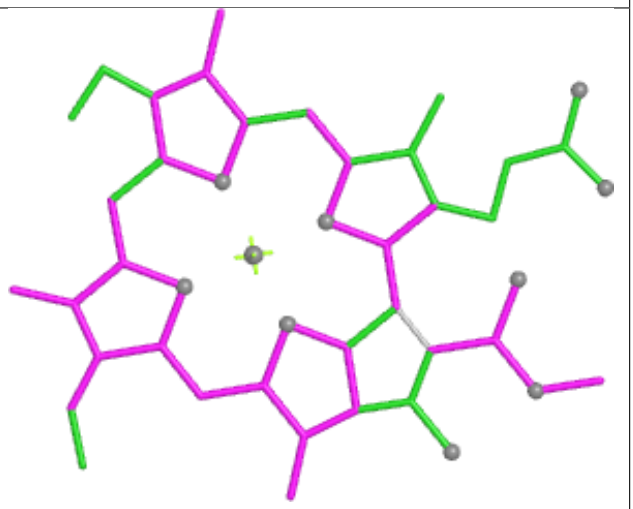
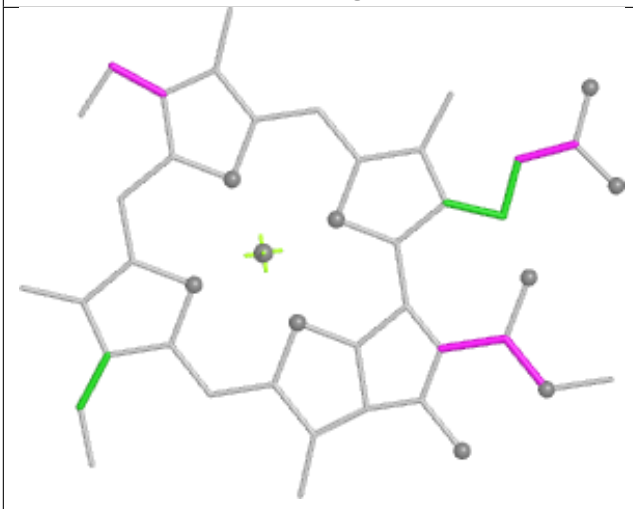


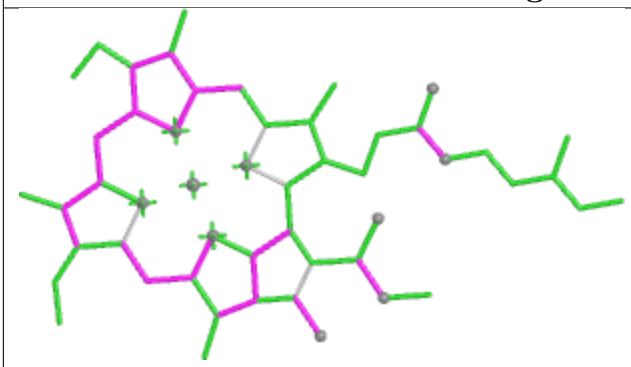
Bond angles



Torsions

Rings

Ligand CLA F 201



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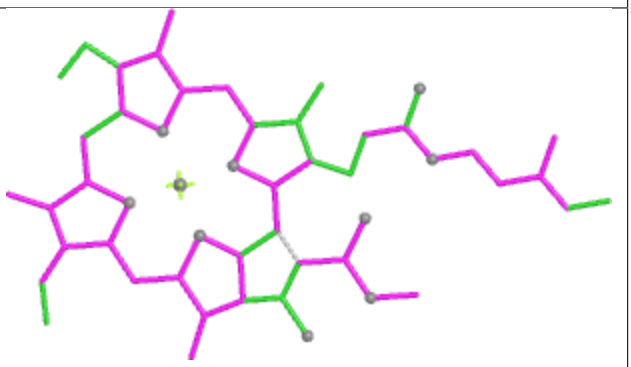
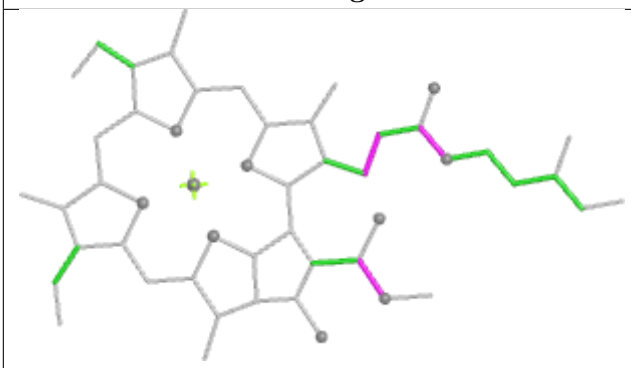


Bond angles



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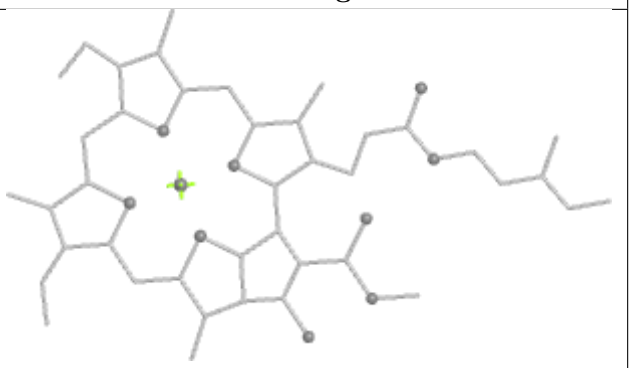
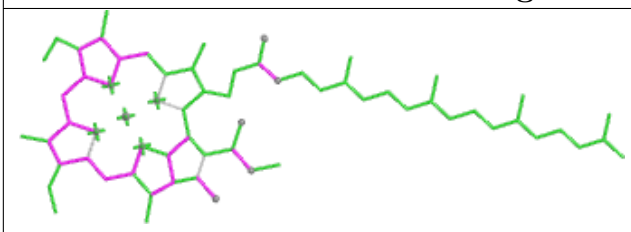


Rings

Ligand CLA cB 827



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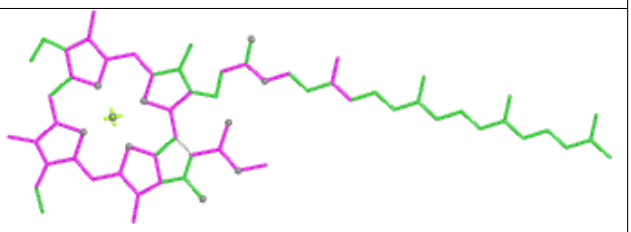

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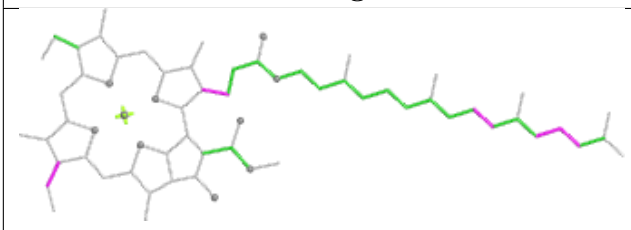

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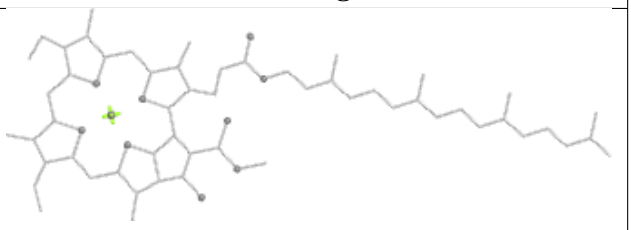
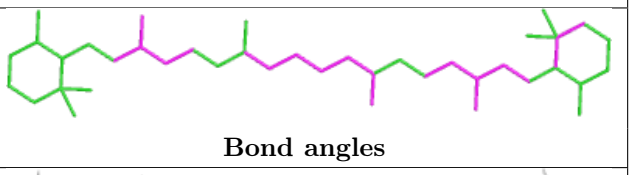


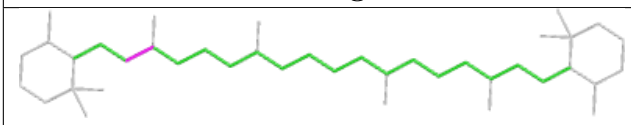
Rings

Ligand BCR B 847

Bond lengths



Bond angles



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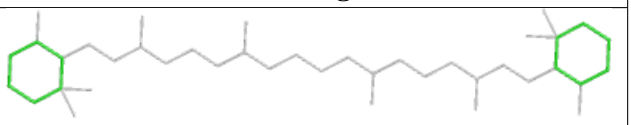
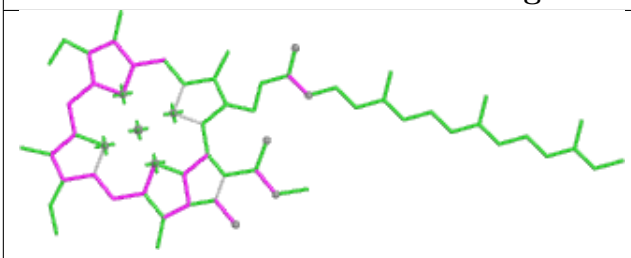


Rings

Ligand CLA A 827



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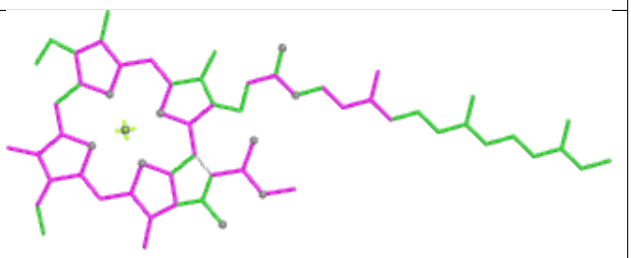

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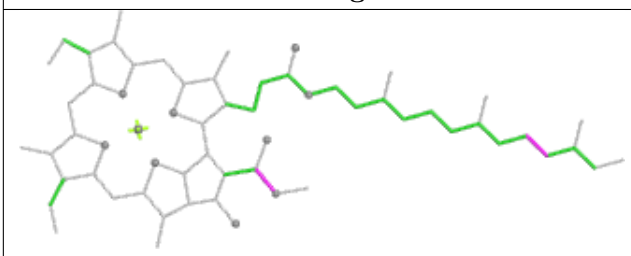

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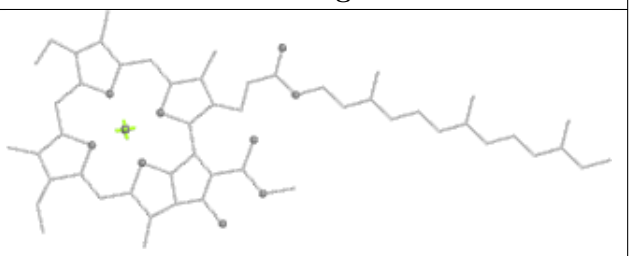
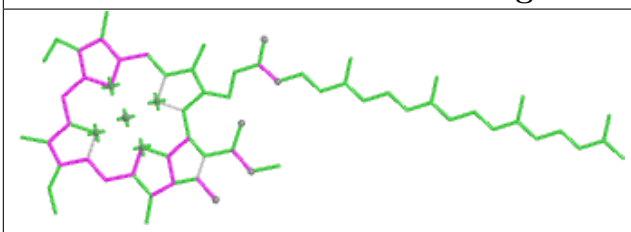


Rings

Ligand CLA cA 837



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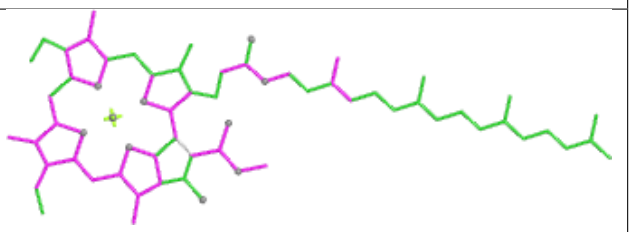
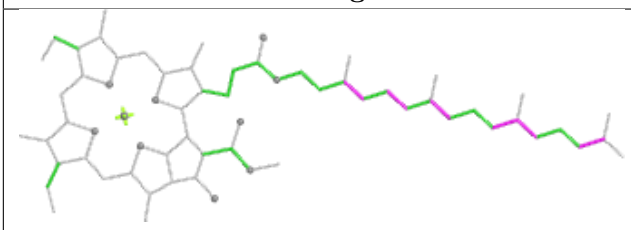


Bond angles



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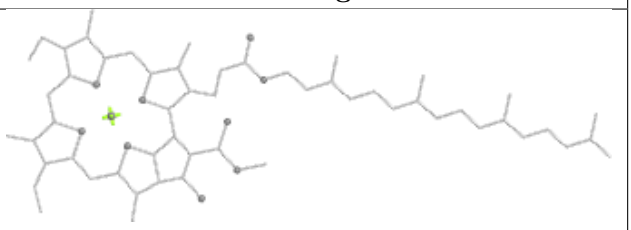
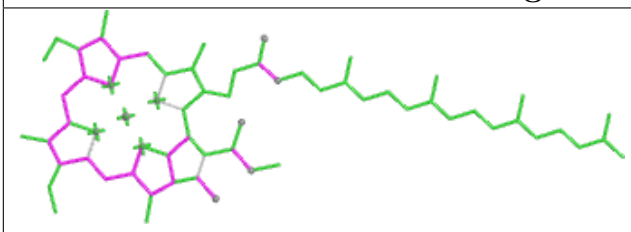


Rings

Ligand CLA B 805



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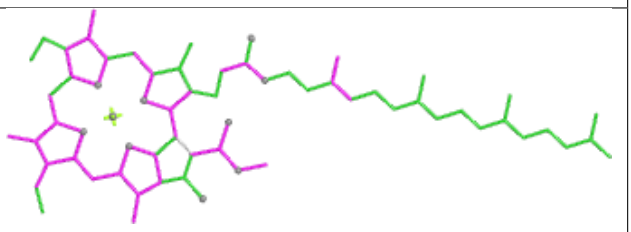
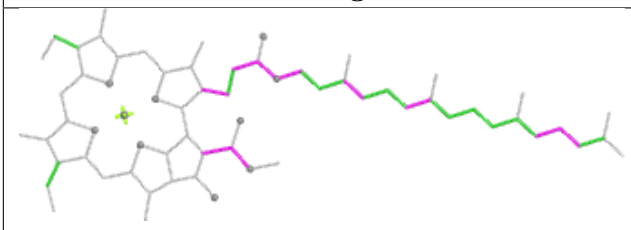


Bond angles



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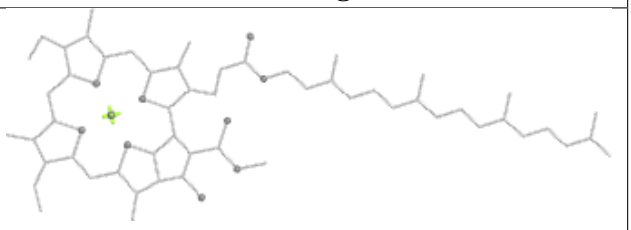
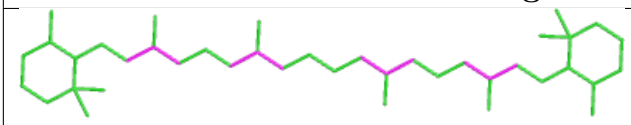


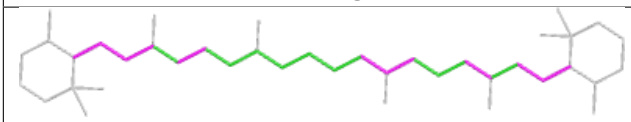
Rings

Ligand BCR B 850



Bond lengths

Bond angles



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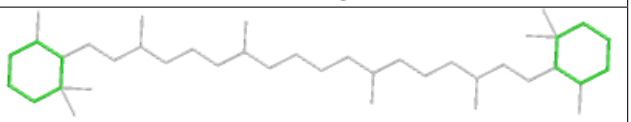
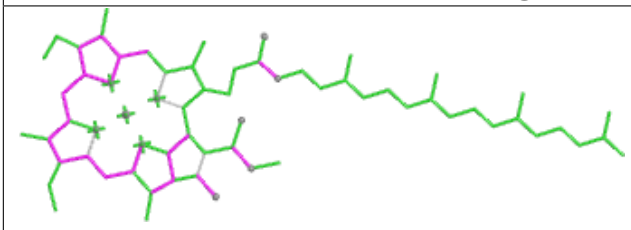
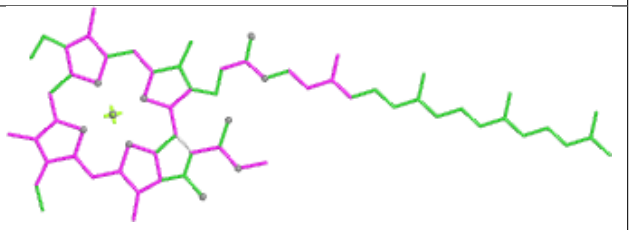


Rings

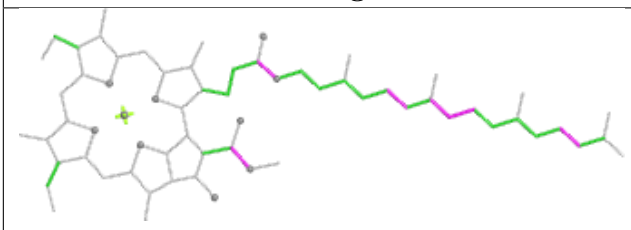
Ligand CLA cA 839



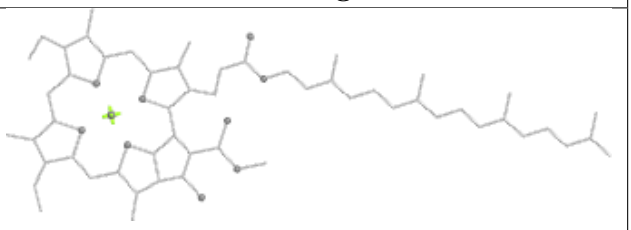
Bond lengths



Bond angles

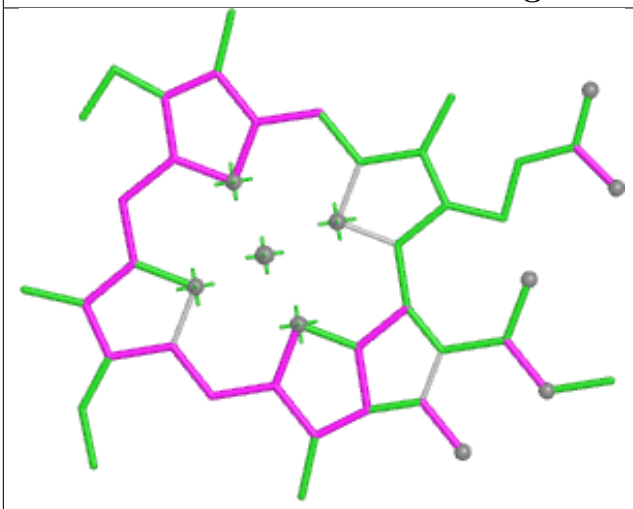


Torsions



Rings

Ligand CLA A 822



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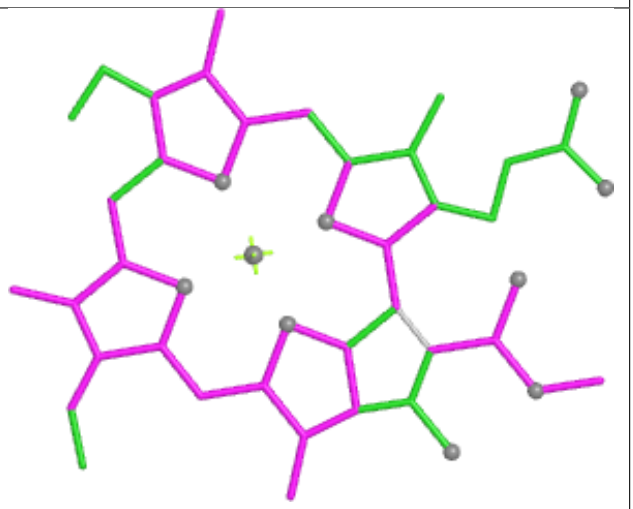
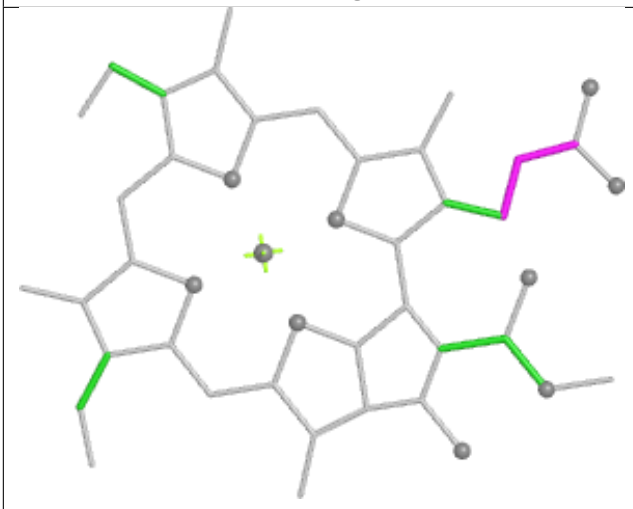


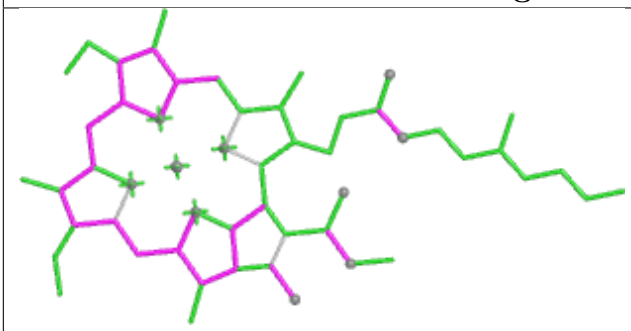
Bond angles



Torsions

Rings

Ligand CLA bA 804



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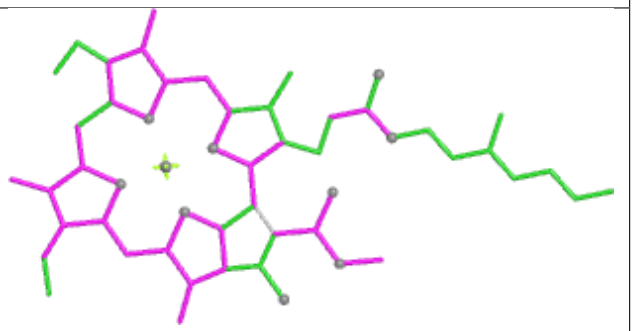
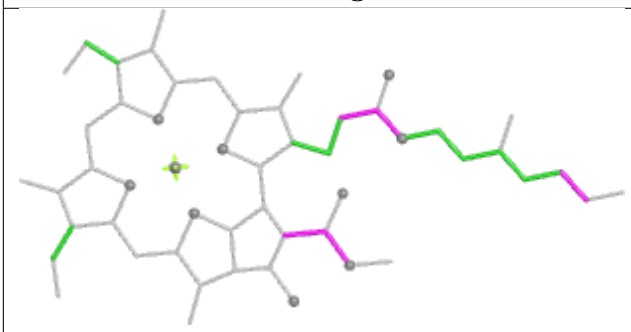
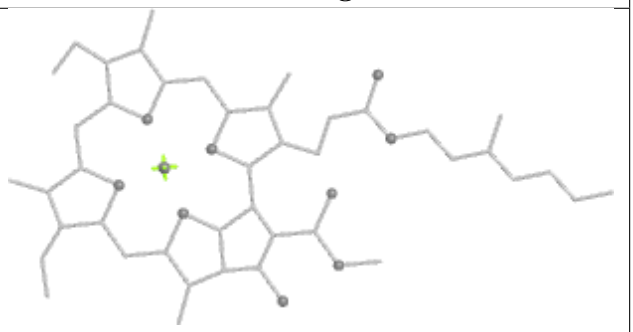


Bond angles

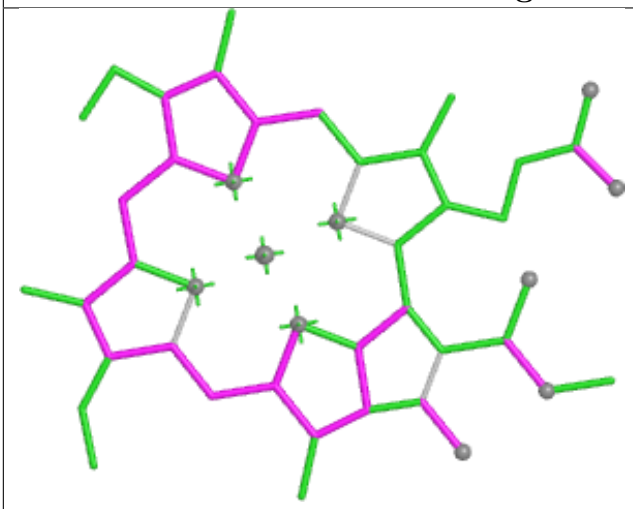


Torsions

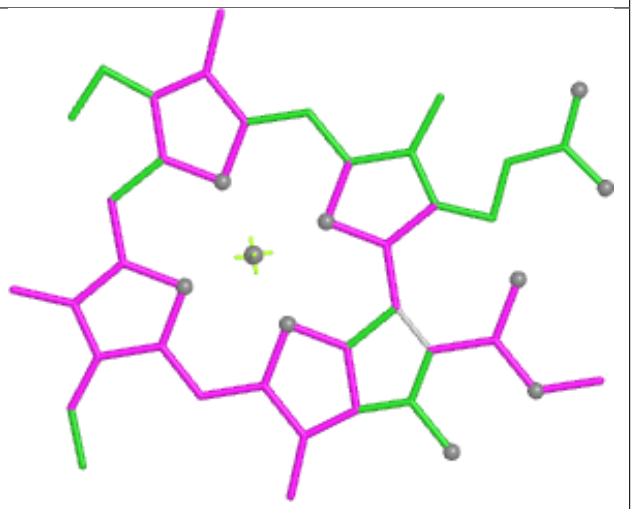


Rings

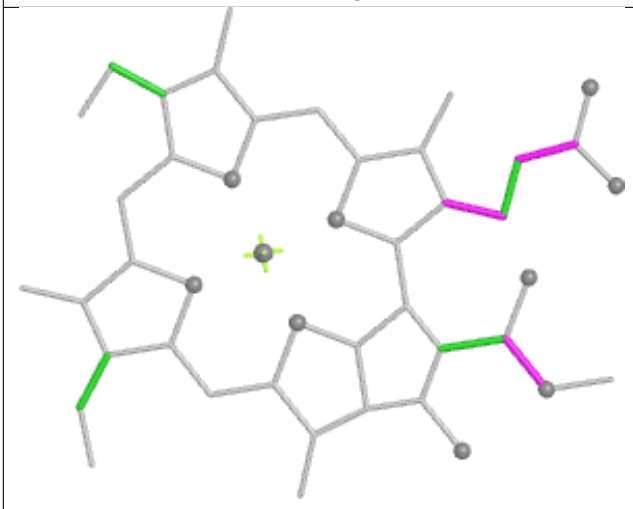
Ligand CLA cA 810



Bond lengths



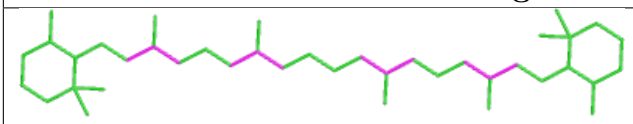
Bond angles



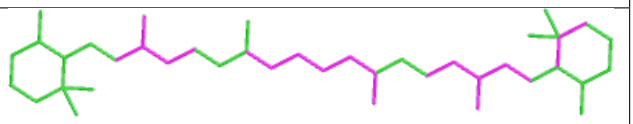
Torsions

Rings

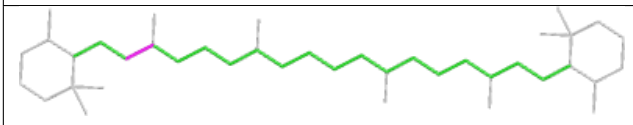
Ligand BCR bB 847



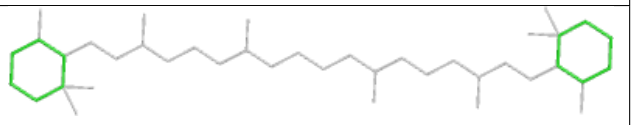
Bond lengths



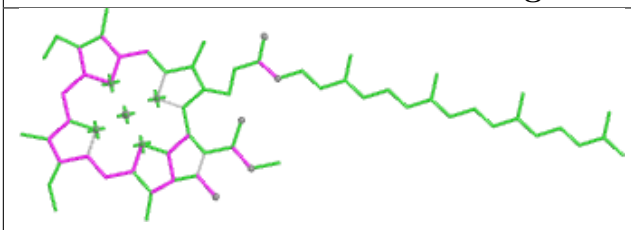
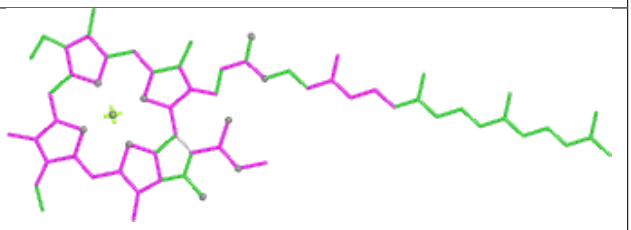
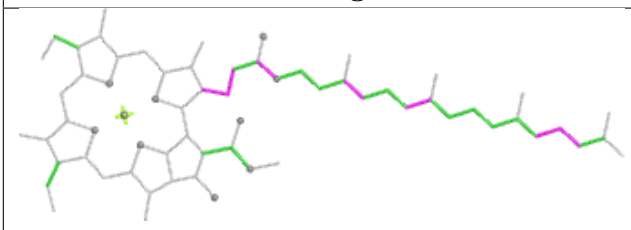
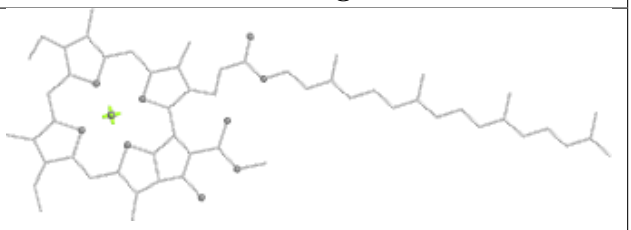
Bond angles

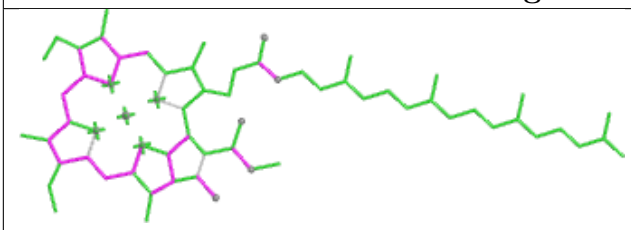
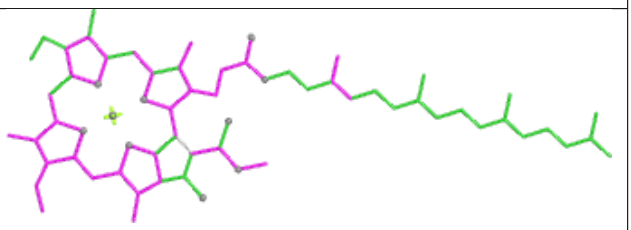
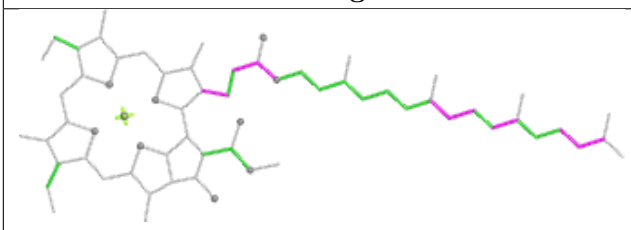
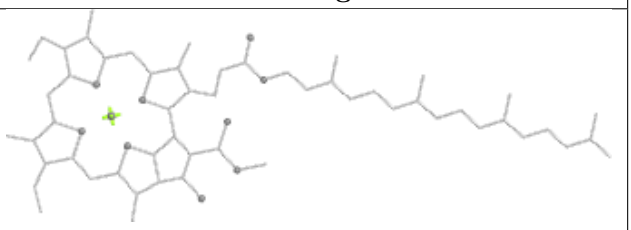


Torsions

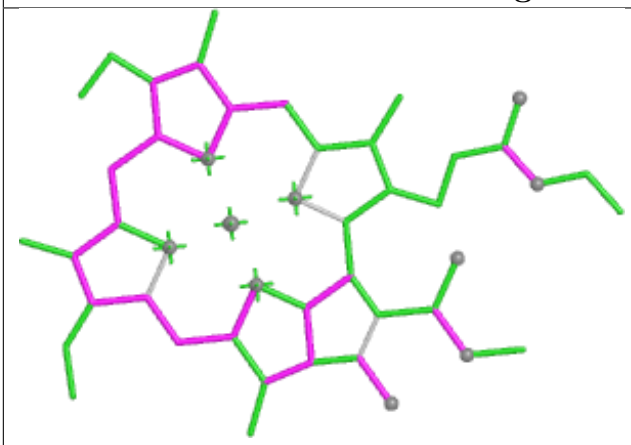


Rings

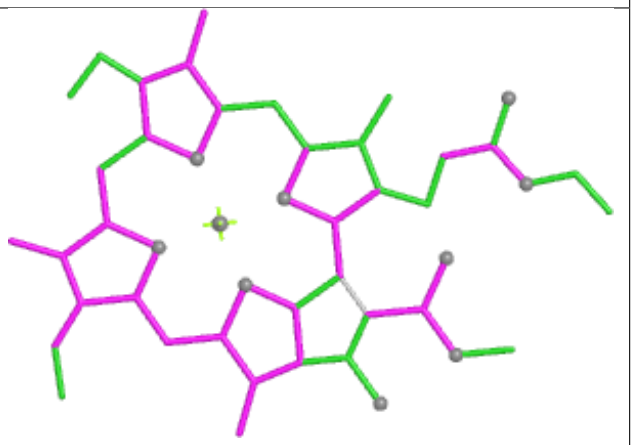
Ligand CLA B 809	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 841	
	
Bond lengths	Bond angles
	
Torsions	Rings

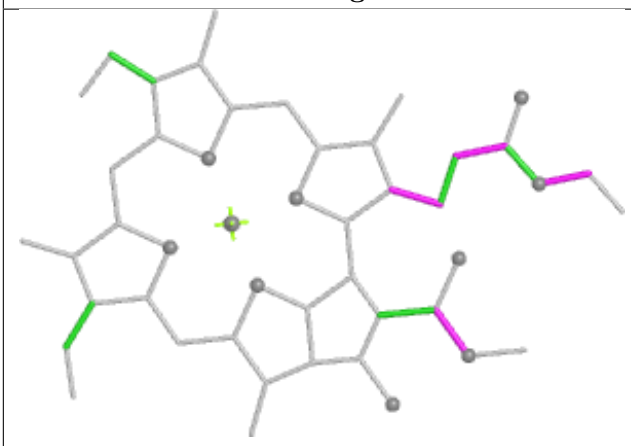
Ligand CLA bB 837



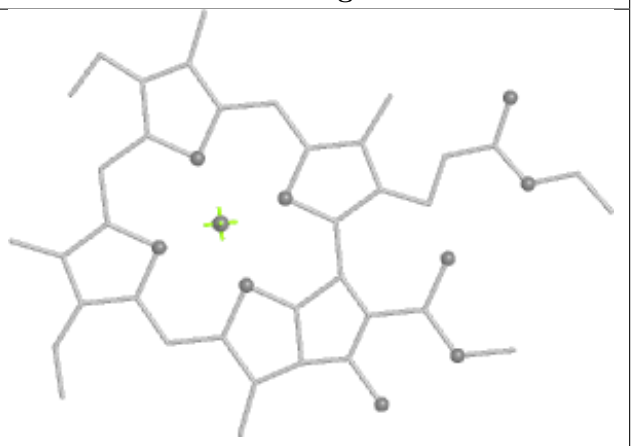
Bond lengths



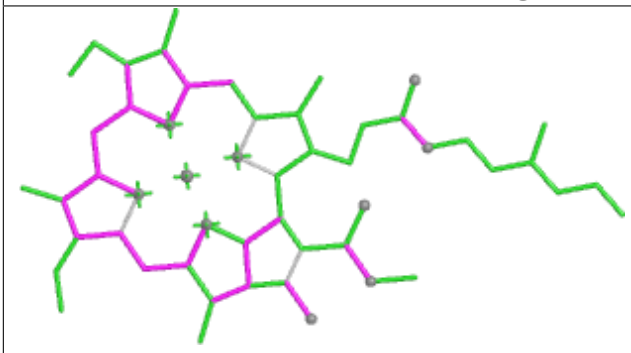
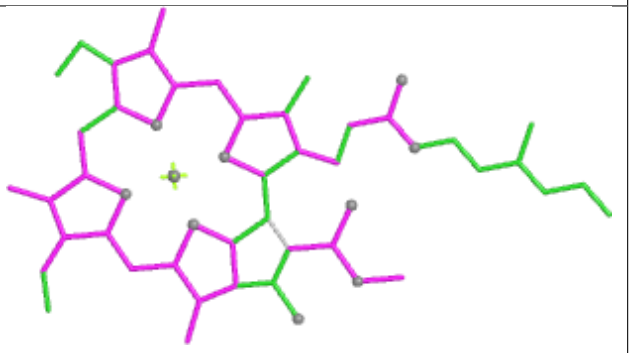
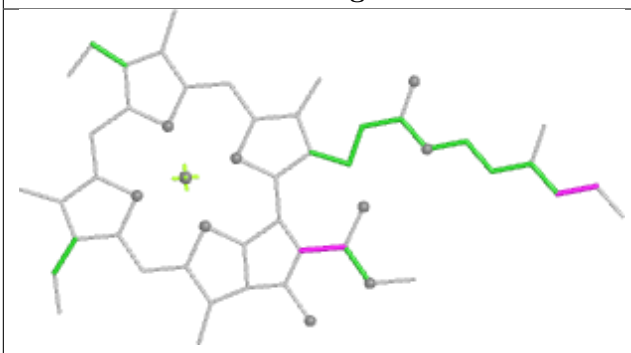
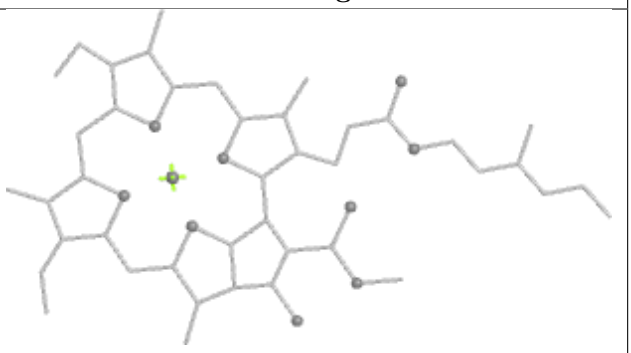
Bond angles

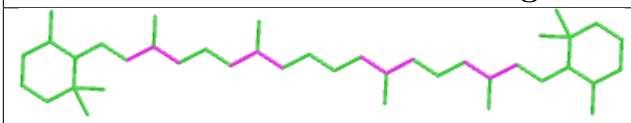
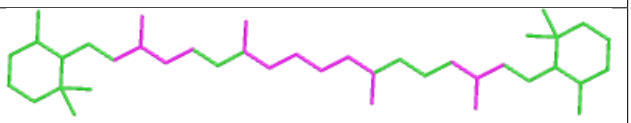
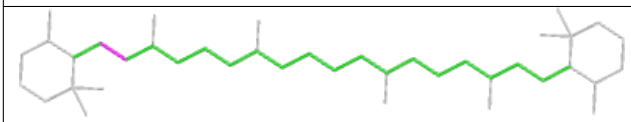
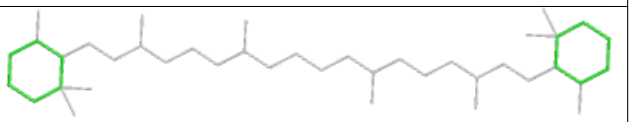


Torsions

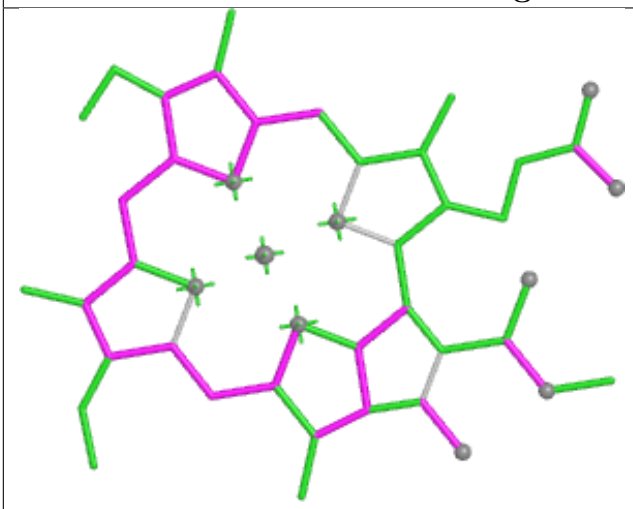


Rings

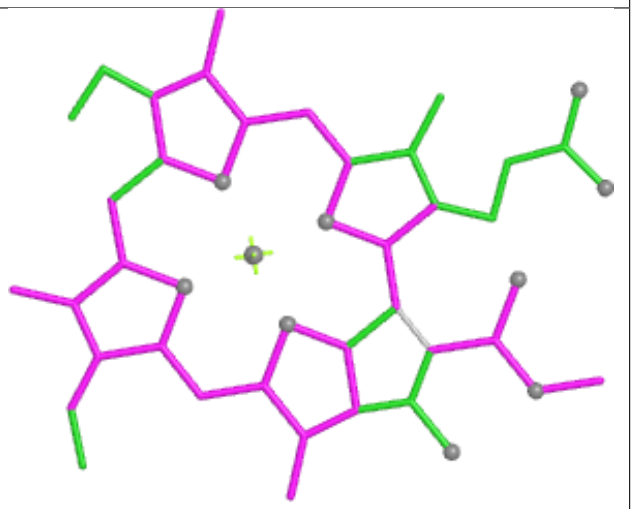
Ligand CLA bB 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR cI 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

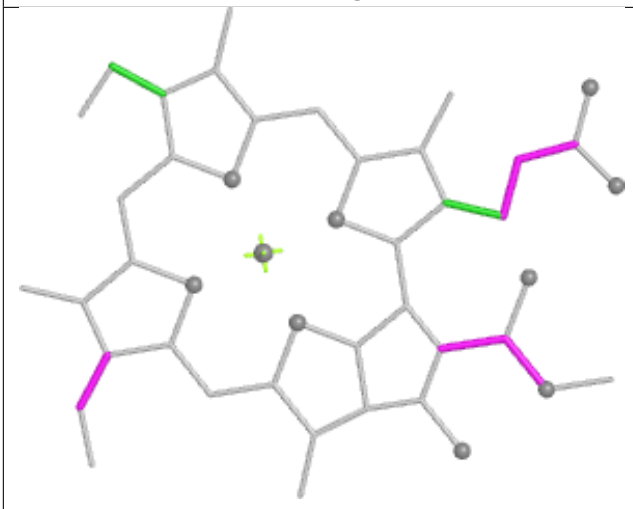
Ligand CLA bA 807



Bond lengths



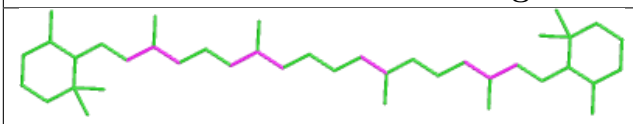
Bond angles



Torsions

Rings

Ligand BCR bA 845



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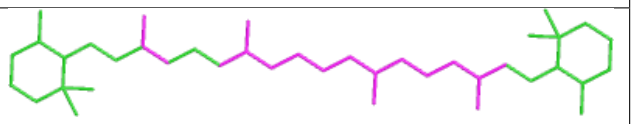
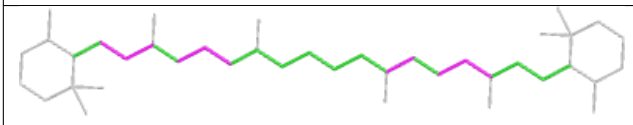
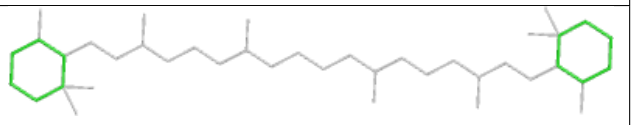


Bond angles

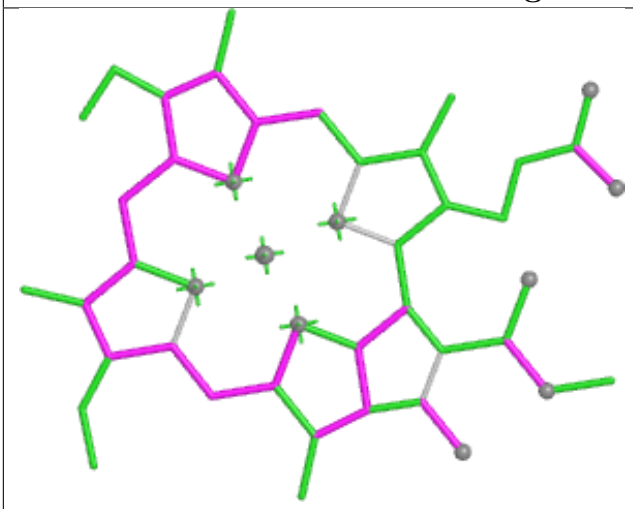


Torsions

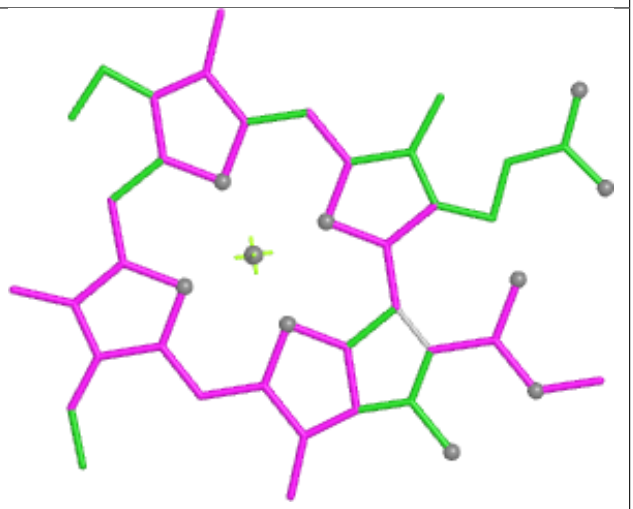


Rings

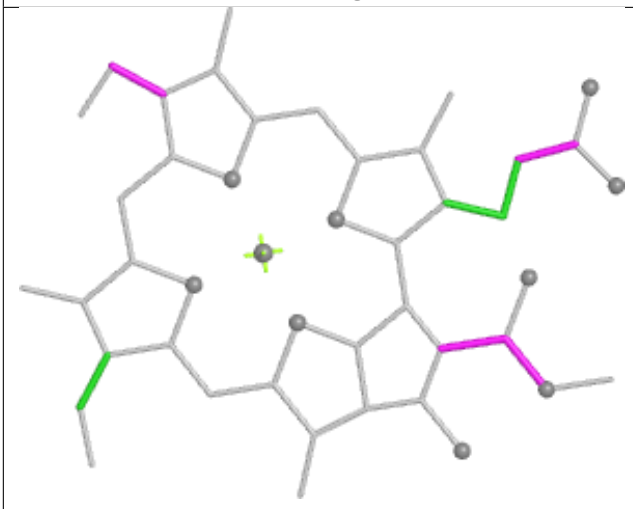
Ligand CLA B 836



Bond lengths



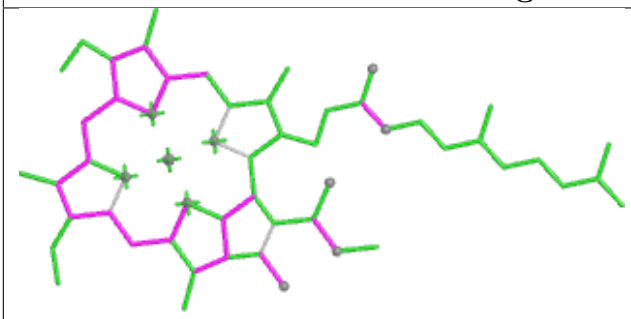
Bond angles



Torsions

Rings

Ligand CLA cB 826



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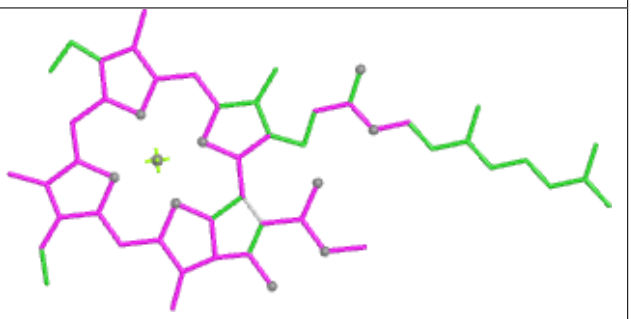
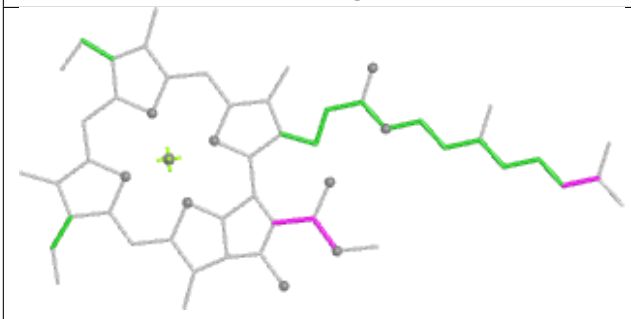
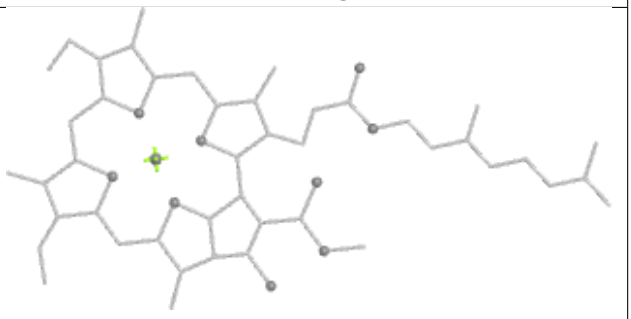


Bond angles

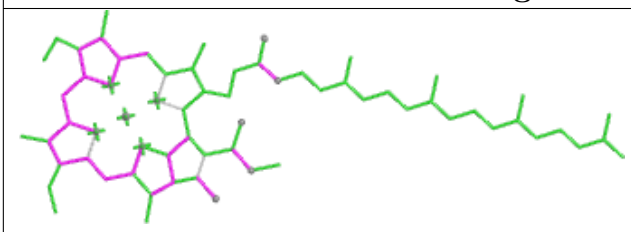


Torsions



Rings

Ligand CLA bA 833



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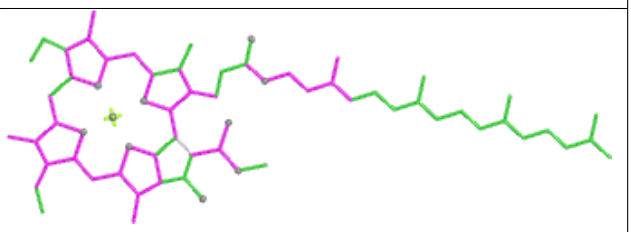
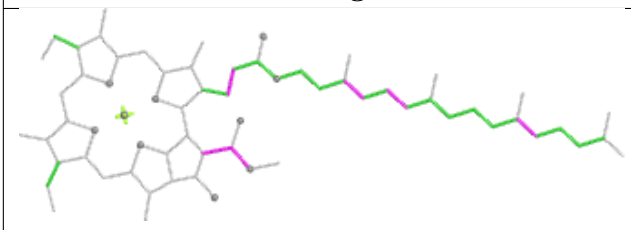
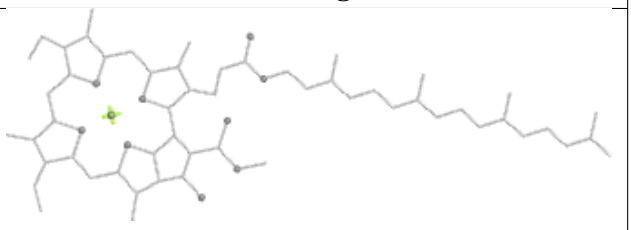


Bond angles

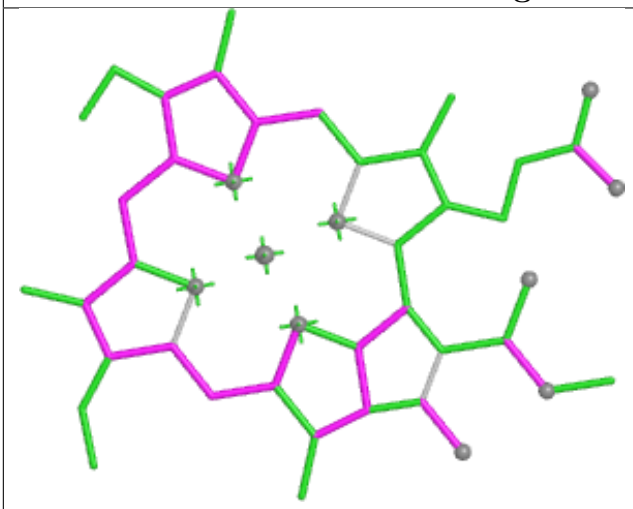


Torsions



Rings

Ligand CLA bA 821



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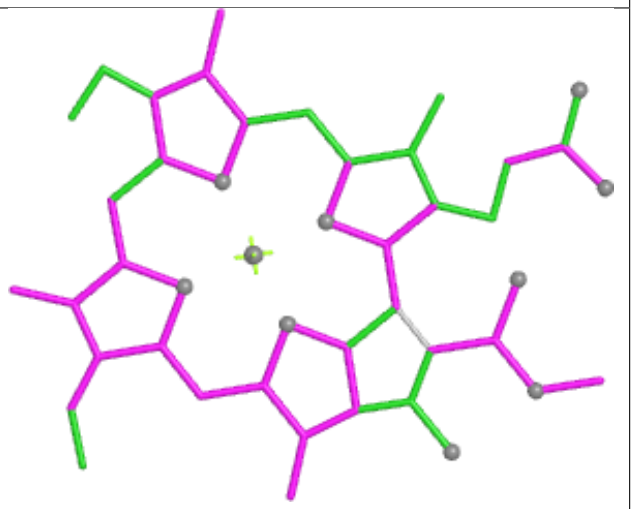
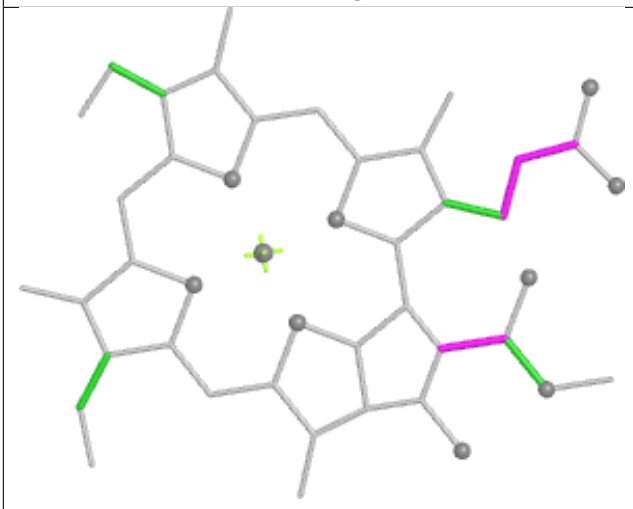


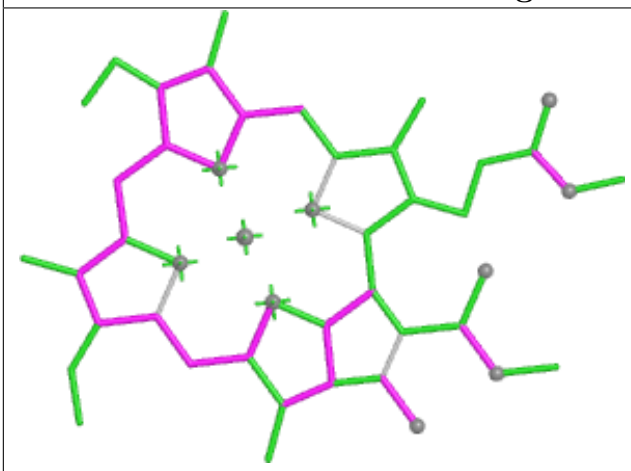
Bond angles



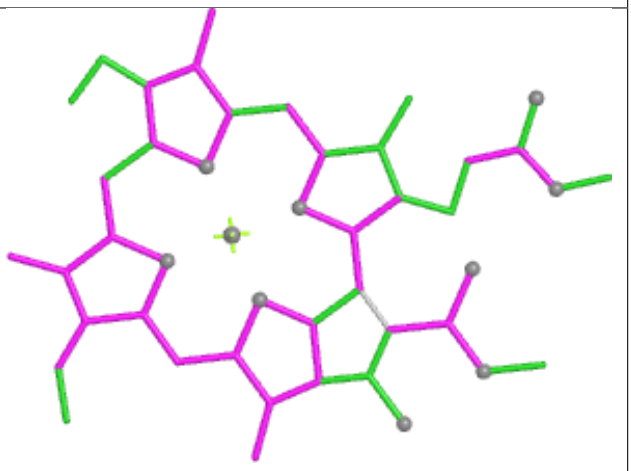
Torsions

Rings

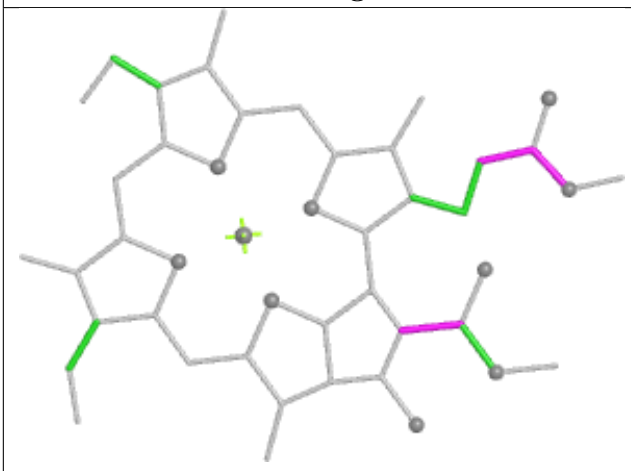
Ligand CLA cA 826



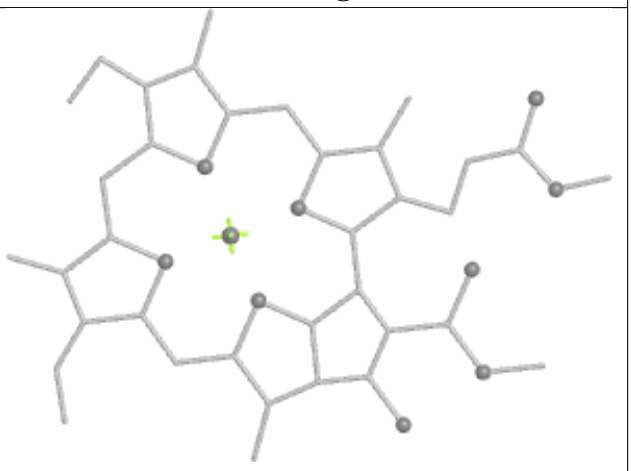
Bond lengths



Bond angles

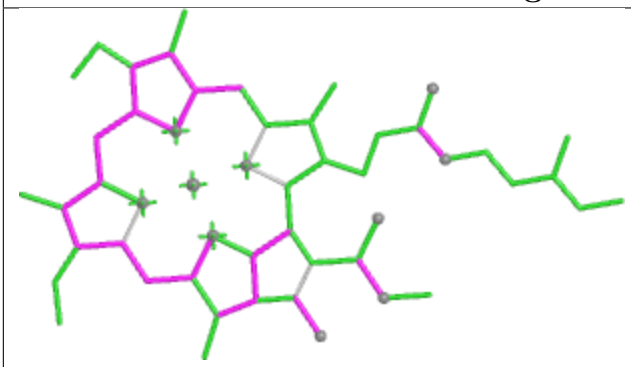


Torsions

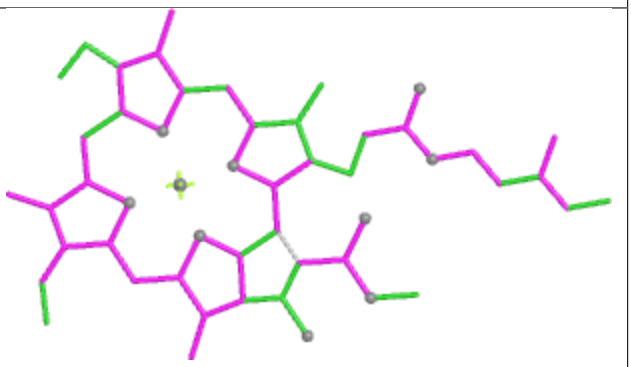


Rings

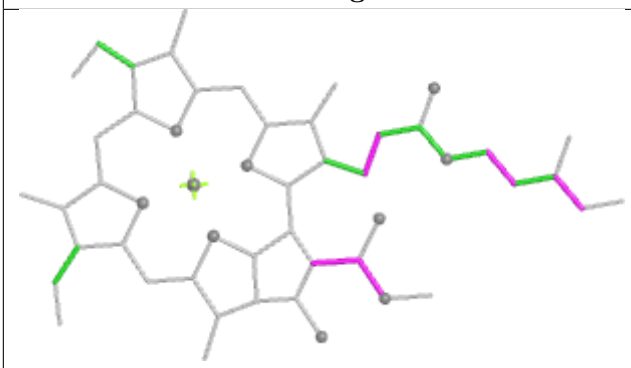
Ligand CLA B 804



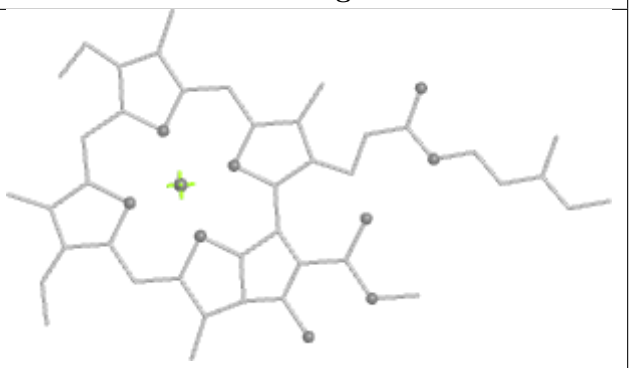
Bond lengths



Bond angles

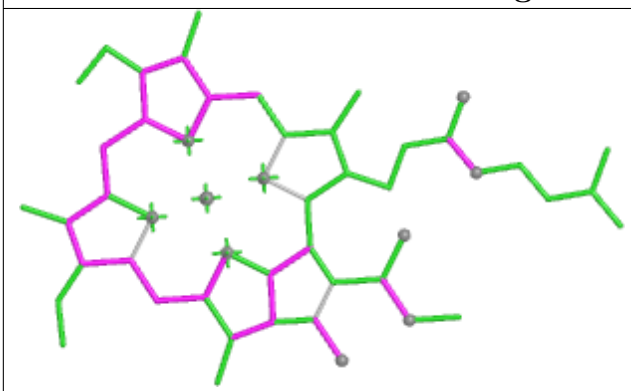


Torsions

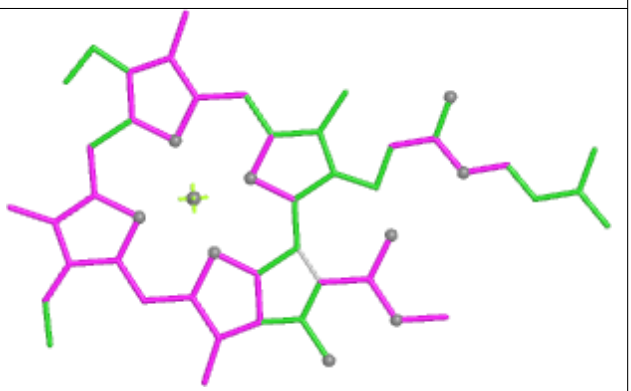


Rings

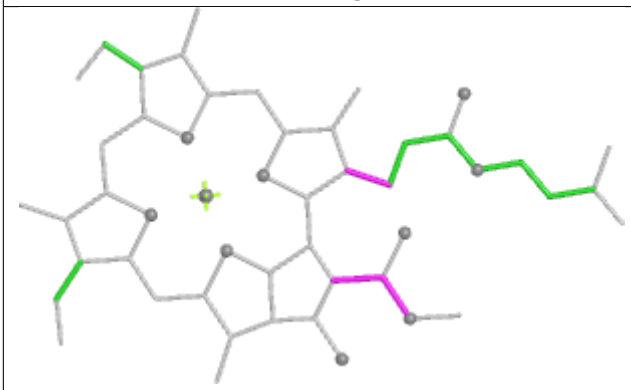
Ligand CLA bB 823



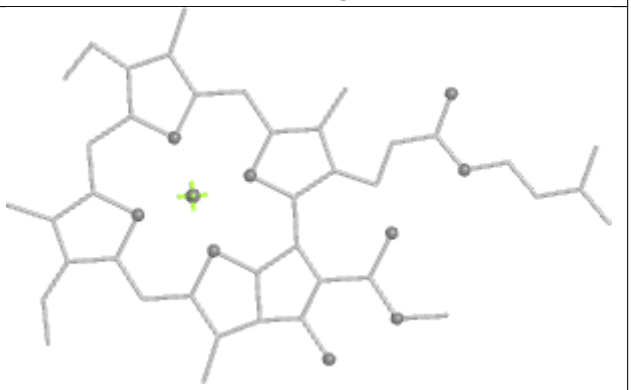
Bond lengths



Bond angles

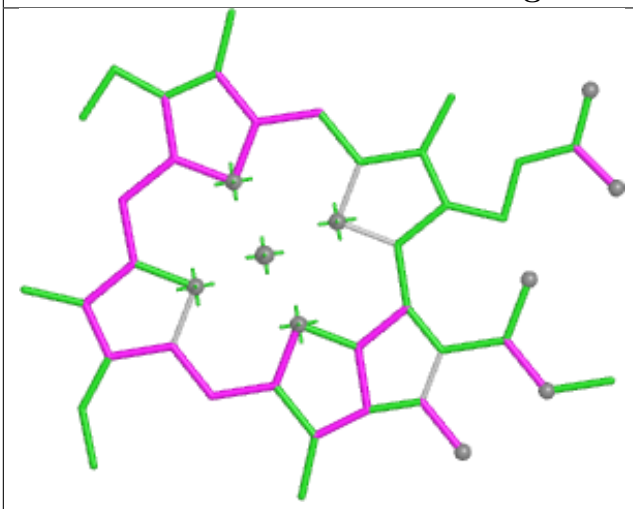


Torsions



Rings

Ligand CLA A 838



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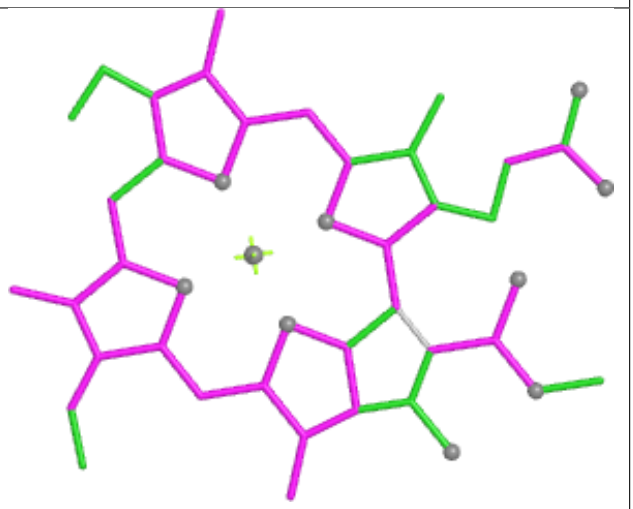
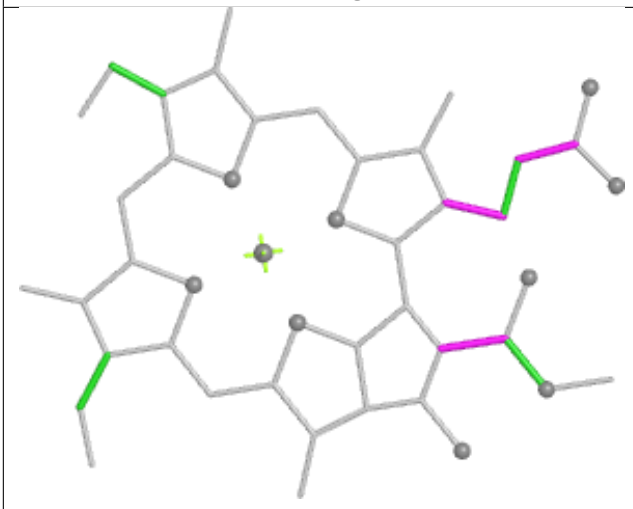


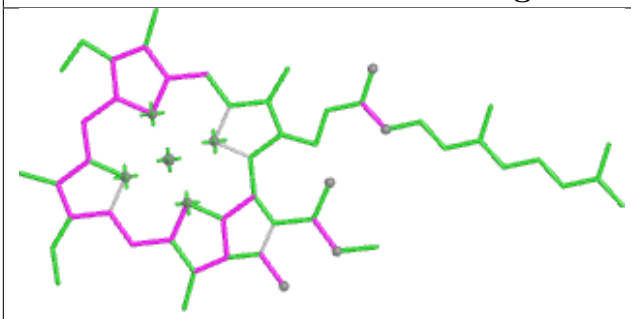
Bond angles



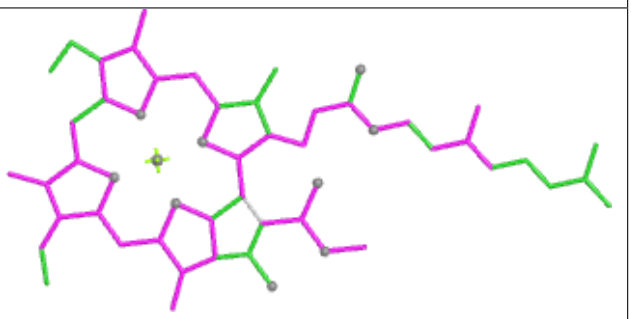
Torsions

Rings

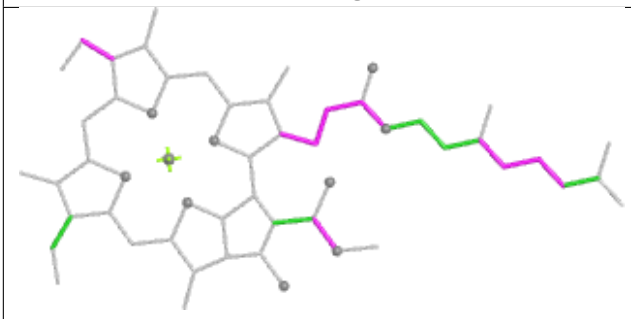
Ligand CLA bA 831



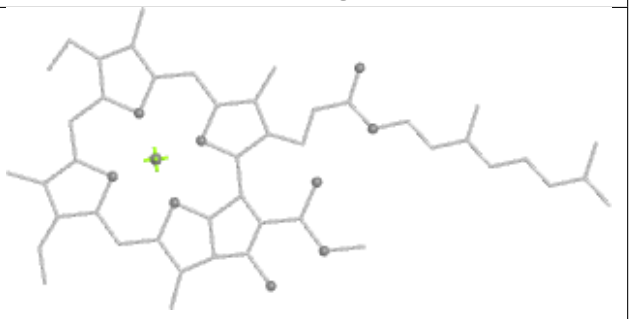
Bond lengths



Bond angles

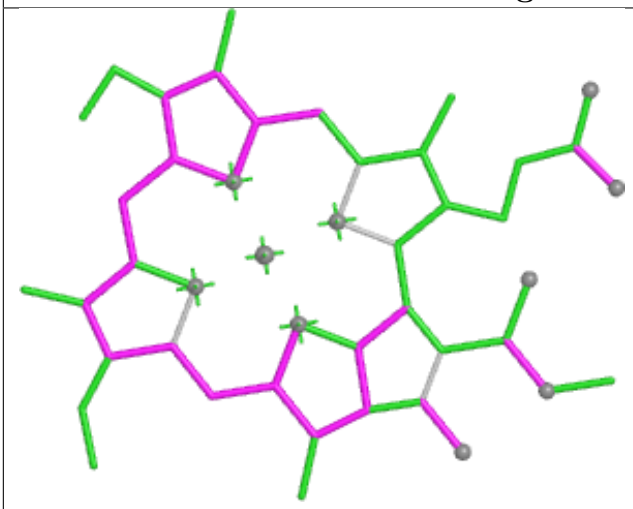


Torsions



Rings

Ligand CLA cB 817



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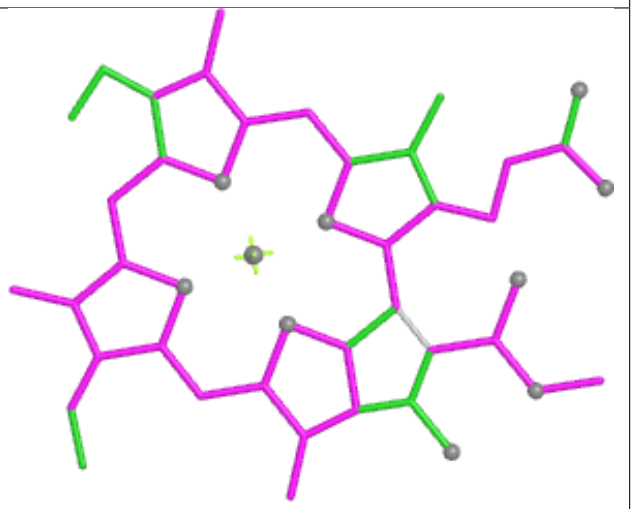
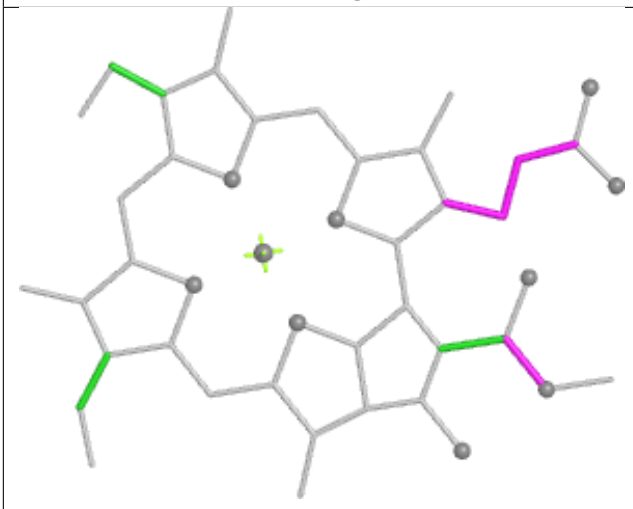


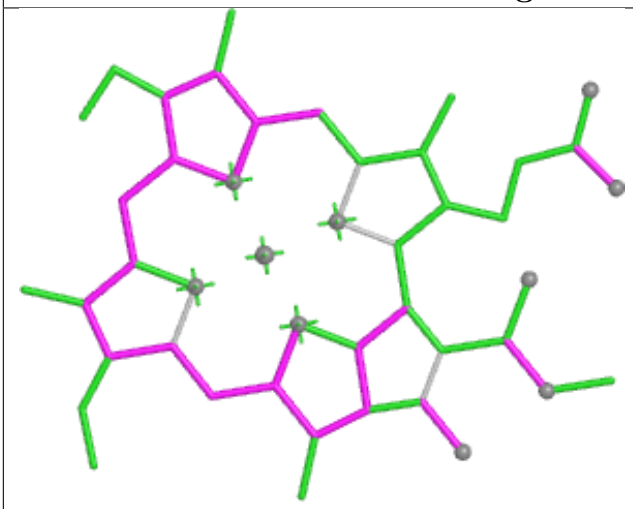
Bond angles



Torsions

Rings

Ligand CLA cX 201



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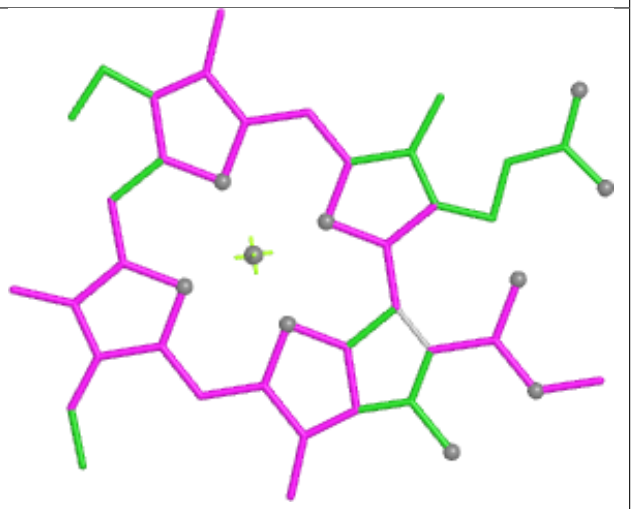
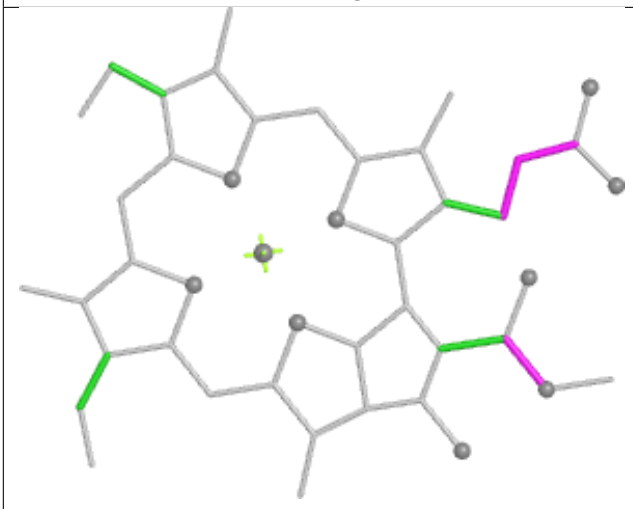


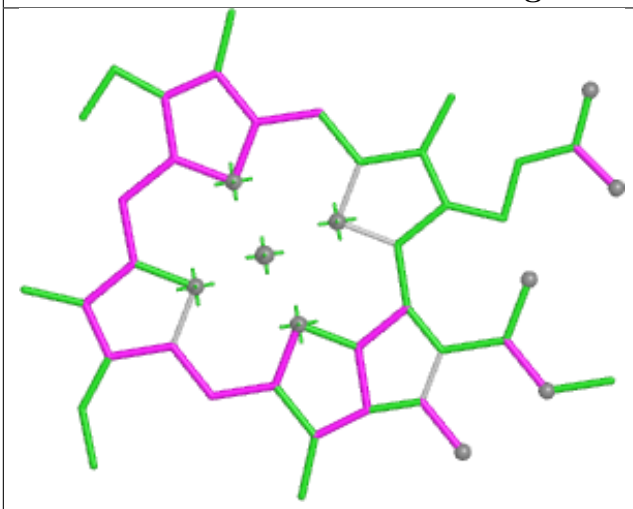
Bond angles



Torsions

Rings

Ligand CLA B 851



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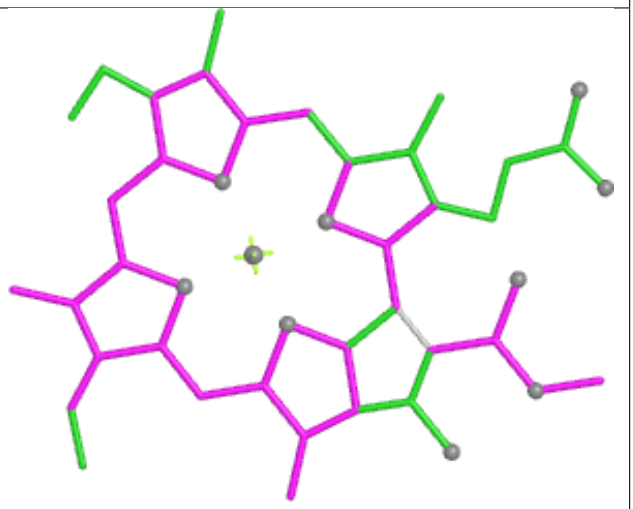
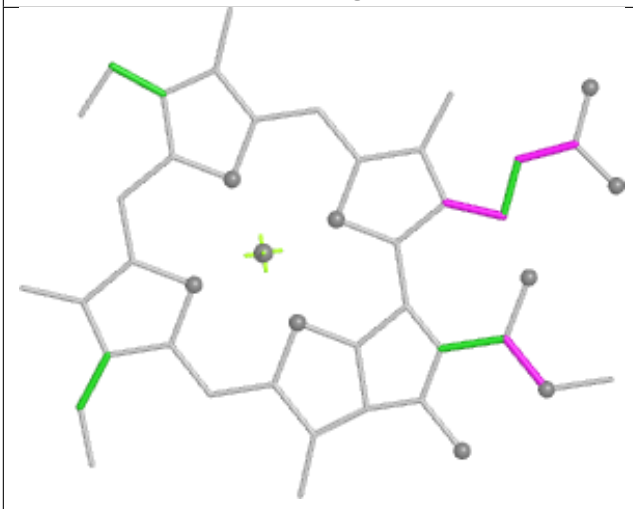


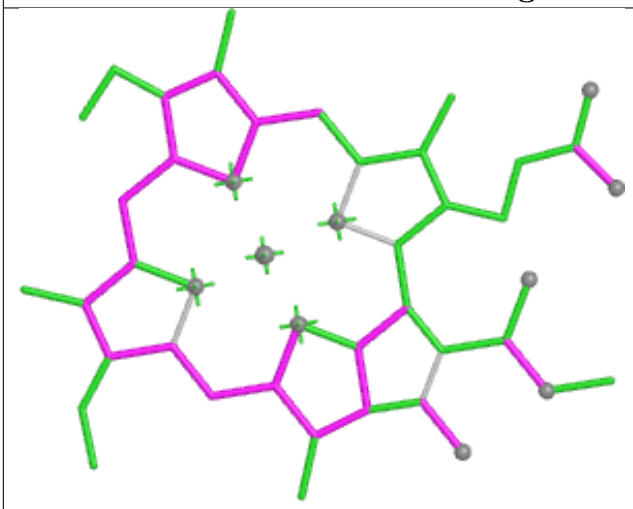
Bond angles



Torsions

Rings

Ligand CLA bJ 102



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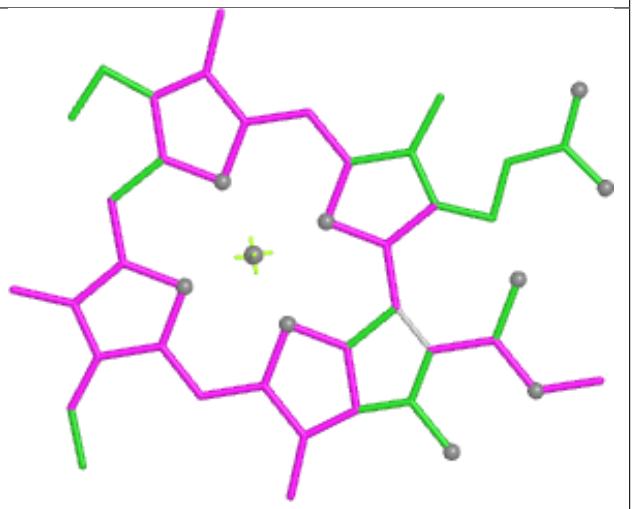
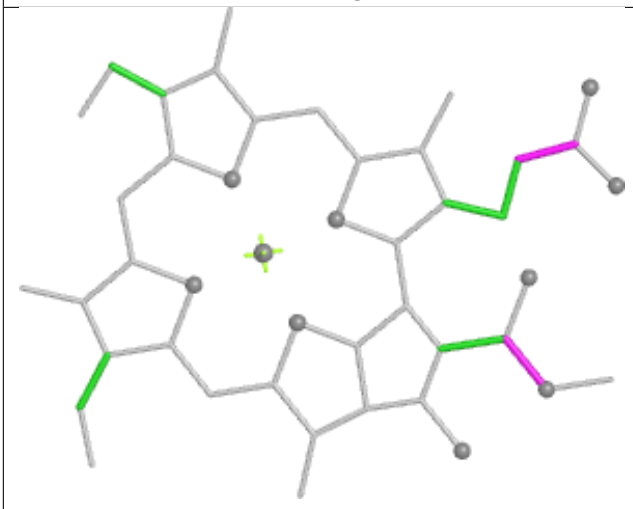


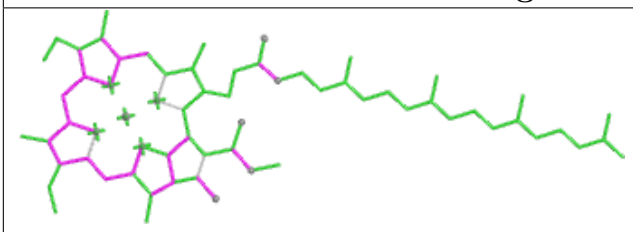
Bond angles



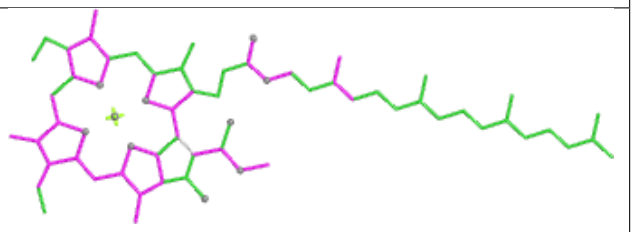
Torsions

Rings

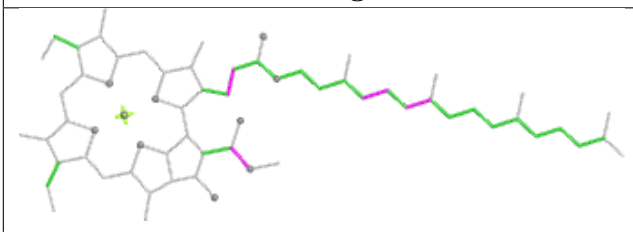
Ligand CLA cB 839



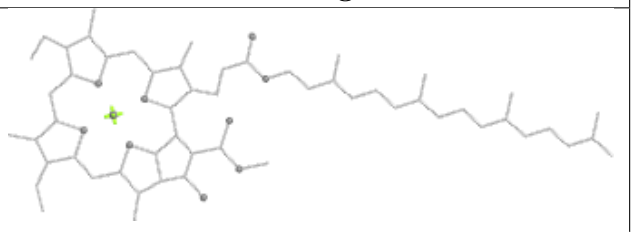
Bond lengths



Bond angles

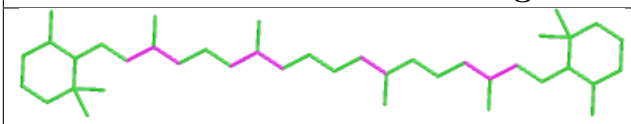


Torsions



Rings

Ligand BCR cA 849



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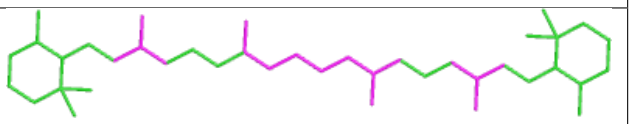
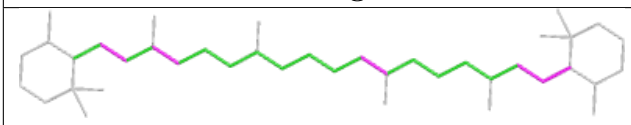


Bond angles



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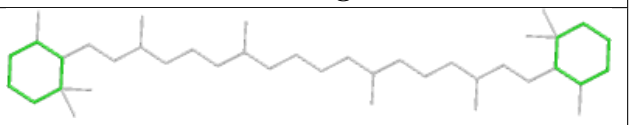
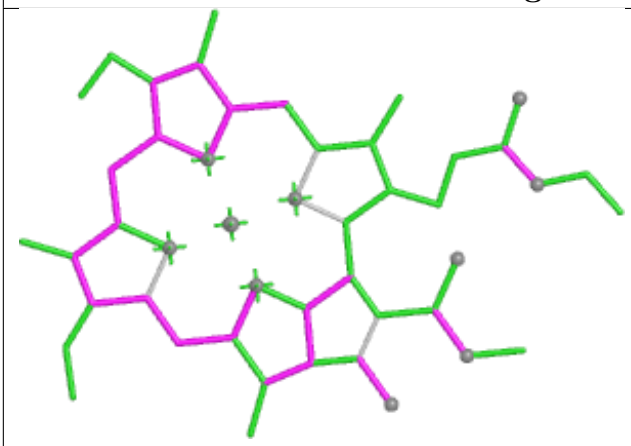


Rings

Ligand CLA B 837



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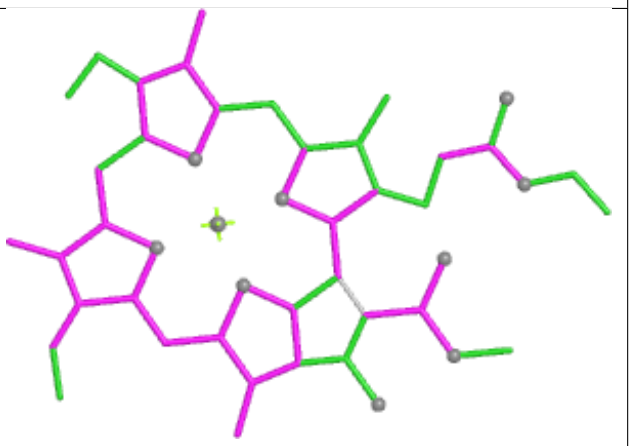
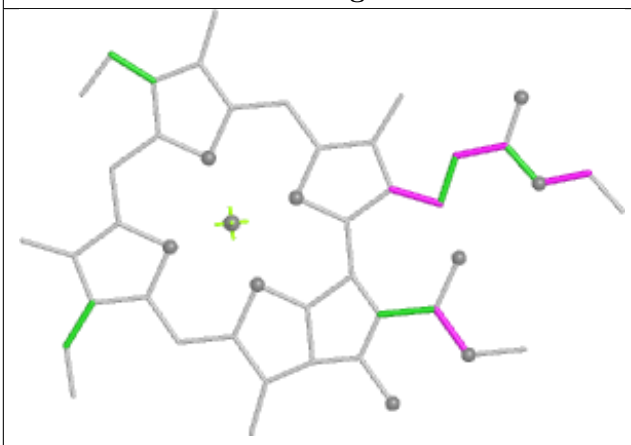
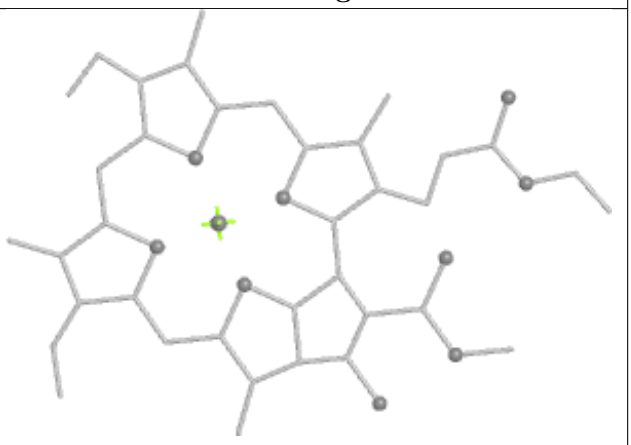


Bond angles

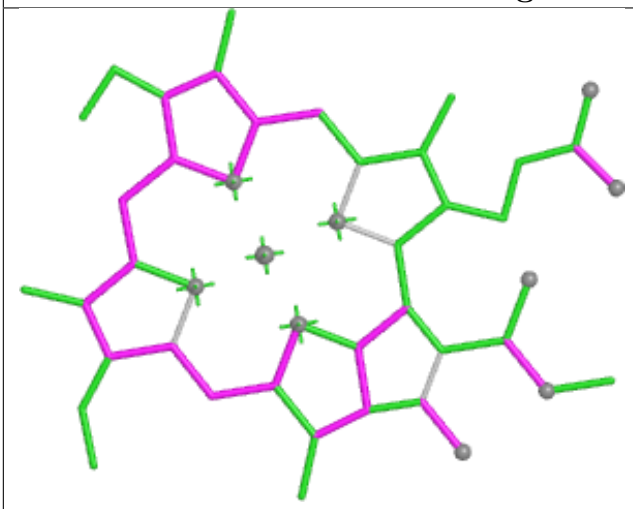


Torsions



Rings

Ligand CLA cB 836



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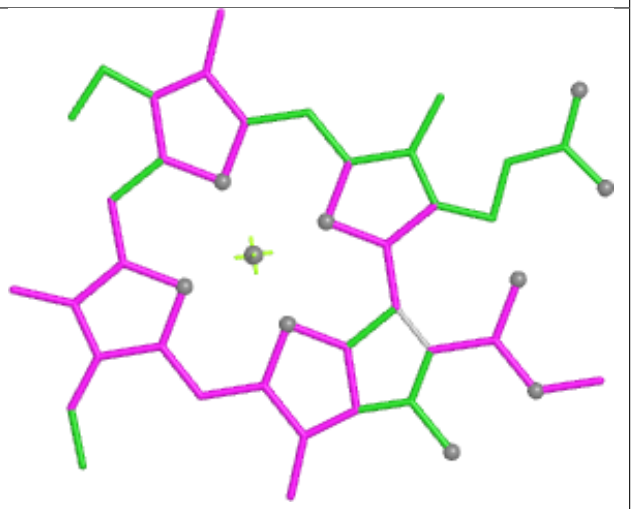
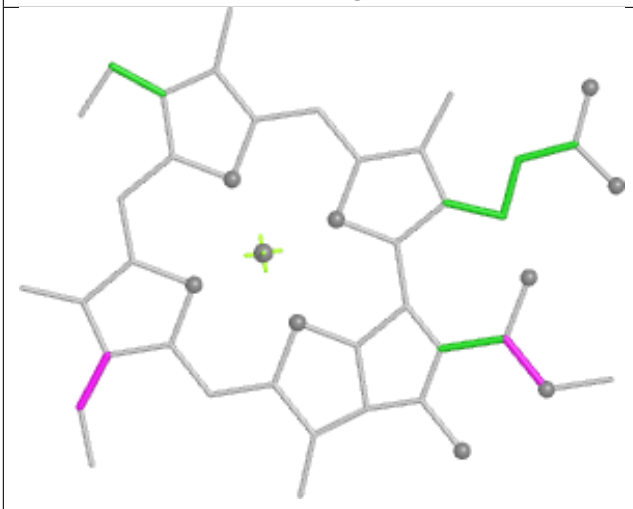


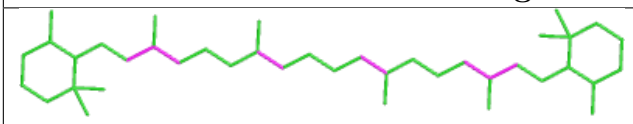
Bond angles



Torsions

Rings

Ligand BCR bF 202



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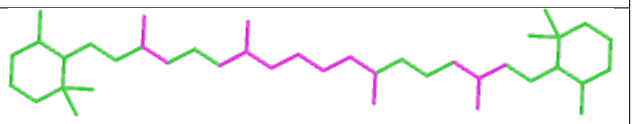
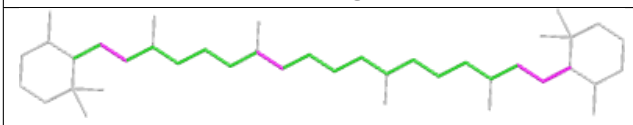
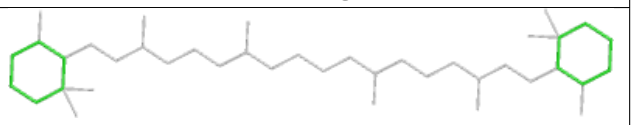


Bond angles

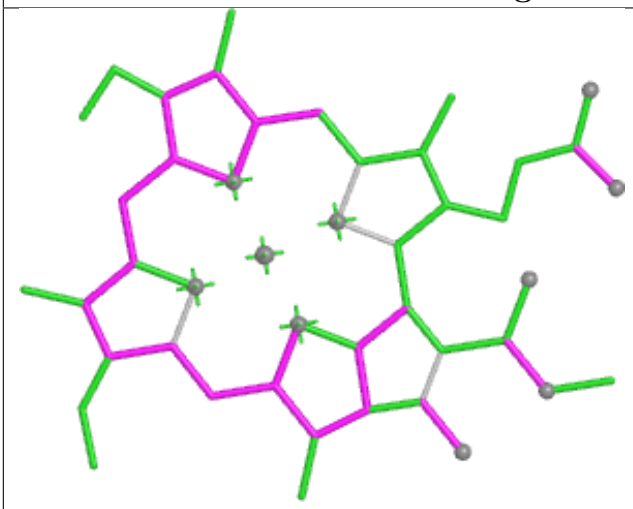


Torsions



Rings

Ligand CLA bB 834



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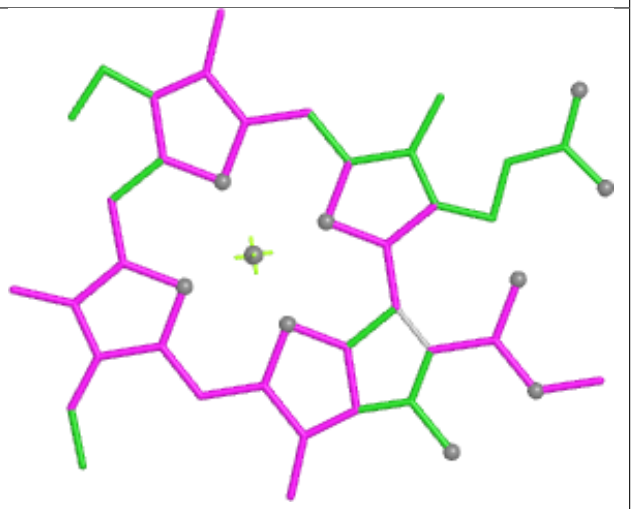
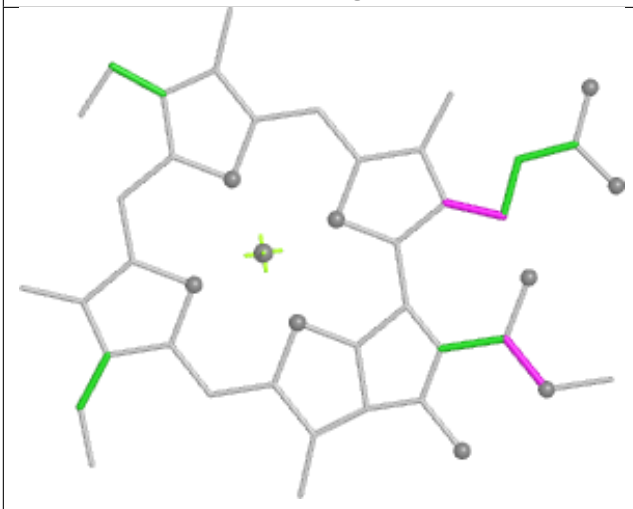


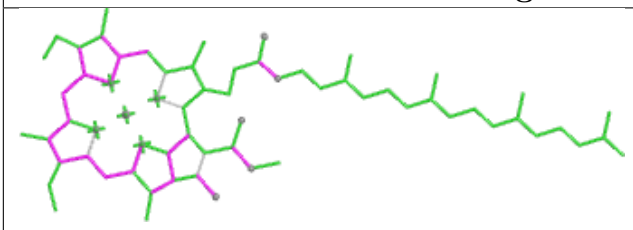
Bond angles



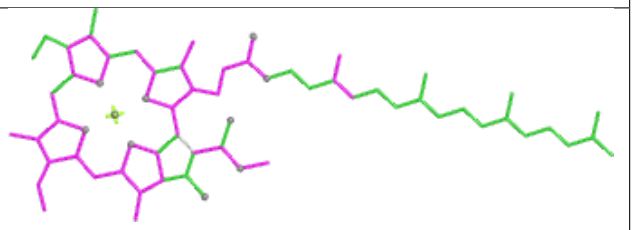
Torsions

Rings

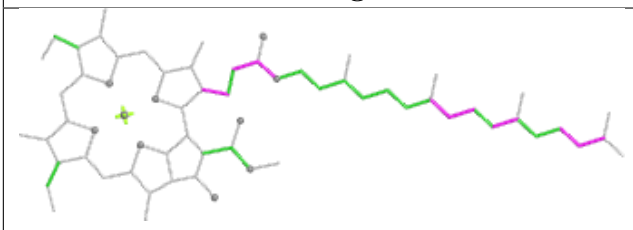
Ligand CLA cA 841



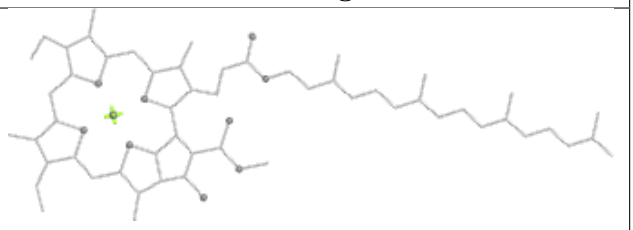
Bond lengths



Bond angles

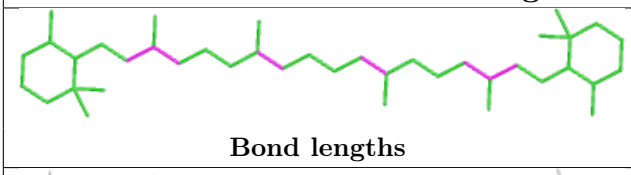


Torsions



Rings

Ligand BCR A 846



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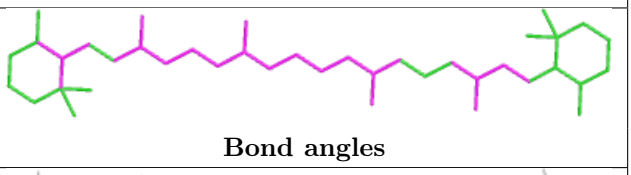

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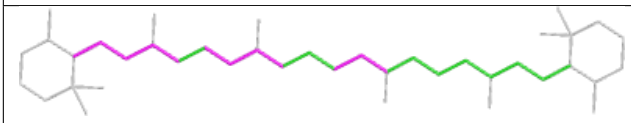

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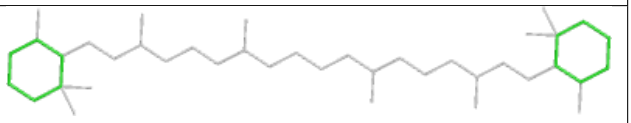
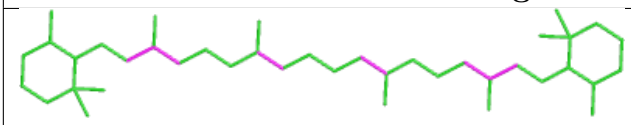


Rings

Ligand BCR bB 841



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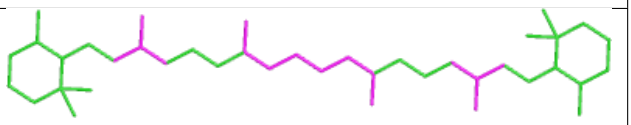
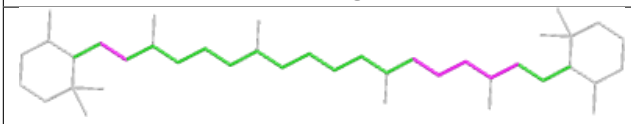


Bond angles



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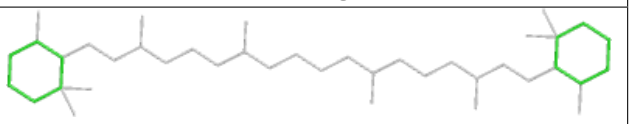
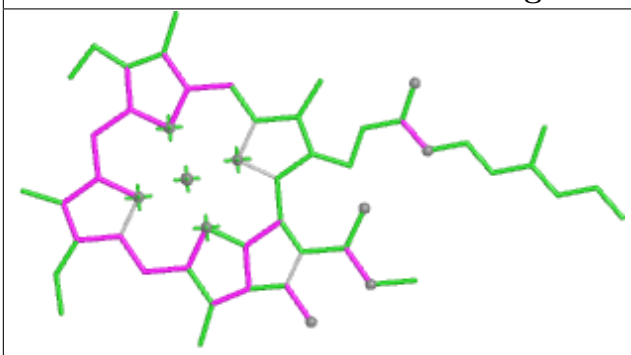


Rings

Ligand CLA B 808



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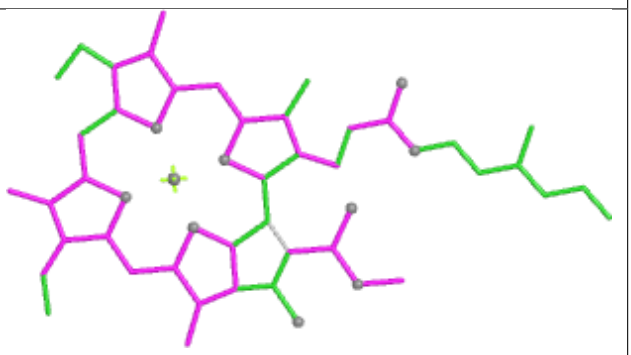
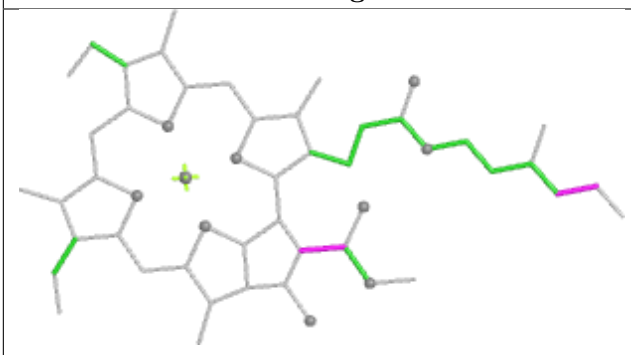


Bond angles



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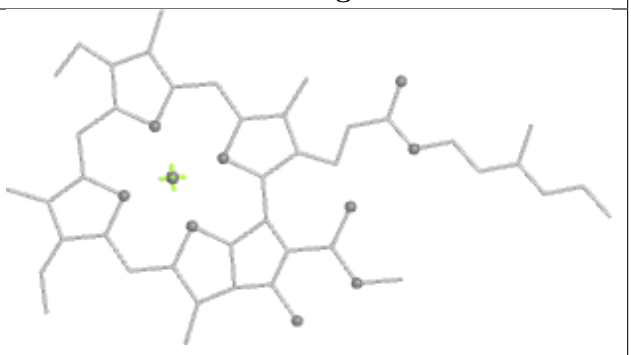
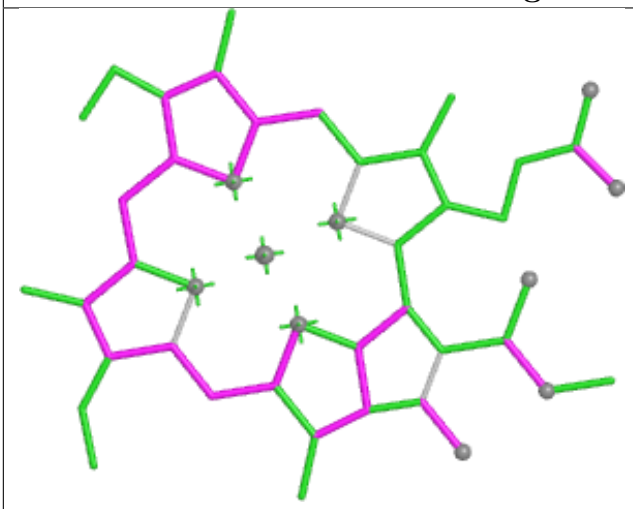


Rings

Ligand CLA A 803



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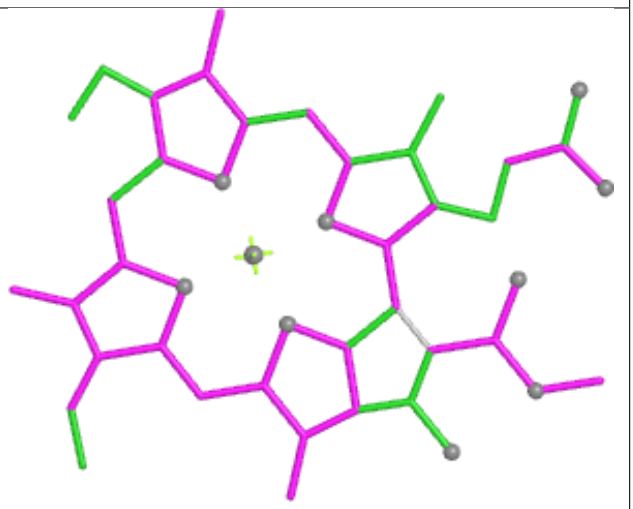
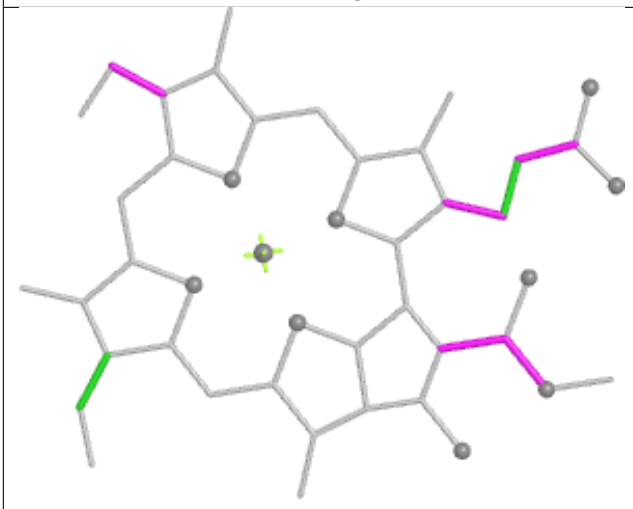


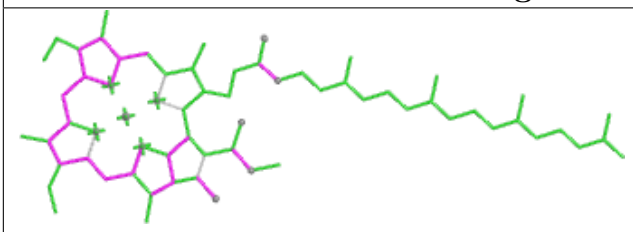
Bond angles



Torsions

Rings

Ligand CLA bB 806



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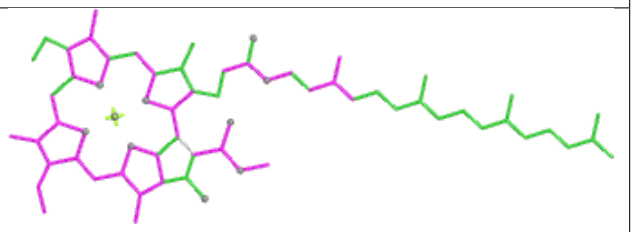
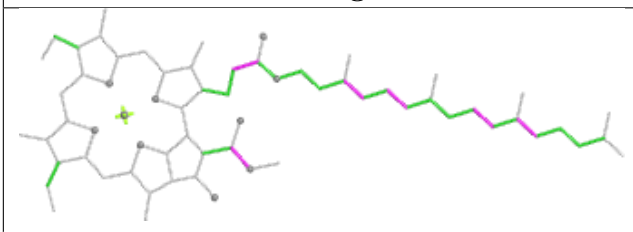


Bond angles



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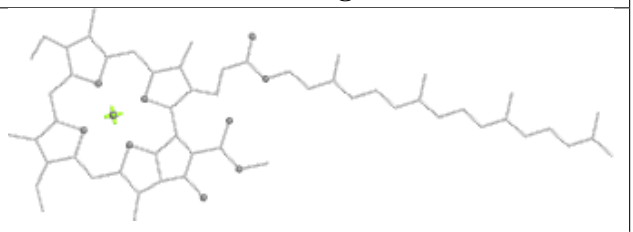
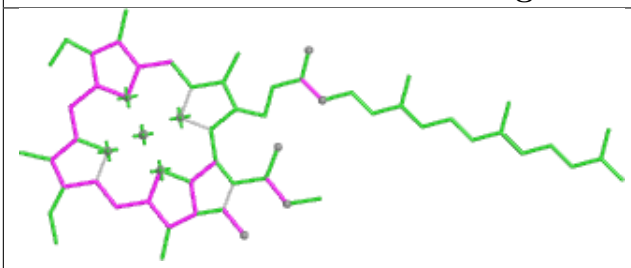


Rings

Ligand CLA cA 818



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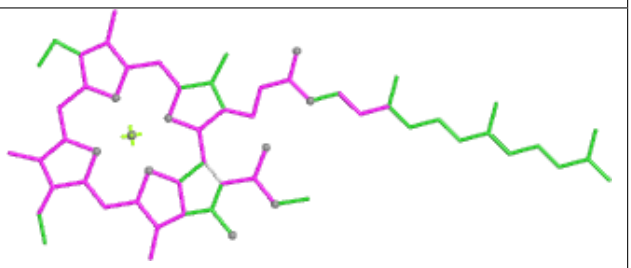
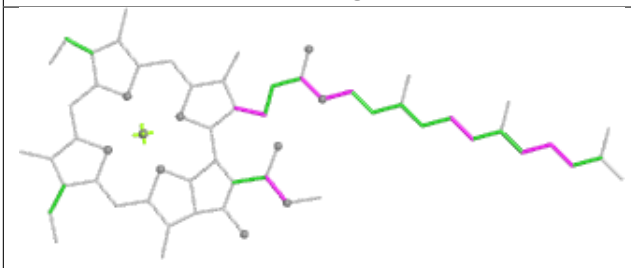


Bond angles



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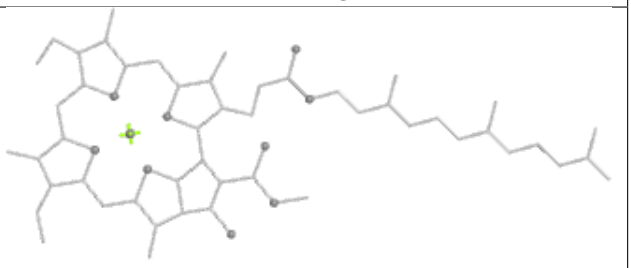
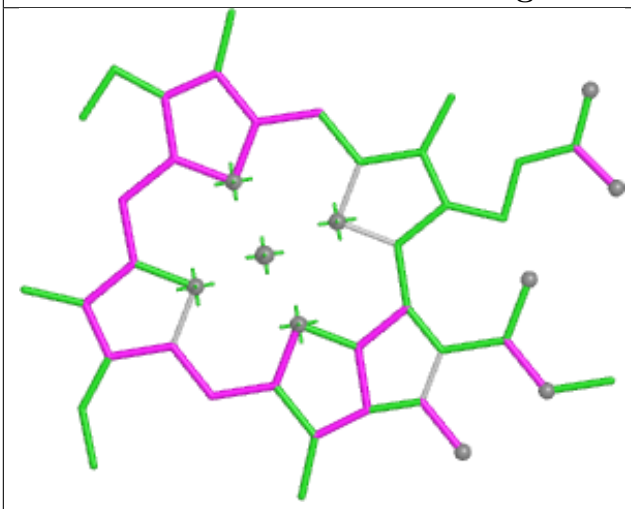


Rings

Ligand CLA cB 812



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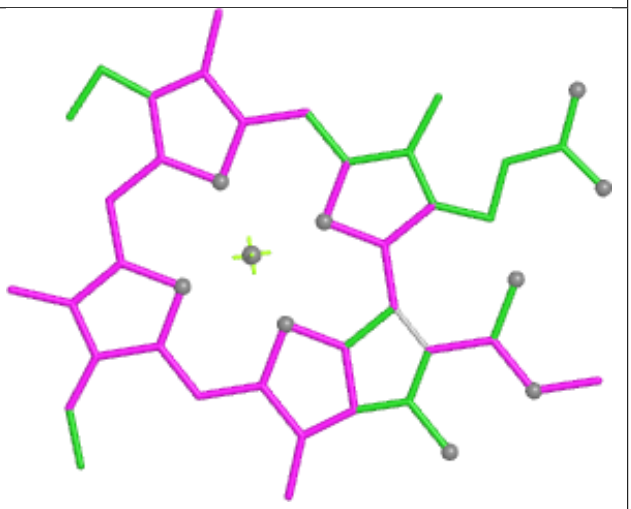
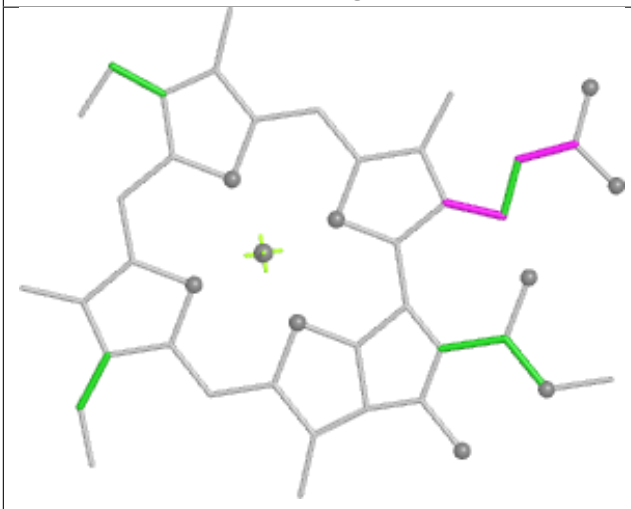


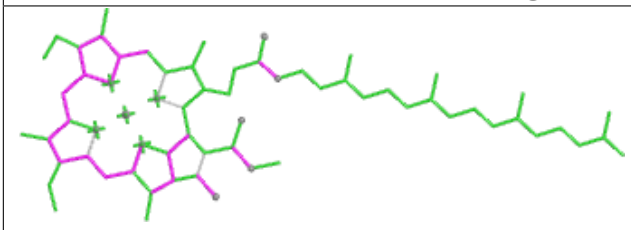
Bond angles



Torsions

Rings

Ligand CLA B 802



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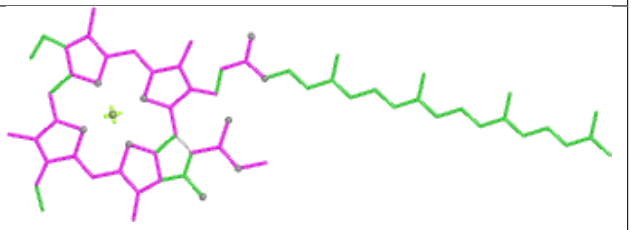
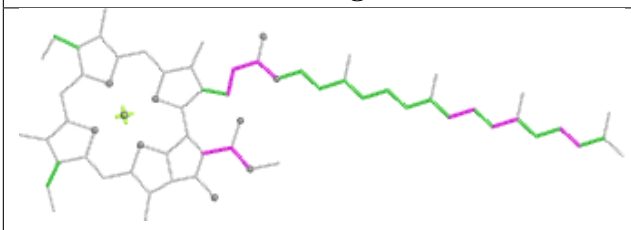
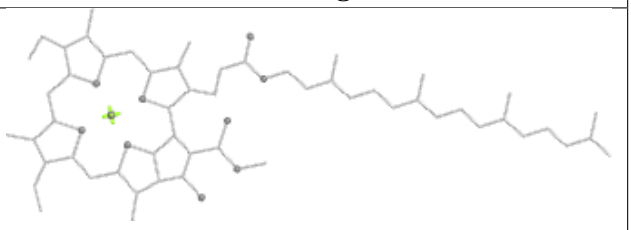


Bond angles

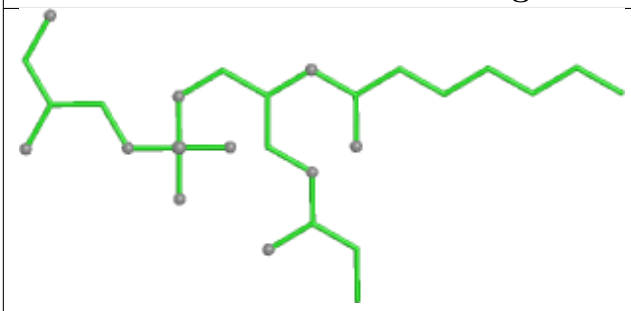


Torsions



Rings

Ligand LHG bA 851



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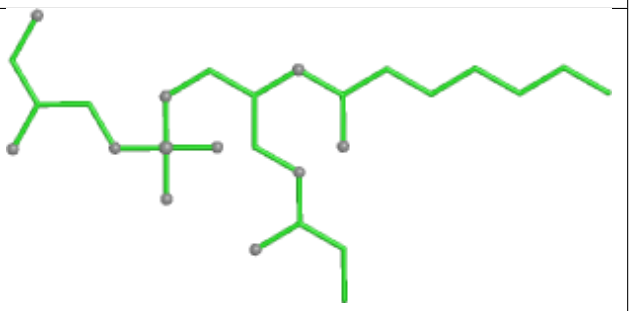
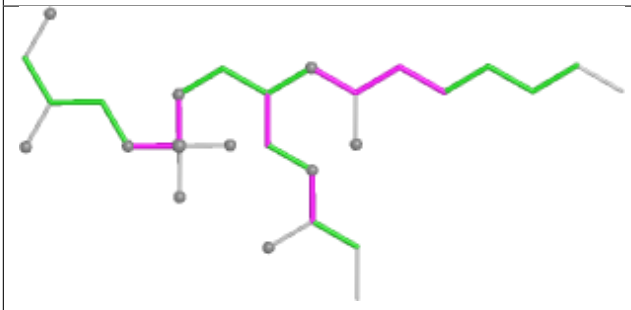


Bond angles



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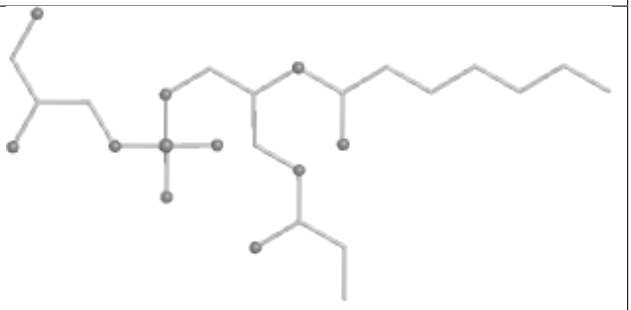
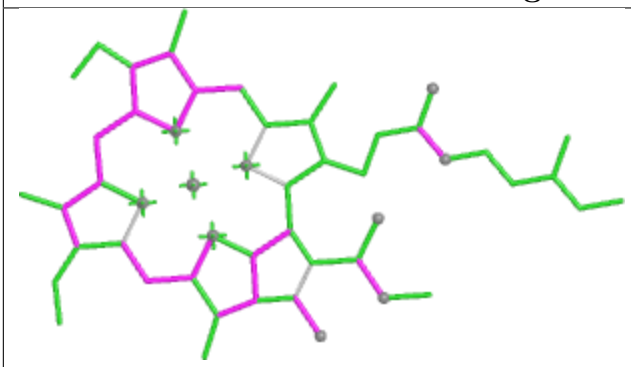


Rings

Ligand CLA A 836



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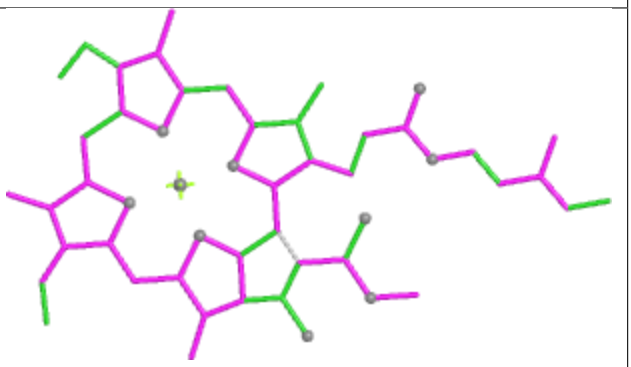

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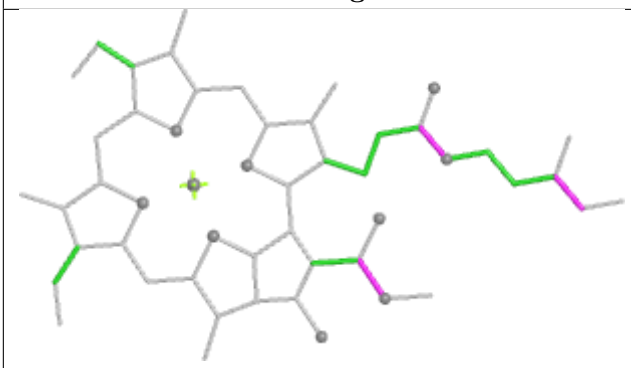

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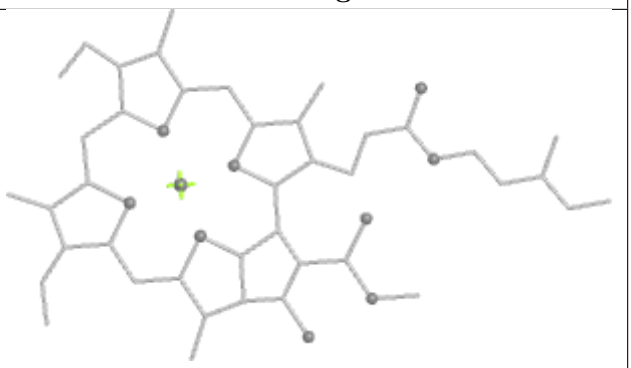
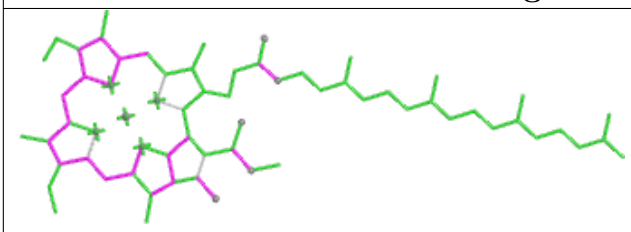


Rings

Ligand CLA A 832



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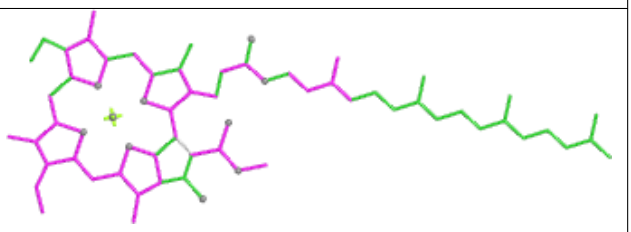
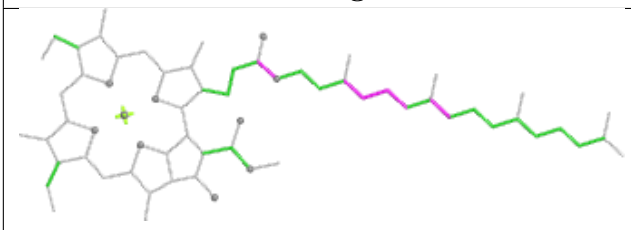


Bond angles



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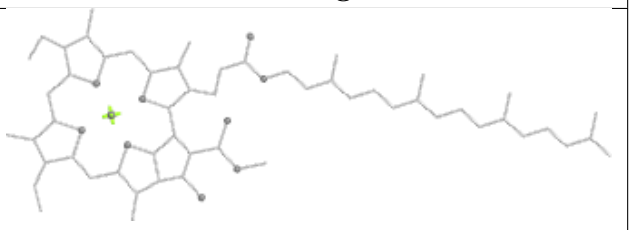
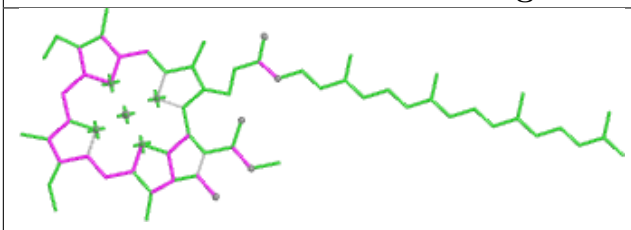
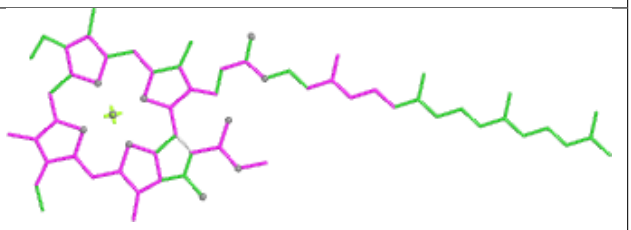


Rings

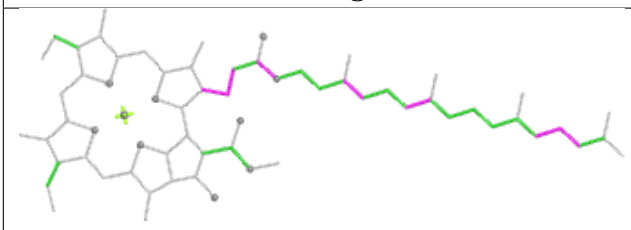
Ligand CLA cB 810



Bond lengths



Bond angles



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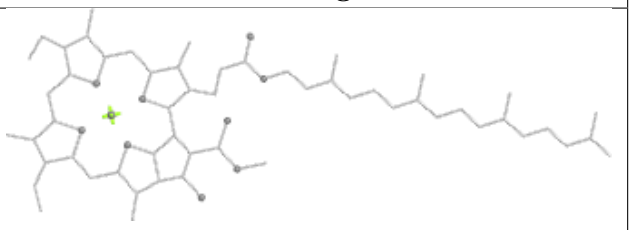
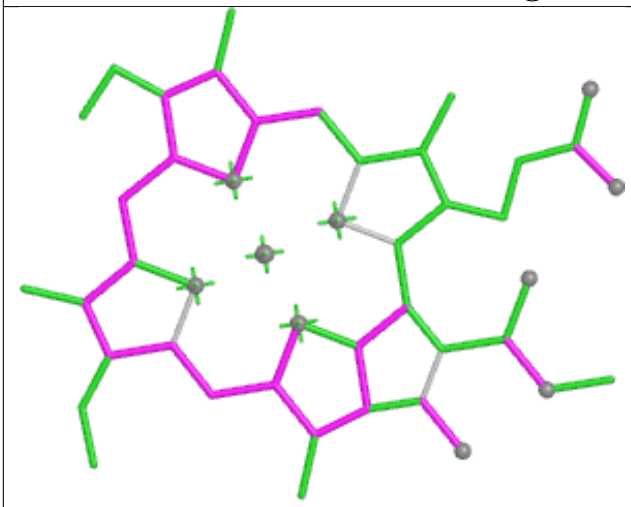


Rings

Ligand CLA A 810



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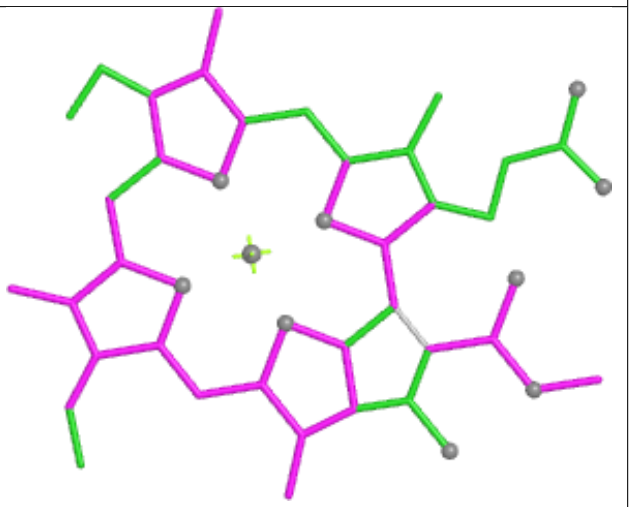
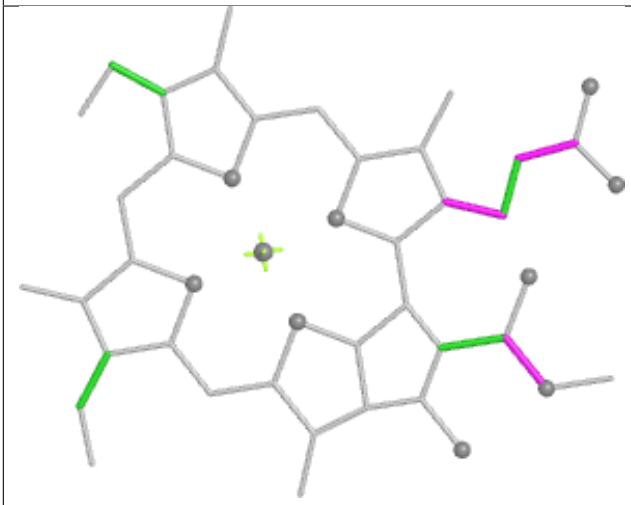
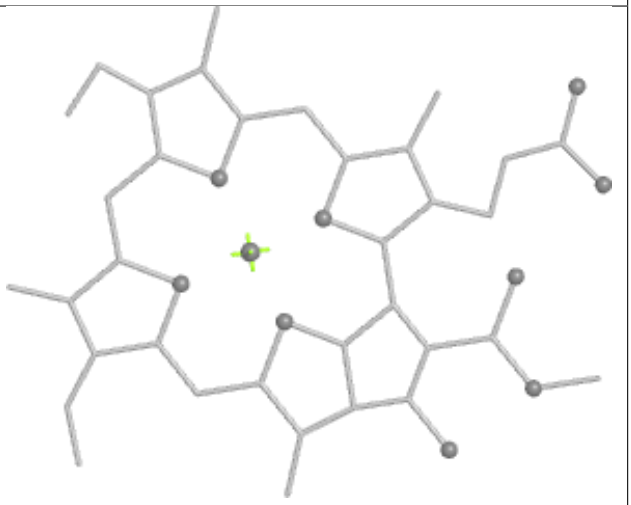


Bond angles

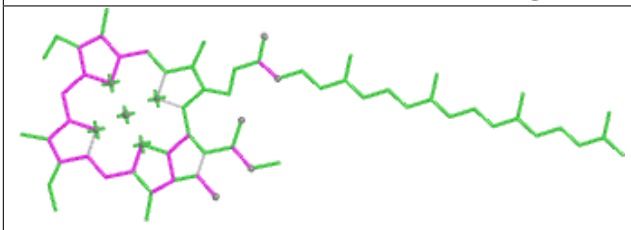


Torsions

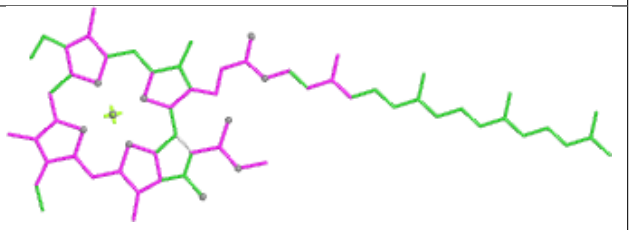


Rings

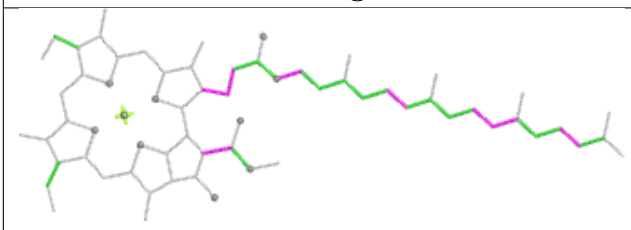
Ligand CLA L 201



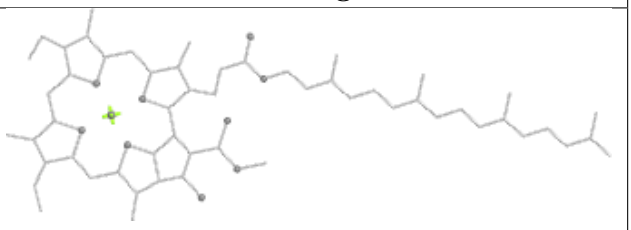
Bond lengths



Bond angles

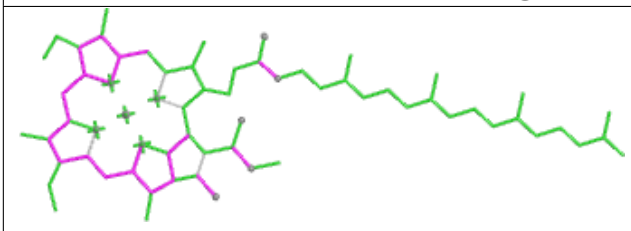


Torsions

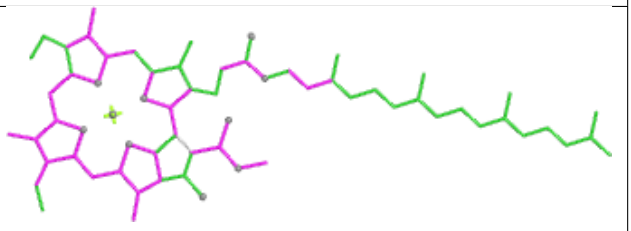


Rings

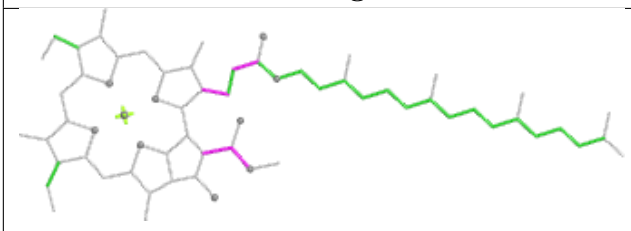
Ligand CLA cB 813



Bond lengths



Bond angles



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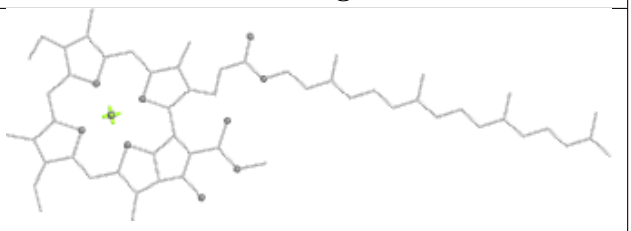
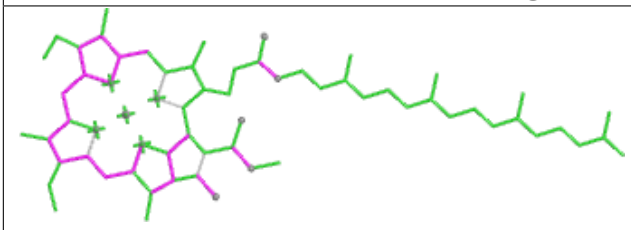


Rings

Ligand CLA B 806



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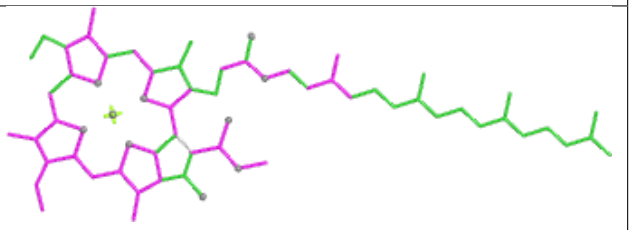
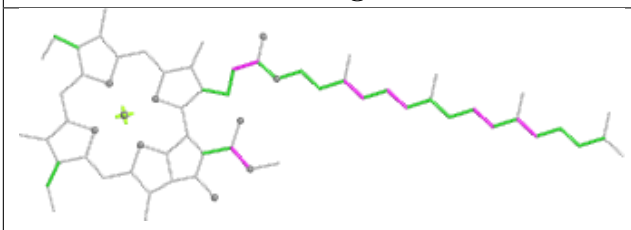


Bond angles



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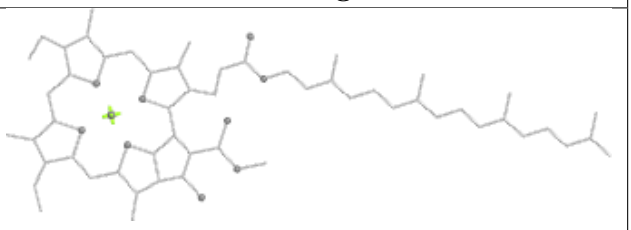
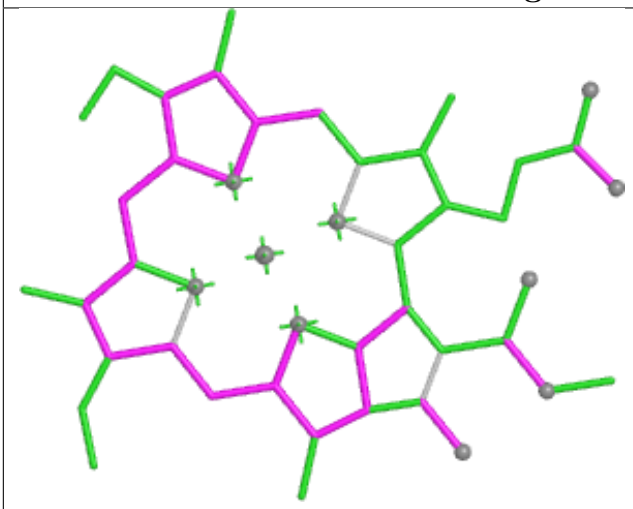


Rings

Ligand CLA B 834



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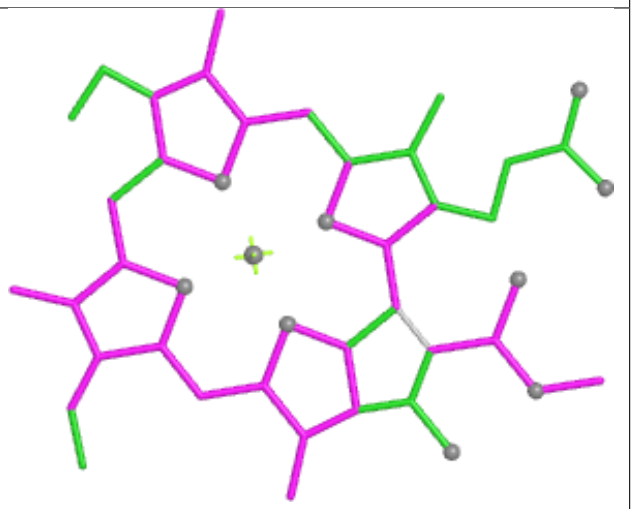
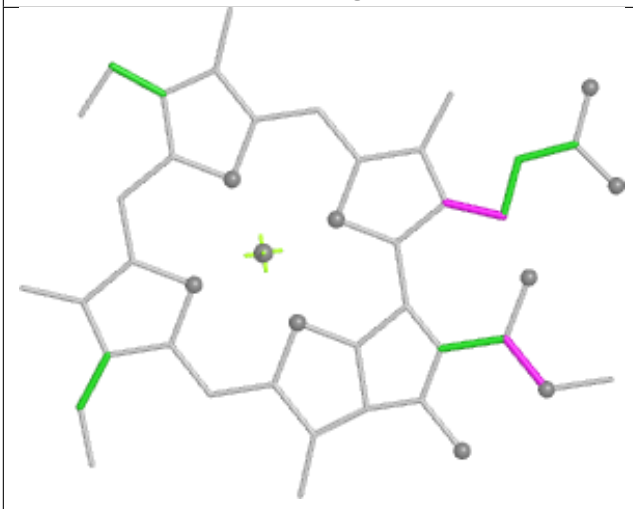


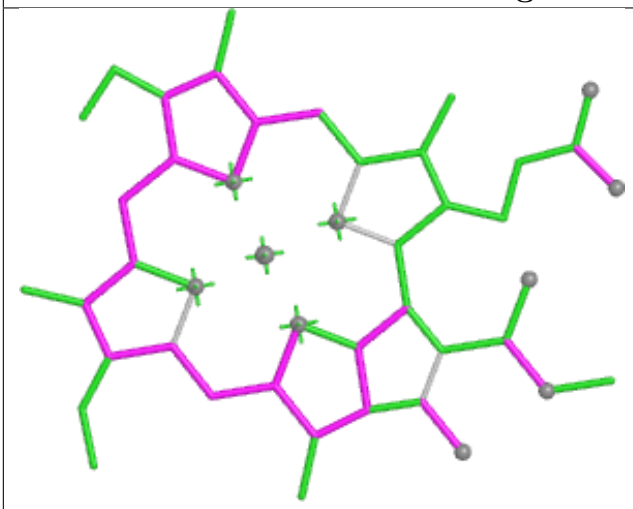
Bond angles



Torsions

Rings

Ligand CLA cB 835



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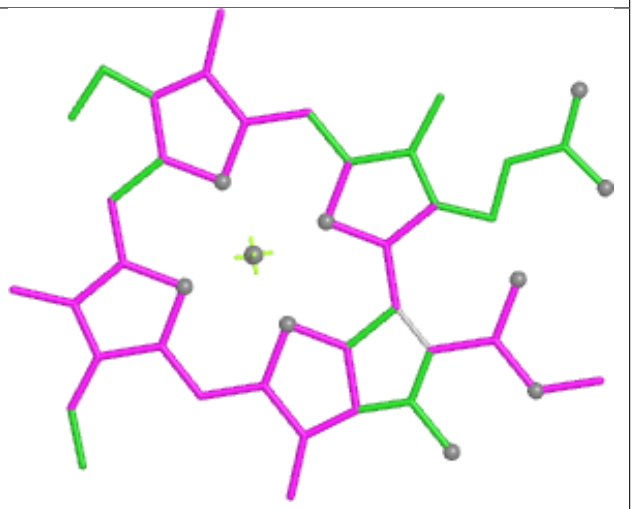
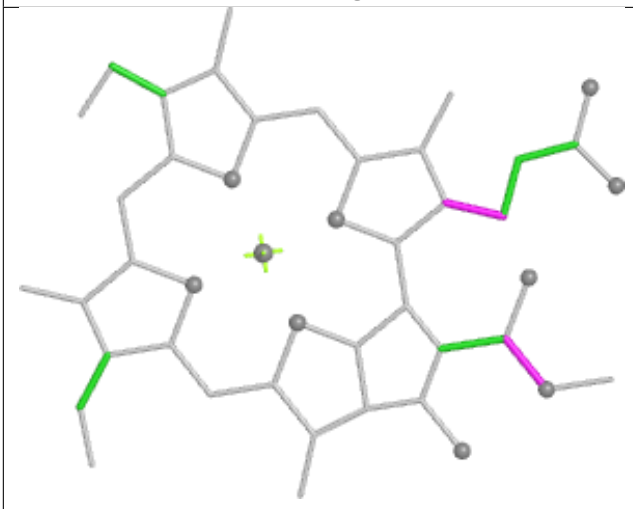


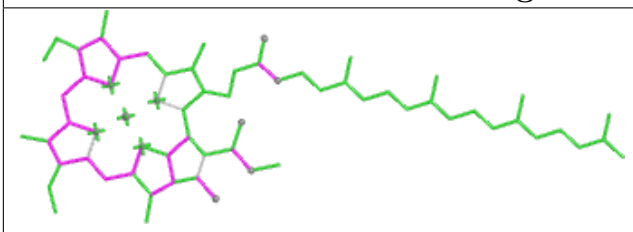
Bond angles



Torsions

Rings

Ligand CLA bL 201



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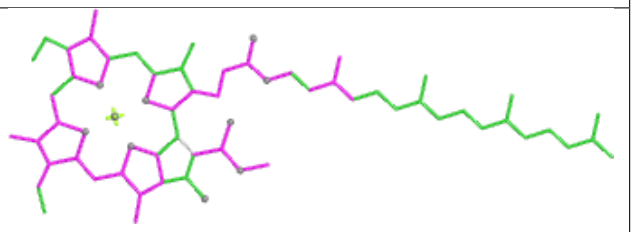
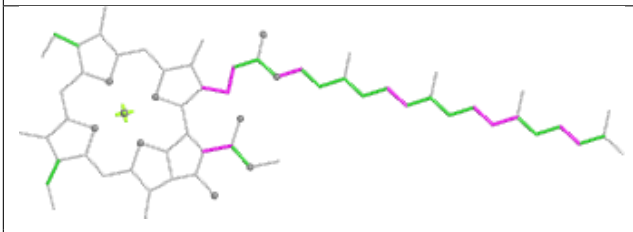
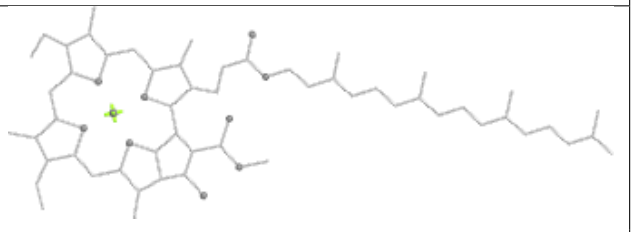


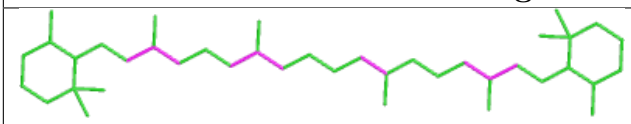
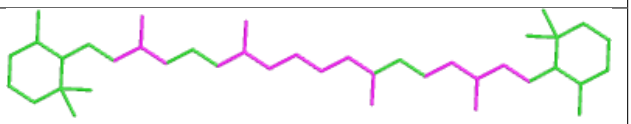
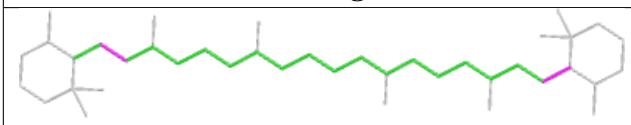
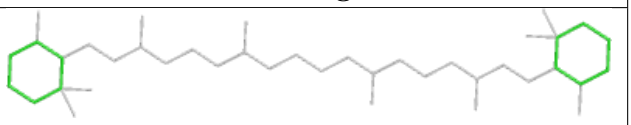
Bond angles

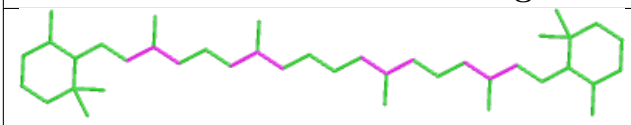
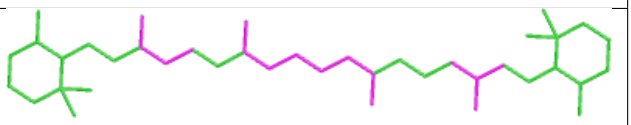
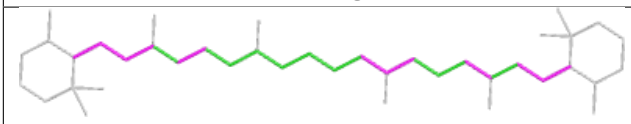
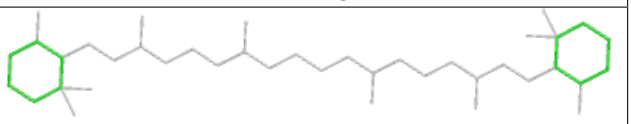


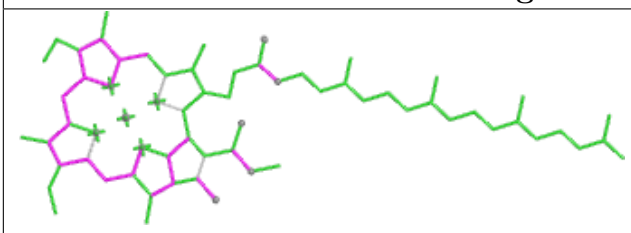
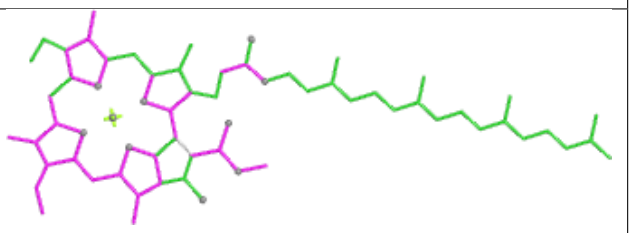
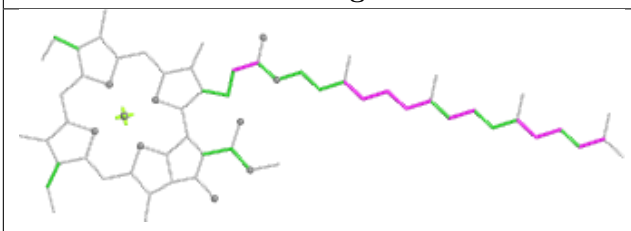
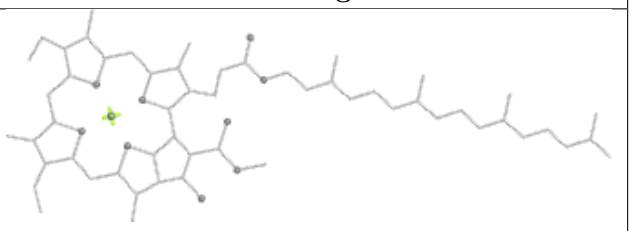
Torsions



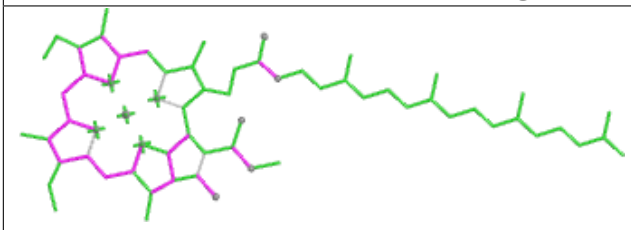
Rings

Ligand BCR cB 846	
 Bond lengths	 Bond angles
 Torsions	 Rings

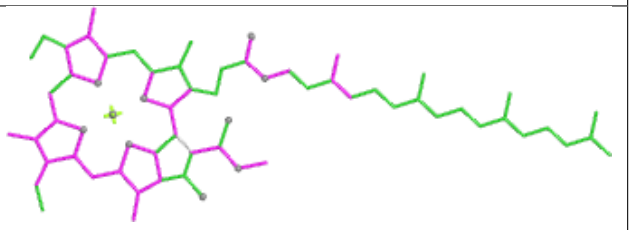
Ligand BCR cB 851	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA cB 808	
 Bond lengths	 Bond angles
 Torsions	 Rings

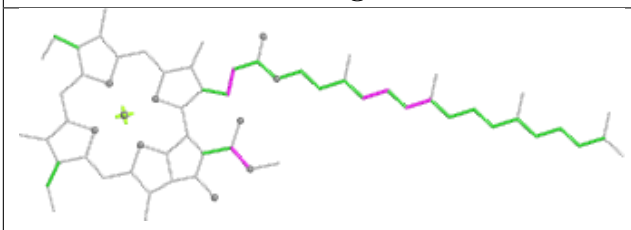
Ligand CLA bB 838



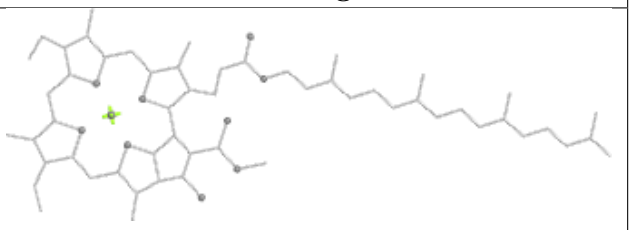
Bond lengths



Bond angles

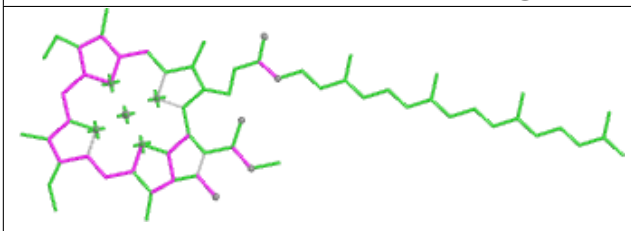


Torsions



Rings

Ligand CLA bL 204



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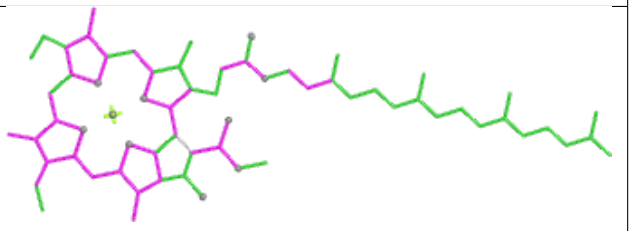
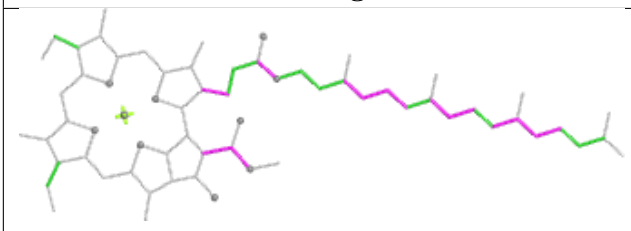
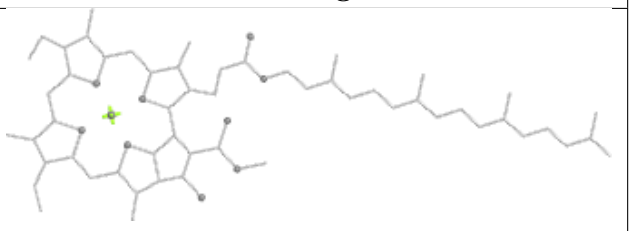


Bond angles

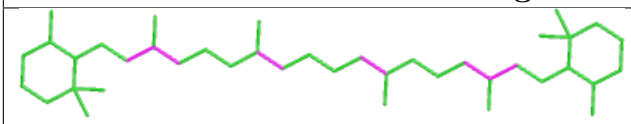


Torsions



Rings

Ligand BCR cA 846



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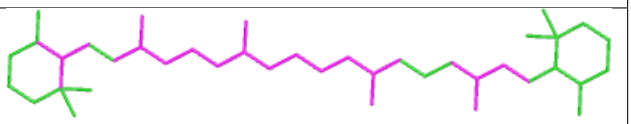
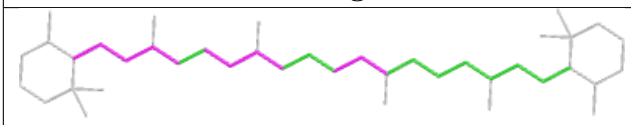
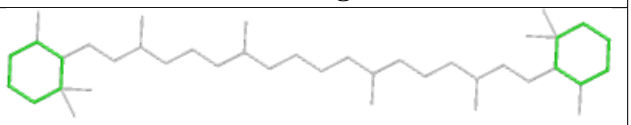


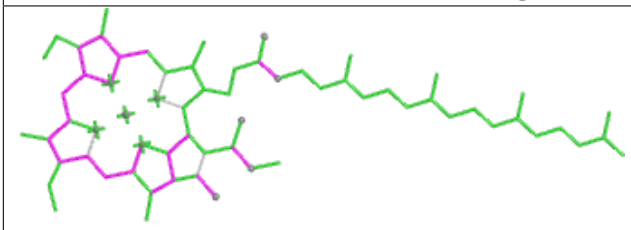
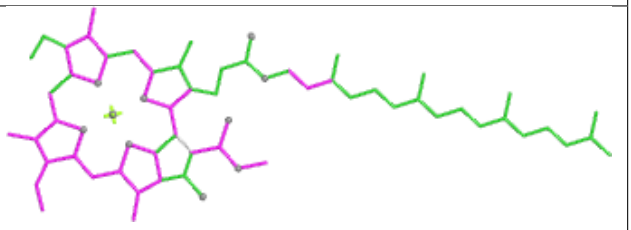
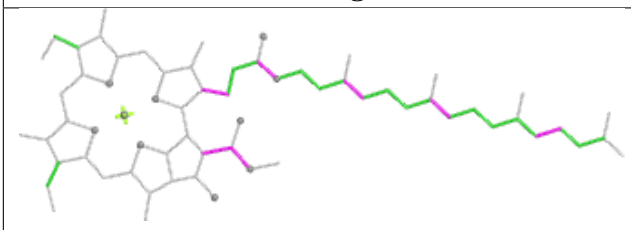
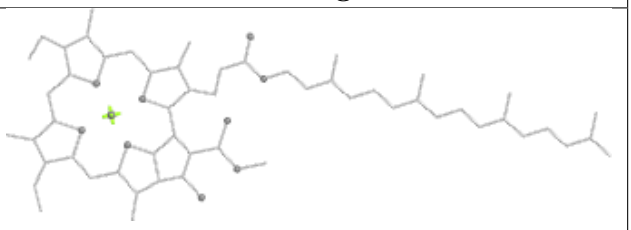
Bond angles

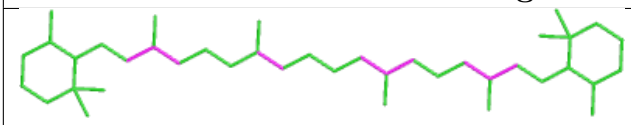
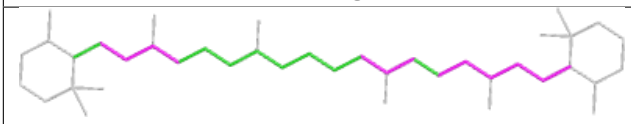
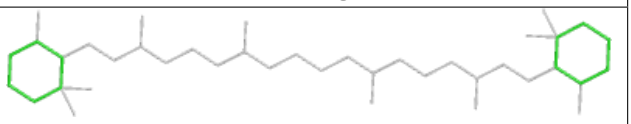


Torsions

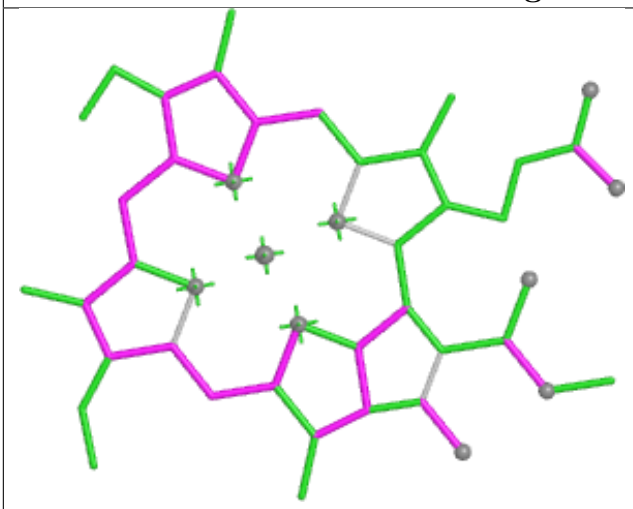


Rings

Ligand CLA bA 829	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR bJ 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 820



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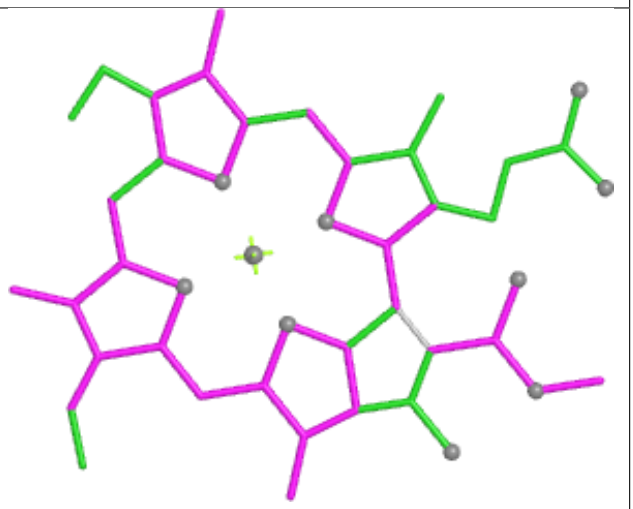

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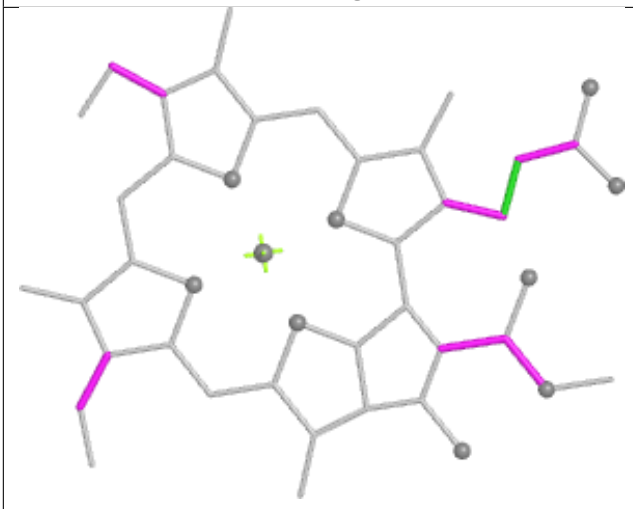
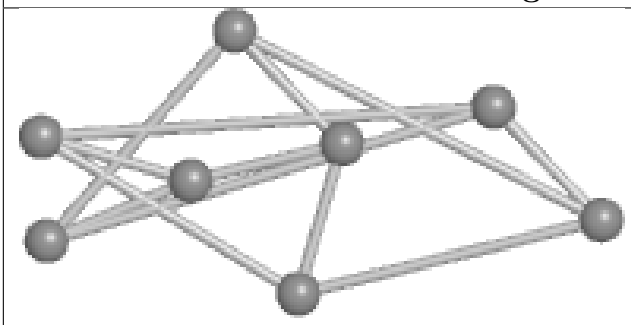


Torsions

Rings

Ligand SF4 cA 844



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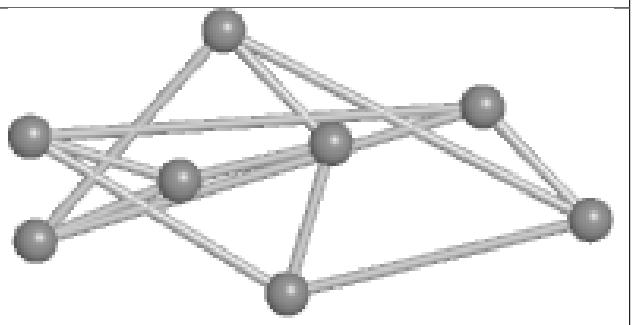

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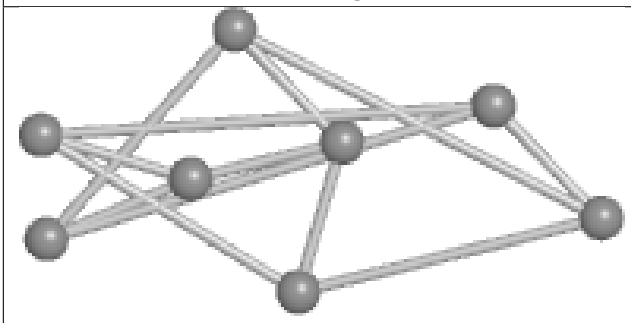

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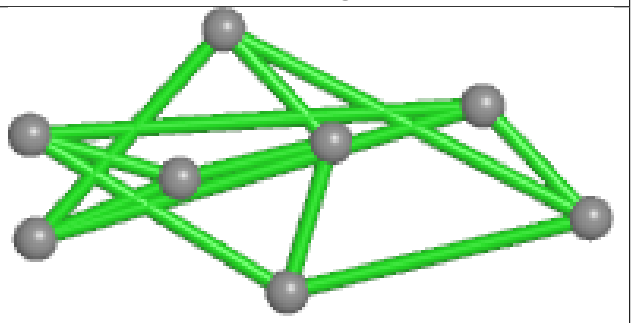
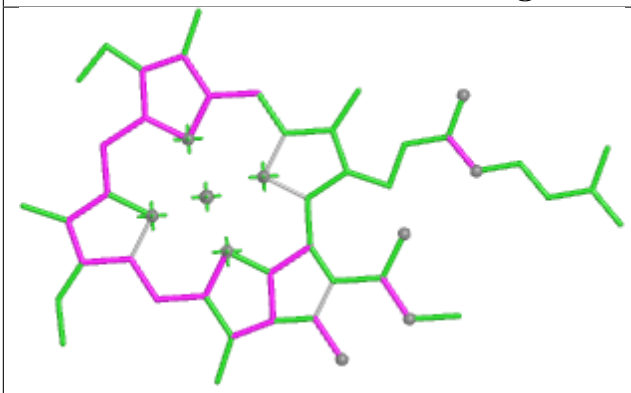


Rings

Ligand CLA cB 824



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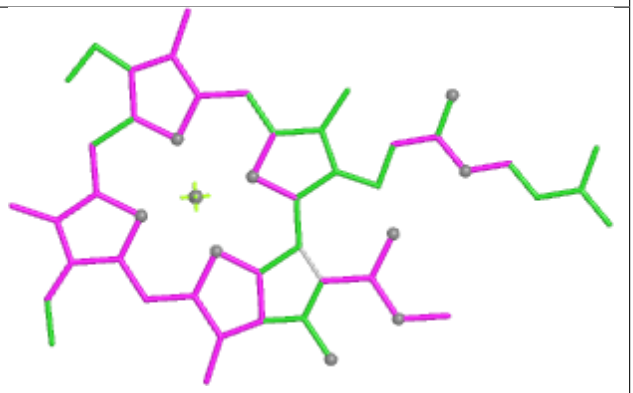
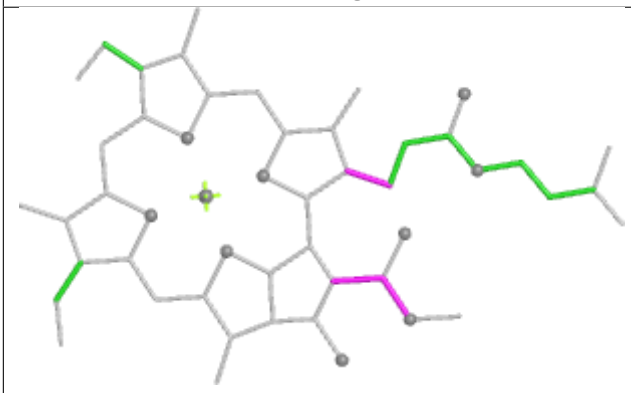


Bond angles



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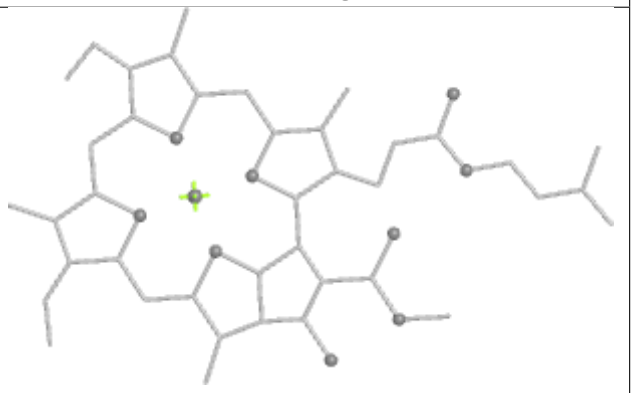
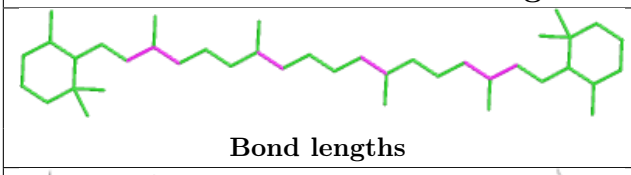


Rings

Ligand BCR F 202



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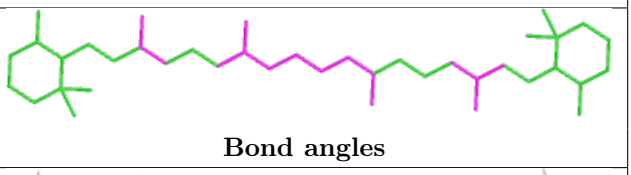

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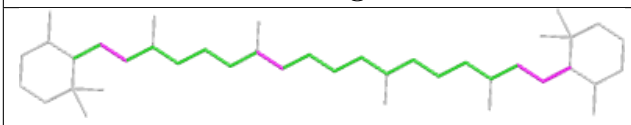

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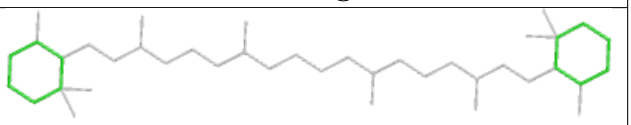
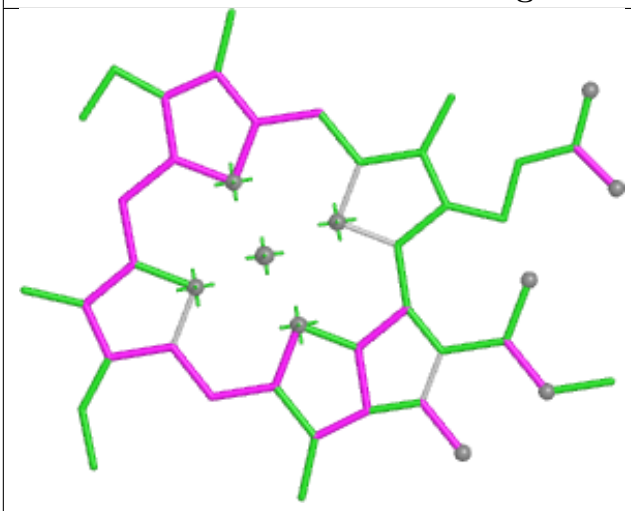


Rings

Ligand CLA cB 801



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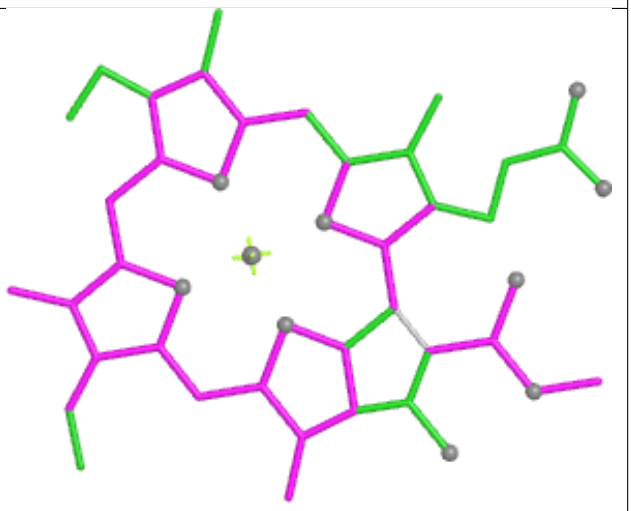

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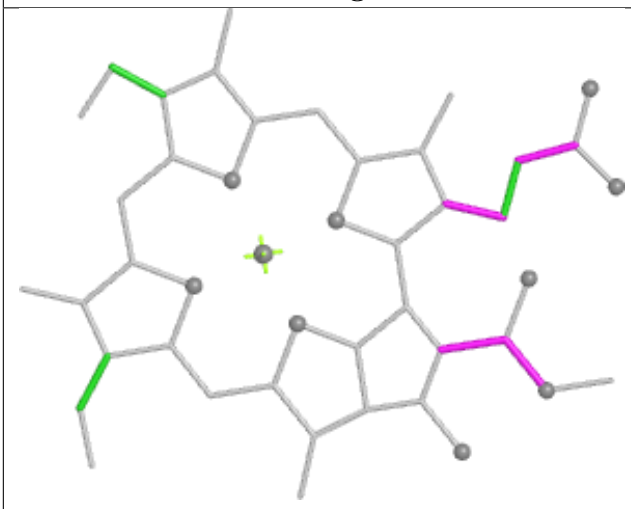

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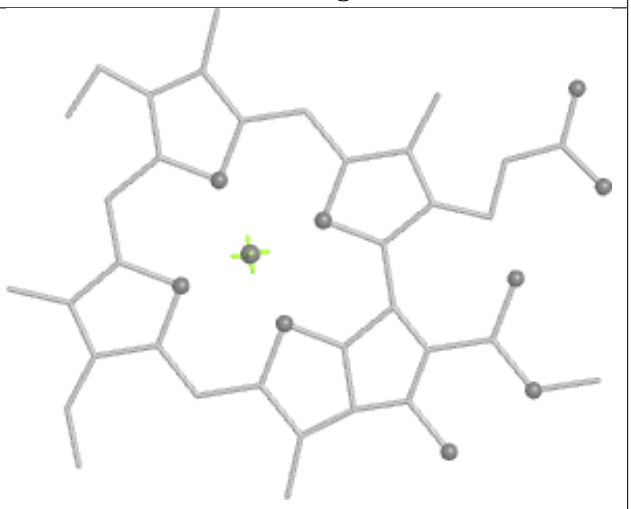

Rings

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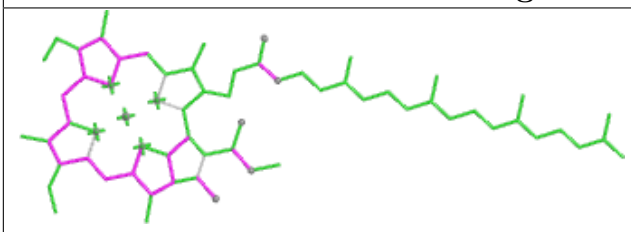

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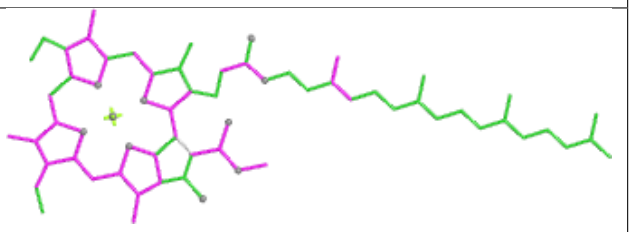

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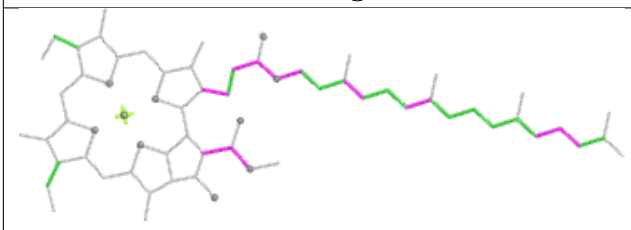

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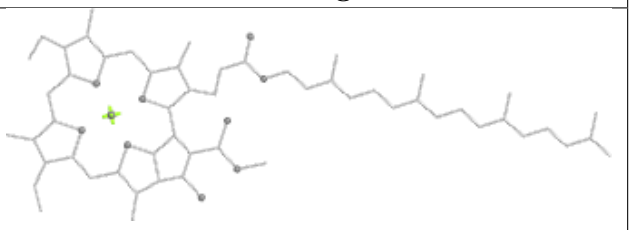
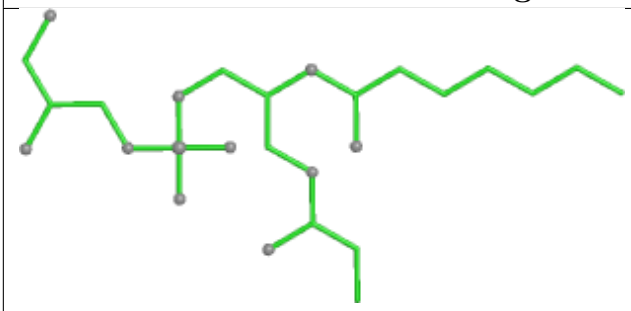


Rings

Ligand LHG cA 851



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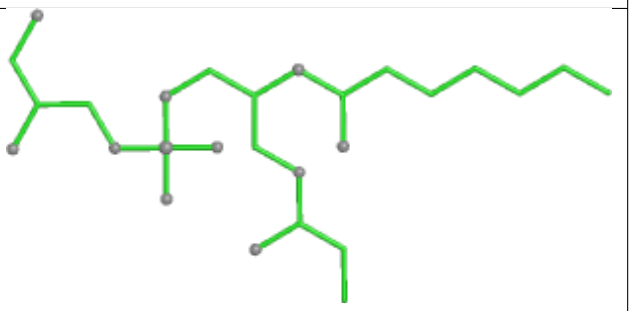

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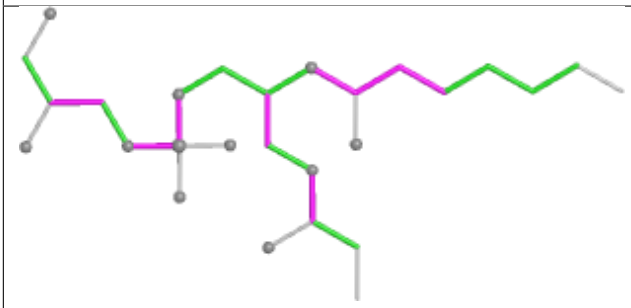

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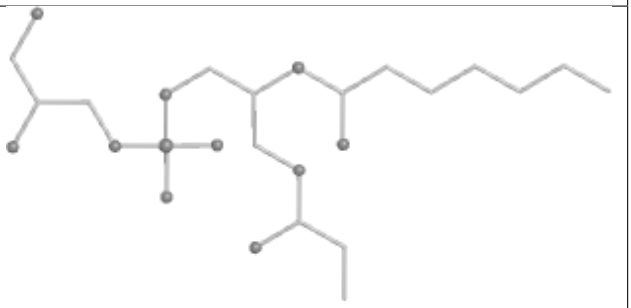
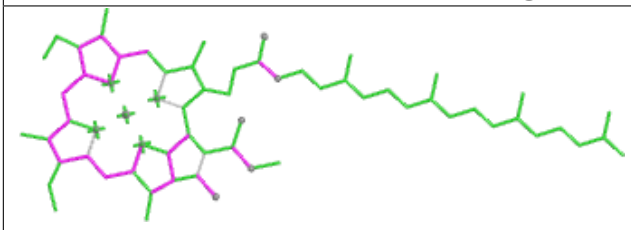


Rings

Ligand CL0 cA 801



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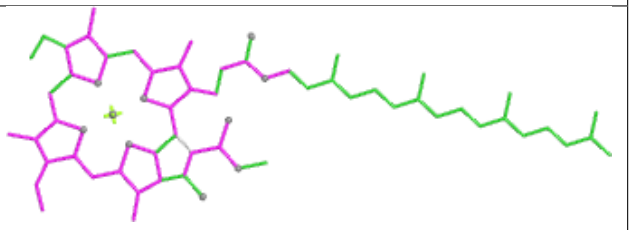

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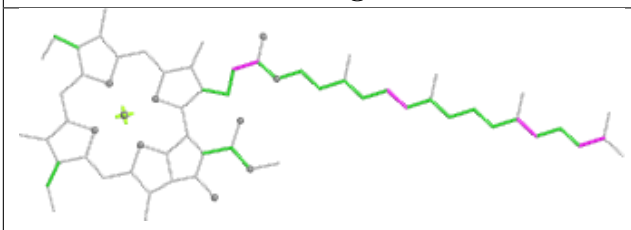

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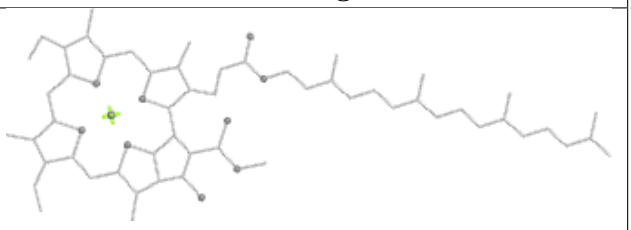
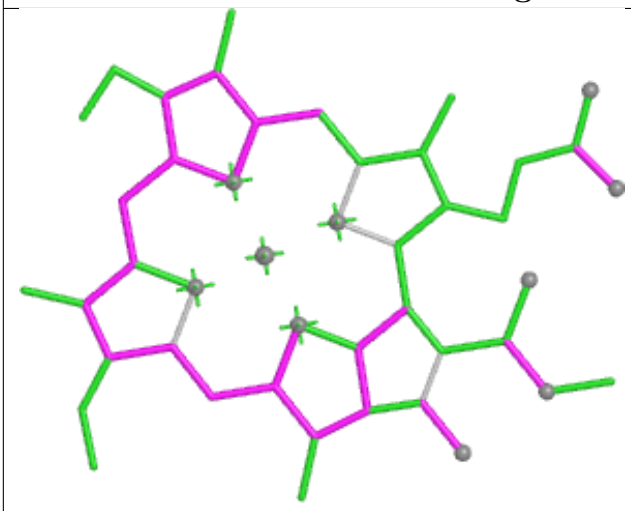


Rings

Ligand CLA bB 816



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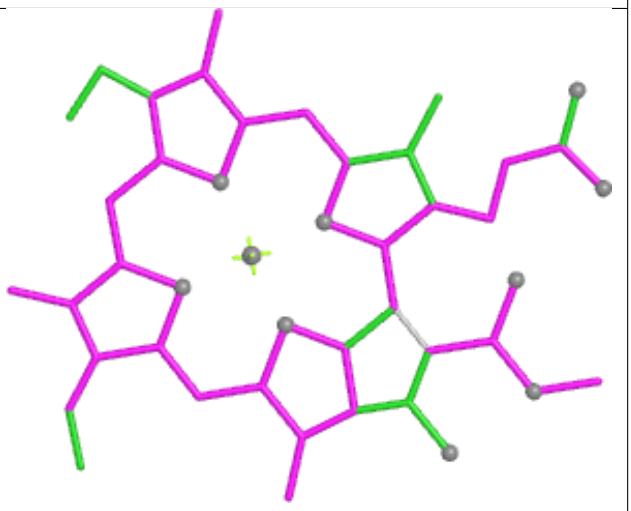
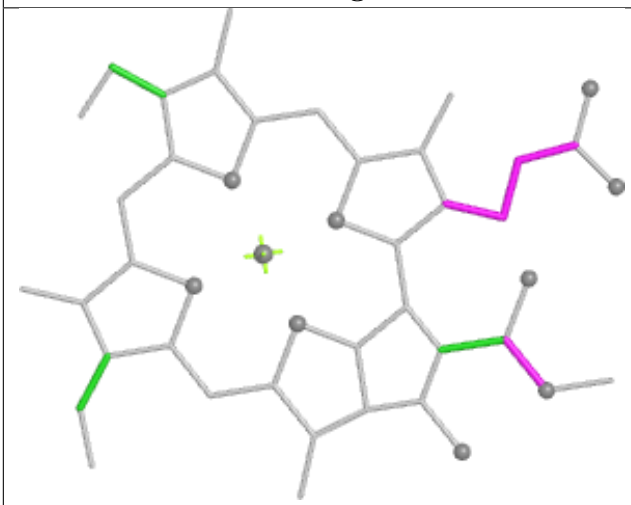


Bond angles



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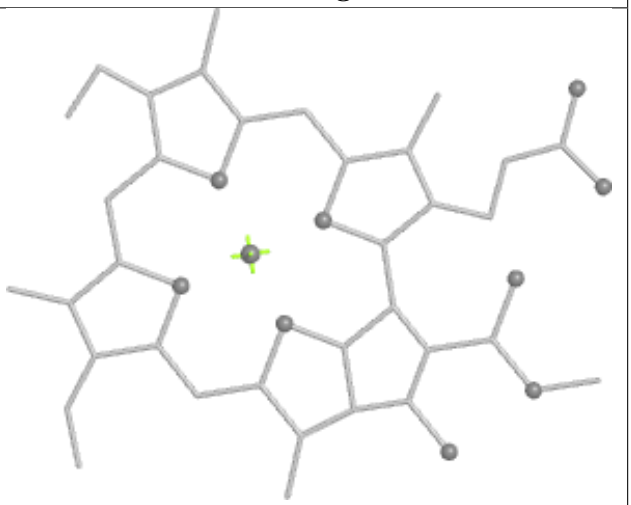
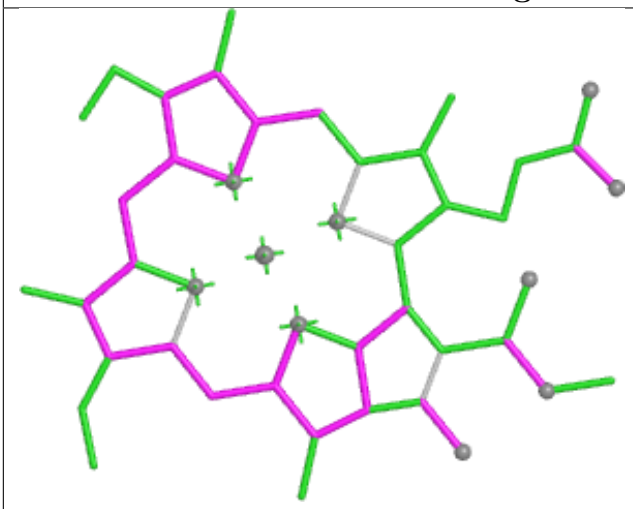


Rings

Ligand CLA bX 201



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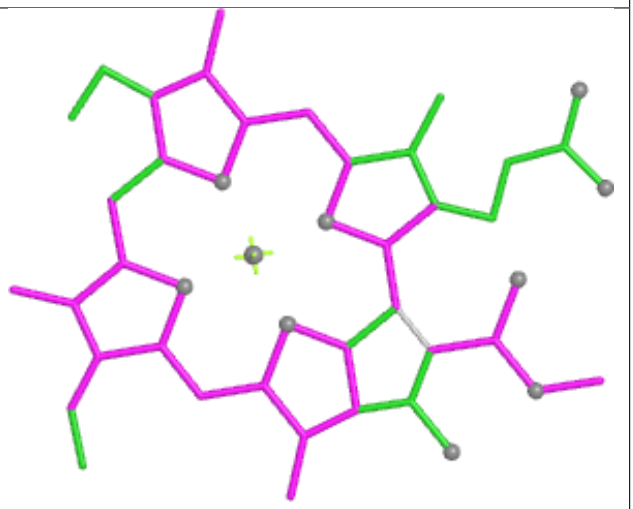

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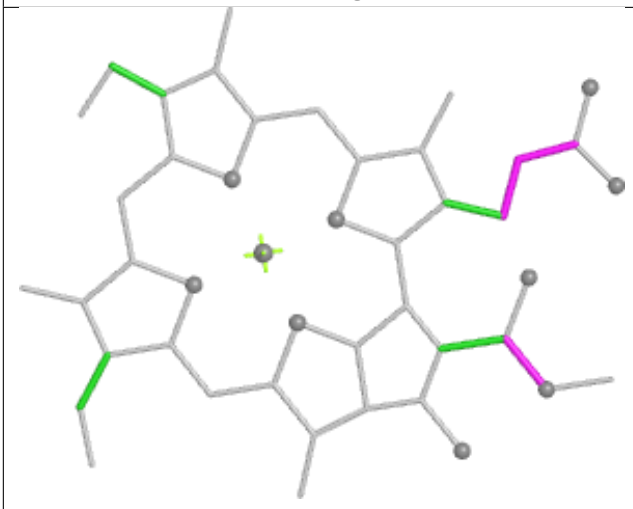
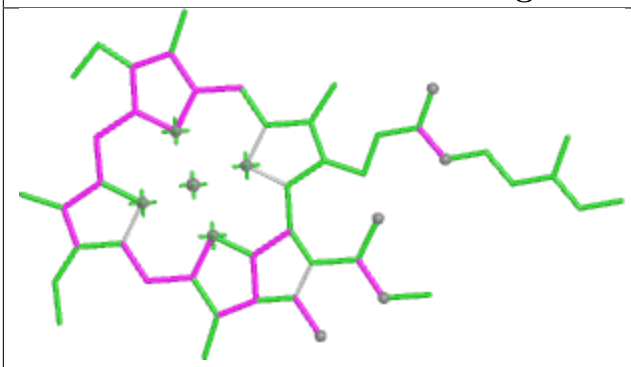


Torsions

Rings

Ligand CLA cA 836



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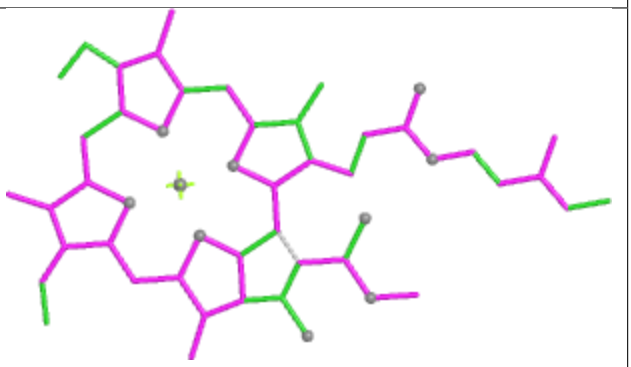
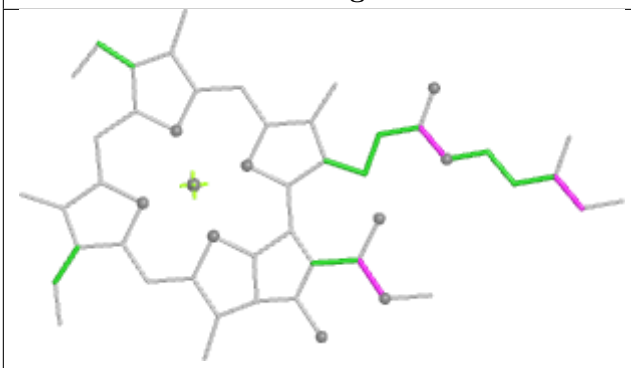


Bond angles



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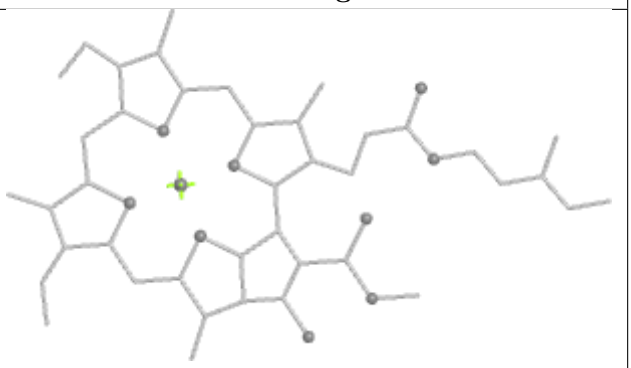
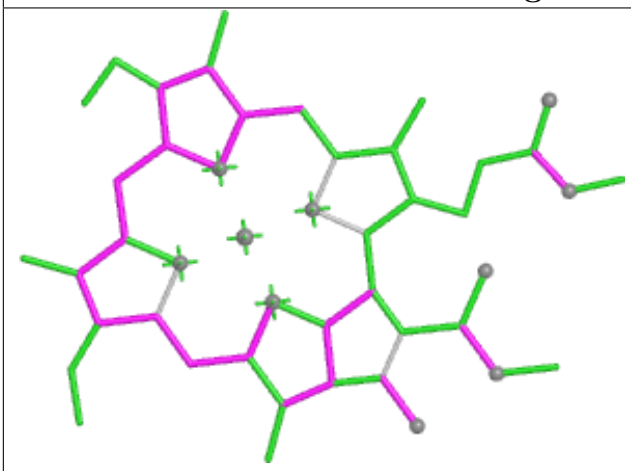


Rings

Ligand CLA B 824



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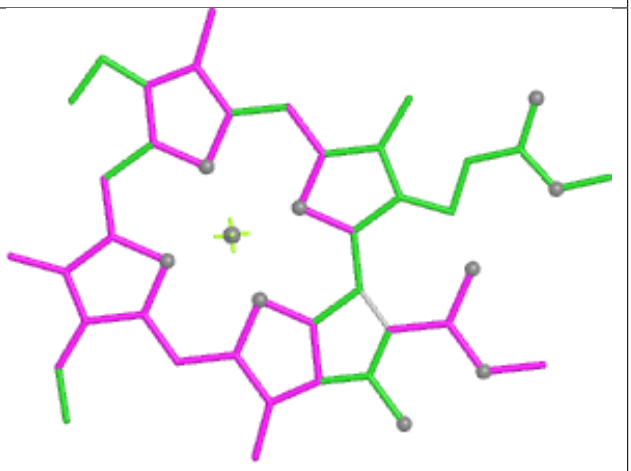
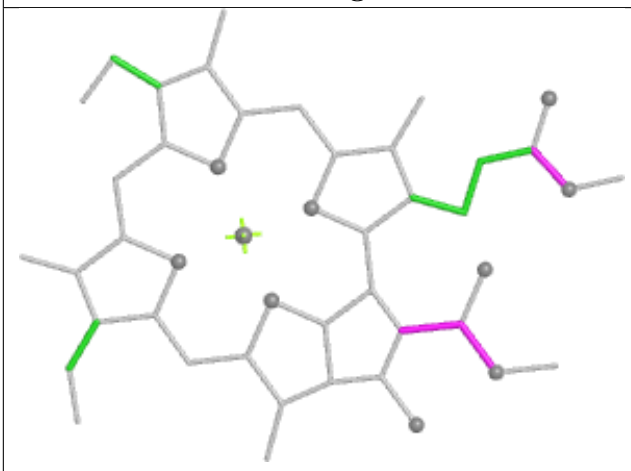


Bond angles



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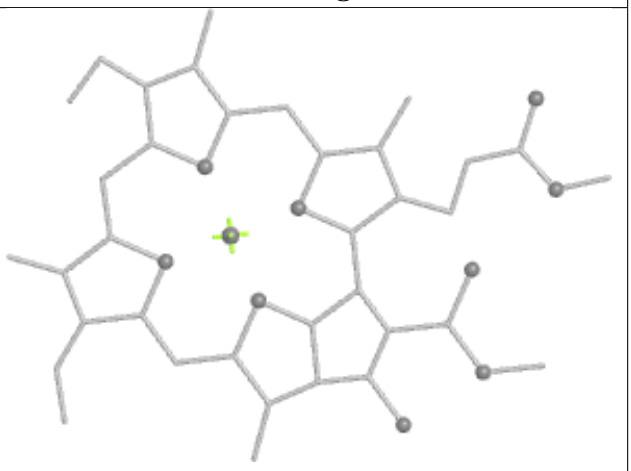
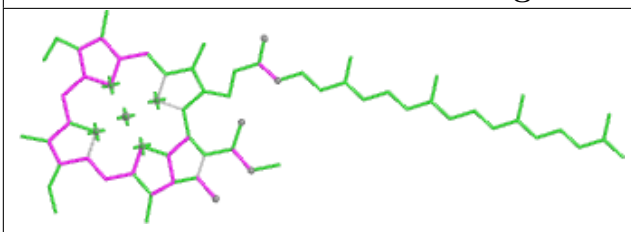


Rings

Ligand CLA bA 840



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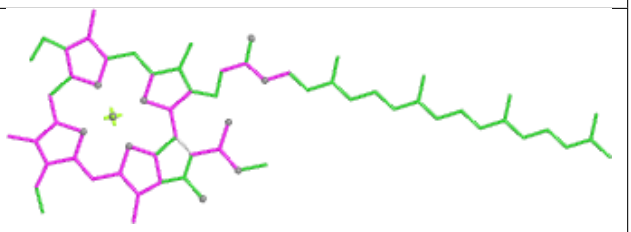
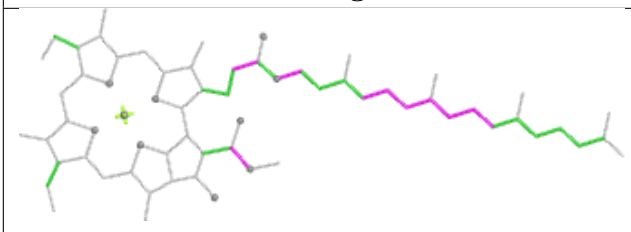


Bond angles



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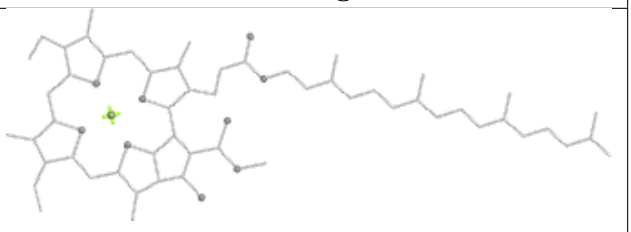
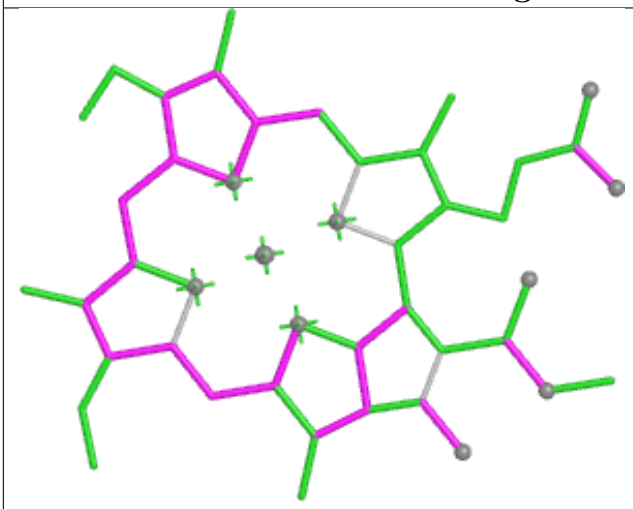
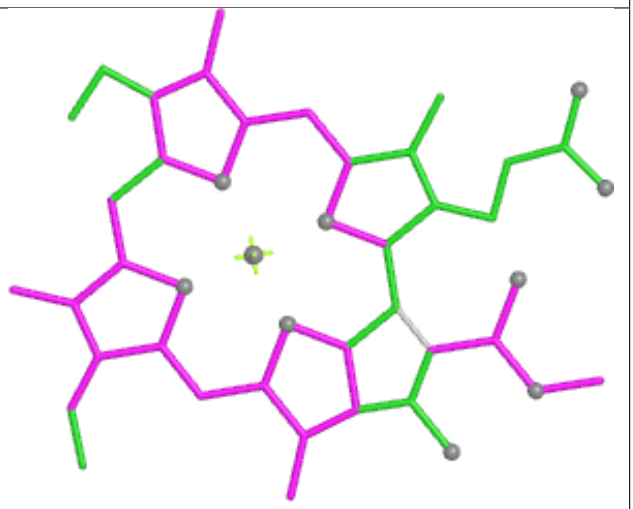


Rings

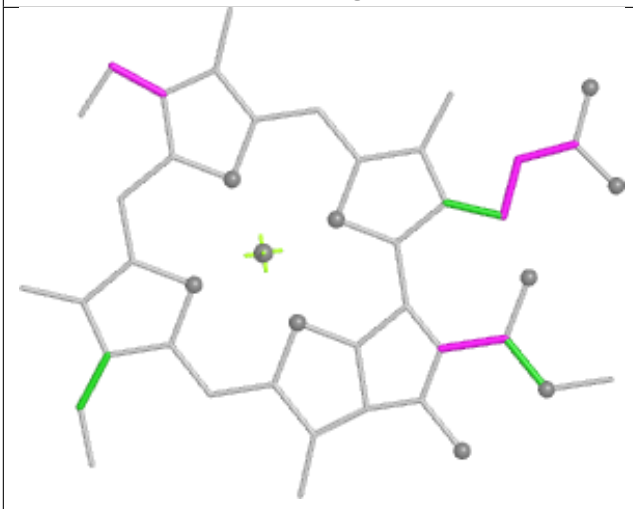
Ligand CLA bA 813



Bond lengths



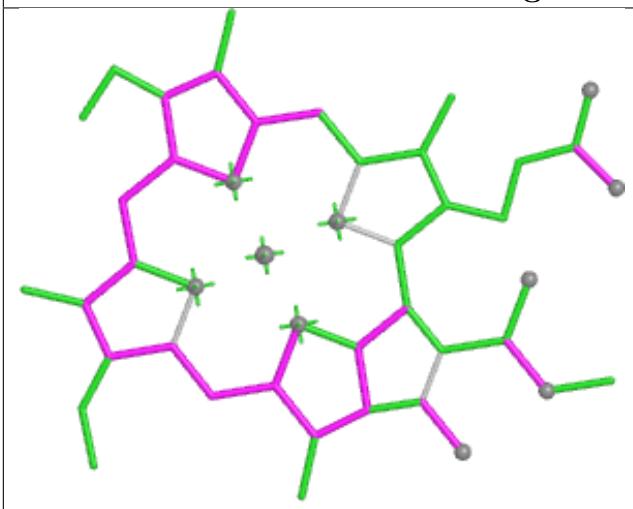
Bond angles



Torsions

Rings

Ligand CLA A 815



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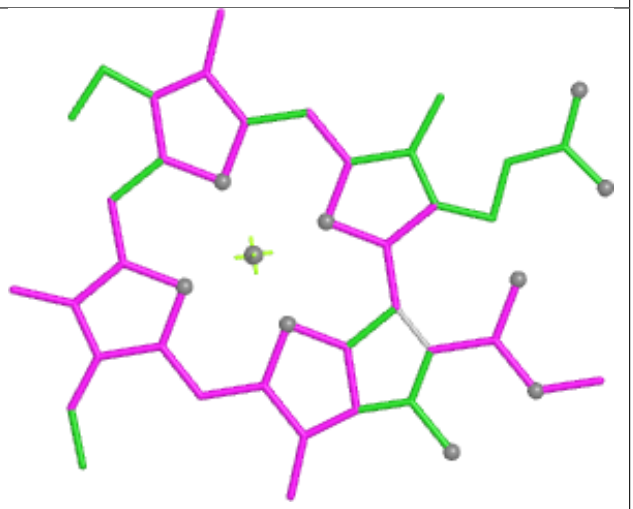

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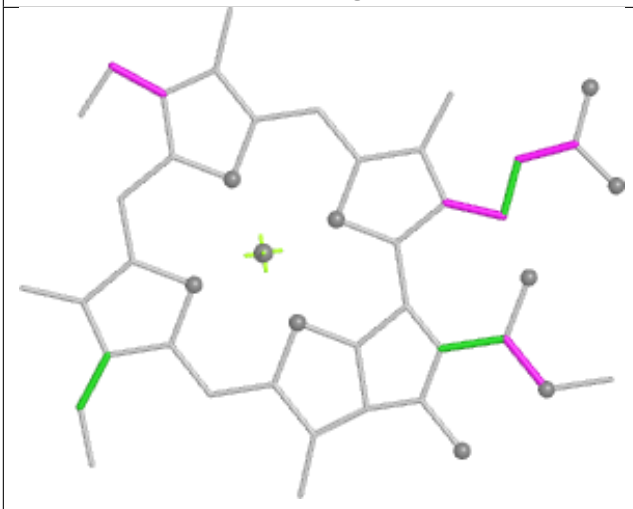
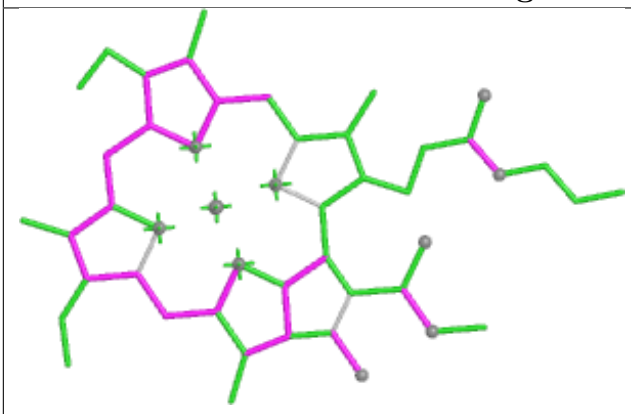


Torsions

Rings

Ligand CLA cB 814



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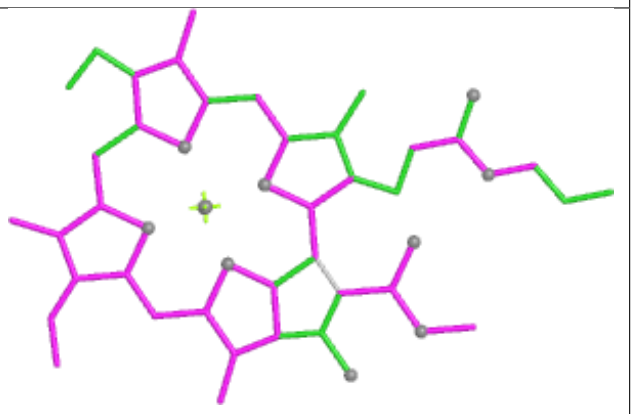

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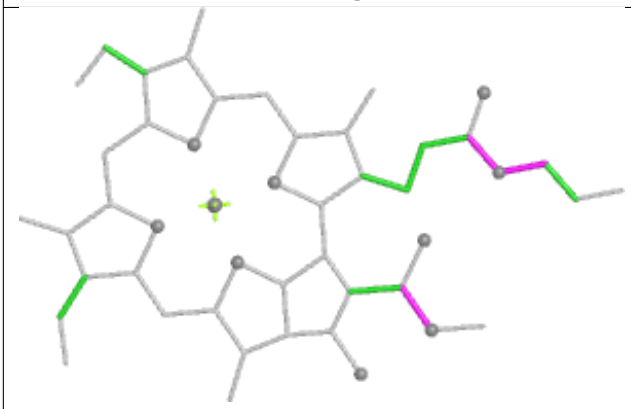
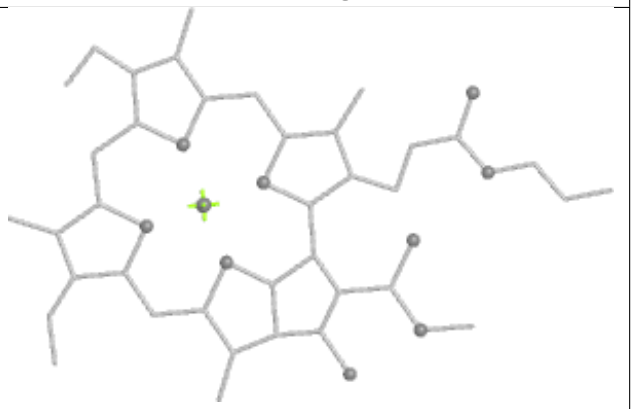
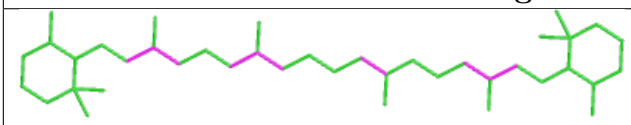


Torsions



Rings

Ligand BCR cB 847



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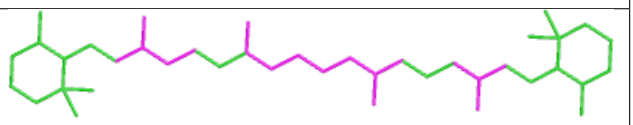
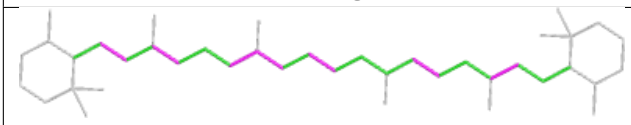


Bond angles



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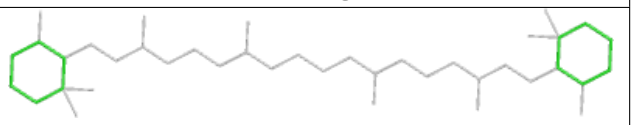
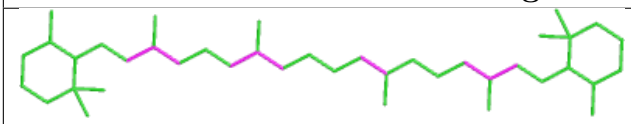


Rings

Ligand BCR A 847



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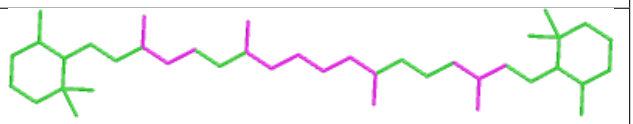
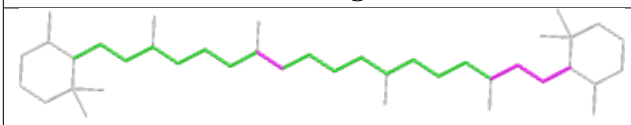


Bond angles



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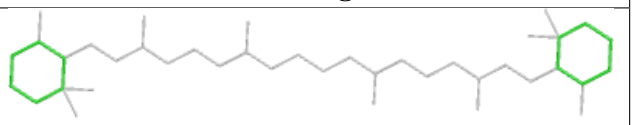
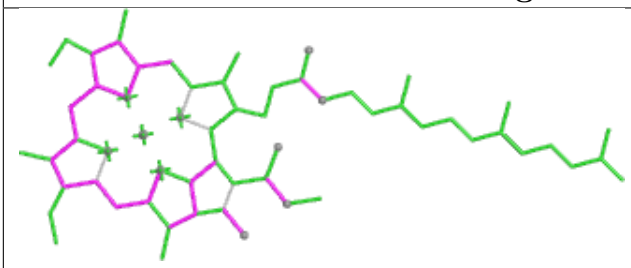


Rings

Ligand CLA cA 828



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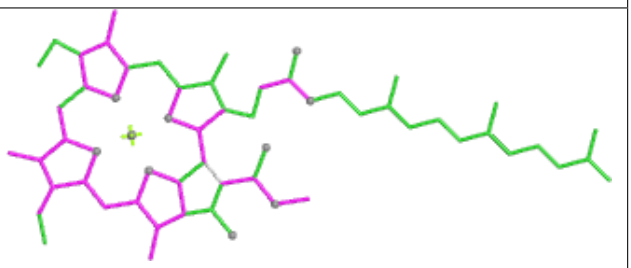
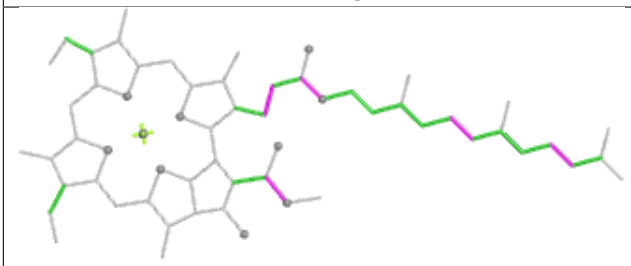


Bond angles



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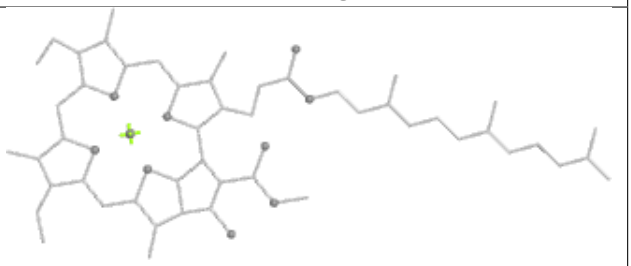
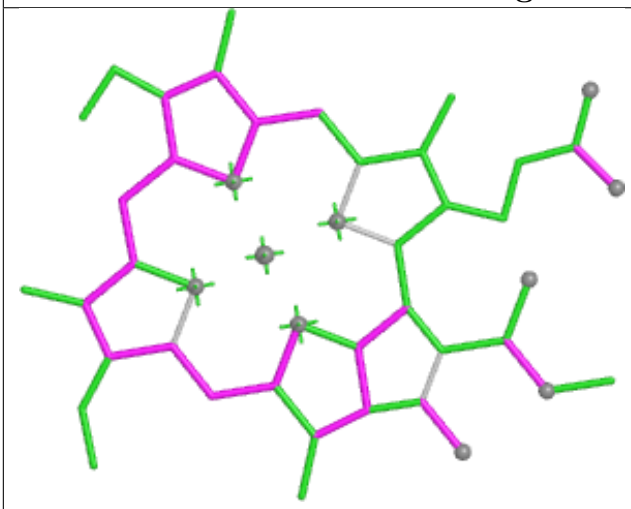


Rings

Ligand CLA cA 834



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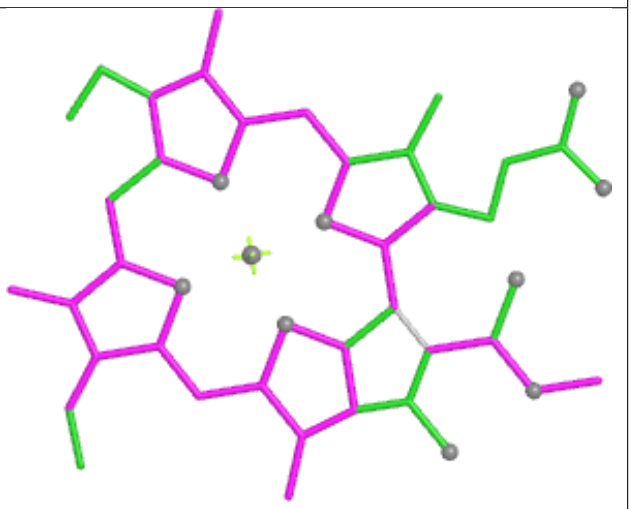

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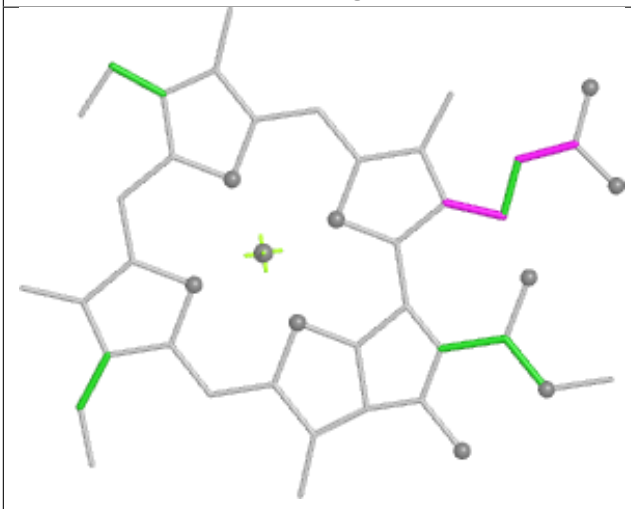
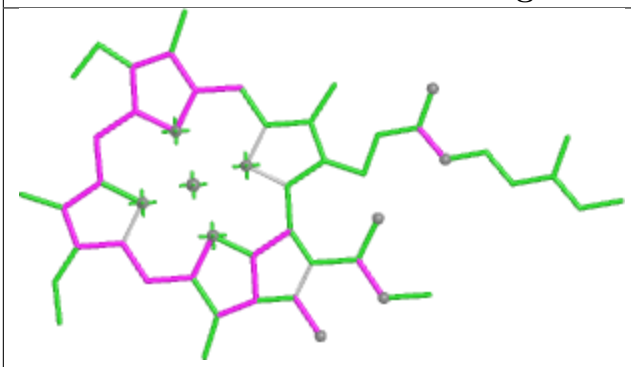


Torsions

Rings

Ligand CLA cB 805



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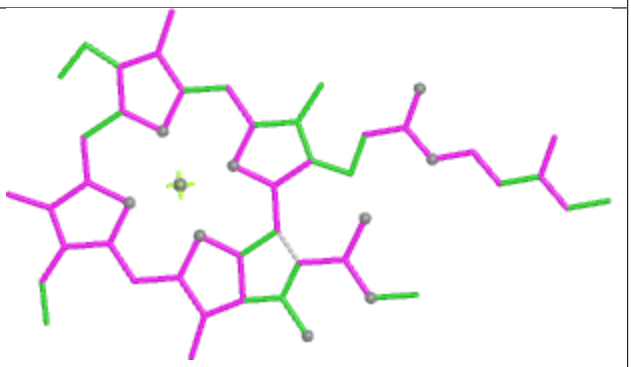
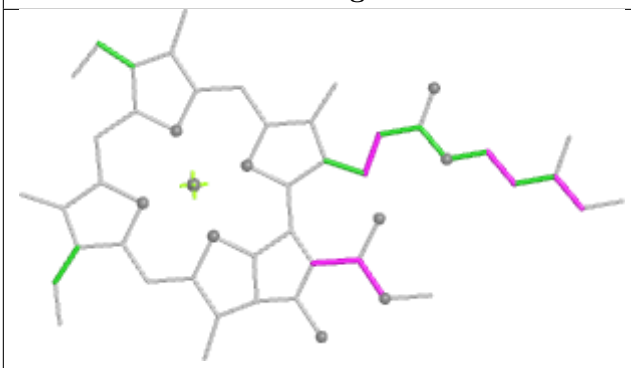
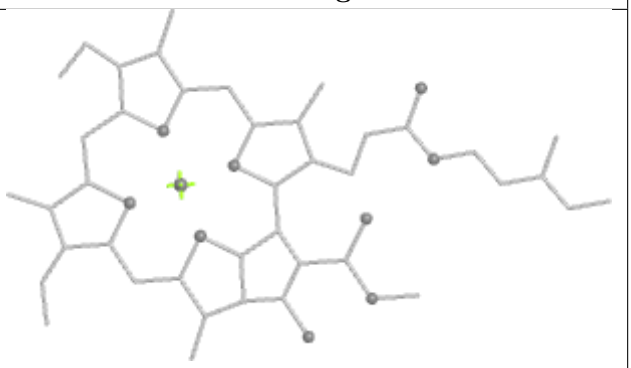


Bond angles

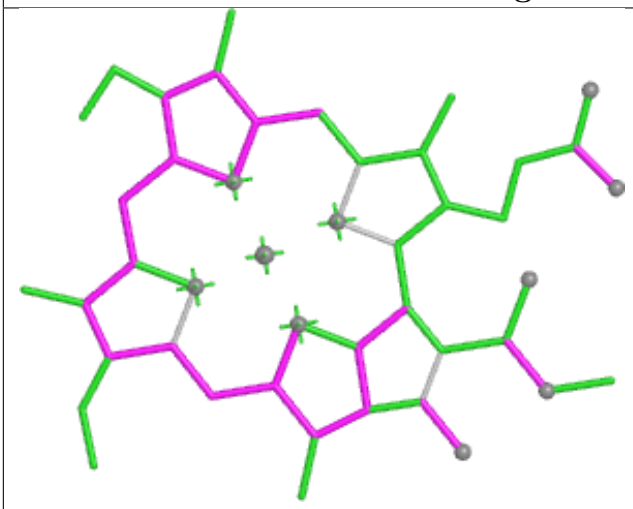


Torsions



Rings

Ligand CLA bB 821



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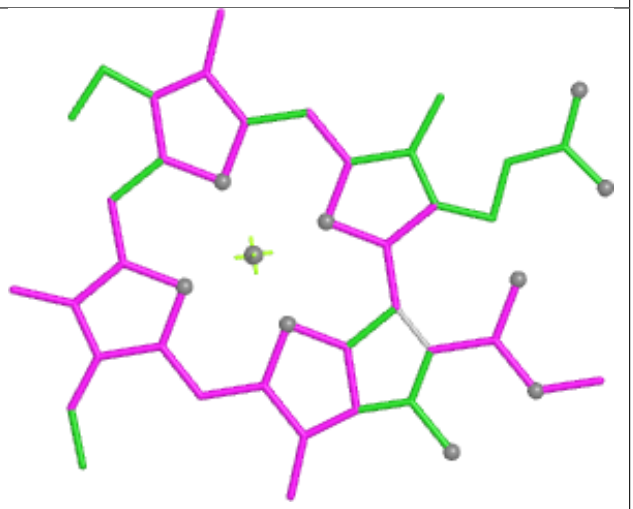

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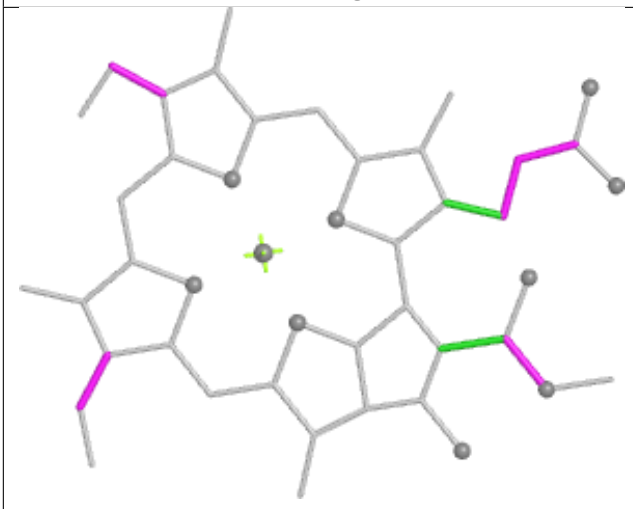
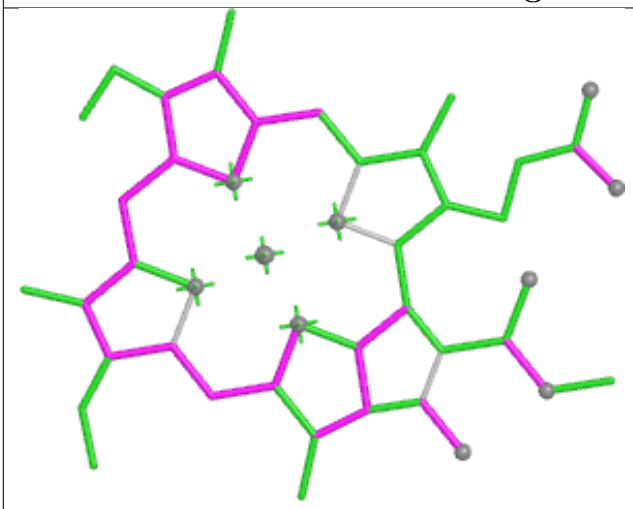


Torsions

Rings

Ligand CLA B 829



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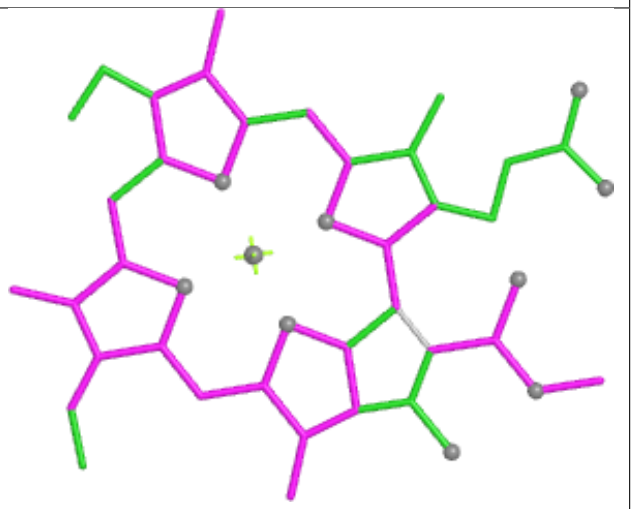

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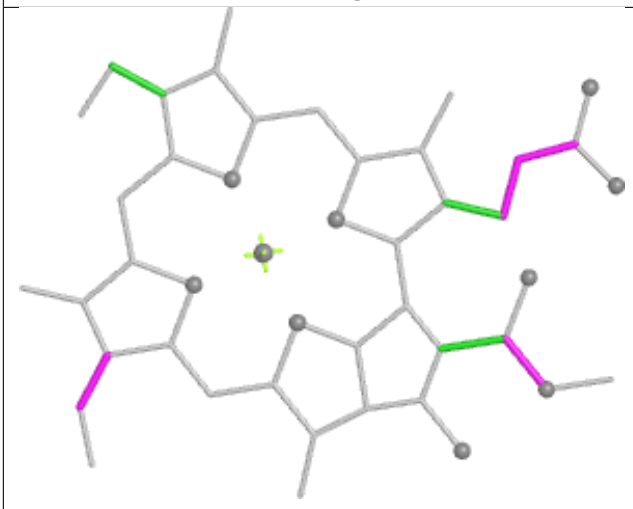
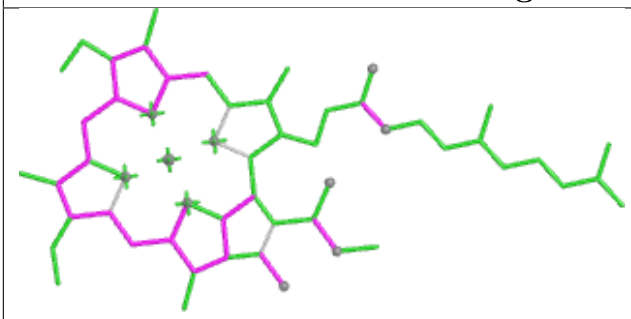


Torsions

Rings

Ligand CLA cA 805



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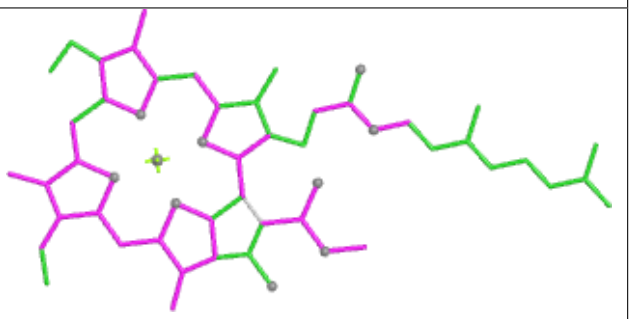
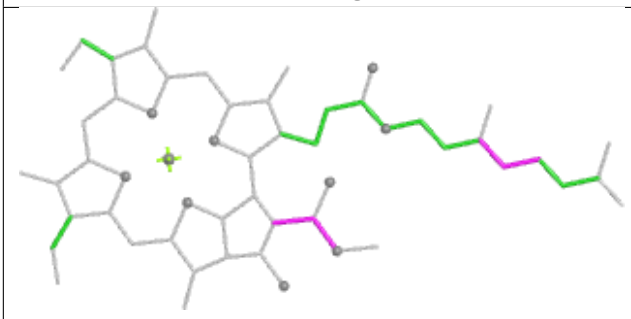


Bond angles



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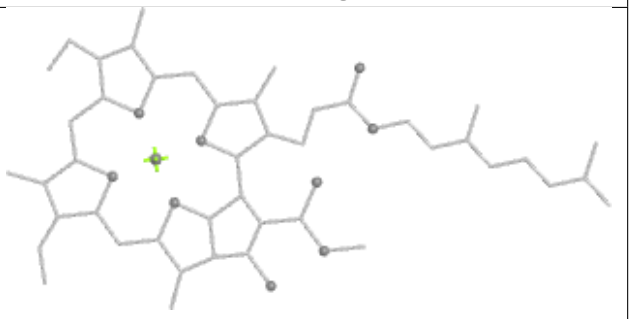
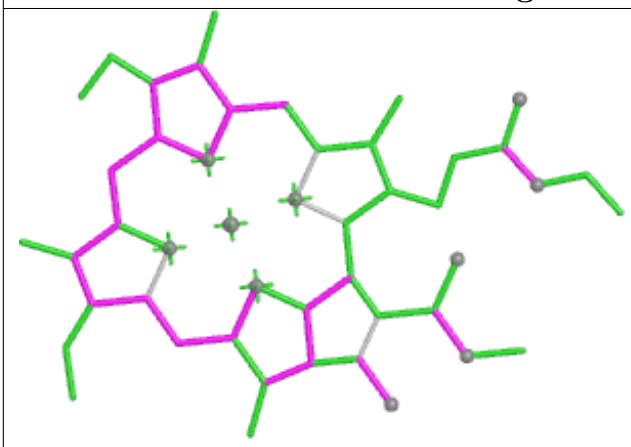


Rings

Ligand CLA cB 820



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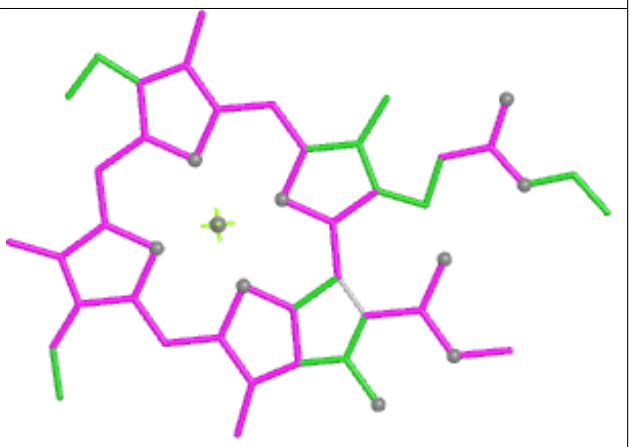
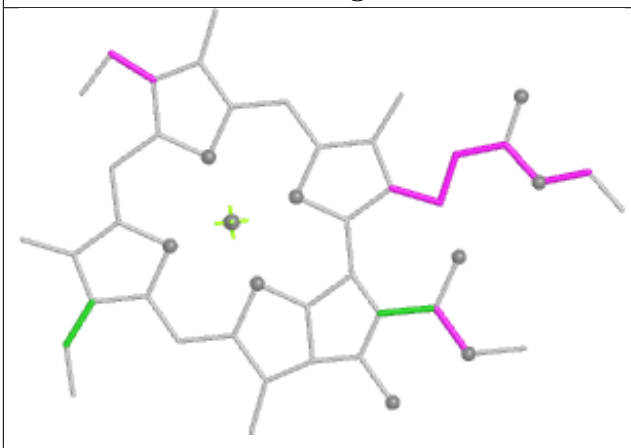


Bond angles



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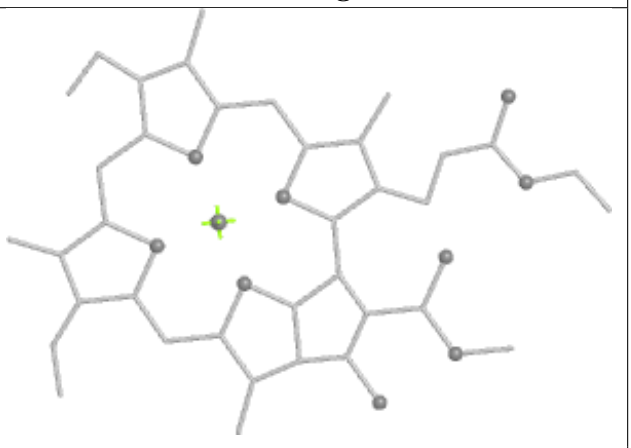
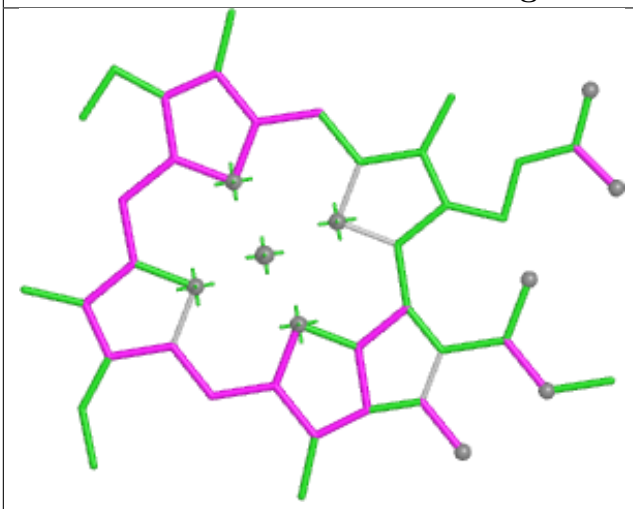


Rings

Ligand CLA cJ 102



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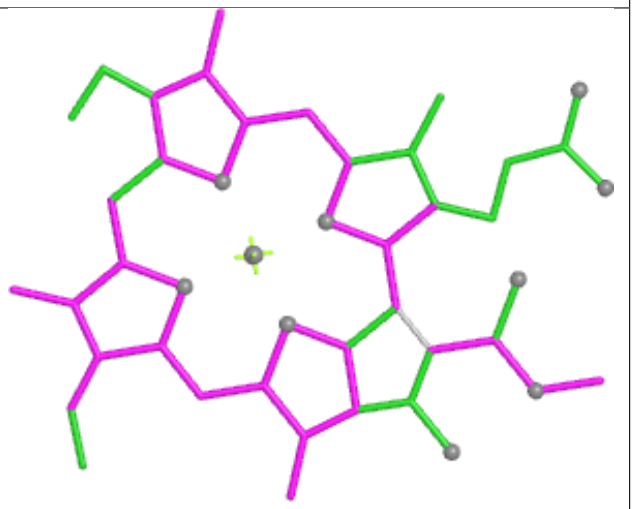
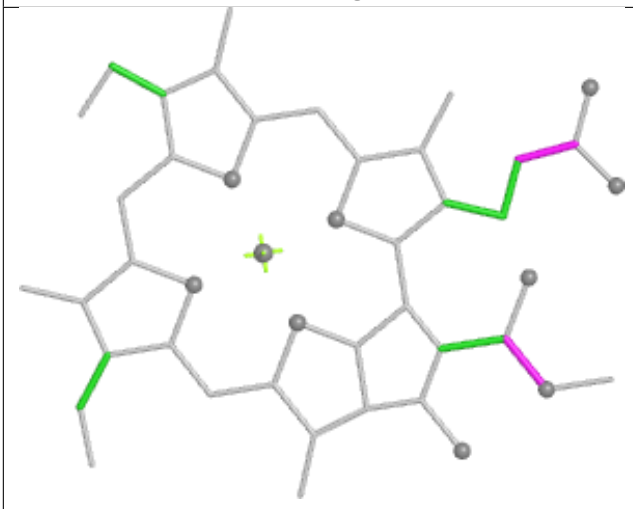


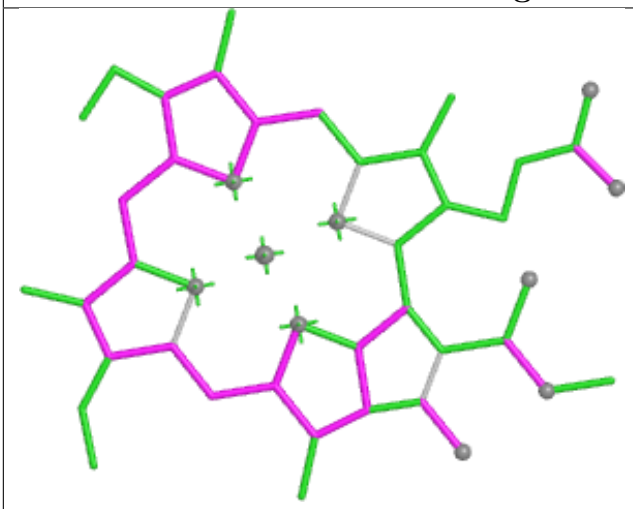
Bond angles



Torsions

Rings

Ligand CLA bA 815



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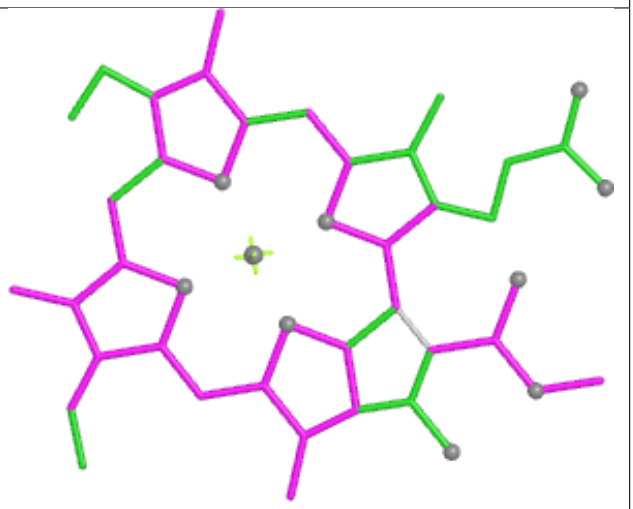
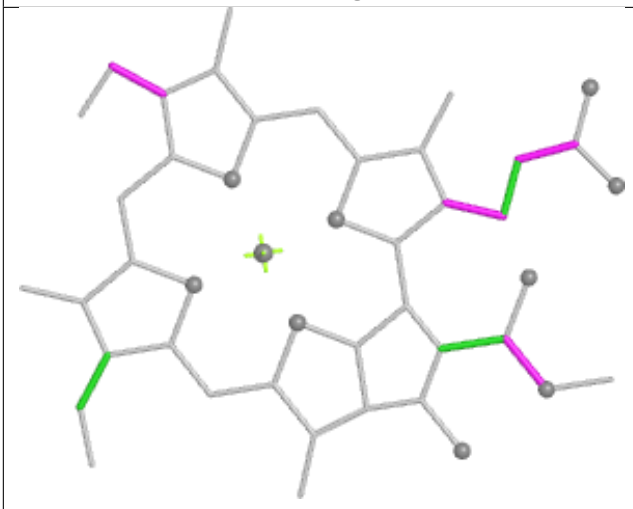


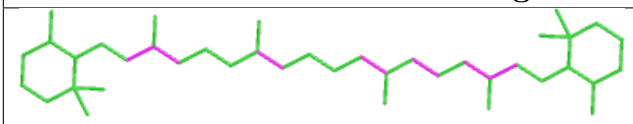
Bond angles



Torsions

Rings

Ligand BCR bB 843



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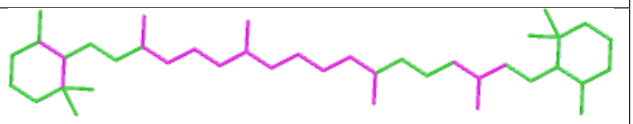
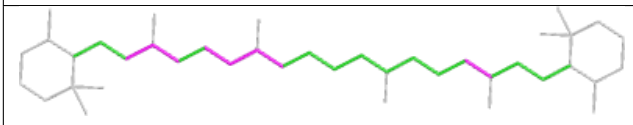
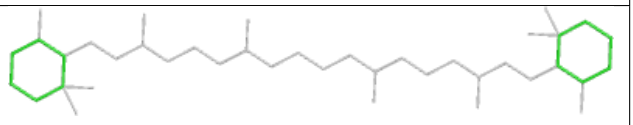


Bond angles



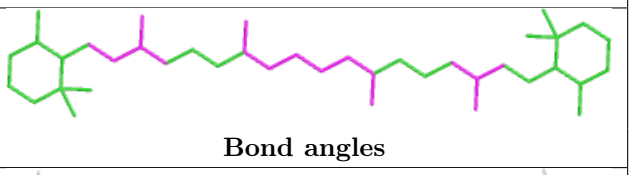
Torsions



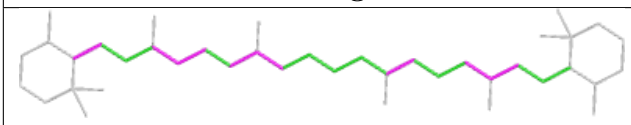
Rings

Ligand BCR B 844

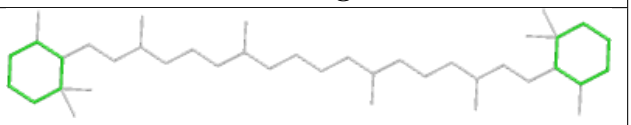
Bond lengths



Bond angles

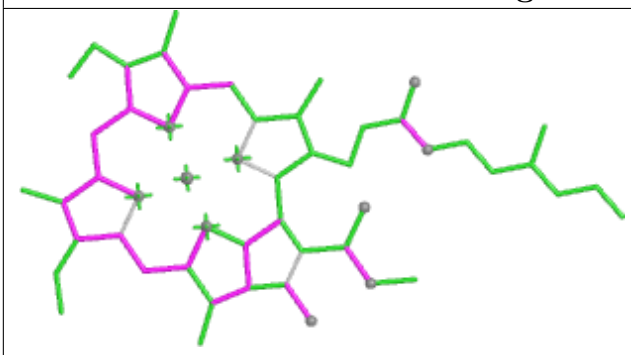


Torsions



Rings

Ligand CLA cB 809



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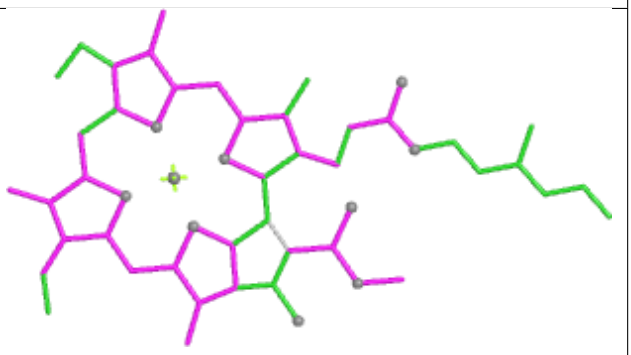
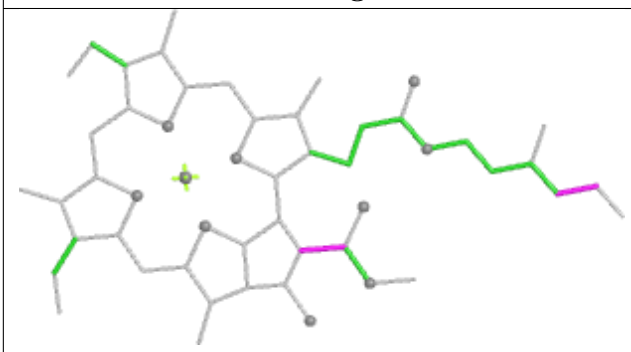


Bond angles



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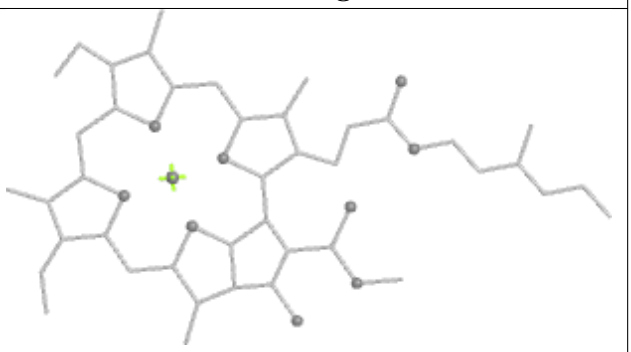
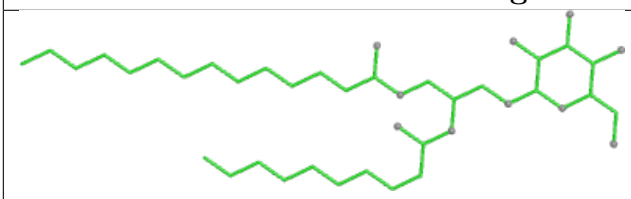


Rings

Ligand LMG bB 848



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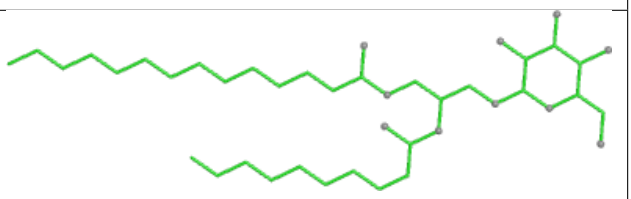
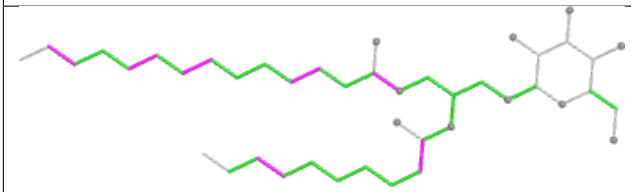
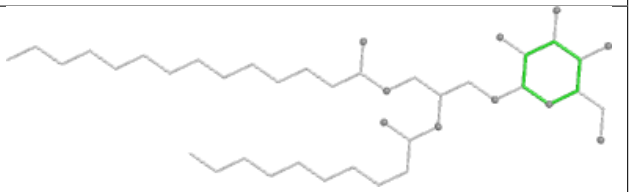


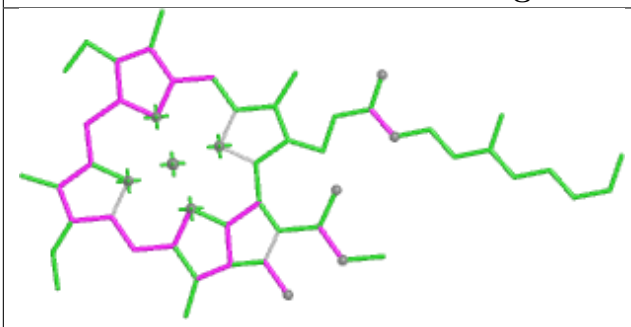
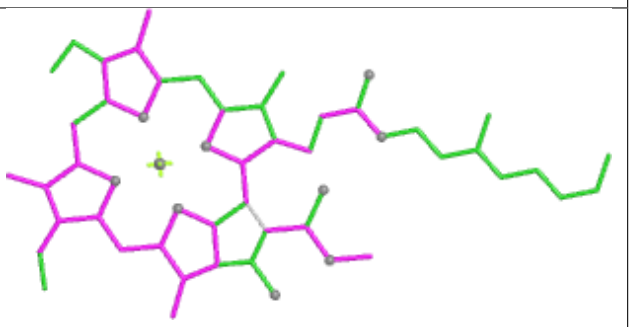
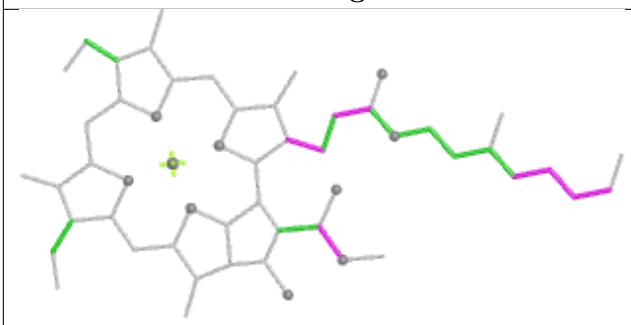
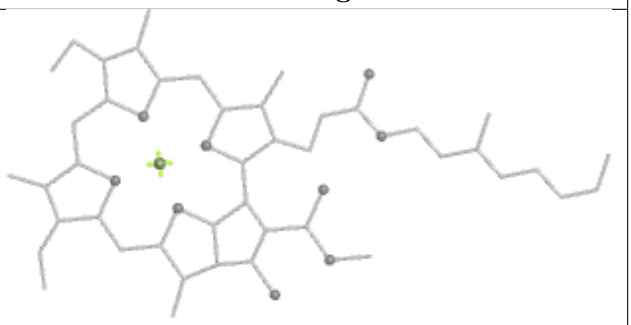
Bond angles



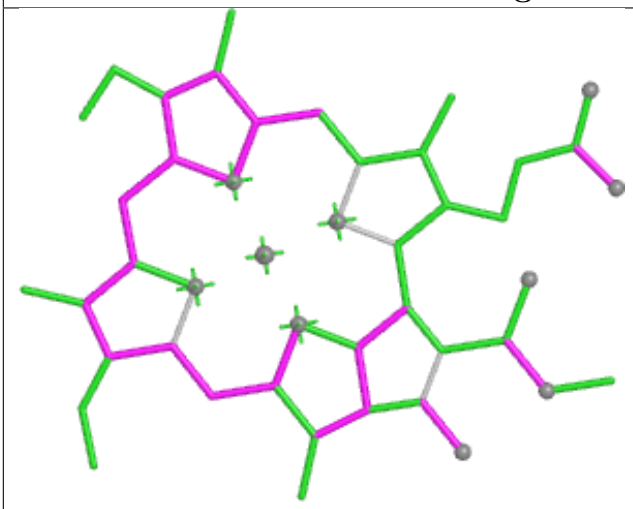
Torsions



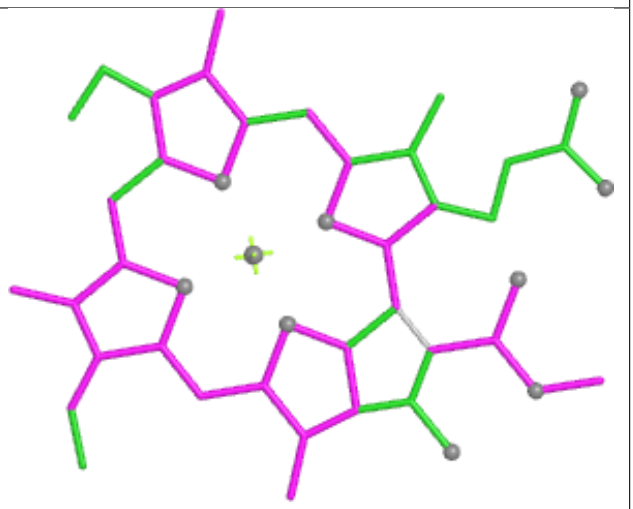
Rings

Ligand CLA bA 817	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

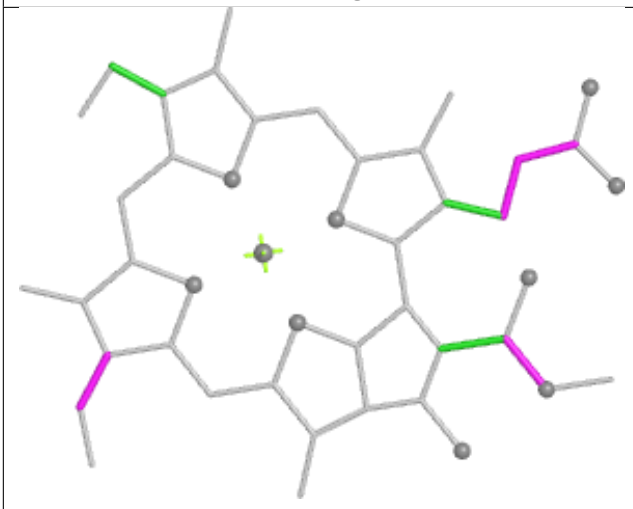
Ligand CLA bB 829



Bond lengths



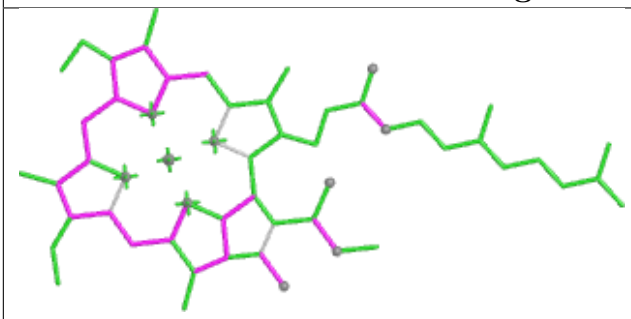
Bond angles



Torsions

Rings

Ligand CLA bB 803



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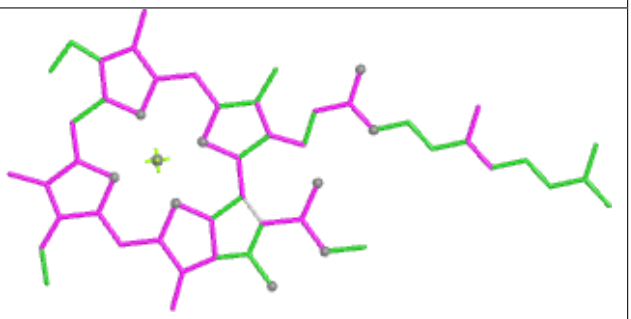
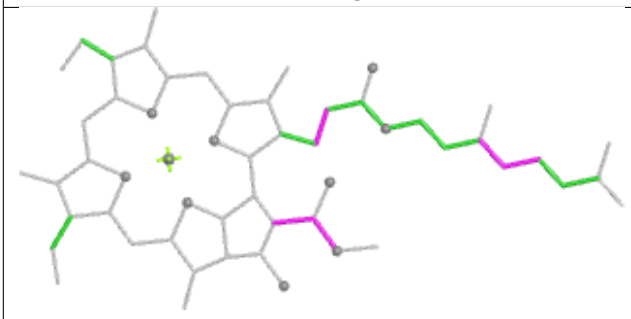
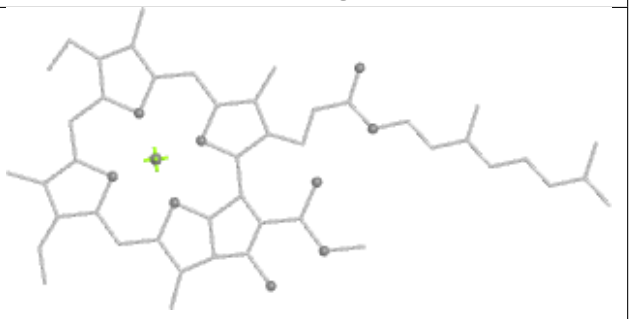


Bond angles

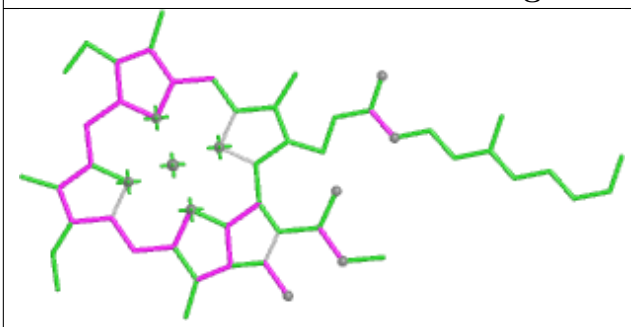


Torsions



Rings

Ligand CLA A 817



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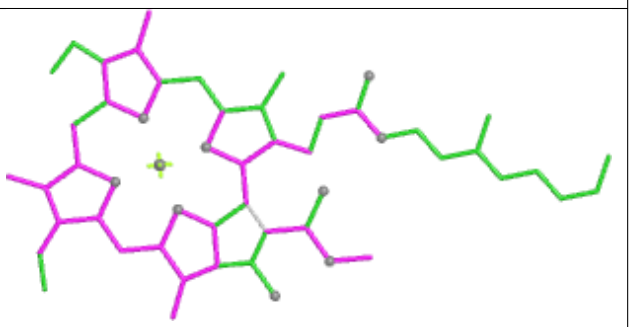

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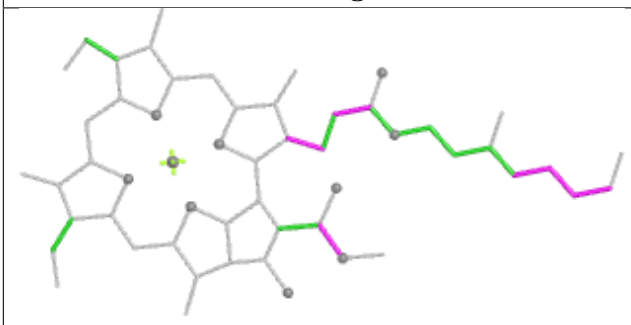

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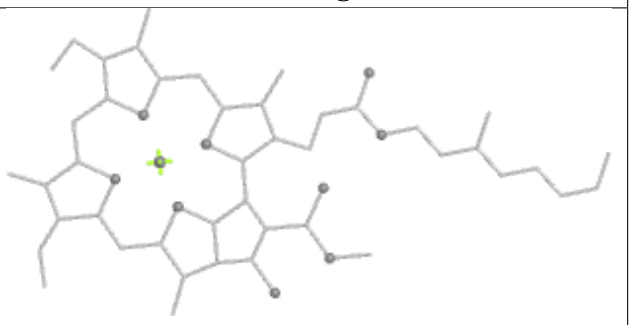
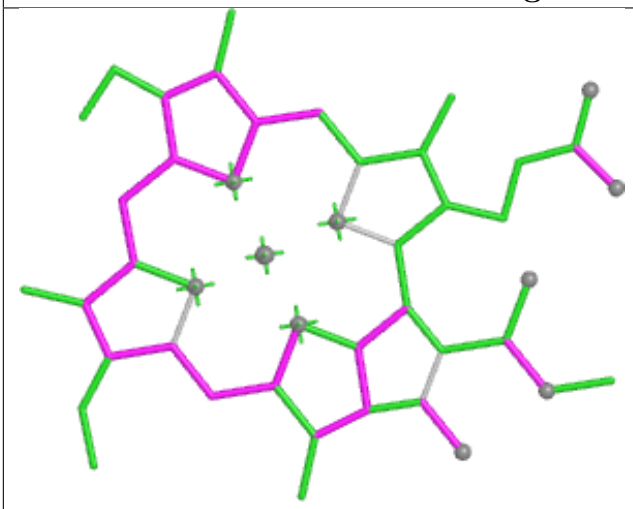


Rings

Ligand CLA A 835



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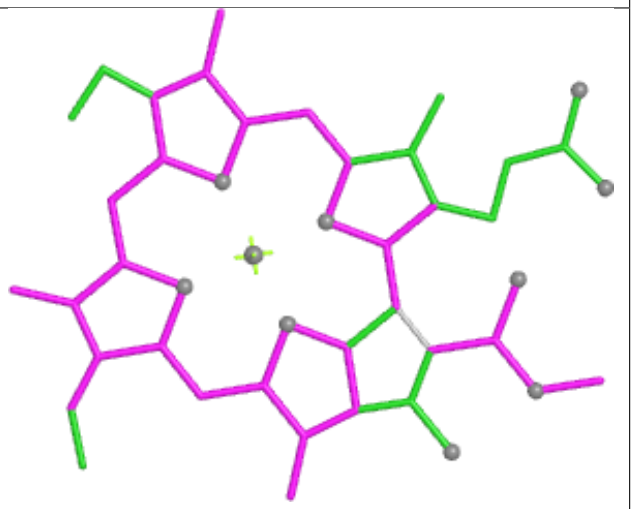
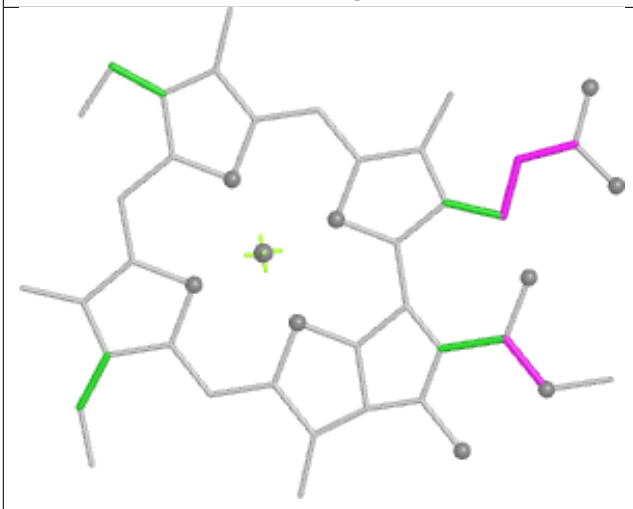


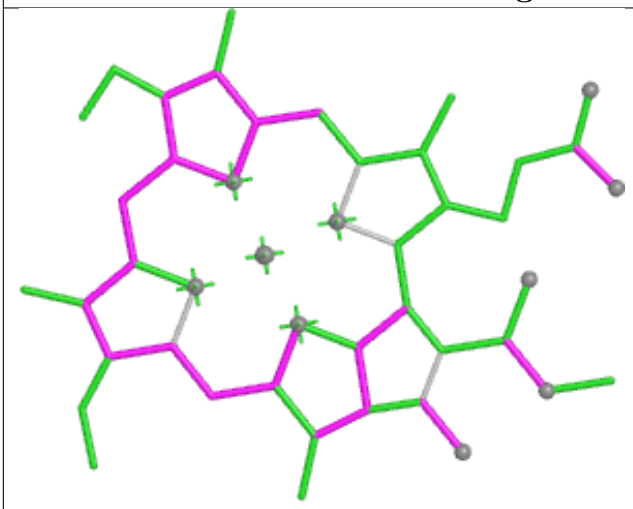
Bond angles



Torsions

Rings

Ligand CLA cA 823



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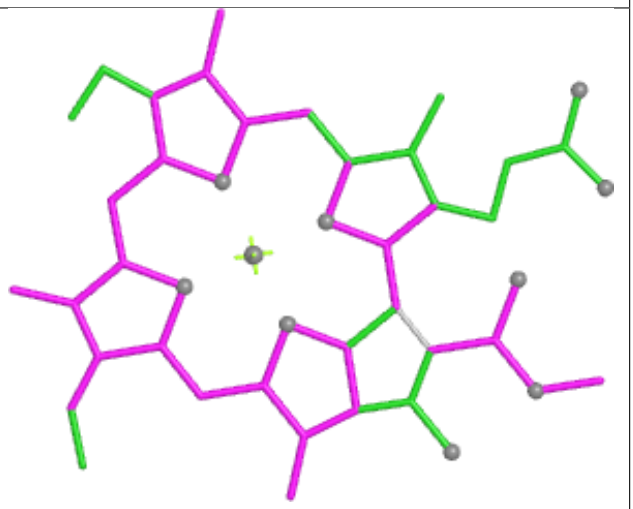
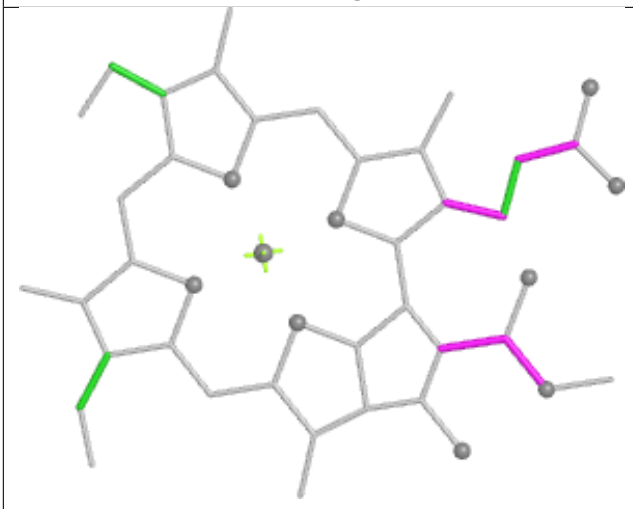


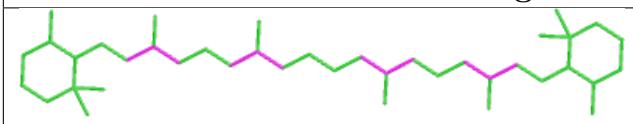
Bond angles



Torsions

Rings

Ligand BCR bL 205



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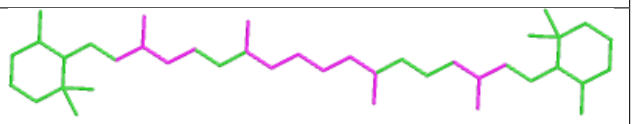

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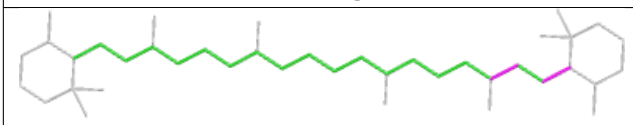

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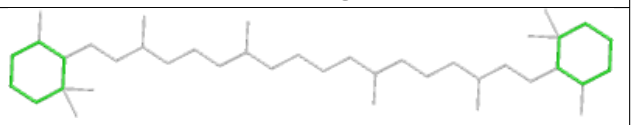
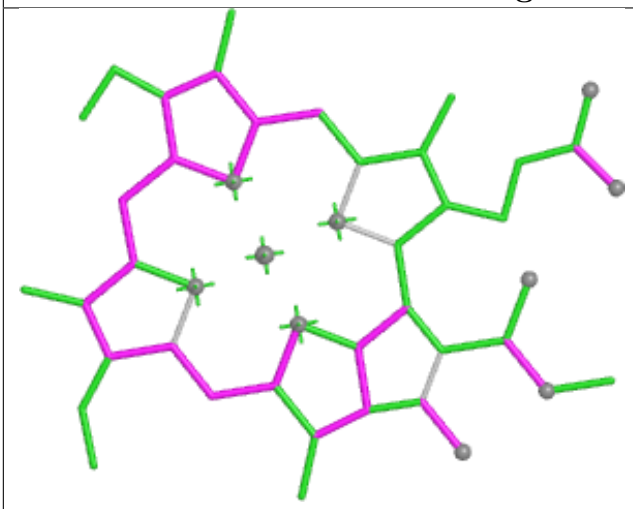


Rings

Ligand CLA cA 803



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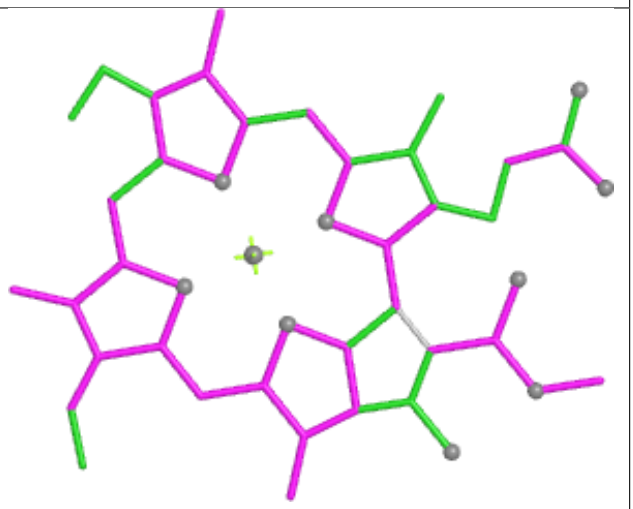
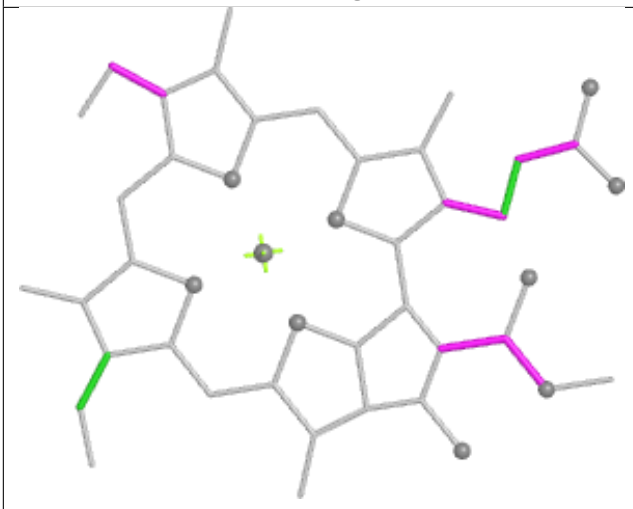


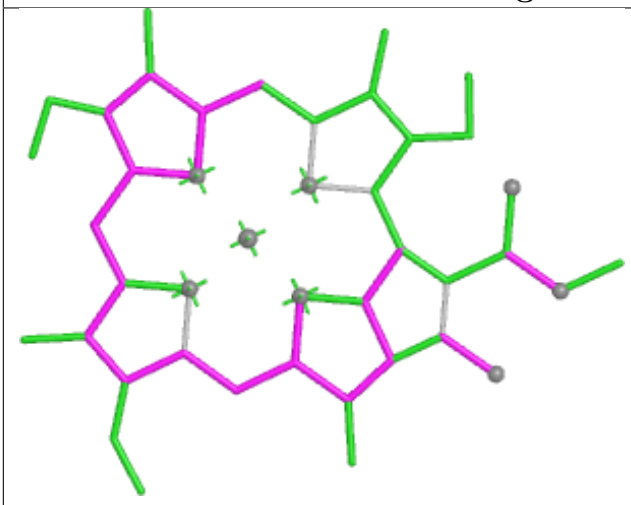
Bond angles



Torsions

Rings

Ligand CLA cB 831



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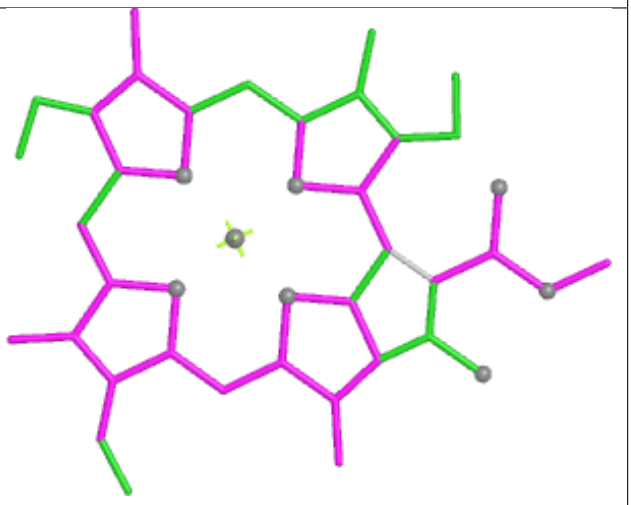
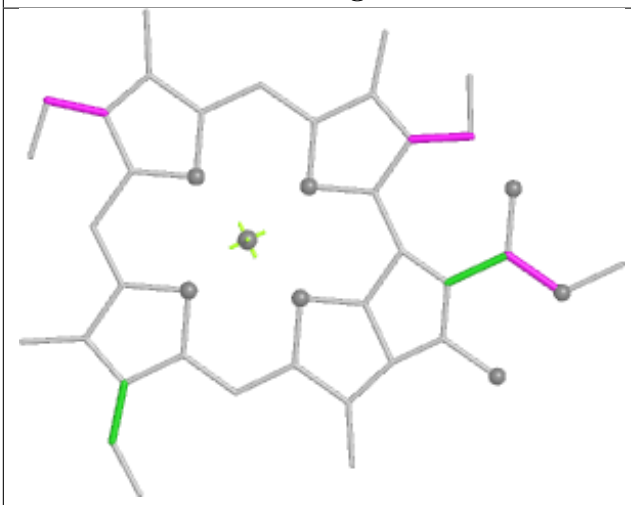


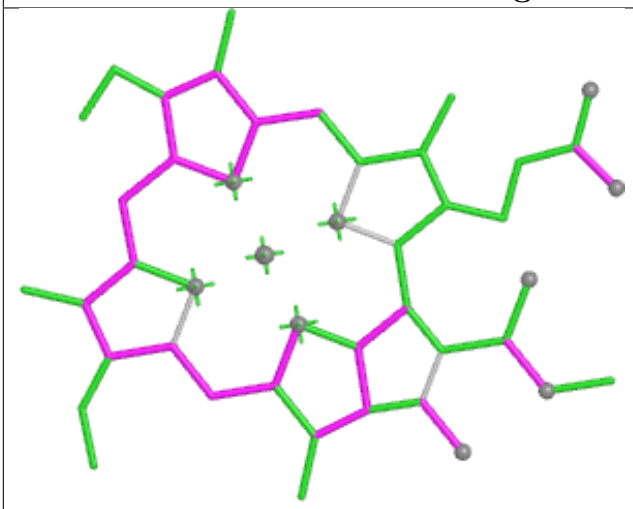
Bond angles



Torsions

Rings

Ligand CLA bA 814



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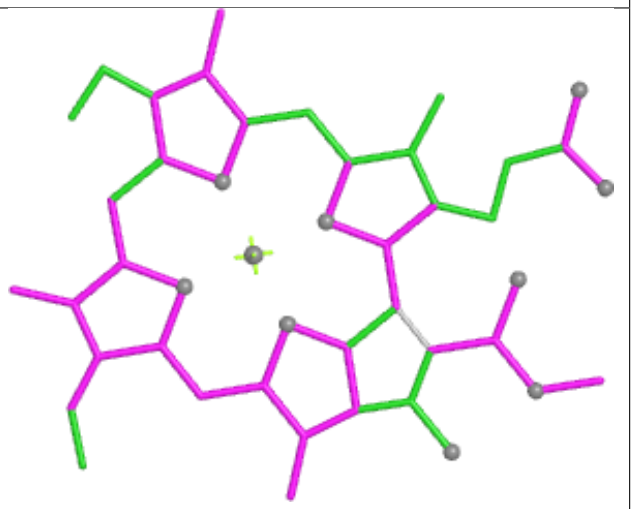
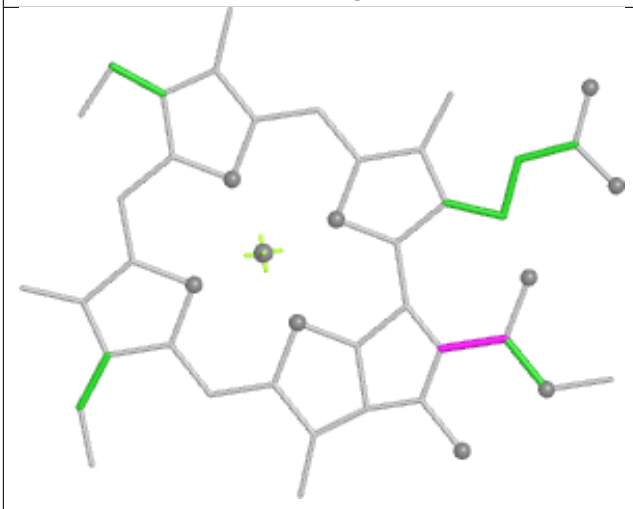


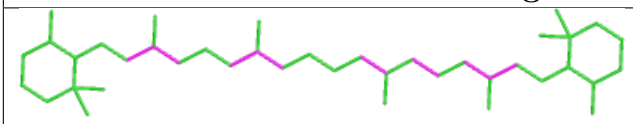
Bond angles



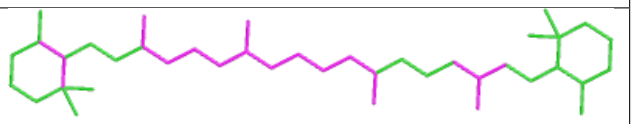
Torsions

Rings

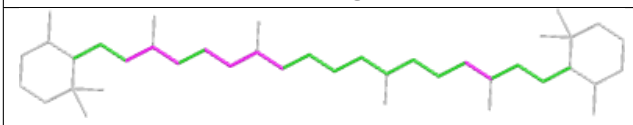
Ligand BCR B 843



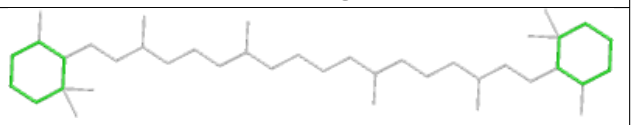
Bond lengths



Bond angles

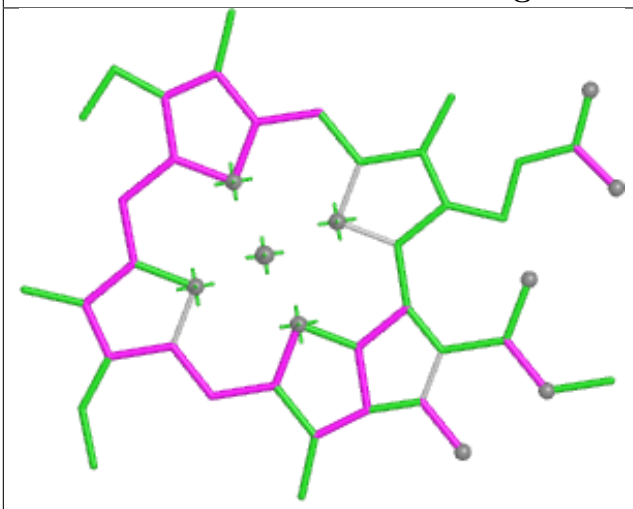


Torsions

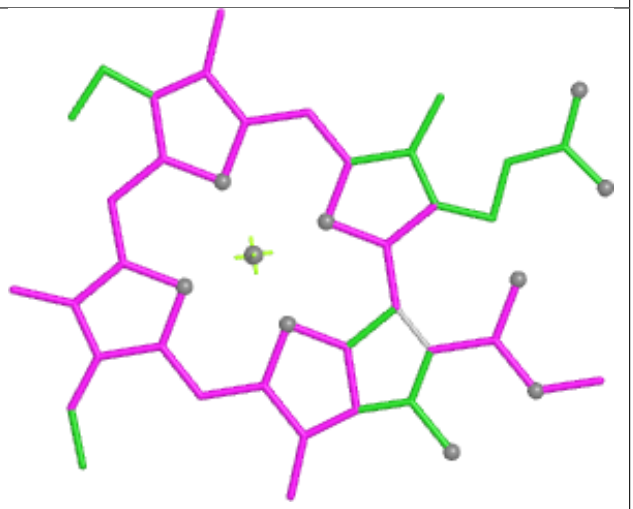


Rings

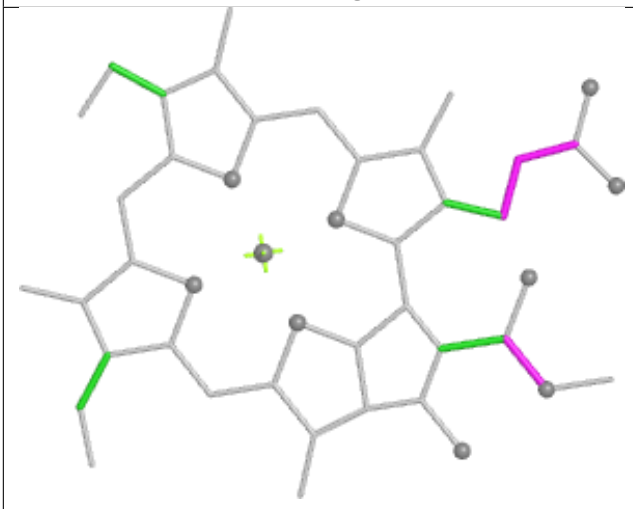
Ligand CLA bA 835



Bond lengths



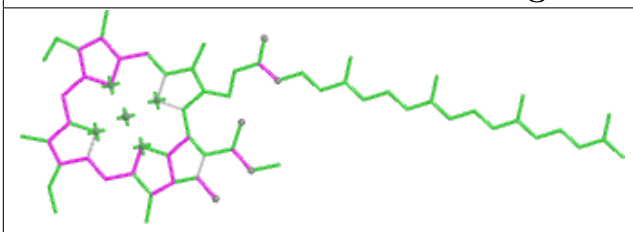
Bond angles



Torsions

Rings

Ligand CL0 A 801



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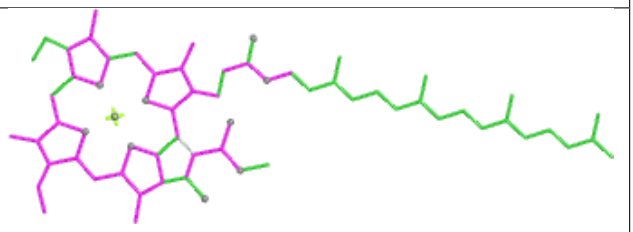
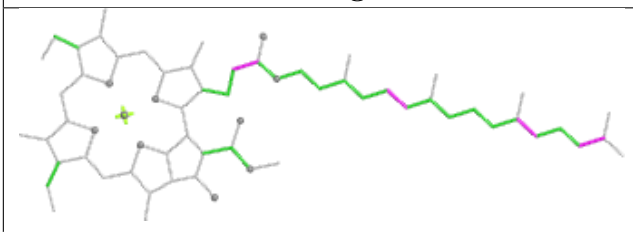
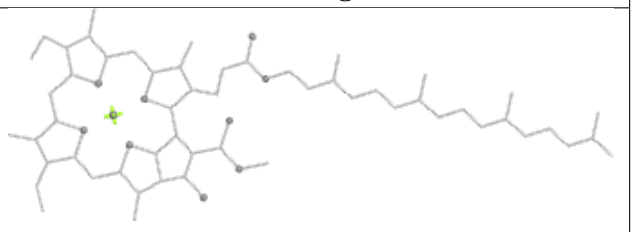


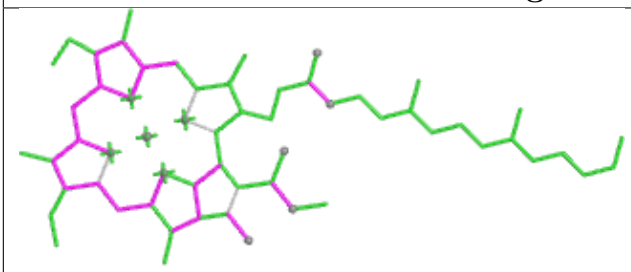
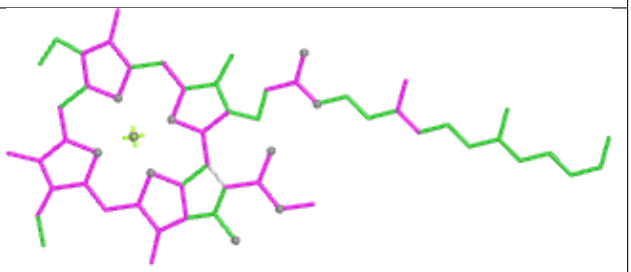
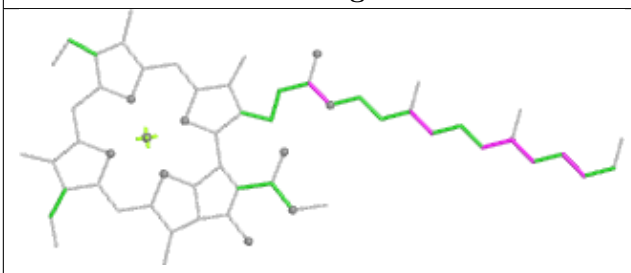
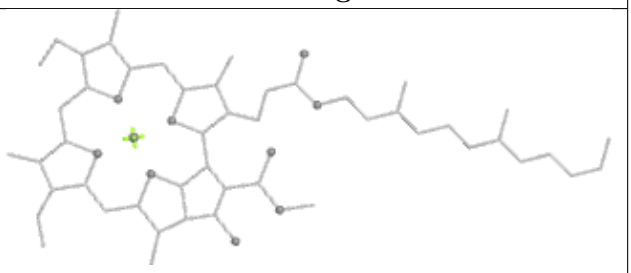
Bond angles

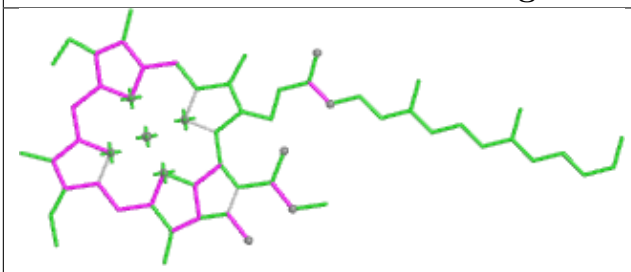
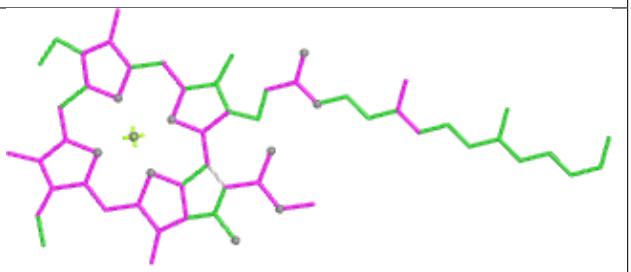
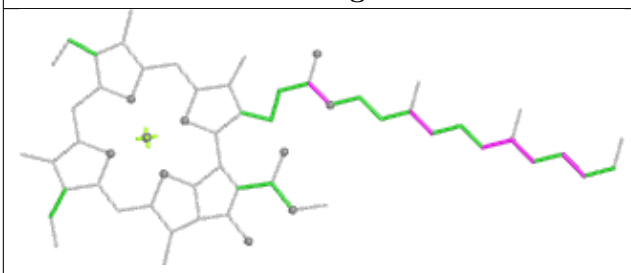
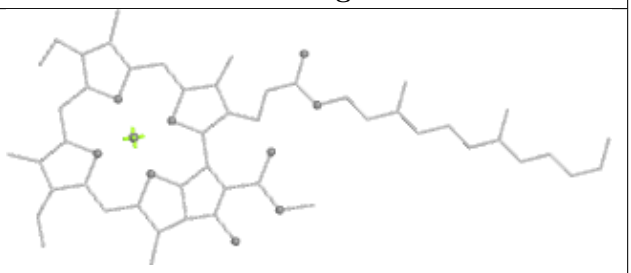


Torsions

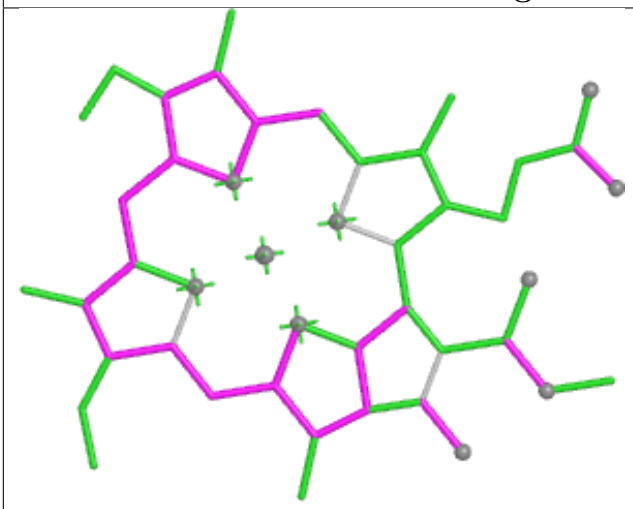


Rings

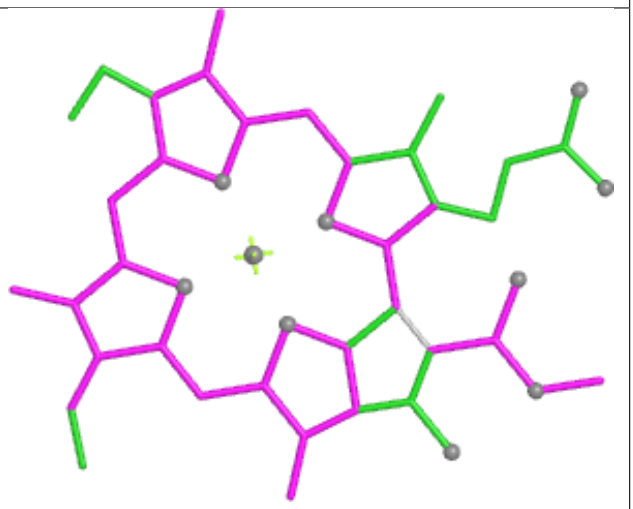
Ligand CLA L 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA cL 204	
	
Bond lengths	Bond angles
	
Torsions	Rings

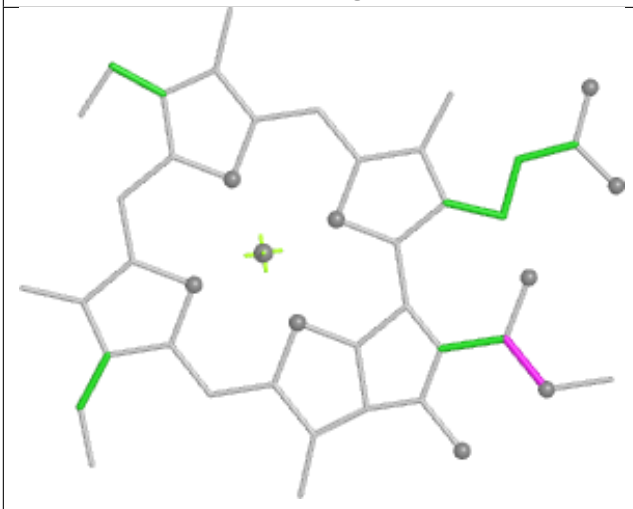
Ligand CLA bB 833



Bond lengths



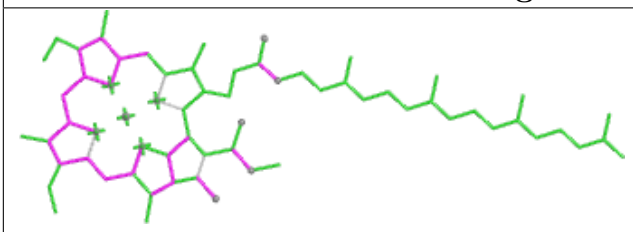
Bond angles



Torsions

Rings

Ligand CLA cA 802



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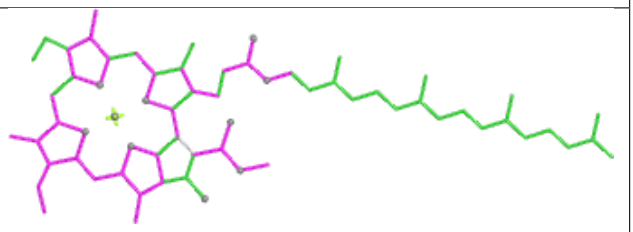
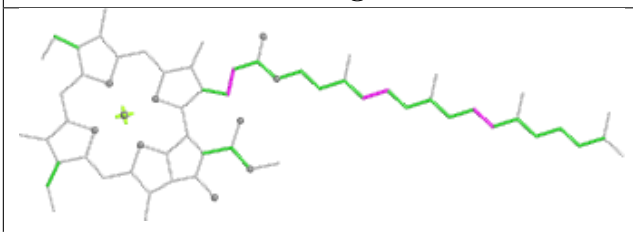


Bond angles



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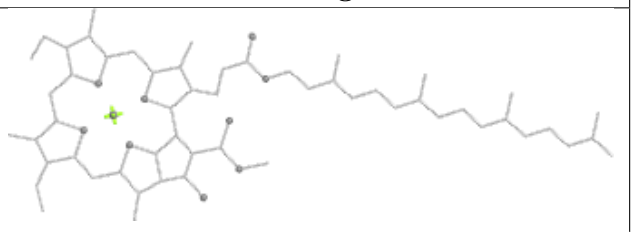

Rings

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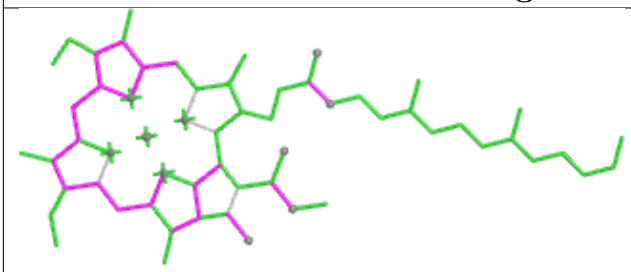

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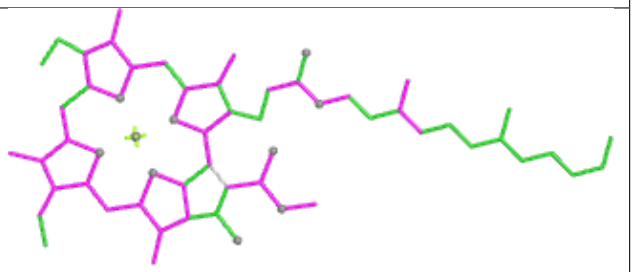
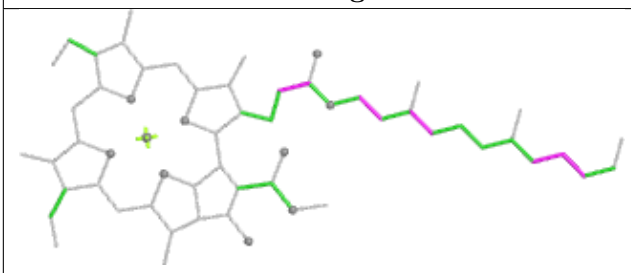


Bond angles



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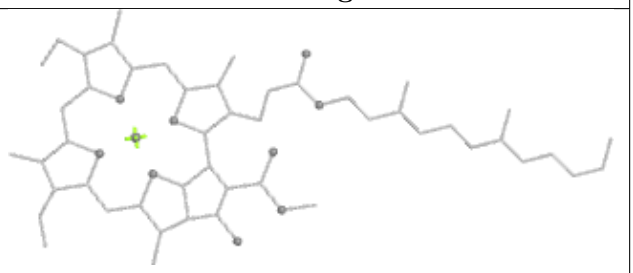
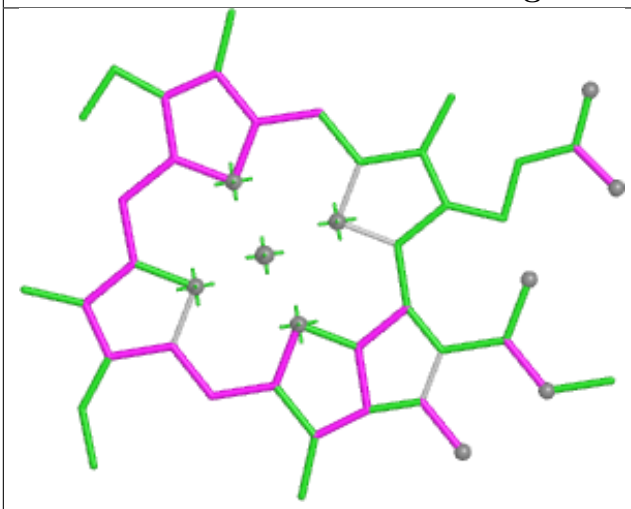


Rings

Ligand CLA A 821



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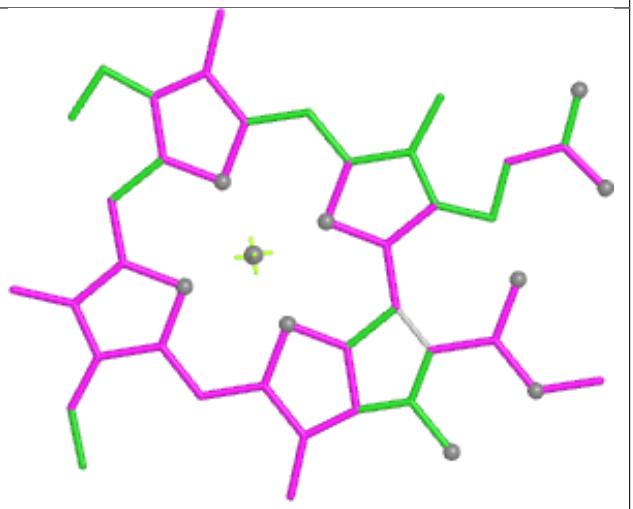
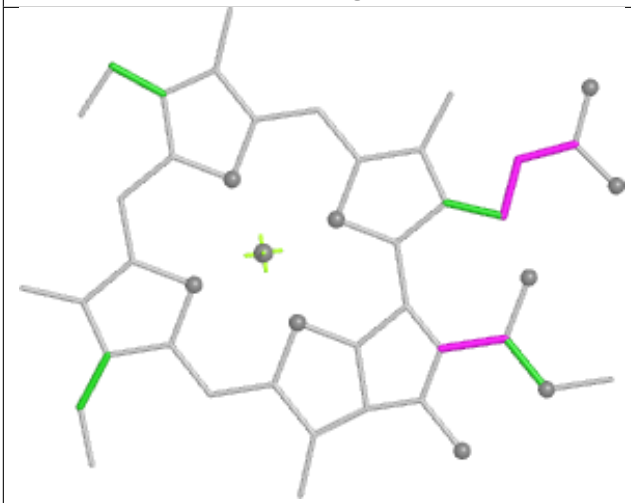


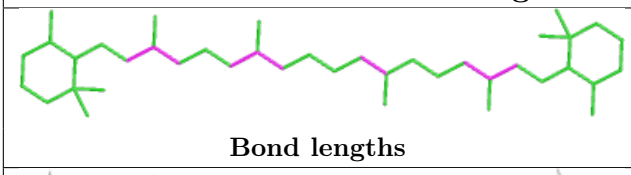
Bond angles



Torsions

Rings

Ligand BCR bA 849



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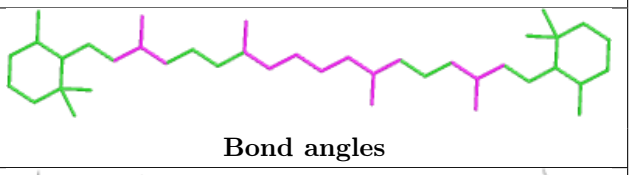
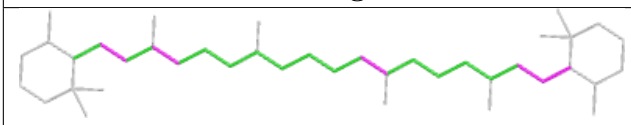
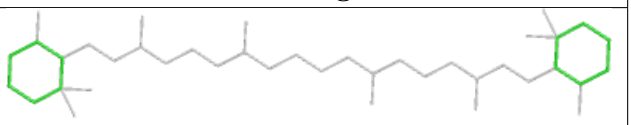


Bond angles

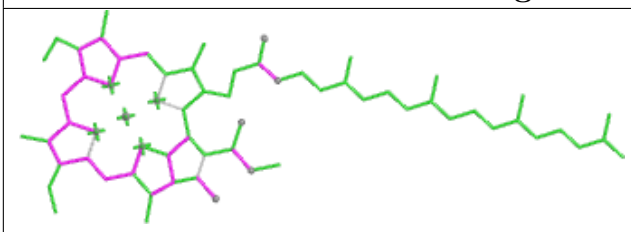


Torsions



Rings

Ligand CLA bB 839



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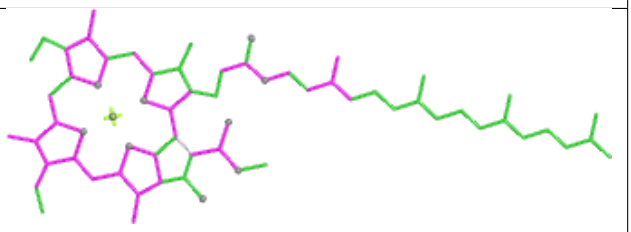
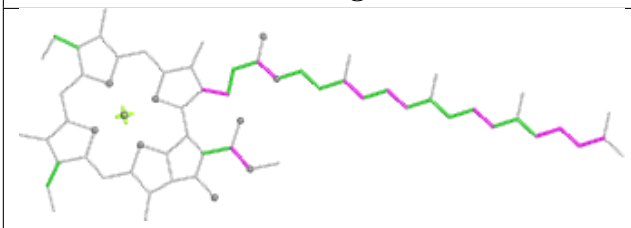


Bond angles



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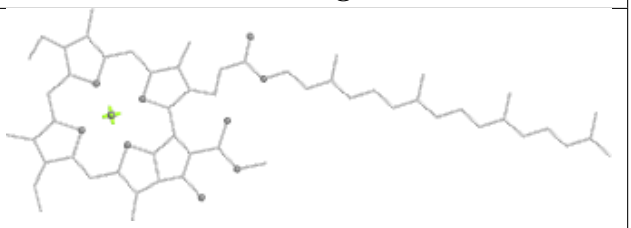
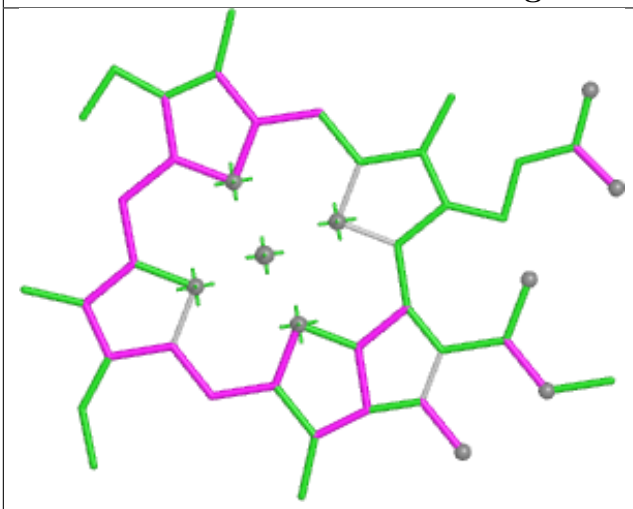


Rings

Ligand CLA B 832



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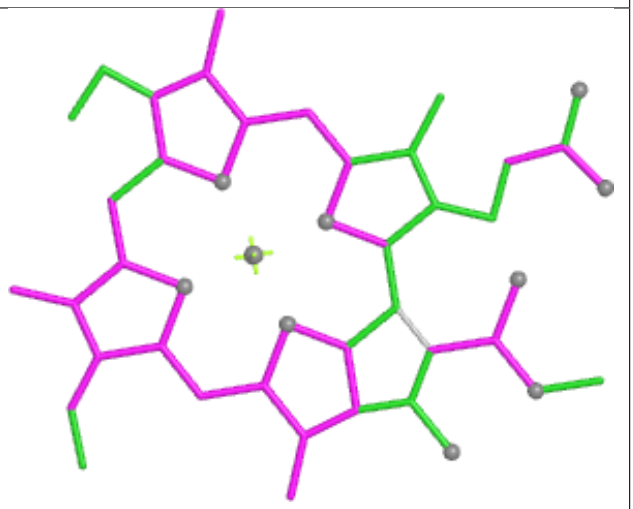
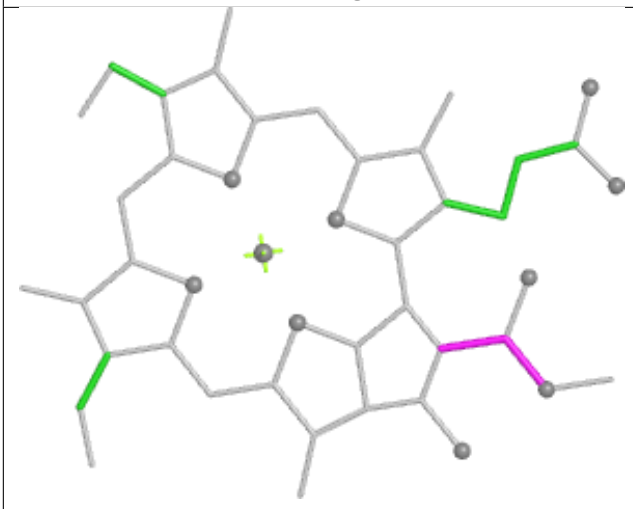


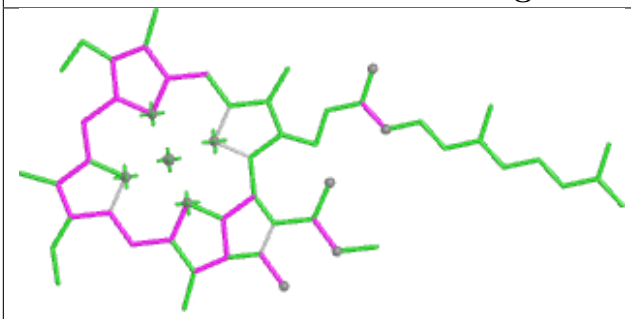
Bond angles



Torsions

Rings

Ligand CLA bB 825



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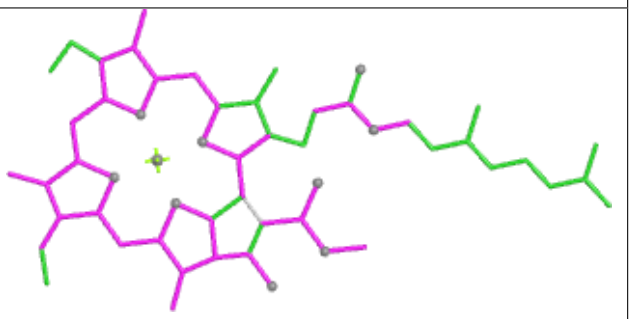
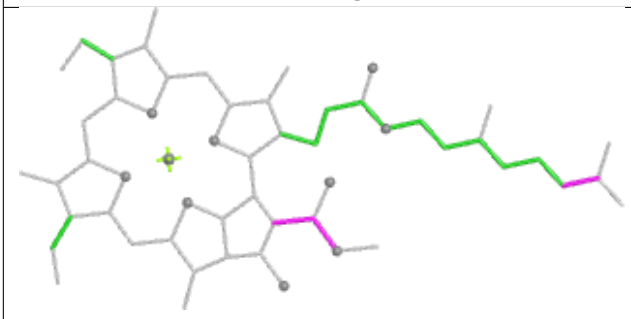
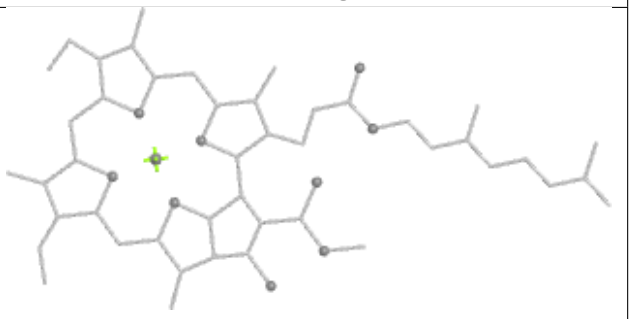


Bond angles

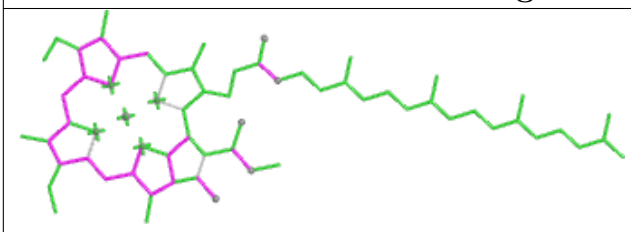


Torsions



Rings

Ligand CLA bL 202



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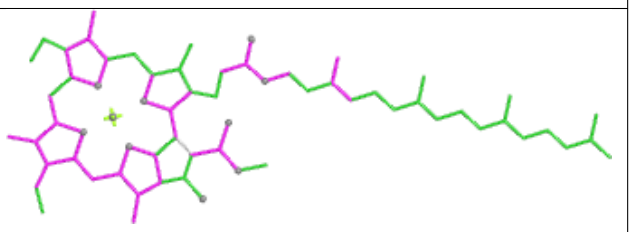
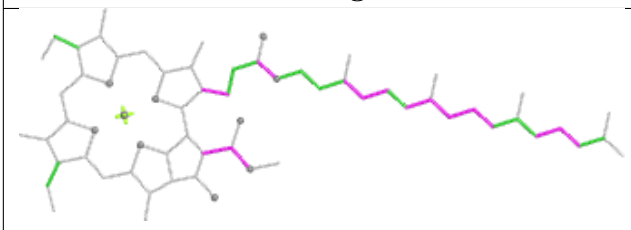


Bond angles



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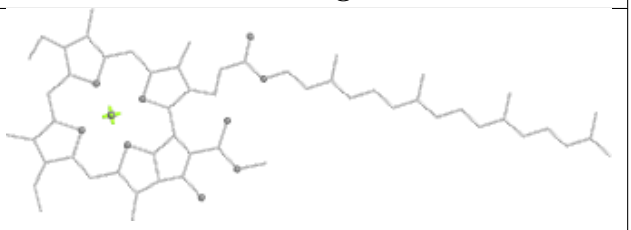
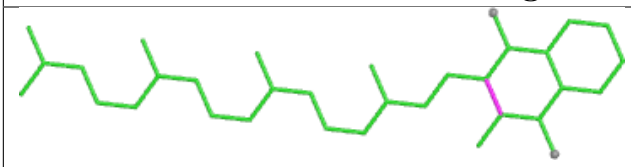
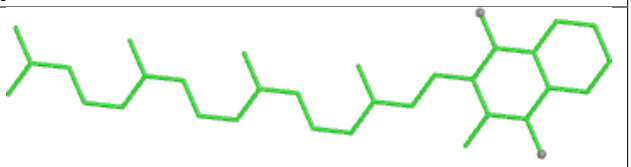


Rings

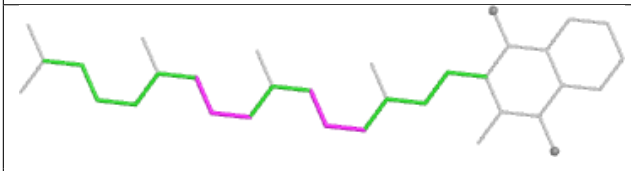
Ligand PQN B 840



Bond lengths



Bond angles



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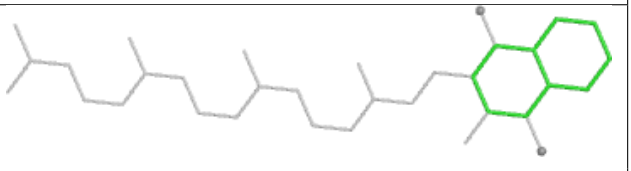
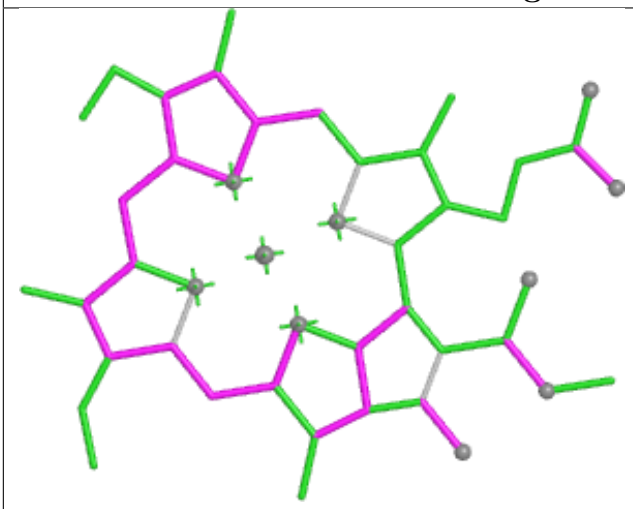


Rings

Ligand CLA A 808



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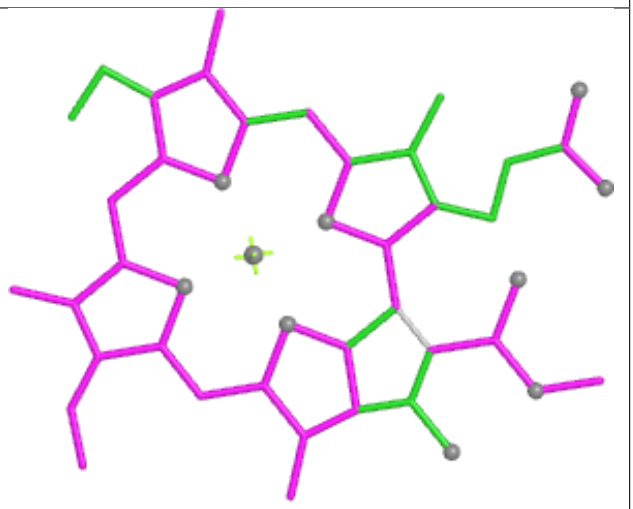
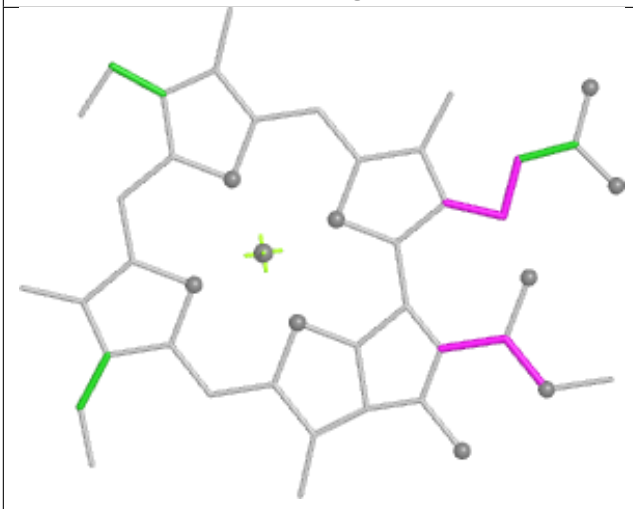


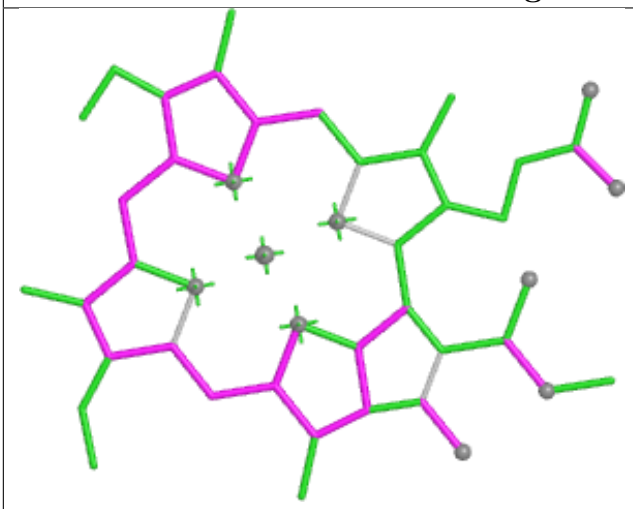
Bond angles



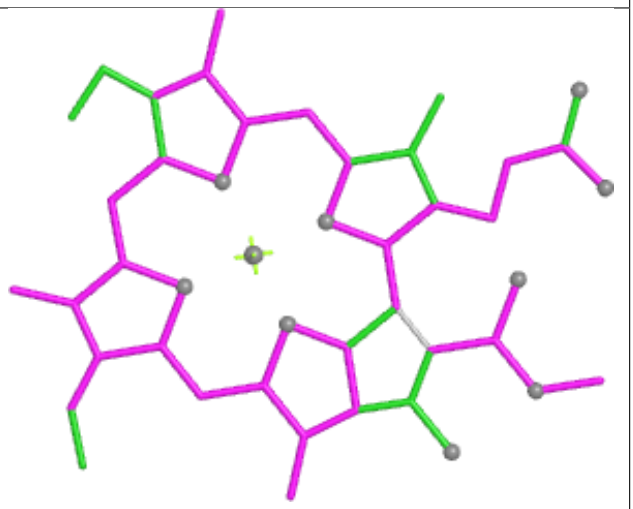
Torsions

Rings

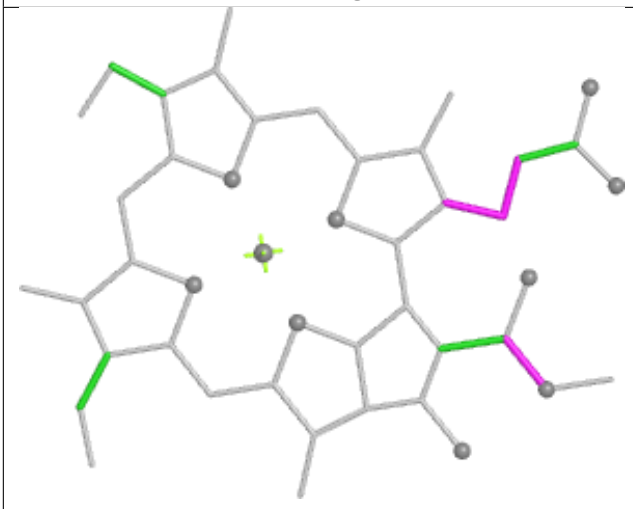
Ligand CLA B 816



Bond lengths



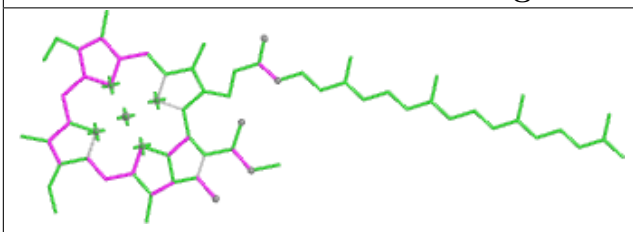
Bond angles



Torsions

Rings

Ligand CLA bA 852



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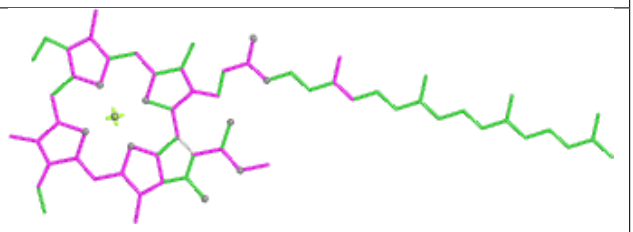
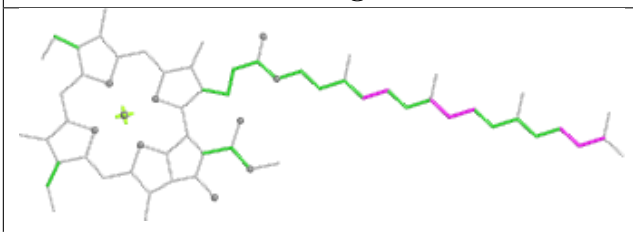
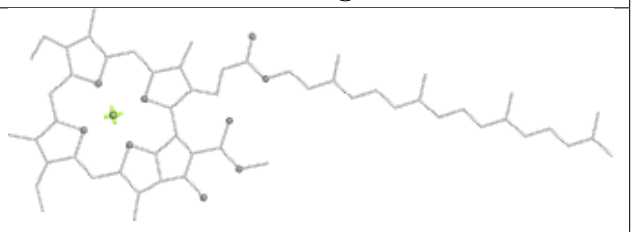


Bond angles

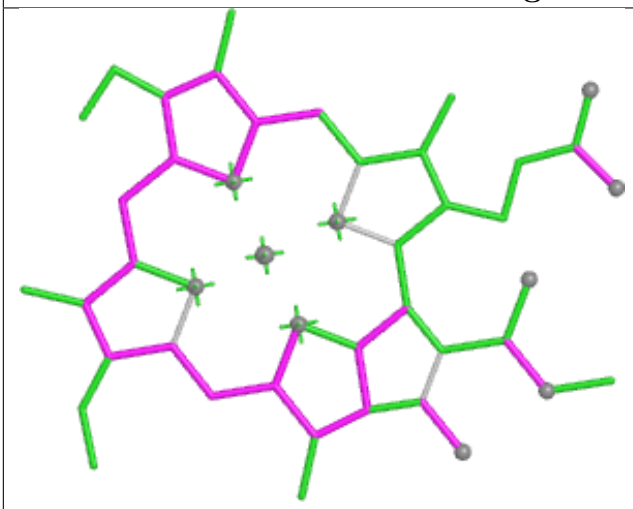


Torsions



Rings

Ligand CLA A 807



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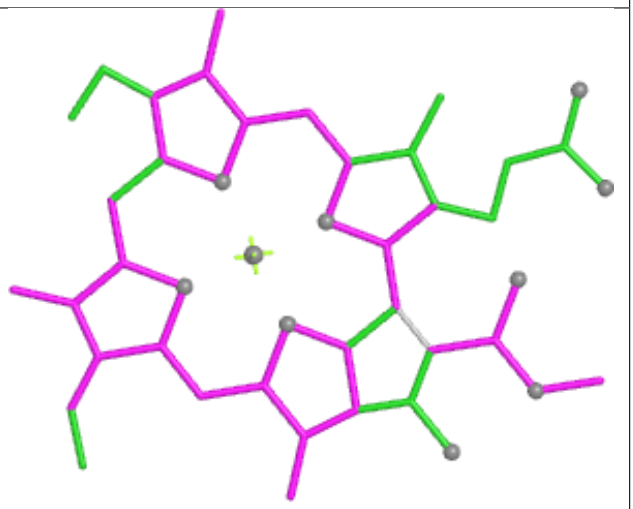
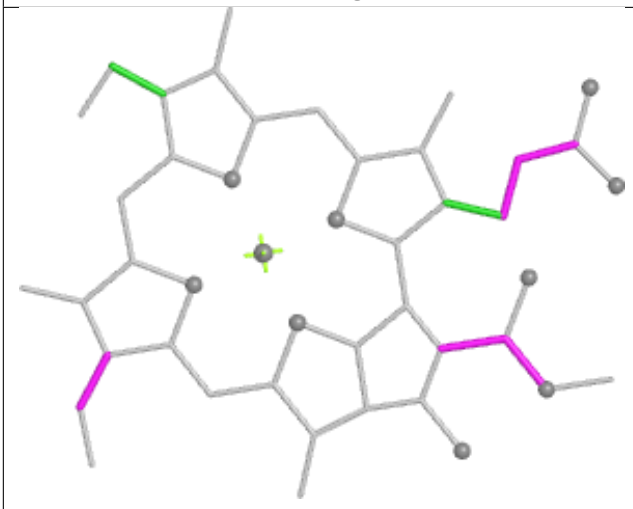


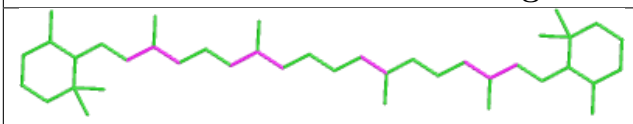
Bond angles



Torsions

Rings

Ligand BCR A 845



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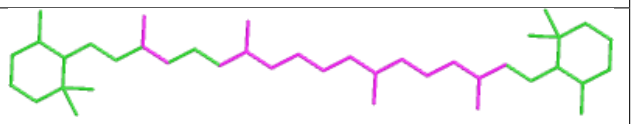
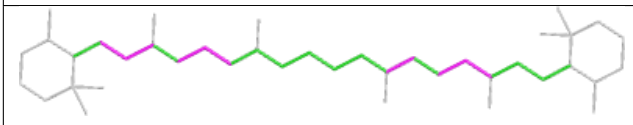
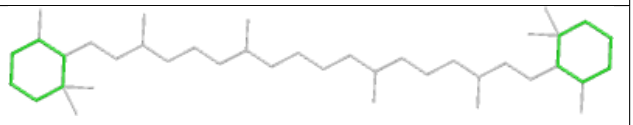


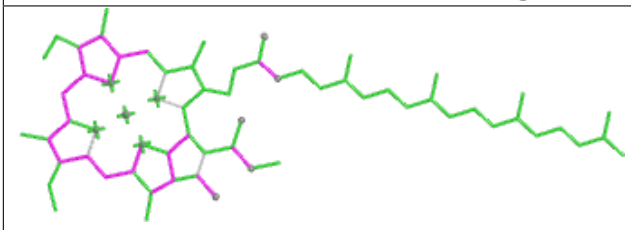
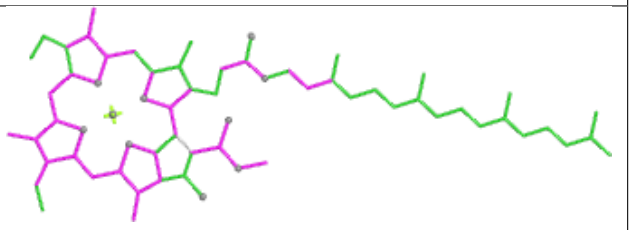
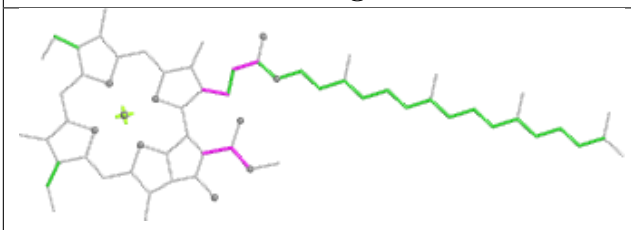
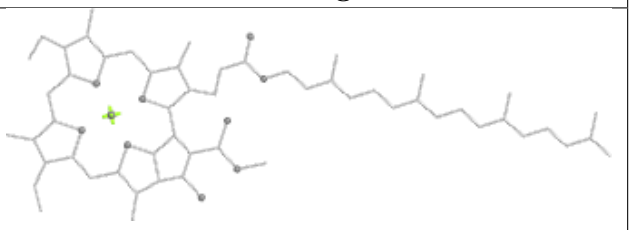
Bond angles

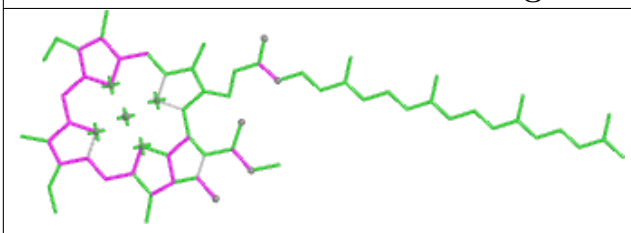
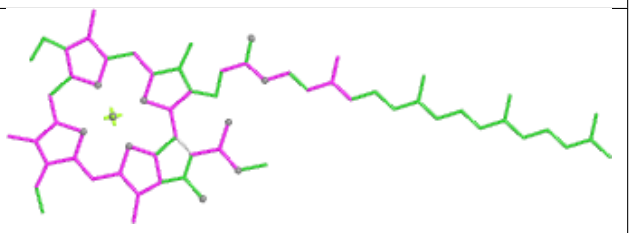
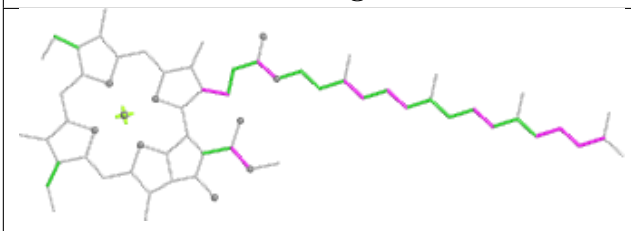
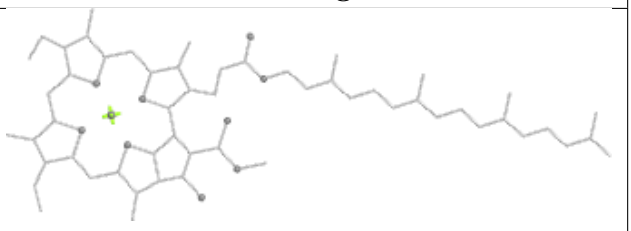


Torsions

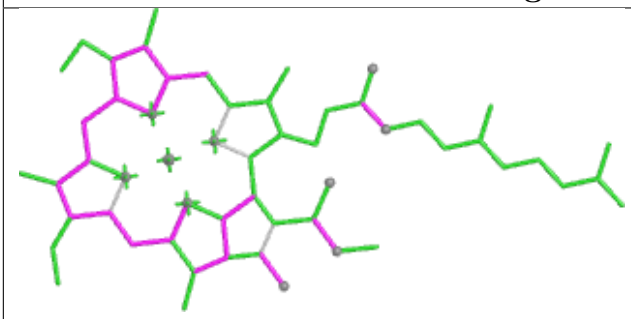


Rings

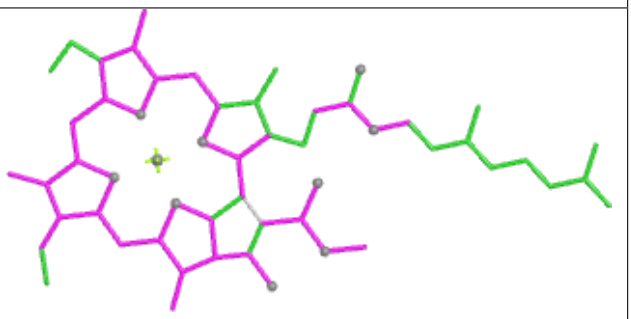
Ligand CLA bB 812	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

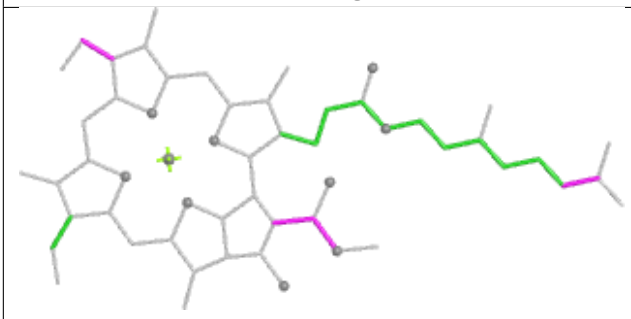
Ligand CLA B 825



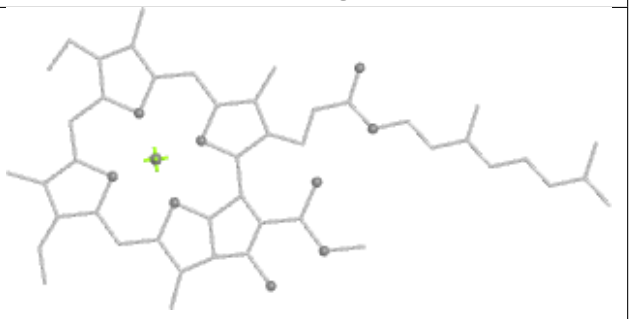
Bond lengths



Bond angles

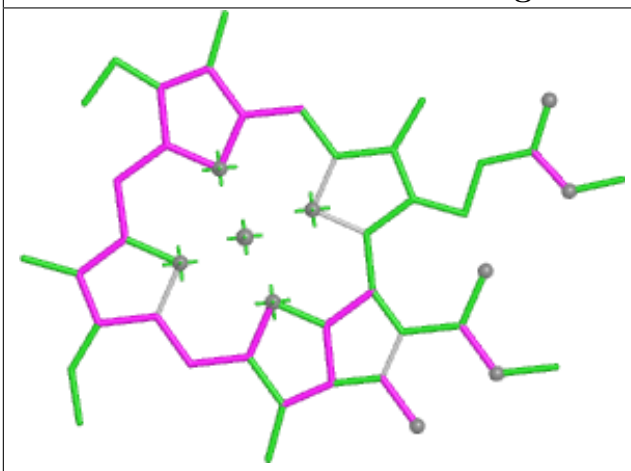


Torsions

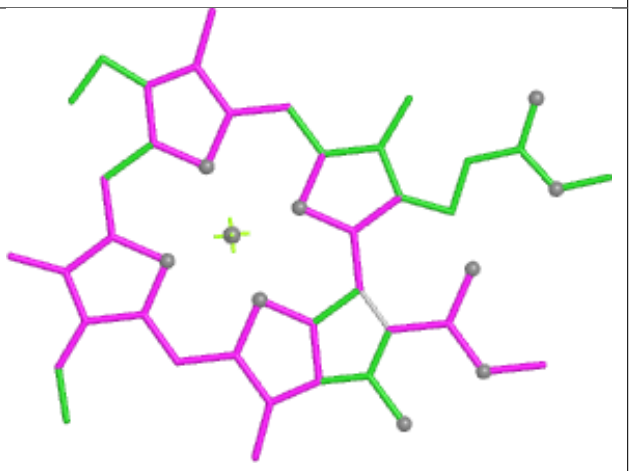


Rings

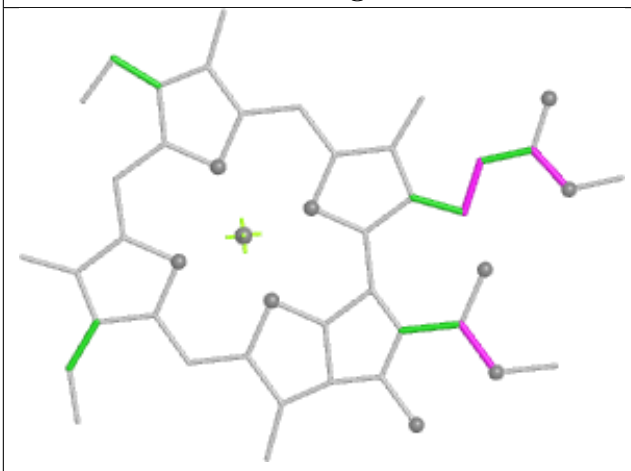
Ligand CLA bB 818



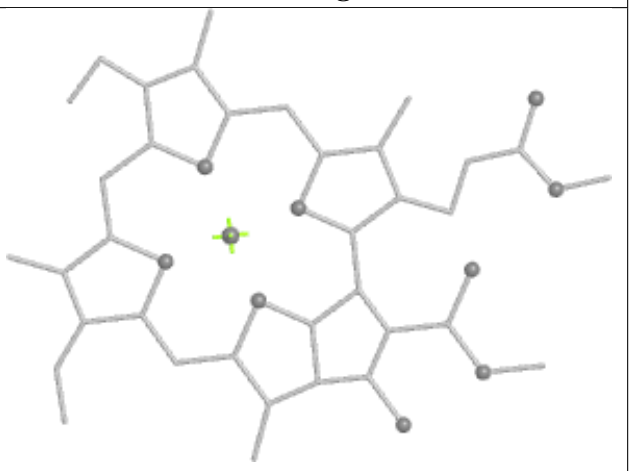
Bond lengths



Bond angles

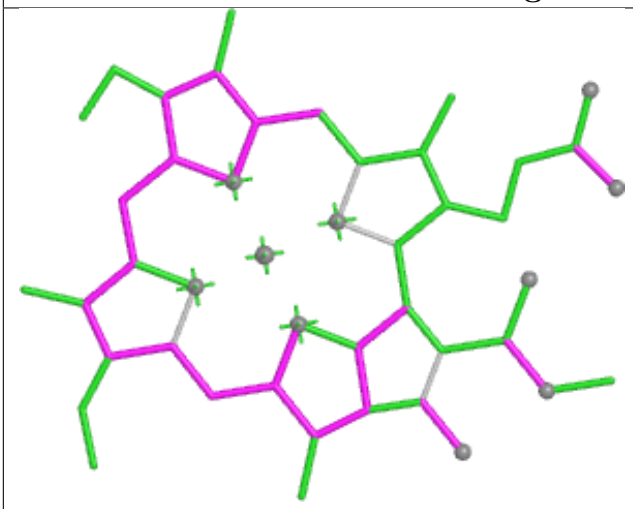


Torsions



Rings

Ligand CLA B 833



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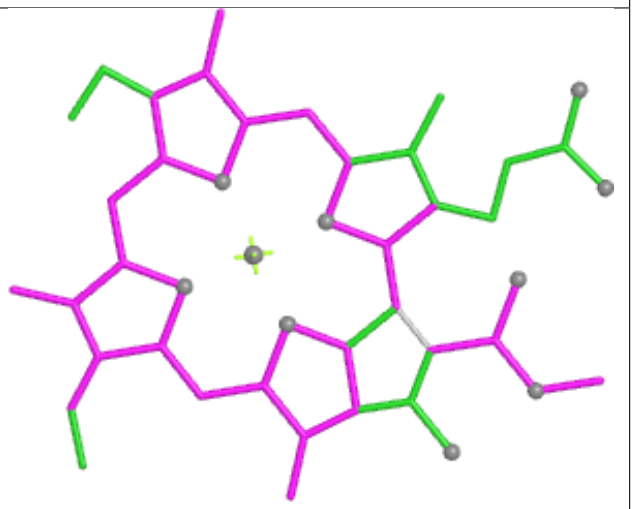
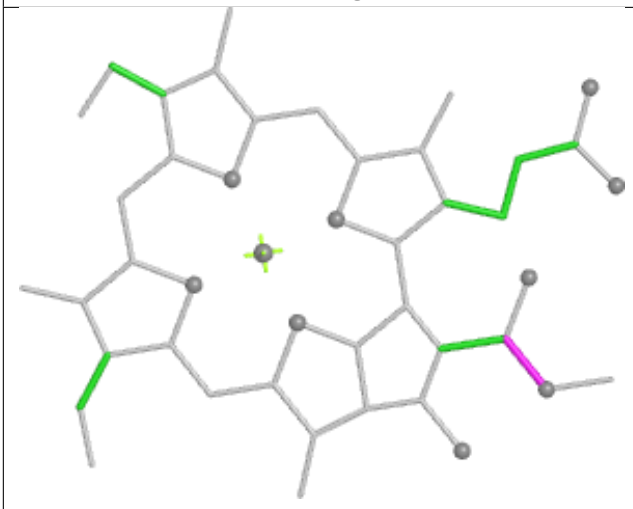


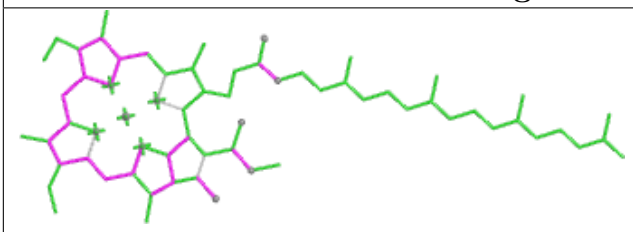
Bond angles



Torsions

Rings

Ligand CLA bA 837



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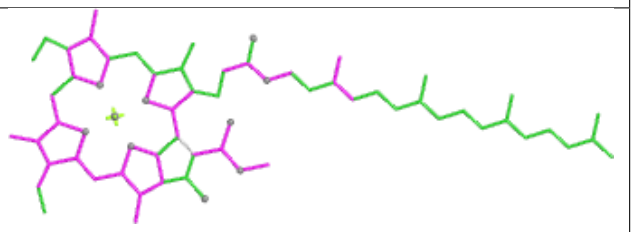
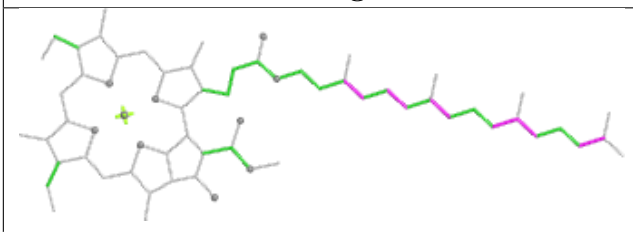


Bond angles



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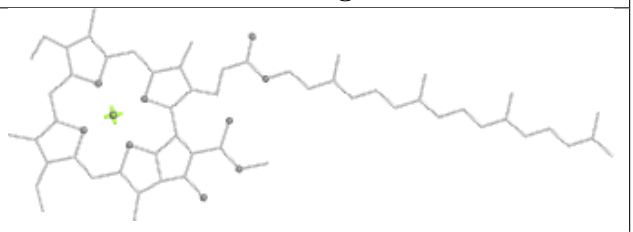
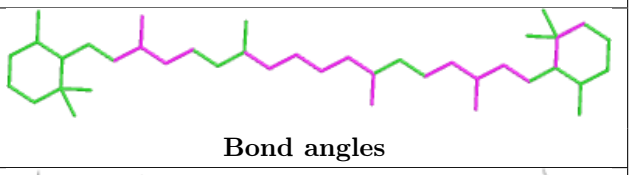


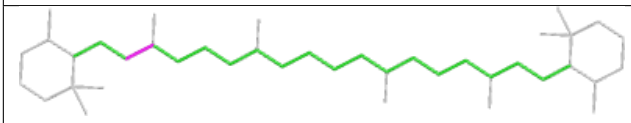
Rings

Ligand BCR cB 848

Bond lengths



Bond angles



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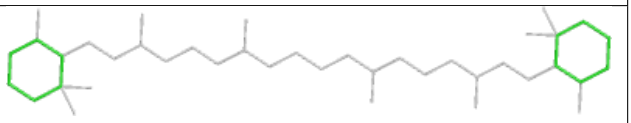
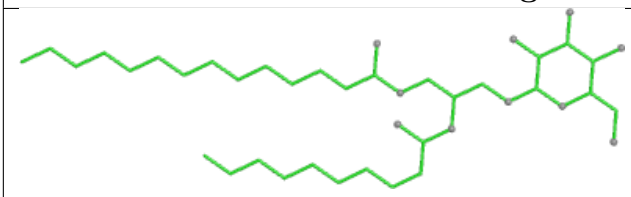
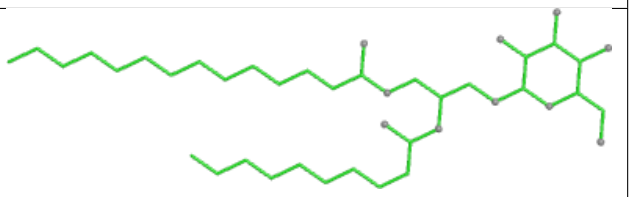


Rings

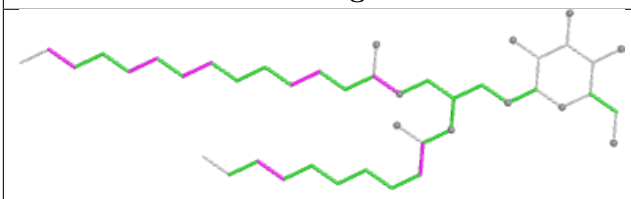
Ligand LMG B 848



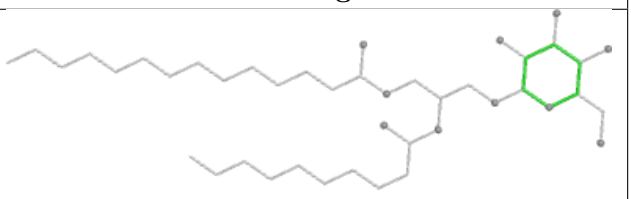
Bond lengths



Bond angles

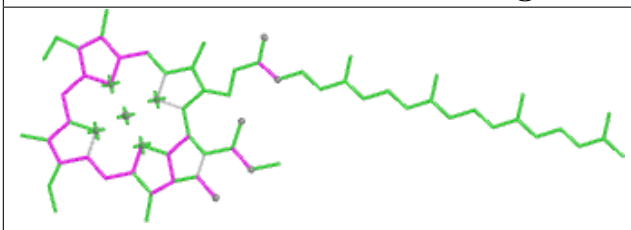


Torsions

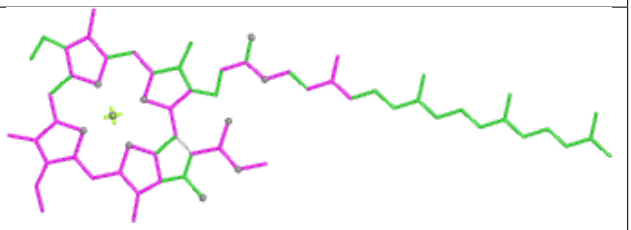


Rings

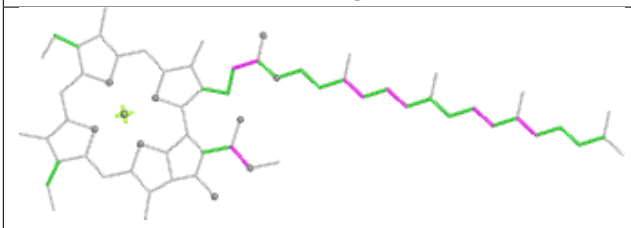
Ligand CLA cB 807



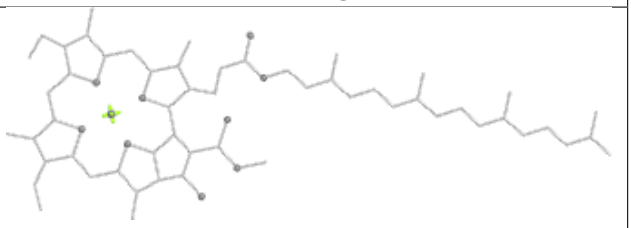
Bond lengths



Bond angles

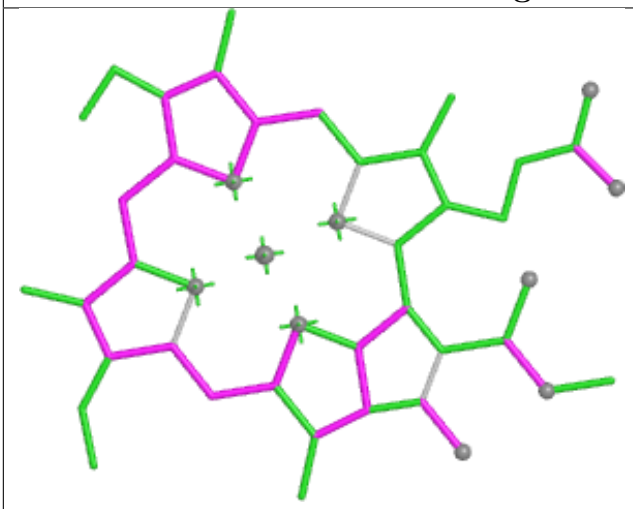


Torsions



Rings

Ligand CLA bA 812



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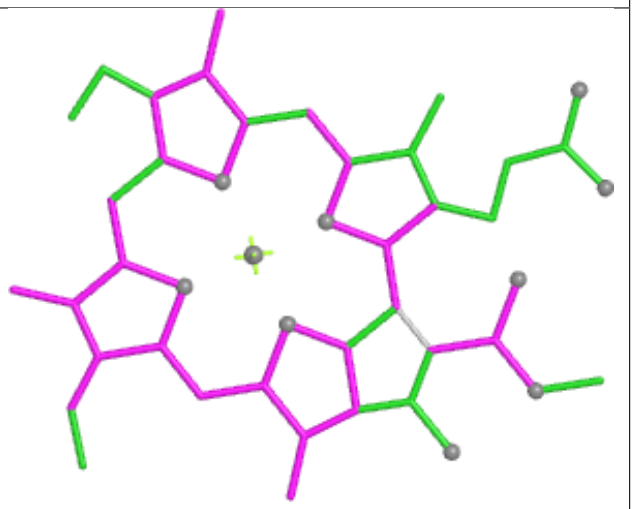
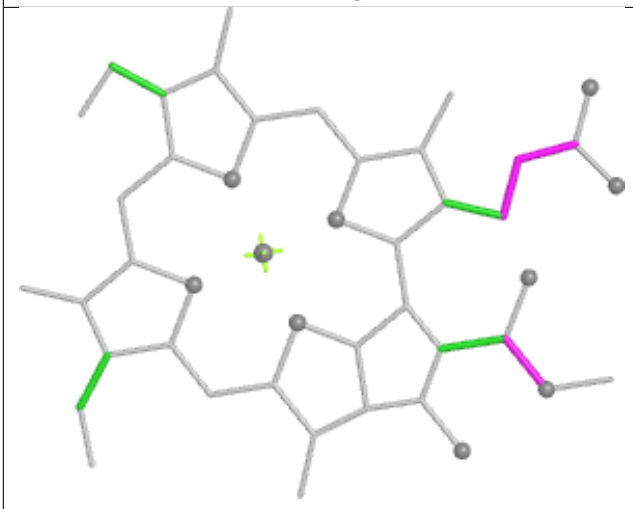


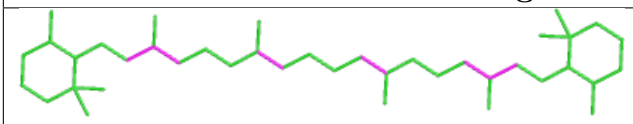
Bond angles



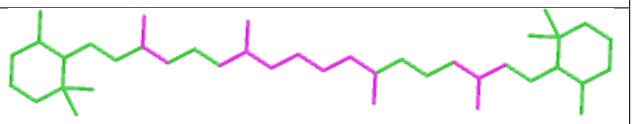
Torsions

Rings

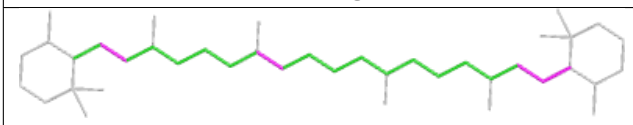
Ligand BCR cF 202



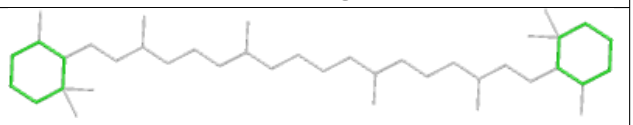
Bond lengths



Bond angles

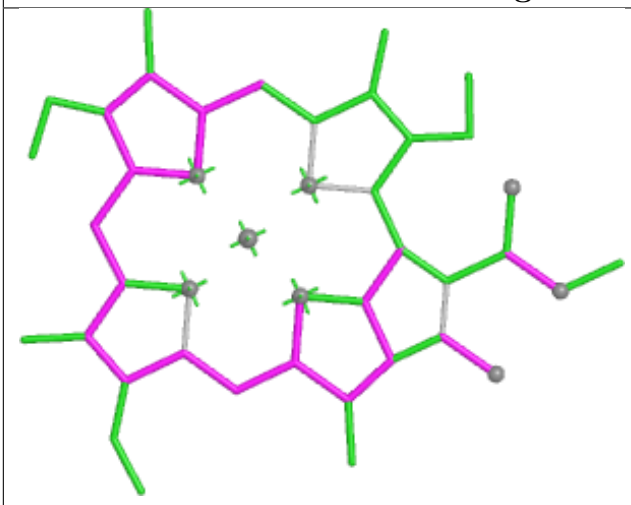


Torsions



Rings

Ligand CLA bB 830



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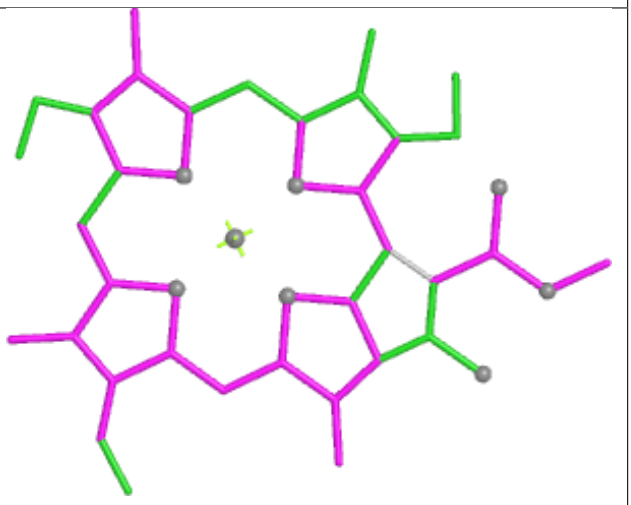
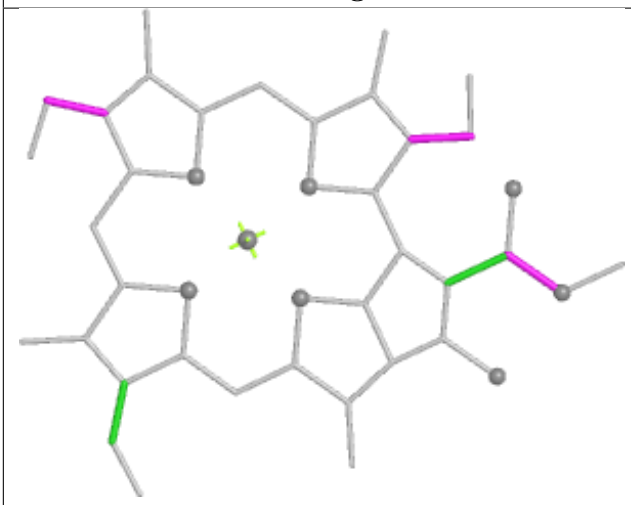


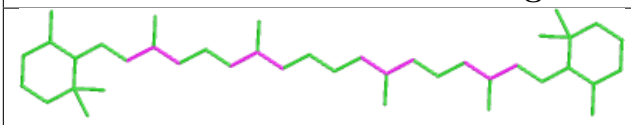
Bond angles



Torsions

Rings

Ligand BCR L 206



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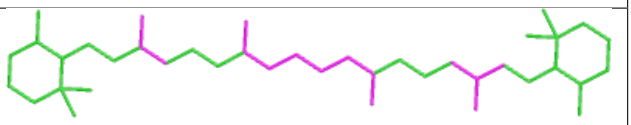
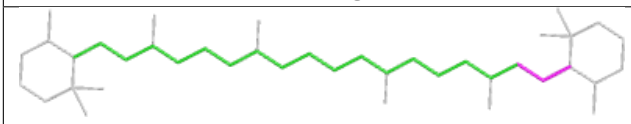
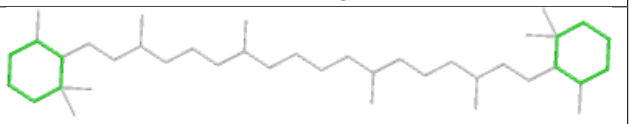


Bond angles

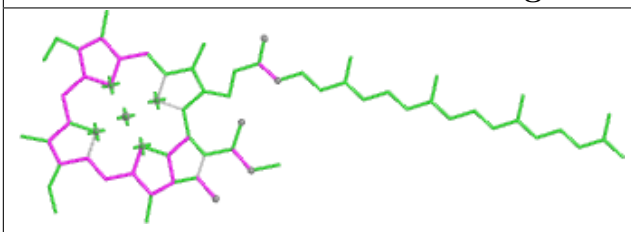


Torsions



Rings

Ligand CLA B 812



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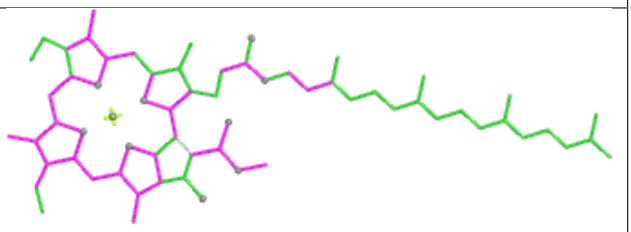
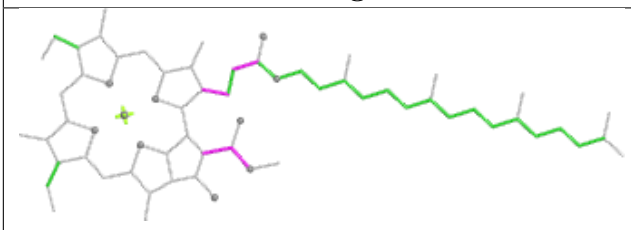


Bond angles



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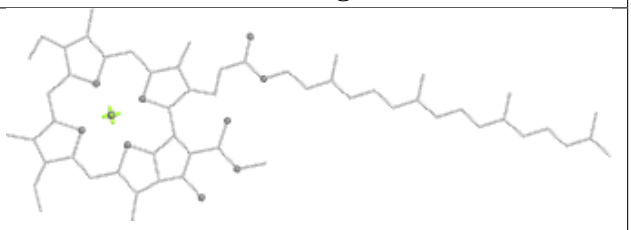
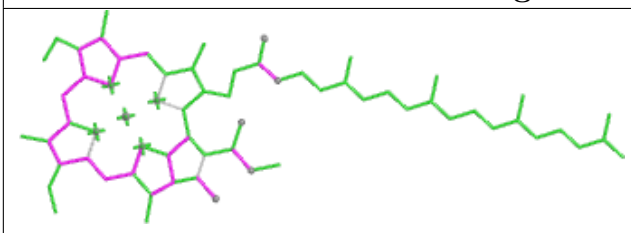


Rings

Ligand CLA bA 832



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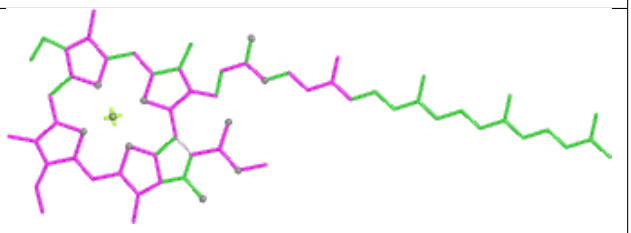
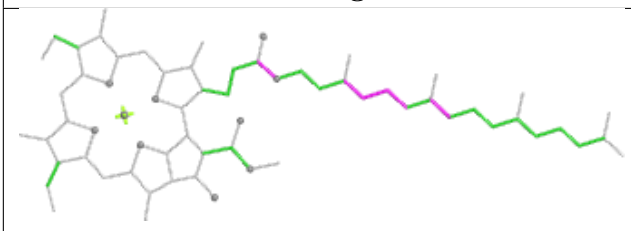


Bond angles



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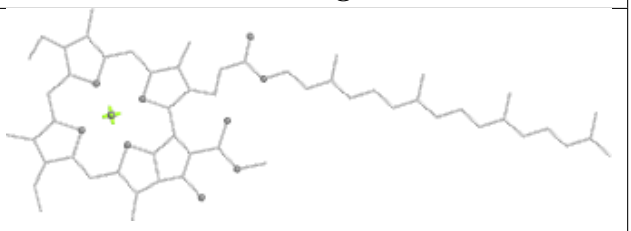
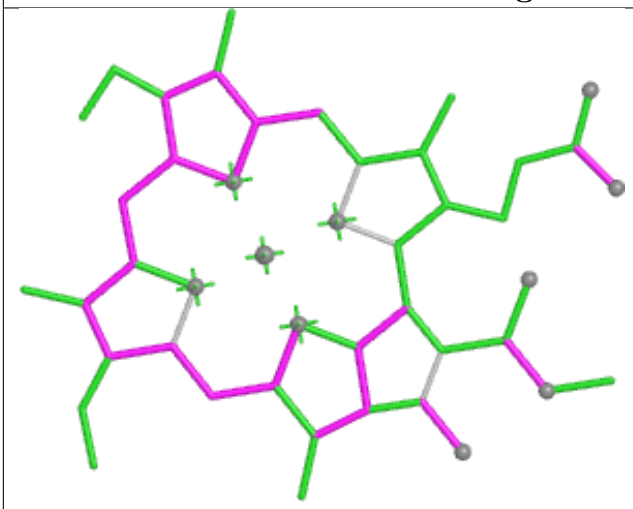


Rings

Ligand CLA cA 813



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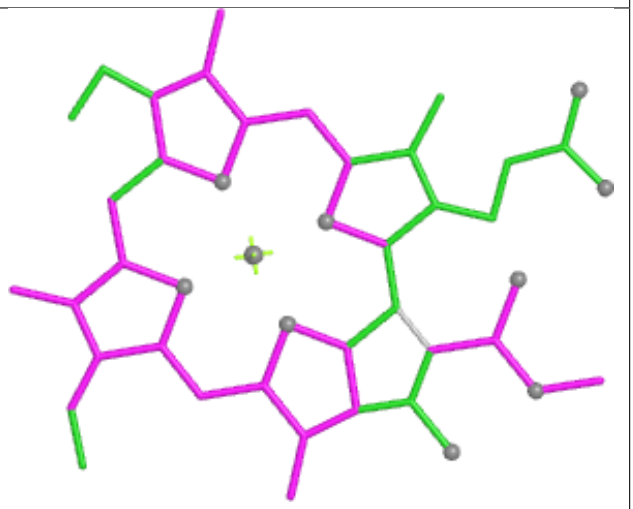

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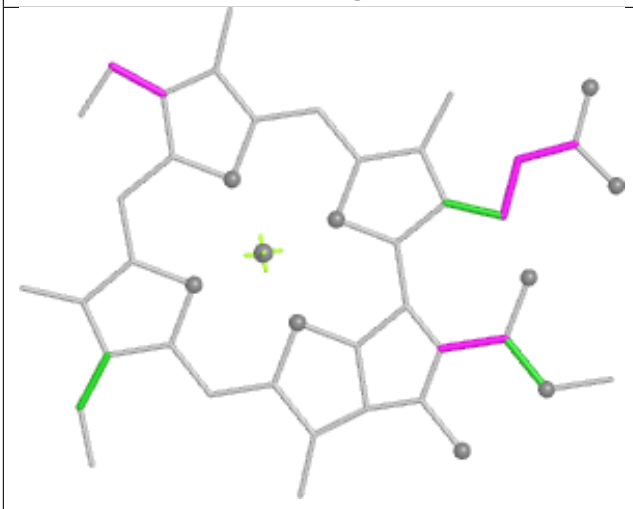
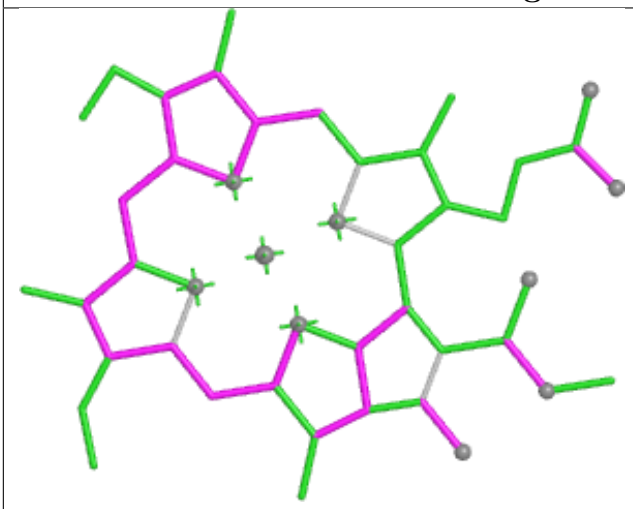


Torsions

Rings

Ligand CLA A 834



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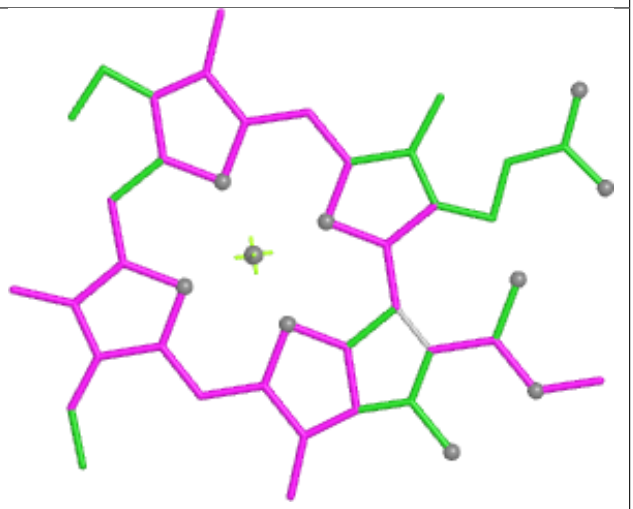
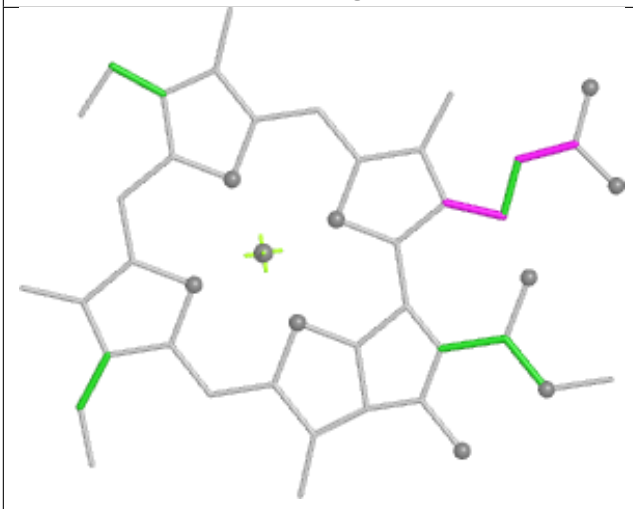


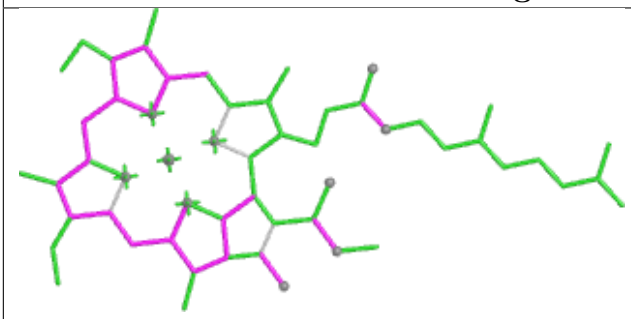
Bond angles



Torsions

Rings

Ligand CLA bA 805



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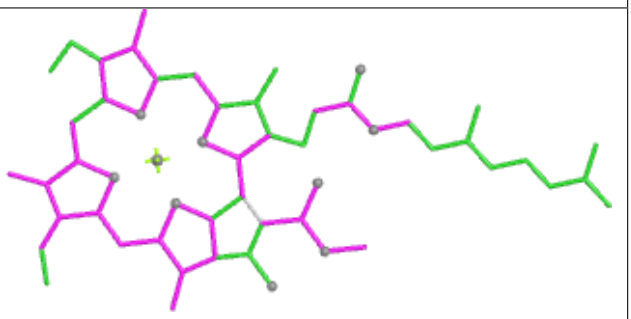
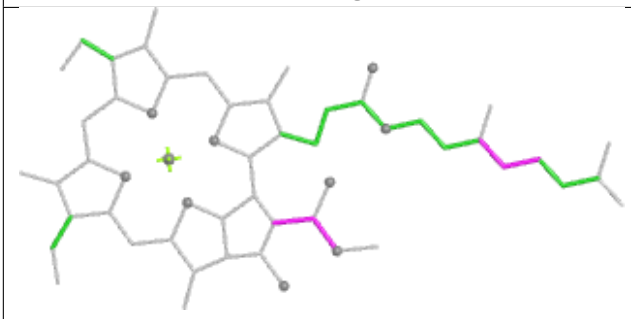


Bond angles



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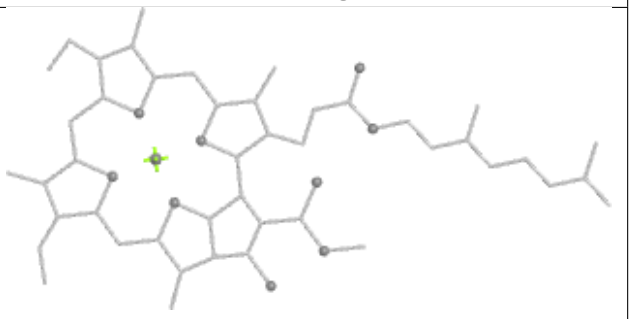
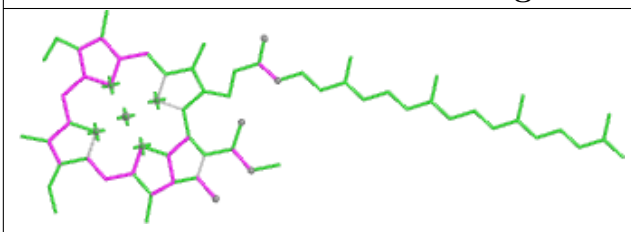


Rings

Ligand CLA bB 828



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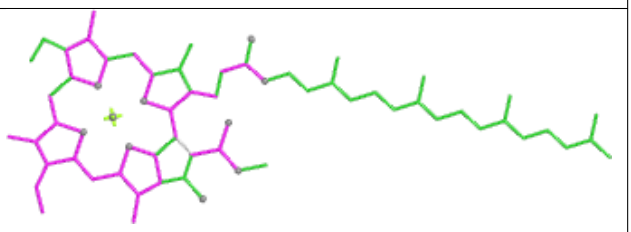
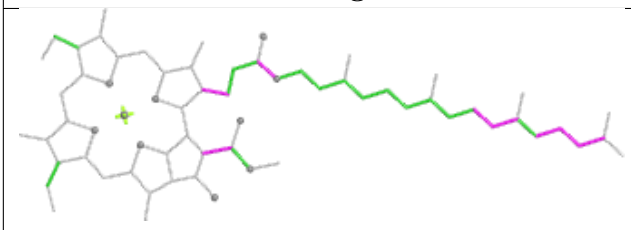


Bond angles



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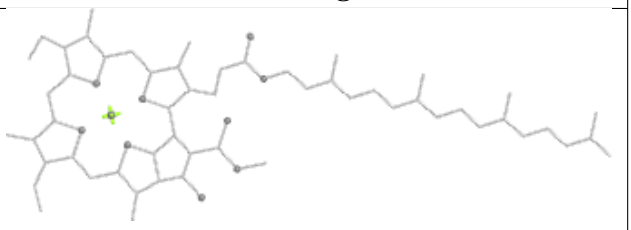
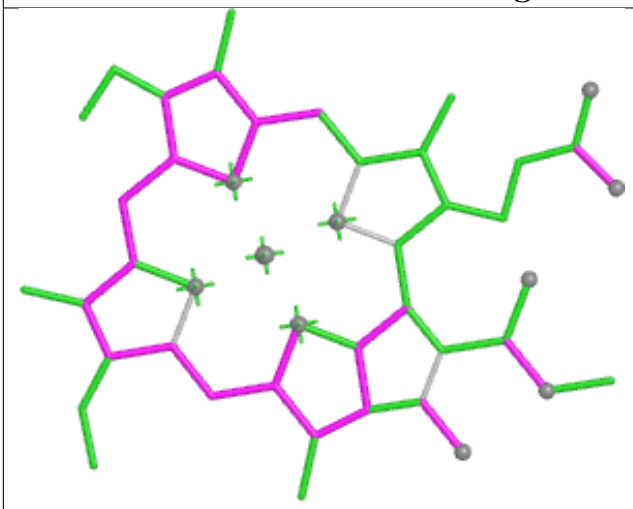


Rings

Ligand CLA bA 820



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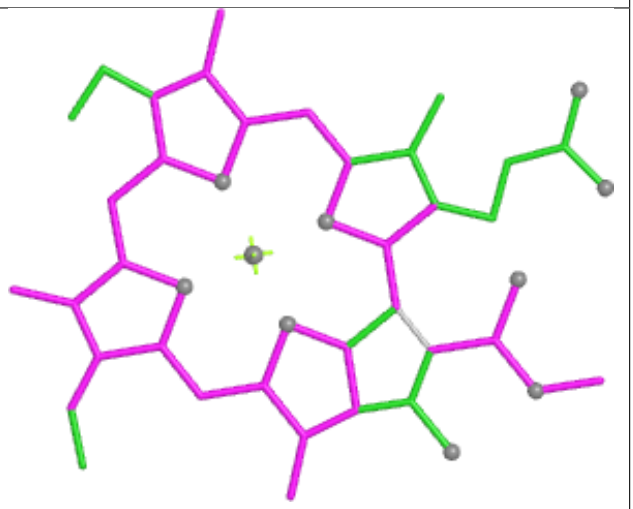
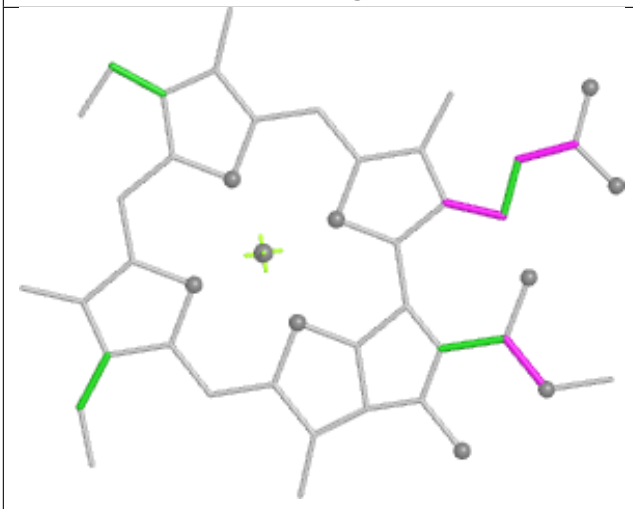


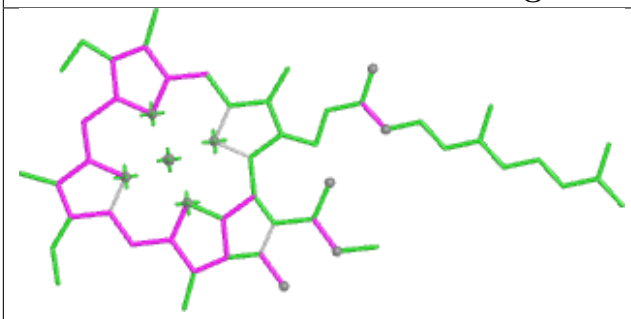
Bond angles



Torsions

Rings

Ligand CLA B 817



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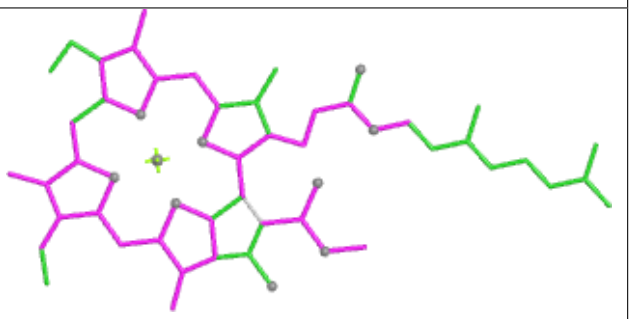
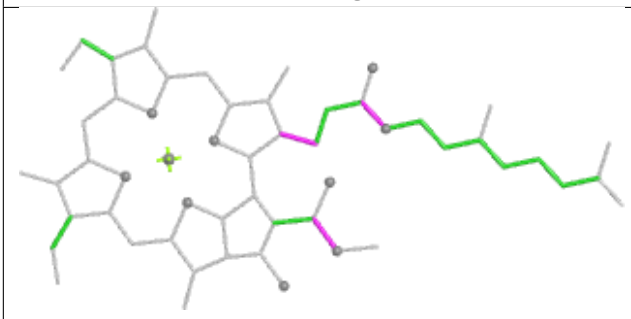


Bond angles



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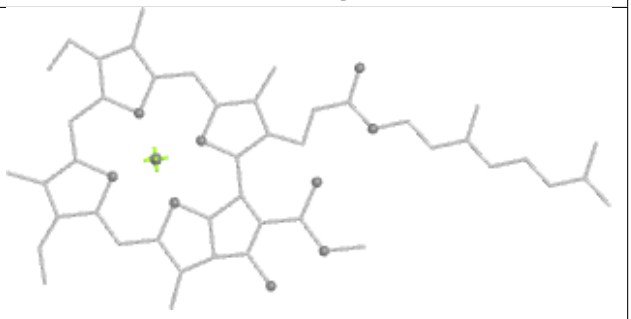
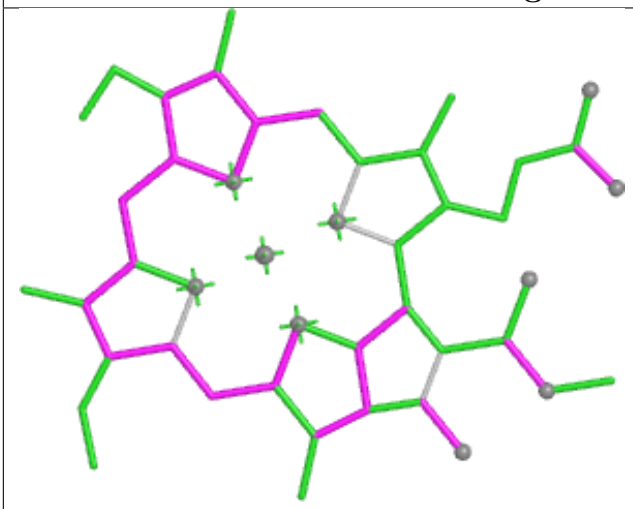


Rings

Ligand CLA B 835



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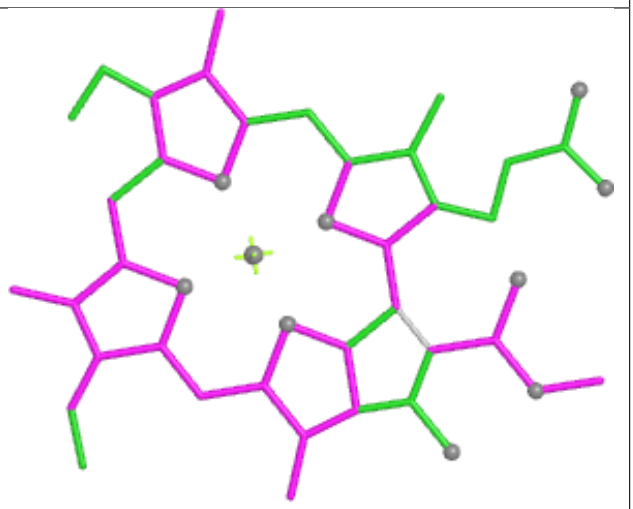
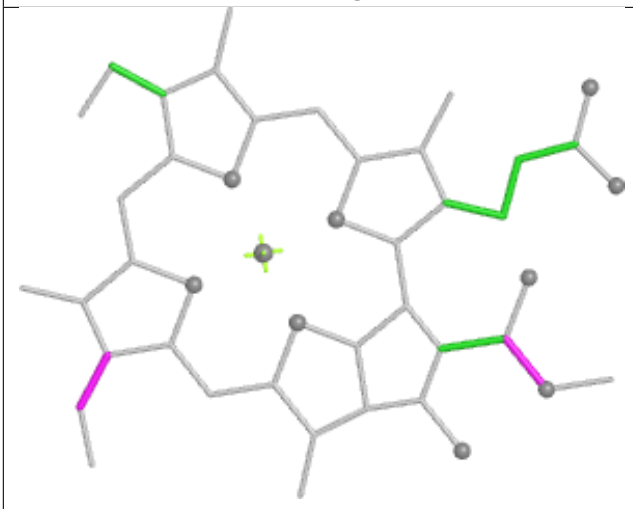


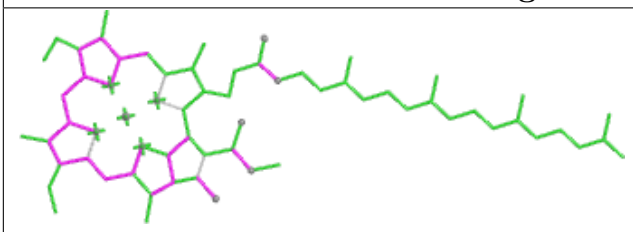
Bond angles



Torsions

Rings

Ligand CLA cL 202



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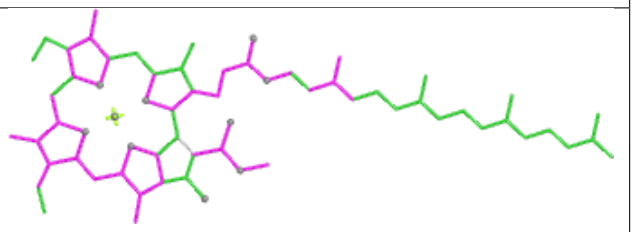

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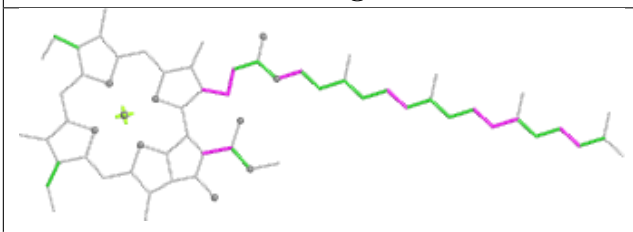
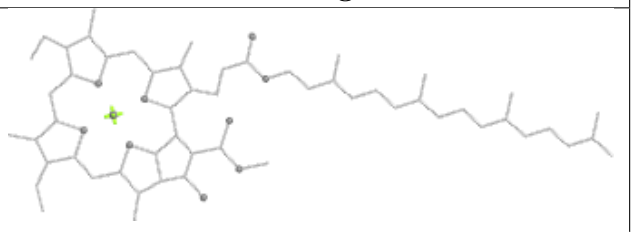
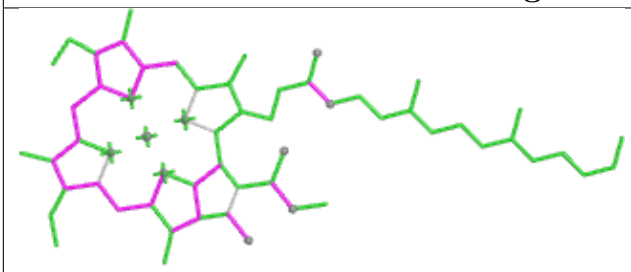


Torsions



Rings

Ligand CLA A 824



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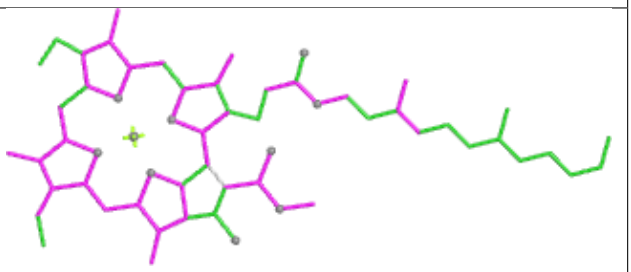
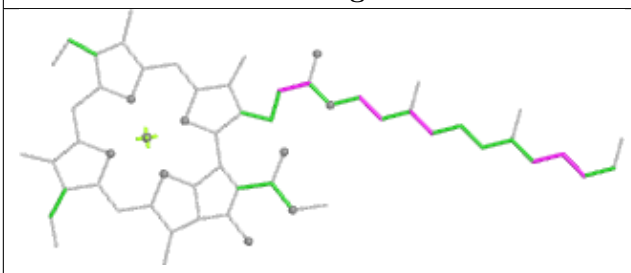


Bond angles



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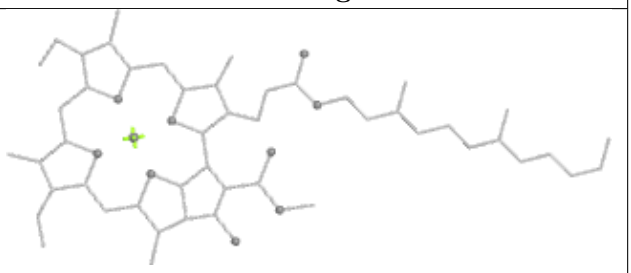
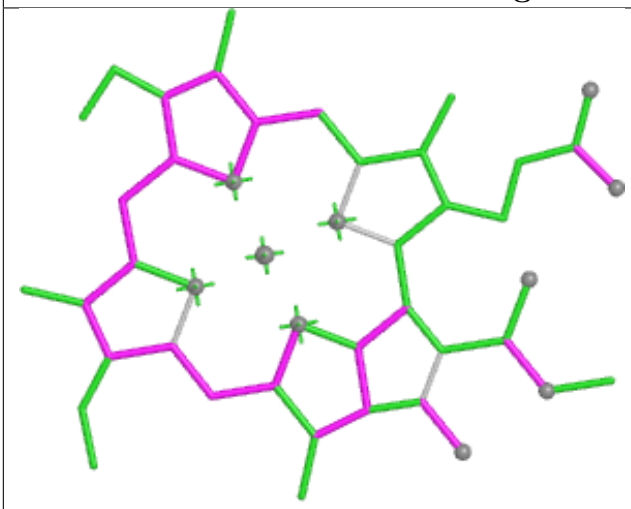


Rings

Ligand CLA bA 808



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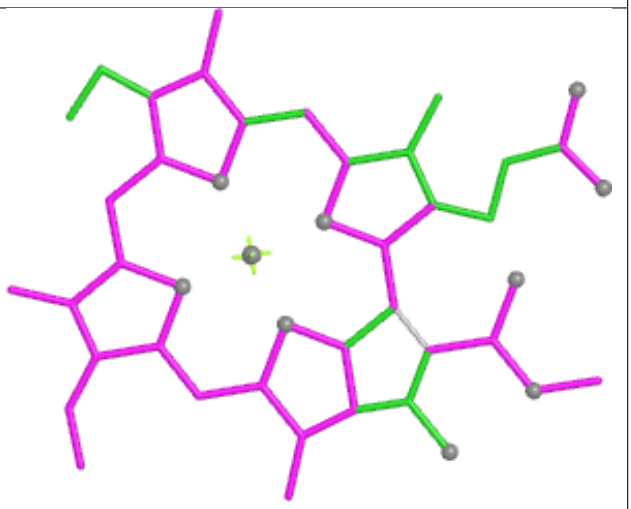
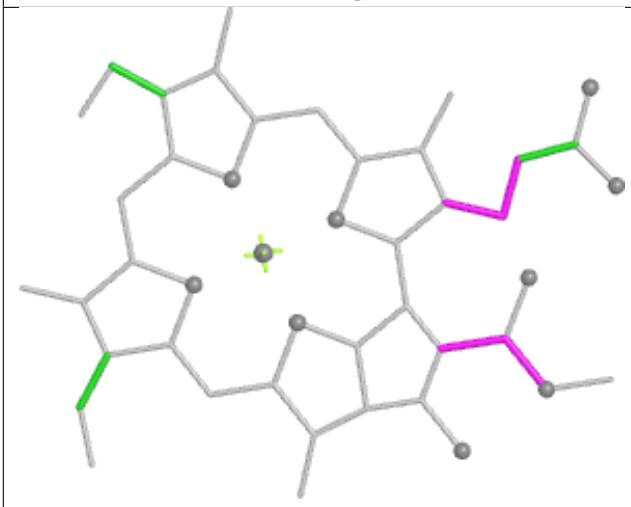


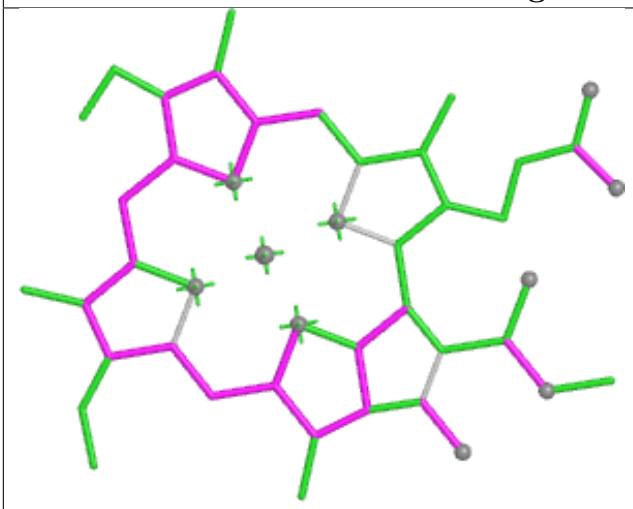
Bond angles



Torsions

Rings

Ligand CLA J 101



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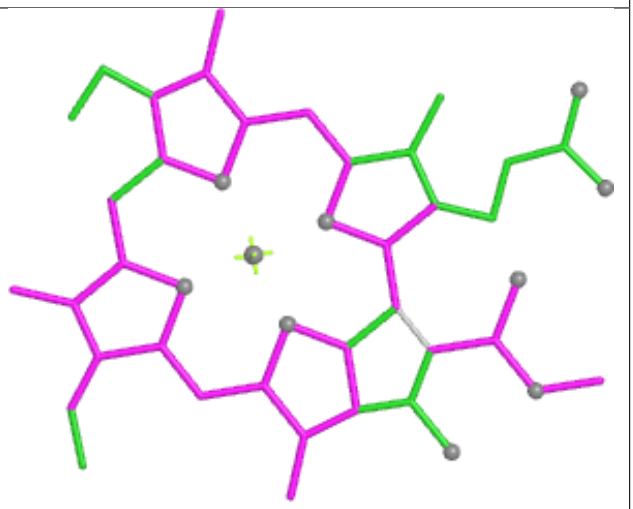

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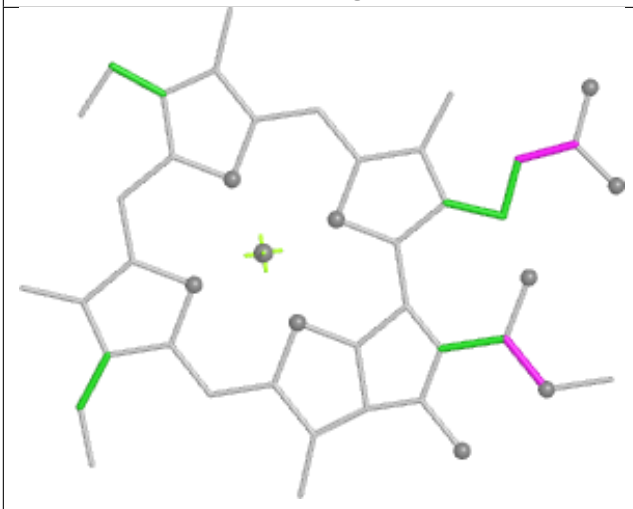
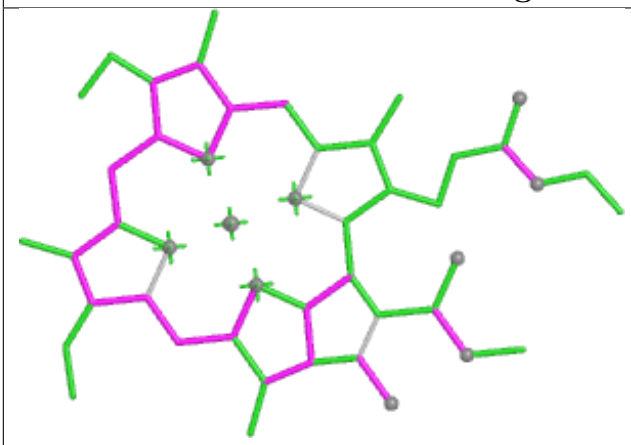


Torsions

Rings

Ligand CLA bB 819



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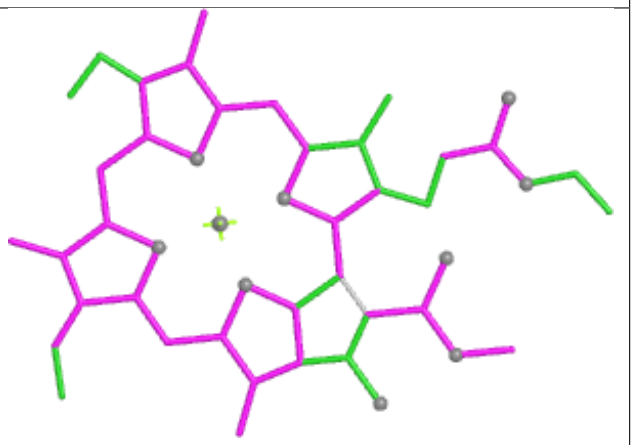

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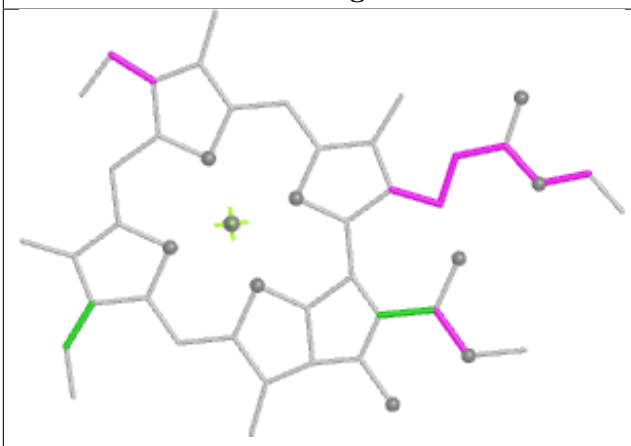
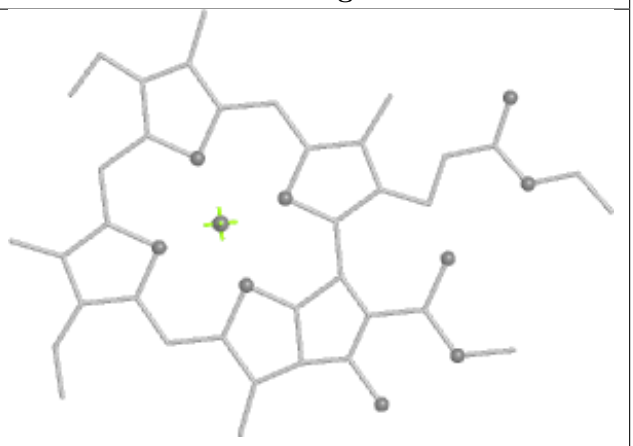
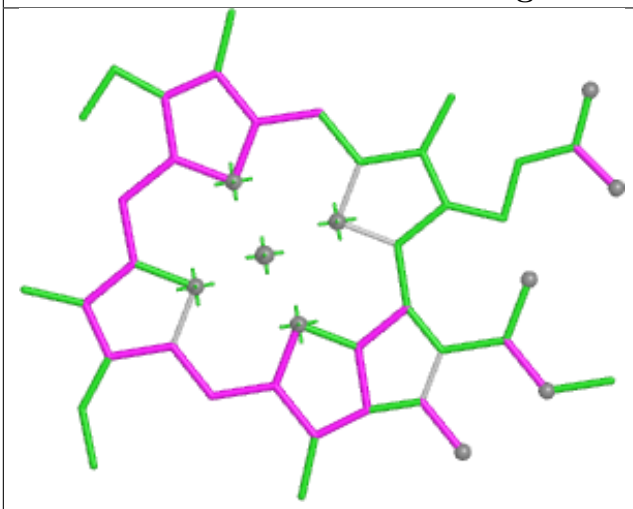


Torsions



Rings

Ligand CLA cB 811



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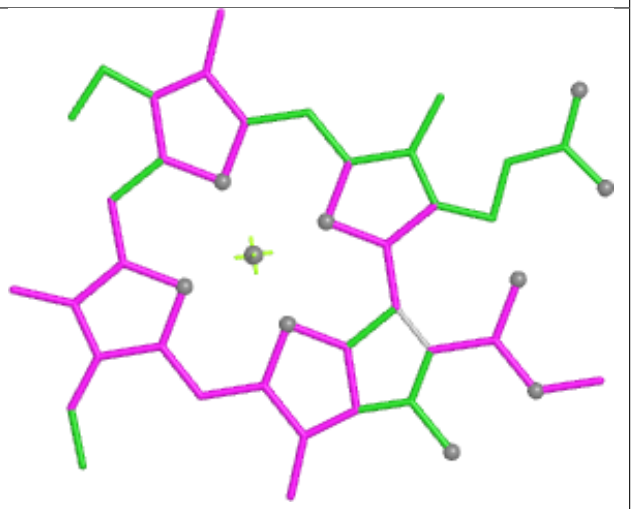

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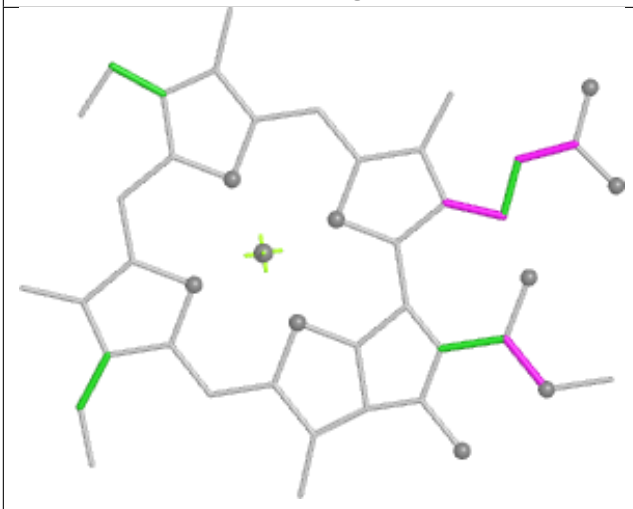
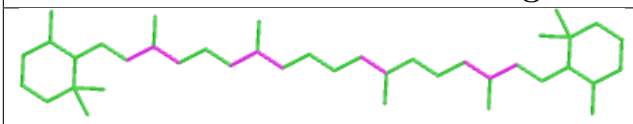


Torsions

Rings

Ligand BCR B 846



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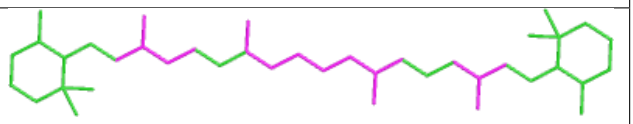
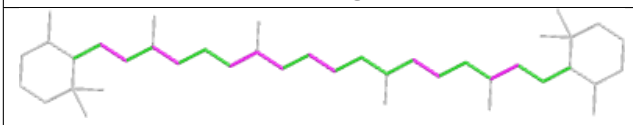


Bond angles



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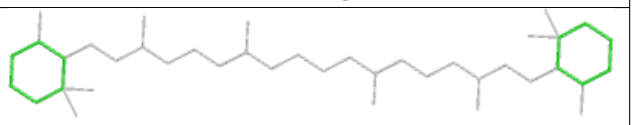

Rings

Ligand BCR I 102

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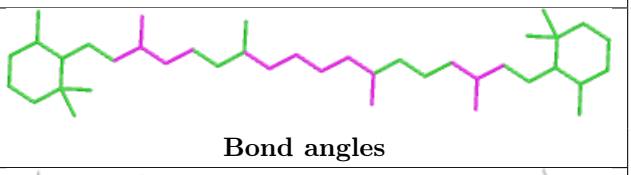

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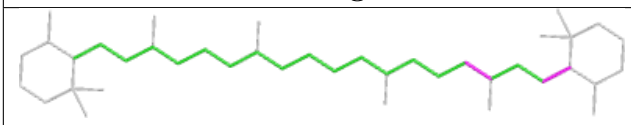

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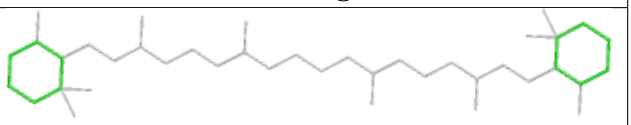
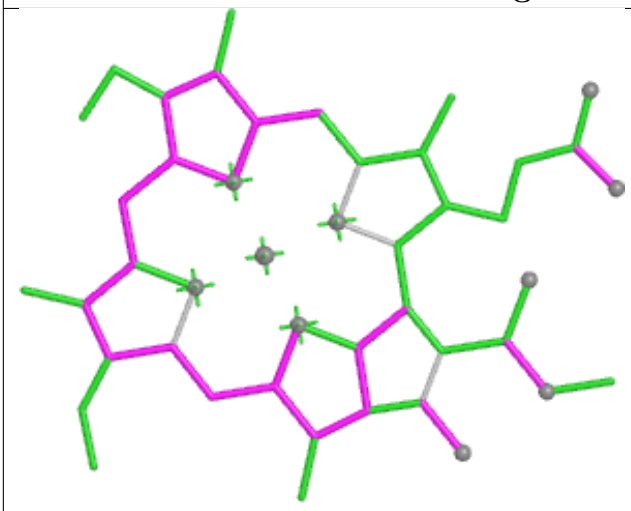


Rings

Ligand CLA bA 822



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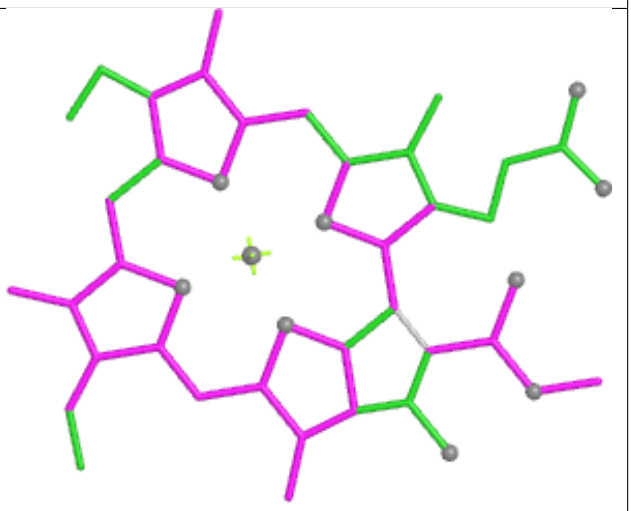

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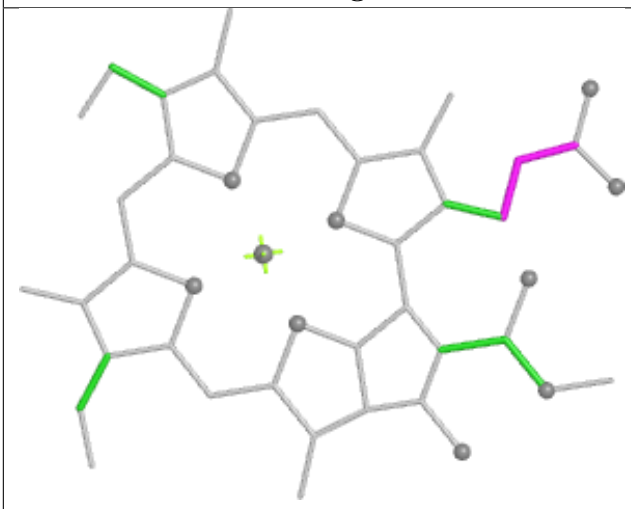

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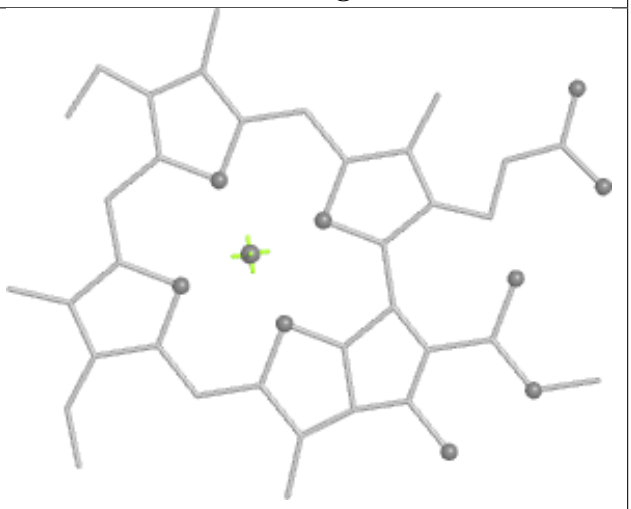
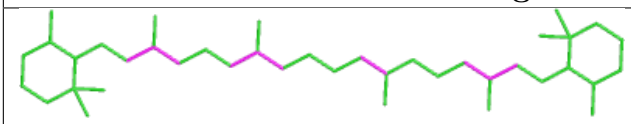


Rings

Ligand BCR bB 845



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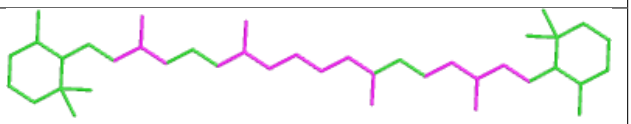

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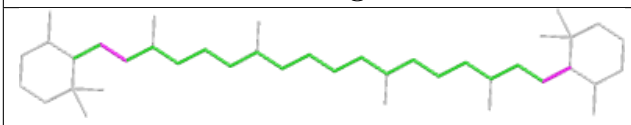

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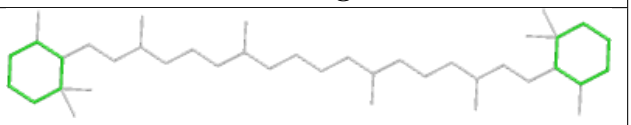
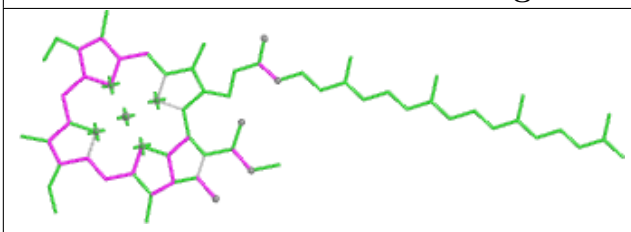


Rings

Ligand CLA bA 806



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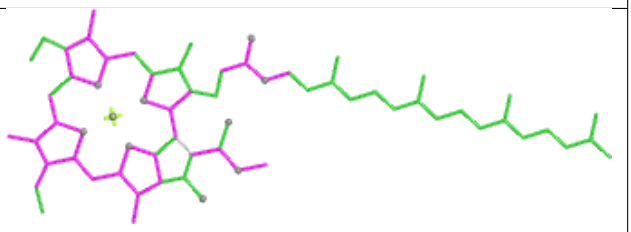

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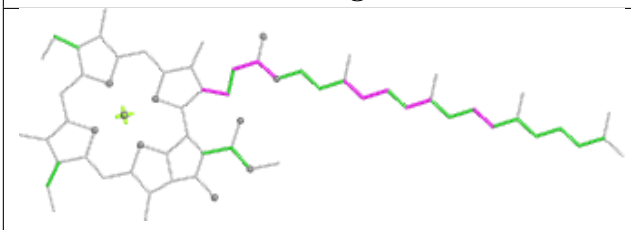

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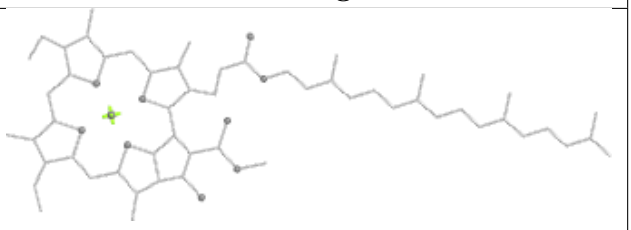
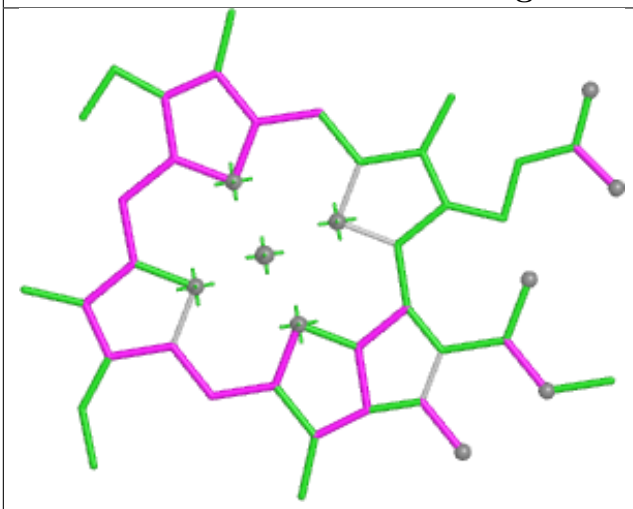


Rings

Ligand CLA cA 821



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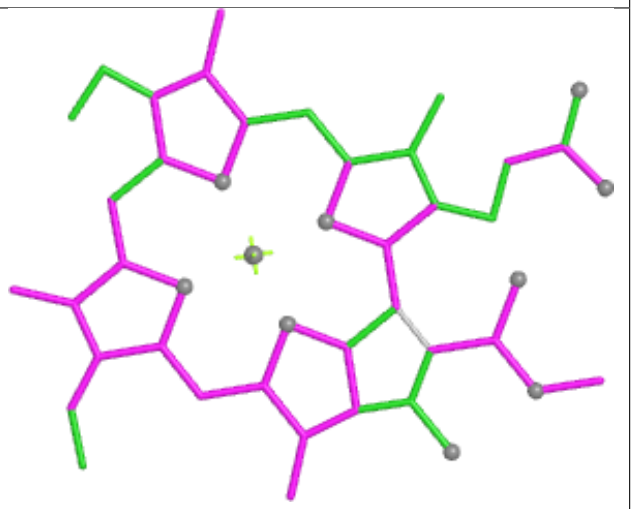

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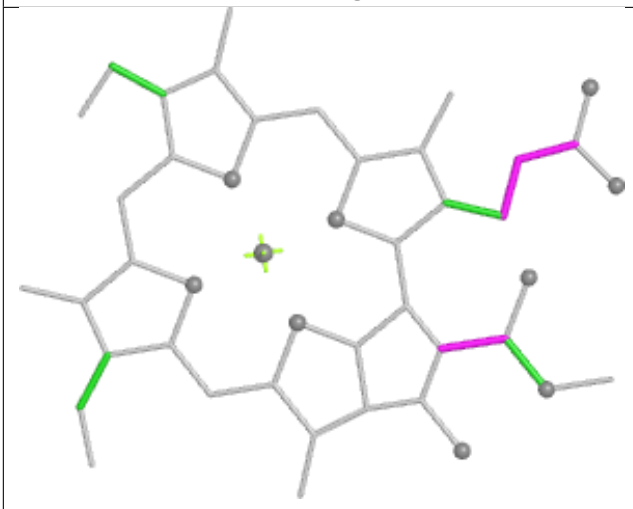

Torsions

Rings

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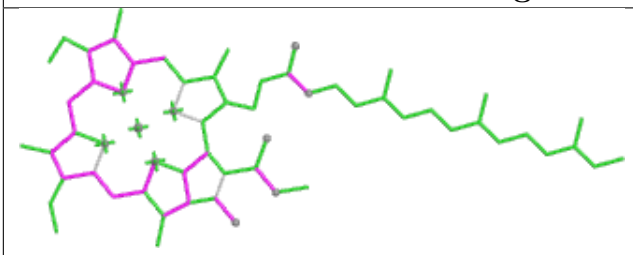

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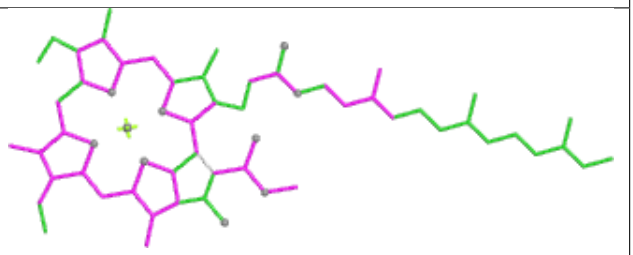

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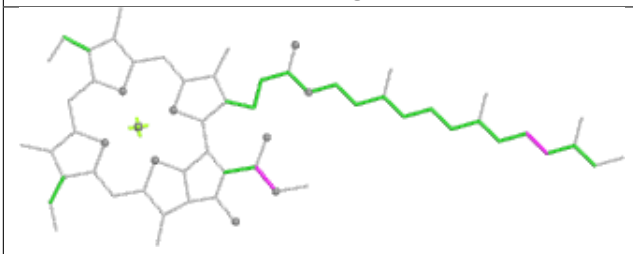

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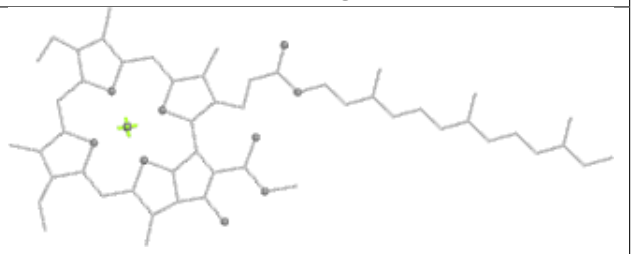
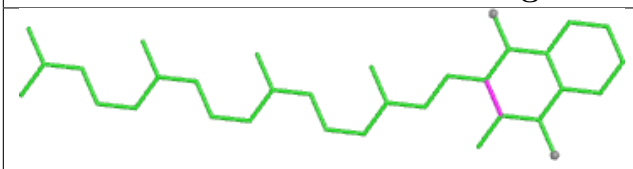


Rings

Ligand PQN A 843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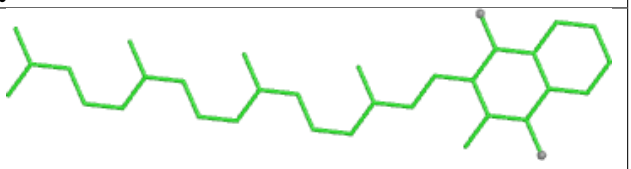
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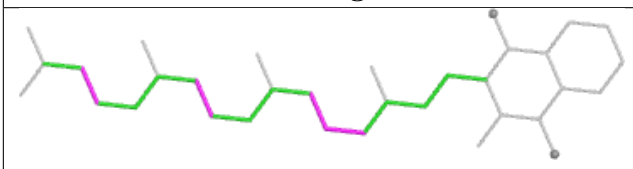
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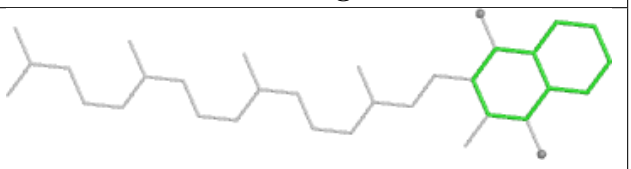
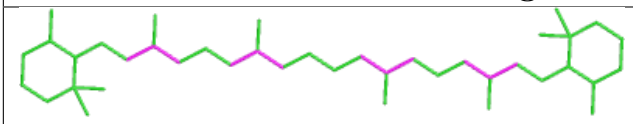

Rings

Ligand BCR bI 101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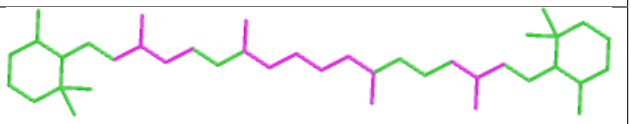
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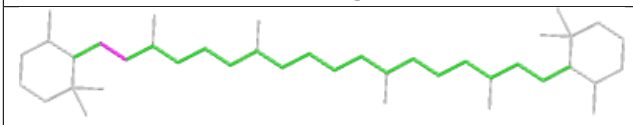
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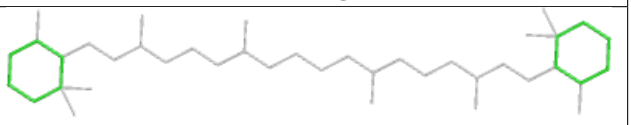
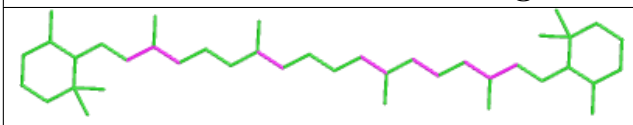

Rings

Ligand BCR cB 844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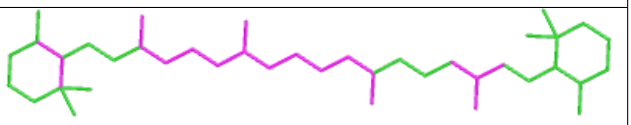
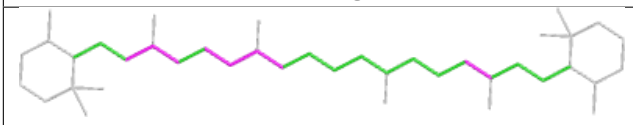

Bond angles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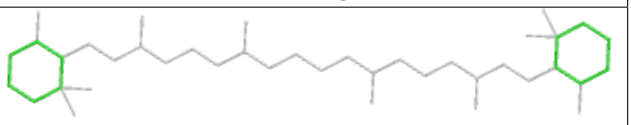
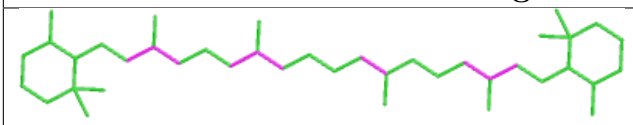

Rings

Ligand BCR bB 846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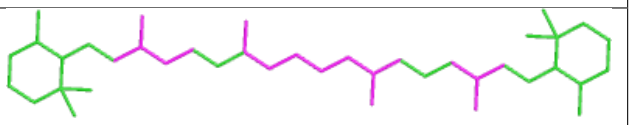
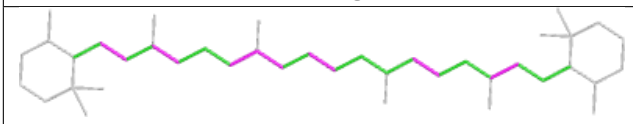
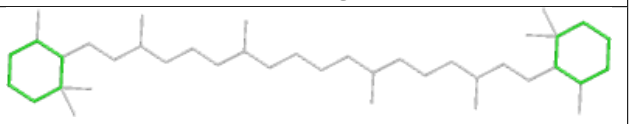
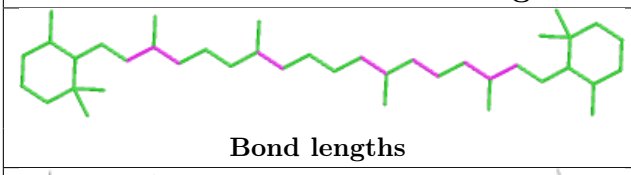

Bond angles

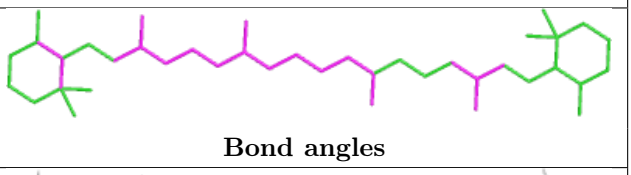

Torsions


Rings

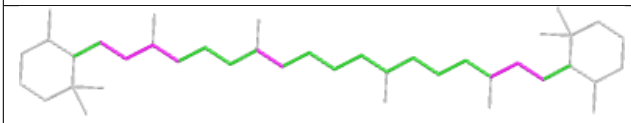
Ligand BCR bB 842



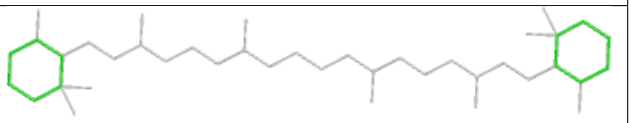
Bond lengths



Bond angles

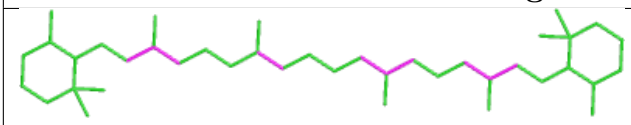


Torsions



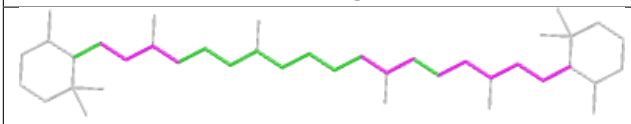
Rings

Ligand BCR J 103



Bond lengths

Bond angles



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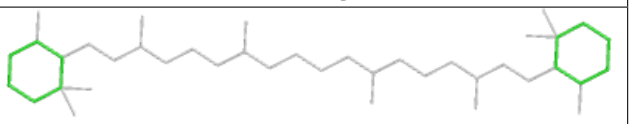
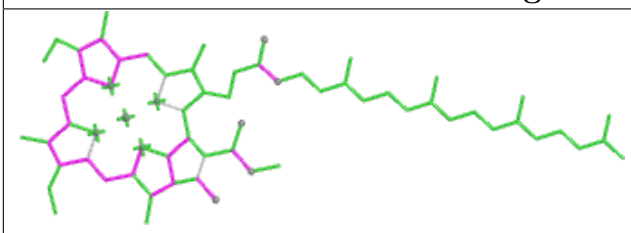


Rings

Ligand CLA A 829



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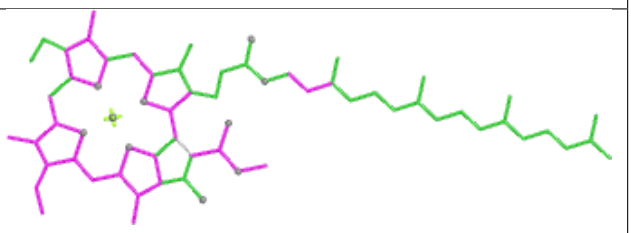
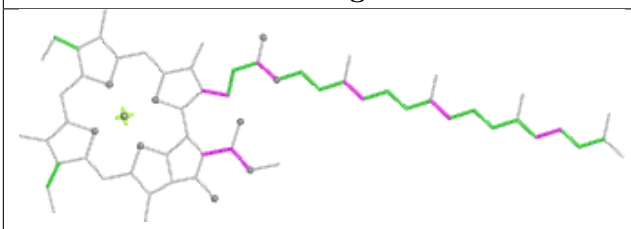


Bond angles



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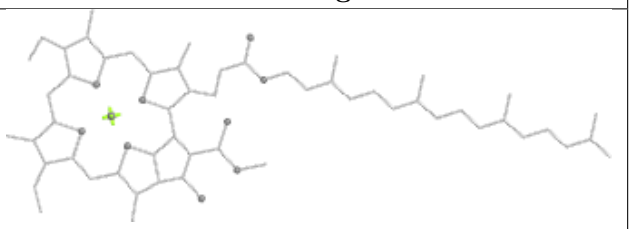
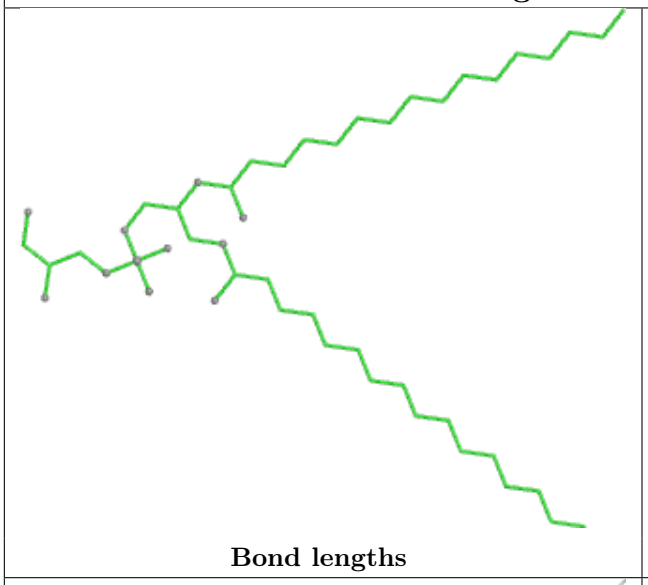


Rings

Ligand LHG bA 850



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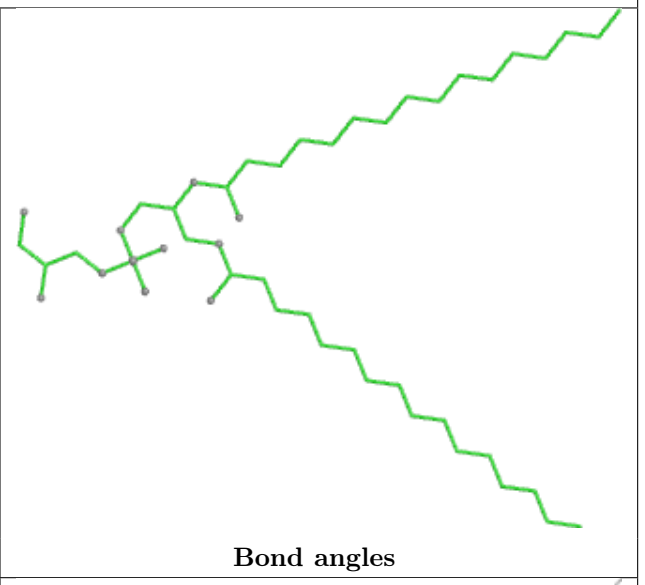
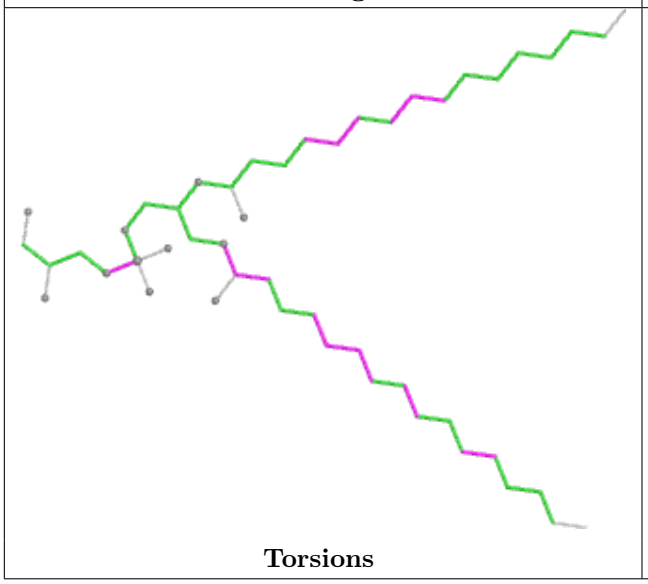


Bond angles



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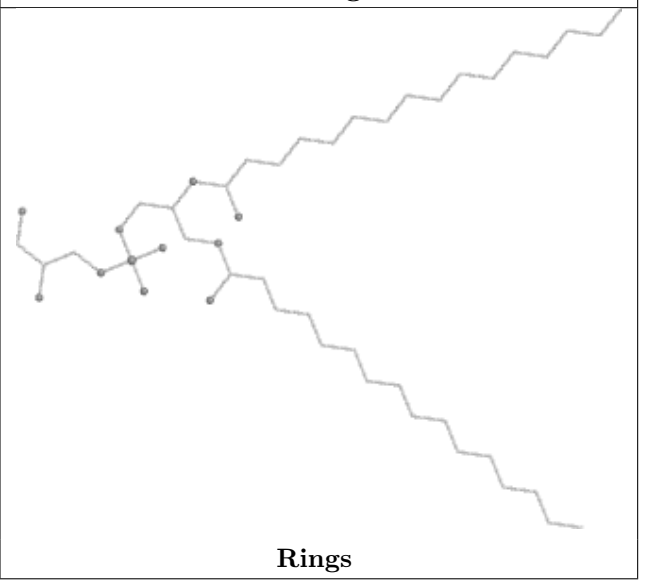
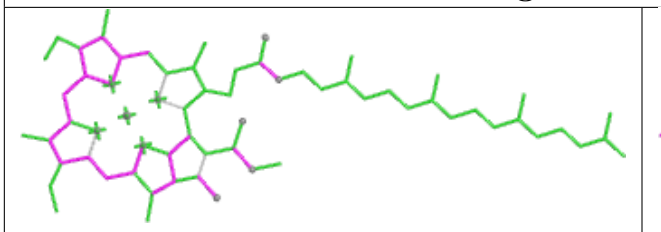


Rings

Ligand CLA cA 840



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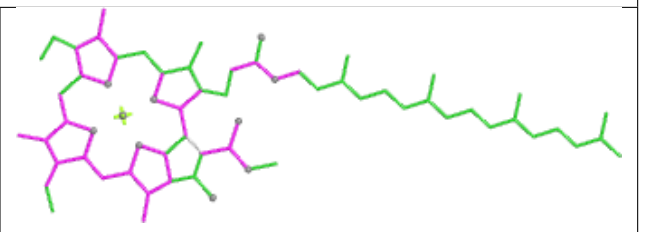
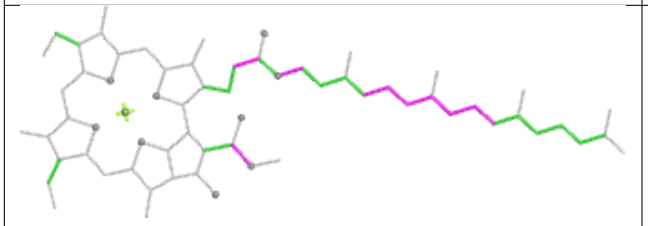


Bond angles



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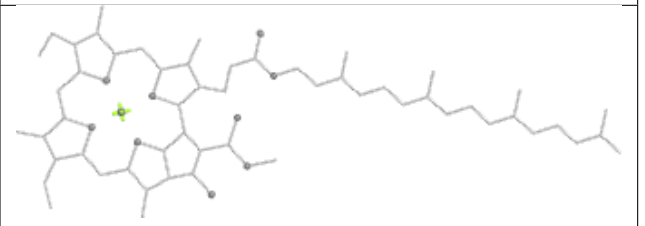
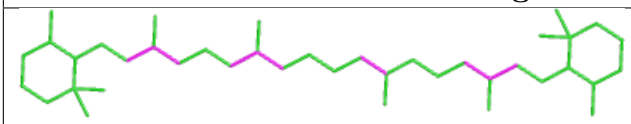


Rings

Ligand BCR bA 847



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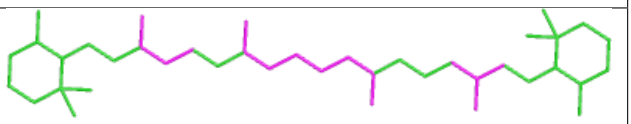
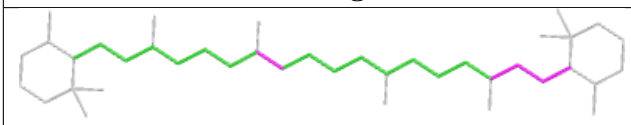


Bond angles



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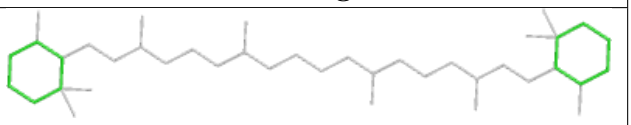
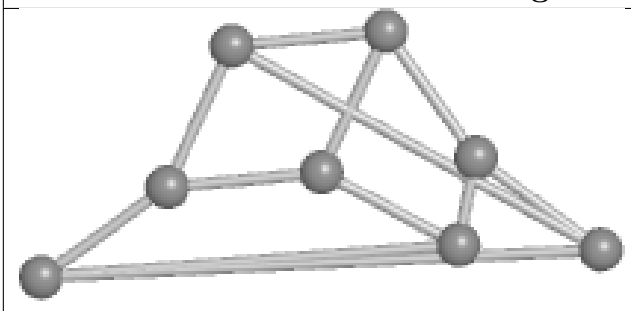


Rings

Ligand SF4 C 102



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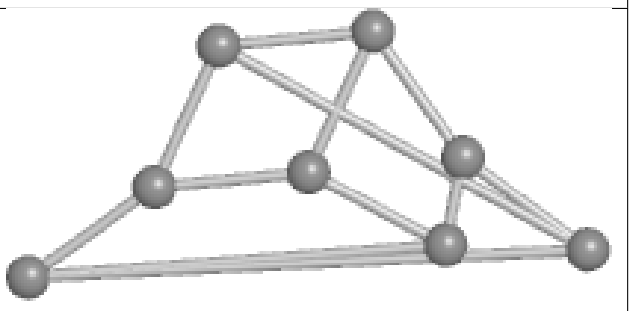

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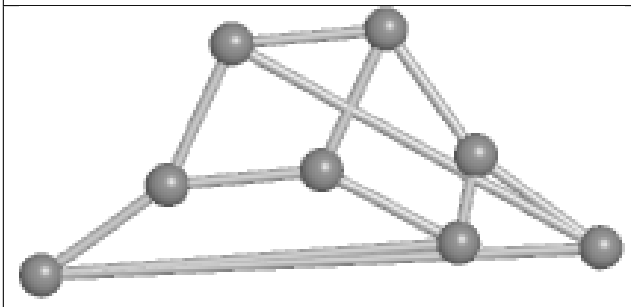

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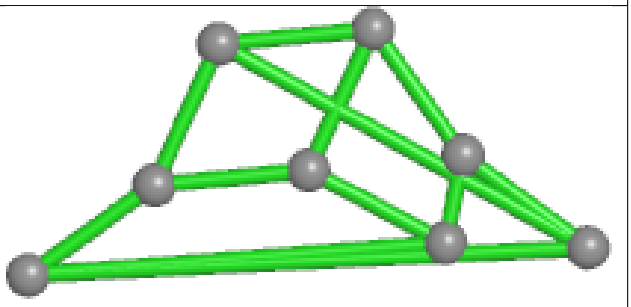
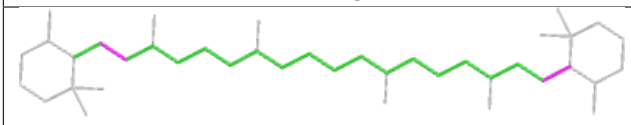


Rings

Ligand BCR B 845

Bond lengths

Bond angles



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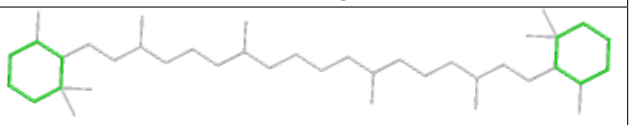
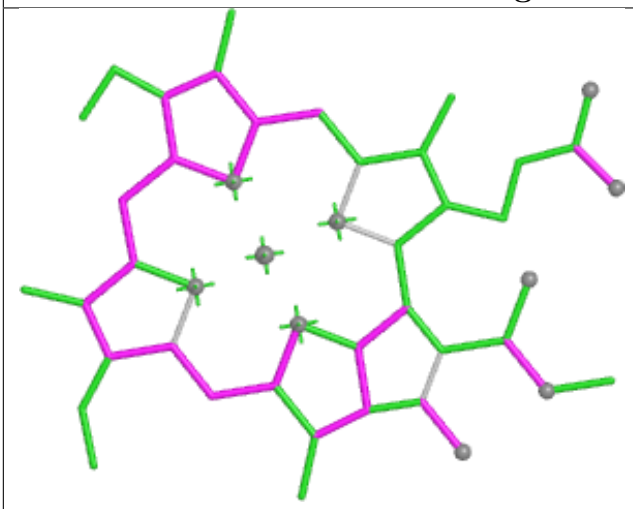


Rings

Ligand CLA bB 836



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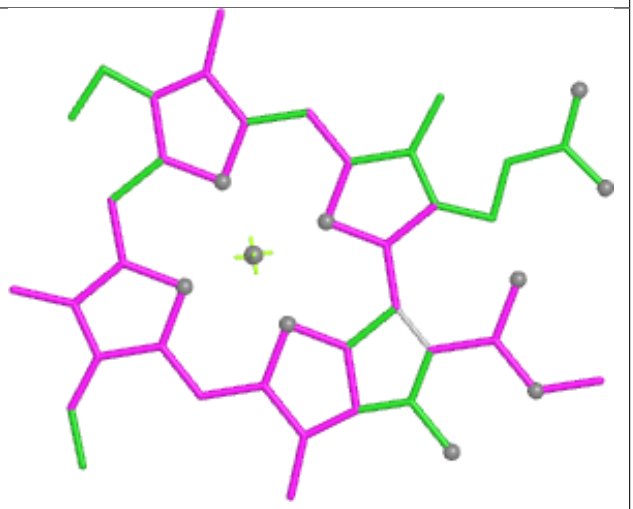
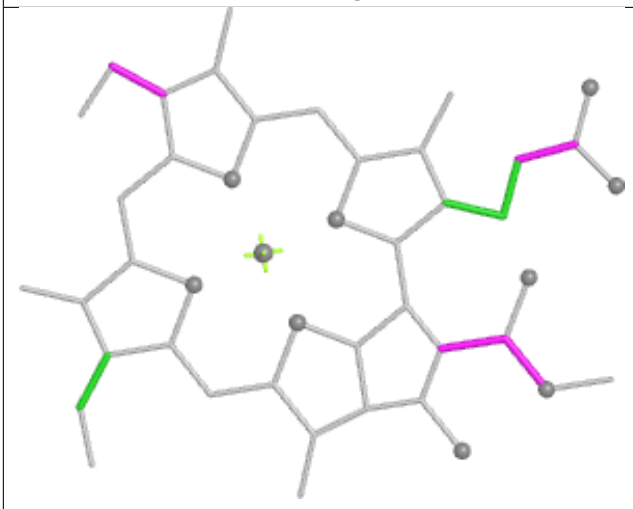


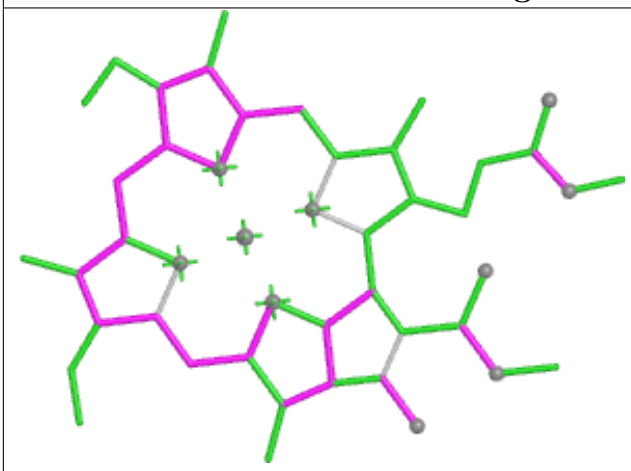
Bond angles



Torsions

Rings

Ligand CLA bA 826



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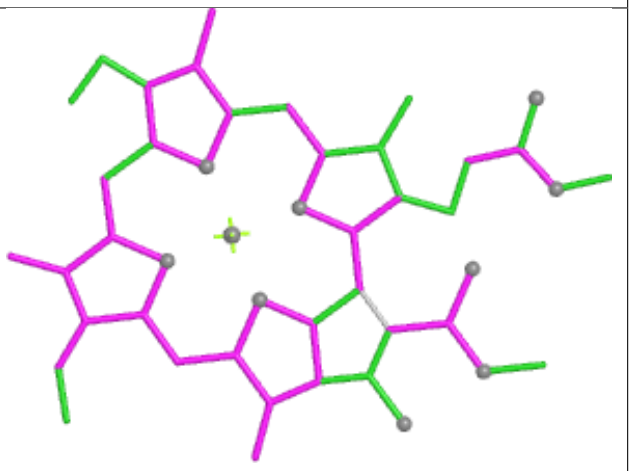
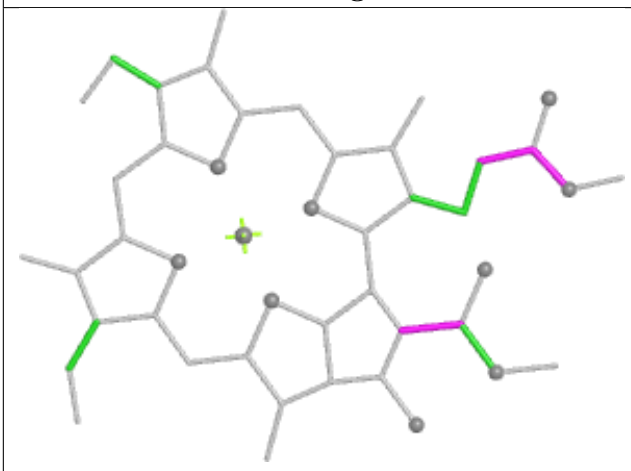


Bond angles



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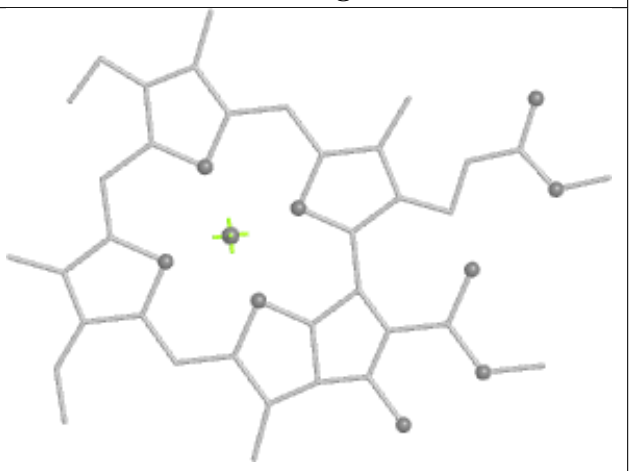
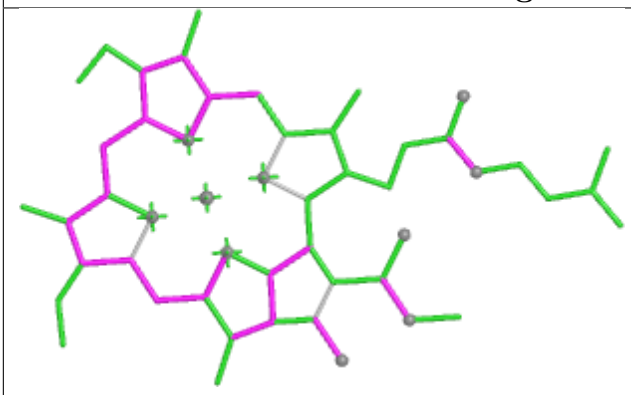


Rings

Ligand CLA cA 825



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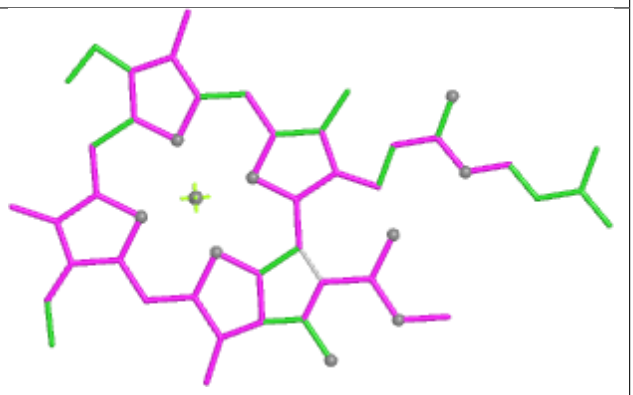
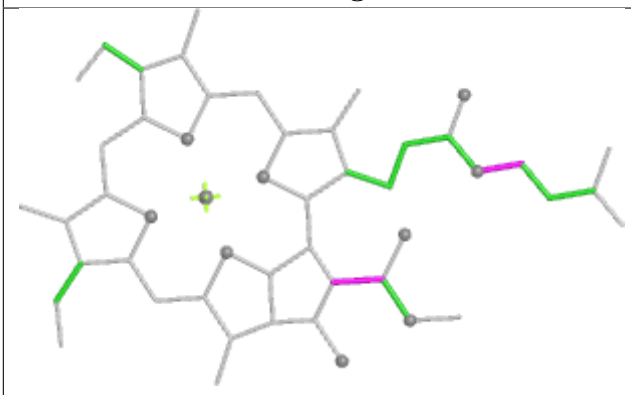


Bond angles



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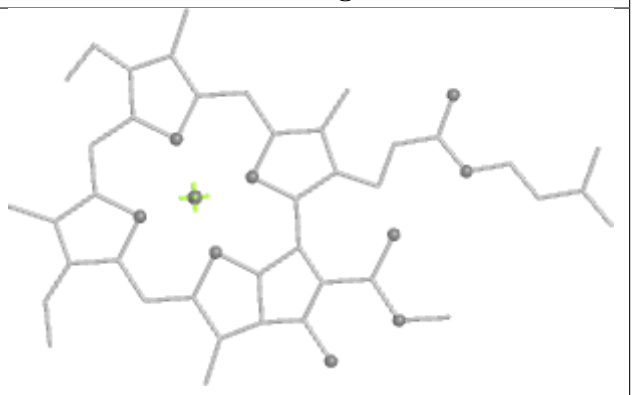
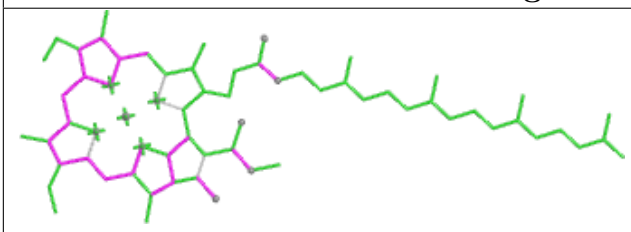


Rings

Ligand CLA A 839



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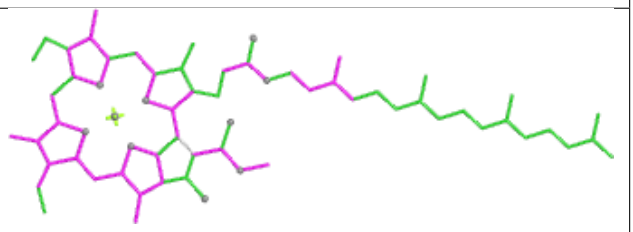
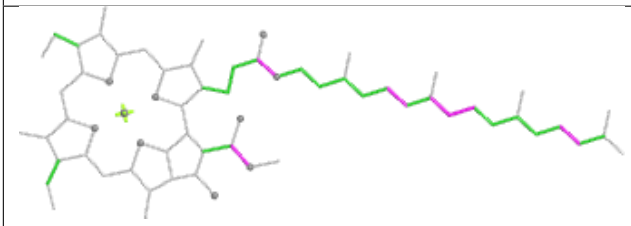


Bond angles



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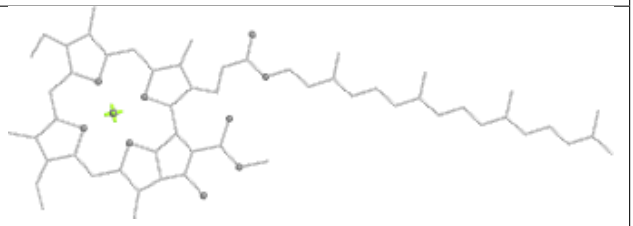
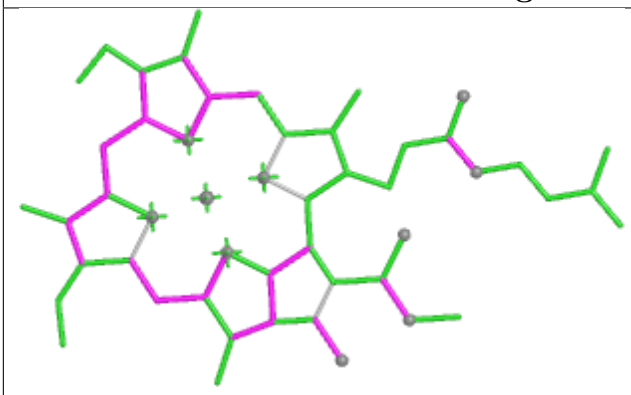


Rings

Ligand CLA cA 830



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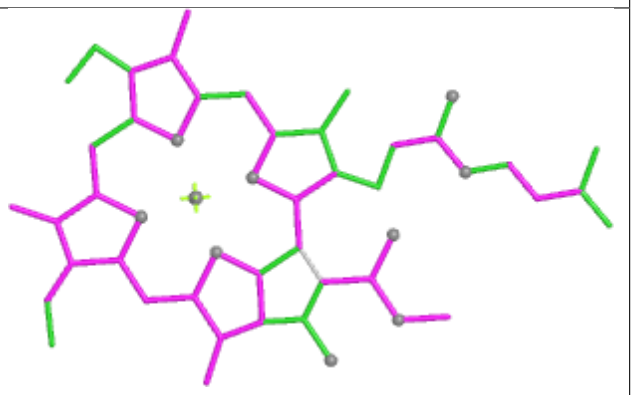
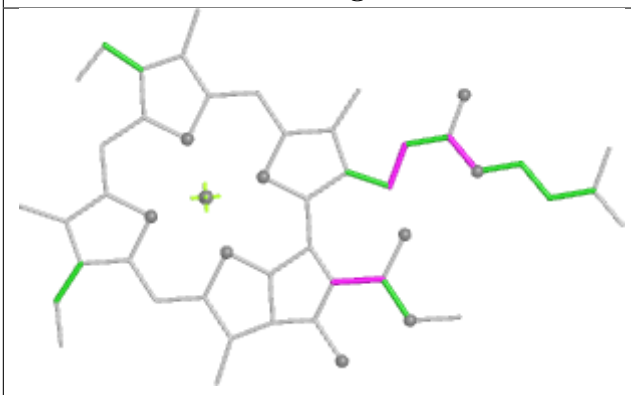
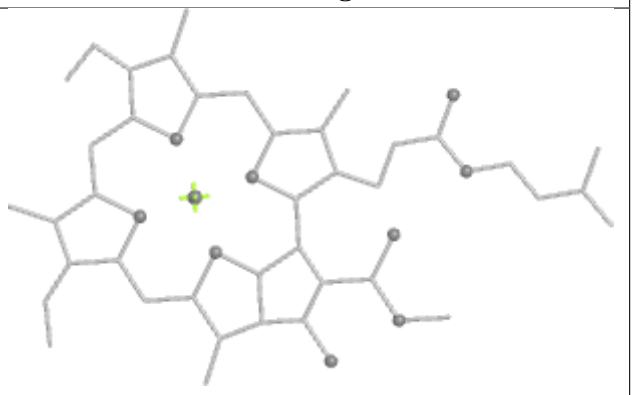


Bond angles

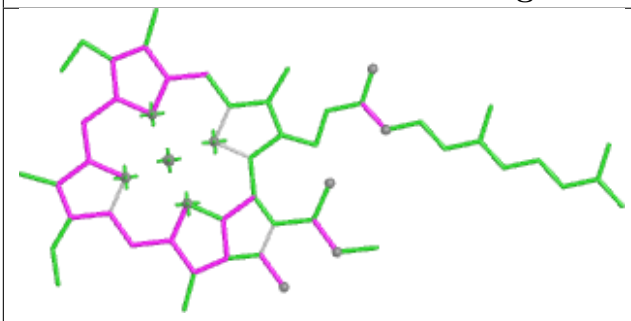


Torsions



Rings

Ligand CLA cB 818



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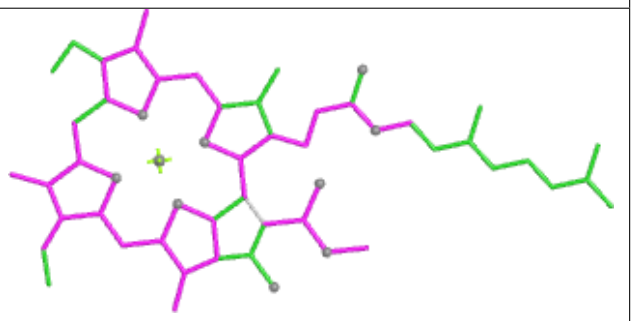
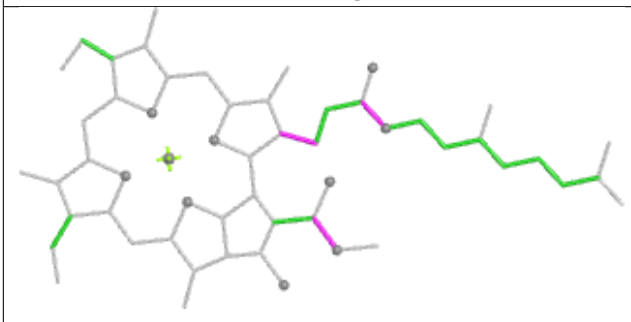
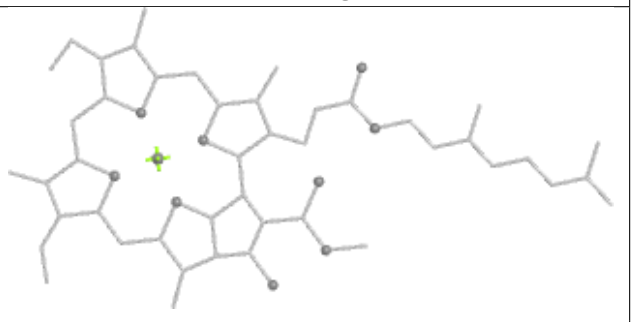


Bond angles

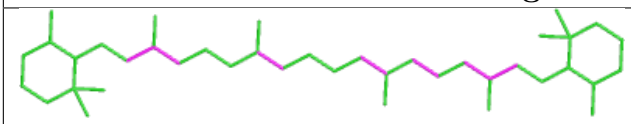


Torsions

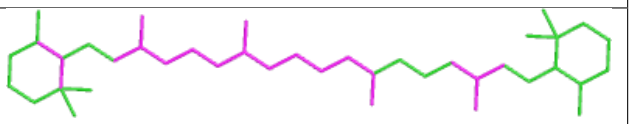


Rings

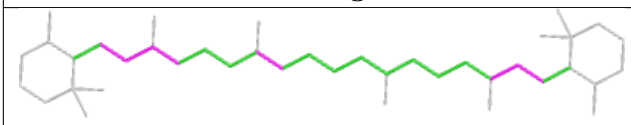
Ligand BCR B 842



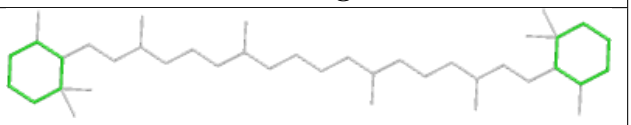
Bond lengths



Bond angles

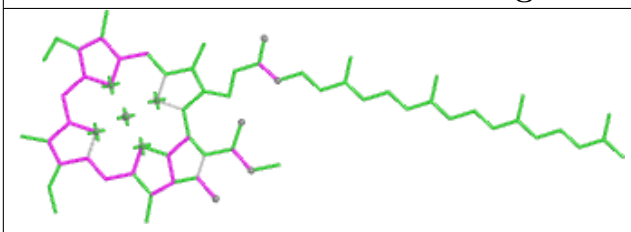


Torsions



Rings

Ligand CLA cA 833



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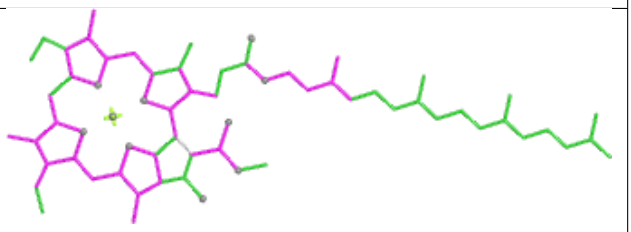
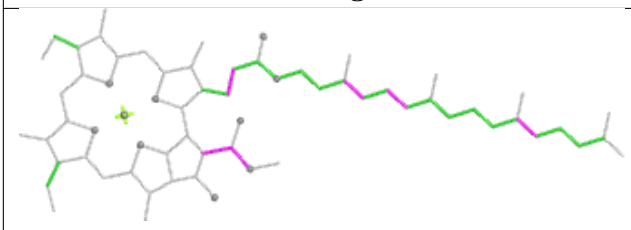
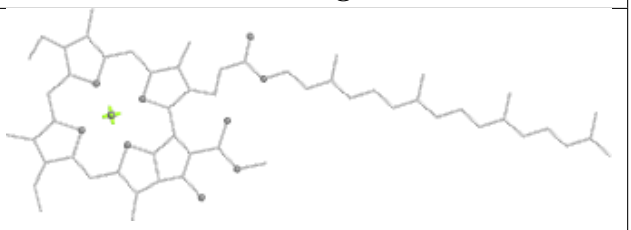


Bond angles

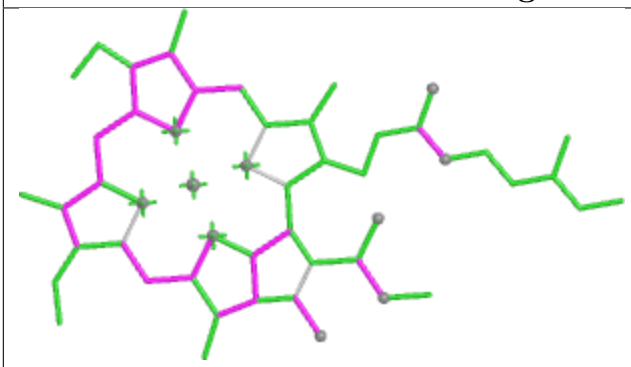


Torsions



Rings

Ligand CLA cF 201



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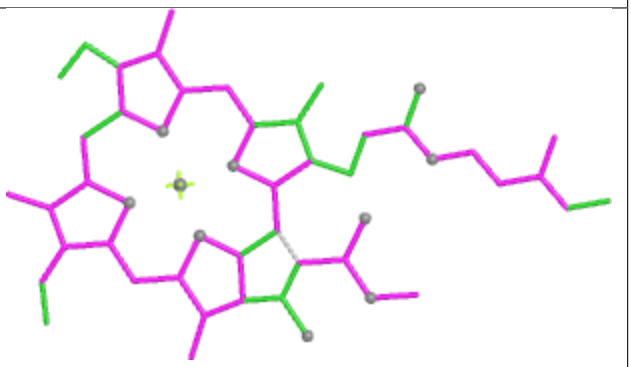
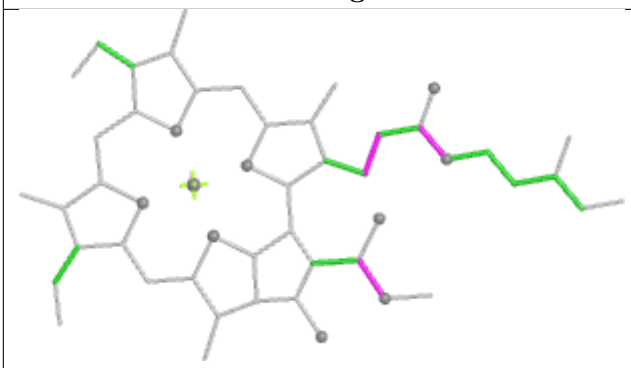


Bond angles



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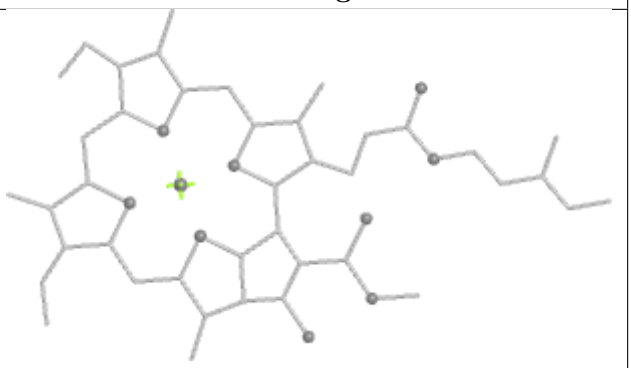
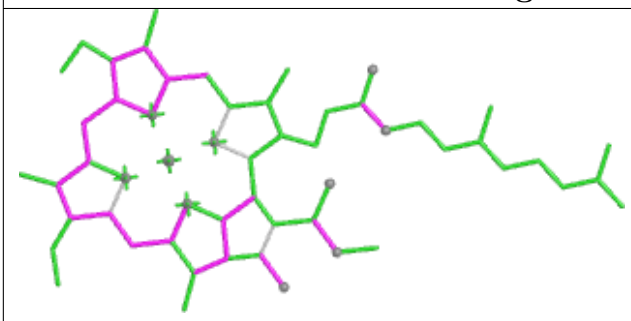
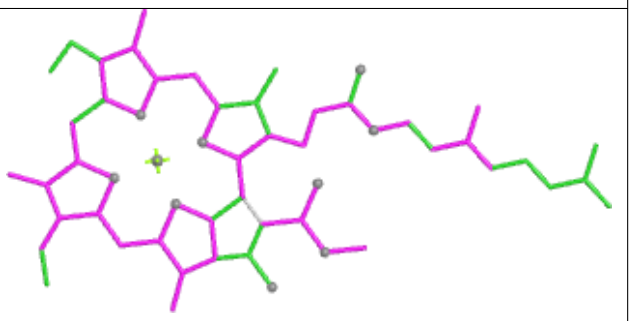


Rings

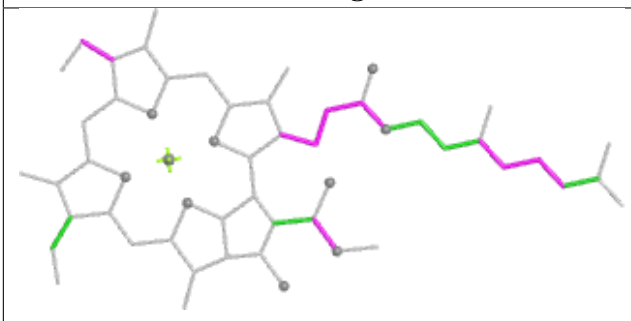
Ligand CLA cA 831



Bond lengths



Bond angles



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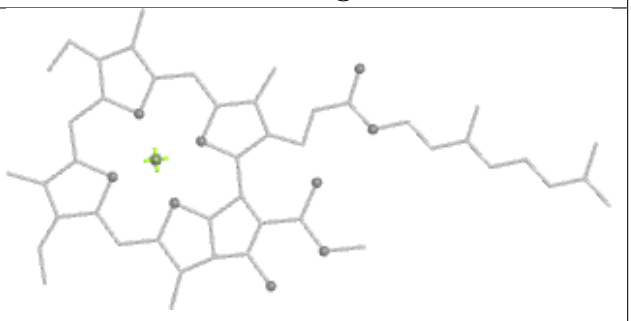
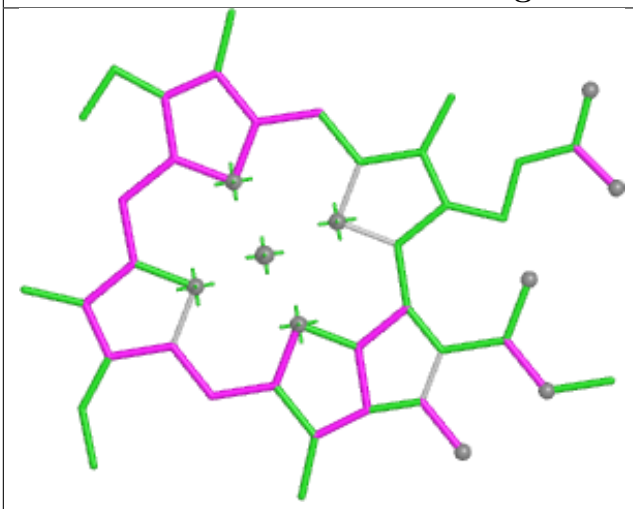


Rings

Ligand CLA bB 849



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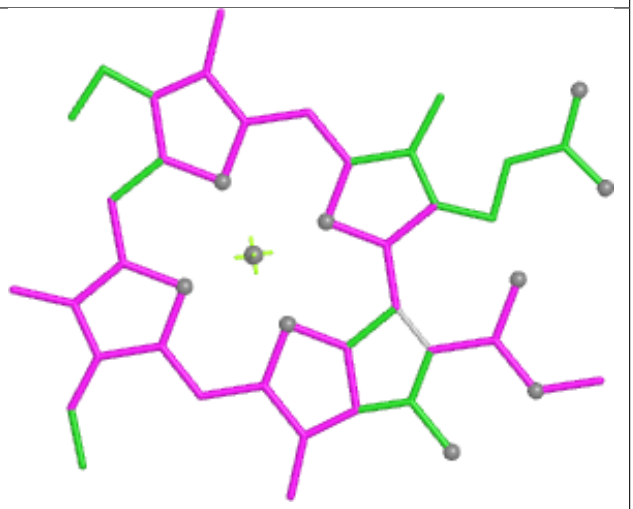
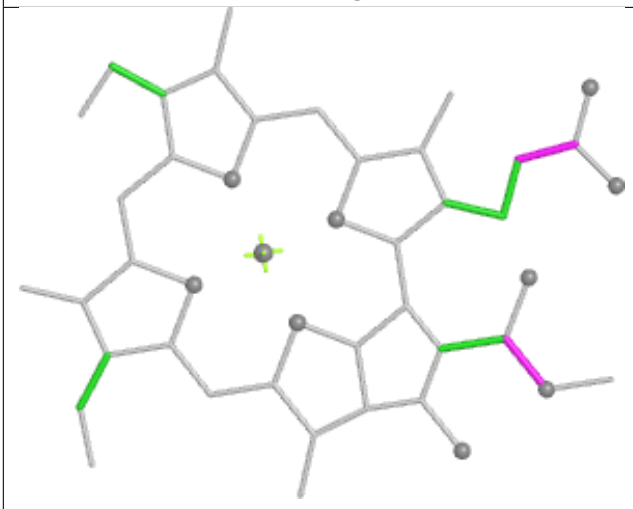


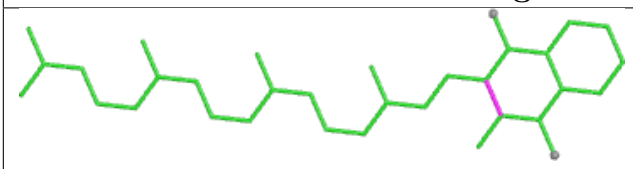
Bond angles



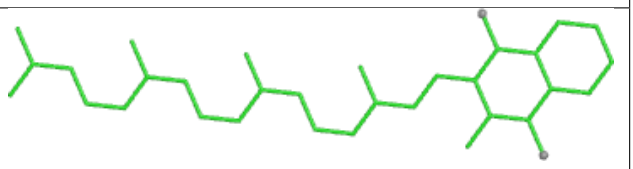
Torsions

Rings

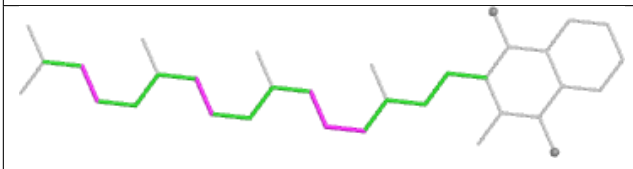
Ligand PQN cA 843



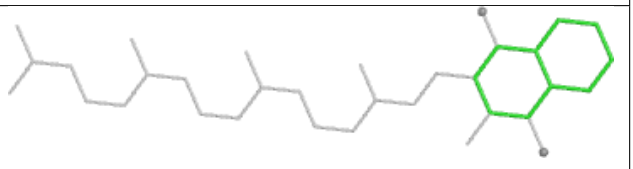
Bond lengths



Bond angles

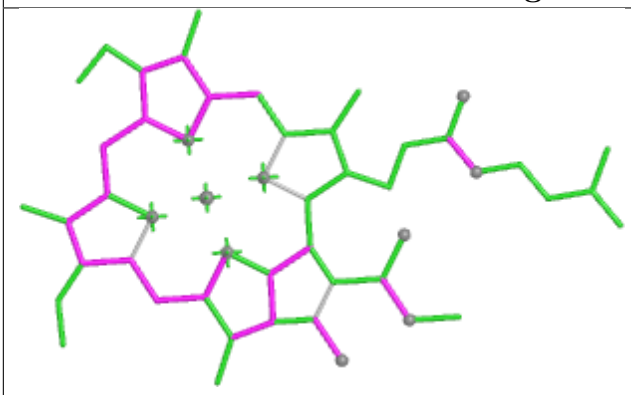


Torsions



Rings

Ligand CLA B 823



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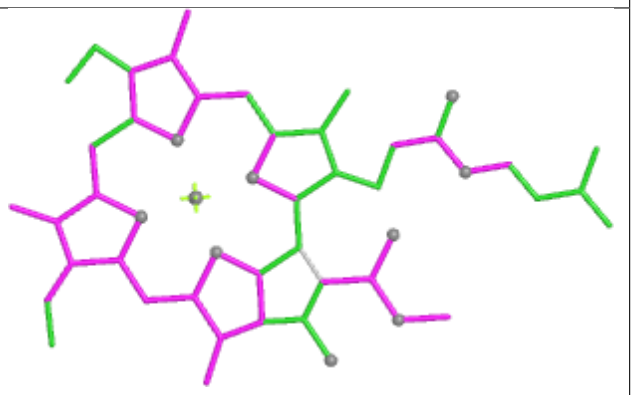

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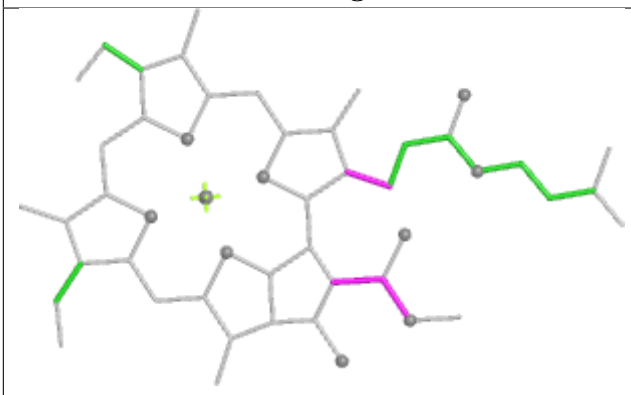

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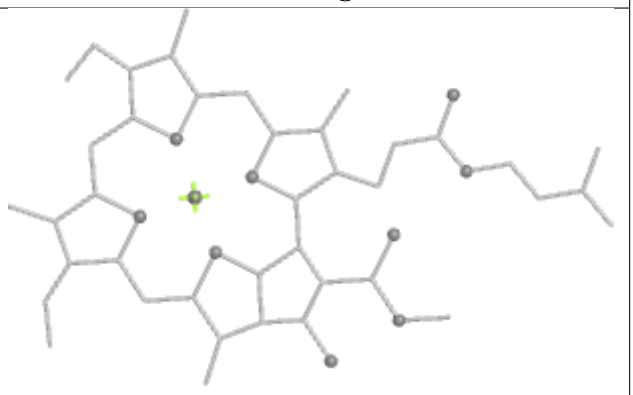
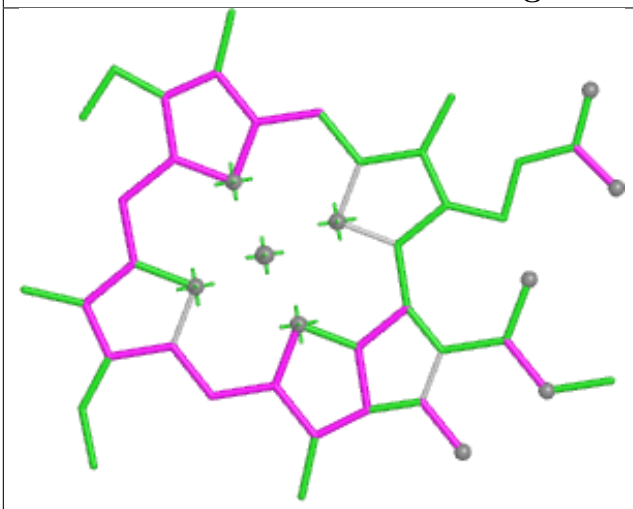


Rings

Ligand CLA A 812



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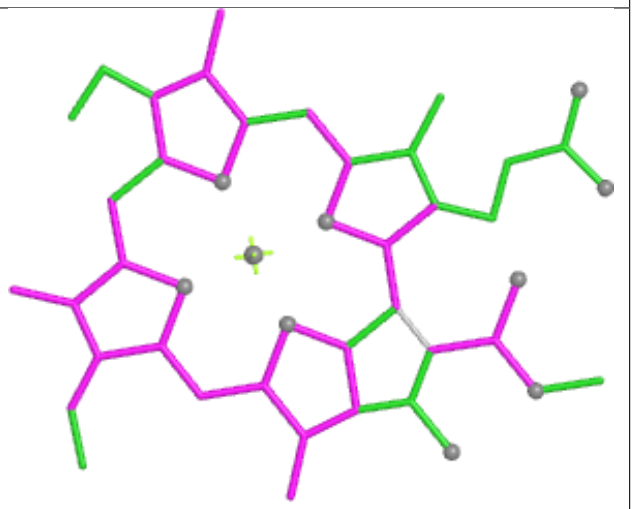
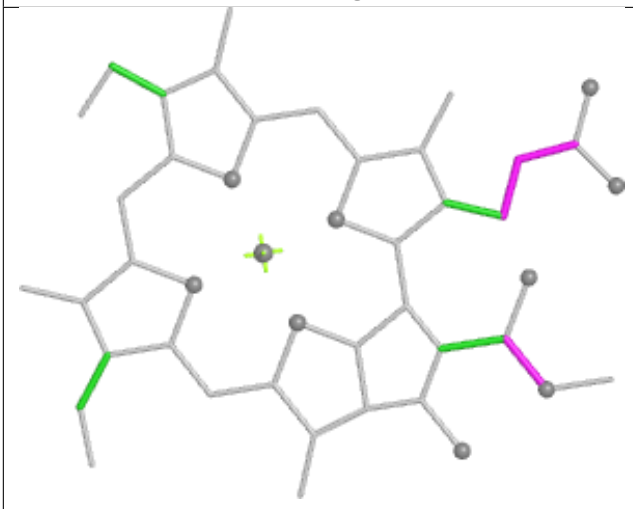


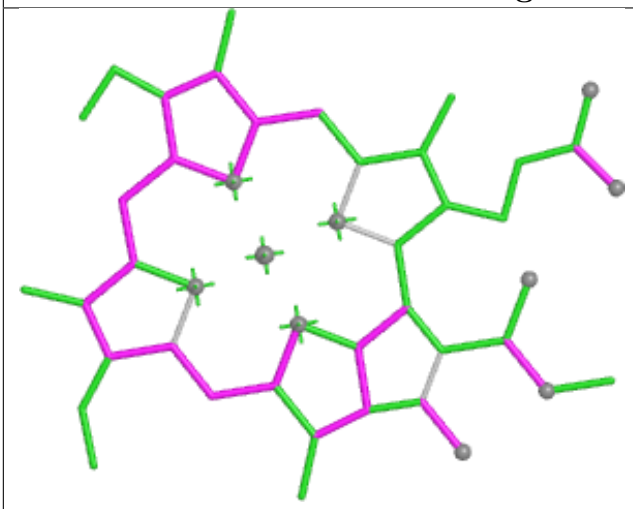
Bond angles



Torsions

Rings

Ligand CLA cA 814



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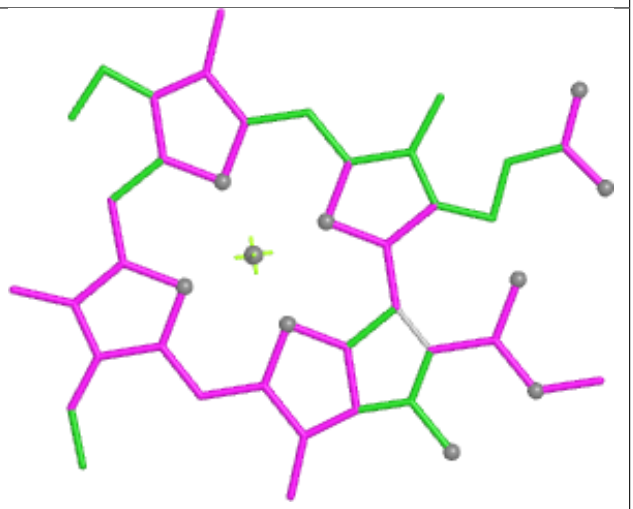

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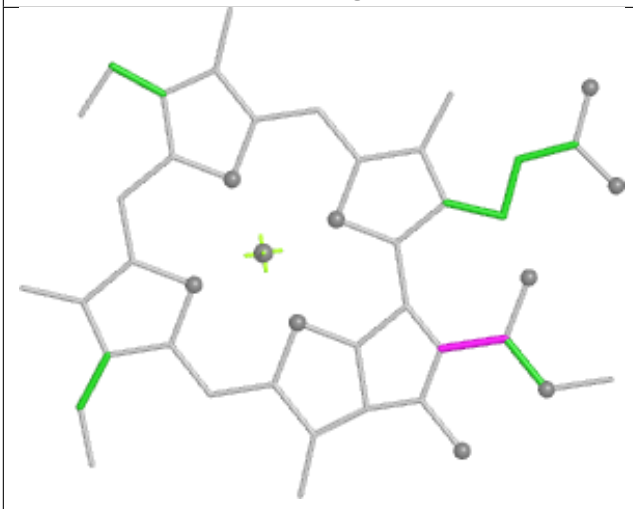
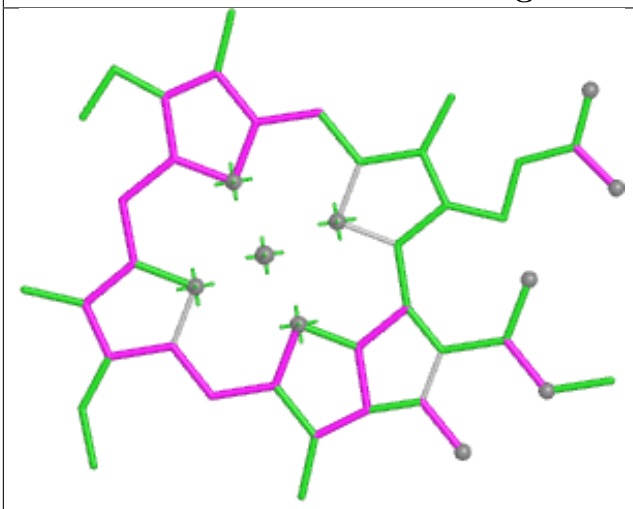


Torsions

Rings

Ligand CLA cA 816



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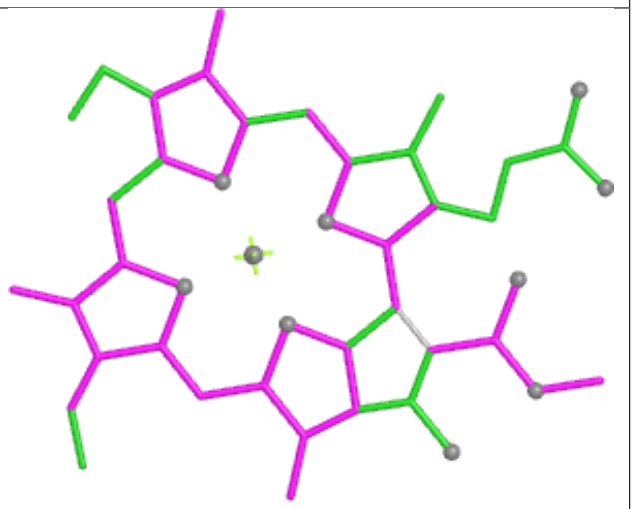
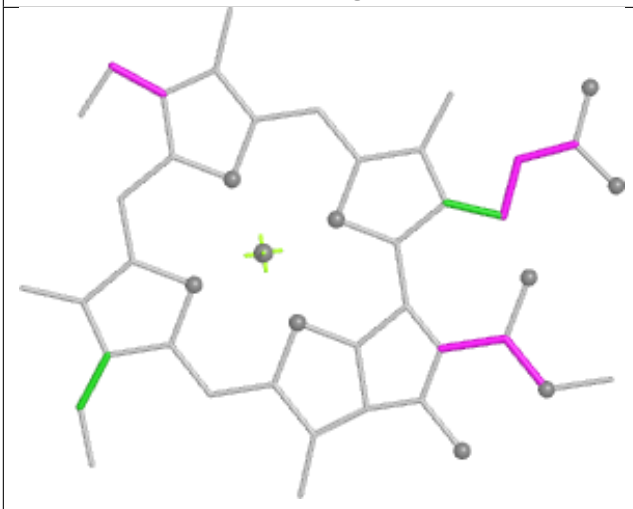


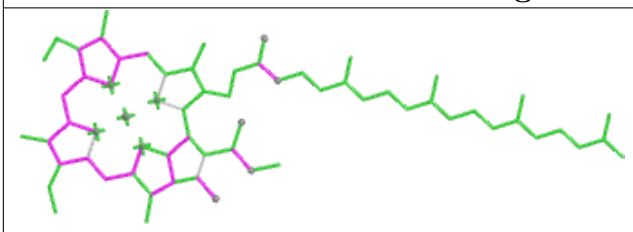
Bond angles



Torsions

Rings

Ligand CLA bB 826



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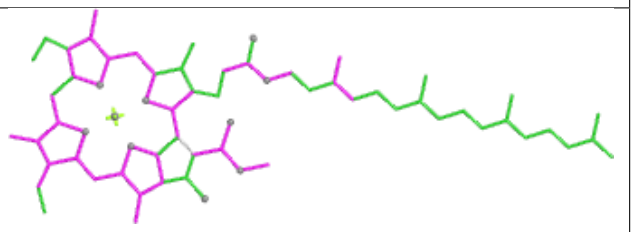

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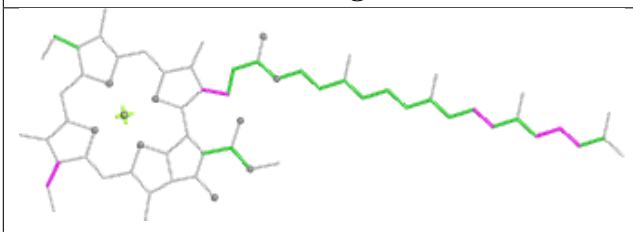
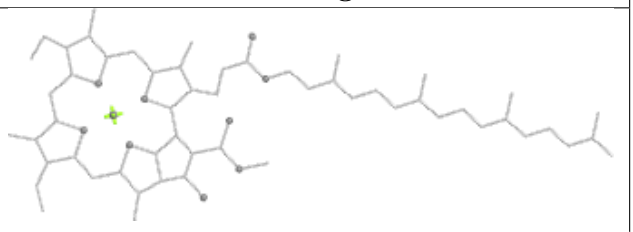
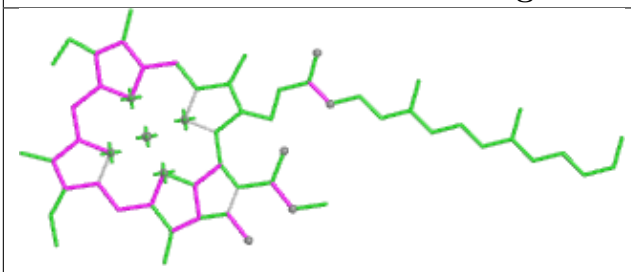
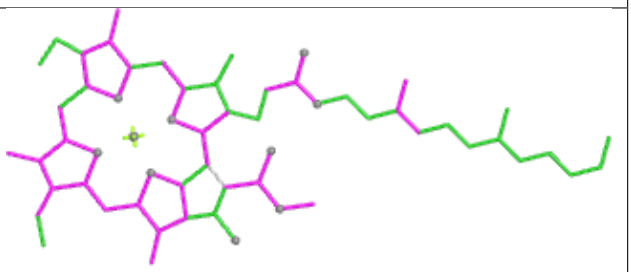
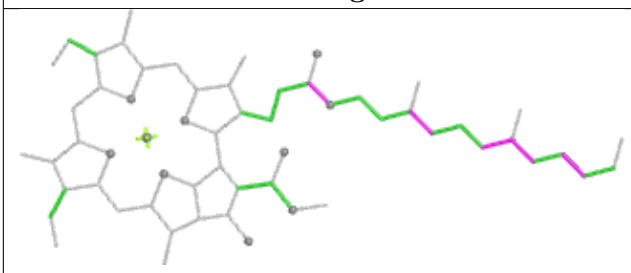
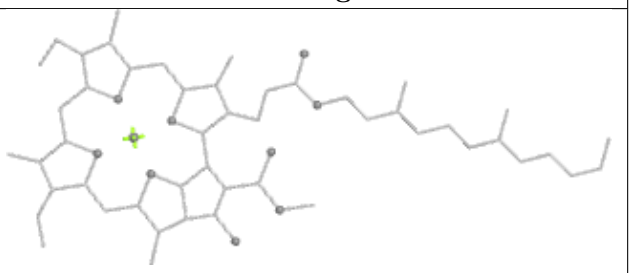
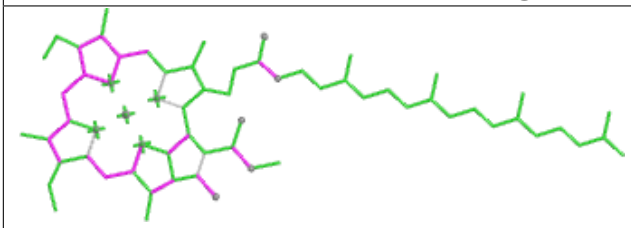
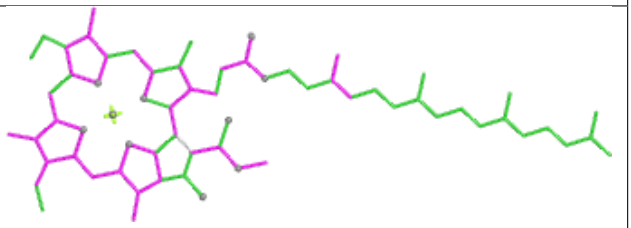
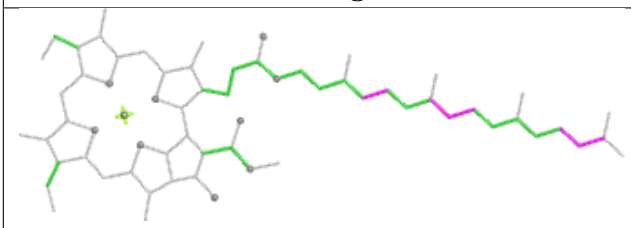
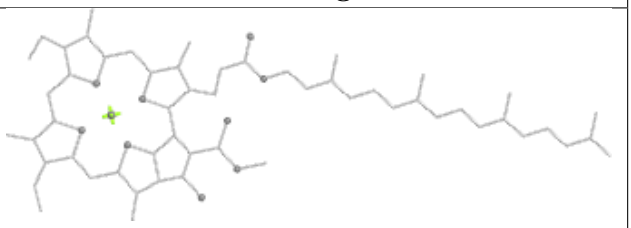


Torsions

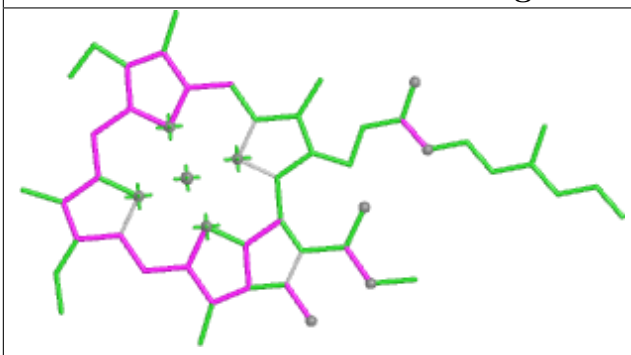


Rings

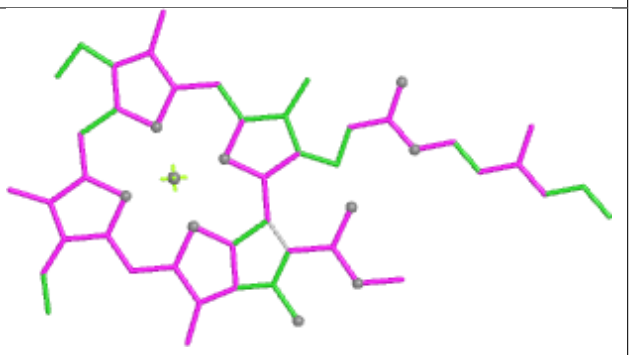
Ligand CLA bL 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA cA 852	
	
Bond lengths	Bond angles
	
Torsions	Rings

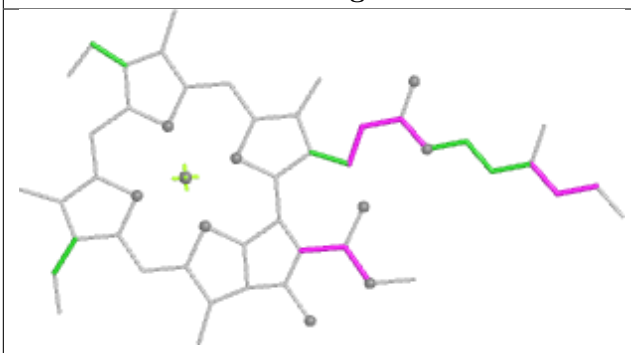
Ligand CLA bB 815



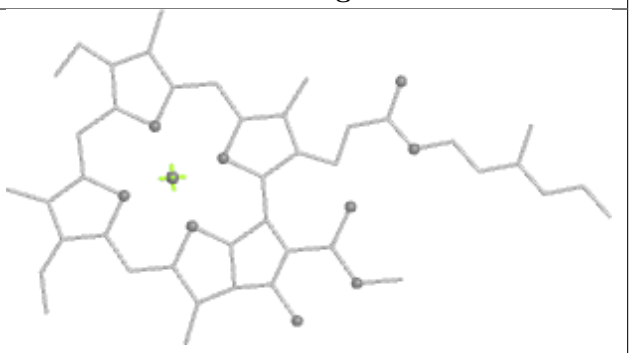
Bond lengths



Bond angles

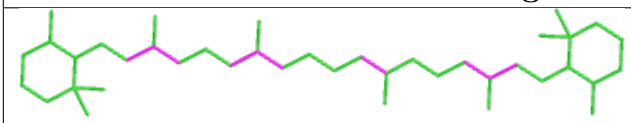


Torsions

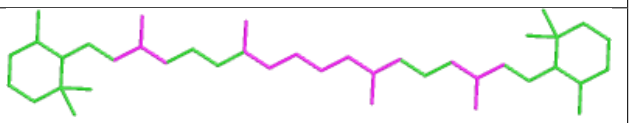


Rings

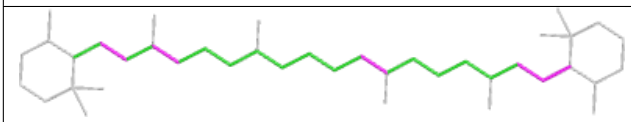
Ligand BCR A 849



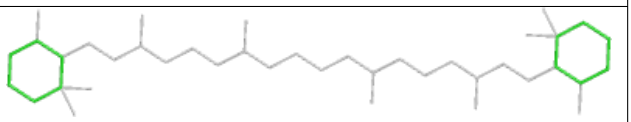
Bond lengths



Bond angles

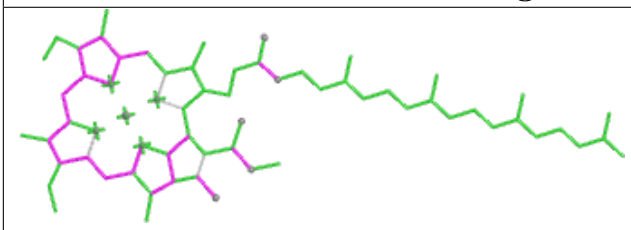


Torsions



Rings

Ligand CLA cB 803



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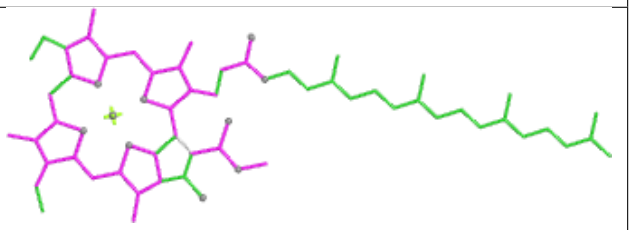
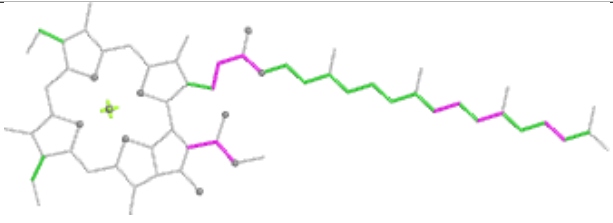


Bond angles



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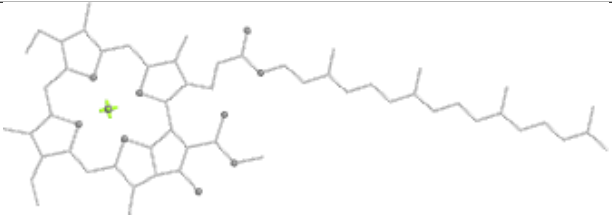
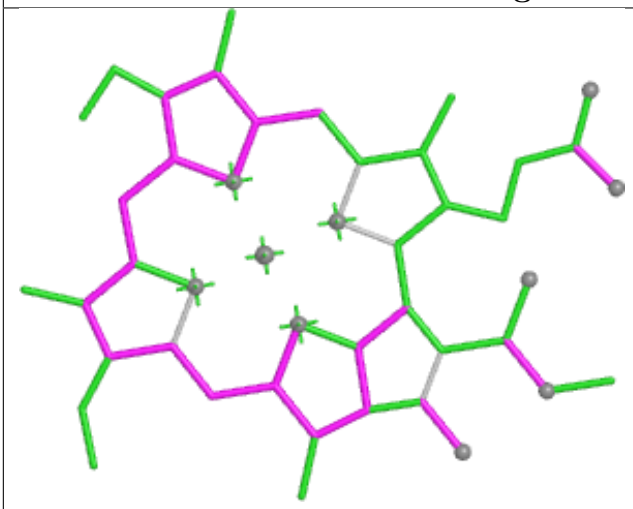


Rings

Ligand CLA bA 810



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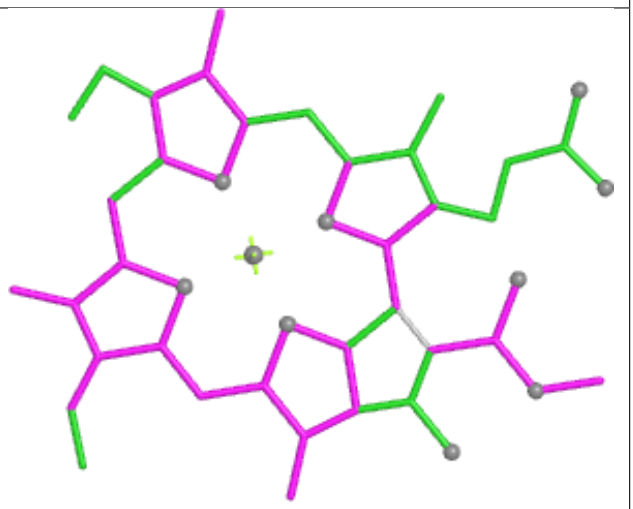
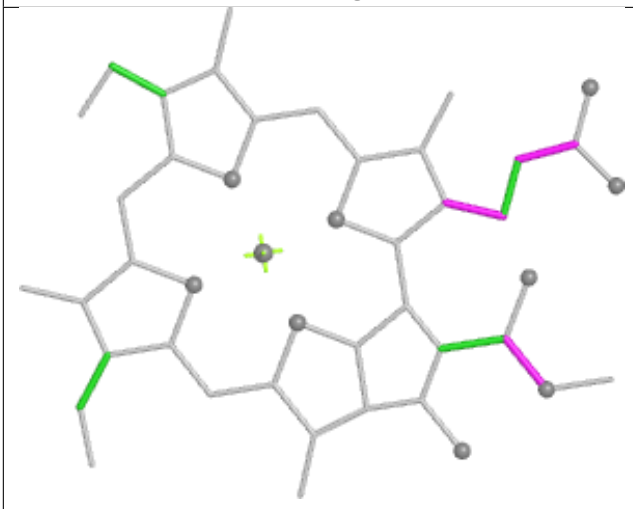


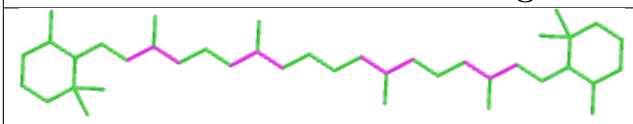
Bond angles



Torsions

Rings

Ligand BCR cL 207



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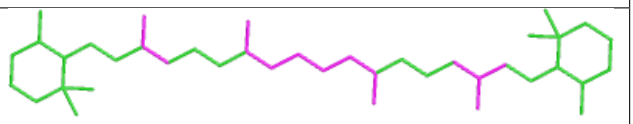
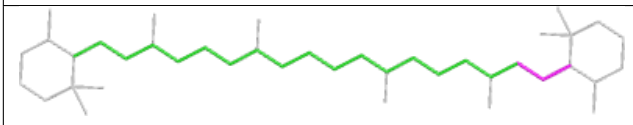


Bond angles



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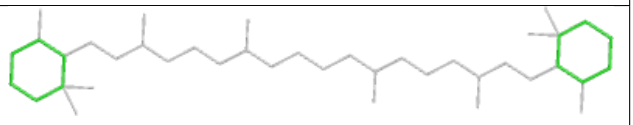
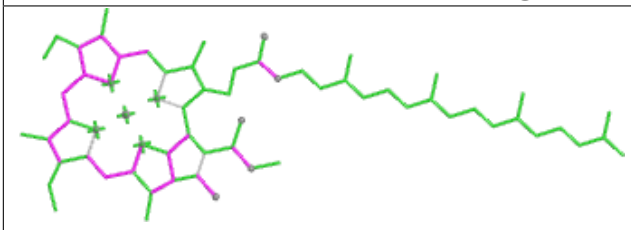


Rings

Ligand CLA cB 802



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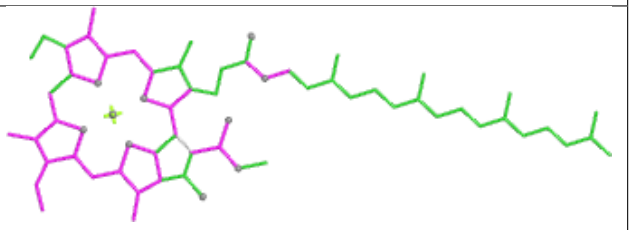
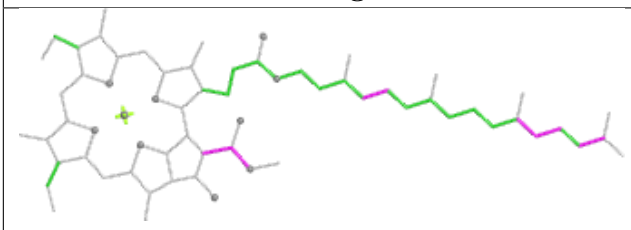


Bond angles



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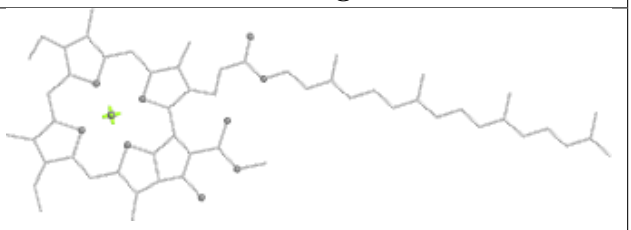
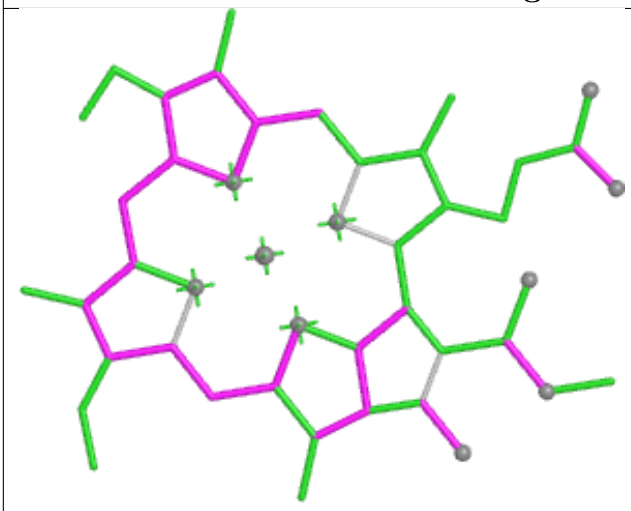


Rings

Ligand CLA A 811



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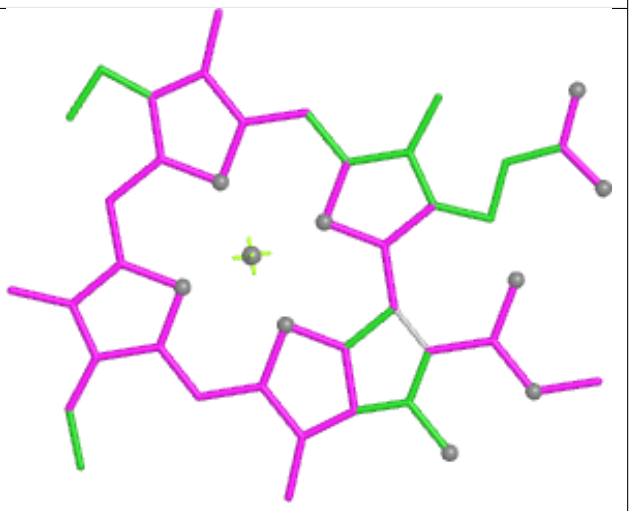
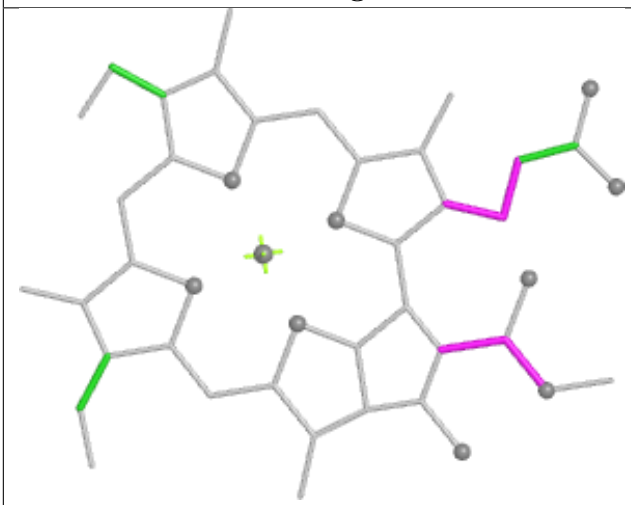


Bond angles



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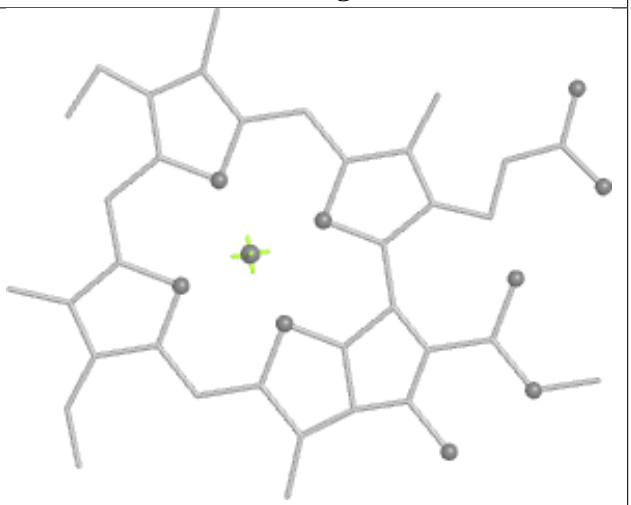
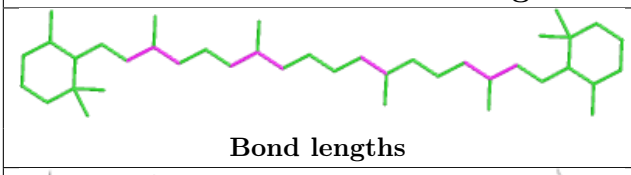


Rings

Ligand BCR bA 846



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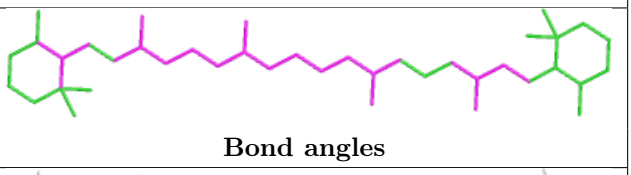
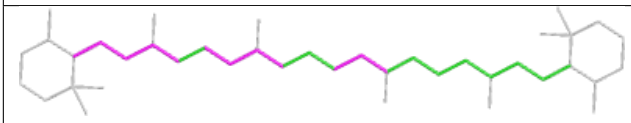


Bond angles



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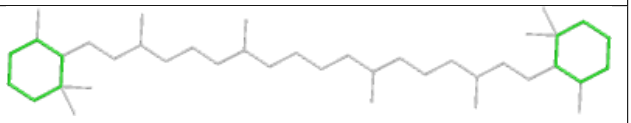
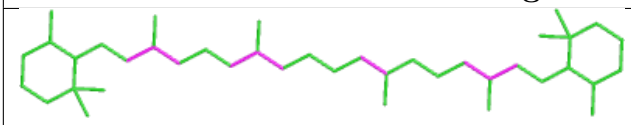


Rings

Ligand BCR B 841



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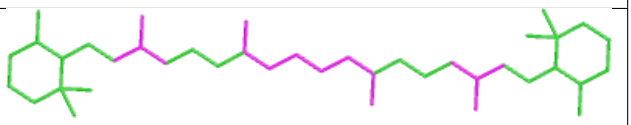
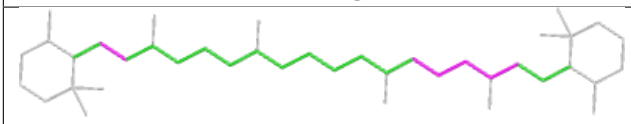


Bond angles



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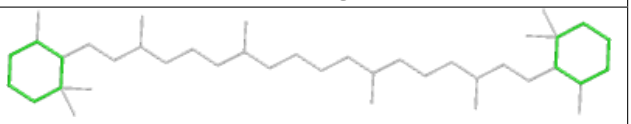
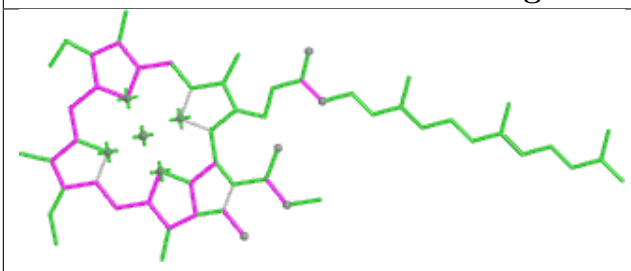


Rings

Ligand CLA A 818



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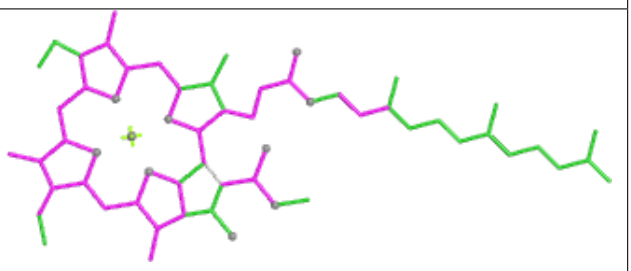
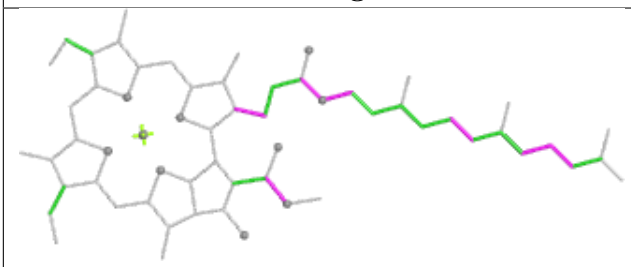


Bond angles



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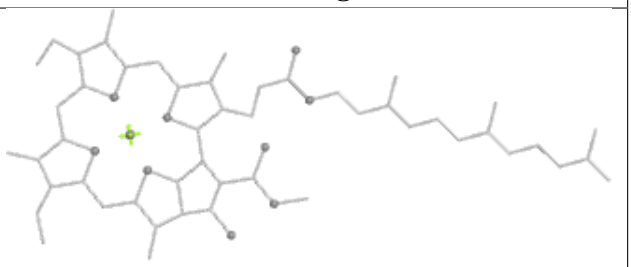
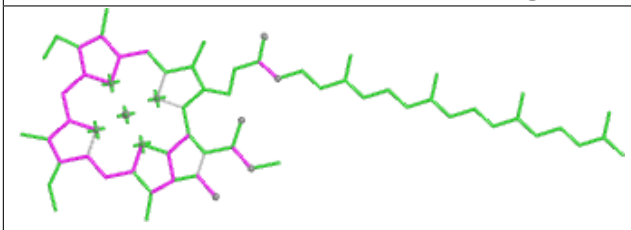


Rings

Ligand CLA A 802



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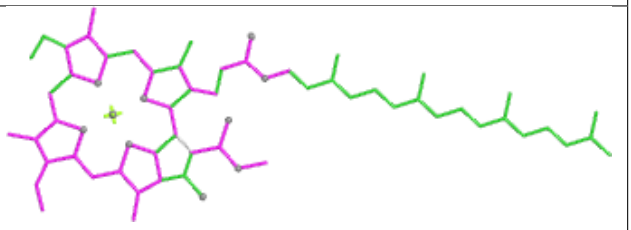

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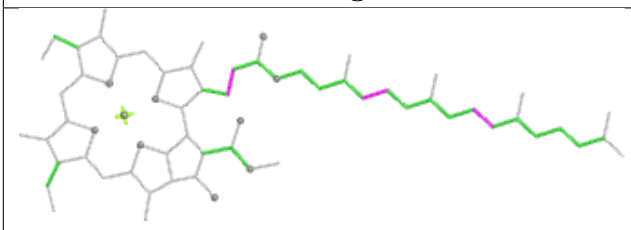

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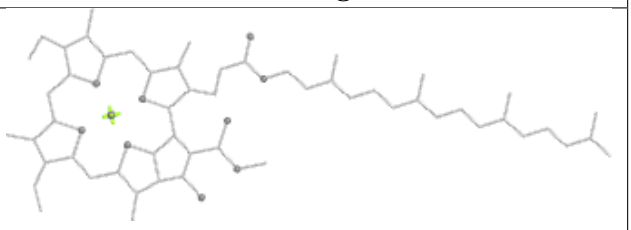
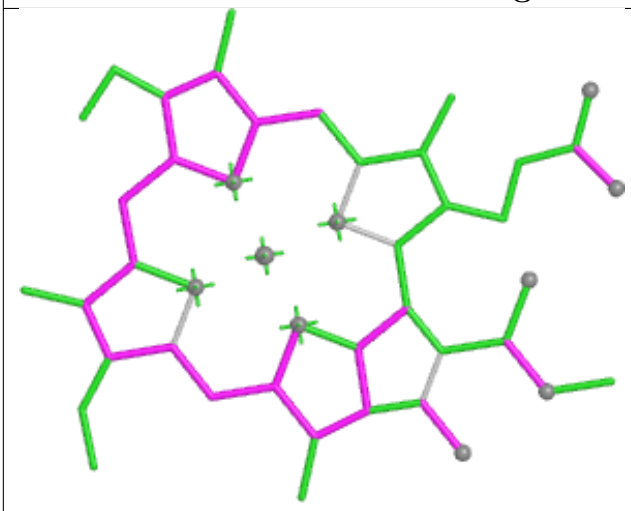


Rings

Ligand CLA bA 811



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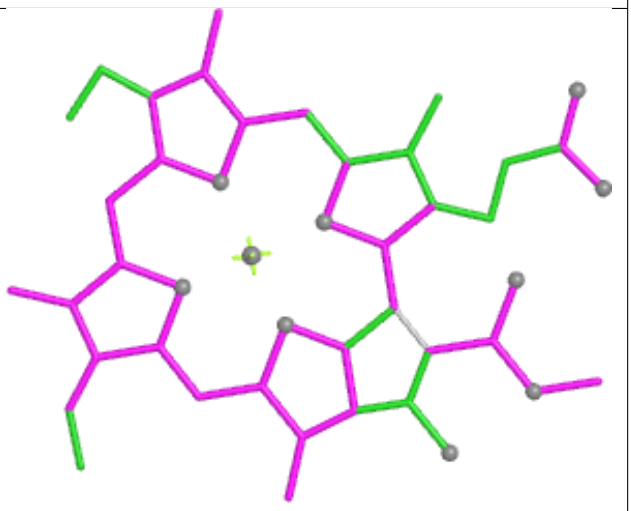
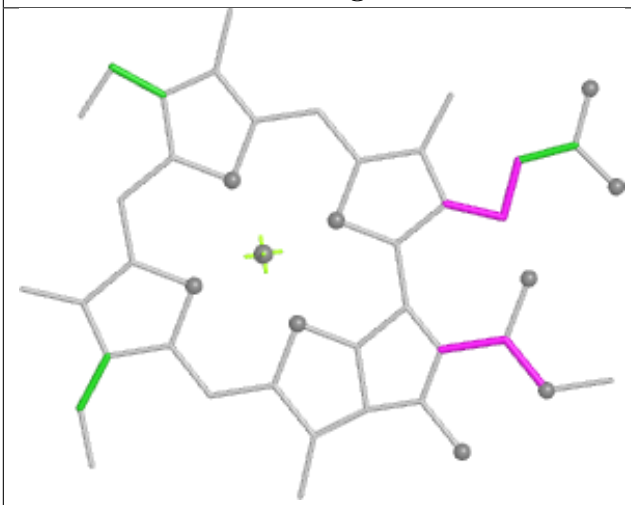


Bond angles



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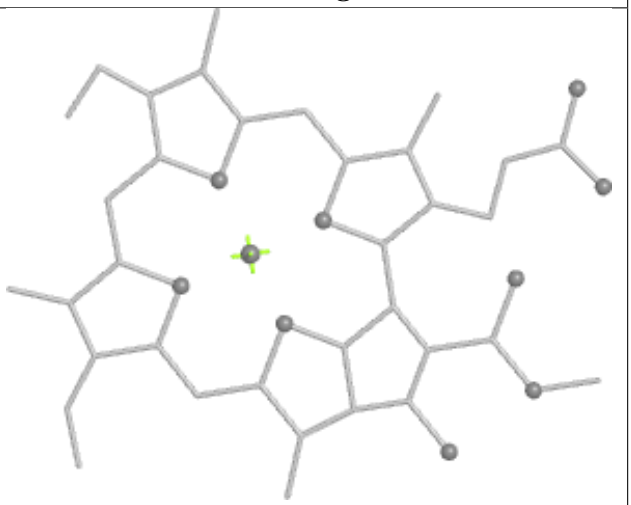
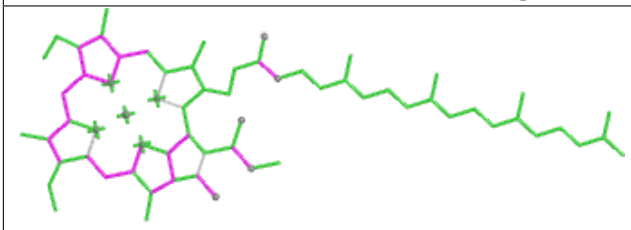


Rings

Ligand CLA bB 801



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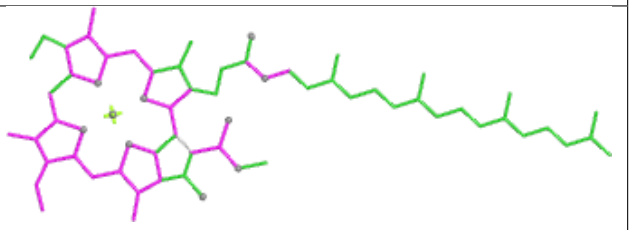
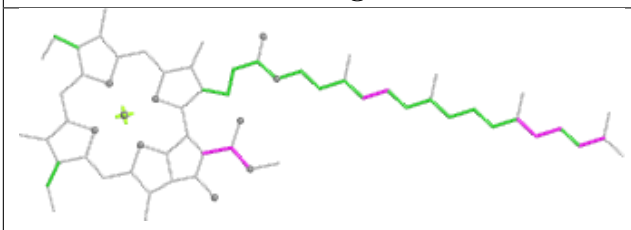


Bond angles



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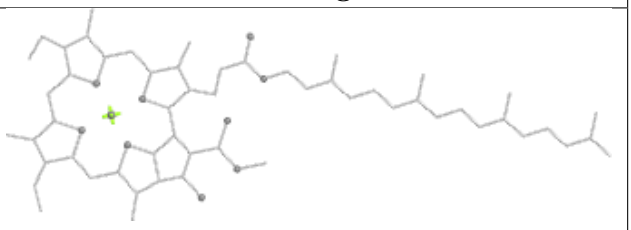
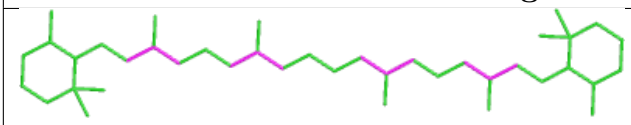


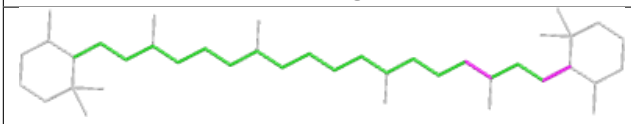
Rings

Ligand BCR cI 102



Bond lengths

Bond angles



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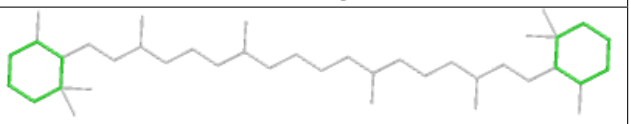
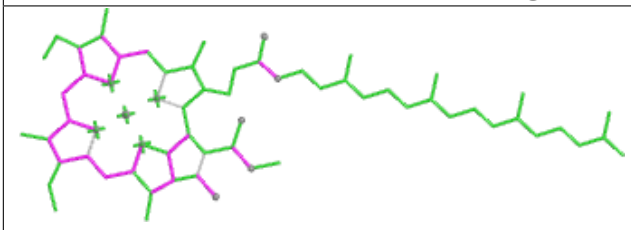
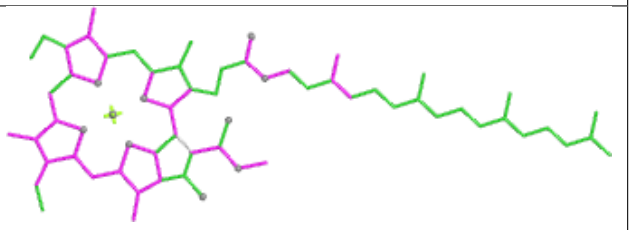


Rings

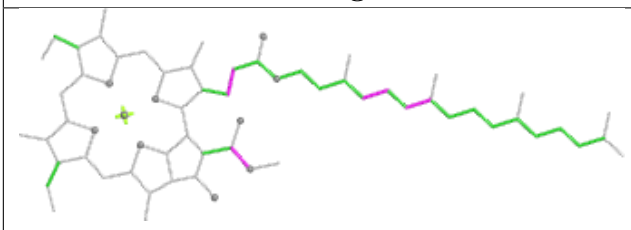
Ligand CLA B 838



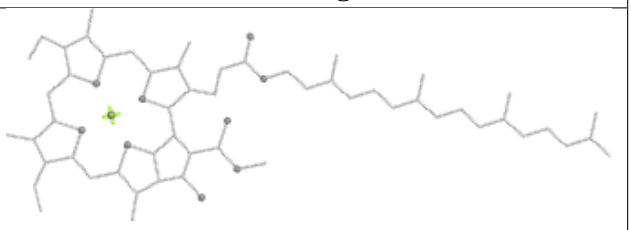
Bond lengths



Bond angles

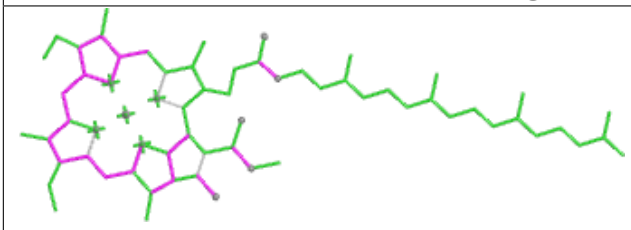


Torsions



Rings

Ligand CLA B 807



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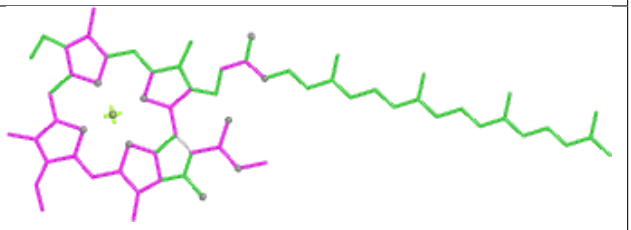

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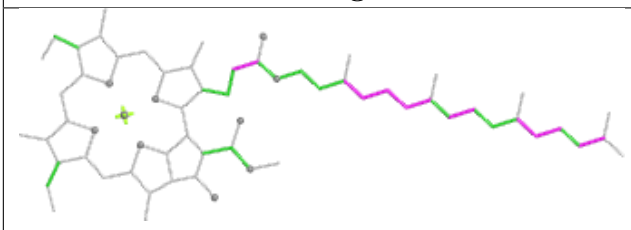

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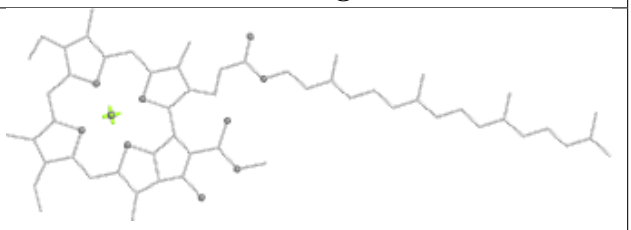
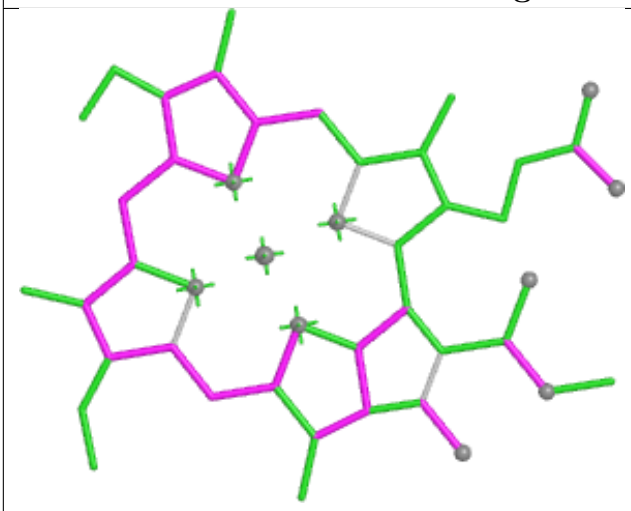


Rings

Ligand CLA bA 803



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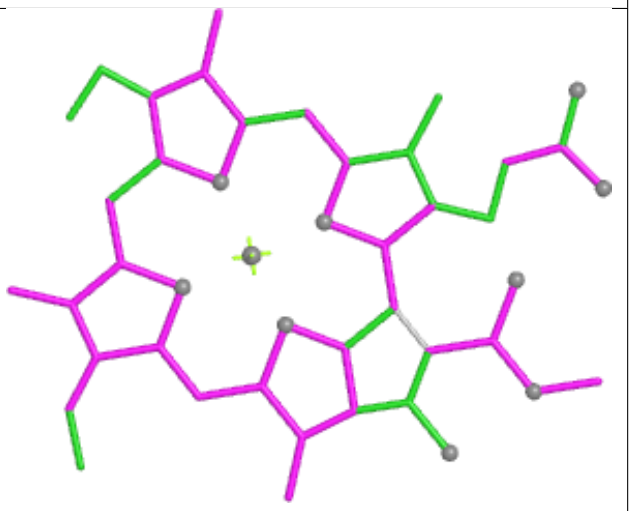
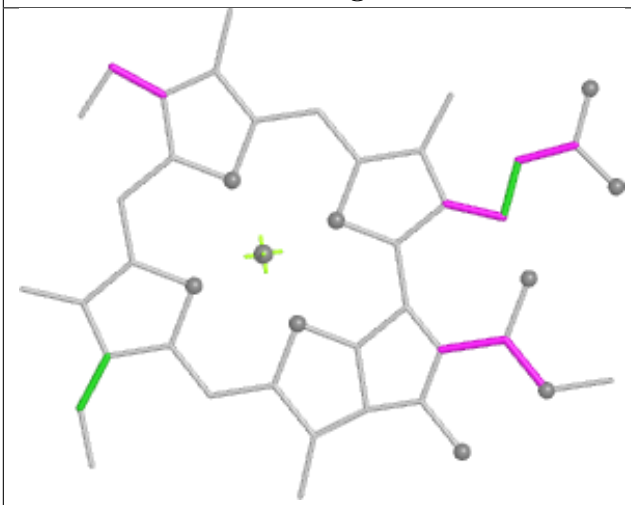


Bond angles



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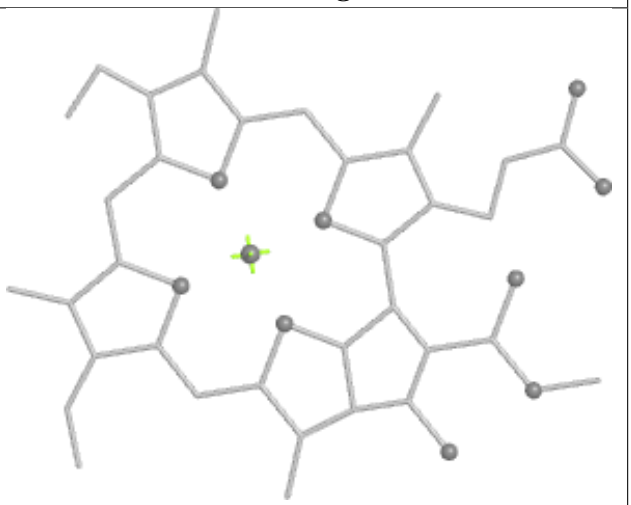
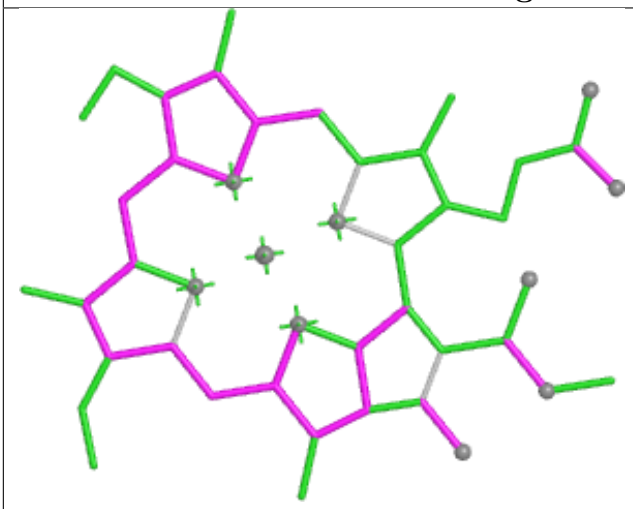


Rings

Ligand CLA cA 820



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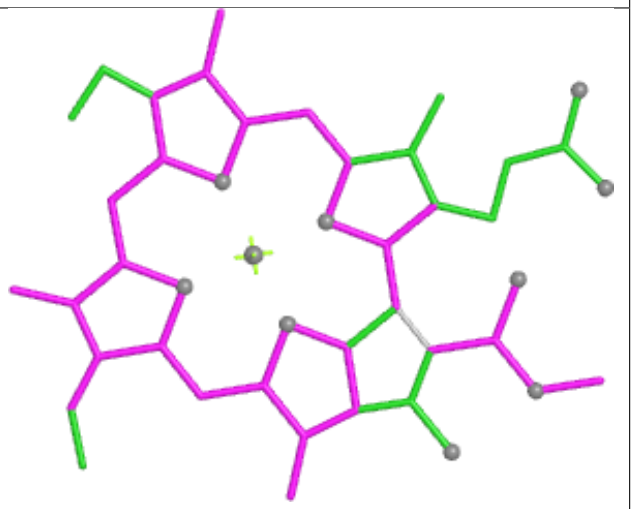
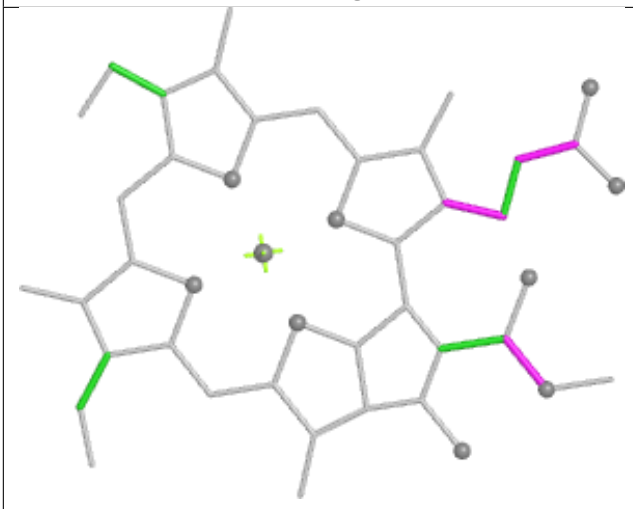


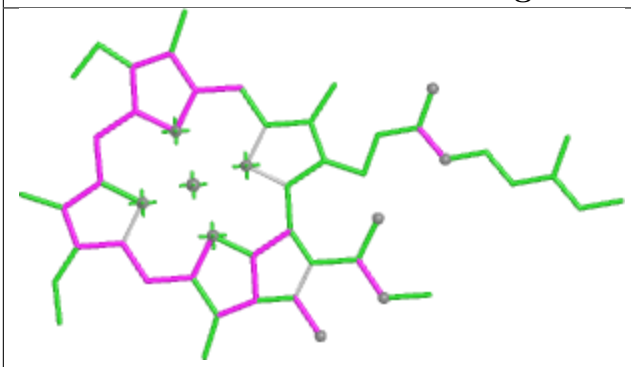
Bond angles



Torsions

Rings

Ligand CLA bB 804



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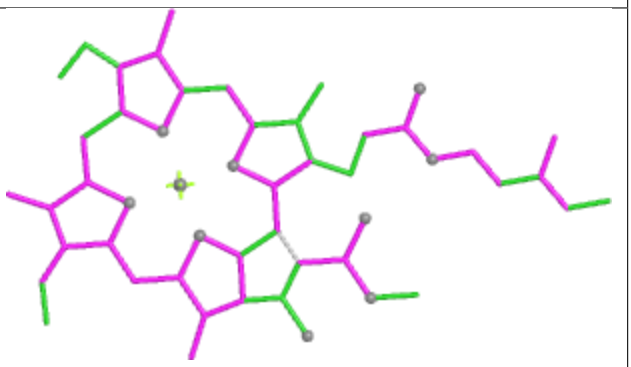
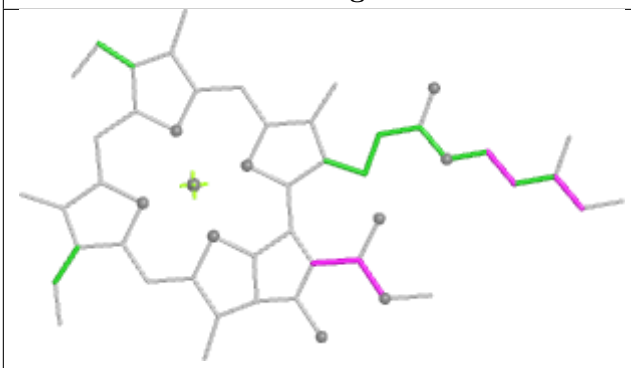
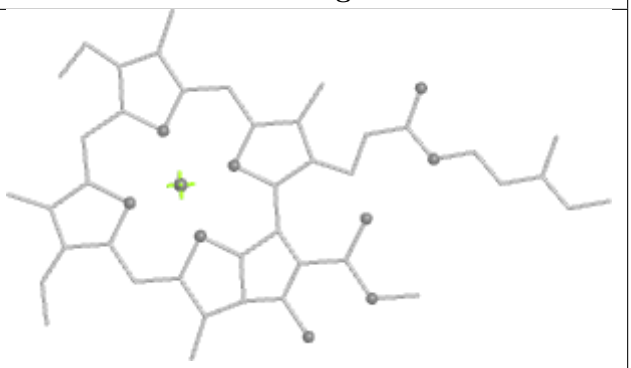


Bond angles

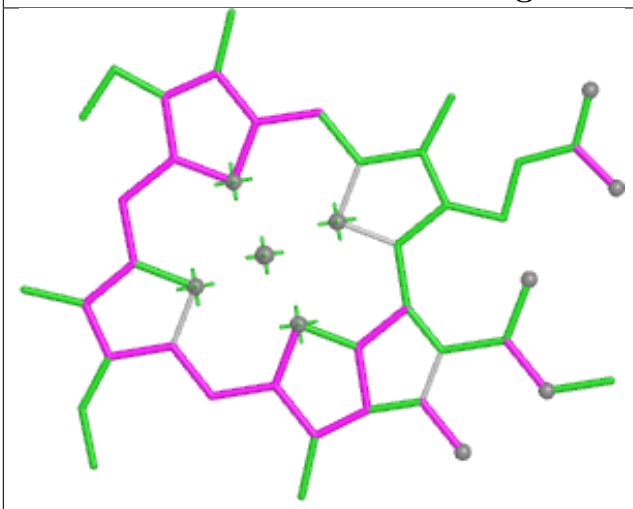


Torsions



Rings

Ligand CLA cA 807



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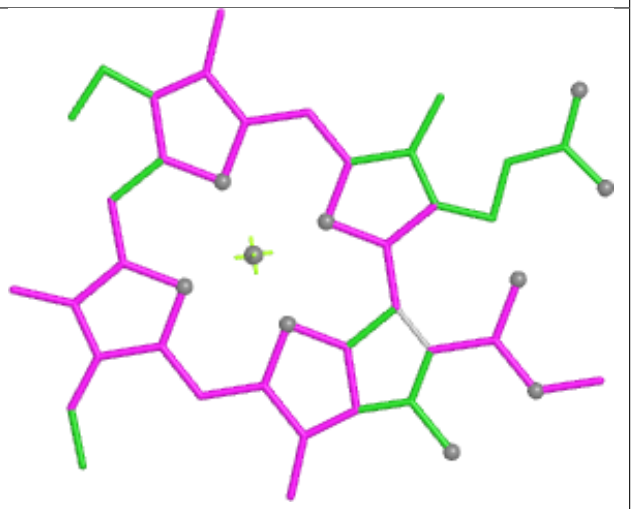
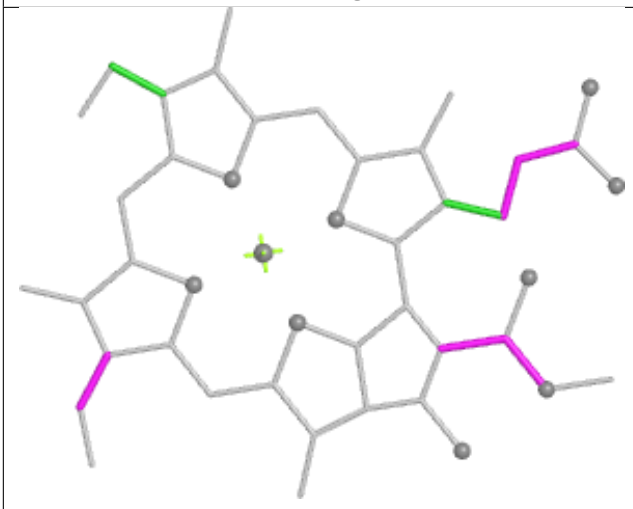


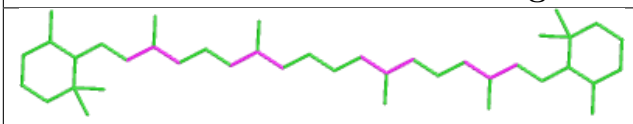
Bond angles



Torsions

Rings

Ligand BCR I 101



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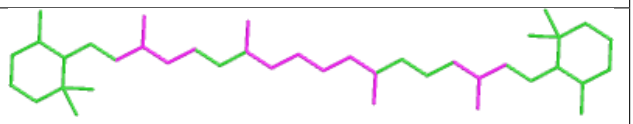
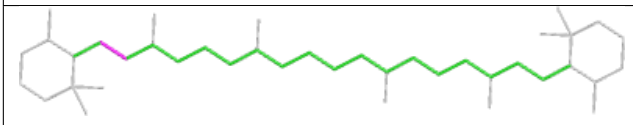
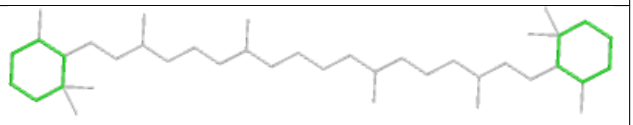


Bond angles

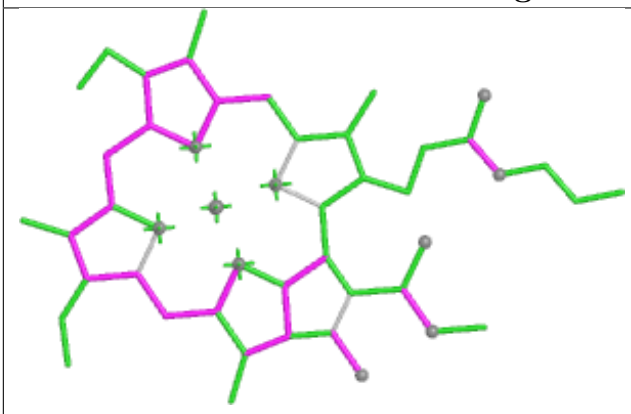


Torsions



Rings

Ligand CLA bB 813



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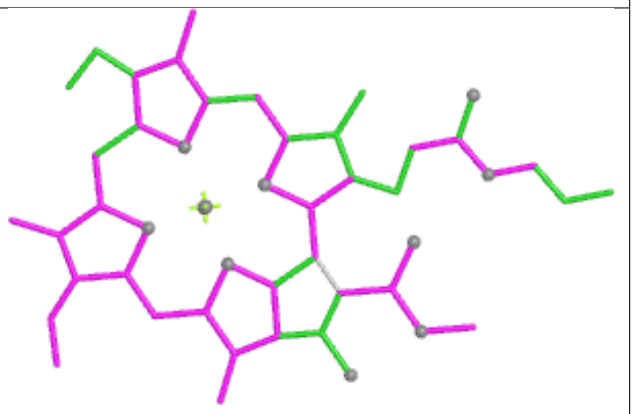

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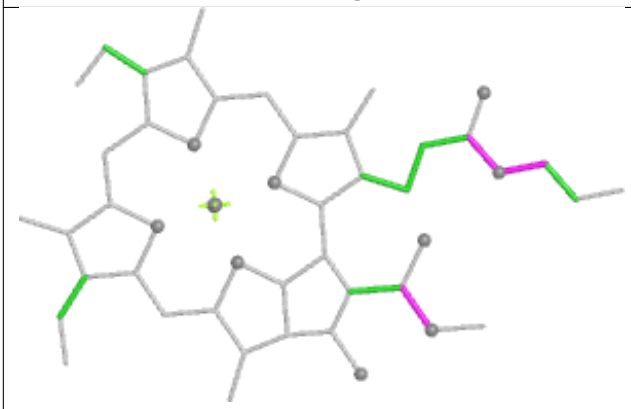

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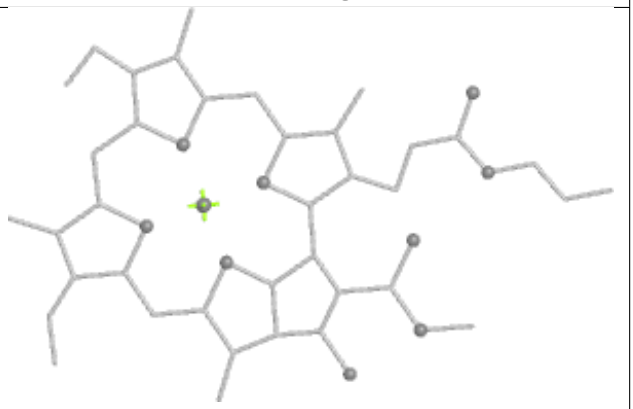
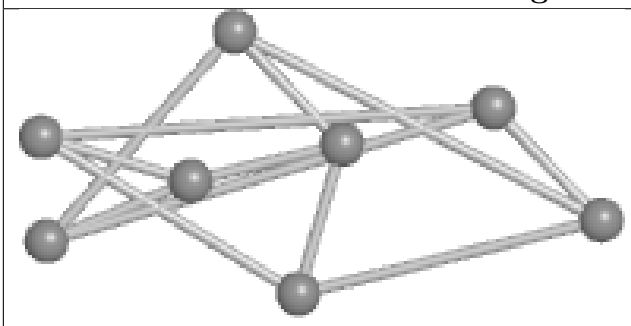


Rings

Ligand SF4 A 844



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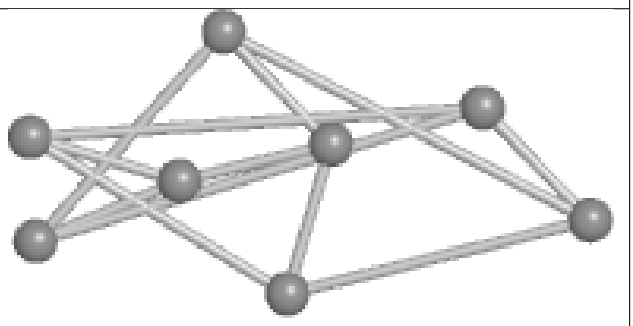
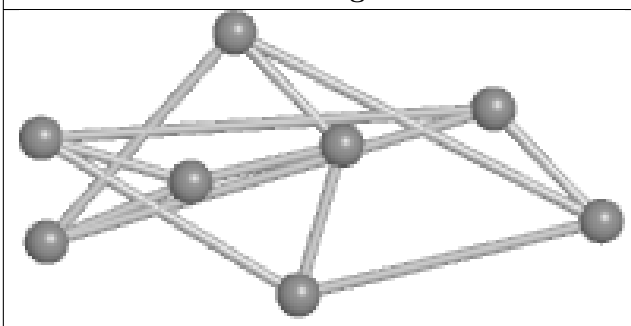
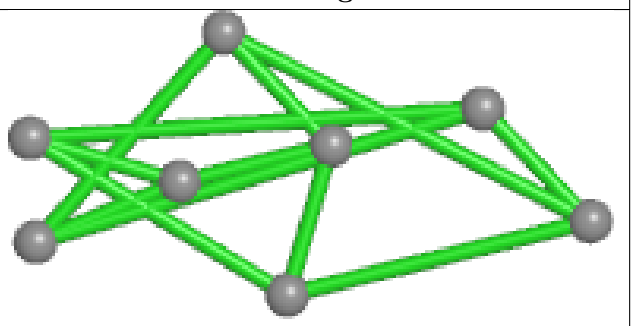


Bond angles

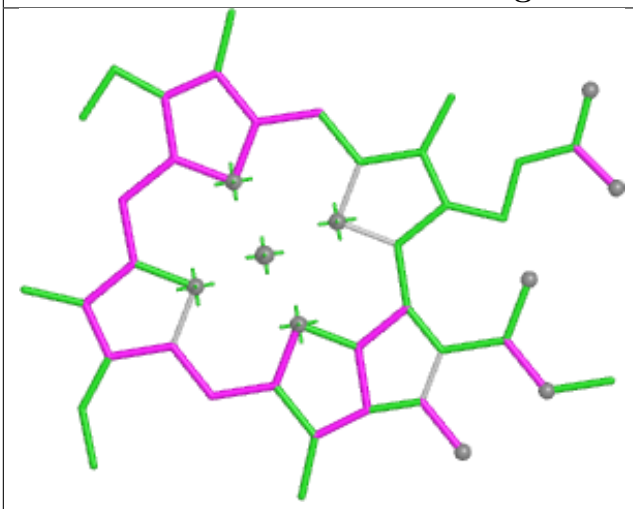


Torsions



Rings

Ligand CLA bB 835



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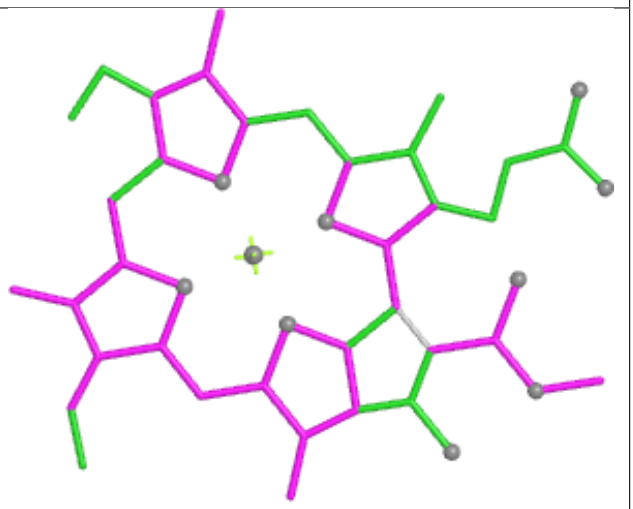
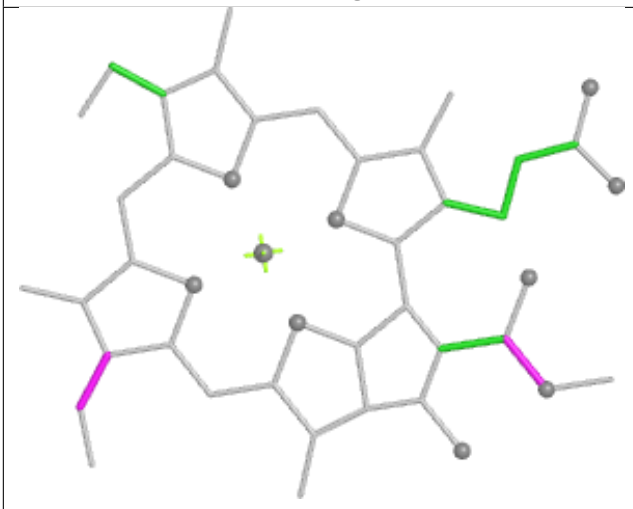


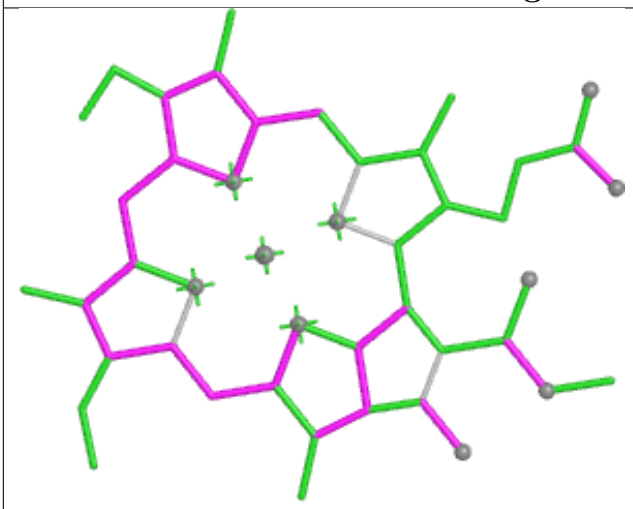
Bond angles



Torsions

Rings

Ligand CLA A 819



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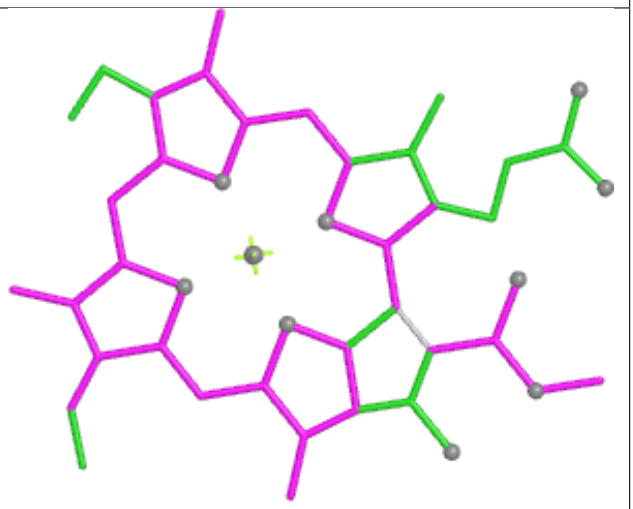
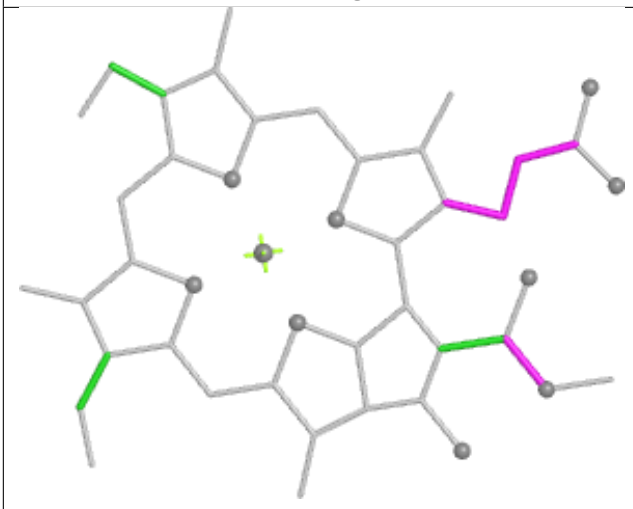


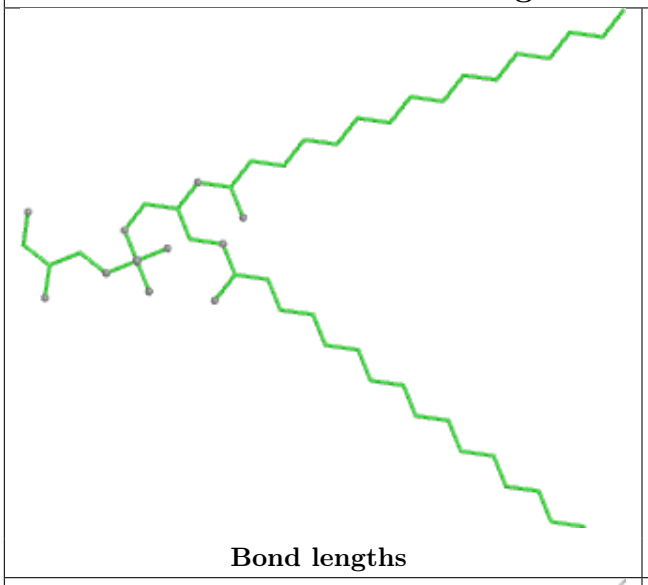
Bond angles



Torsions

Rings

Ligand LHG cA 850



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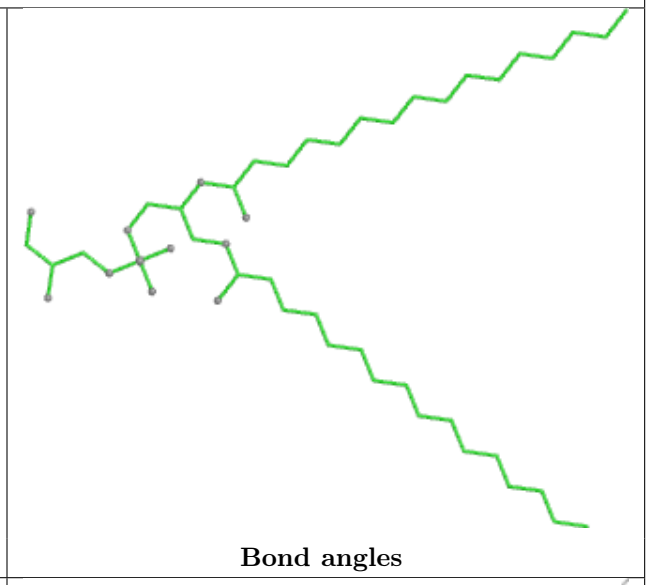
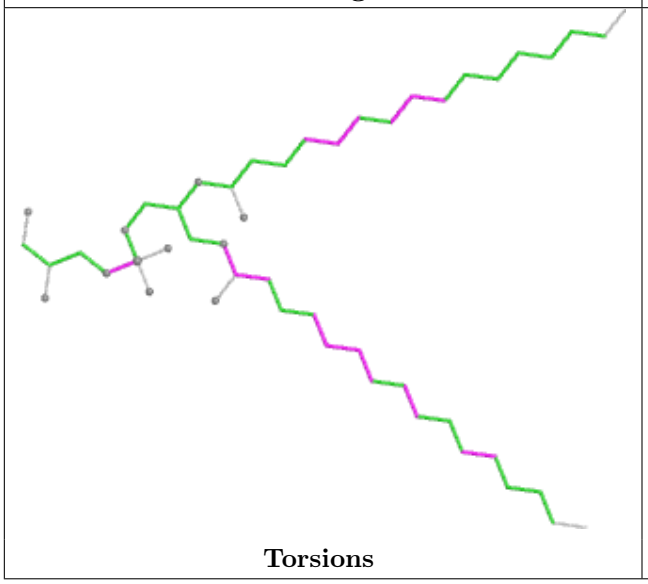


Bond angles



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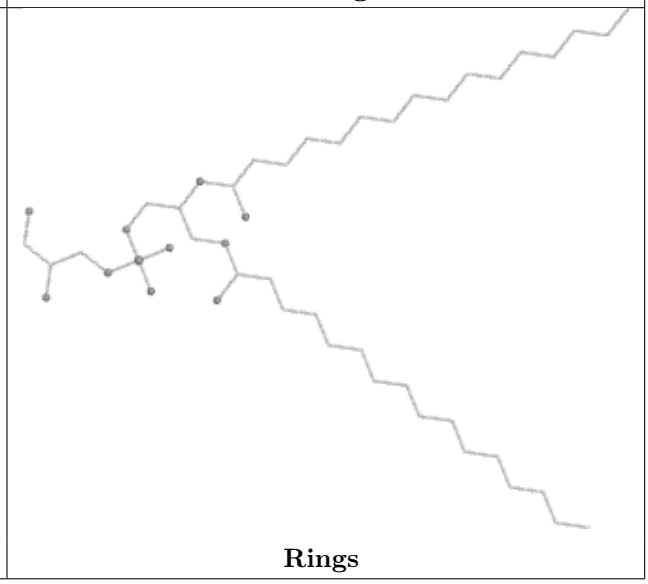
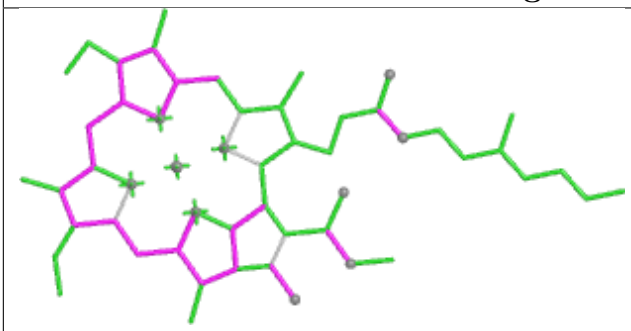


Rings

Ligand CLA A 804



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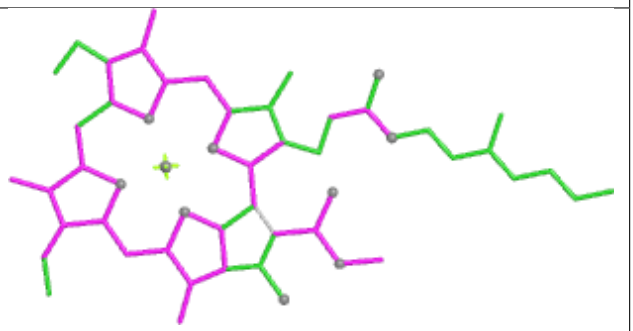
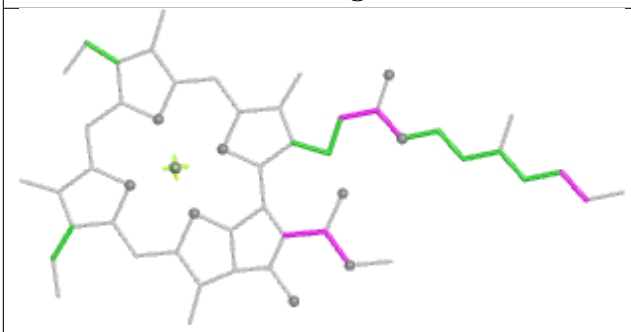
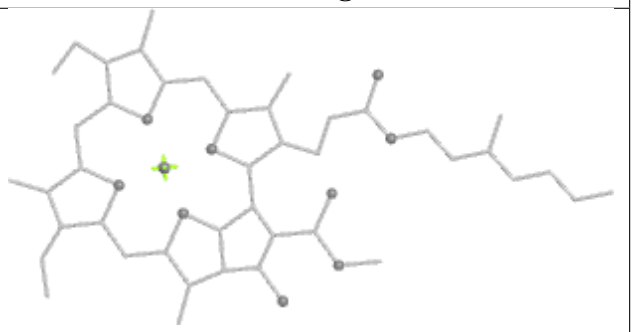


Bond angles

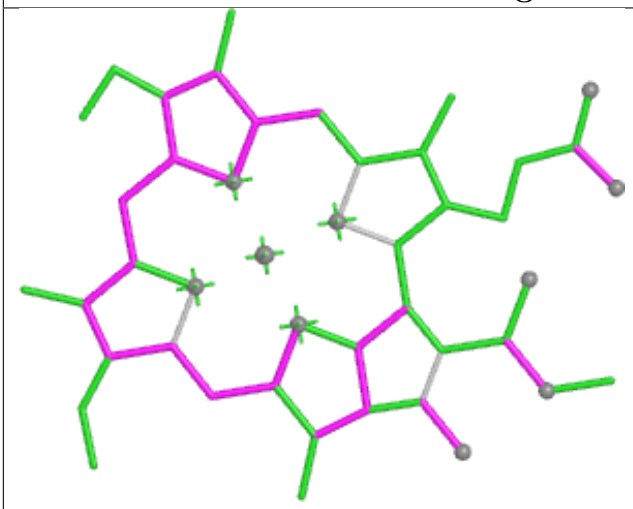


Torsions

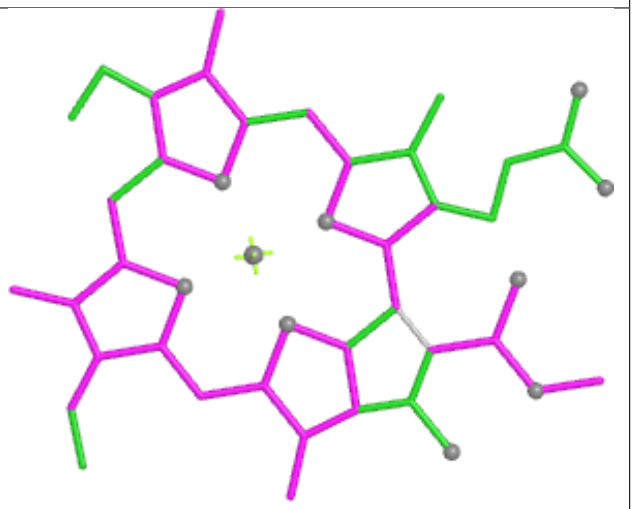


Rings

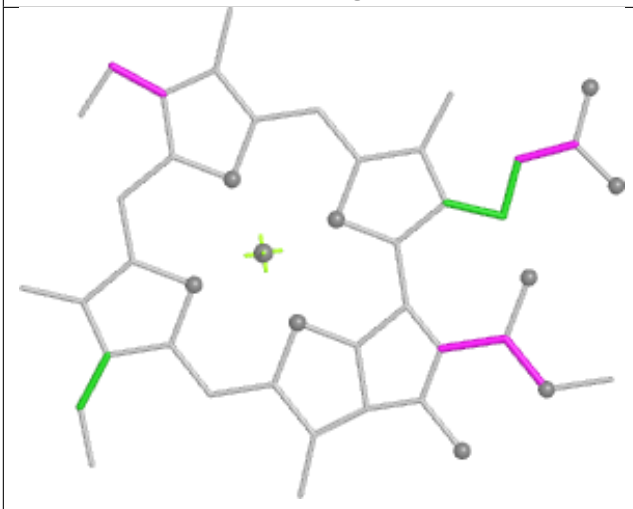
Ligand CLA cA 809



Bond lengths



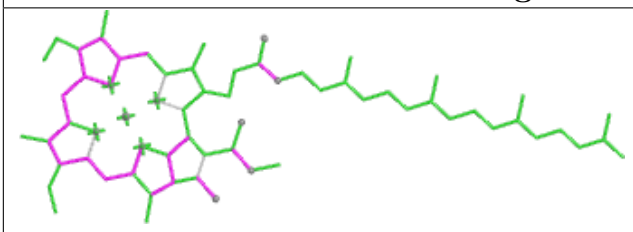
Bond angles



Torsions

Rings

Ligand CLA bB 807



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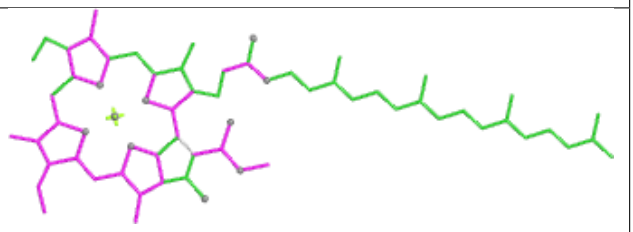
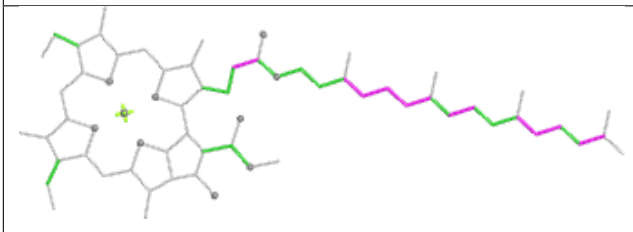
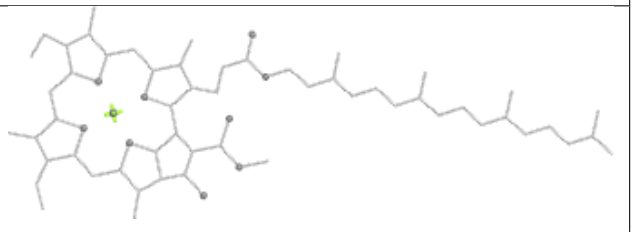


Bond angles

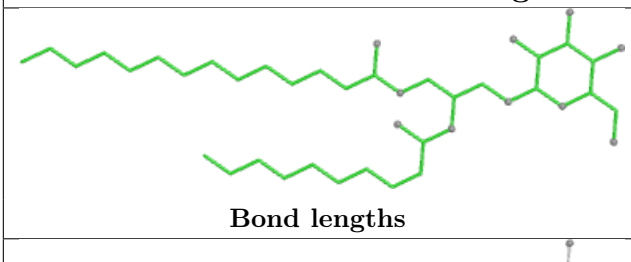


Torsions



Rings

Ligand LMG cB 849



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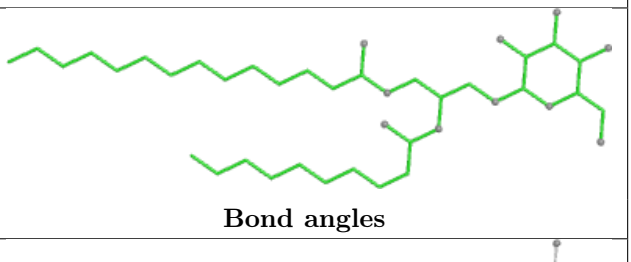
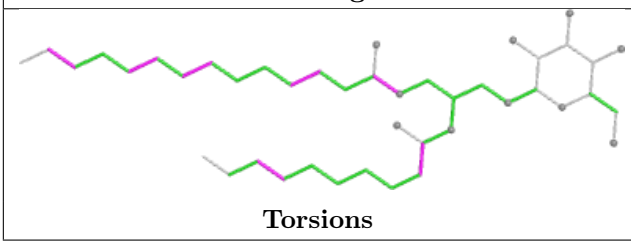


Bond angles



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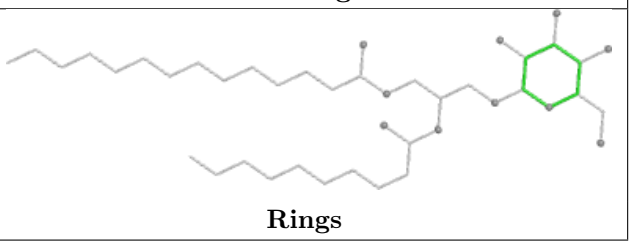
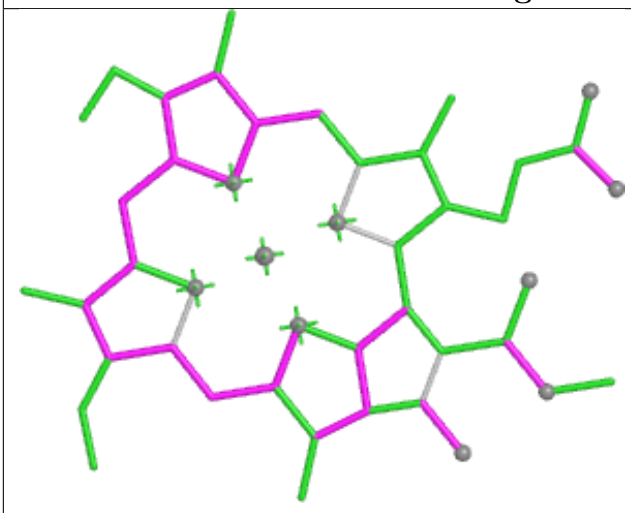


Rings

Ligand CLA bB 822



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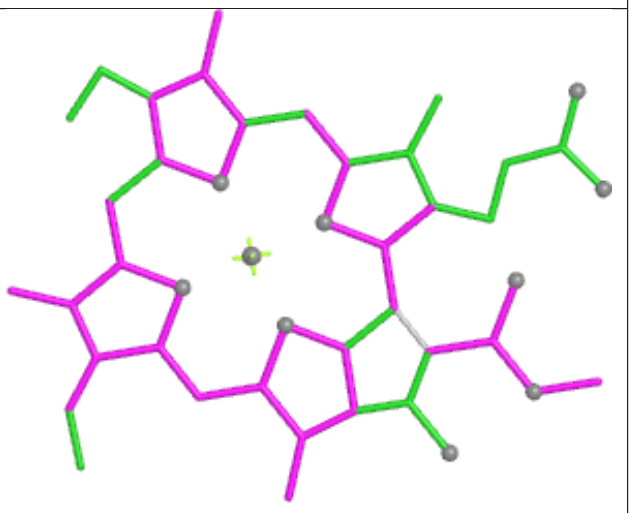
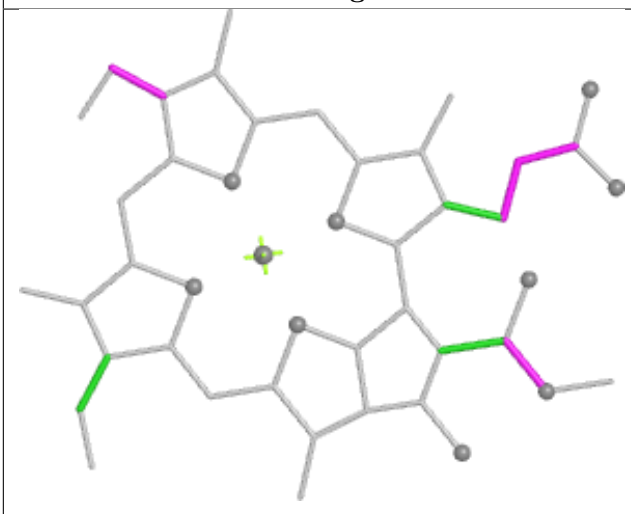


Bond angles



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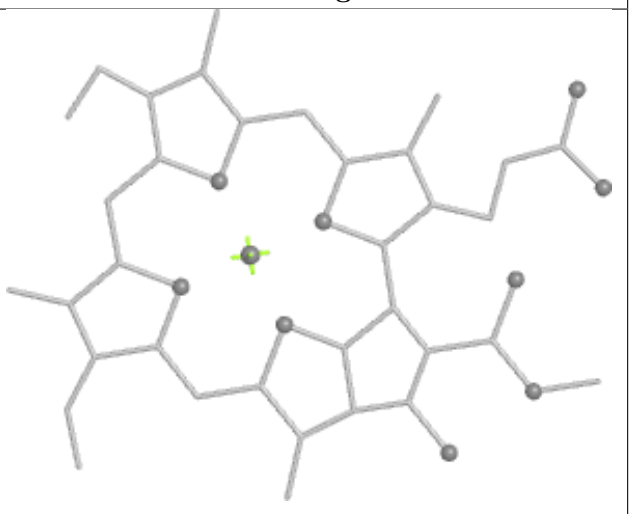
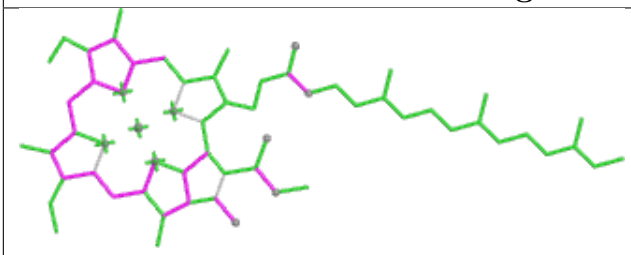


Rings

Ligand CLA cA 827



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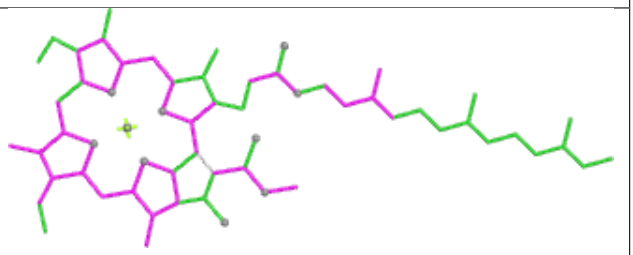
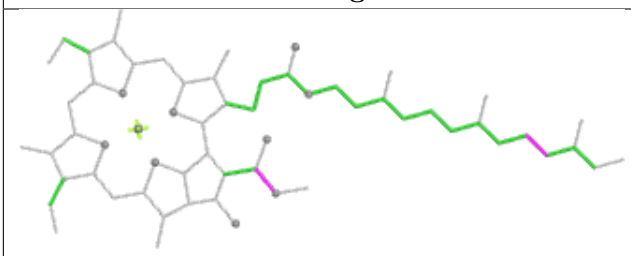


Bond angles



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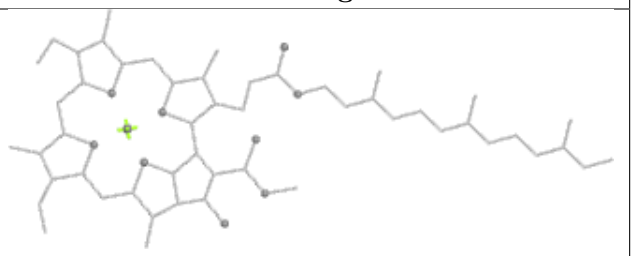
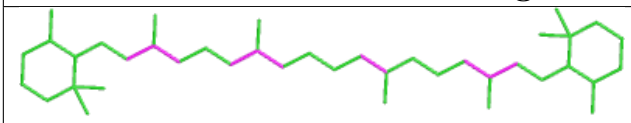


Rings

Ligand BCR cB 842



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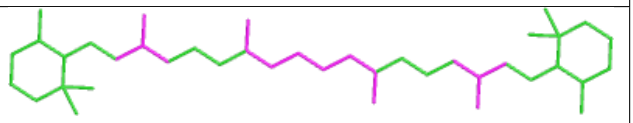
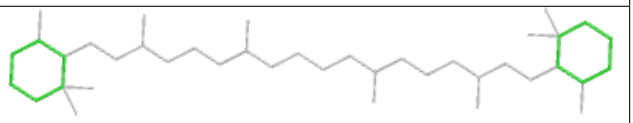


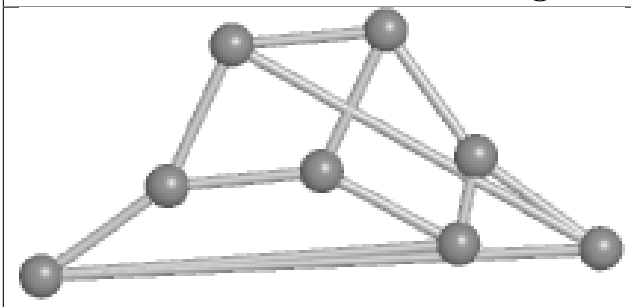
Bond angles

Torsions



Rings

Ligand SF4 C 101



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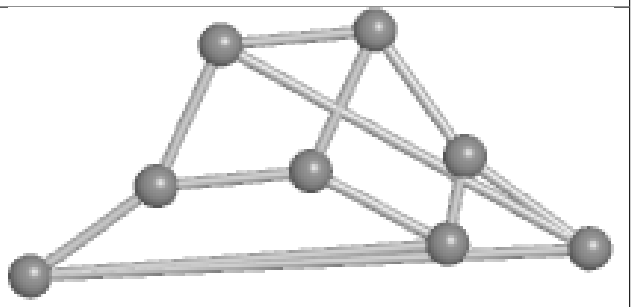
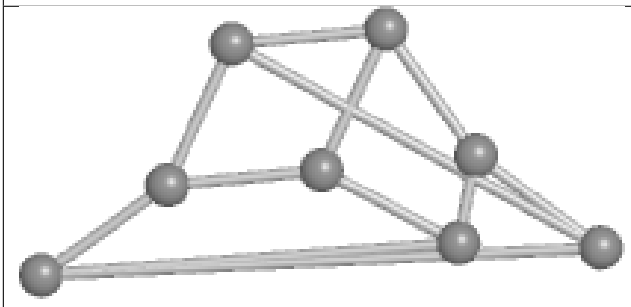


Bond angles



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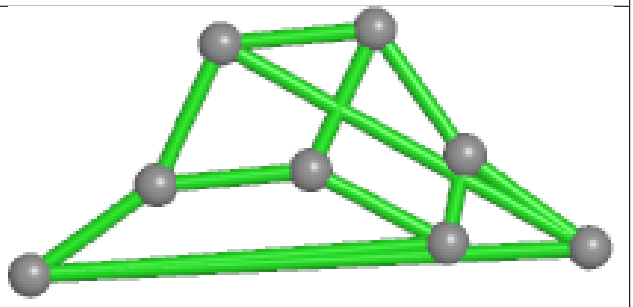
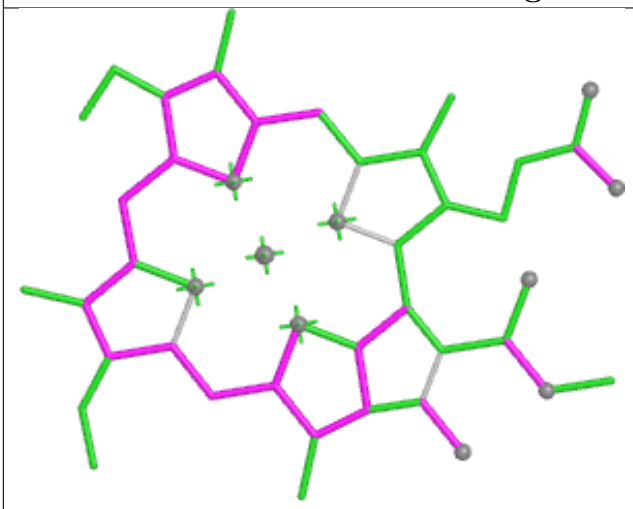


Rings

Ligand CLA B 814



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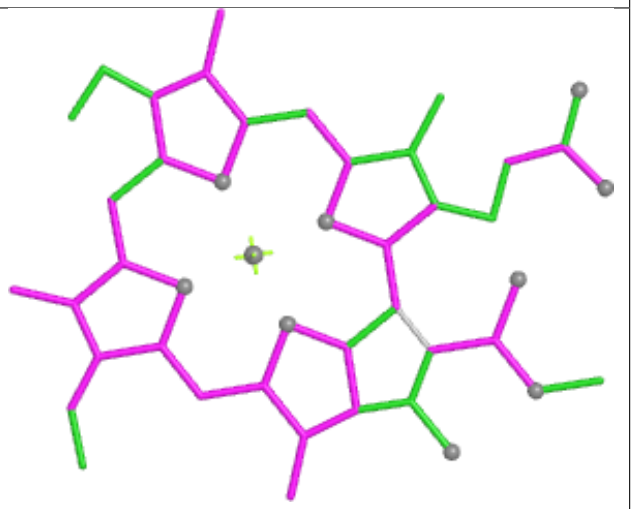
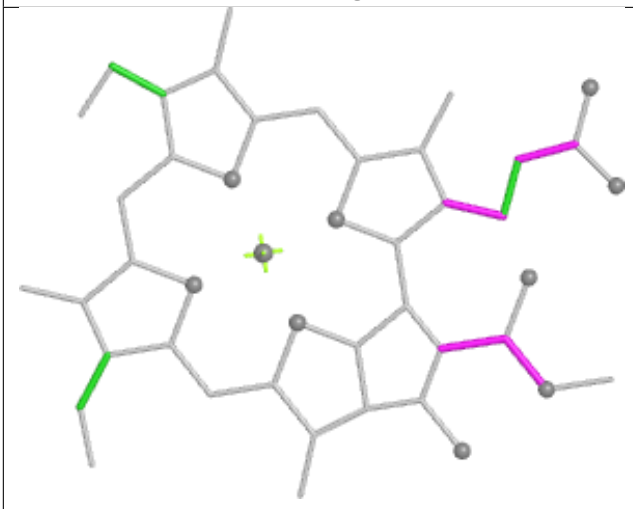


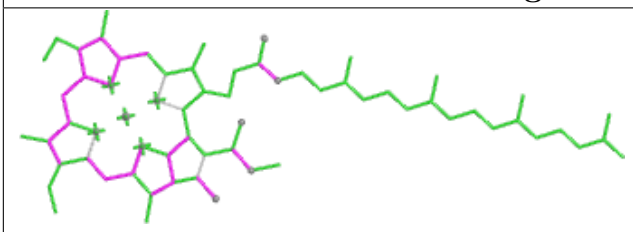
Bond angles



Torsions

Rings

Ligand CLA B 828



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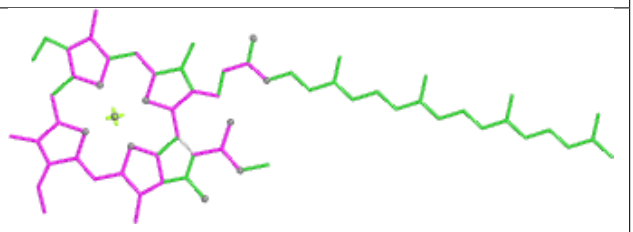

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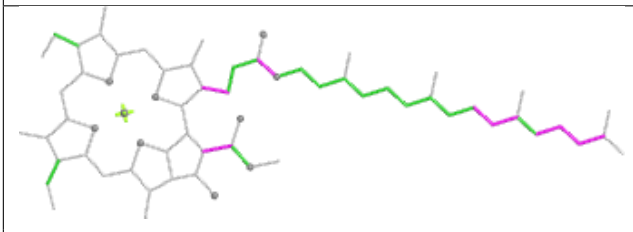

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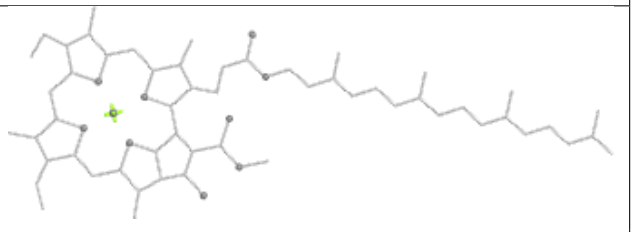
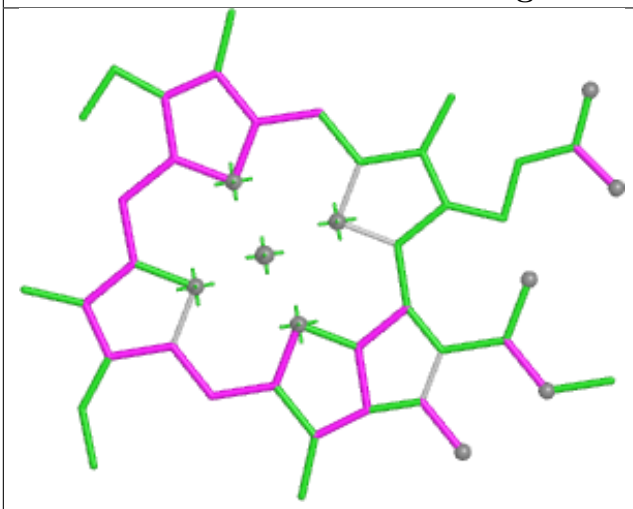


Rings

Ligand CLA cB 837



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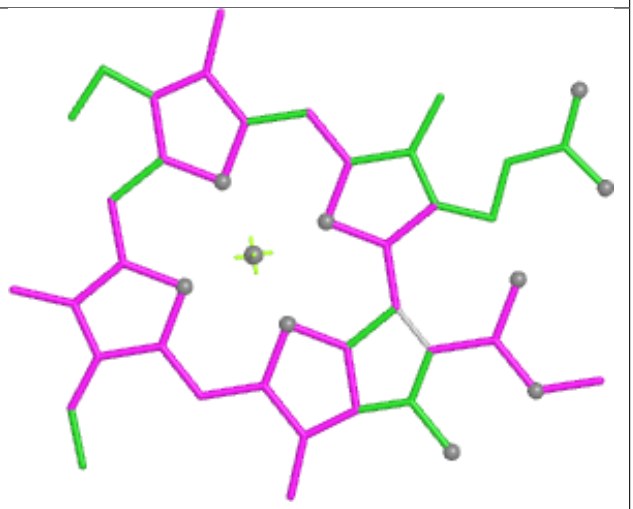
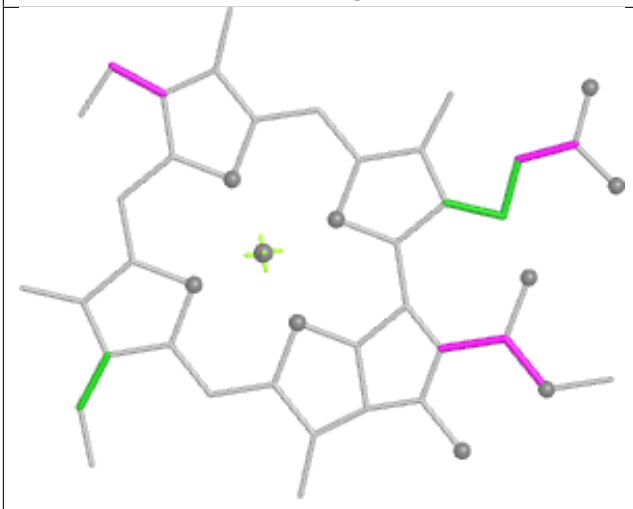


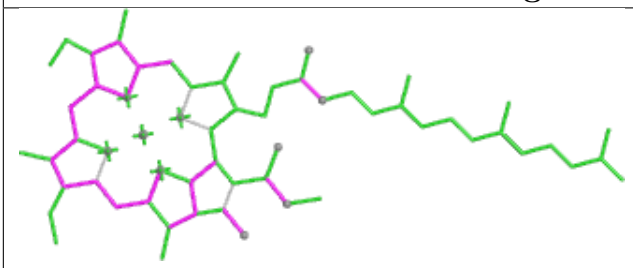
Bond angles



Torsions

Rings

Ligand CLA A 828



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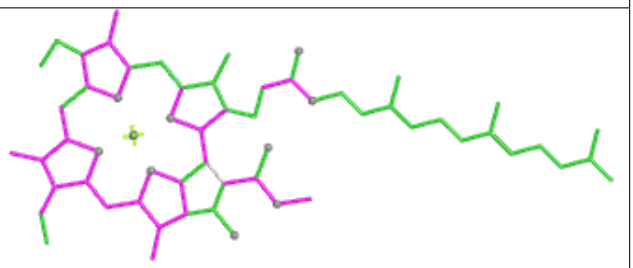
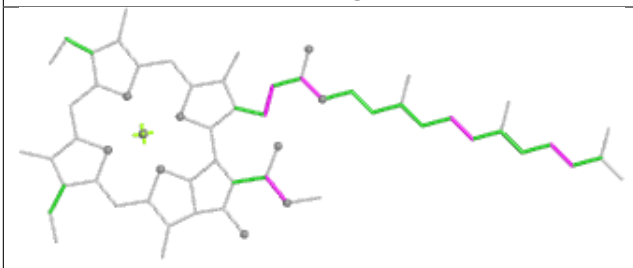
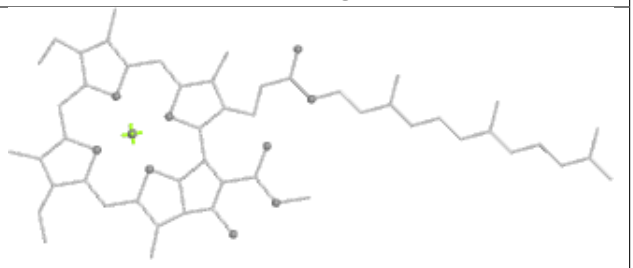


Bond angles

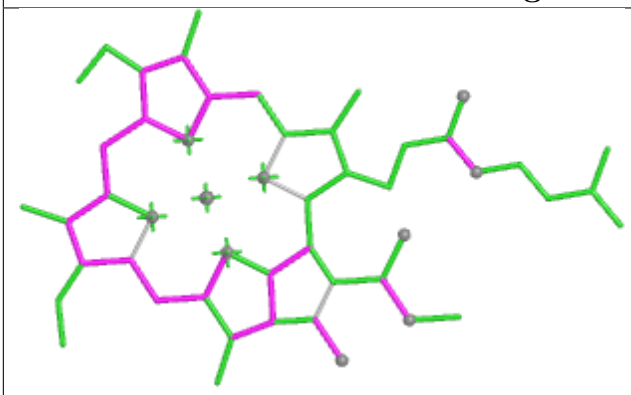


Torsions



Rings

Ligand CLA A 825



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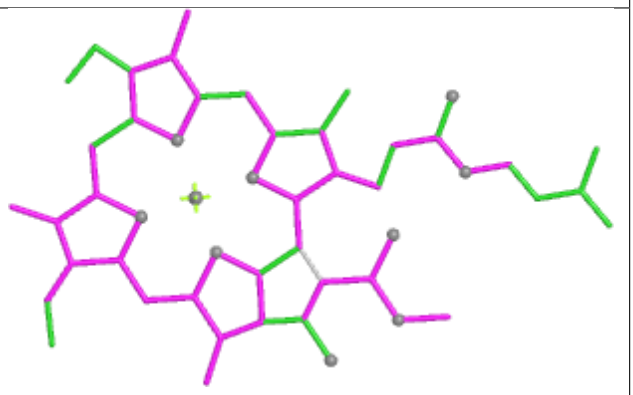
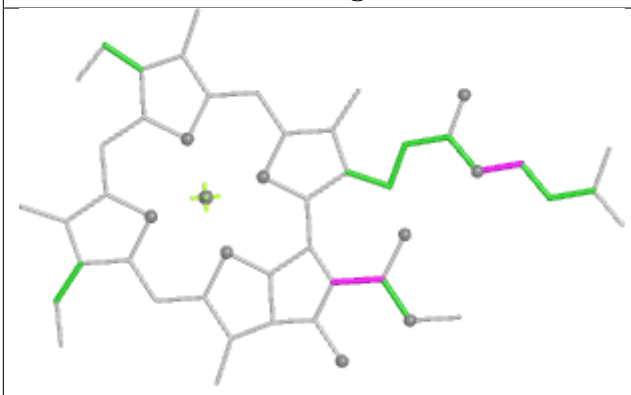


Bond angles



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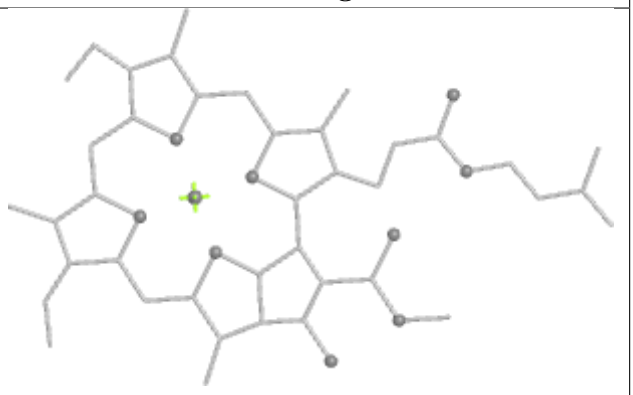
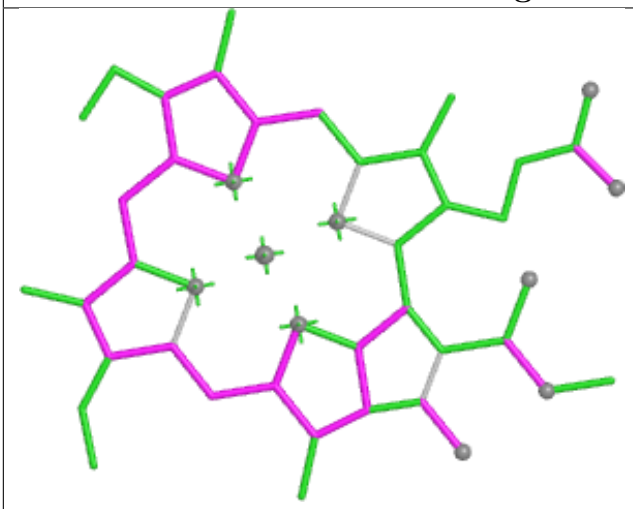


Rings

Ligand CLA bB 814



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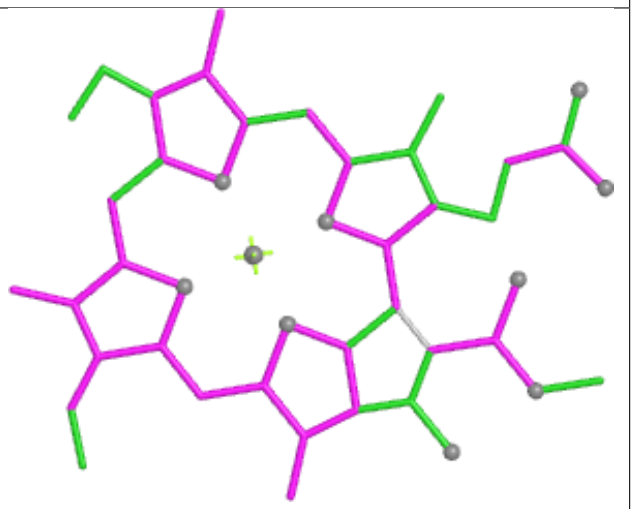
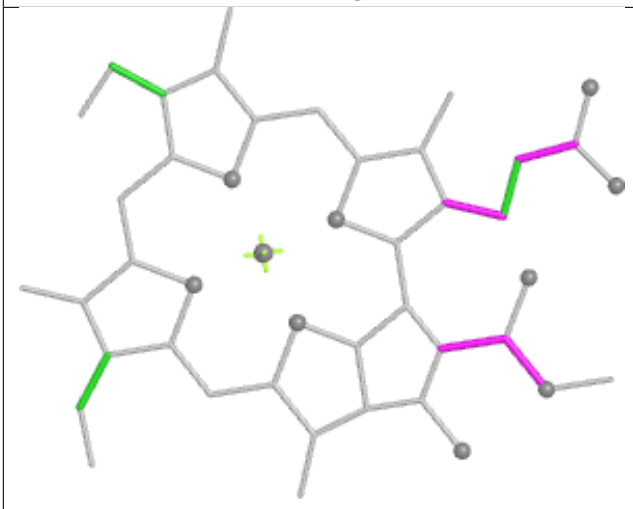


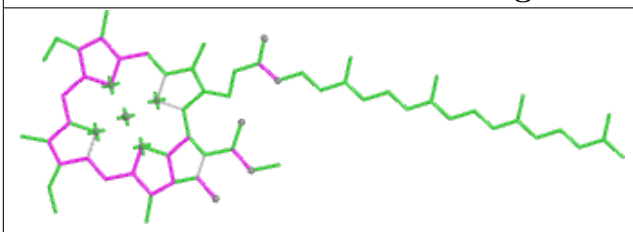
Bond angles



Torsions

Rings

Ligand CLA bB 805



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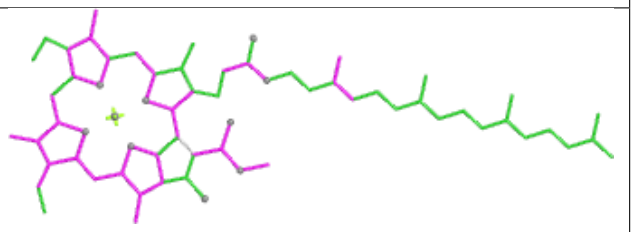
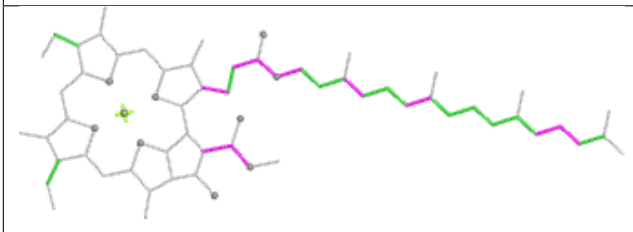
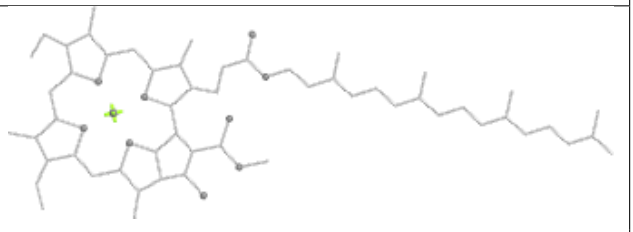


Bond angles

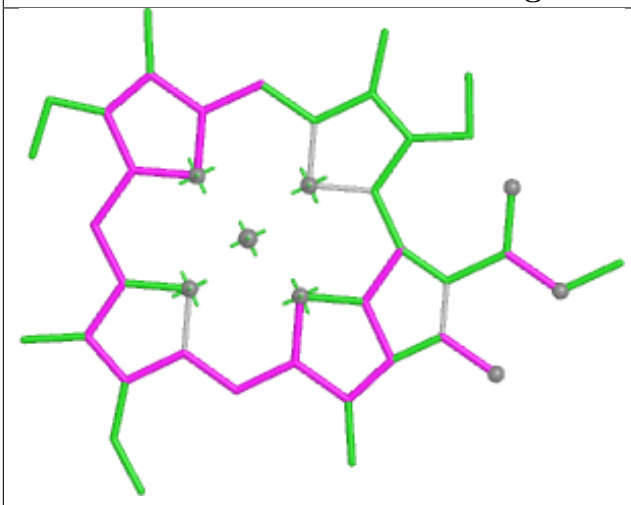


Torsions



Rings

Ligand CLA B 830



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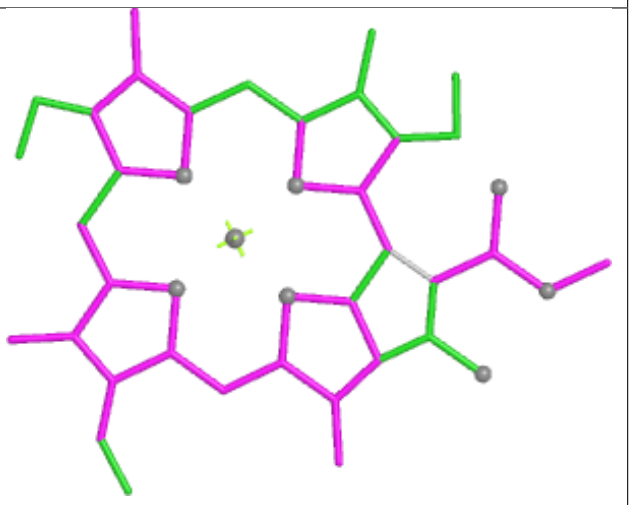
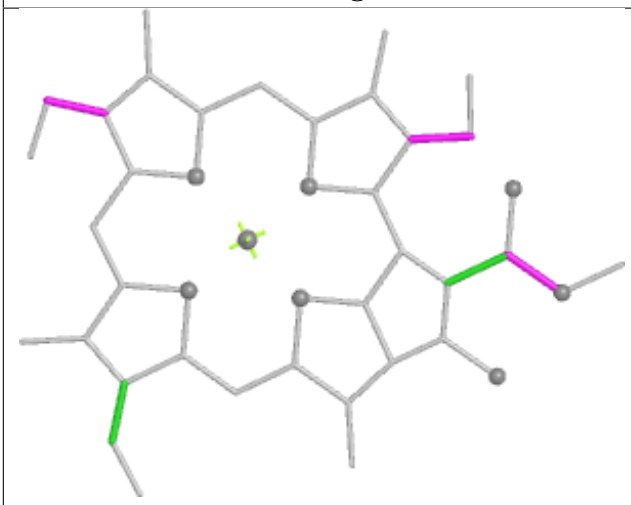


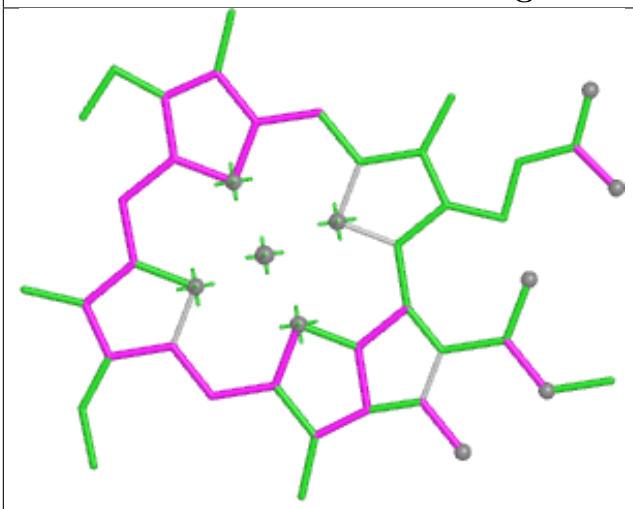
Bond angles



Torsions

Rings

Ligand CLA cA 819



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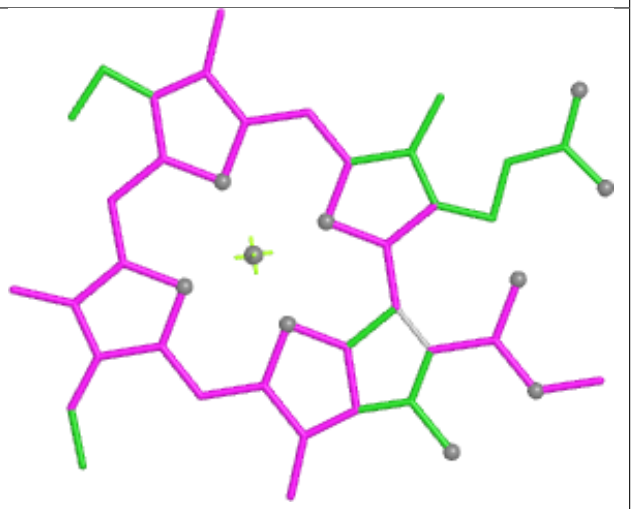
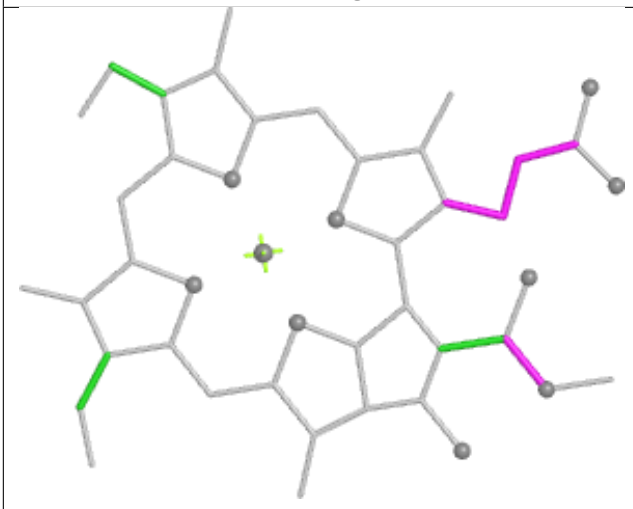


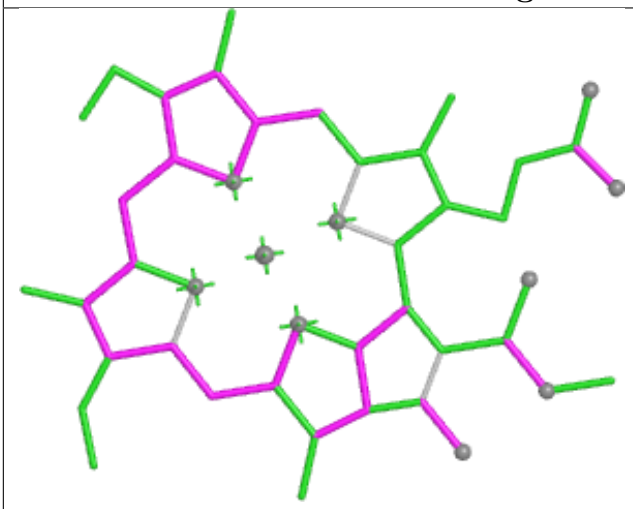
Bond angles



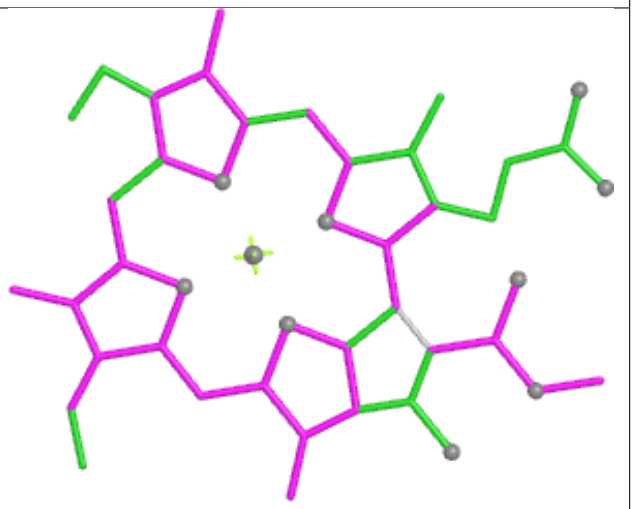
Torsions

Rings

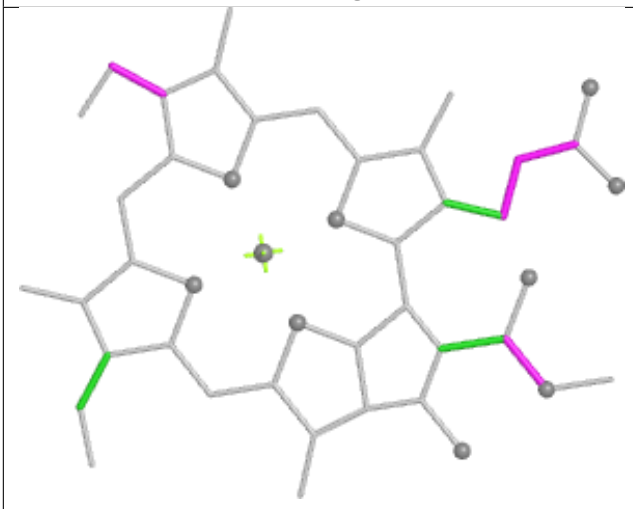
Ligand CLA cB 823



Bond lengths



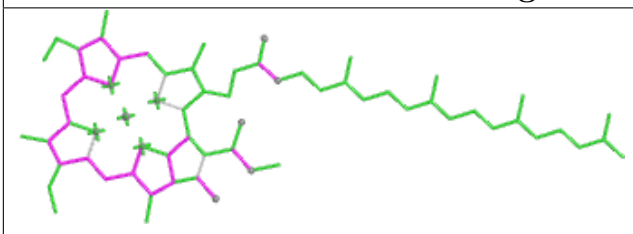
Bond angles



Torsions

Rings

Ligand CLA cL 203



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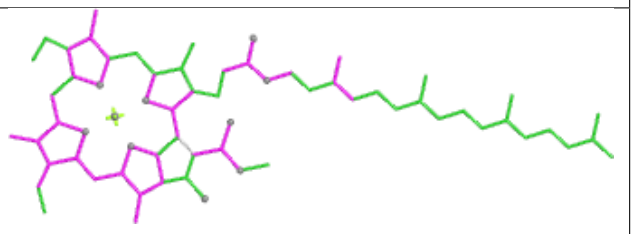
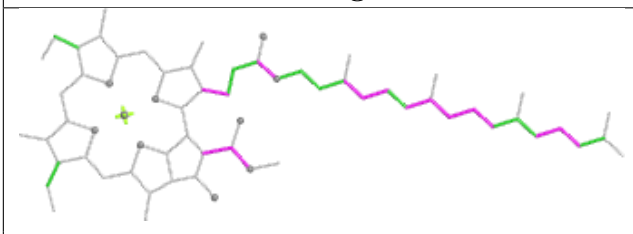
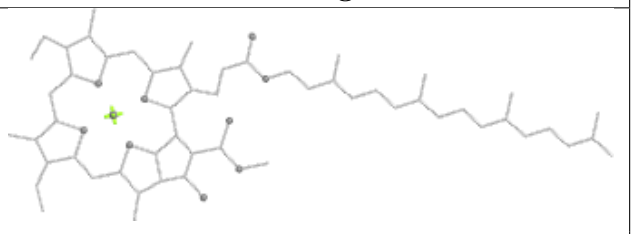


Bond angles

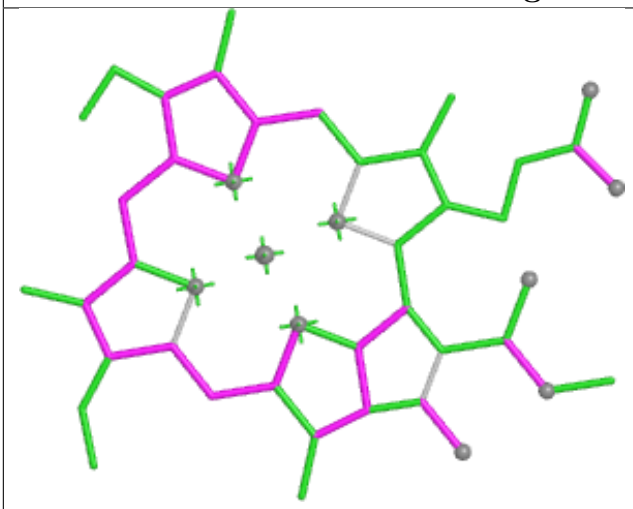


Torsions



Rings

Ligand CLA A 823



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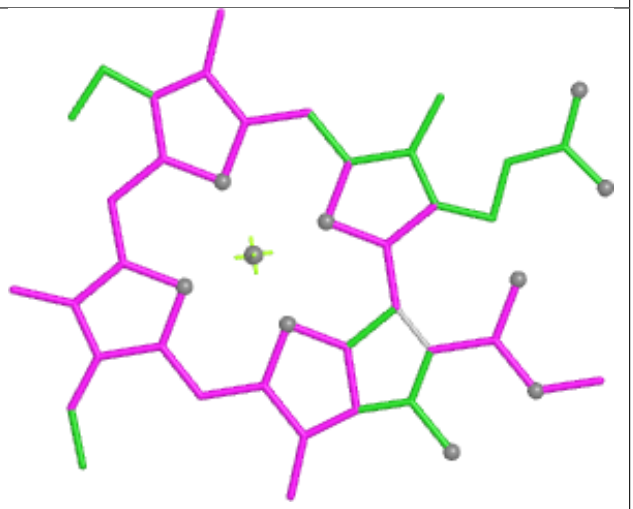
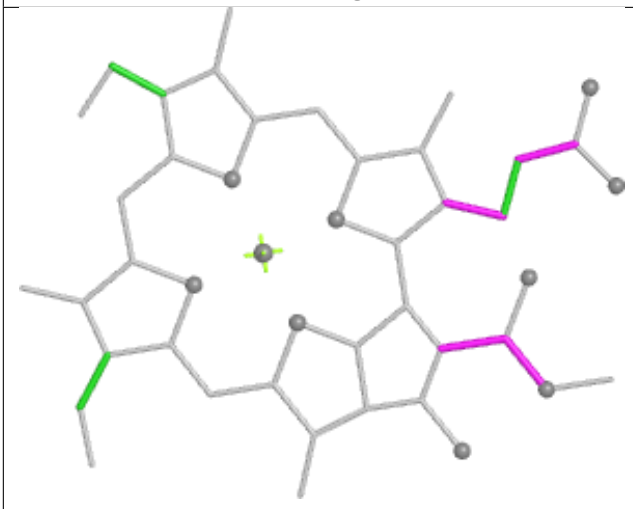


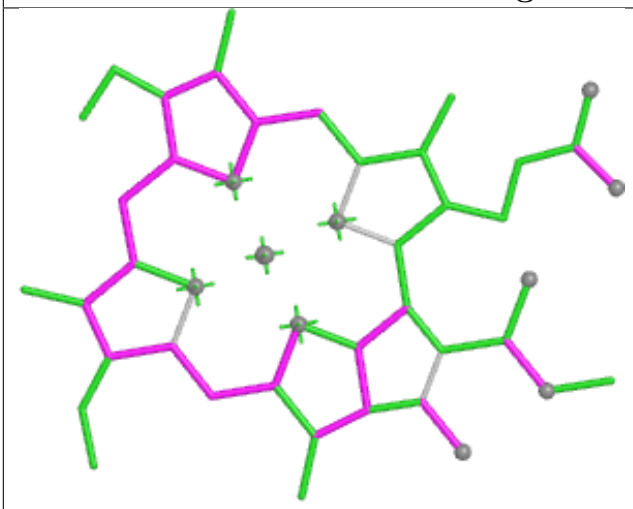
Bond angles



Torsions

Rings

Ligand CLA cB 821



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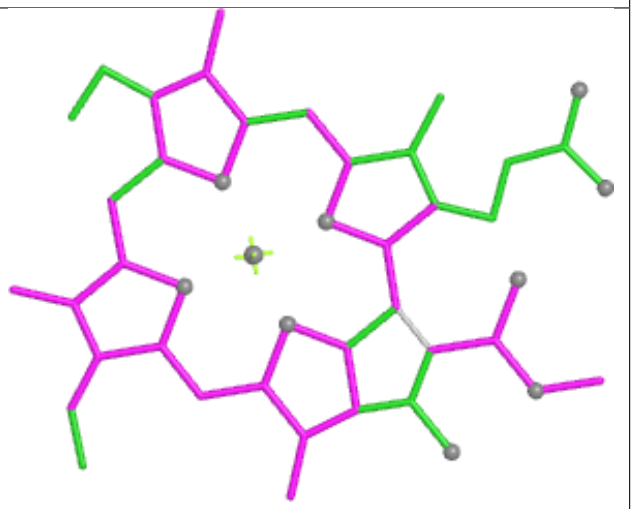
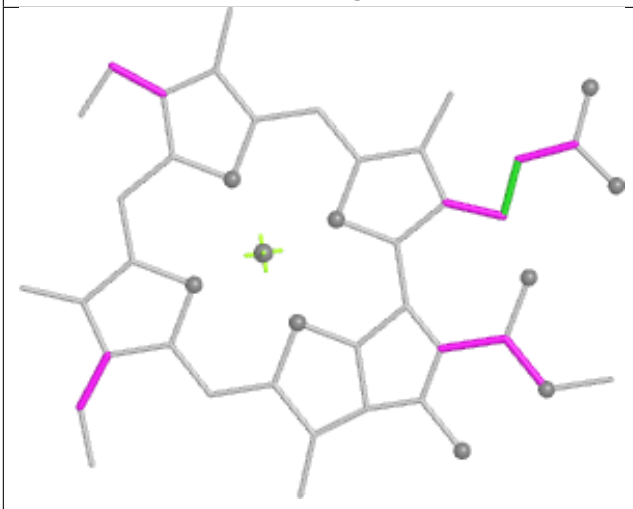


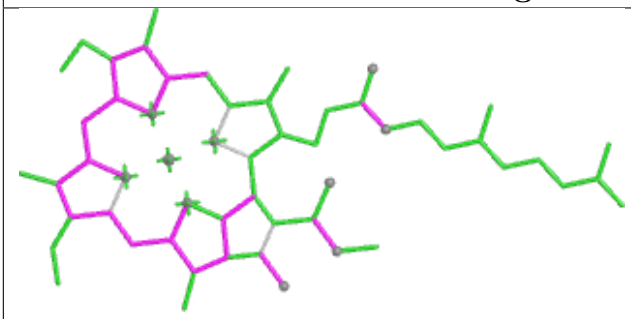
Bond angles



Torsions

Rings

Ligand CLA bB 817



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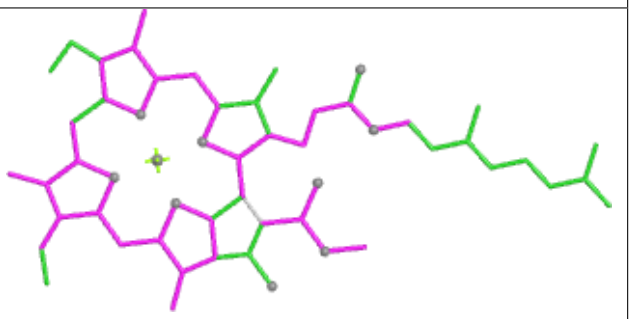
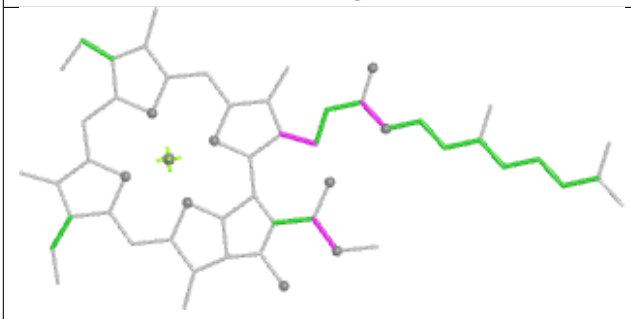


Bond angles



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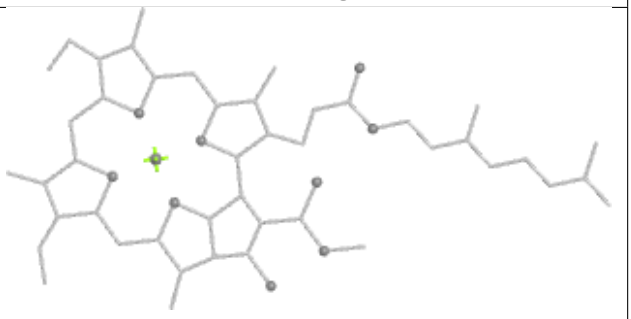
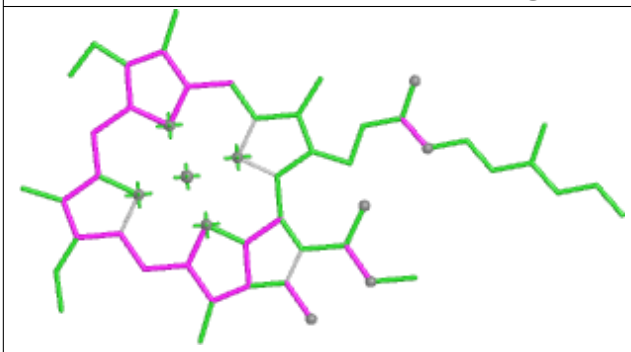


Rings

Ligand CLA B 815



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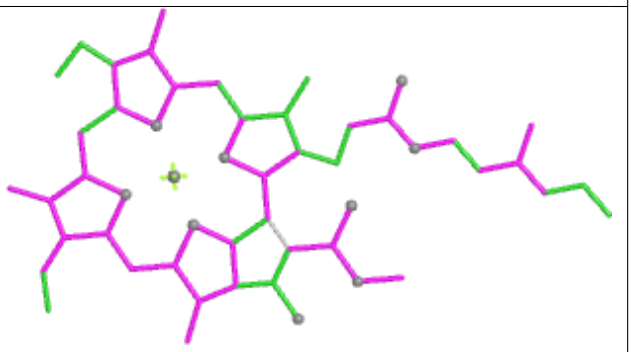
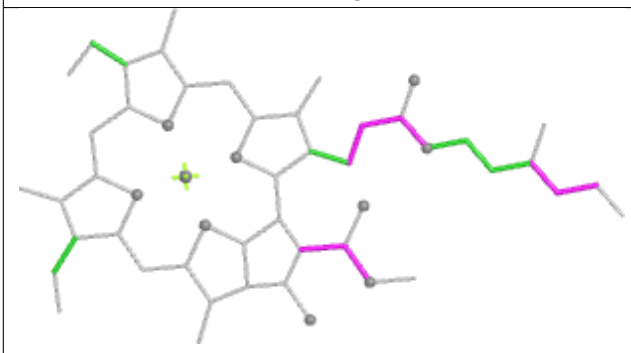


Bond angles



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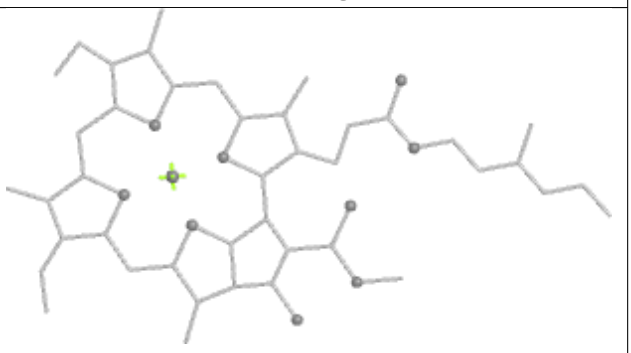
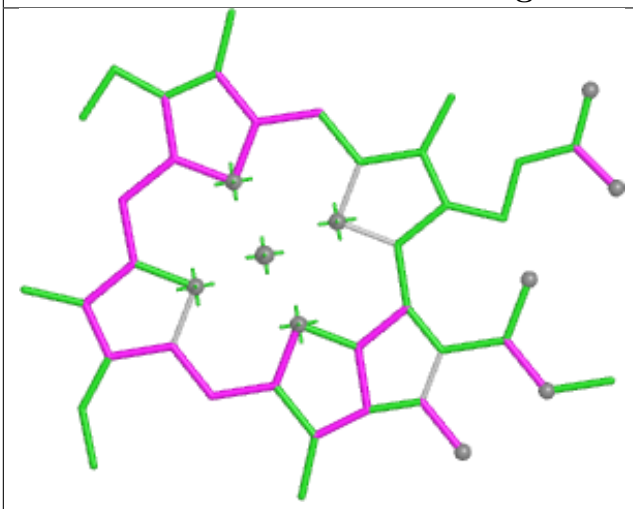


Rings

Ligand CLA cA 838



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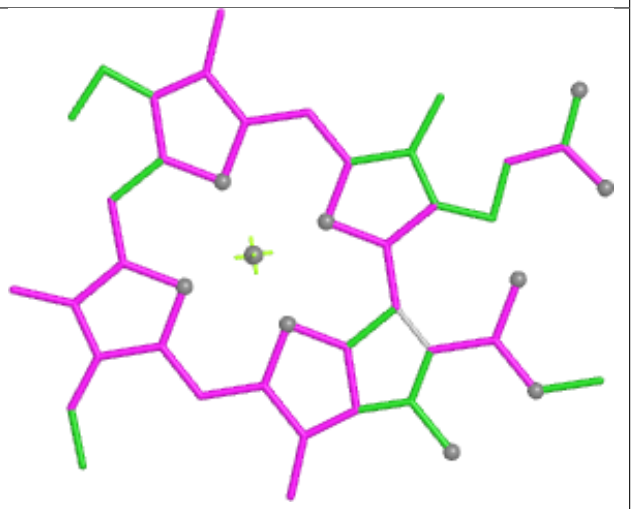

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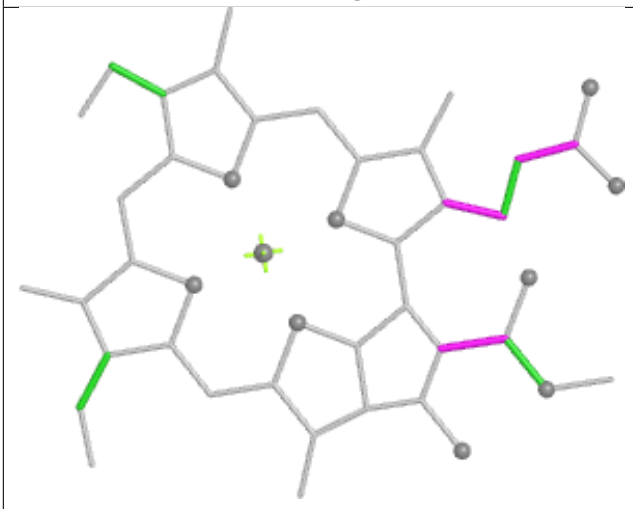
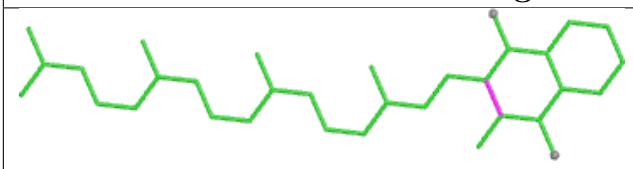


Torsions

Rings

Ligand PQN cB 841



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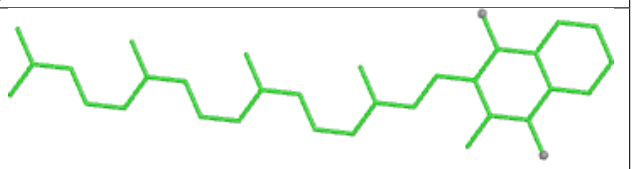
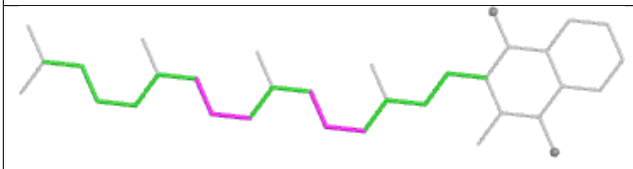
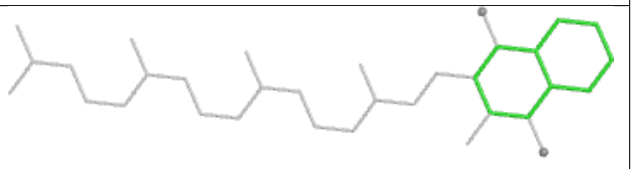


Bond angles

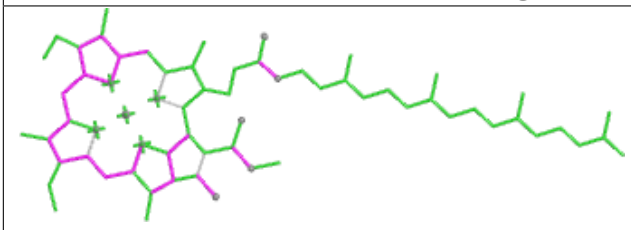


Torsions



Rings

Ligand CLA bB 831



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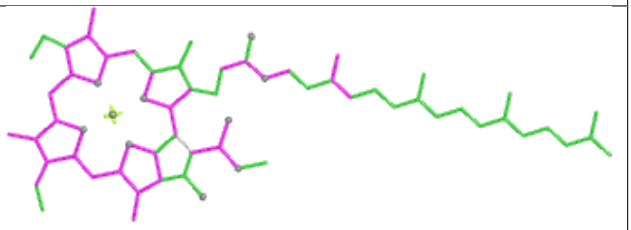
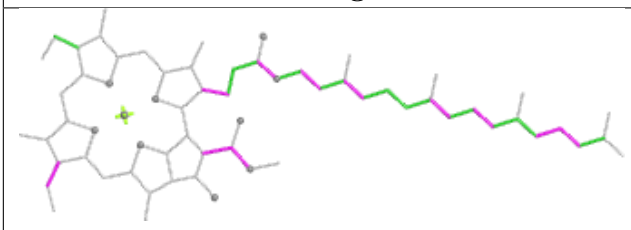


Bond angles



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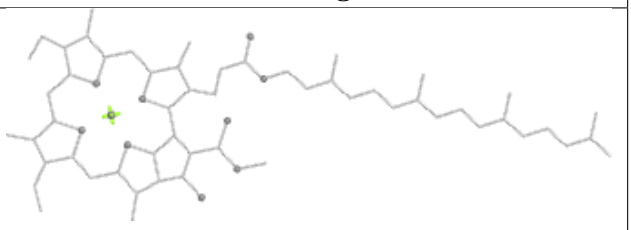
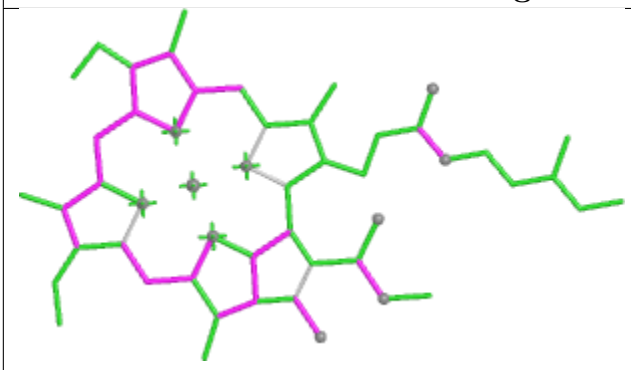


Rings

Ligand CLA bA 836



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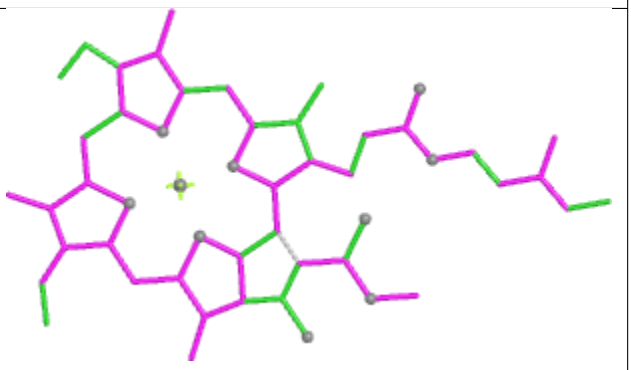

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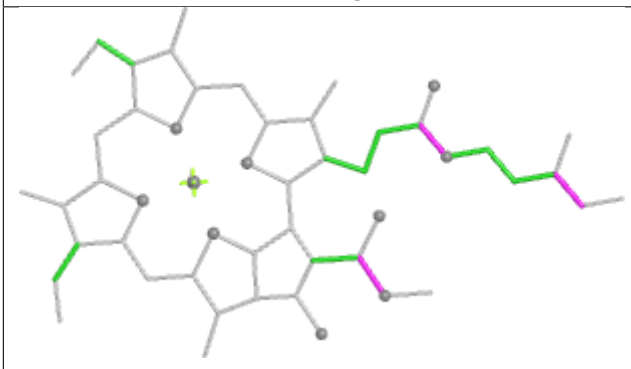

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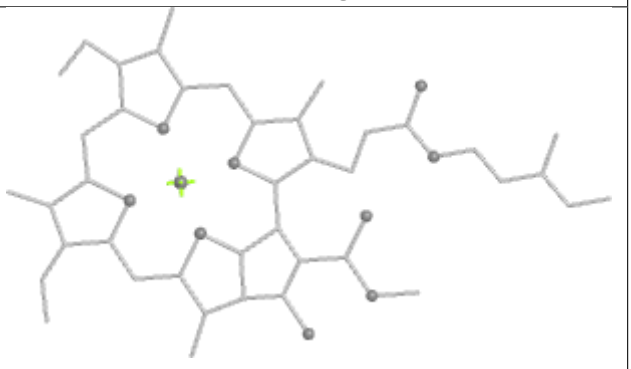
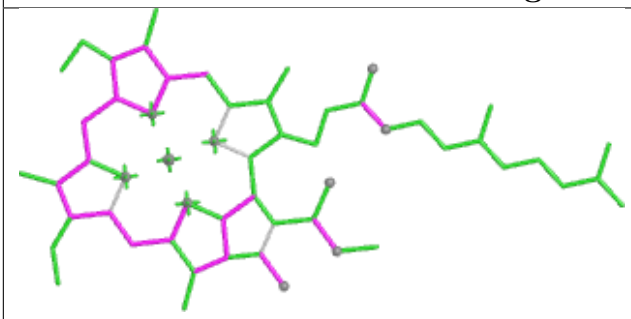


Rings

Ligand CLA B 803



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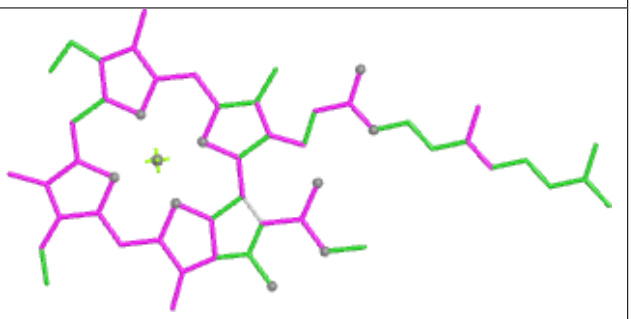
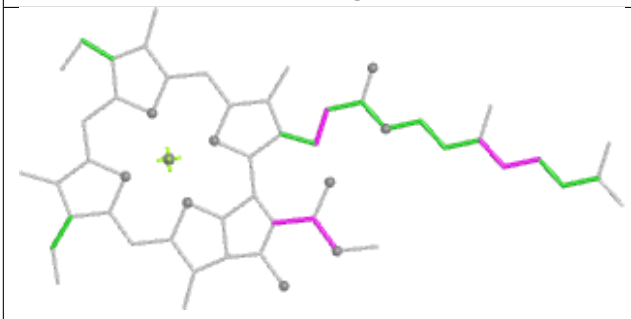


Bond angles



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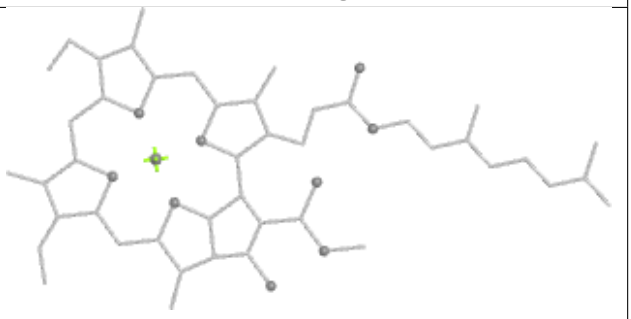
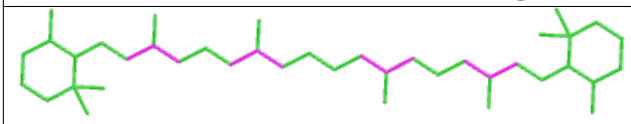


Rings

Ligand BCR bA 848



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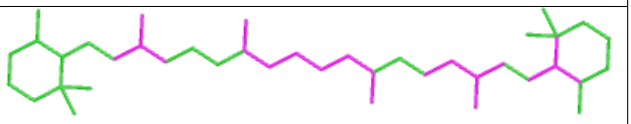
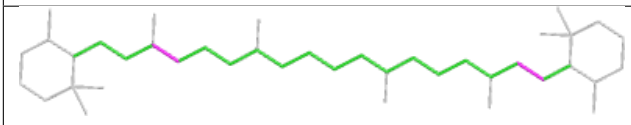
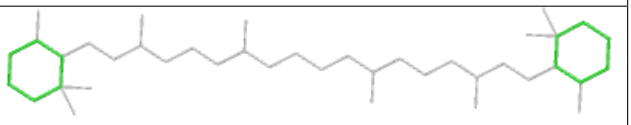


Bond angles

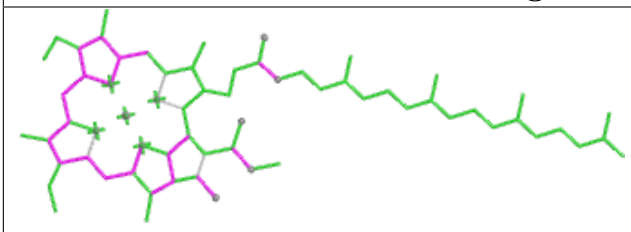


Torsions



Rings

Ligand CLA L 204



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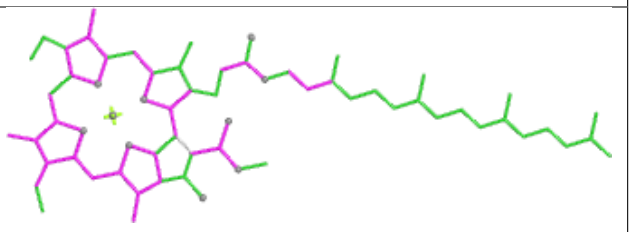
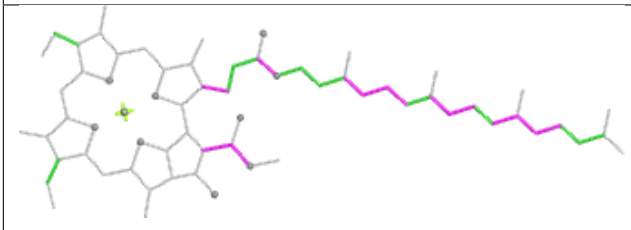


Bond angles



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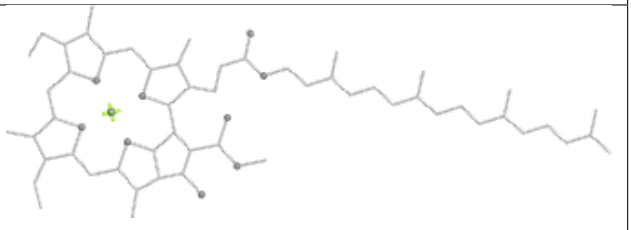
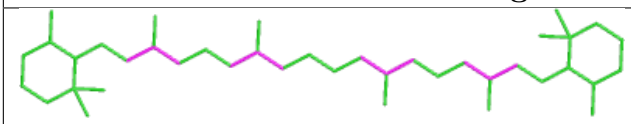


Rings

Ligand BCR cM 101



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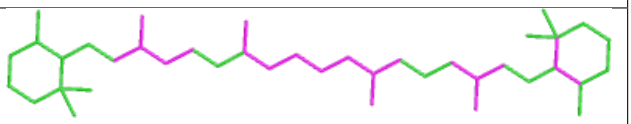
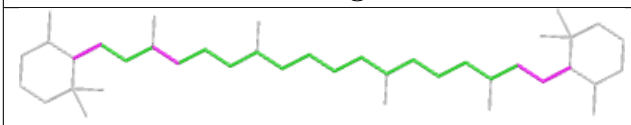
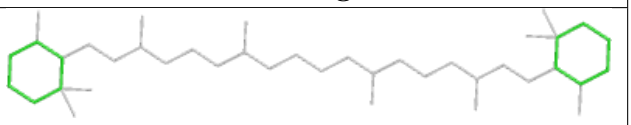


Bond angles

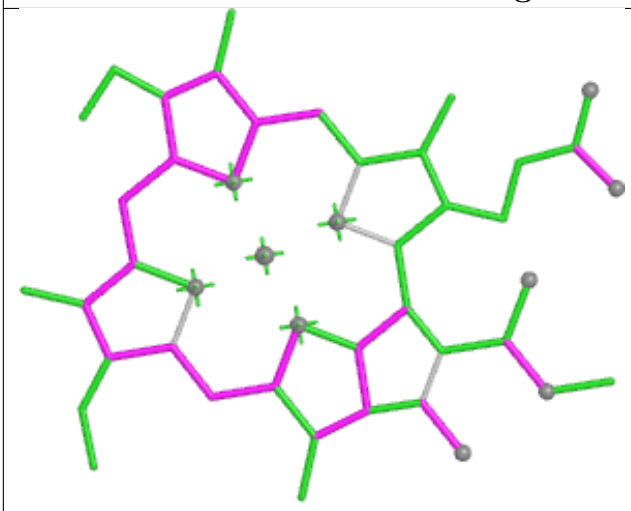


Torsions

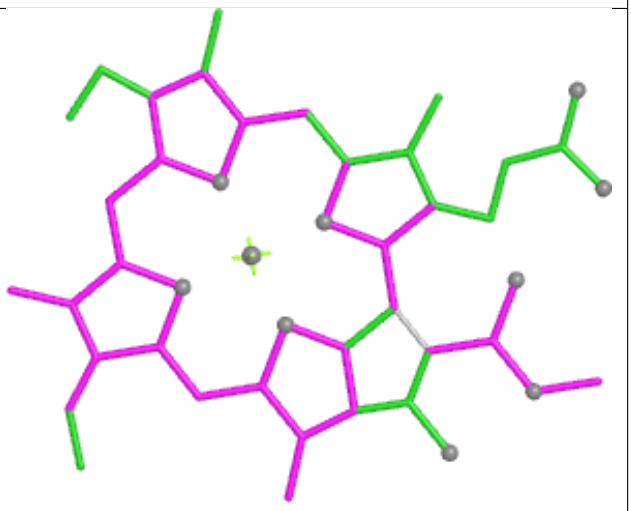


Rings

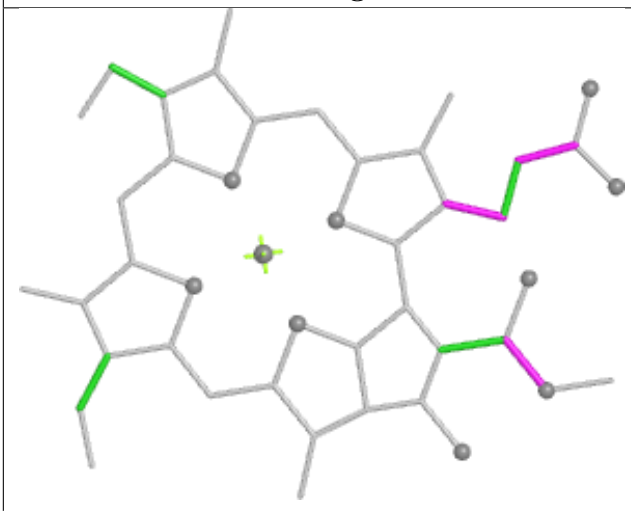
Ligand CLA bB 851



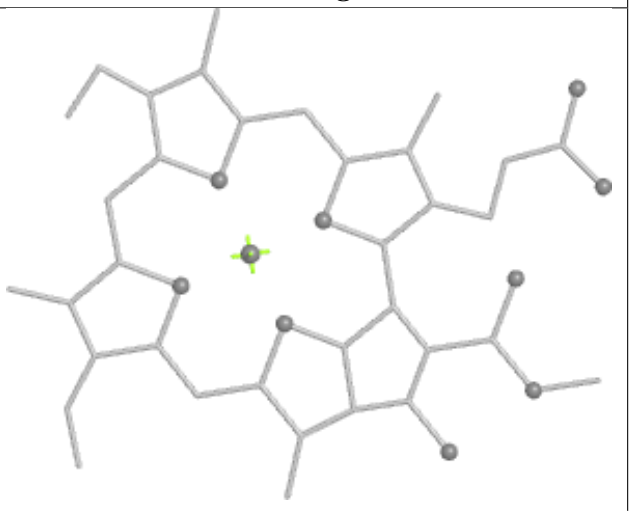
Bond lengths



Bond angles

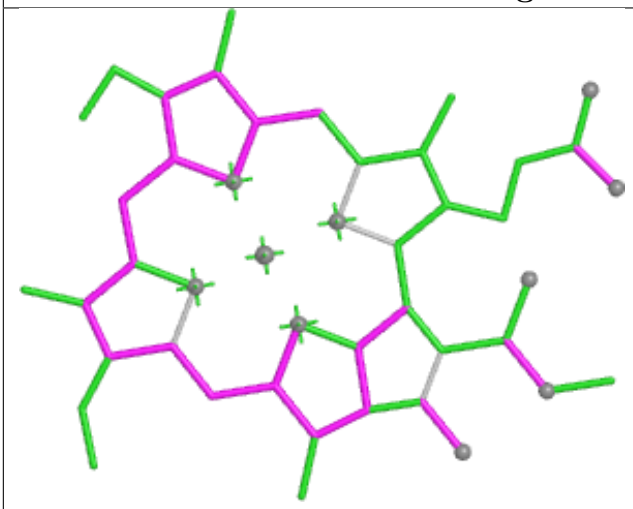


Torsions



Rings

Ligand CLA cB 822



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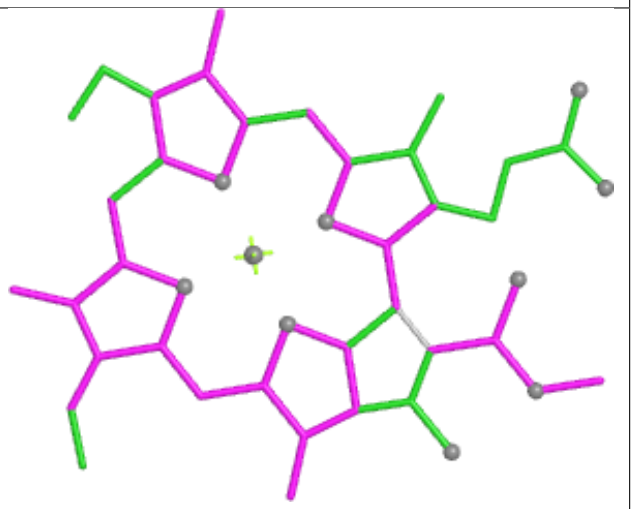
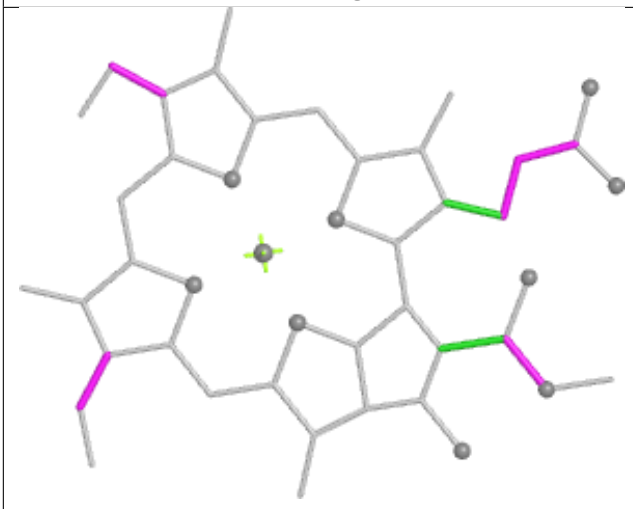


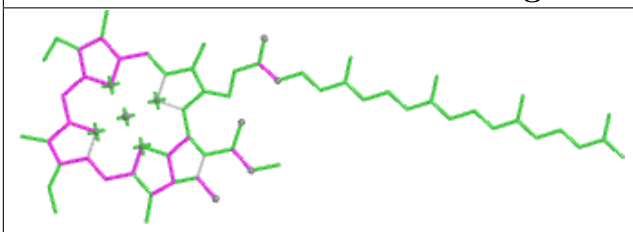
Bond angles



Torsions

Rings

Ligand CLA A 833



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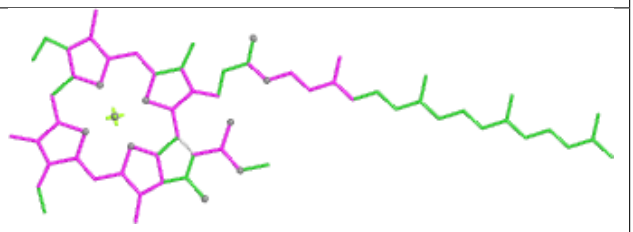
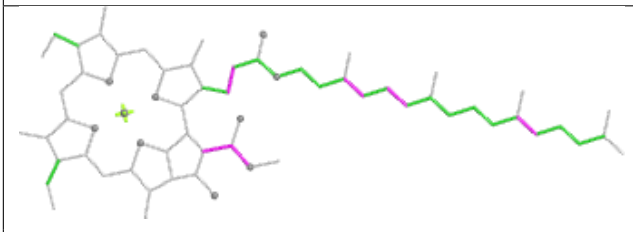
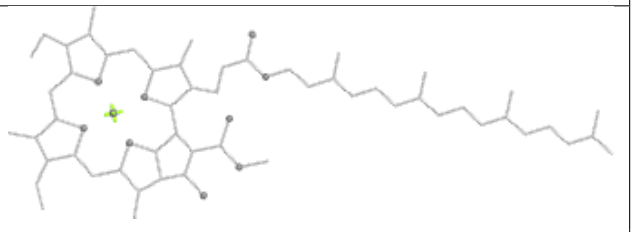


Bond angles

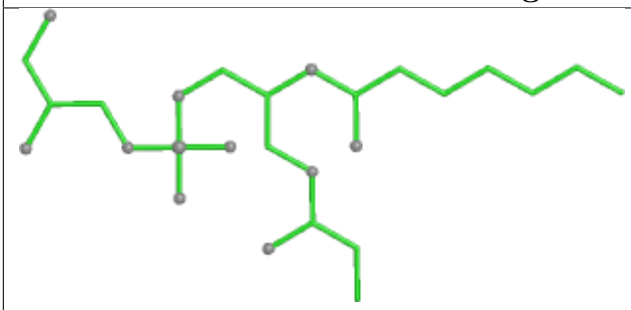


Torsions



Rings

Ligand LHG A 851



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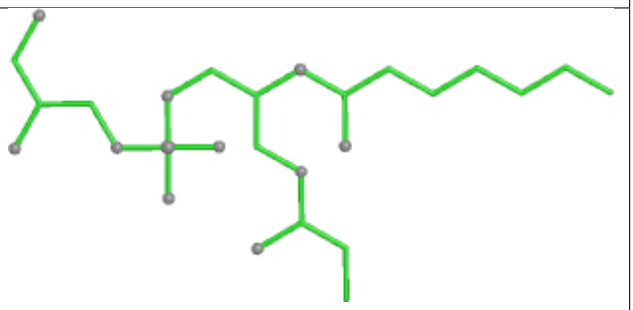
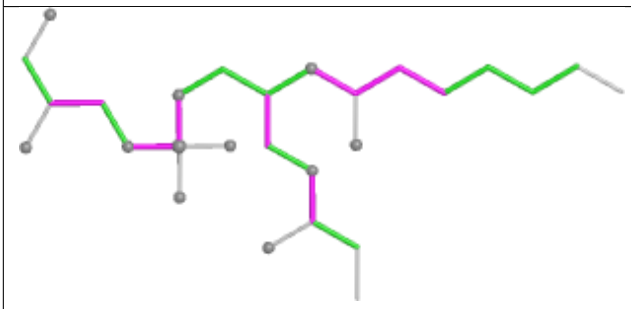
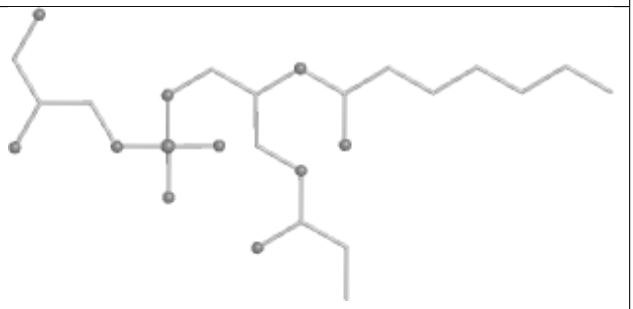


Bond angles

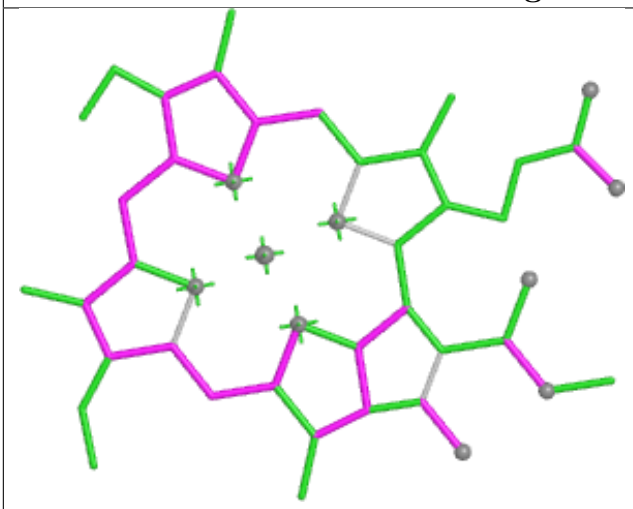


Torsions



Rings

Ligand CLA B 822



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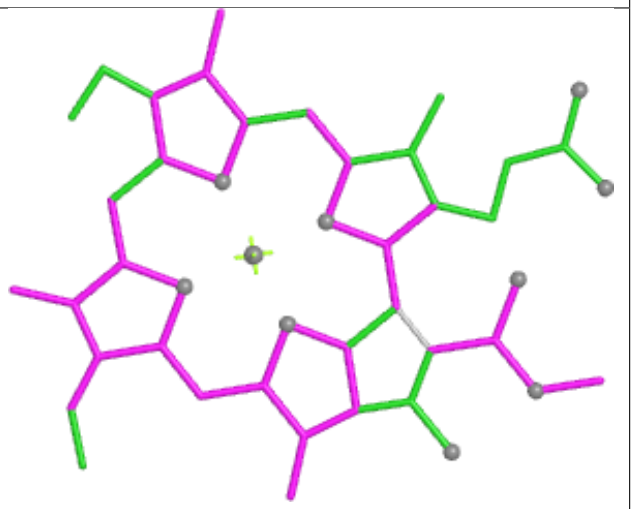
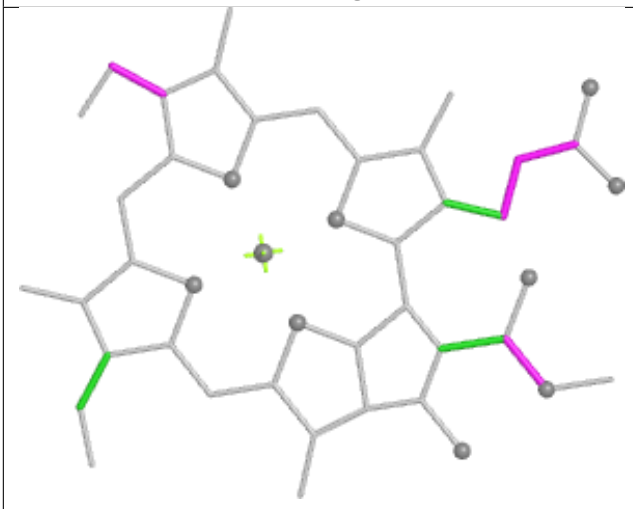


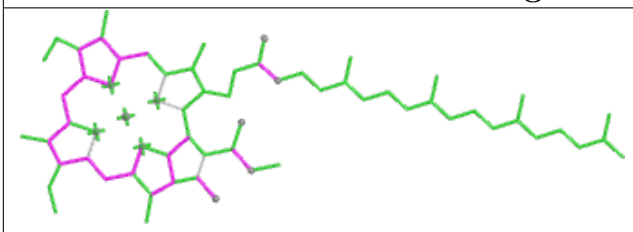
Bond angles



Torsions

Rings

Ligand CLA B 831



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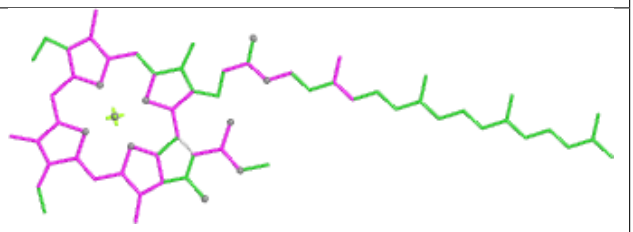
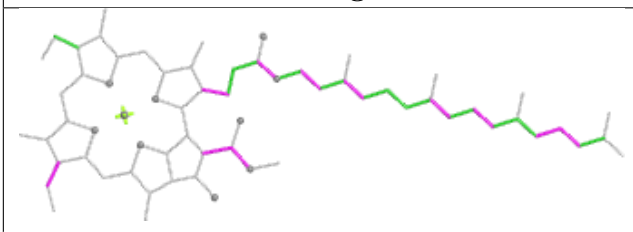


Bond angles



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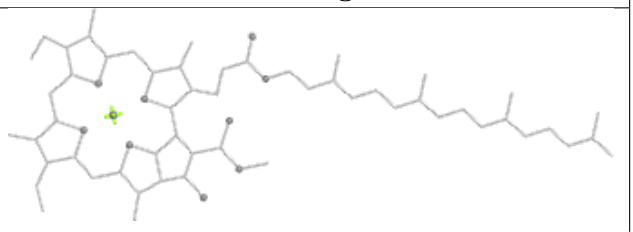
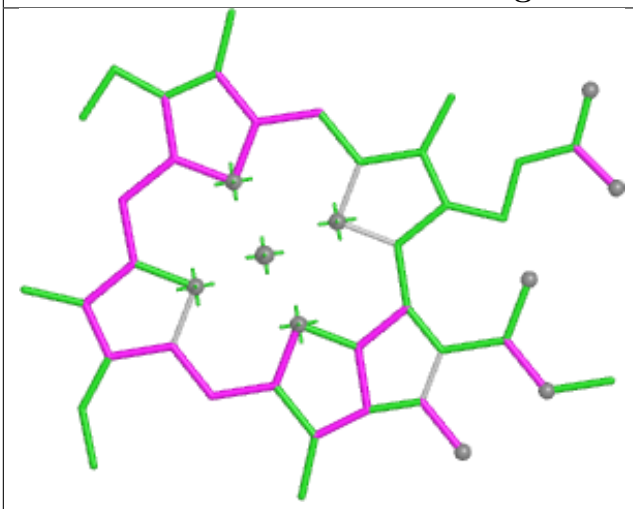


Rings

Ligand CLA bB 832



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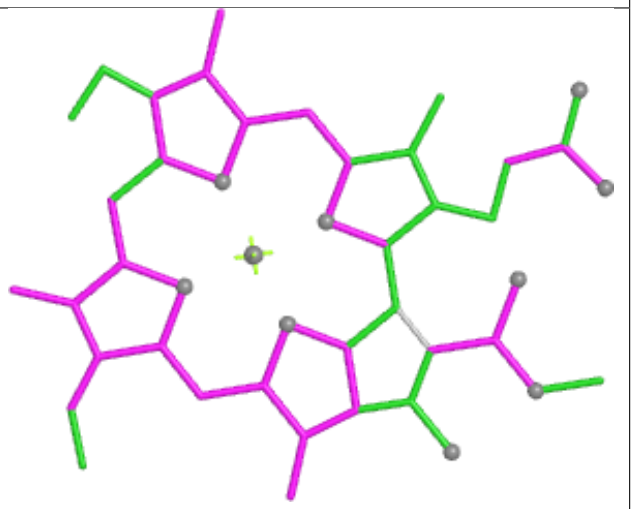
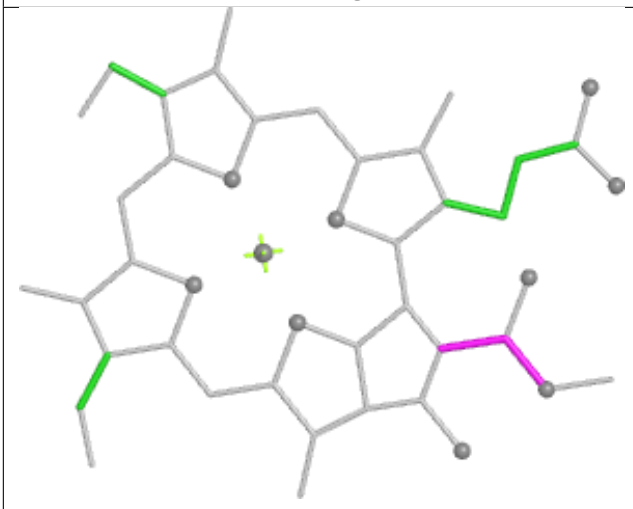


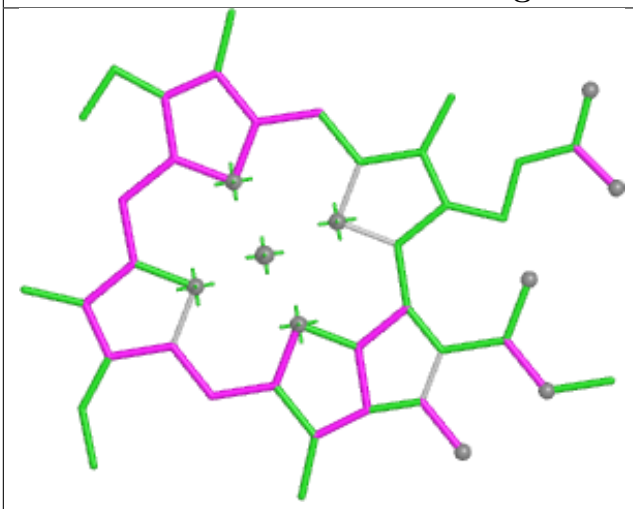
Bond angles



Torsions

Rings

Ligand CLA bA 834



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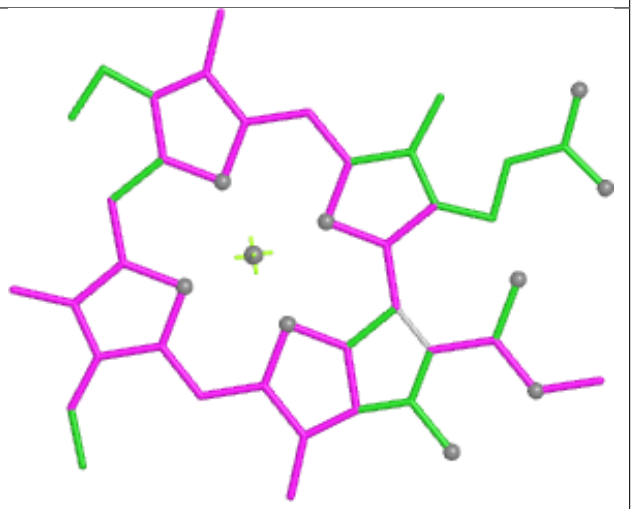
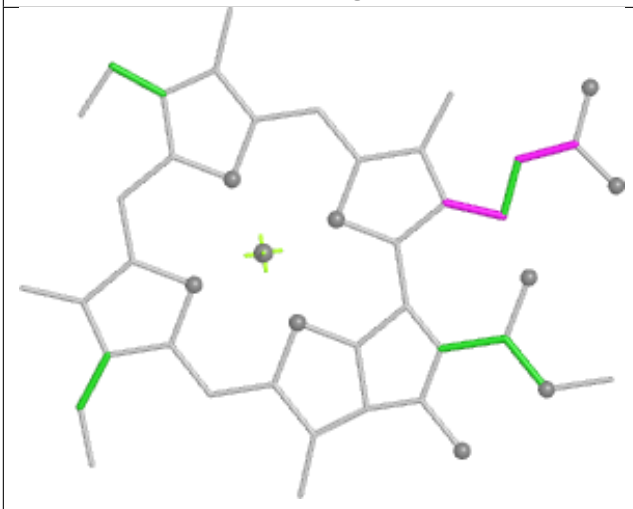


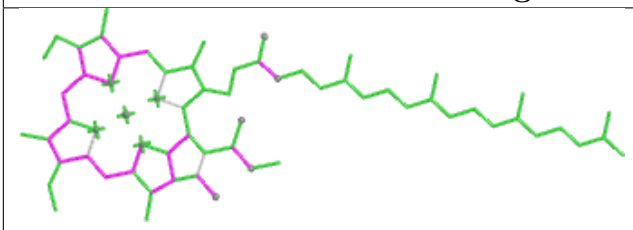
Bond angles



Torsions

Rings

Ligand CLA bA 841



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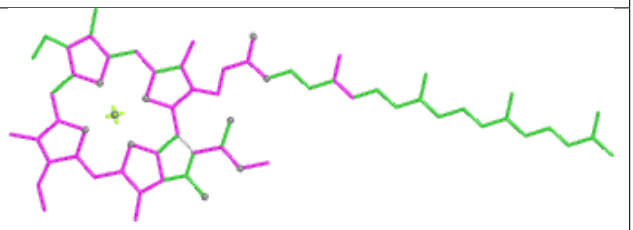
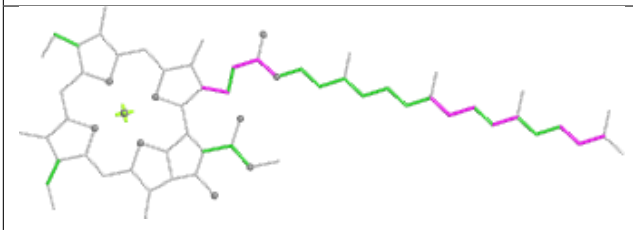
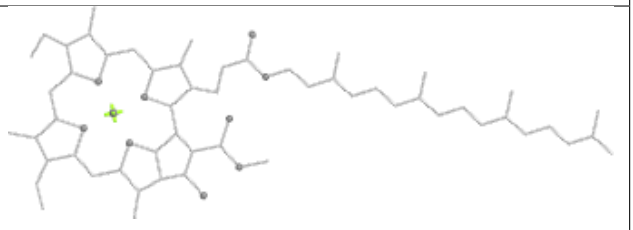


Bond angles

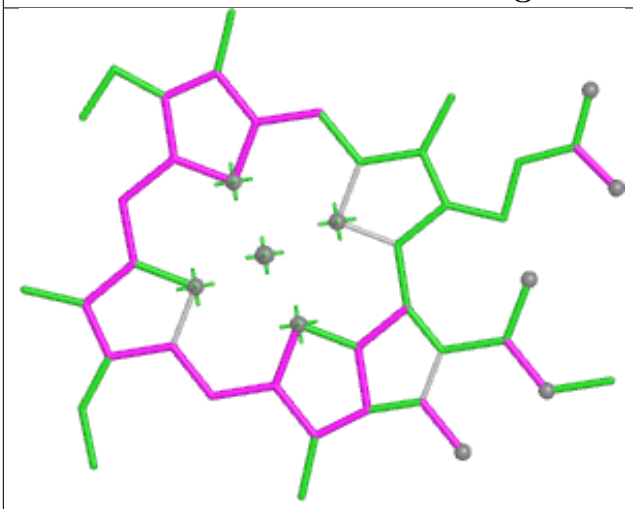


Torsions



Rings

Ligand CLA bB 810



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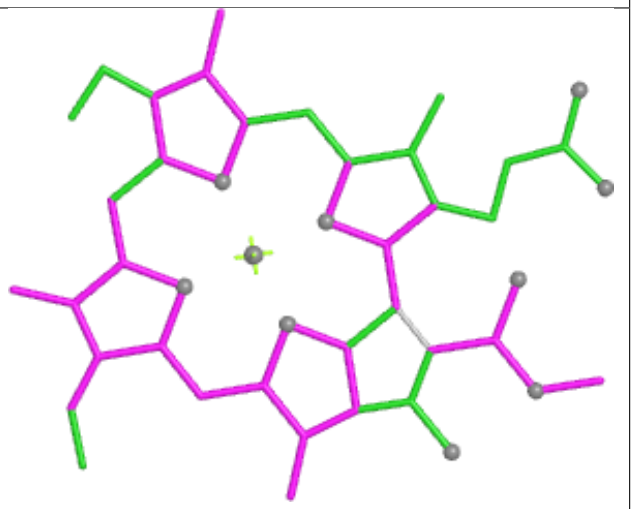
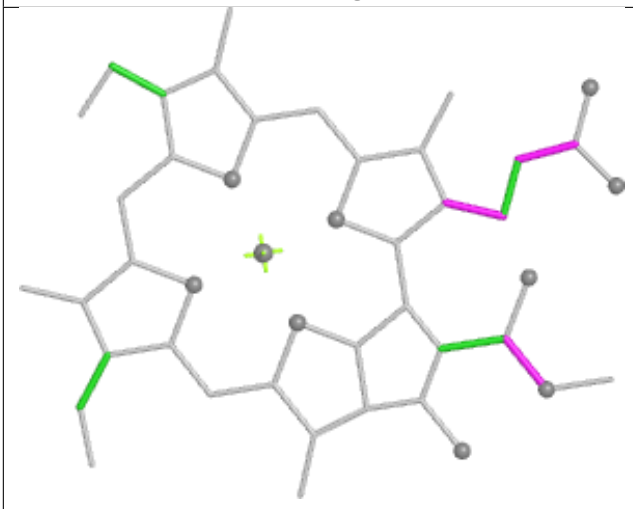


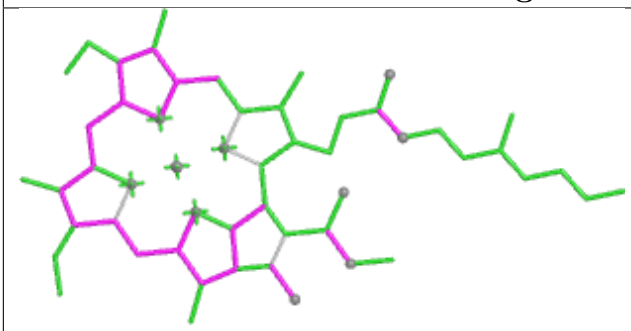
Bond angles



Torsions

Rings

Ligand CLA cA 804



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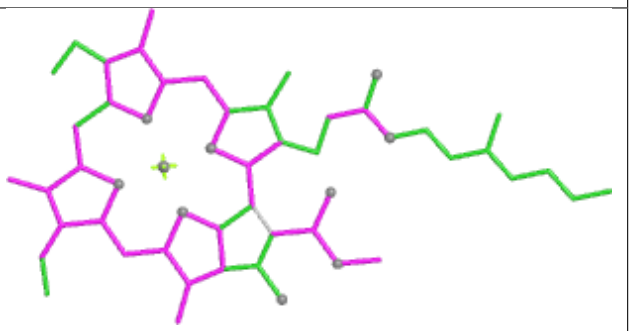
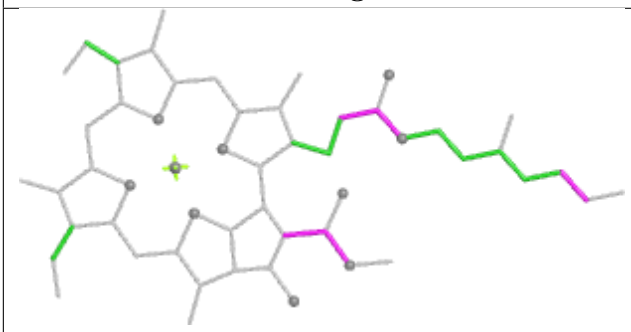
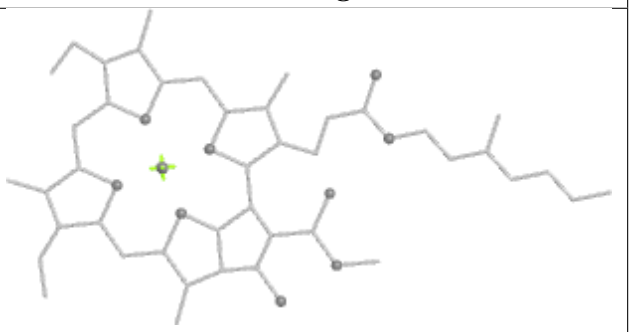


Bond angles

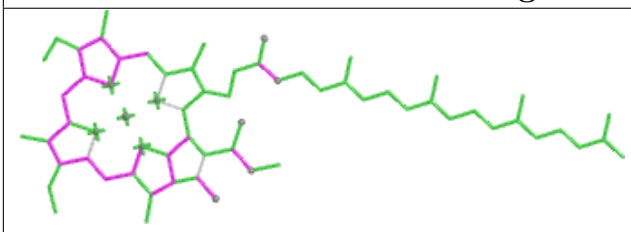


Torsions



Rings

Ligand CLA cL 205



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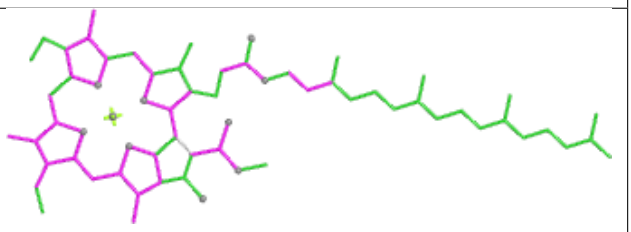
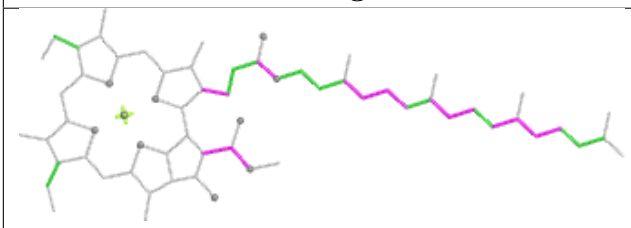


Bond angles



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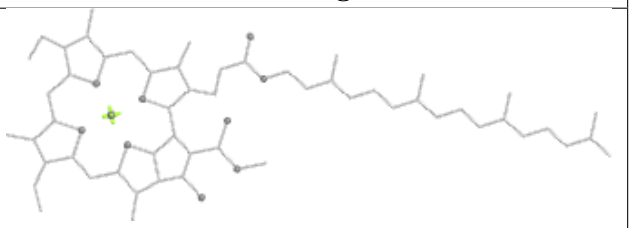
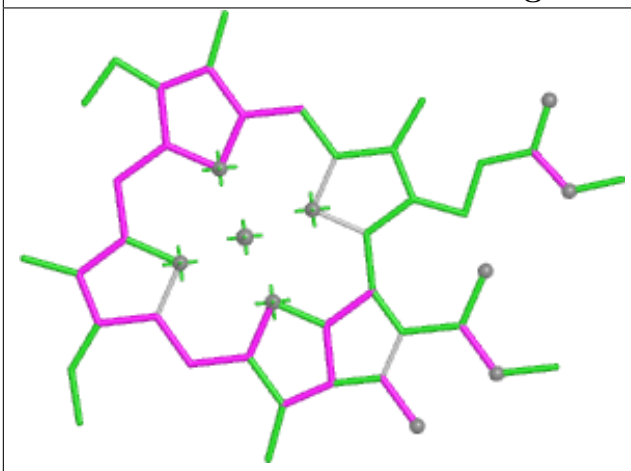


Rings

Ligand CLA B 818



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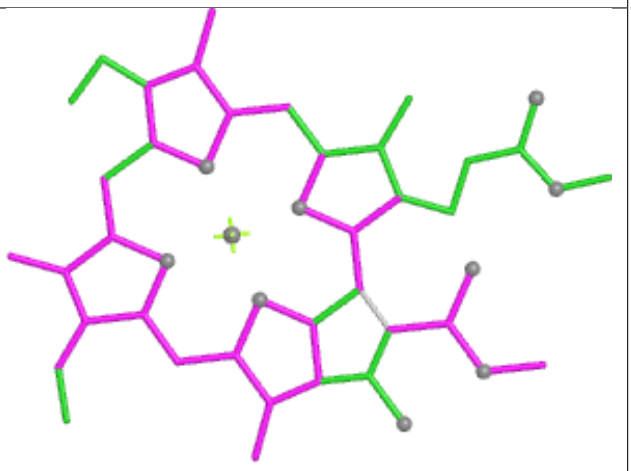
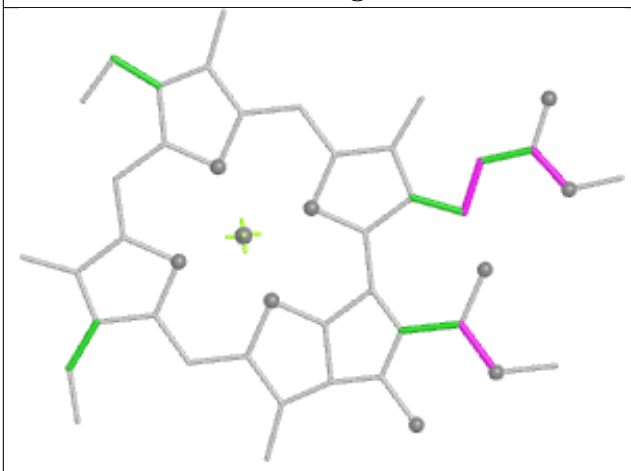


Bond angles



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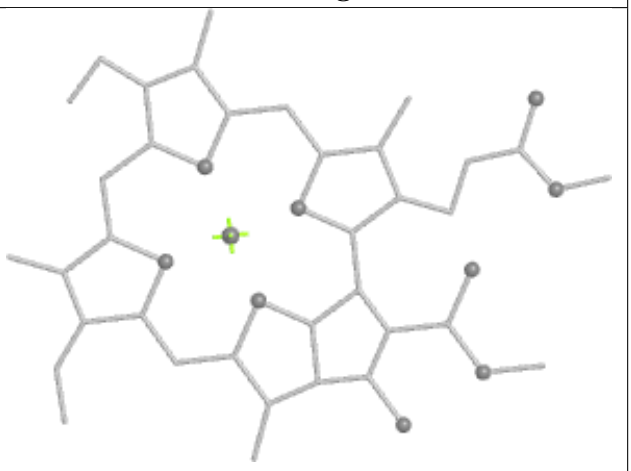
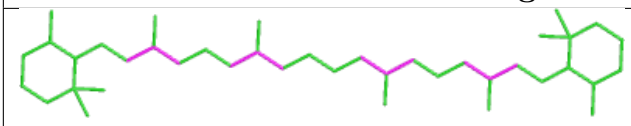


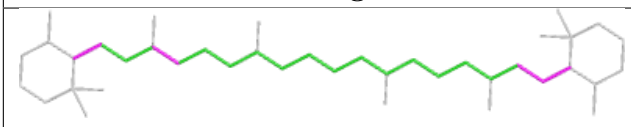
Rings

Ligand BCR M 101

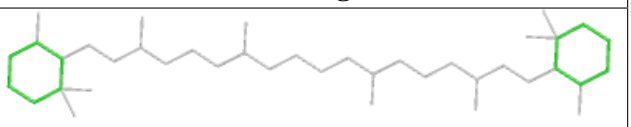


Bond lengths

Bond angles

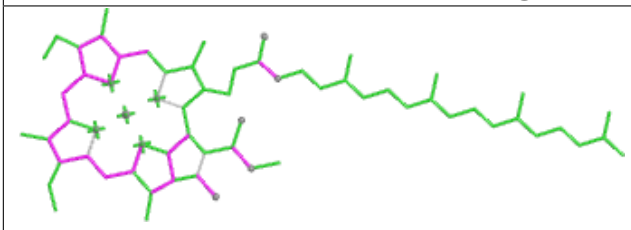


Torsions

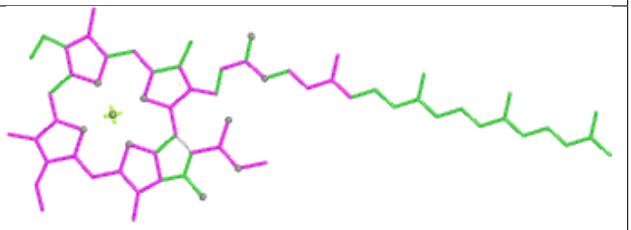


Rings

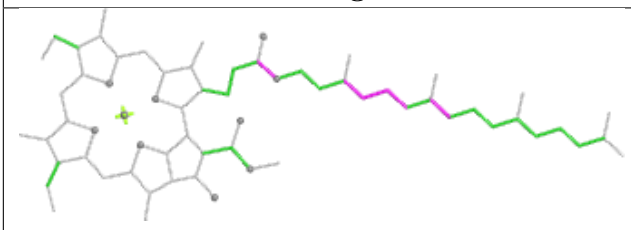
Ligand CLA cA 832



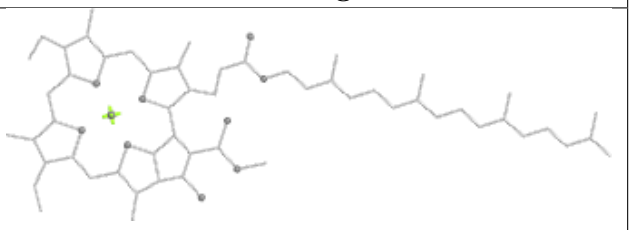
Bond lengths



Bond angles

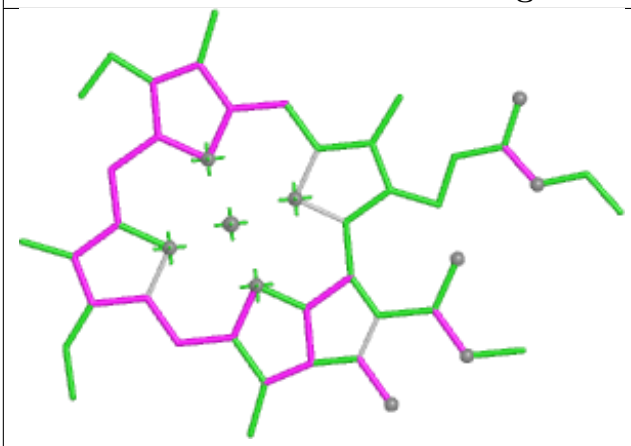


Torsions

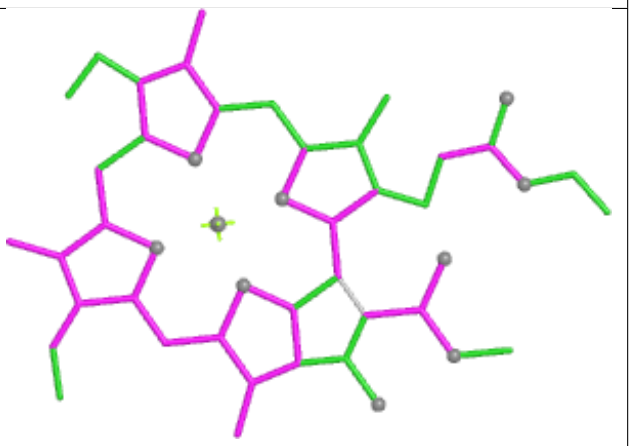


Rings

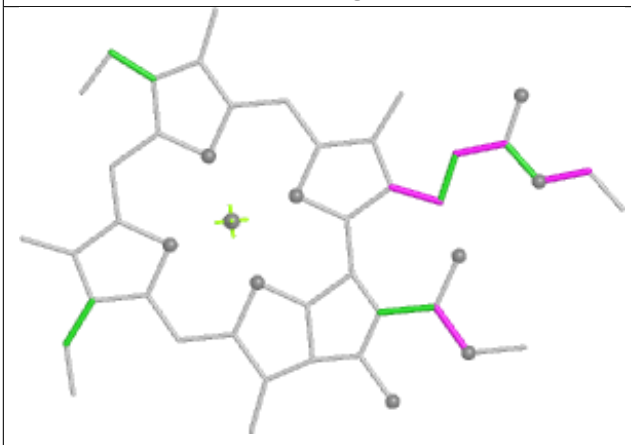
Ligand CLA cB 838



Bond lengths



Bond angles



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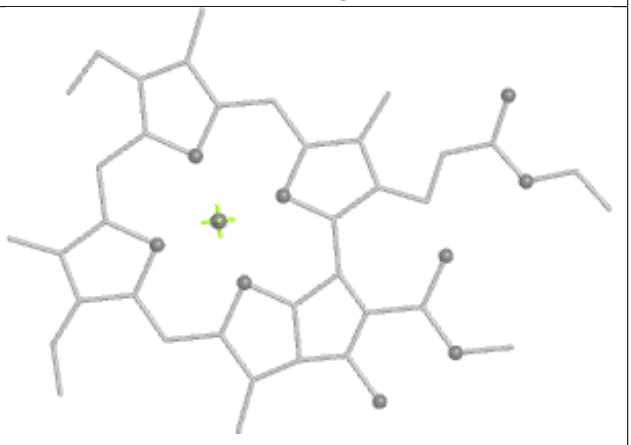
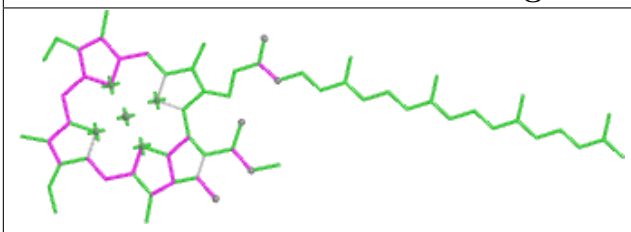


Rings

Ligand CLA B 801



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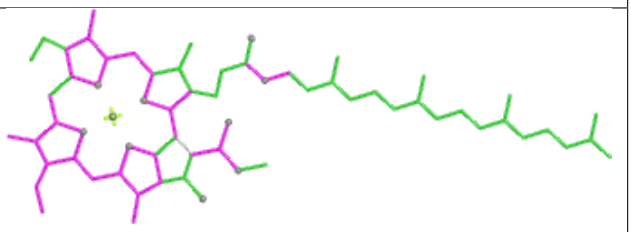
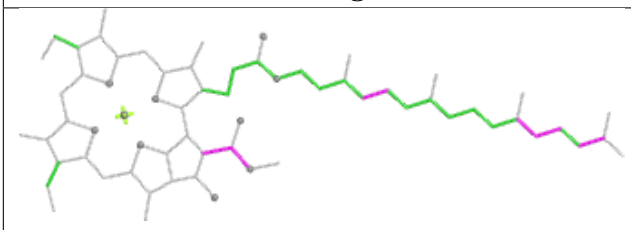
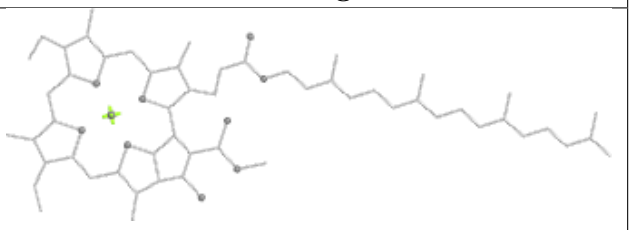


Bond angles

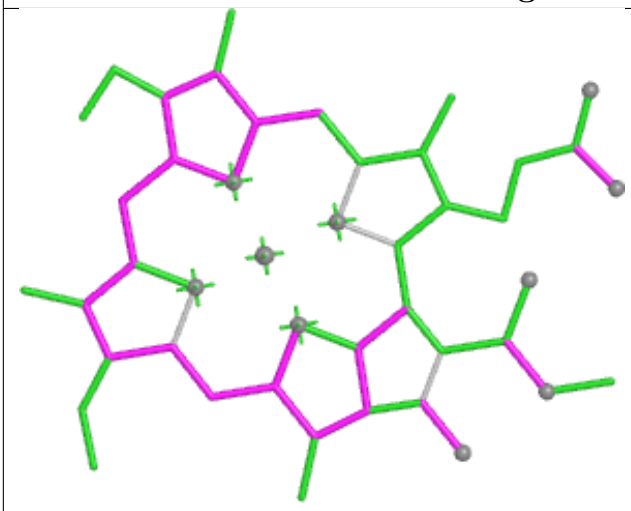


Torsions



Rings

Ligand CLA bJ 101



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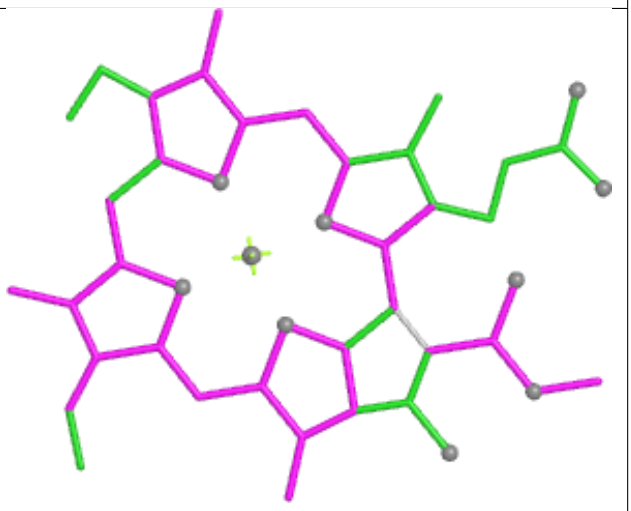
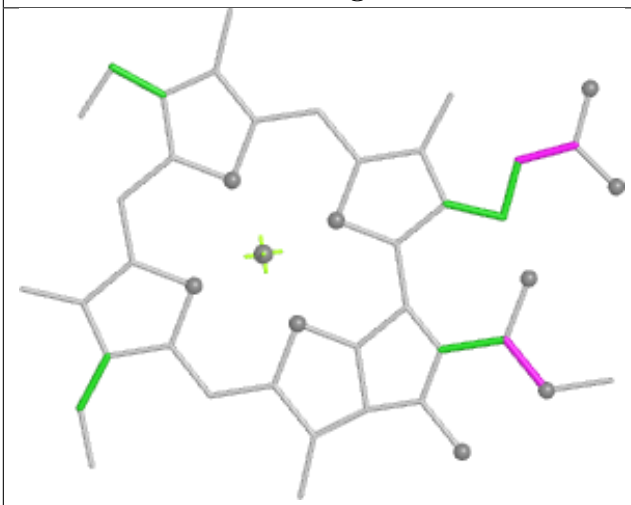


Bond angles



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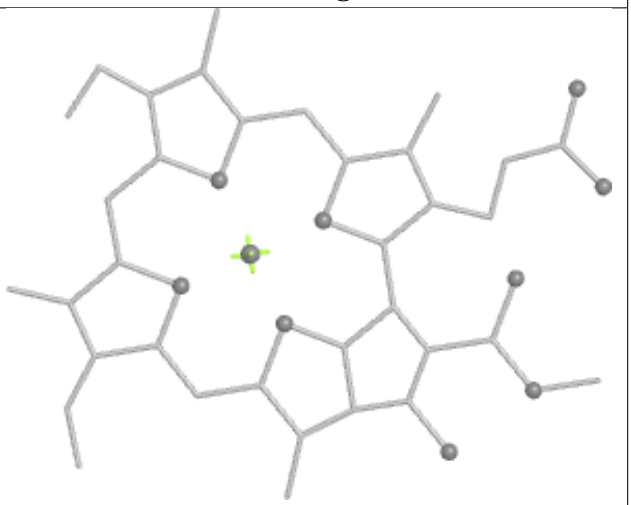
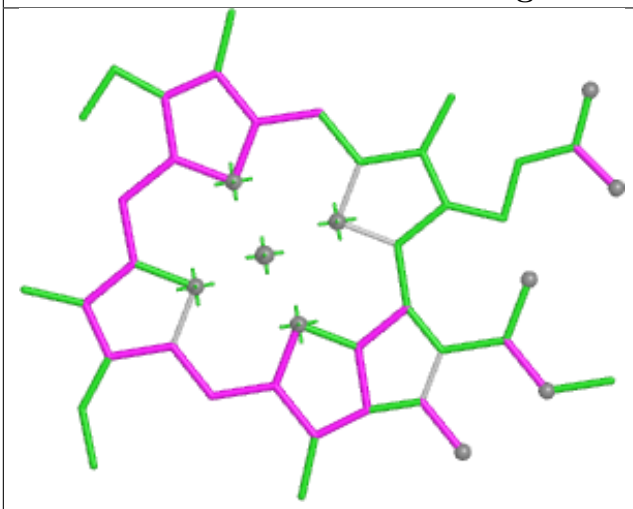


Rings

Ligand CLA cB 850



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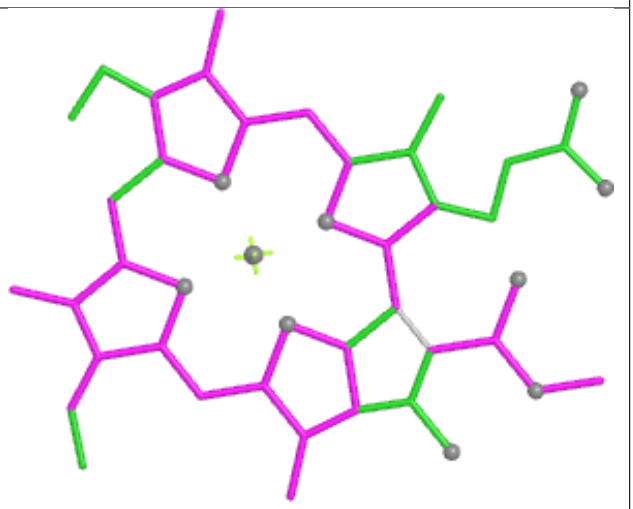
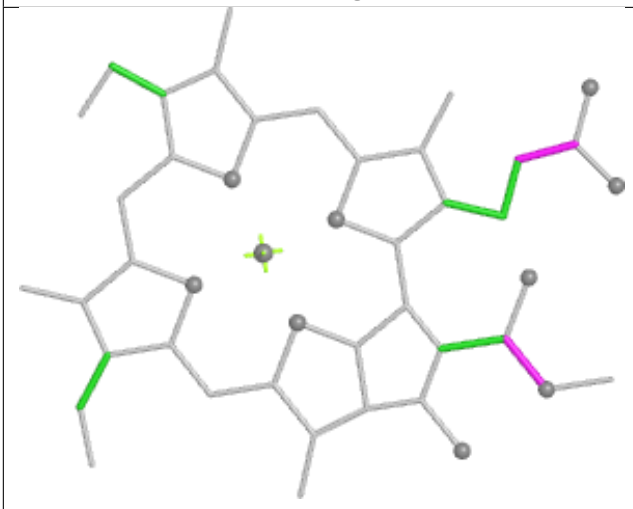


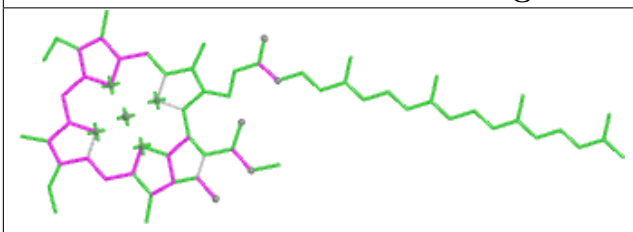
Bond angles



Torsions

Rings

Ligand CLA bA 802



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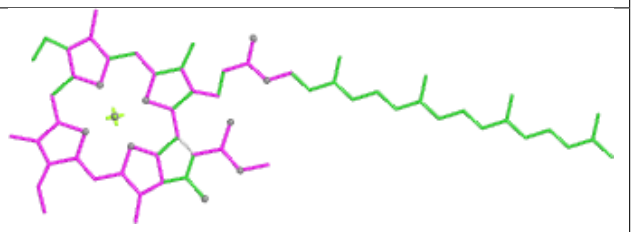
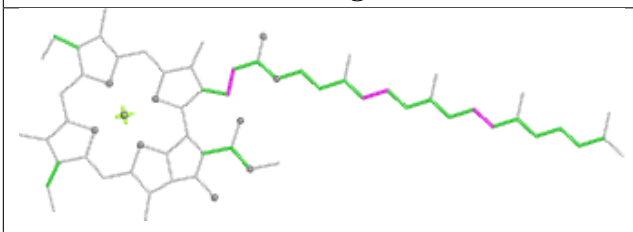


Bond angles



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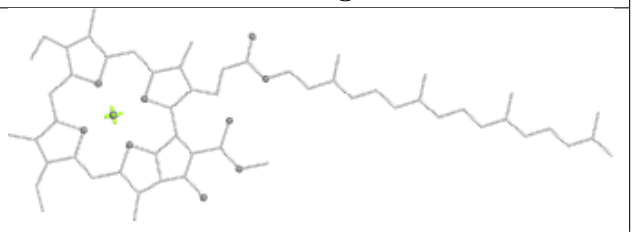
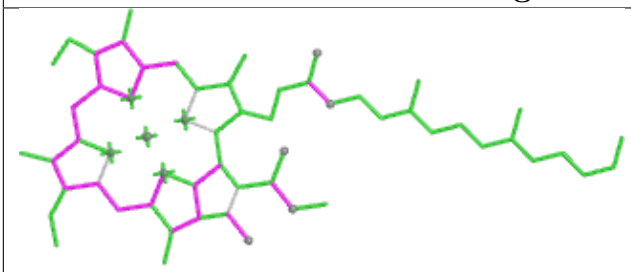


Rings

Ligand CLA bA 824



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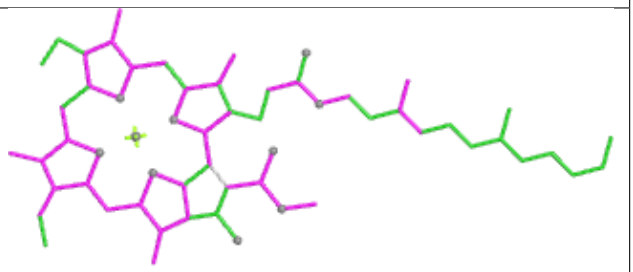
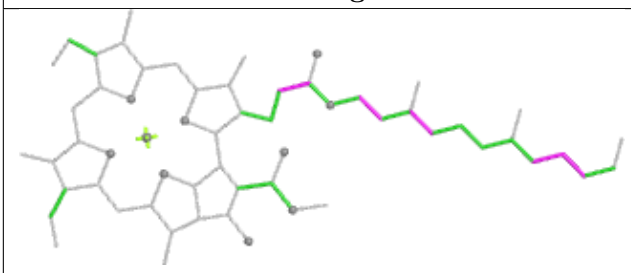


Bond angles



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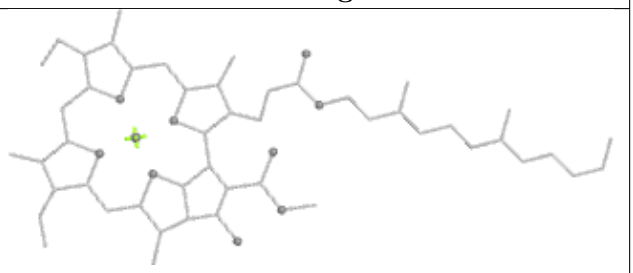
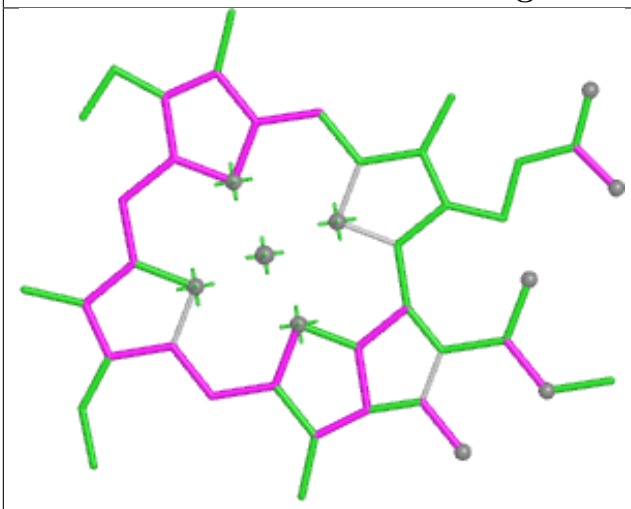


Rings

Ligand CLA cB 834



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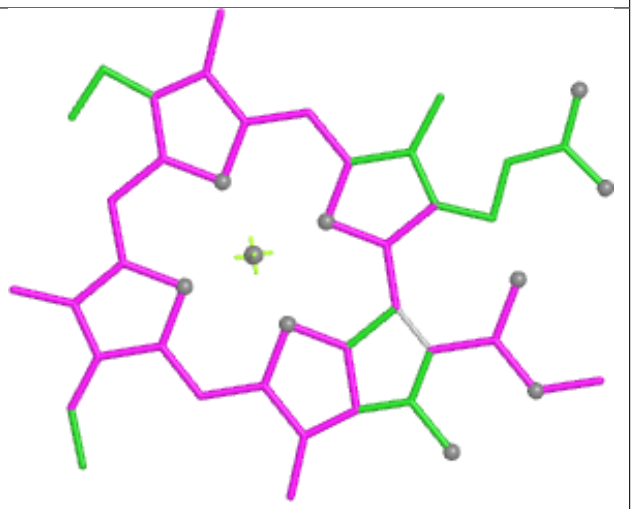
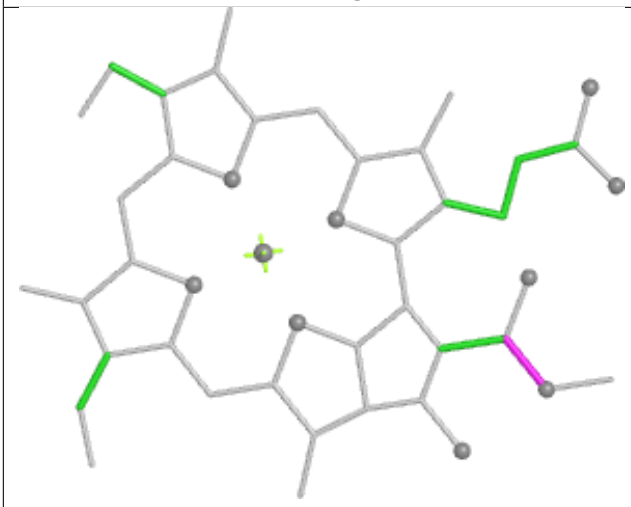


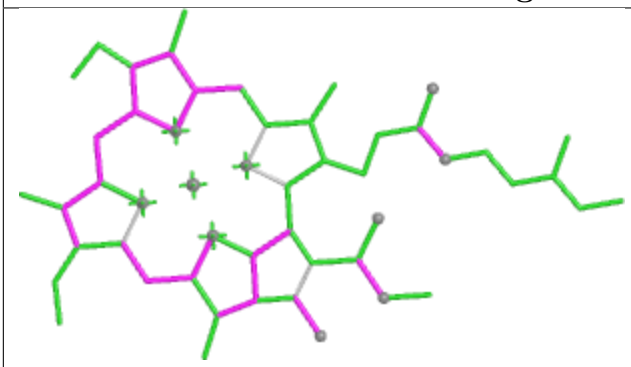
Bond angles



Torsions

Rings

Ligand CLA bF 201



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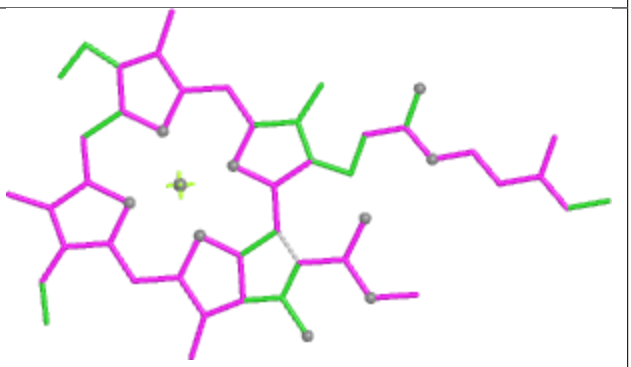
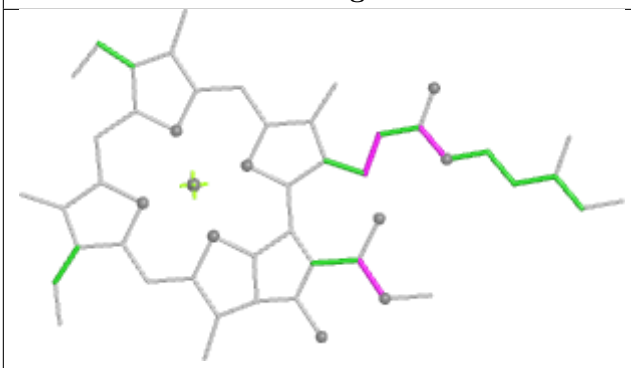
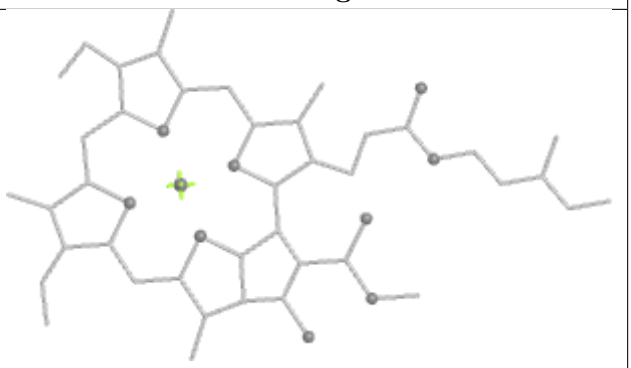


Bond angles

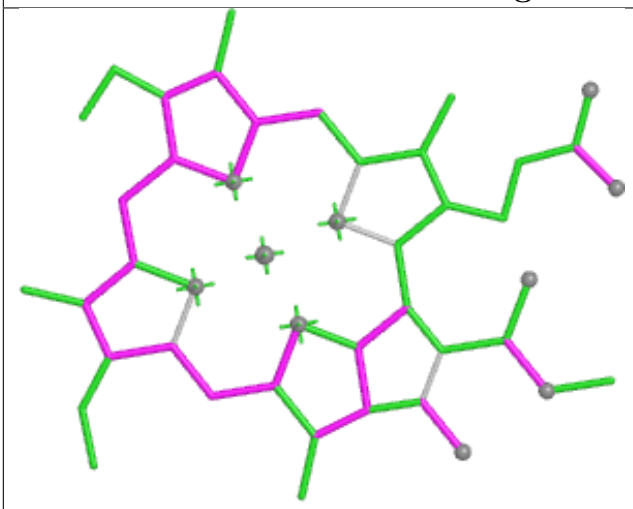


Torsions



Rings

Ligand CLA bB 811



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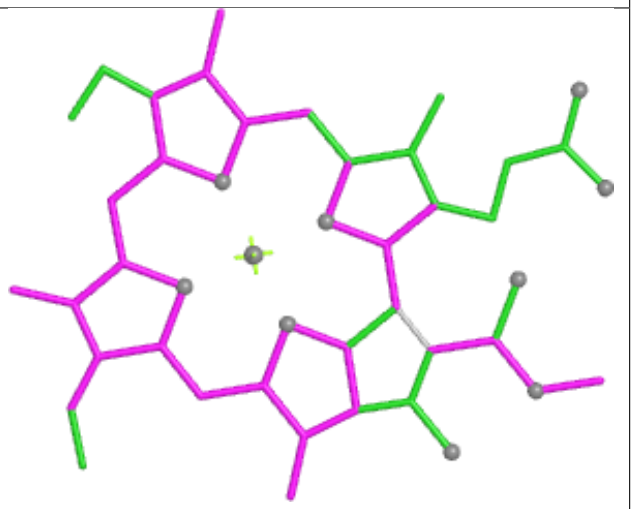
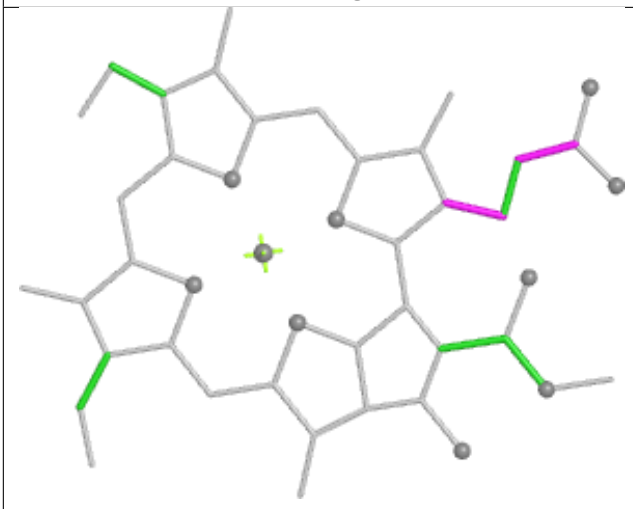


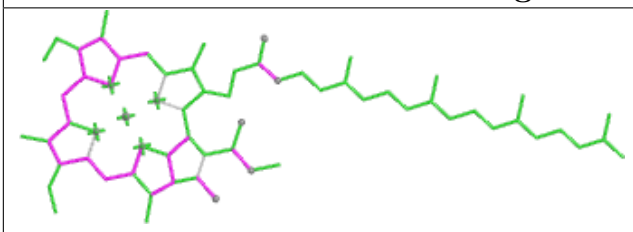
Bond angles



Torsions

Rings

Ligand CLA bB 802



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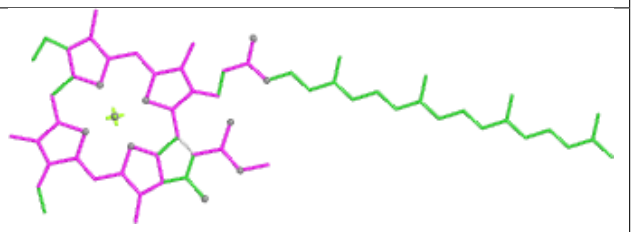

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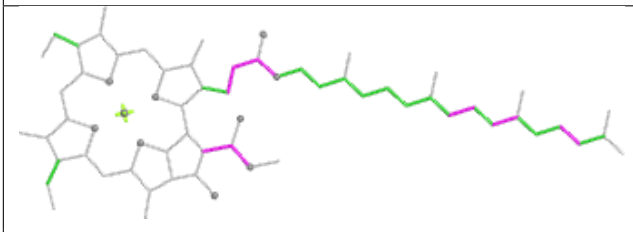
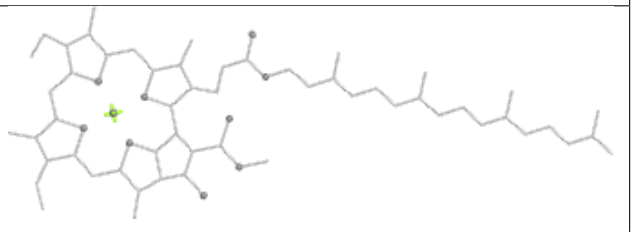
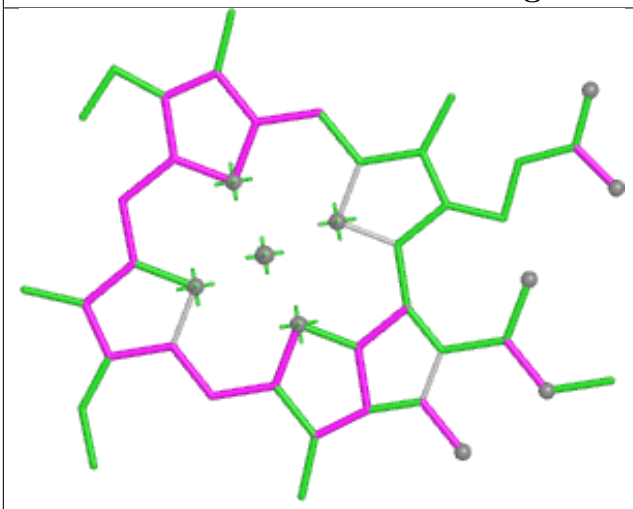


Torsions



Rings

Ligand CLA A 813



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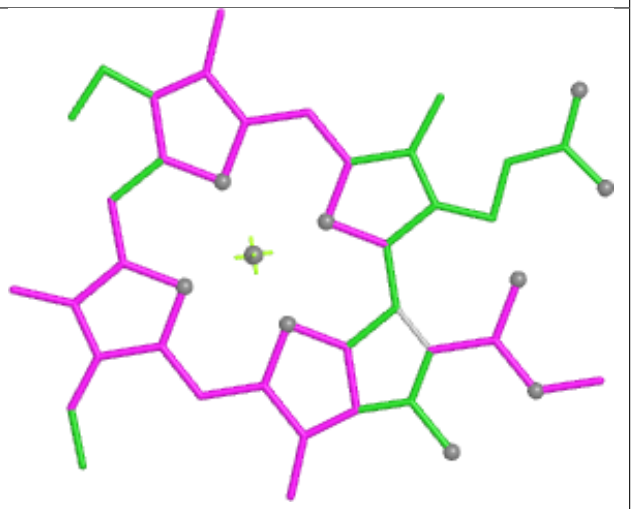
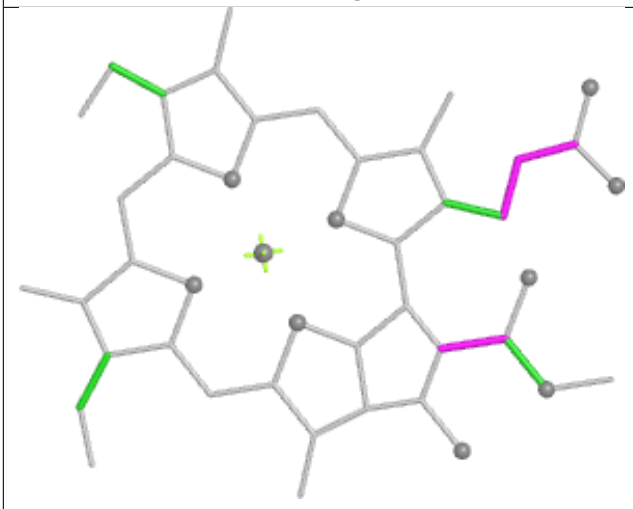


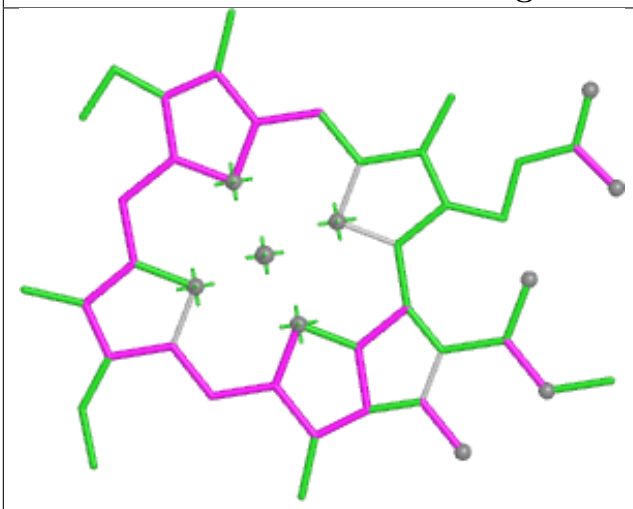
Bond angles



Torsions

Rings

Ligand CLA cA 822



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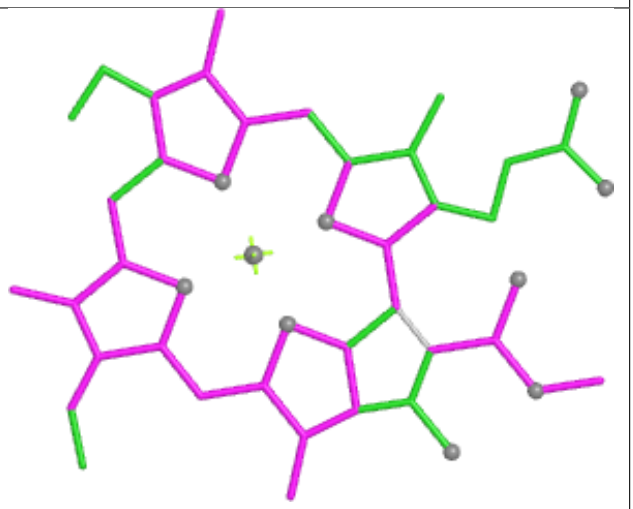
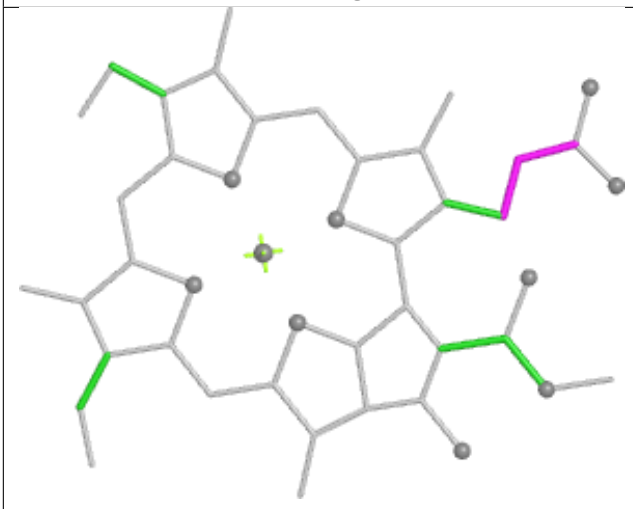


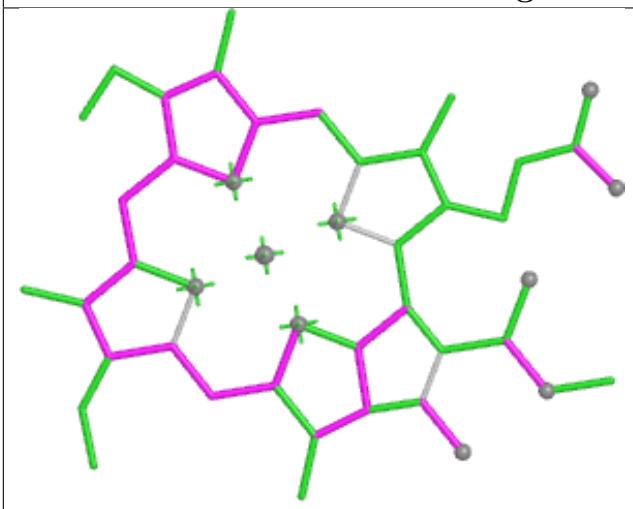
Bond angles



Torsions

Rings

Ligand CLA cB 830



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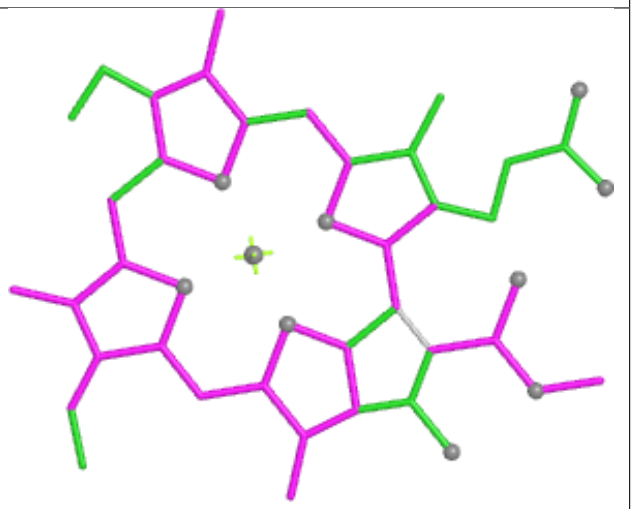
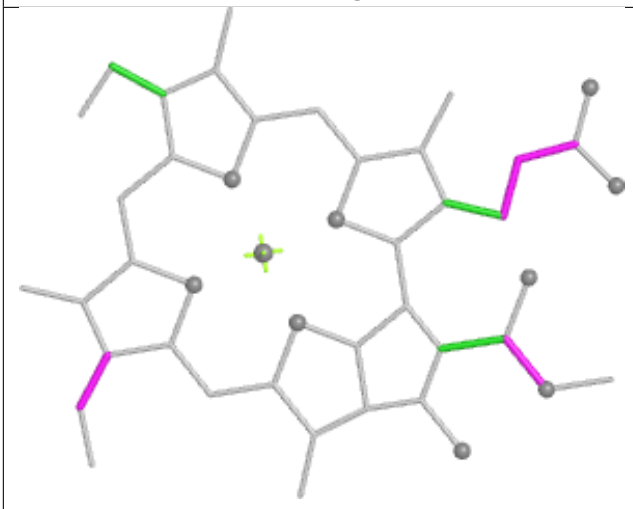


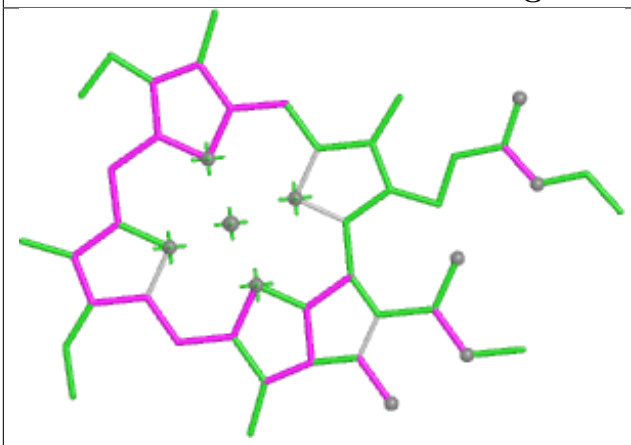
Bond angles



Torsions

Rings

Ligand CLA B 819



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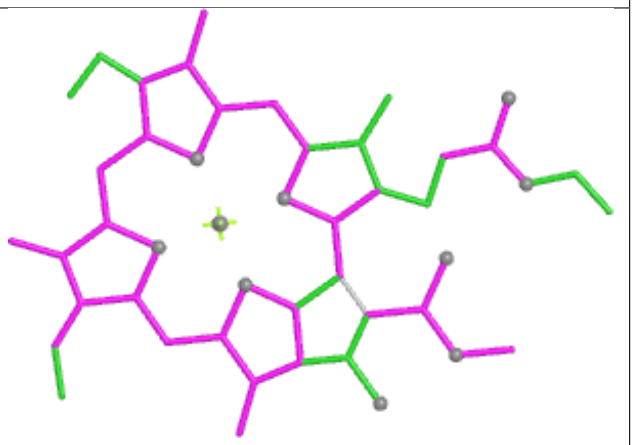
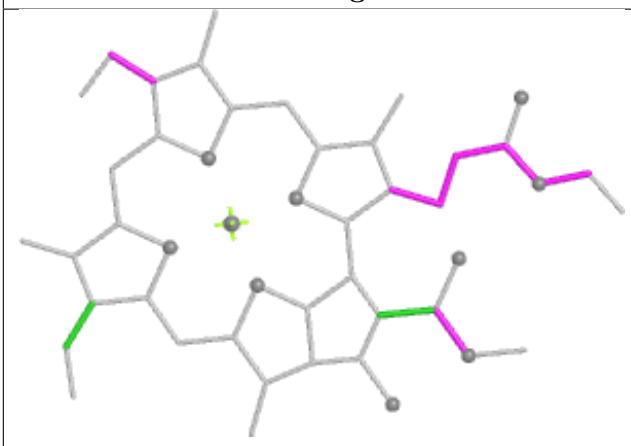
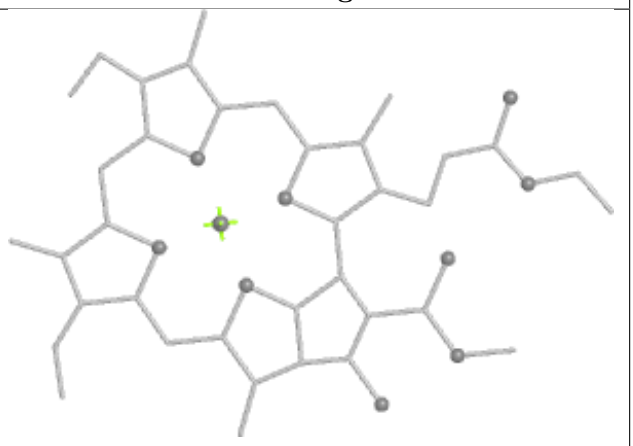


Bond angles

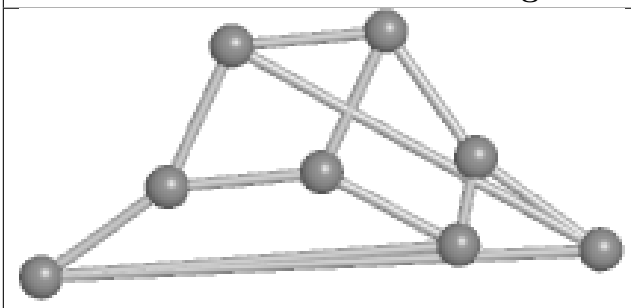


Torsions

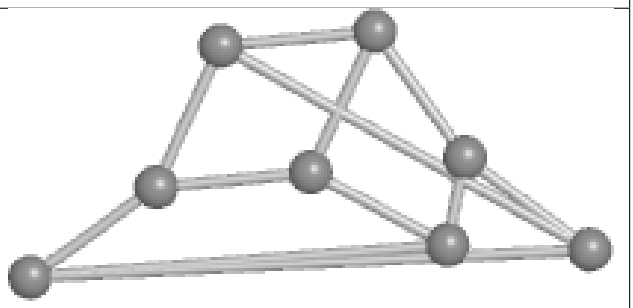


Rings

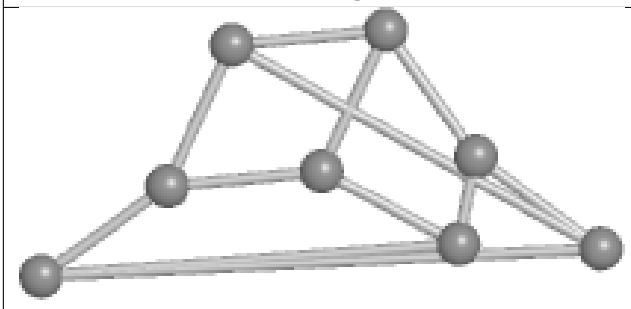
Ligand SF4 bC 102



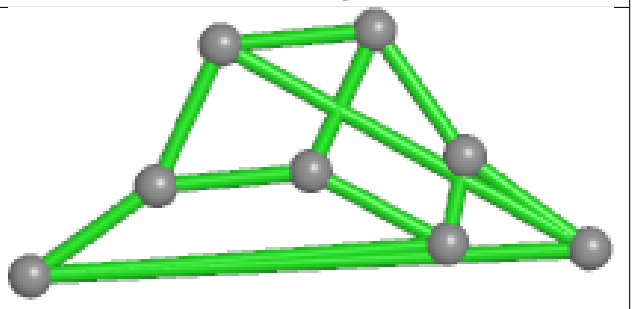
Bond lengths



Bond angles

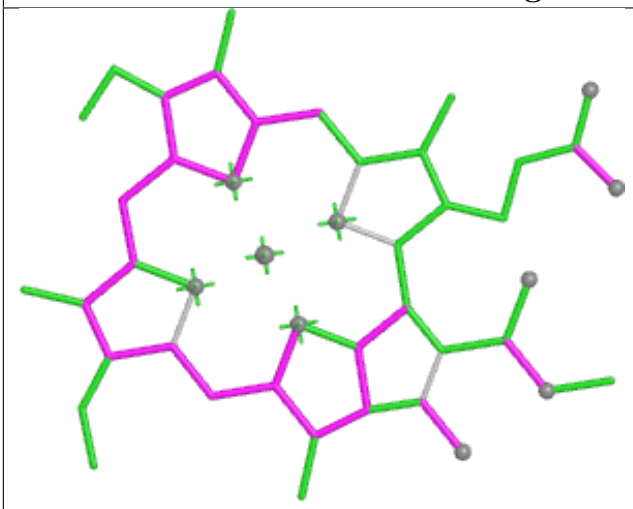


Torsions



Rings

Ligand CLA B 810



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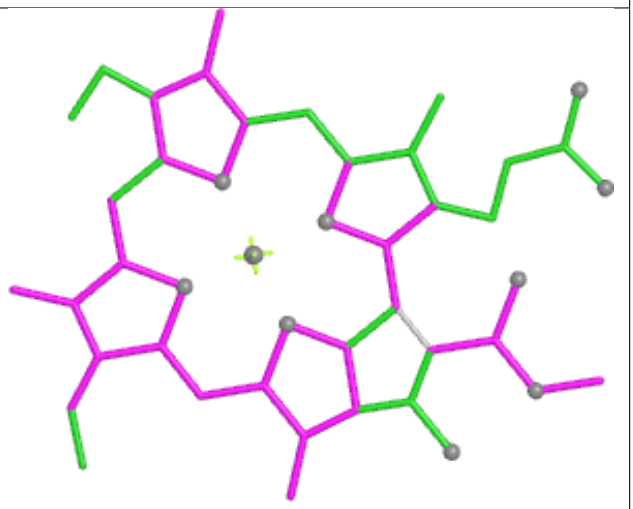
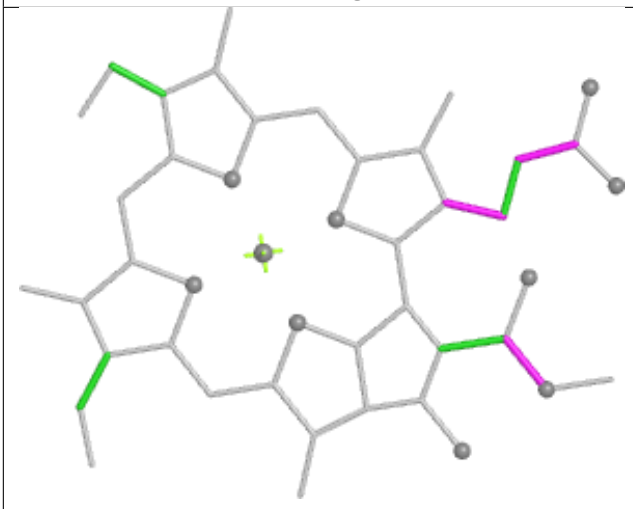


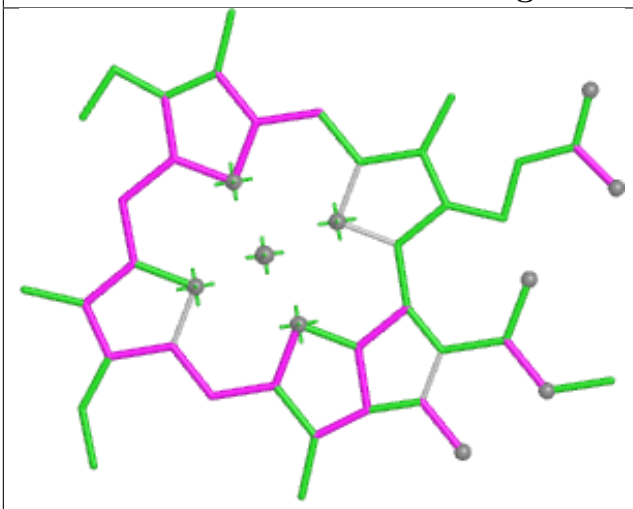
Bond angles



Torsions

Rings

Ligand CLA cB 833



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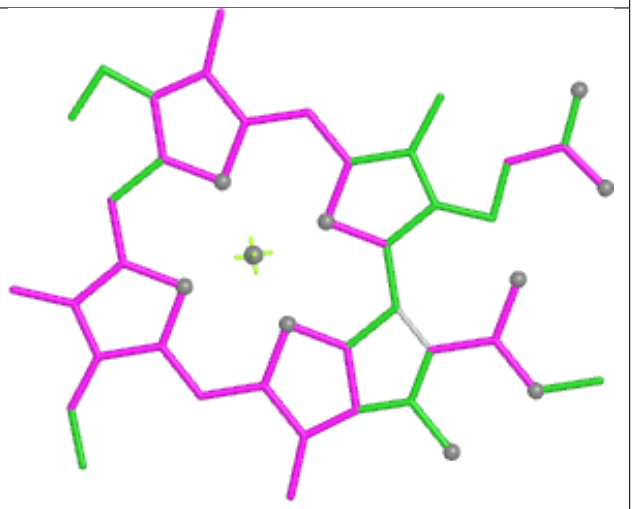
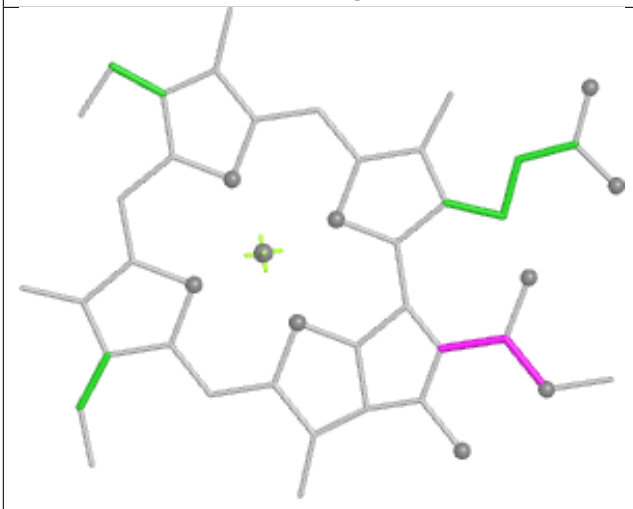


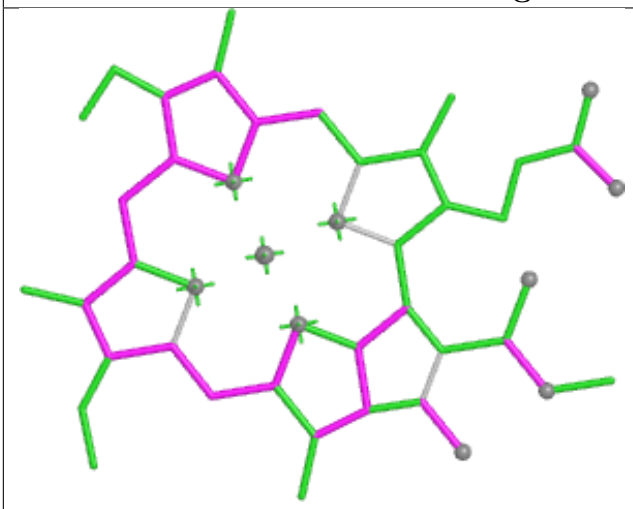
Bond angles



Torsions

Rings

Ligand CLA bA 809



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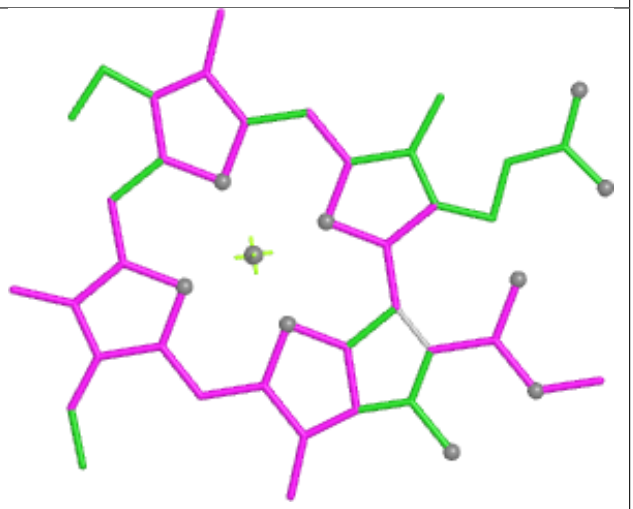
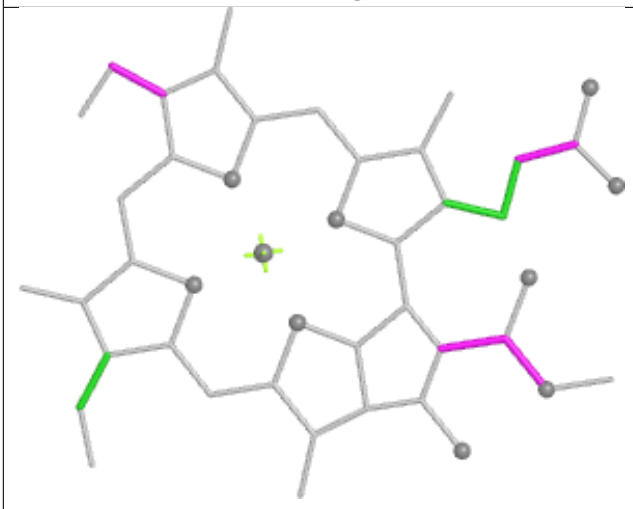


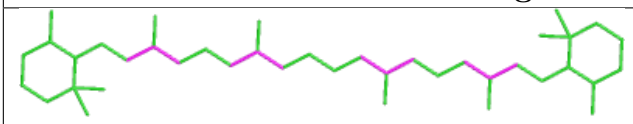
Bond angles



Torsions

Rings

Ligand BCR bL 206



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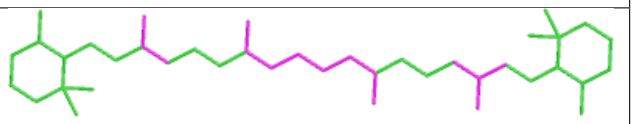
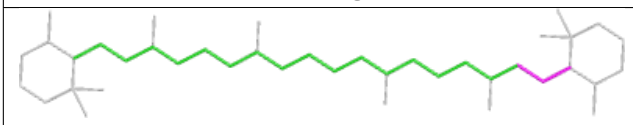
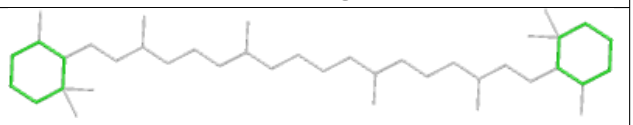


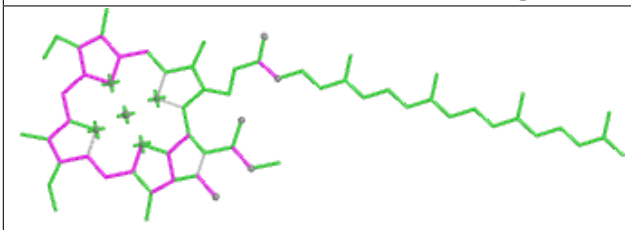
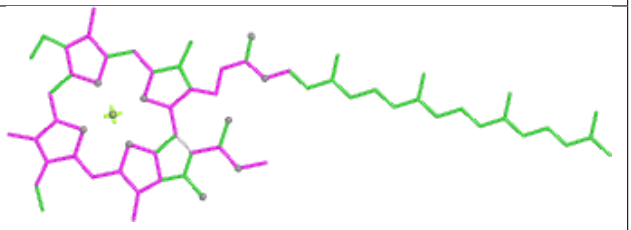
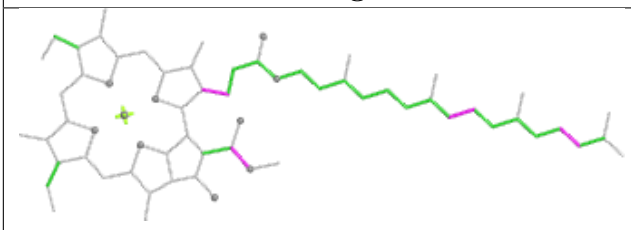
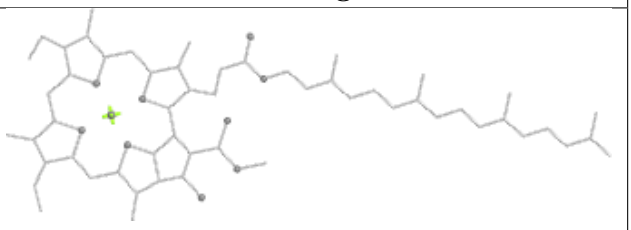
Bond angles

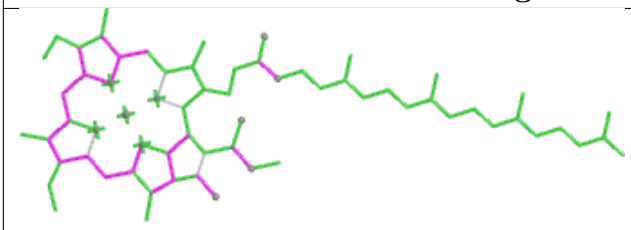
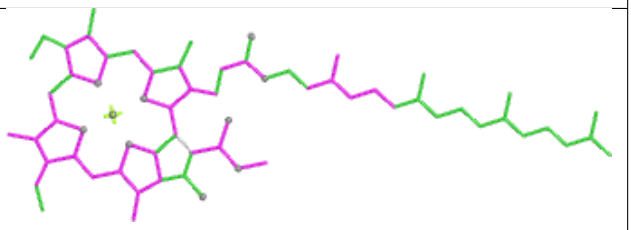
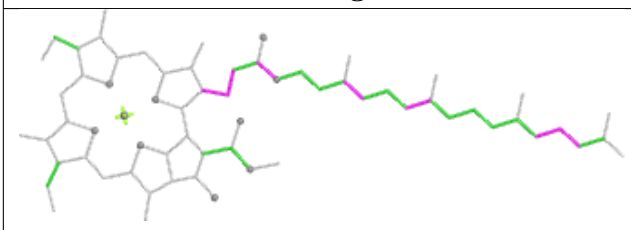
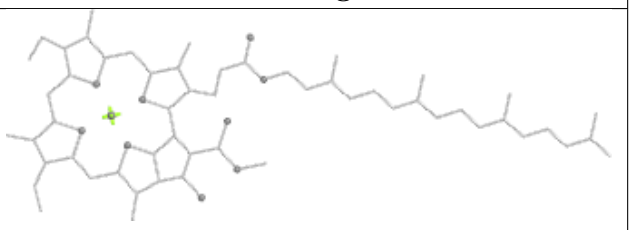


Torsions

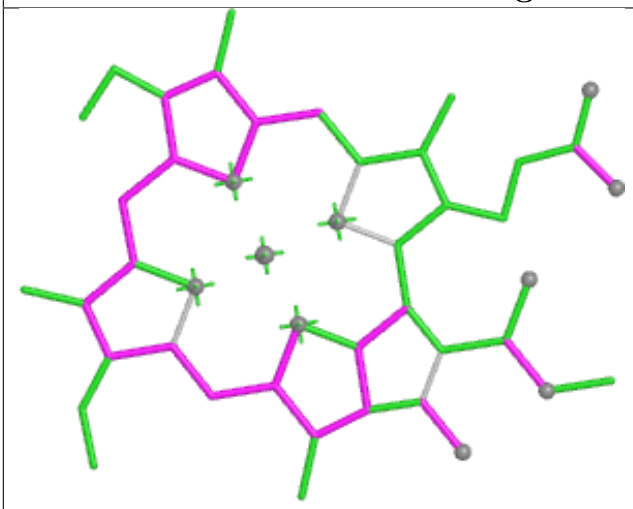


Rings

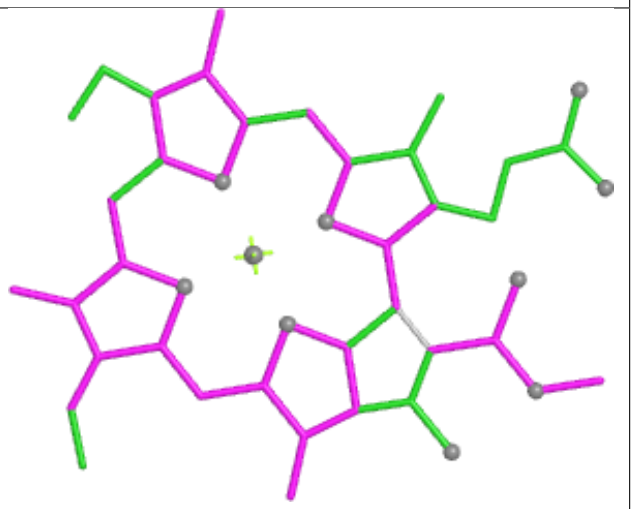
Ligand CLA bB 827	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA bB 809	
	
Bond lengths	Bond angles
	
Torsions	Rings

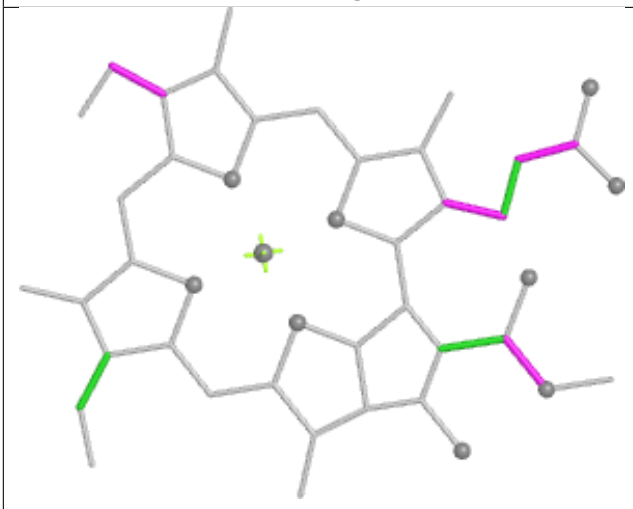
Ligand CLA cA 815



Bond lengths



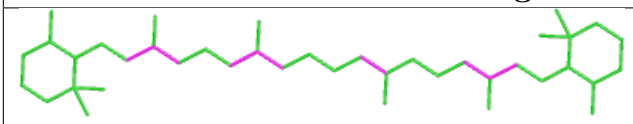
Bond angles



Torsions

Rings

Ligand BCR cA 847



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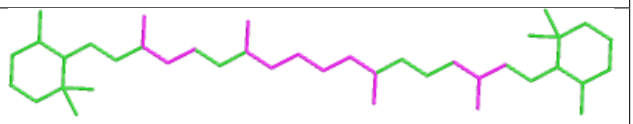
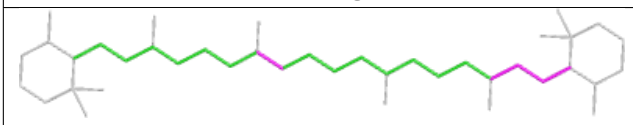
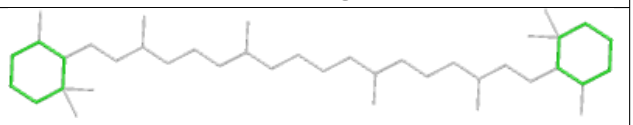


Bond angles

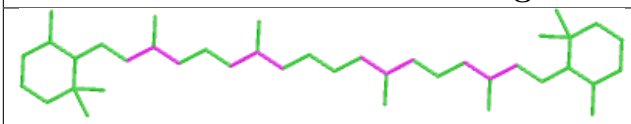


Torsions

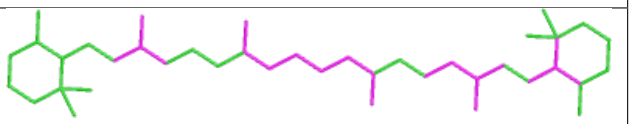


Rings

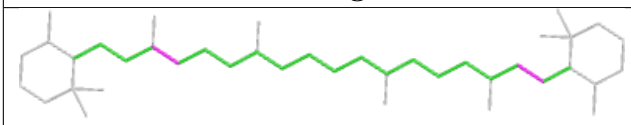
Ligand BCR cA 848



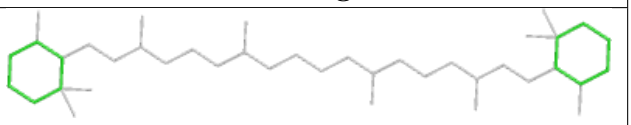
Bond lengths



Bond angles

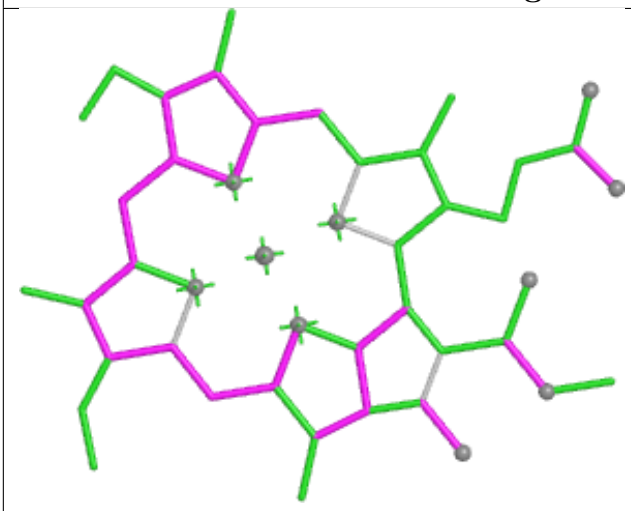


Torsions



Rings

Ligand CLA B 811



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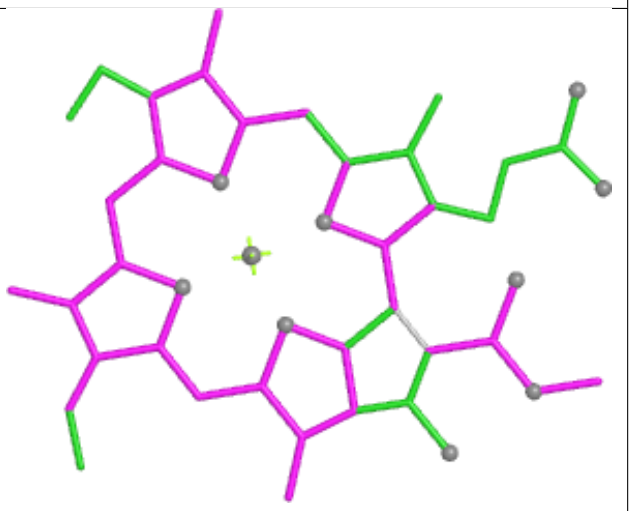
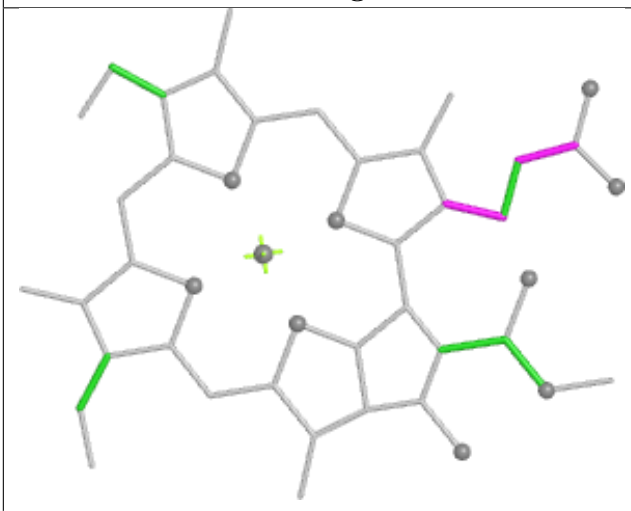


Bond angles



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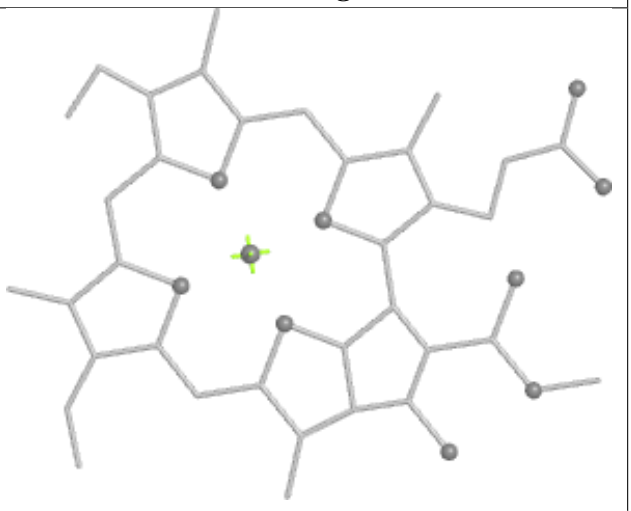
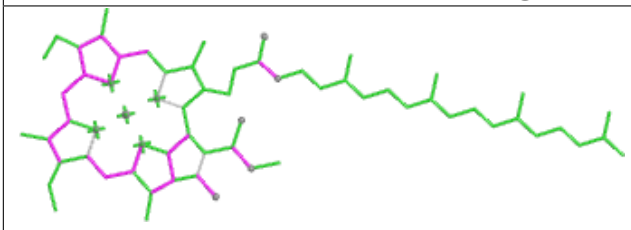


Rings

Ligand CLA cB 829



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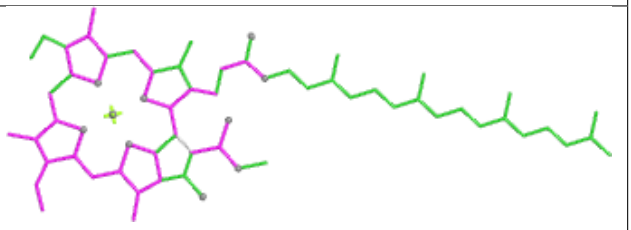
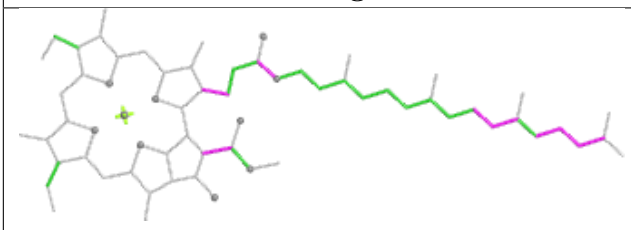
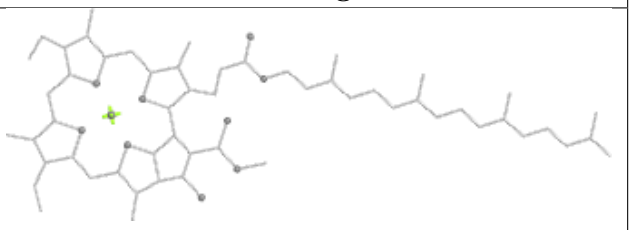


Bond angles

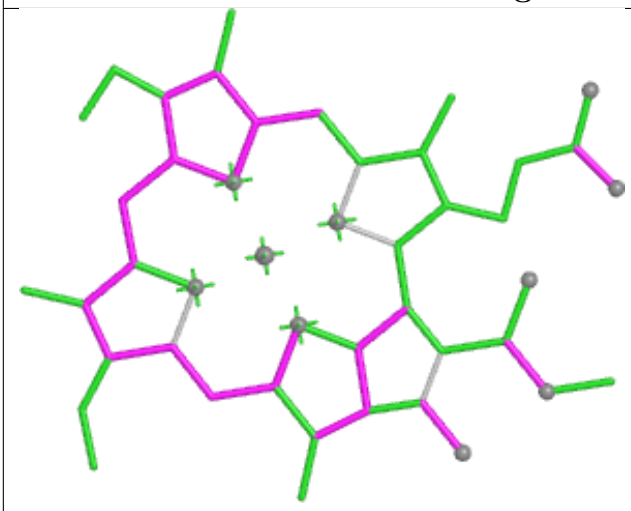


Torsions

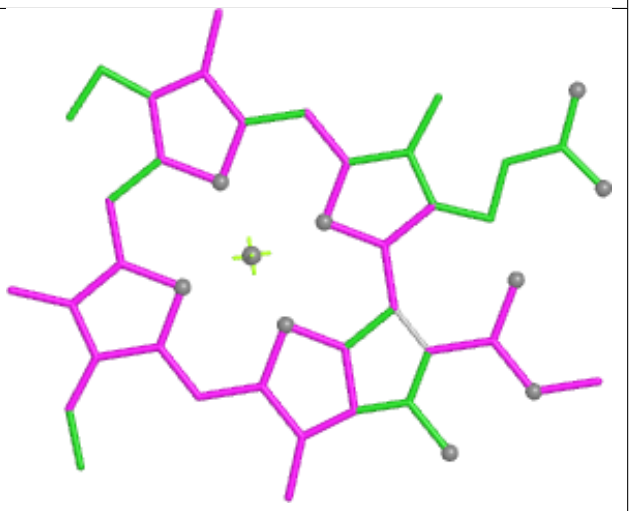


Rings

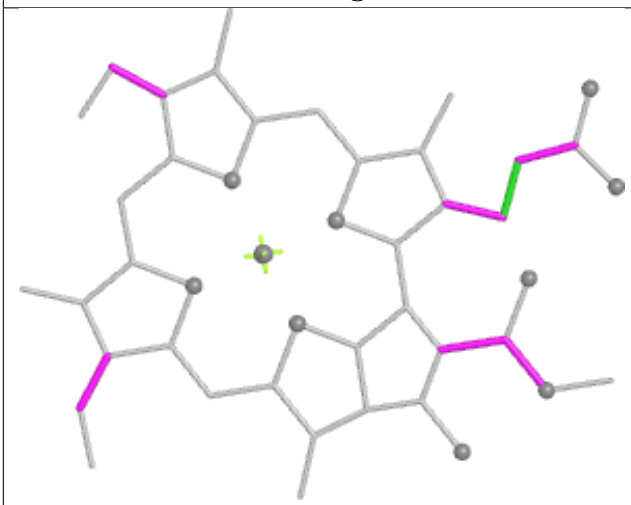
Ligand CLA bB 820



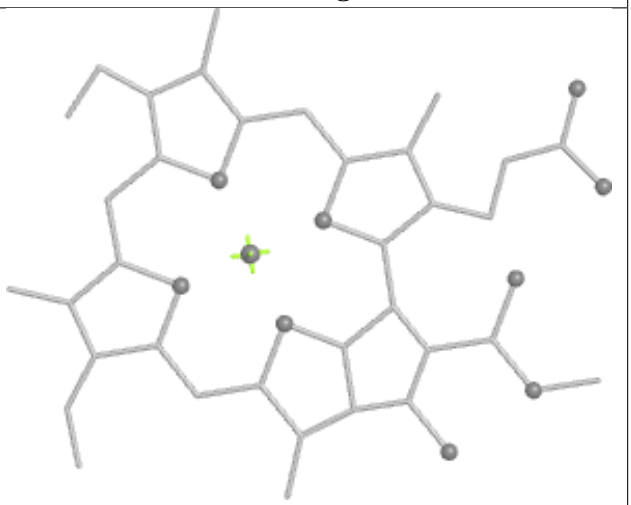
Bond lengths



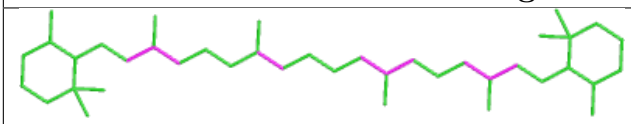
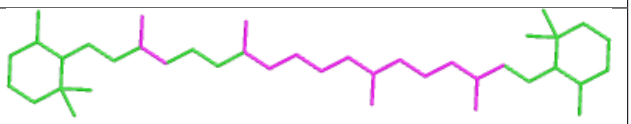
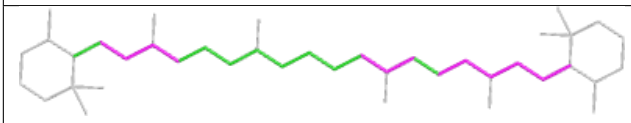
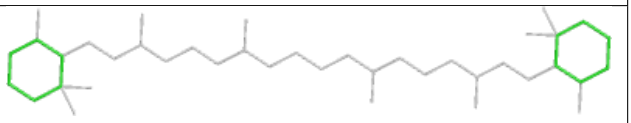
Bond angles

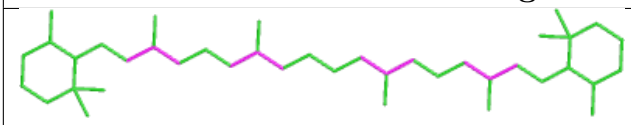
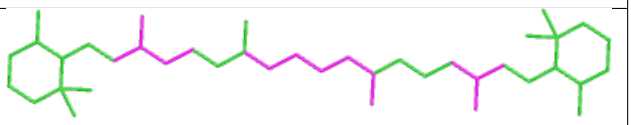
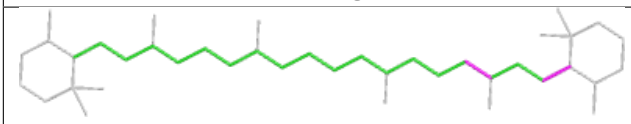
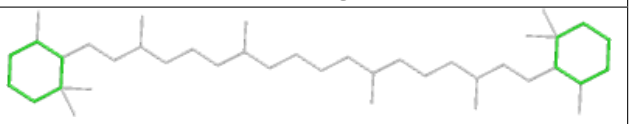


Torsions

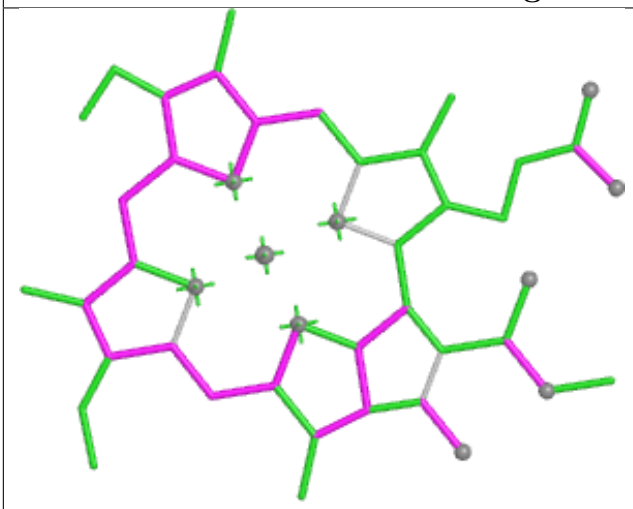


Rings

Ligand BCR cJ 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR bI 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 842



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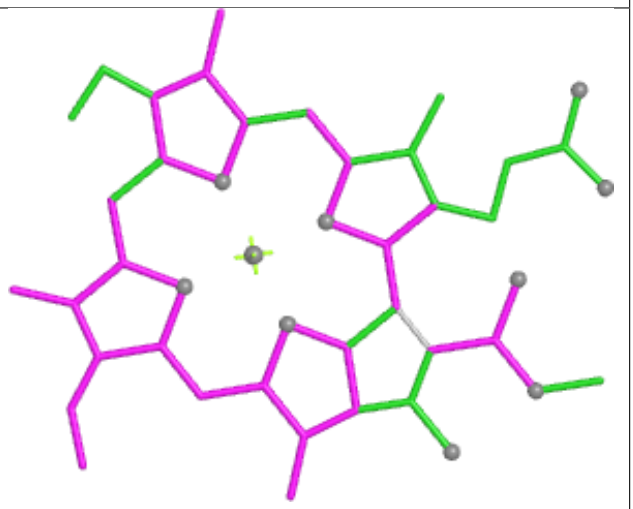
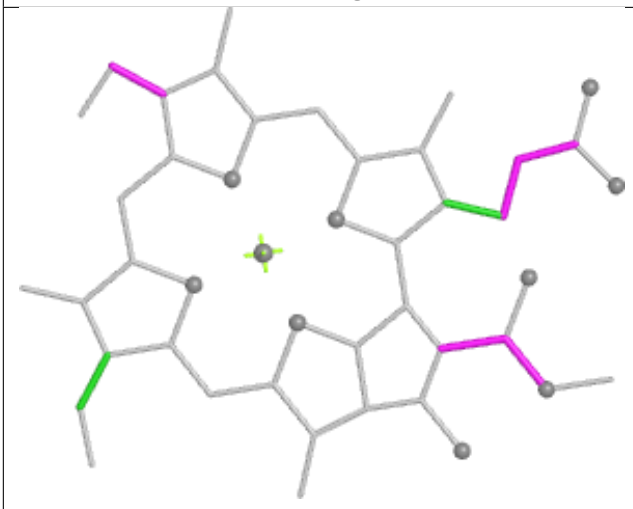


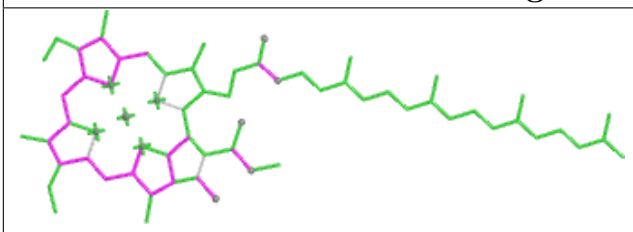
Bond angles



Torsions

Rings

Ligand CLA L 202



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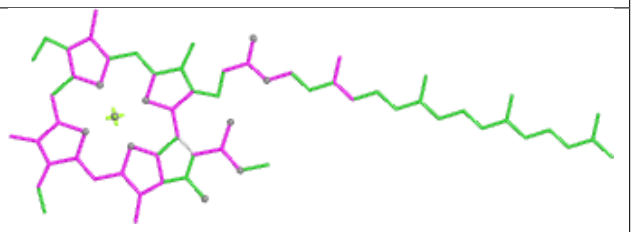
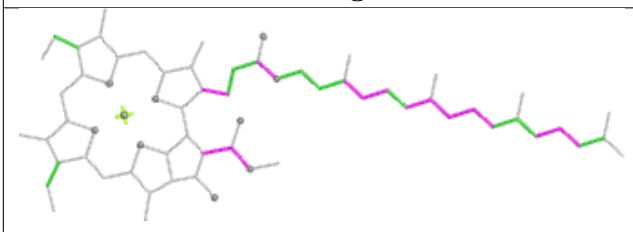


Bond angles



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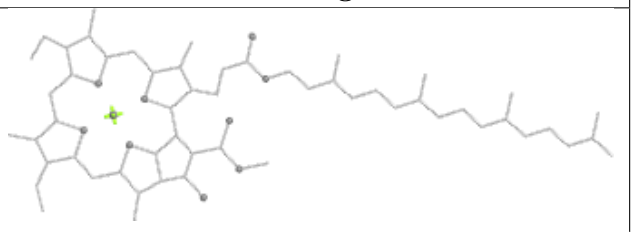
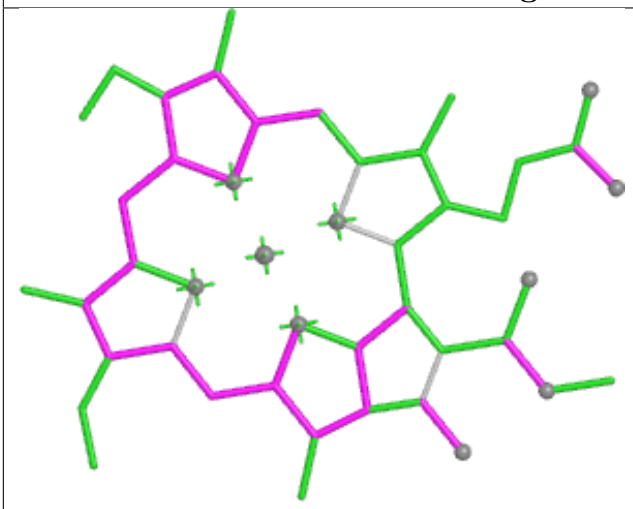


Rings

Ligand CLA cJ 101



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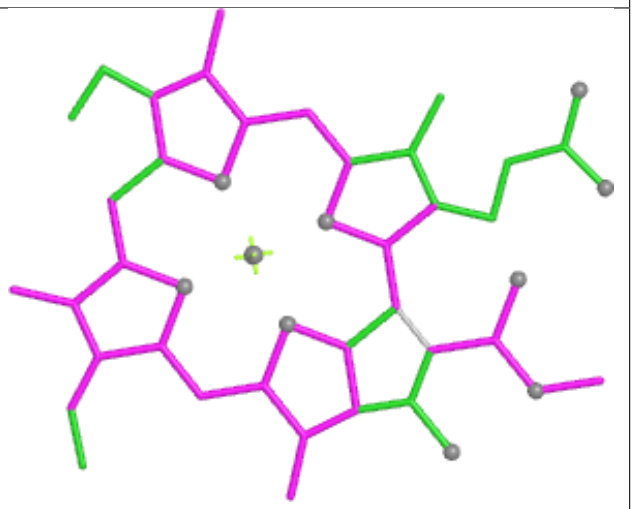
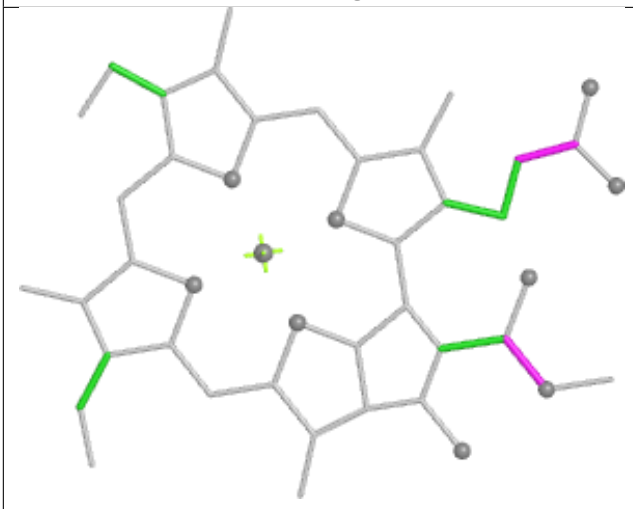
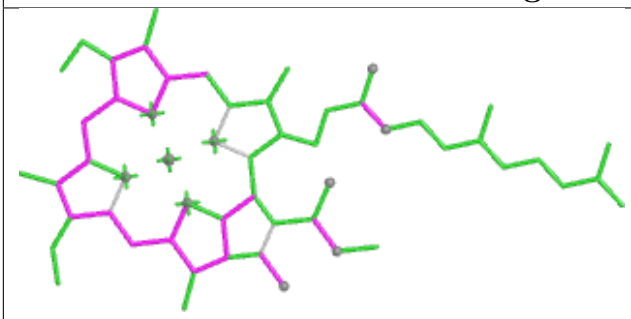
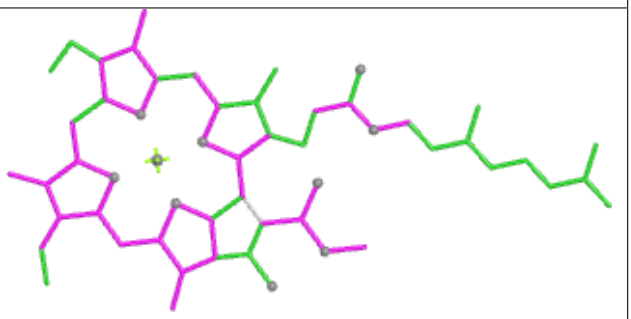
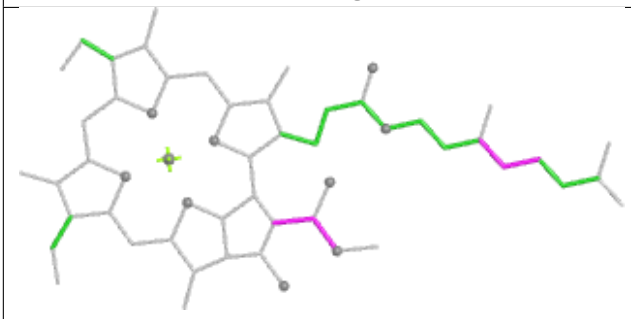
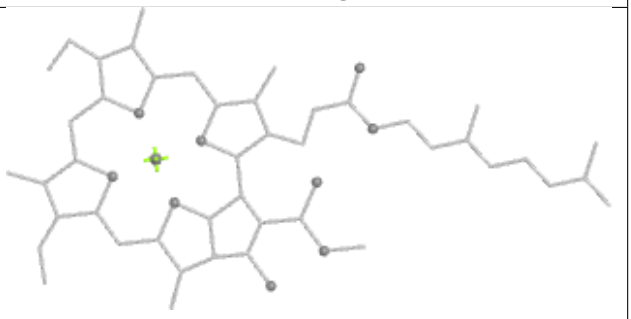


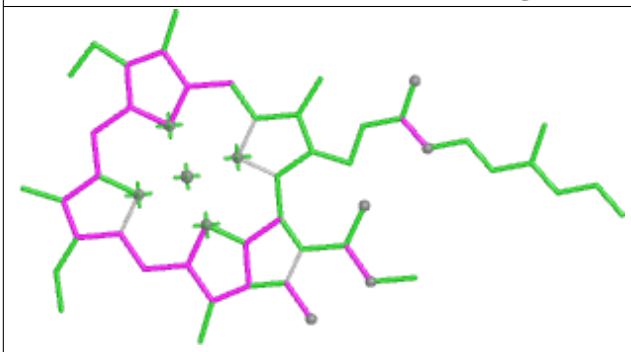
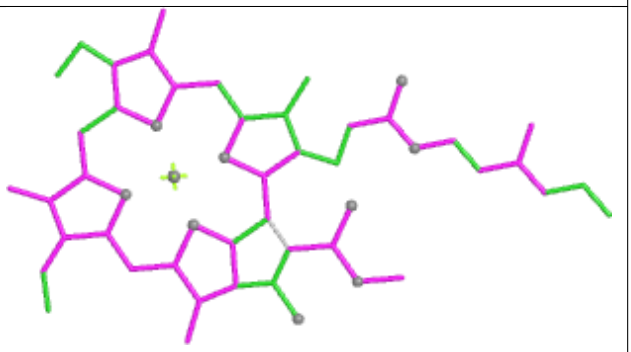
Bond angles



Torsions

Rings

Ligand CLA A 805	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA cB 816	
	
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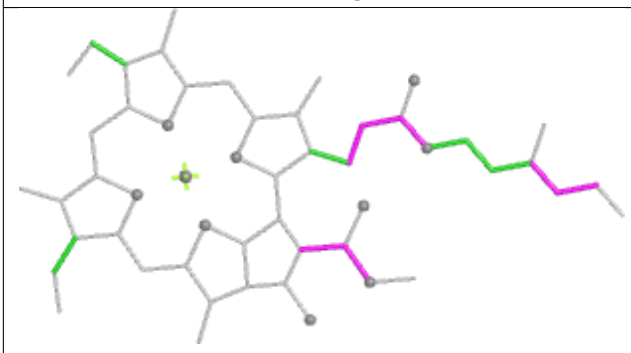
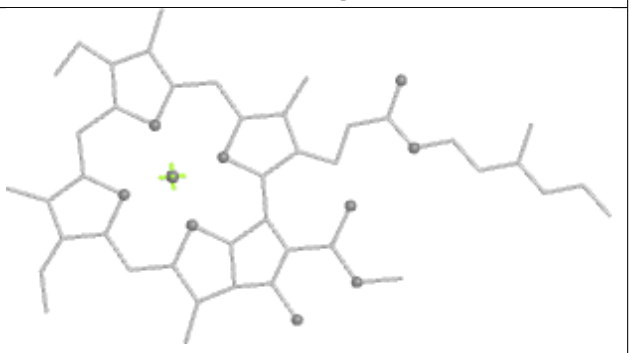
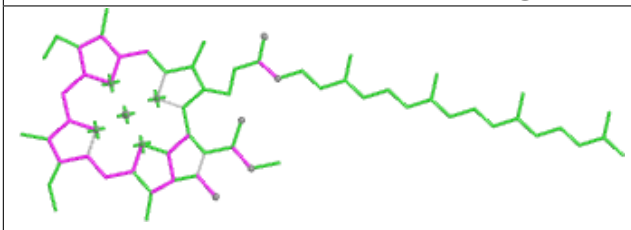
	
Torsions	Rings

Ligand CLA cB 840



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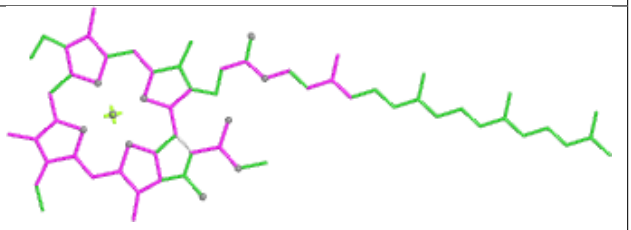
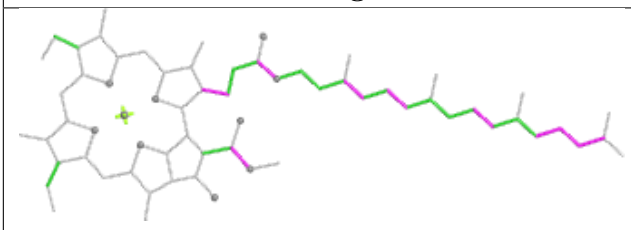
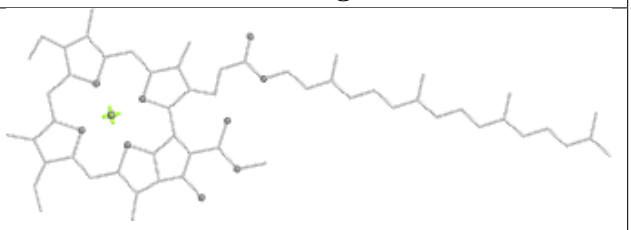


Bond angles

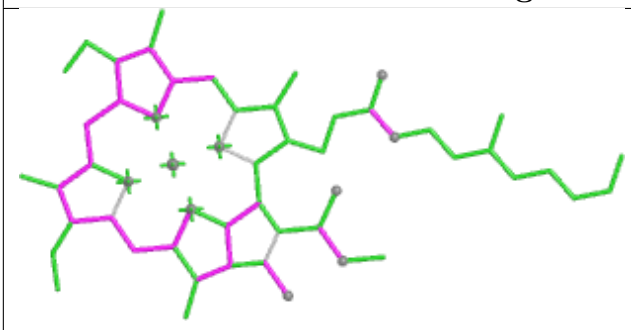


Torsions



Rings

Ligand CLA cA 817



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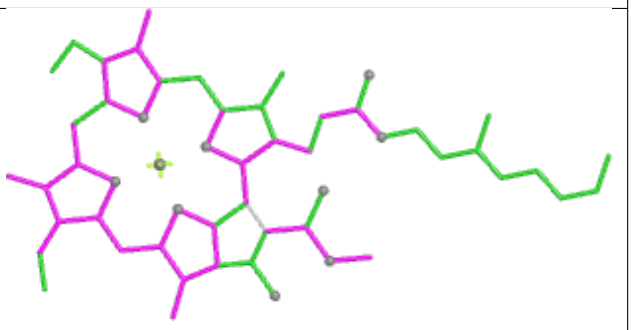

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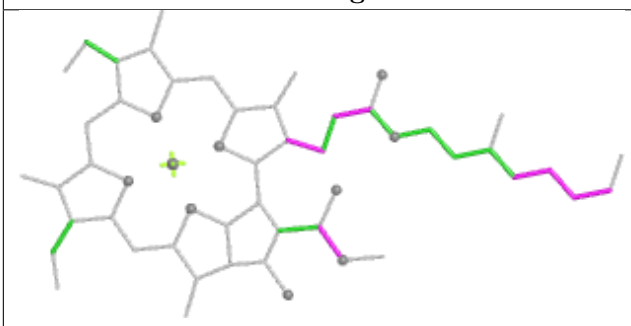

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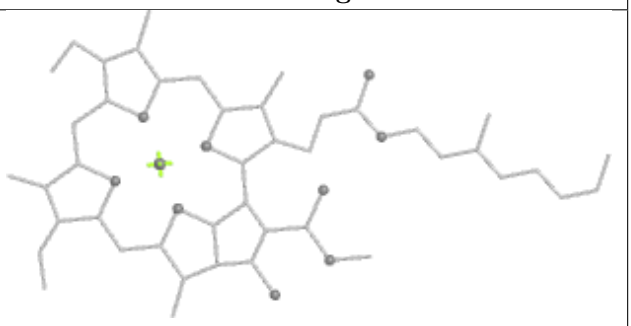
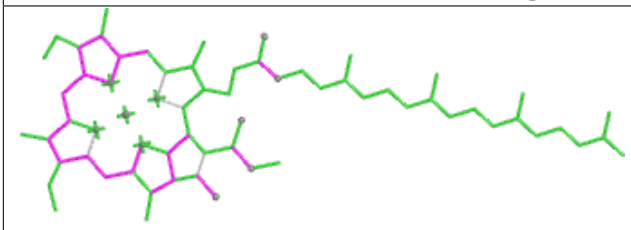


Rings

Ligand CLA A 840



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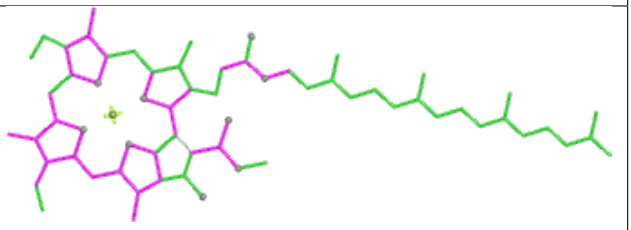

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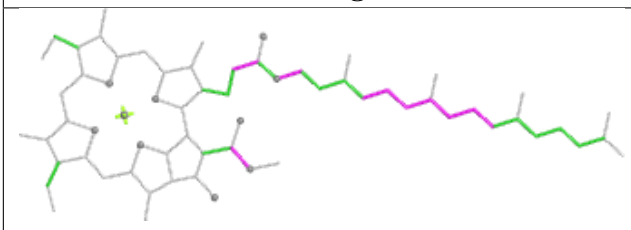

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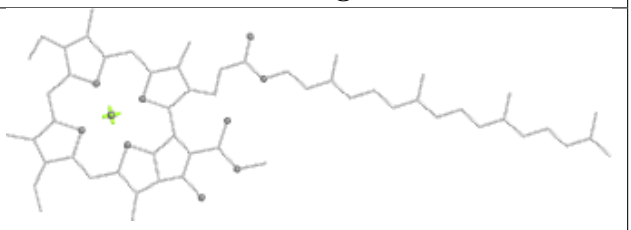
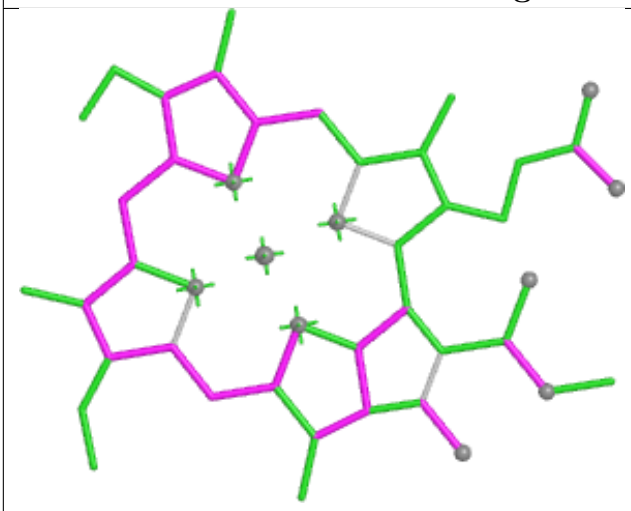


Rings

Ligand CLA bA 842



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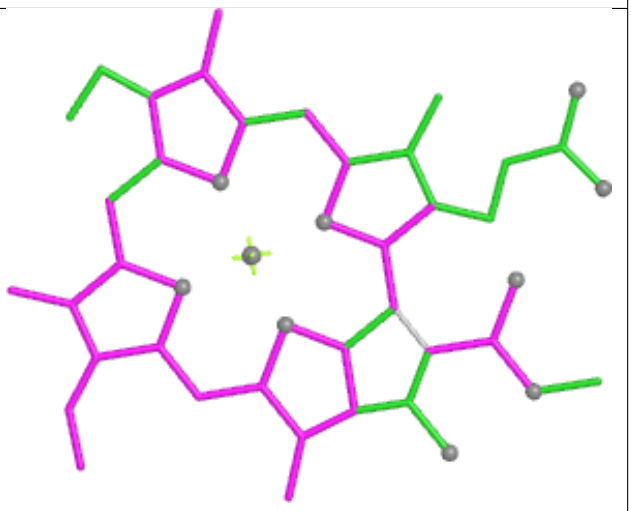
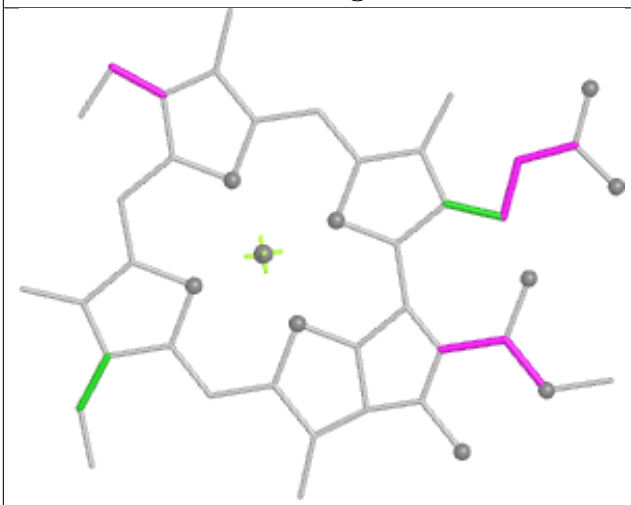


Bond angles



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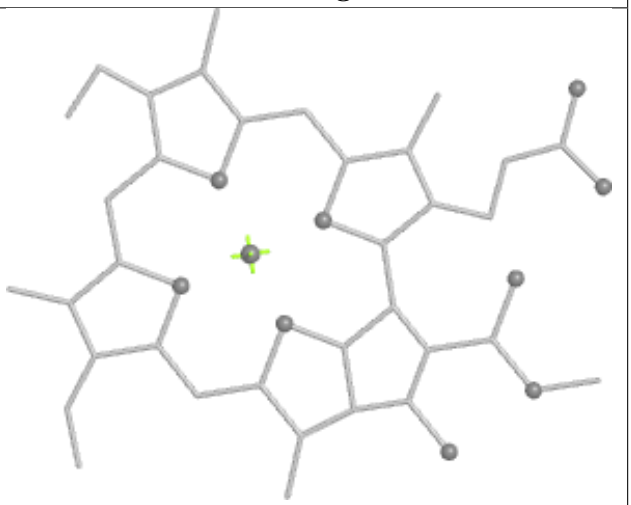
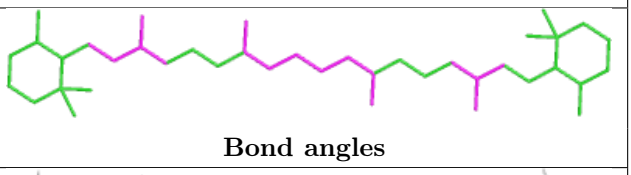
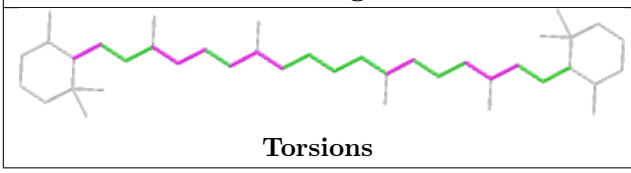


Rings

Ligand BCR cB 845

Bond lengths


Bond angles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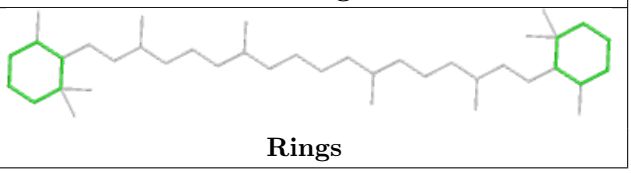
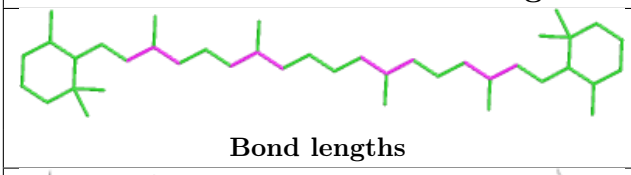

Rings

Ligand BCR L 205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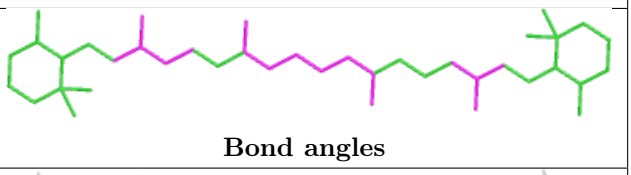
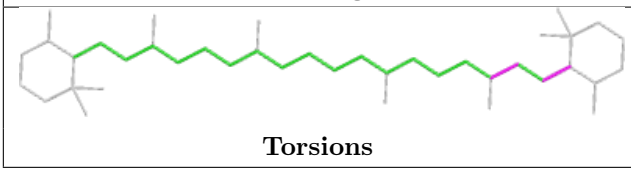
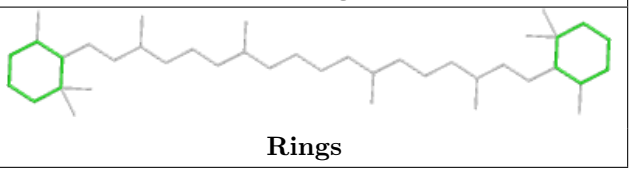
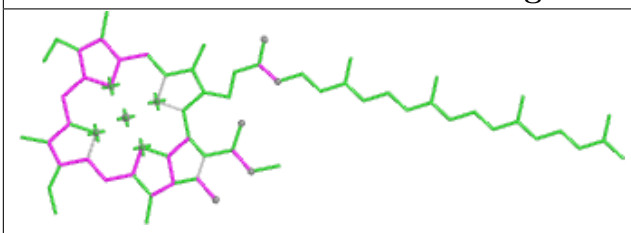

Bond angles


Torsions


Rings

Ligand CLA B 827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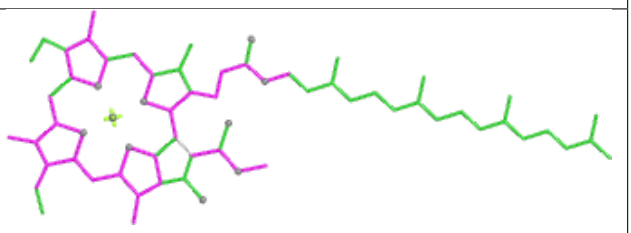
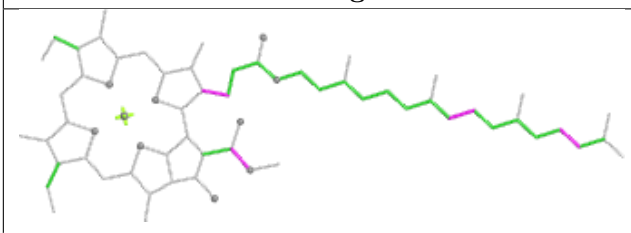

Bond angles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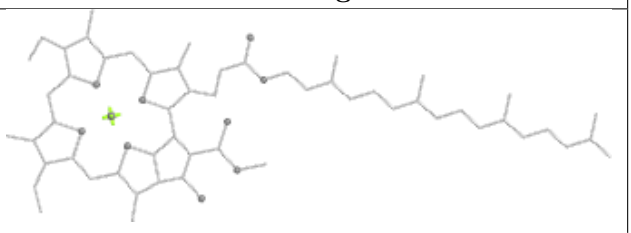
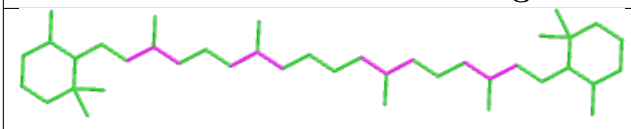

Rings

Ligand BCR bB 844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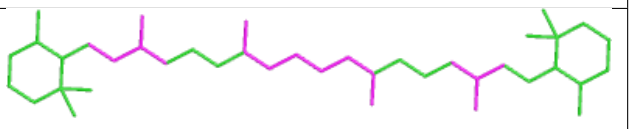
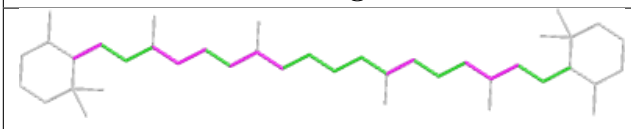
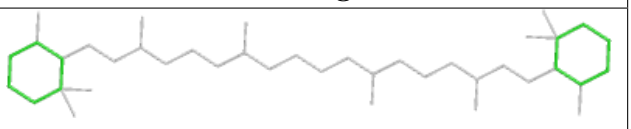
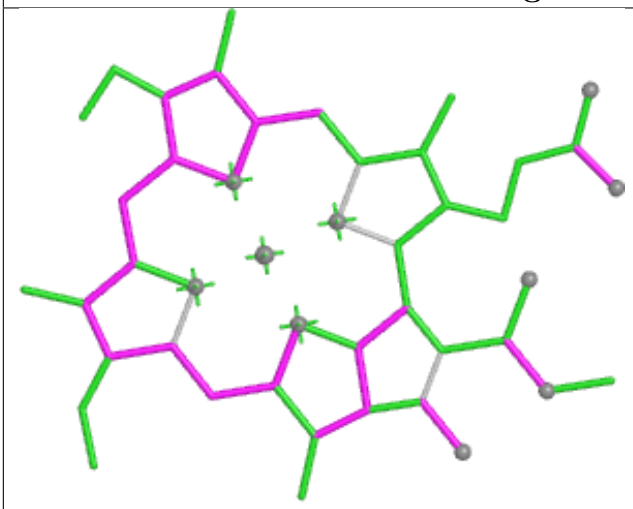

Bond angles


Torsions


Rings

Ligand CLA A 816



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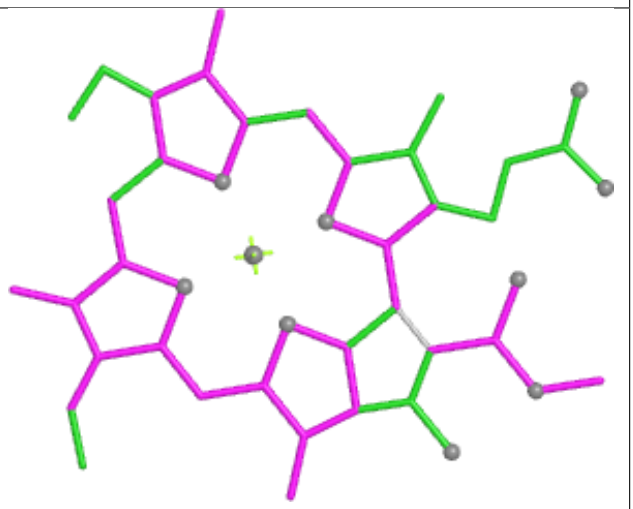
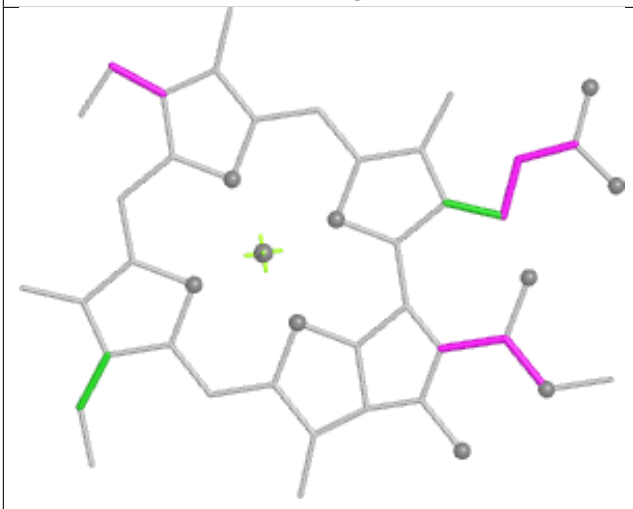


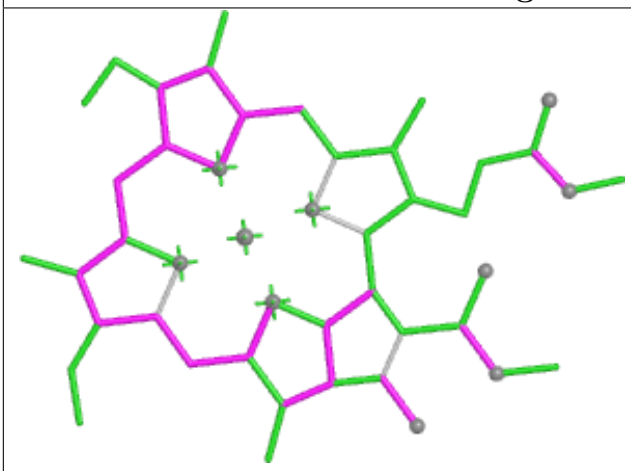
Bond angles



Torsions

Rings

Ligand CLA cB 825



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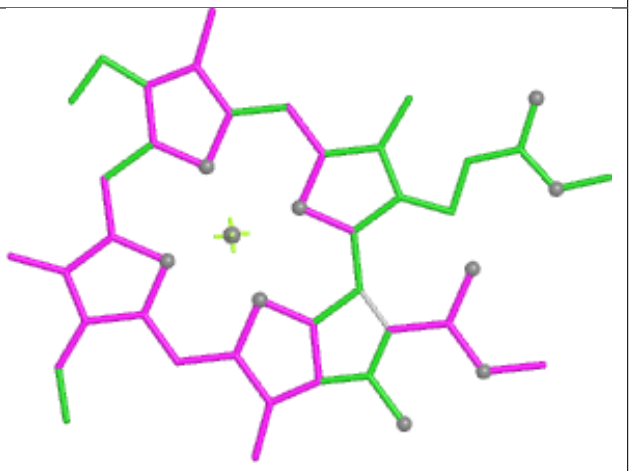

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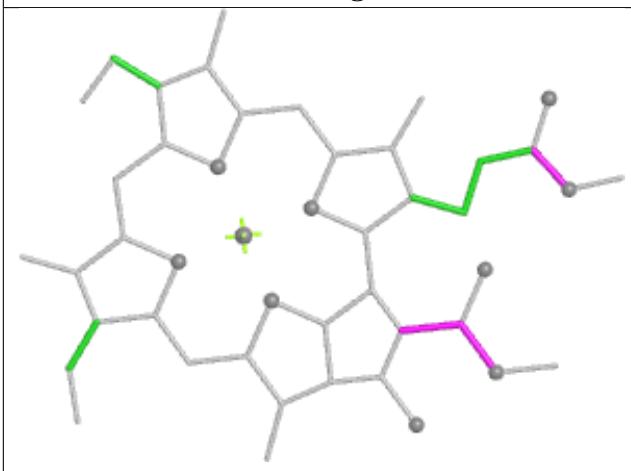

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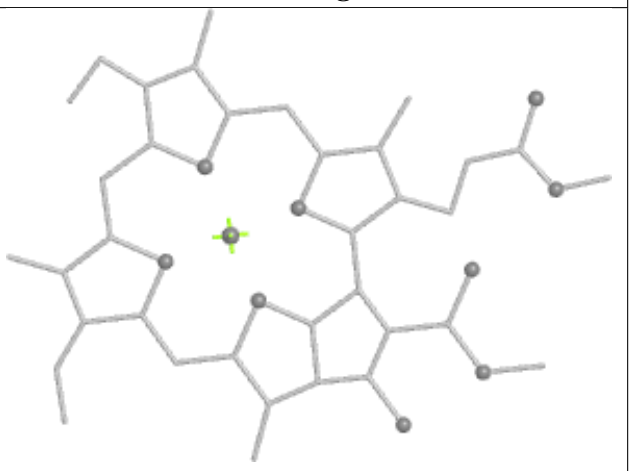
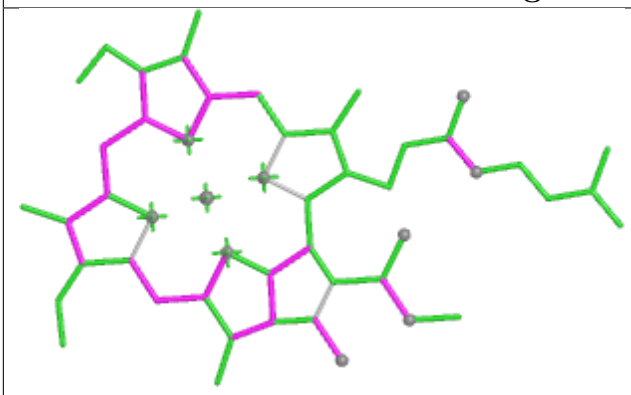


Rings

Ligand CLA A 830



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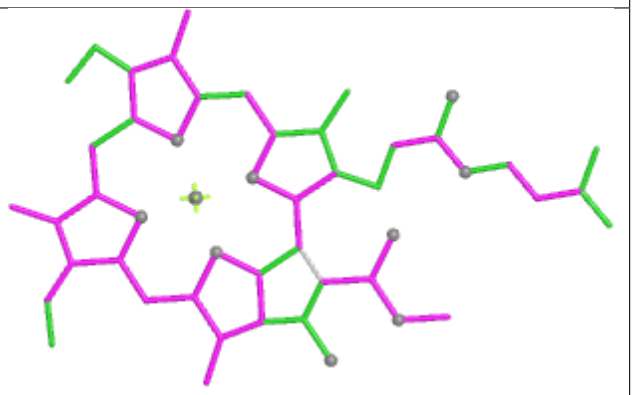

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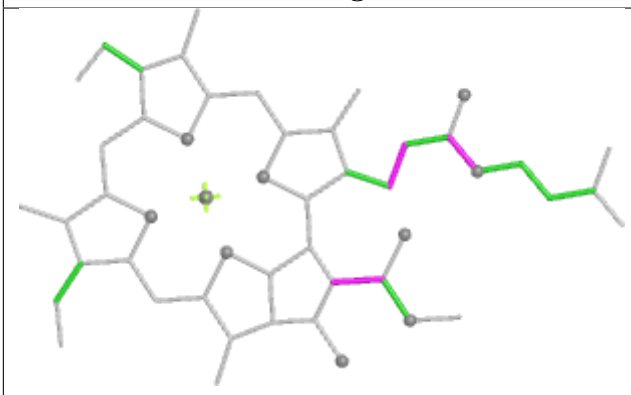

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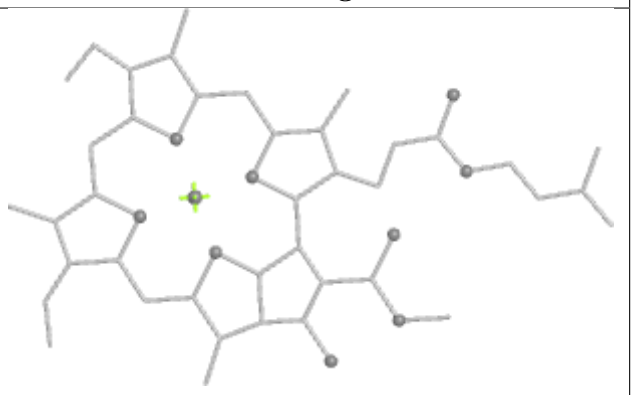
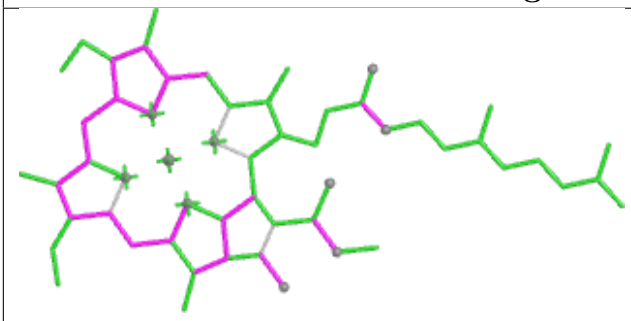


Rings

Ligand CLA A 831



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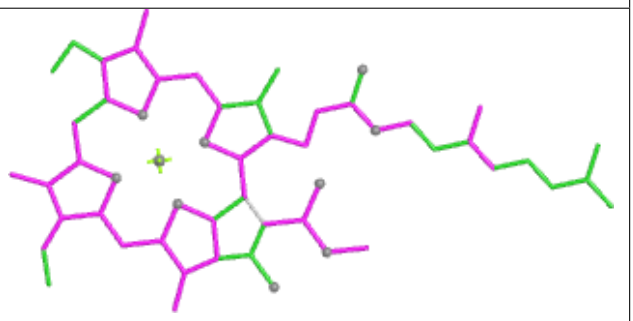
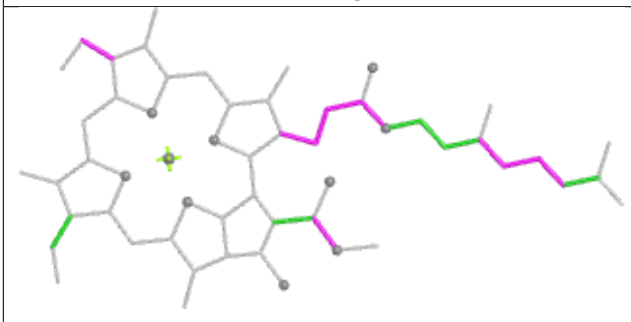


Bond angles



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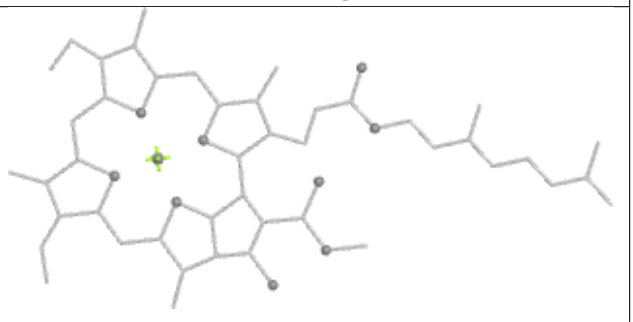
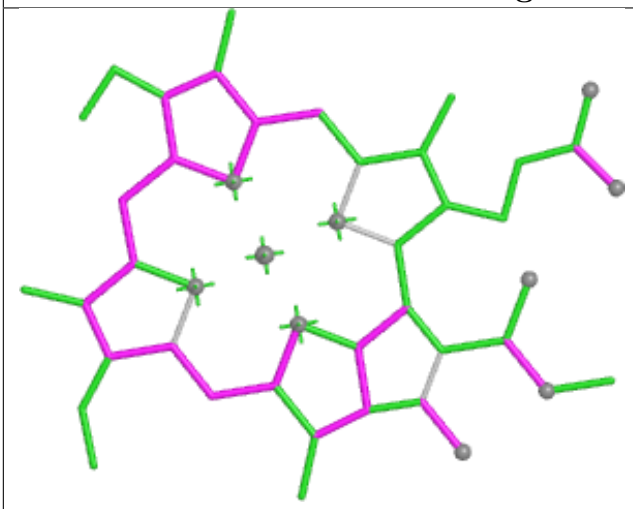


Rings

Ligand CLA cA 812



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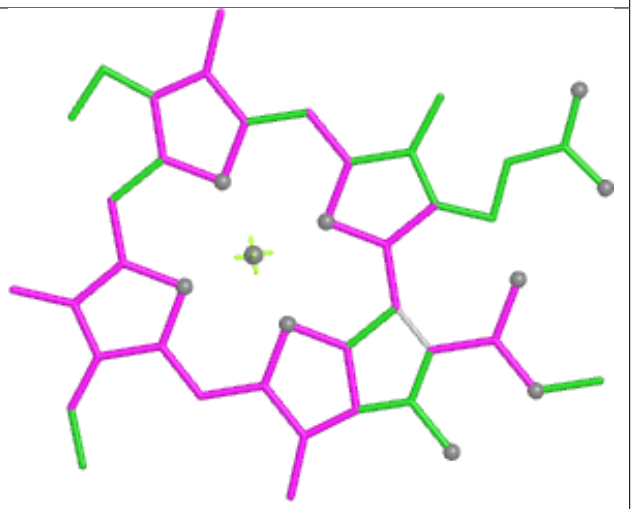
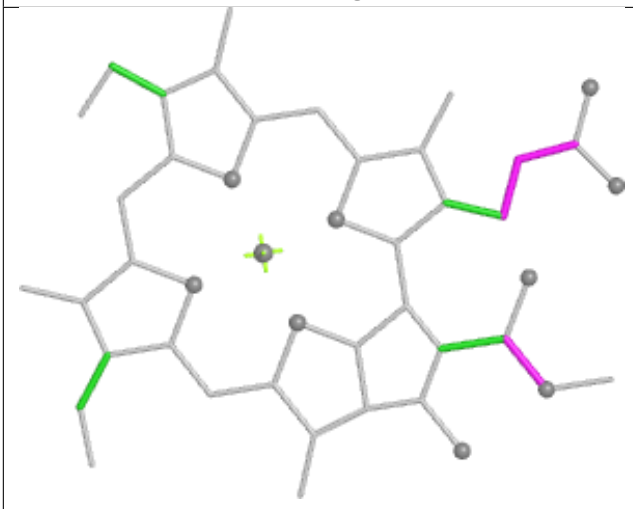


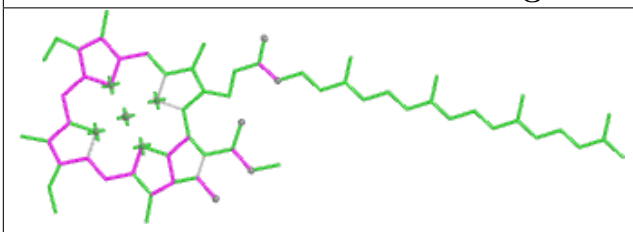
Bond angles



Torsions

Rings

Ligand CLA A 806



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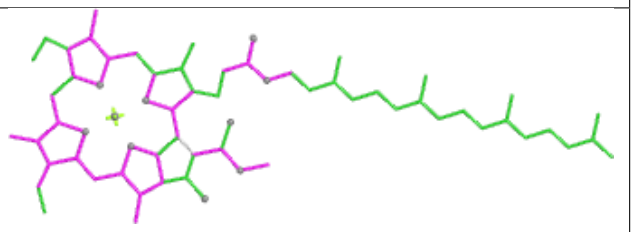
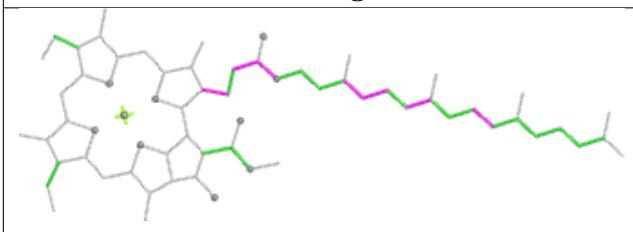


Bond angles



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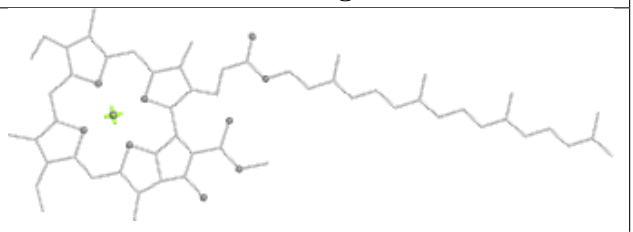
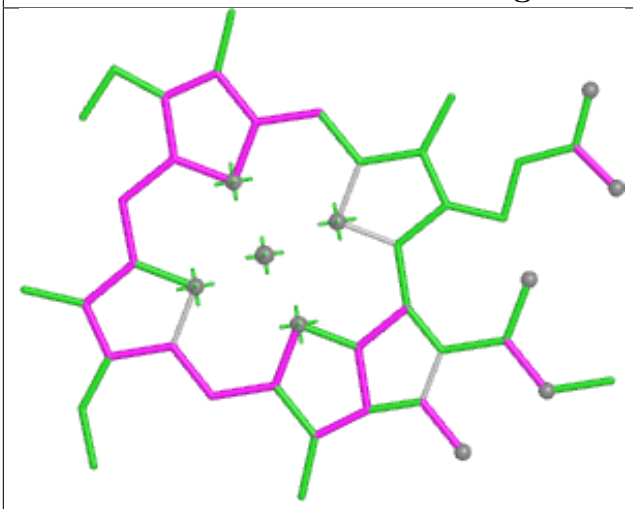


Rings

Ligand CLA bA 823



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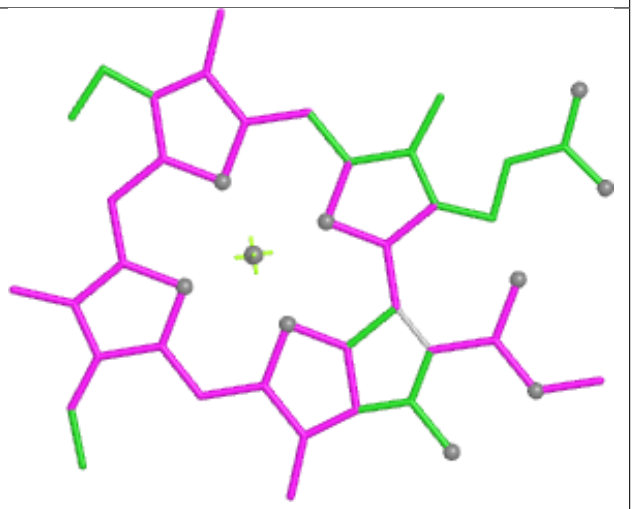
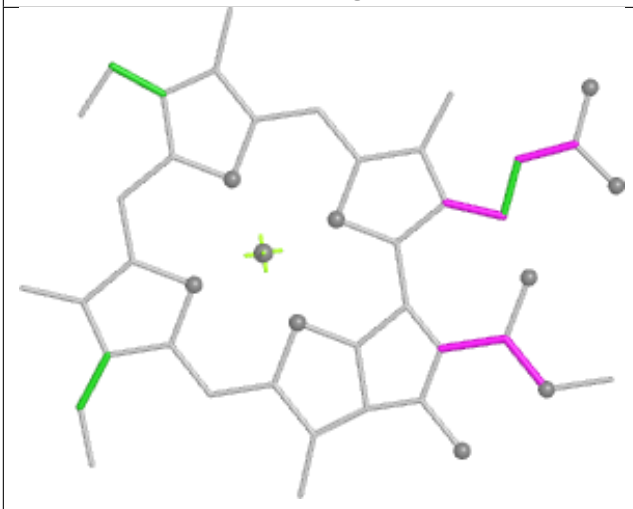


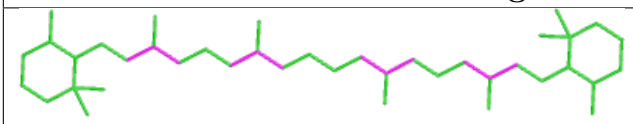
Bond angles



Torsions

Rings

Ligand BCR bM 101



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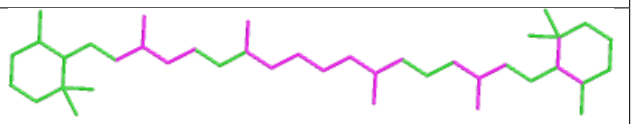
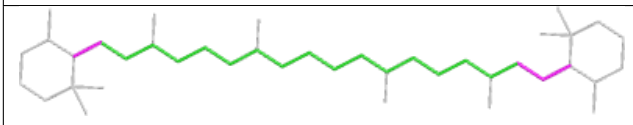


Bond angles



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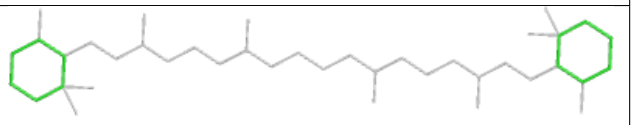
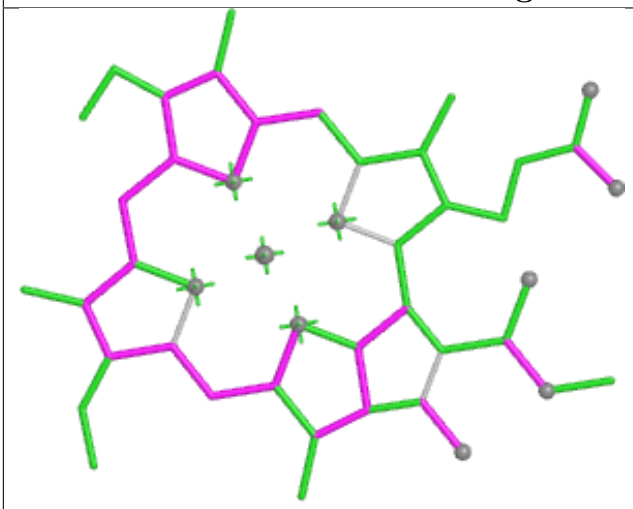


Rings

Ligand CLA cA 842



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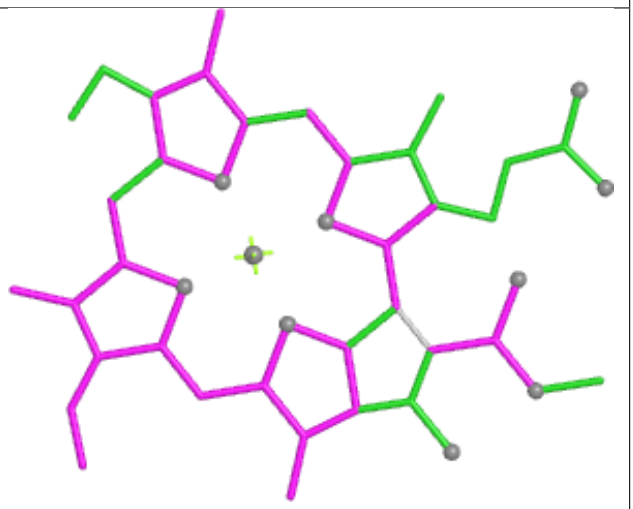
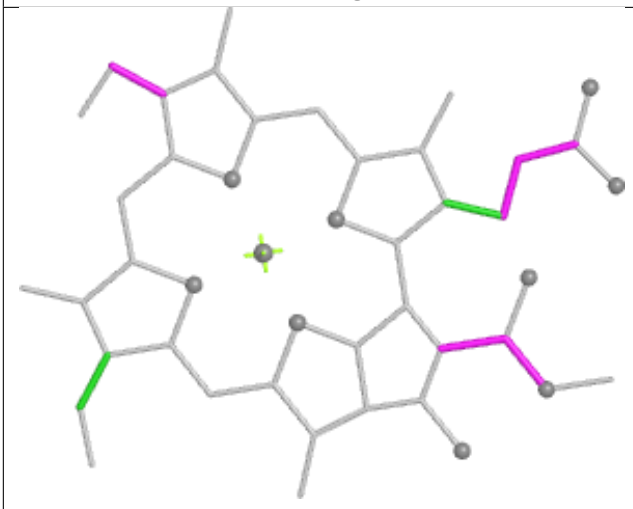


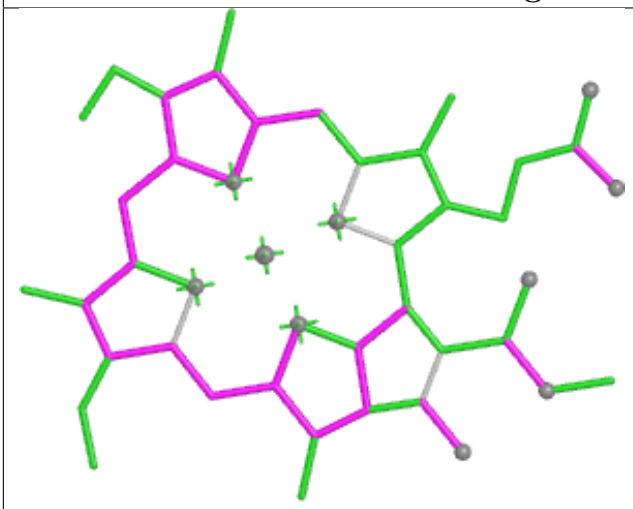
Bond angles



Torsions

Rings

Ligand CLA B 849



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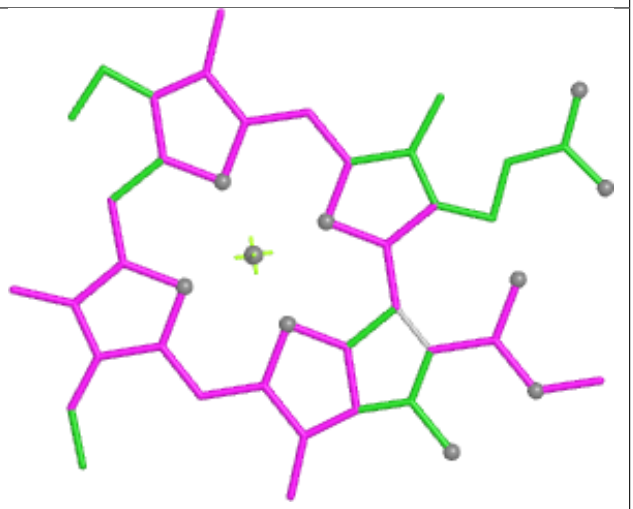
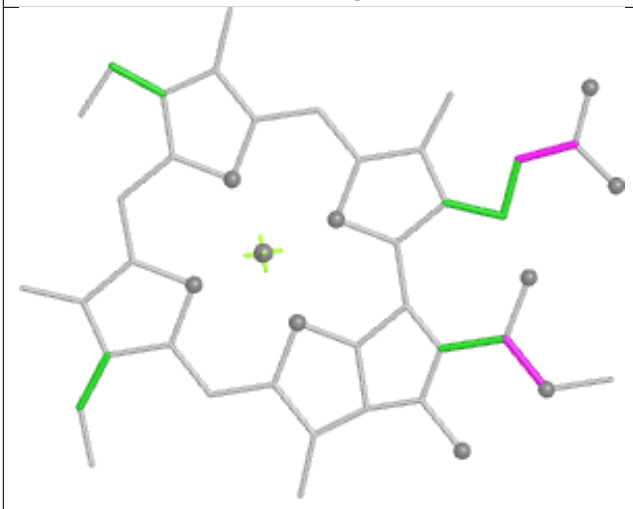


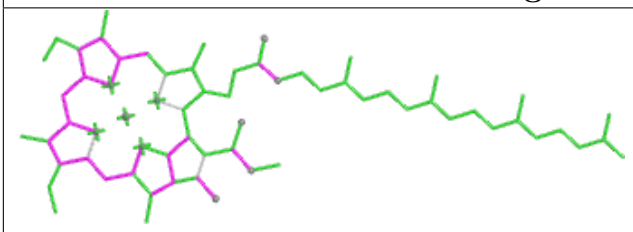
Bond angles



Torsions

Rings

Ligand CLA B 826



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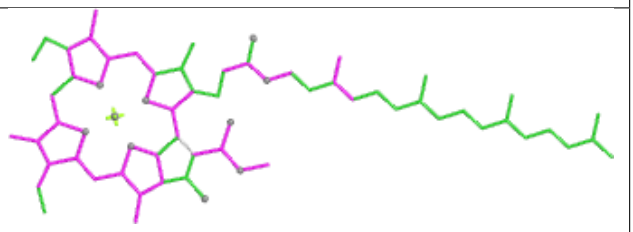

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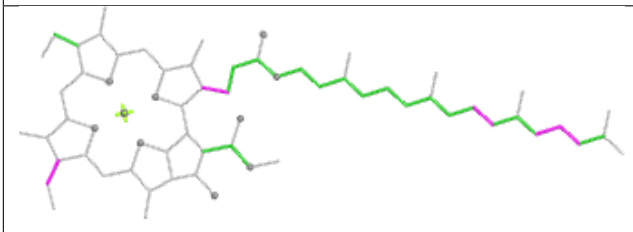
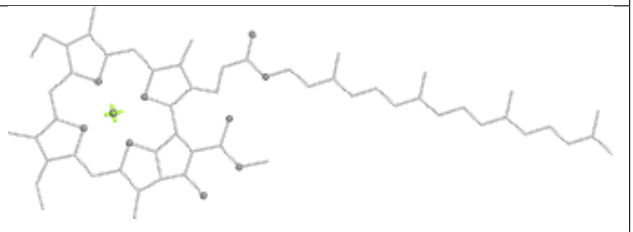
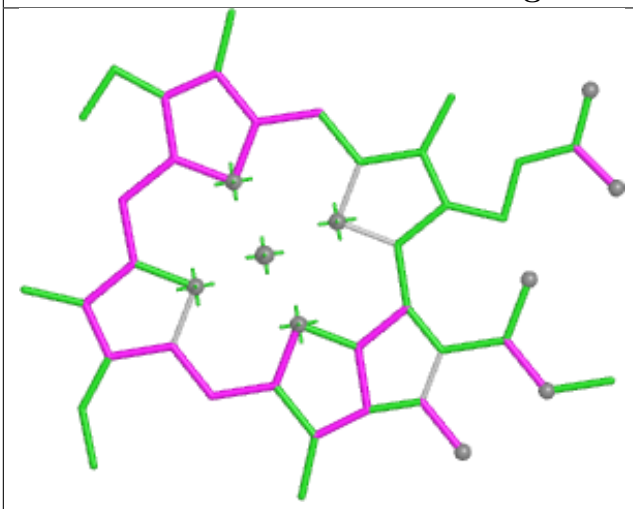


Torsions



Rings

Ligand CLA A 814



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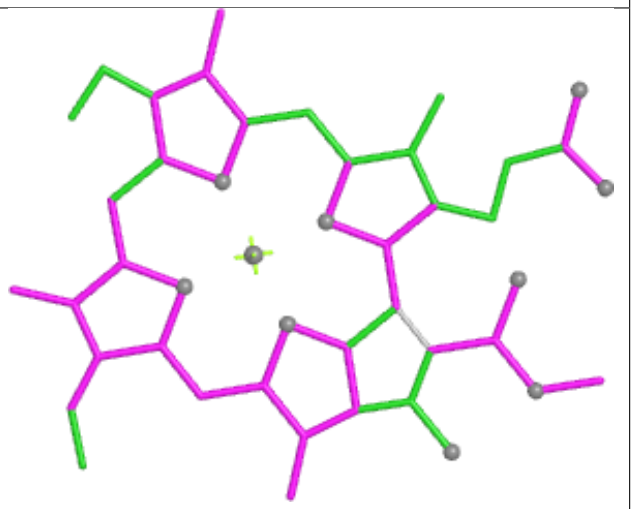
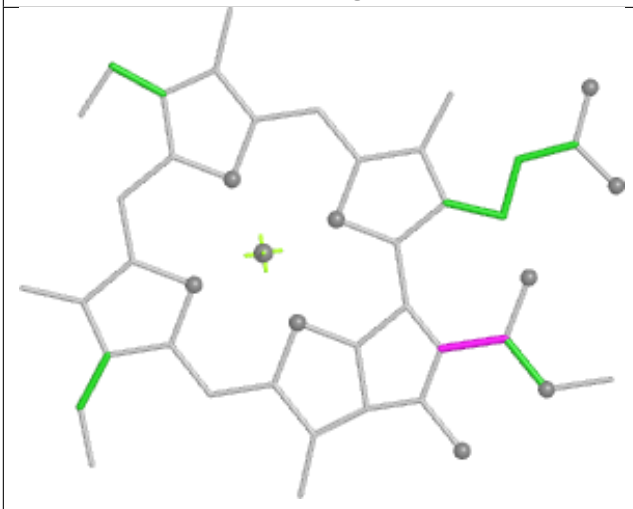


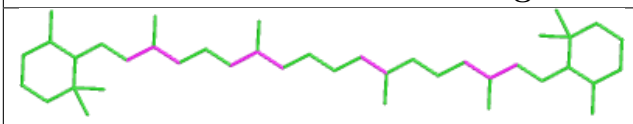
Bond angles



Torsions

Rings

Ligand BCR cA 845



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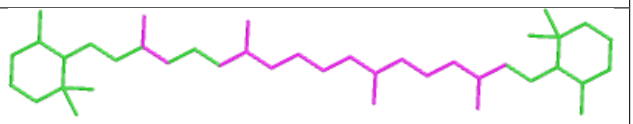
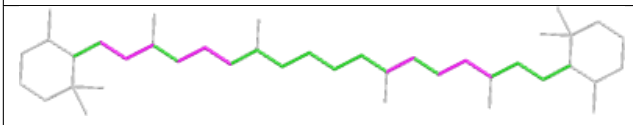


Bond angles



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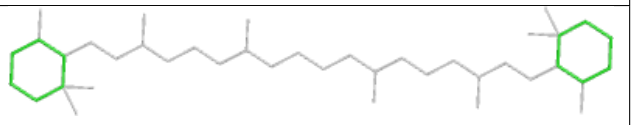
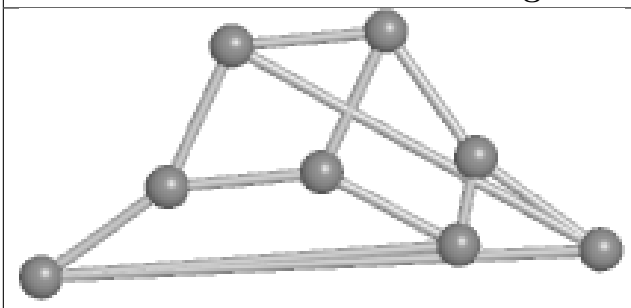


Rings

Ligand SF4 cC 101



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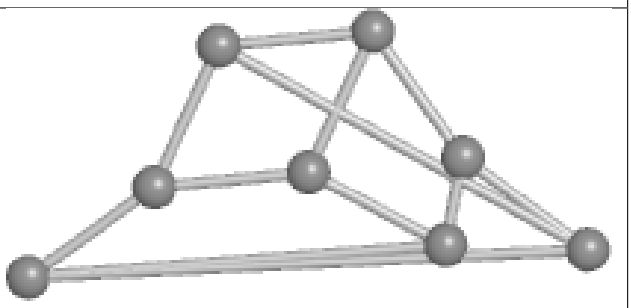
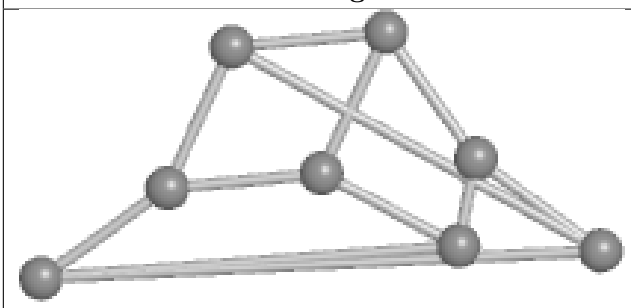


Bond angles



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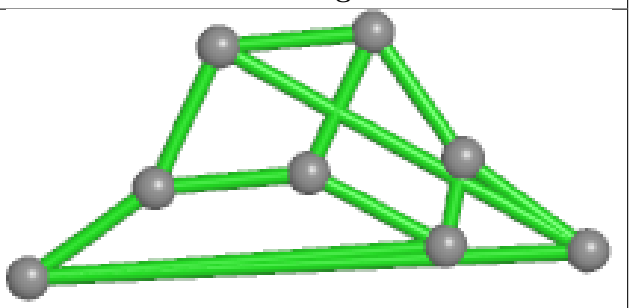
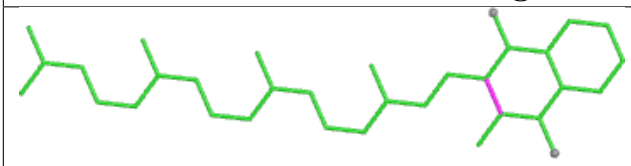
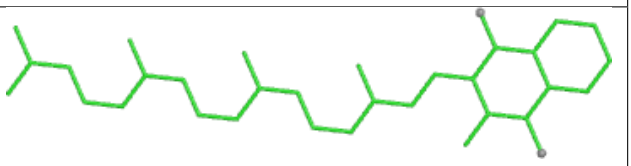


Rings

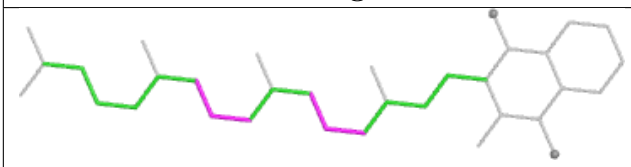
Ligand PQN bB 840



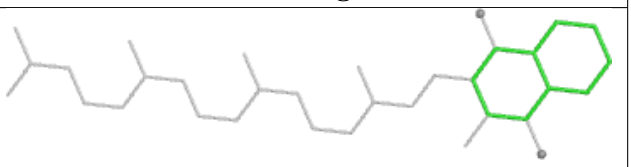
Bond lengths



Bond angles

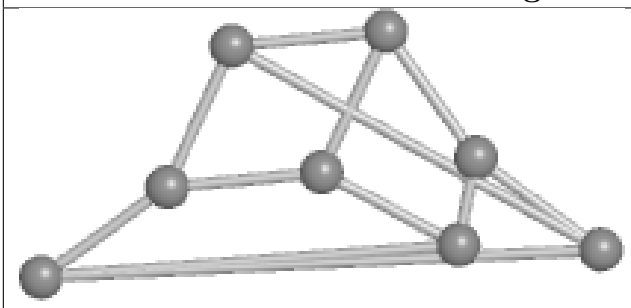


Torsions

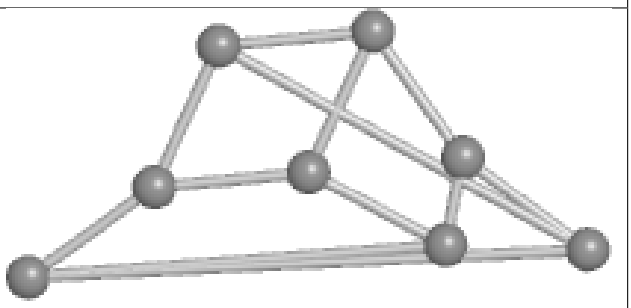


Rings

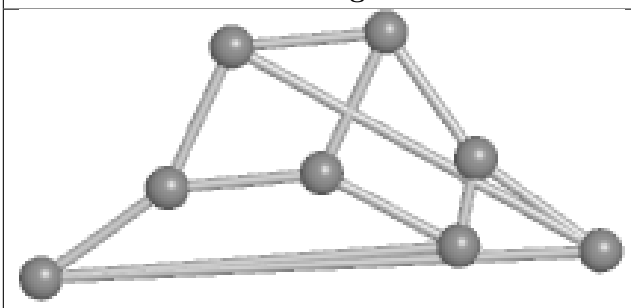
Ligand SF4 cC 102



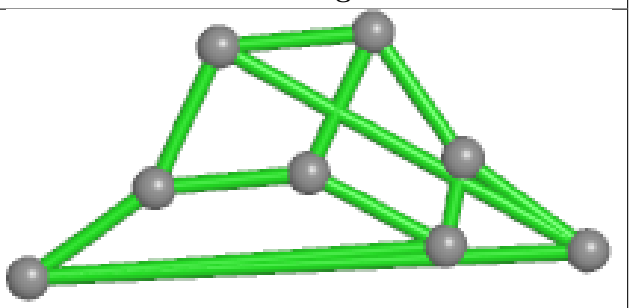
Bond lengths



Bond angles

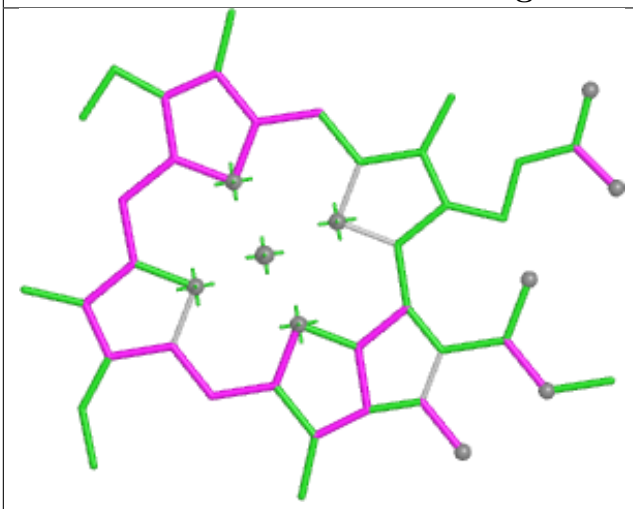


Torsions

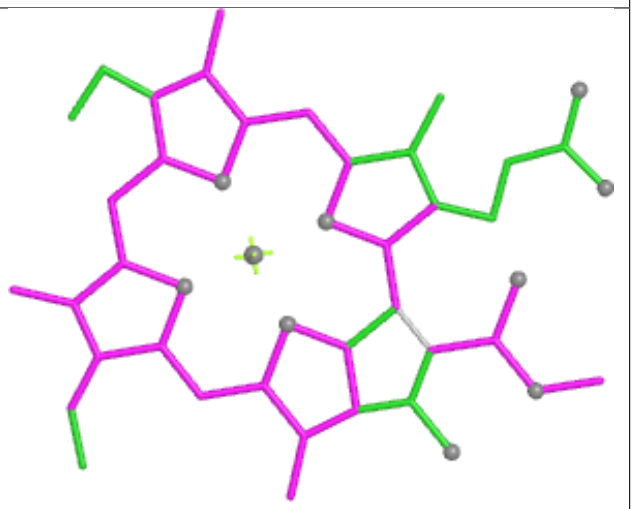


Rings

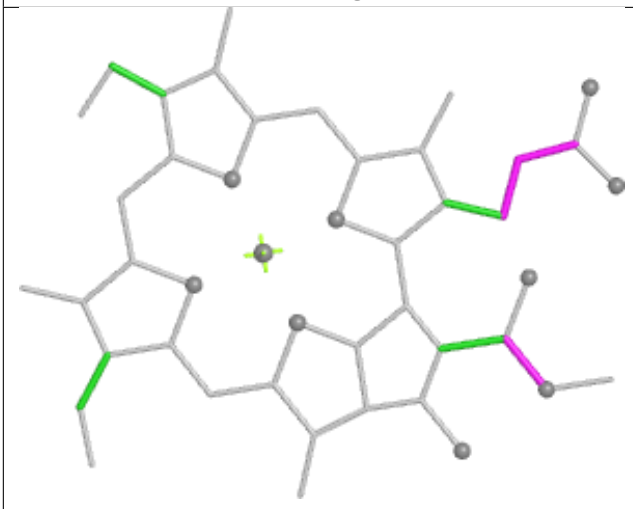
Ligand CLA cA 835



Bond lengths



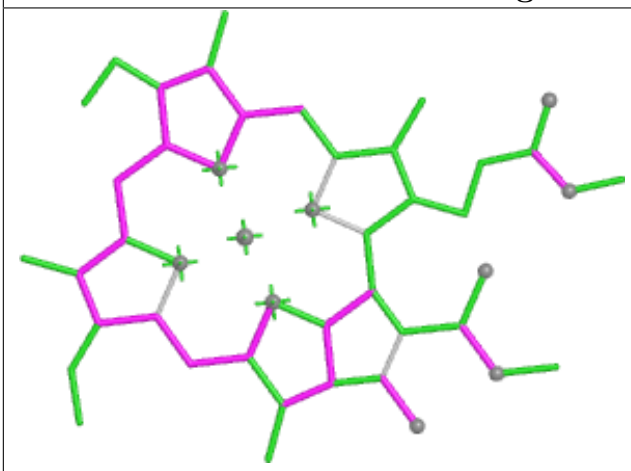
Bond angles



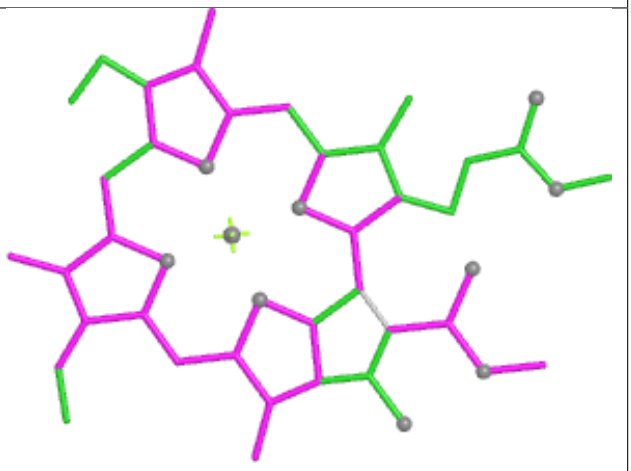
Torsions

Rings

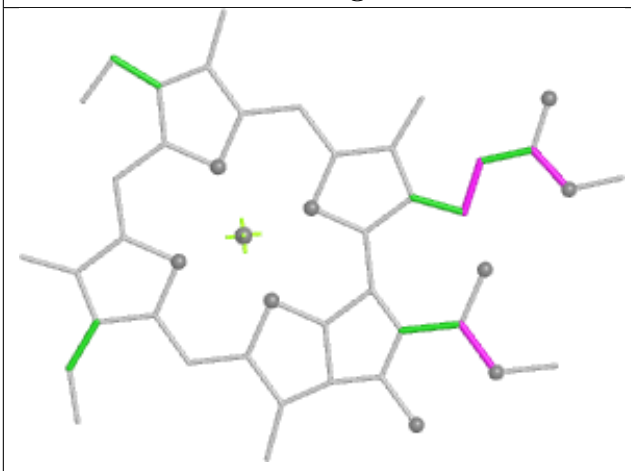
Ligand CLA cB 819



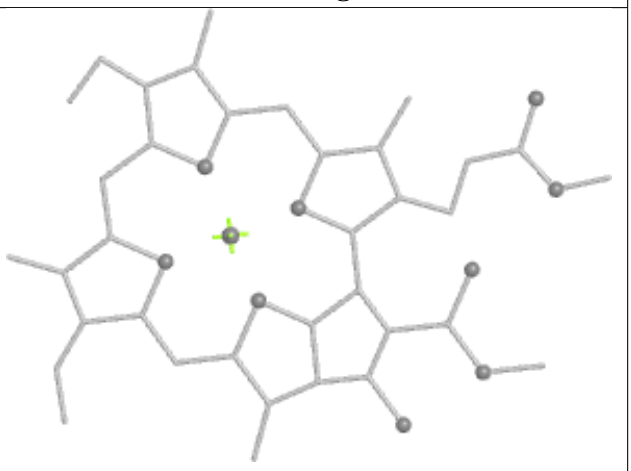
Bond lengths



Bond angles

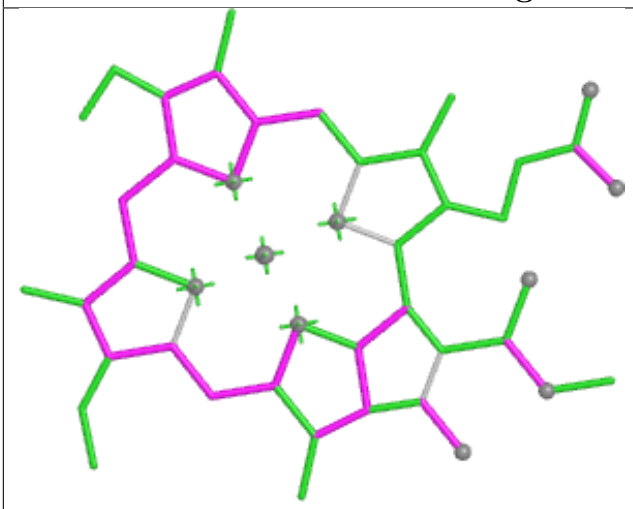


Torsions

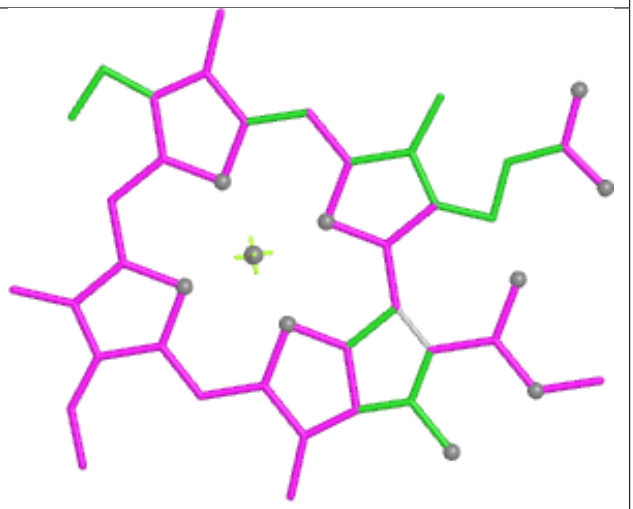


Rings

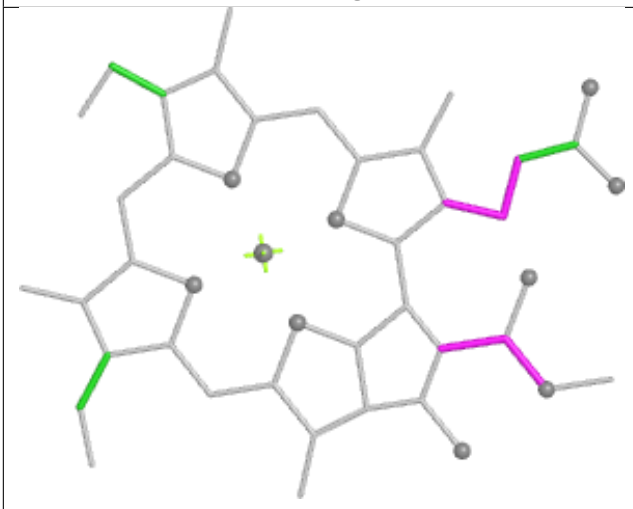
Ligand CLA cA 808



Bond lengths



Bond angles



Torsions

Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

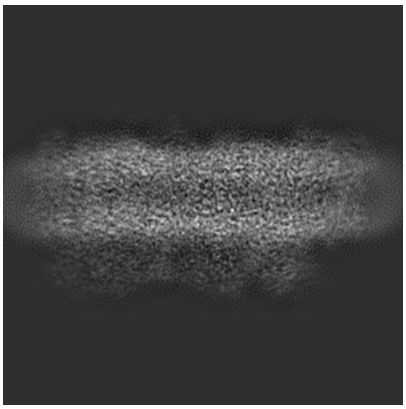
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-62693. These allow visual inspection of the internal detail of the map and identification of artifacts.

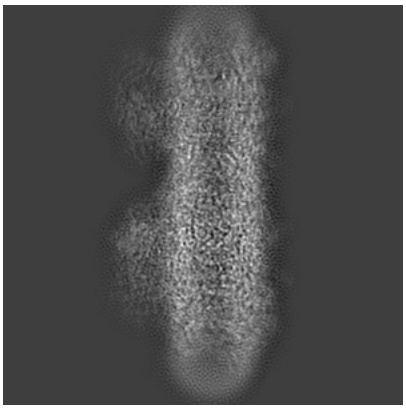
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

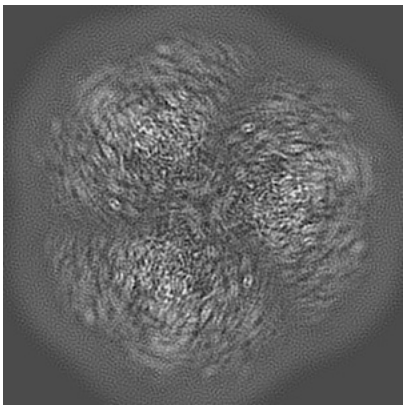
6.1.1 Primary map



X

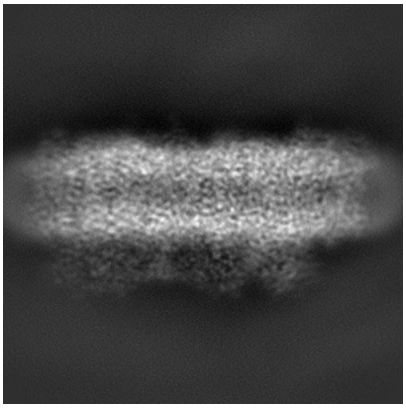


Y

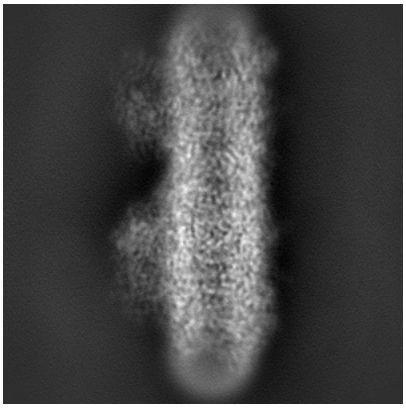


Z

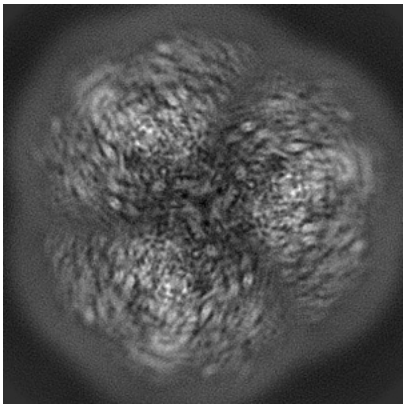
6.1.2 Raw map



X



Y

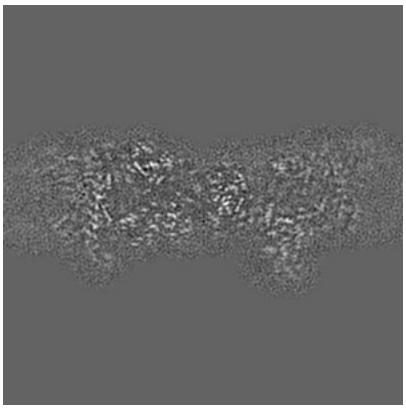


Z

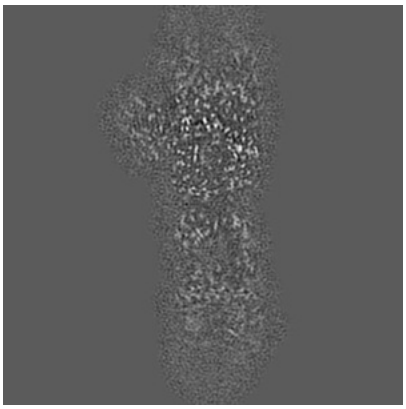
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

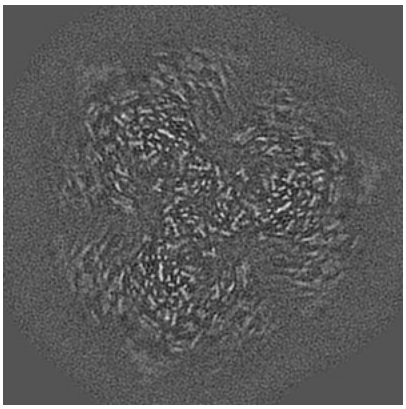
6.2.1 Primary map



X Index: 148

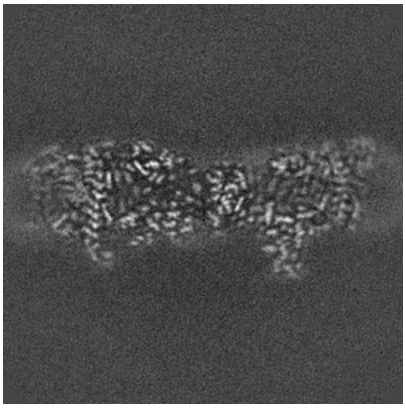


Y Index: 148

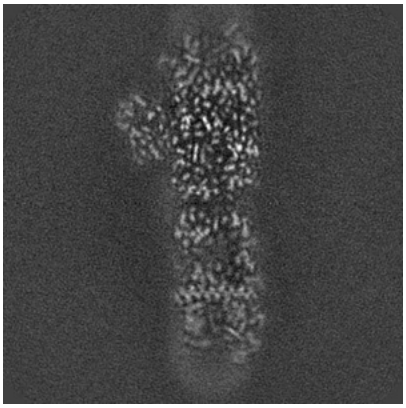


Z Index: 148

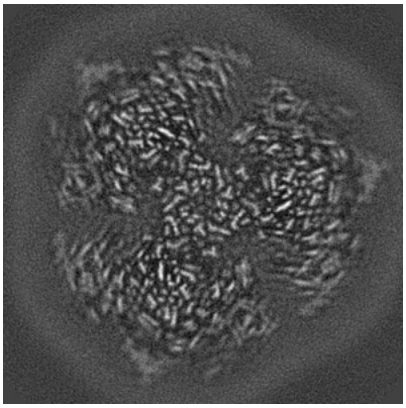
6.2.2 Raw map



X Index: 148



Y Index: 148

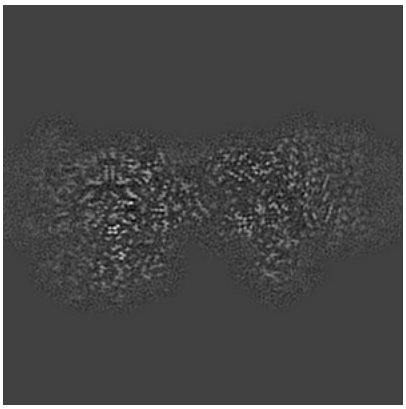


Z Index: 148

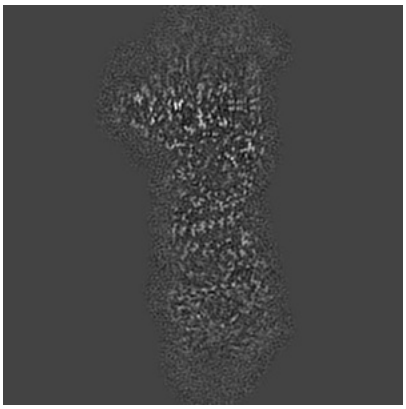
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

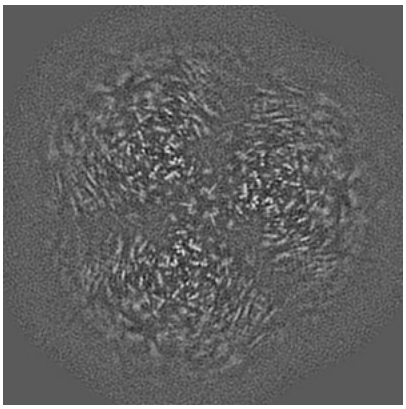
6.3.1 Primary map



X Index: 122

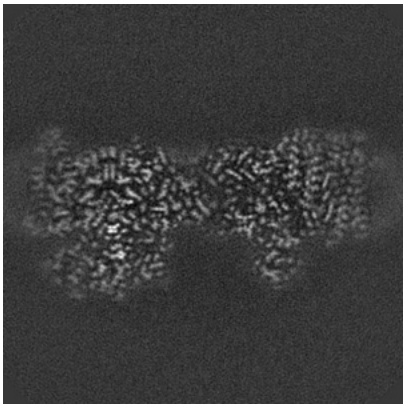


Y Index: 160

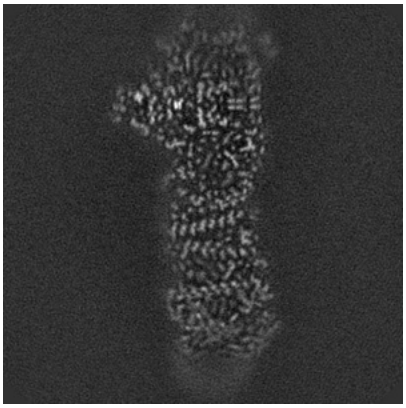


Z Index: 171

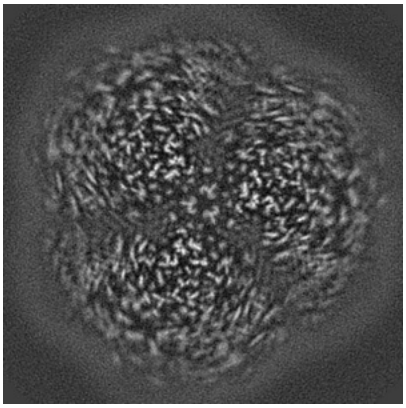
6.3.2 Raw map



X Index: 122



Y Index: 160

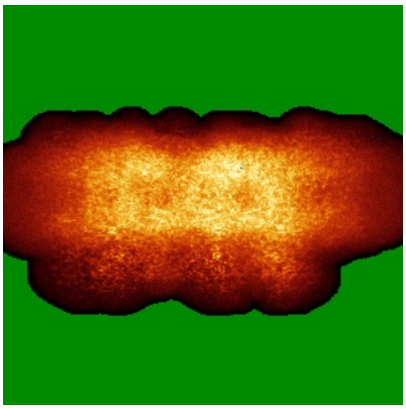


Z Index: 171

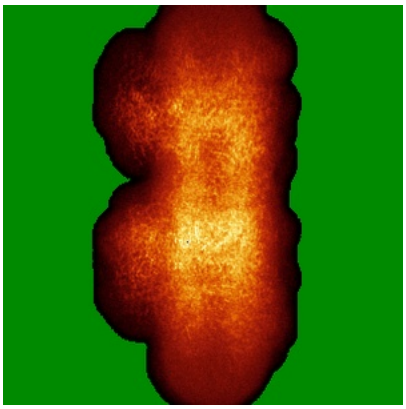
The images above show the largest variance slices of the map in three orthogonal directions.

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

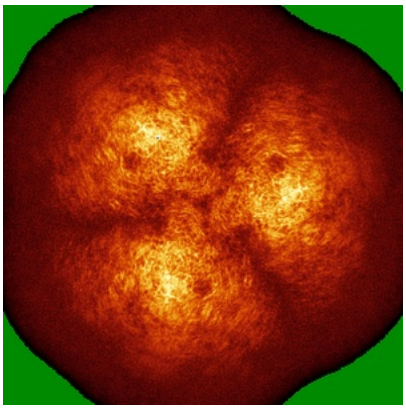
6.4.1 Primary map



X

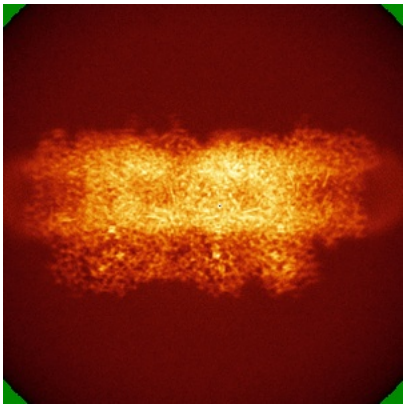


Y

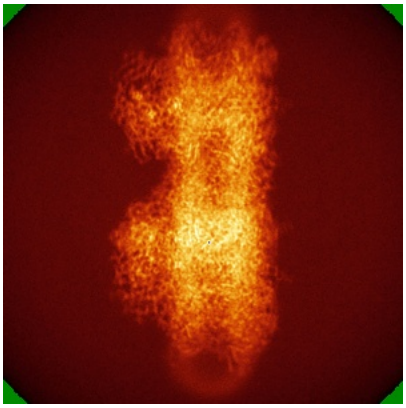


Z

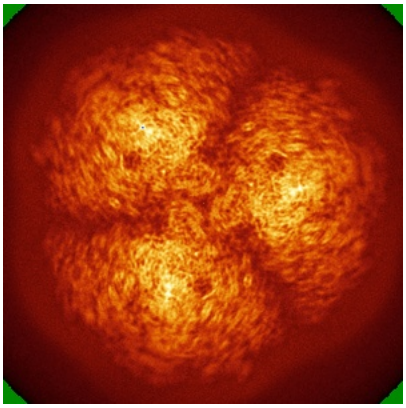
6.4.2 Raw map



X



Y

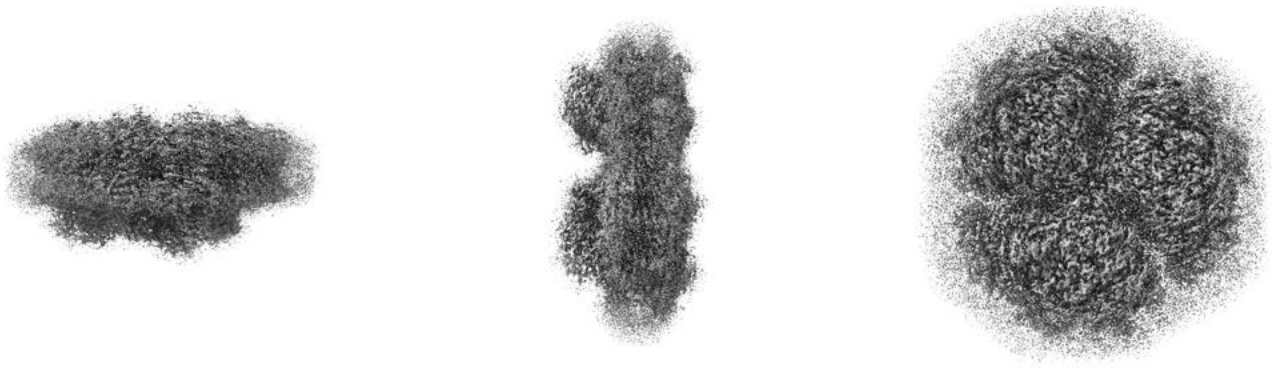


Z

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

6.5 Orthogonal surface views (i)

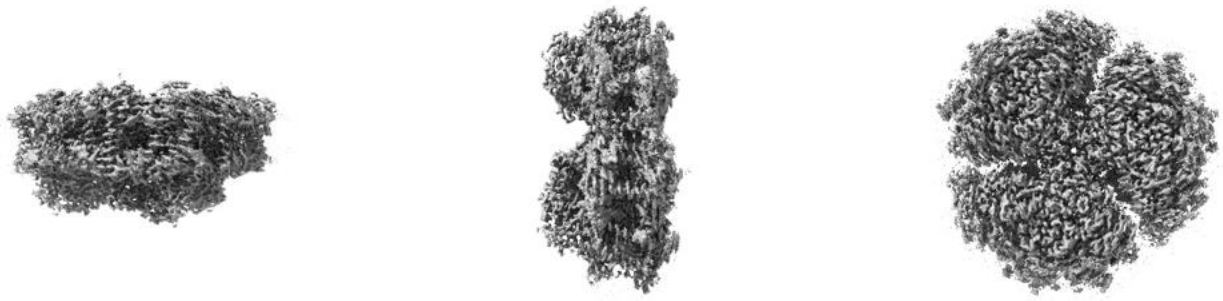
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

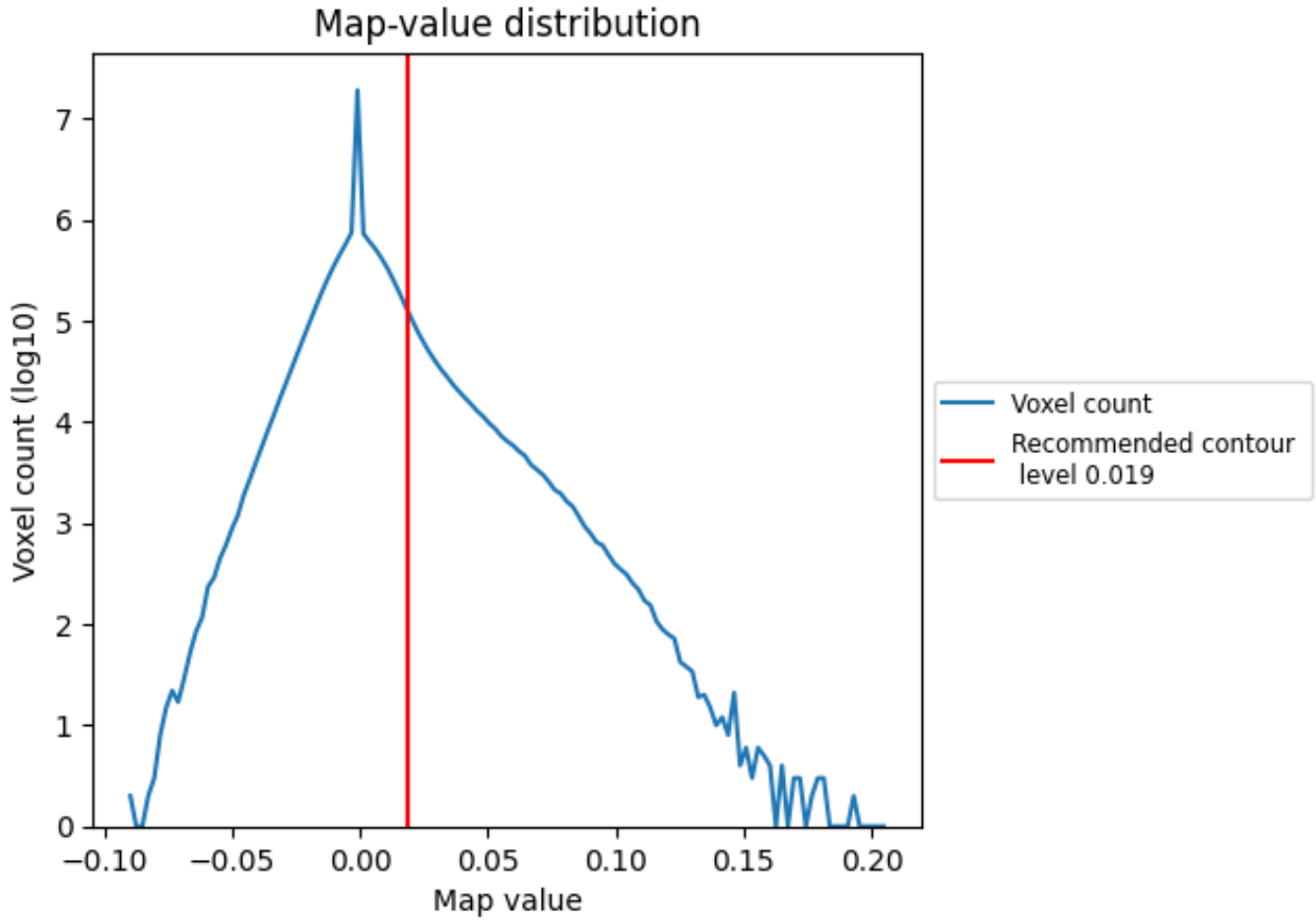
6.6 Mask visualisation (i)

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

7 Map analysis

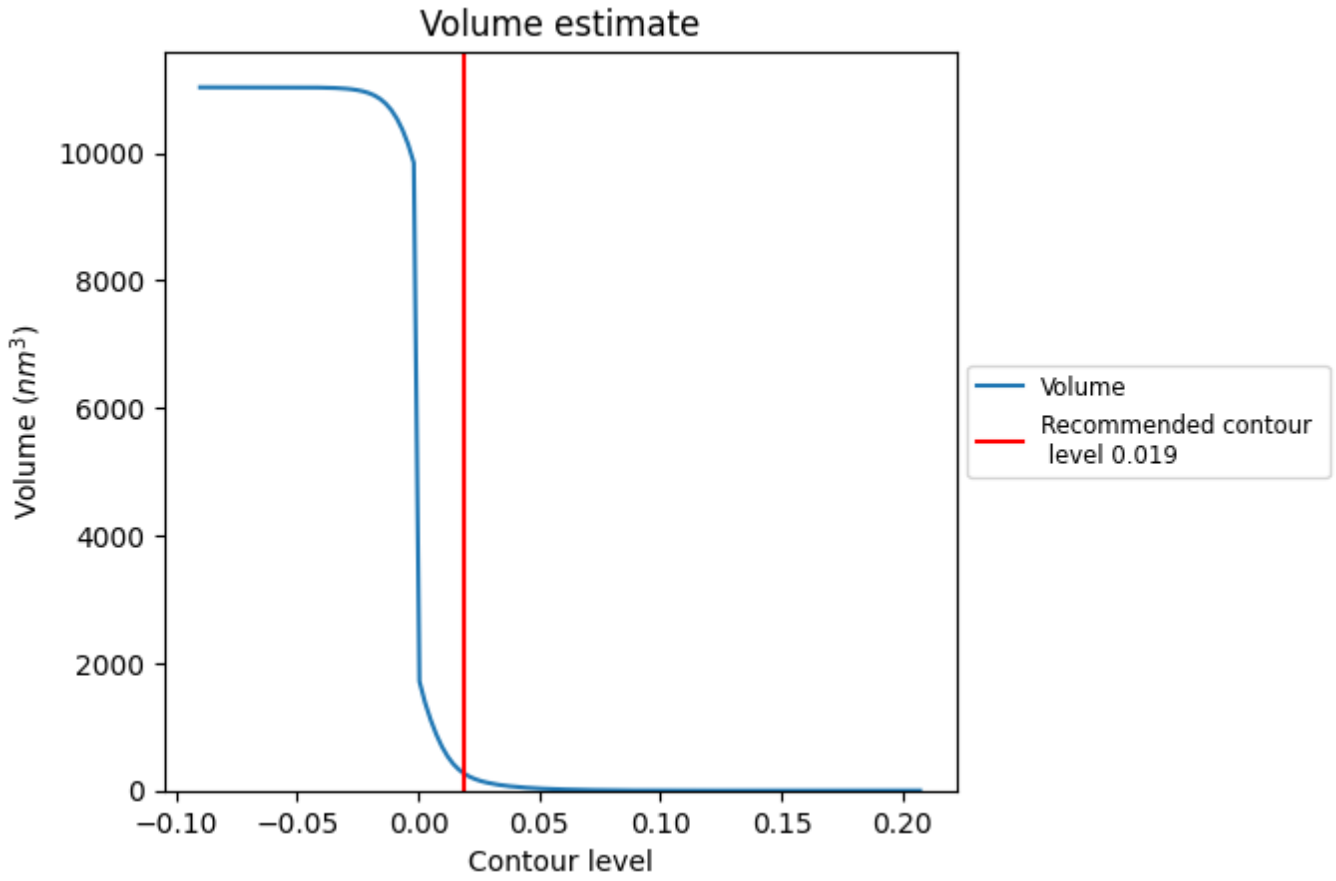
This section contains the results of statistical analysis of the map.

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.

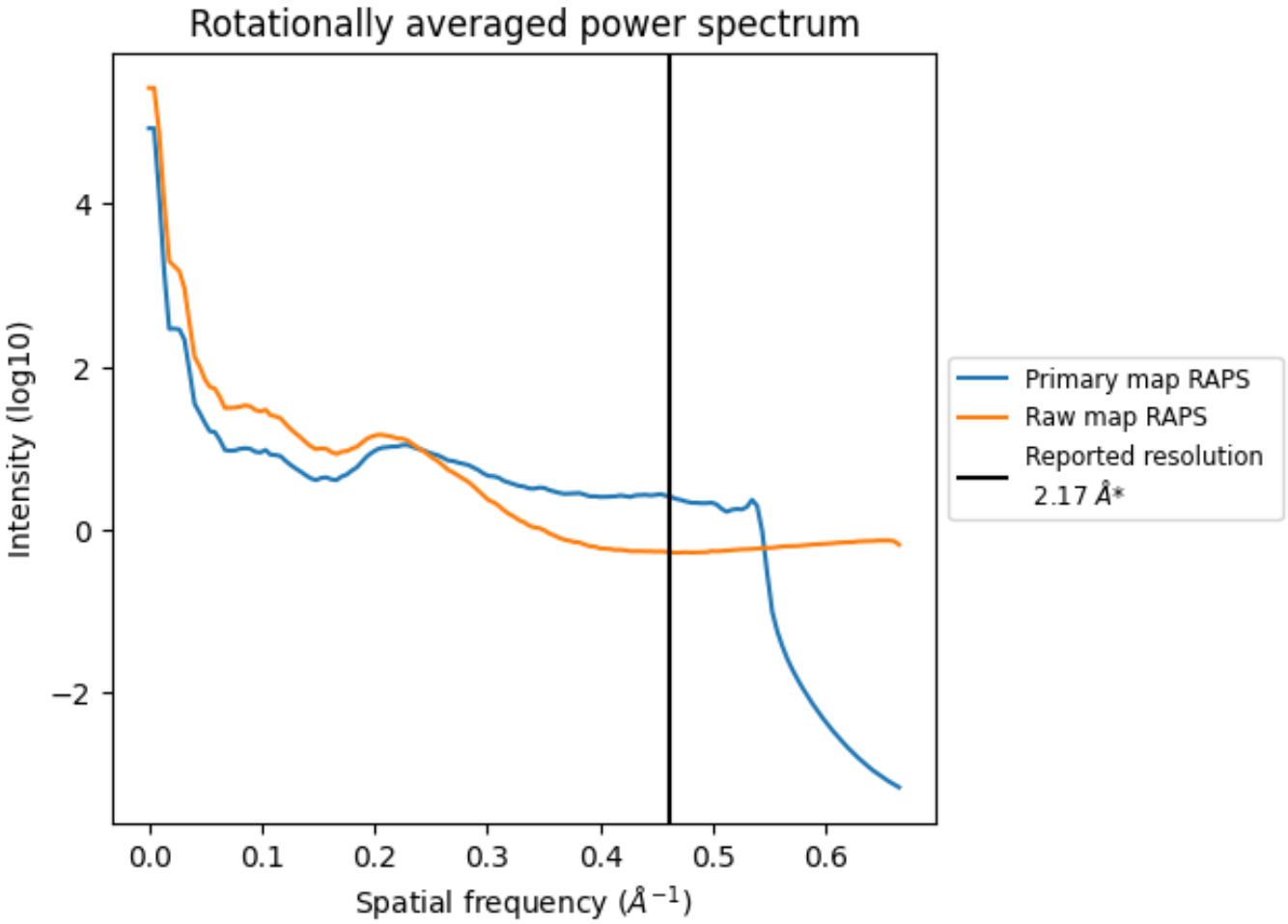
7.2 Volume estimate



The volume at the recommended contour level is 268 nm^3; this corresponds to an approximate mass of 242 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)

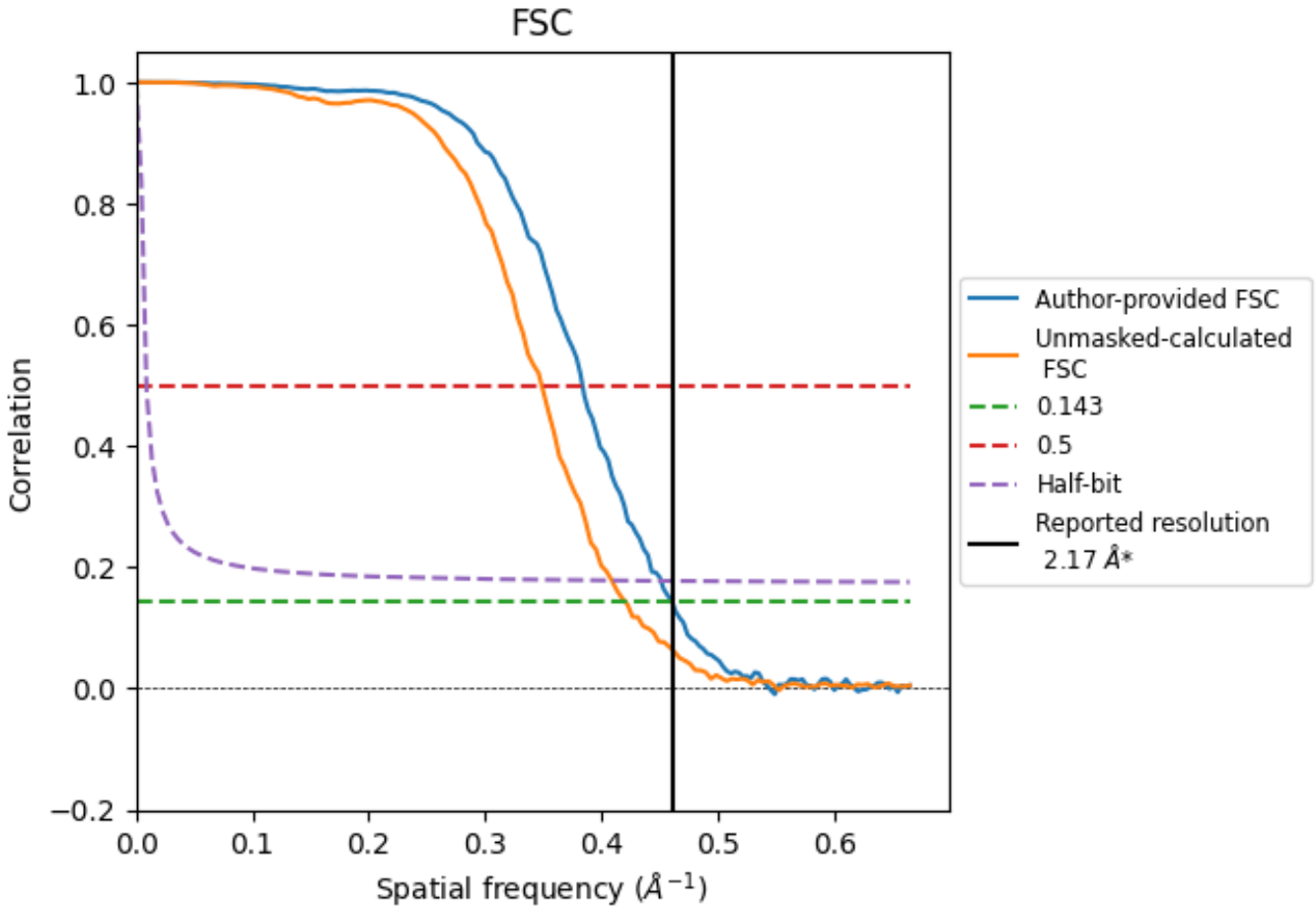


*Reported resolution corresponds to spatial frequency of 0.461 Å^{-1}

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 0.461 Å^{-1}

8.2 Resolution estimates (i)

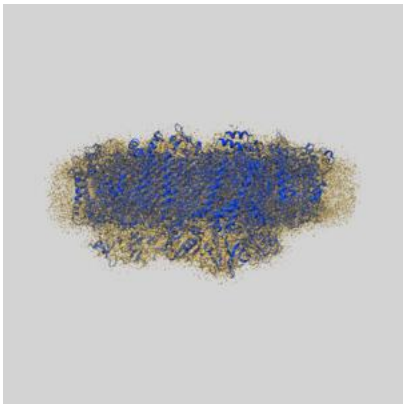
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.17	-	-
Author-provided FSC curve	2.17	2.61	2.22
Unmasked-calculated*	2.38	2.87	2.44

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

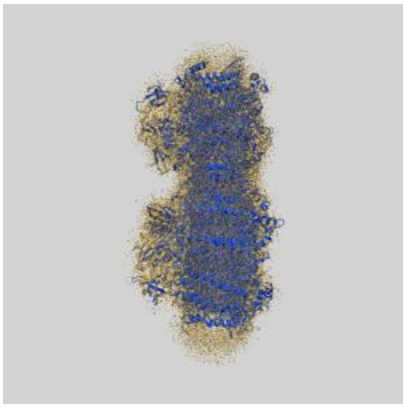
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-62693 and PDB model 9L0A. Per-residue inclusion information can be found in section 3 on page 31.

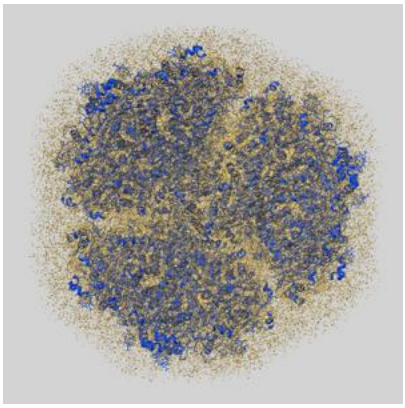
9.1 Map-model overlay



X



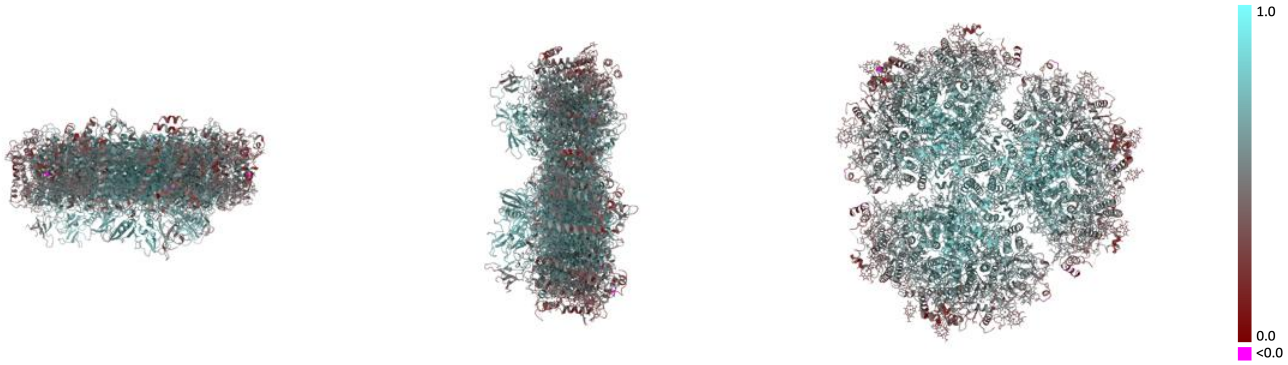
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

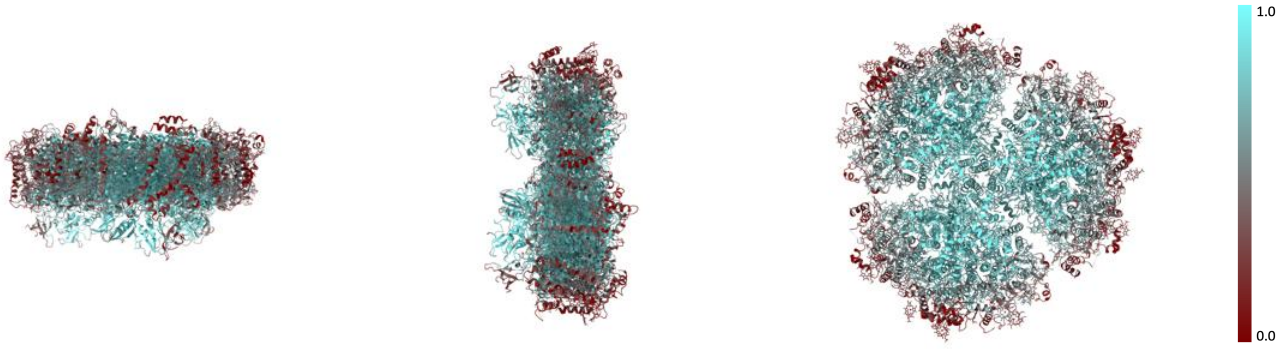
9.2 Q-score mapped to coordinate model (i)



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.

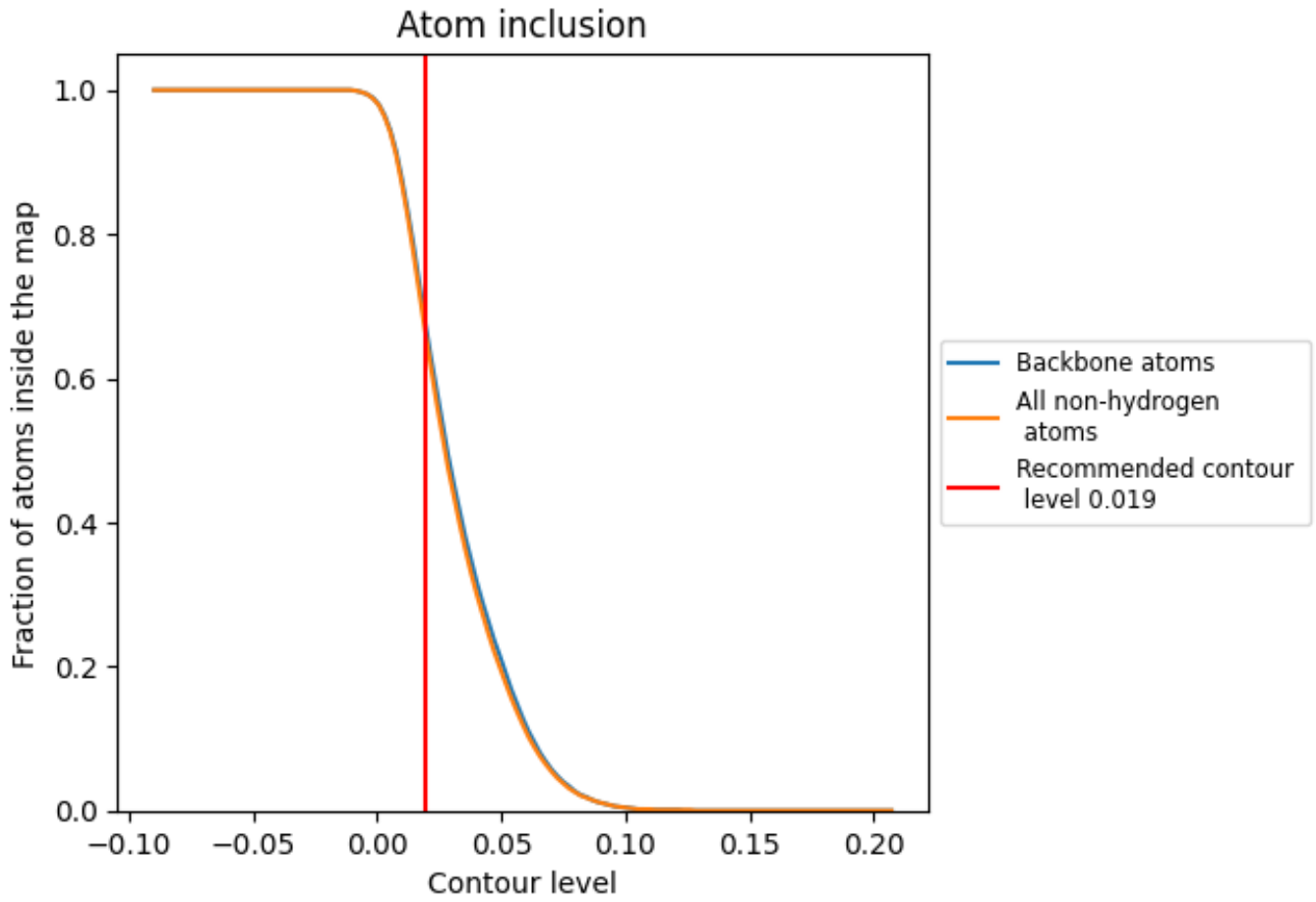
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.019).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 67% 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 (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6710	0.5840
A	0.6890	0.5940
B	0.6950	0.5840
C	0.9380	0.7320
D	0.7640	0.6450
E	0.5290	0.5390
F	0.2250	0.3800
I	0.9190	0.7320
J	0.2450	0.3840
K	0.1490	0.3020
L	0.8660	0.7020
M	0.6010	0.5210
X	0.1430	0.3040
bA	0.6870	0.5940
bB	0.6970	0.5870
bC	0.9320	0.7320
bD	0.7610	0.6440
bE	0.5290	0.5400
bF	0.2240	0.3840
bI	0.9070	0.7310
bJ	0.2280	0.3770
bK	0.1680	0.2930
bL	0.8660	0.7030
bM	0.6120	0.5180
bX	0.1430	0.3090
cA	0.6890	0.5940
cB	0.6930	0.5830
cC	0.9350	0.7290
cD	0.7600	0.6450
cE	0.5350	0.5410
cF	0.2230	0.3790
cI	0.9090	0.7320
cJ	0.2300	0.3770
cK	0.1730	0.2970
cL	0.8650	0.7020

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Chain	Atom inclusion	Q-score
cM	0.6150	0.5240
cX	0.1430	0.3130