Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 06:18 PM UTC

PDB ID	:	7F4V / pdb_00007f4v
EMDB ID	:	EMD-31455
Title	:	Cryo-EM structure of a primordial cyanobacterial photosystem I
Authors	:	Kato, K.; Hamaguchi, T.; Nagao, R.; Kawakami, K.; Yonekura, K.; Shen, J.R.
Deposited on	:	2021-06-21
Resolution	:	2.04 Å(reported)

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

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

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

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

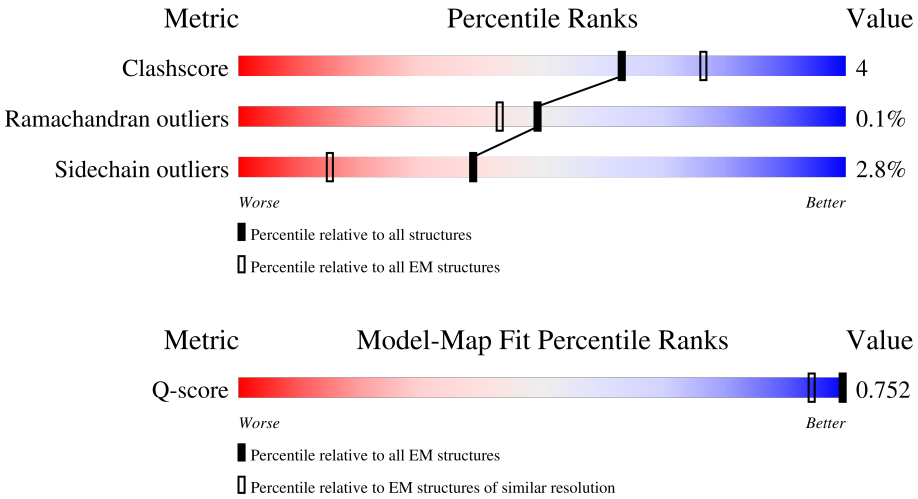
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.04 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	1810 (1.55 - 2.54)

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

Mol	Chain	Length	Quality of chain
1	aA	783	7% 90% 8%
1	bA	783	7% 90% 8%
1	cA	783	7% 90% 8%
2	aB	872	77% 6% 17%

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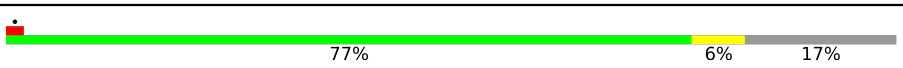
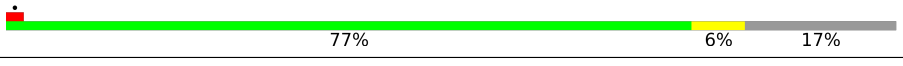
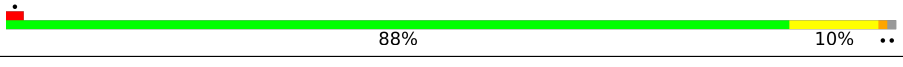
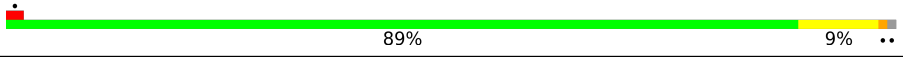
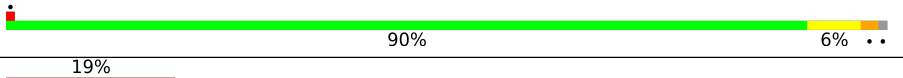
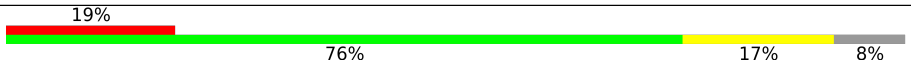
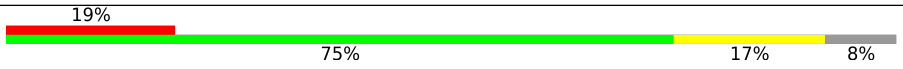
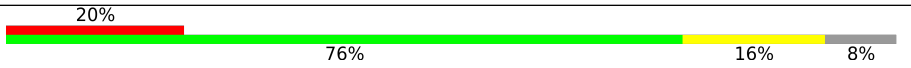
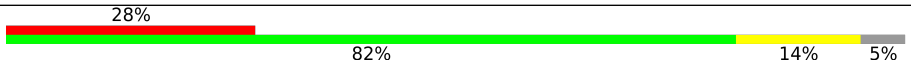
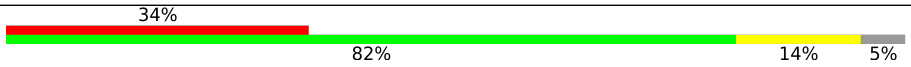
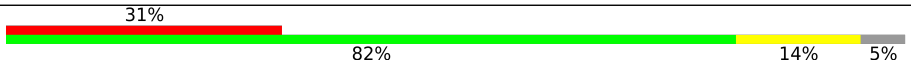
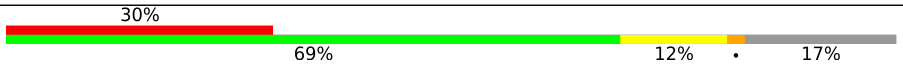
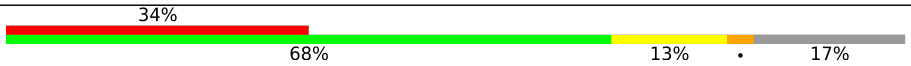
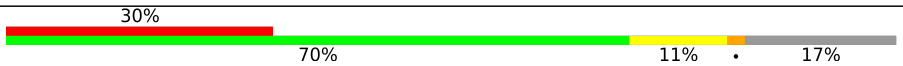
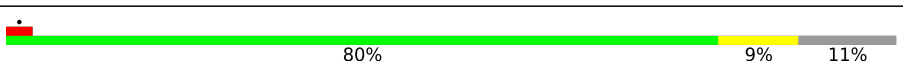
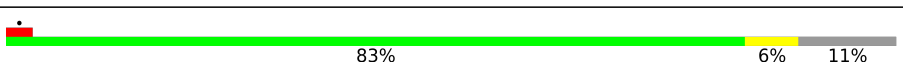
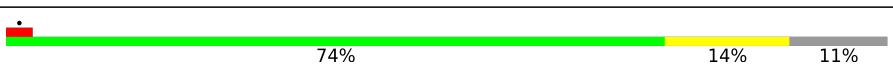
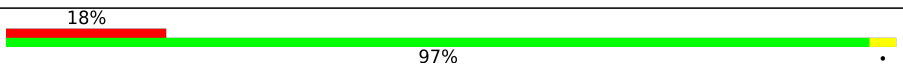
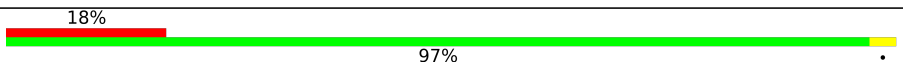
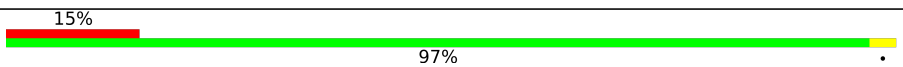
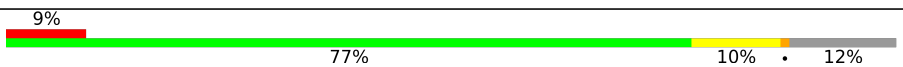
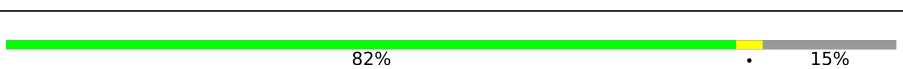
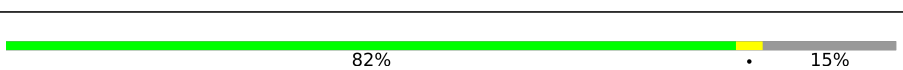
Mol	Chain	Length	Quality of chain
2	bB	872	
2	cB	872	
3	aC	81	
3	bC	81	
3	cC	81	
4	aD	144	
4	bD	144	
4	cD	144	
5	aE	65	
5	bE	65	
5	cE	65	
6	aF	181	
6	bF	181	
6	cF	181	
7	aI	35	
7	bI	35	
7	cI	35	
8	aJ	33	
8	bJ	33	
8	cJ	33	
9	aL	147	
9	bL	147	
9	cL	147	
10	aM	34	
10	bM	34	

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Mol	Chain	Length	Quality of chain
10	cM	34	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CL0	aA	801	X	-	-	-
11	CL0	bA	801	X	-	-	-
11	CL0	cA	801	X	-	-	-
12	CLA	aA	802	X	-	-	-
12	CLA	aA	803	X	-	-	-
12	CLA	aA	804	X	-	-	-
12	CLA	aA	805	X	-	-	-
12	CLA	aA	806	X	-	-	-
12	CLA	aA	807	X	-	-	-
12	CLA	aA	808	X	-	-	-
12	CLA	aA	809	X	-	-	-
12	CLA	aA	810	X	-	-	-
12	CLA	aA	811	X	-	-	-
12	CLA	aA	812	X	-	-	-
12	CLA	aA	813	X	-	-	-
12	CLA	aA	814	X	-	-	-
12	CLA	aA	816	X	-	-	-
12	CLA	aA	818	X	-	-	-
12	CLA	aA	819	X	-	-	-
12	CLA	aA	820	X	-	-	-
12	CLA	aA	821	X	-	-	-
12	CLA	aA	823	X	-	-	-
12	CLA	aA	825	X	-	-	-
12	CLA	aA	826	X	-	-	-
12	CLA	aA	827	X	-	-	-
12	CLA	aA	828	X	-	-	-
12	CLA	aA	829	X	-	-	-
12	CLA	aA	830	X	-	-	-
12	CLA	aA	832	X	-	-	-
12	CLA	aA	833	X	-	-	-
12	CLA	aA	834	X	-	-	-
12	CLA	aA	835	X	-	-	-
12	CLA	aA	836	X	-	-	-
12	CLA	aA	837	X	-	-	-
12	CLA	aA	838	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	aA	839	X	-	-	-
12	CLA	aA	840	X	-	-	-
12	CLA	aA	841	X	-	-	-
12	CLA	aA	842	X	-	-	-
12	CLA	aA	843	X	-	-	-
12	CLA	aA	854	X	-	-	-
12	CLA	aB	901	X	-	-	-
12	CLA	aB	902	X	-	-	-
12	CLA	aB	903	X	-	-	-
12	CLA	aB	904	X	-	-	-
12	CLA	aB	905	X	-	-	-
12	CLA	aB	906	X	-	-	-
12	CLA	aB	907	X	-	-	-
12	CLA	aB	908	X	-	-	-
12	CLA	aB	909	X	-	-	-
12	CLA	aB	910	X	-	-	-
12	CLA	aB	912	X	-	-	-
12	CLA	aB	913	X	-	-	-
12	CLA	aB	914	X	-	-	-
12	CLA	aB	917	X	-	-	-
12	CLA	aB	918	X	-	-	-
12	CLA	aB	919	X	-	-	-
12	CLA	aB	922	X	-	-	-
12	CLA	aB	923	X	-	-	-
12	CLA	aB	924	X	-	-	-
12	CLA	aB	925	X	-	-	-
12	CLA	aB	926	X	-	-	-
12	CLA	aB	927	X	-	-	-
12	CLA	aB	928	X	-	-	-
12	CLA	aB	930	X	-	-	-
12	CLA	aB	931	X	-	-	-
12	CLA	aB	933	X	-	-	-
12	CLA	aB	934	X	-	-	-
12	CLA	aB	935	X	-	-	-
12	CLA	aB	936	X	-	-	-
12	CLA	aB	937	X	-	-	-
12	CLA	aB	938	X	-	-	-
12	CLA	aB	939	X	-	-	-
12	CLA	aB	949	X	-	-	-
12	CLA	aF	202	X	-	-	-
12	CLA	bA	802	X	-	-	-
12	CLA	bA	803	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	bA	804	X	-	-	-
12	CLA	bA	805	X	-	-	-
12	CLA	bA	806	X	-	-	-
12	CLA	bA	807	X	-	-	-
12	CLA	bA	808	X	-	-	-
12	CLA	bA	809	X	-	-	-
12	CLA	bA	810	X	-	-	-
12	CLA	bA	811	X	-	-	-
12	CLA	bA	812	X	-	-	-
12	CLA	bA	813	X	-	-	-
12	CLA	bA	814	X	-	-	-
12	CLA	bA	816	X	-	-	-
12	CLA	bA	818	X	-	-	-
12	CLA	bA	819	X	-	-	-
12	CLA	bA	820	X	-	-	-
12	CLA	bA	821	X	-	-	-
12	CLA	bA	823	X	-	-	-
12	CLA	bA	825	X	-	-	-
12	CLA	bA	826	X	-	-	-
12	CLA	bA	827	X	-	-	-
12	CLA	bA	828	X	-	-	-
12	CLA	bA	829	X	-	-	-
12	CLA	bA	830	X	-	-	-
12	CLA	bA	832	X	-	-	-
12	CLA	bA	833	X	-	-	-
12	CLA	bA	834	X	-	-	-
12	CLA	bA	835	X	-	-	-
12	CLA	bA	836	X	-	-	-
12	CLA	bA	837	X	-	-	-
12	CLA	bA	838	X	-	-	-
12	CLA	bA	839	X	-	-	-
12	CLA	bA	840	X	-	-	-
12	CLA	bA	841	X	-	-	-
12	CLA	bA	842	X	-	-	-
12	CLA	bA	843	X	-	-	-
12	CLA	bA	853	X	-	-	-
12	CLA	bB	901	X	-	-	-
12	CLA	bB	902	X	-	-	-
12	CLA	bB	903	X	-	-	-
12	CLA	bB	904	X	-	-	-
12	CLA	bB	905	X	-	-	-
12	CLA	bB	906	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	bB	907	X	-	-	-
12	CLA	bB	908	X	-	-	-
12	CLA	bB	909	X	-	-	-
12	CLA	bB	910	X	-	-	-
12	CLA	bB	912	X	-	-	-
12	CLA	bB	913	X	-	-	-
12	CLA	bB	914	X	-	-	-
12	CLA	bB	917	X	-	-	-
12	CLA	bB	918	X	-	-	-
12	CLA	bB	919	X	-	-	-
12	CLA	bB	922	X	-	-	-
12	CLA	bB	923	X	-	-	-
12	CLA	bB	924	X	-	-	-
12	CLA	bB	925	X	-	-	-
12	CLA	bB	926	X	-	-	-
12	CLA	bB	927	X	-	-	-
12	CLA	bB	928	X	-	-	-
12	CLA	bB	930	X	-	-	-
12	CLA	bB	931	X	-	-	-
12	CLA	bB	933	X	-	-	-
12	CLA	bB	934	X	-	-	-
12	CLA	bB	935	X	-	-	-
12	CLA	bB	936	X	-	-	-
12	CLA	bB	937	X	-	-	-
12	CLA	bB	938	X	-	-	-
12	CLA	bB	939	X	-	-	-
12	CLA	bB	949	X	-	-	-
12	CLA	bF	202	X	-	-	-
12	CLA	cA	802	X	-	-	-
12	CLA	cA	803	X	-	-	-
12	CLA	cA	804	X	-	-	-
12	CLA	cA	805	X	-	-	-
12	CLA	cA	806	X	-	-	-
12	CLA	cA	807	X	-	-	-
12	CLA	cA	808	X	-	-	-
12	CLA	cA	809	X	-	-	-
12	CLA	cA	810	X	-	-	-
12	CLA	cA	811	X	-	-	-
12	CLA	cA	812	X	-	-	-
12	CLA	cA	813	X	-	-	-
12	CLA	cA	814	X	-	-	-
12	CLA	cA	816	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	cA	818	X	-	-	-
12	CLA	cA	819	X	-	-	-
12	CLA	cA	820	X	-	-	-
12	CLA	cA	821	X	-	-	-
12	CLA	cA	823	X	-	-	-
12	CLA	cA	825	X	-	-	-
12	CLA	cA	826	X	-	-	-
12	CLA	cA	827	X	-	-	-
12	CLA	cA	828	X	-	-	-
12	CLA	cA	829	X	-	-	-
12	CLA	cA	830	X	-	-	-
12	CLA	cA	832	X	-	-	-
12	CLA	cA	833	X	-	-	-
12	CLA	cA	834	X	-	-	-
12	CLA	cA	835	X	-	-	-
12	CLA	cA	836	X	-	-	-
12	CLA	cA	837	X	-	-	-
12	CLA	cA	838	X	-	-	-
12	CLA	cA	839	X	-	-	-
12	CLA	cA	840	X	-	-	-
12	CLA	cA	841	X	-	-	-
12	CLA	cA	842	X	-	-	-
12	CLA	cA	843	X	-	-	-
12	CLA	cA	853	X	-	-	-
12	CLA	cB	901	X	-	-	-
12	CLA	cB	902	X	-	-	-
12	CLA	cB	903	X	-	-	-
12	CLA	cB	904	X	-	-	-
12	CLA	cB	905	X	-	-	-
12	CLA	cB	906	X	-	-	-
12	CLA	cB	907	X	-	-	-
12	CLA	cB	908	X	-	-	-
12	CLA	cB	909	X	-	-	-
12	CLA	cB	910	X	-	-	-
12	CLA	cB	912	X	-	-	-
12	CLA	cB	913	X	-	-	-
12	CLA	cB	914	X	-	-	-
12	CLA	cB	917	X	-	-	-
12	CLA	cB	918	X	-	-	-
12	CLA	cB	919	X	-	-	-
12	CLA	cB	922	X	-	-	-
12	CLA	cB	923	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	cB	924	X	-	-	-
12	CLA	cB	925	X	-	-	-
12	CLA	cB	926	X	-	-	-
12	CLA	cB	927	X	-	-	-
12	CLA	cB	928	X	-	-	-
12	CLA	cB	930	X	-	-	-
12	CLA	cB	931	X	-	-	-
12	CLA	cB	933	X	-	-	-
12	CLA	cB	934	X	-	-	-
12	CLA	cB	935	X	-	-	-
12	CLA	cB	936	X	-	-	-
12	CLA	cB	937	X	-	-	-
12	CLA	cB	938	X	-	-	-
12	CLA	cB	939	X	-	-	-
12	CLA	cB	949	X	-	-	-
12	CLA	cF	202	X	-	-	-

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 67641 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	aA	772	Total	C	N	O	S	0	0
			6038	3957	1031	1025	25		
1	bA	772	Total	C	N	O	S	0	0
			6038	3957	1031	1025	25		
1	cA	772	Total	C	N	O	S	0	0
			6038	3957	1031	1025	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	aB	725	Total	C	N	O	S	0	0
			5701	3761	954	968	18		
2	bB	725	Total	C	N	O	S	0	0
			5701	3761	954	968	18		
2	cB	725	Total	C	N	O	S	0	0
			5701	3761	954	968	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	aC	80	Total	C	N	O	S	0	0
			599	368	103	118	10		
3	bC	80	Total	C	N	O	S	0	0
			599	368	103	118	10		
3	cC	80	Total	C	N	O	S	0	0
			599	368	103	118	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	aD	133	Total	C	N	O	S	0	0
			1038	660	180	194	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	bD	133	Total	C	N	O	S	0	0
			1038	660	180	194	4		
4	cD	133	Total	C	N	O	S	0	0
			1038	660	180	194	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	aE	62	Total	C	N	O	0	0
			507	321	87	99		
5	bE	62	Total	C	N	O	0	0
			507	321	87	99		
5	cE	62	Total	C	N	O	0	0
			507	321	87	99		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	aF	151	Total	C	N	O	S	0	0
			1182	761	200	218	3		
6	bF	151	Total	C	N	O	S	0	0
			1182	761	200	218	3		
6	cF	151	Total	C	N	O	S	0	0
			1182	761	200	218	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	aI	31	Total	C	N	O	S	0	0
			240	164	35	40	1		
7	bI	31	Total	C	N	O	S	0	0
			240	164	35	40	1		
7	cI	31	Total	C	N	O	S	0	0
			240	164	35	40	1		

- Molecule 8 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	aJ	33	Total	C	N	O	0	0
			164	98	33	33		
8	bJ	33	Total	C	N	O	0	0
			164	98	33	33		

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Mol	Chain	Residues	Atoms				AltConf	Trace
8	cJ	33	Total	C	N	O	0	0
			164	98	33	33		

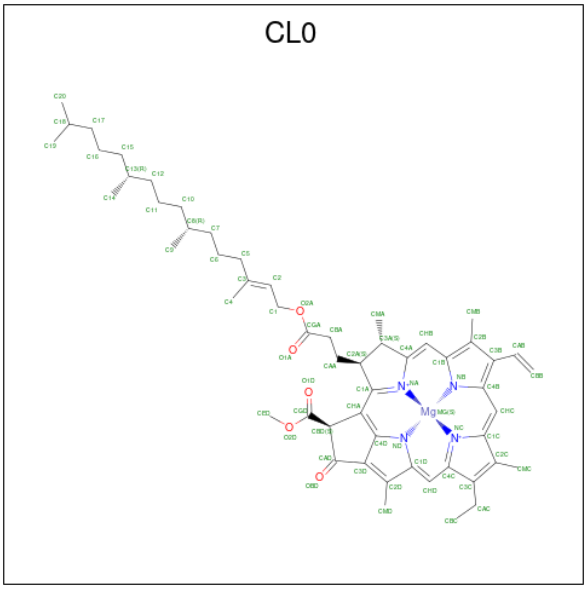
- Molecule 9 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	aL	129	Total	C	N	O	S	0	0
			974	641	162	169	2		
9	bL	129	Total	C	N	O	S	0	0
			974	641	162	169	2		
9	cL	129	Total	C	N	O	S	0	0
			974	641	162	169	2		

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

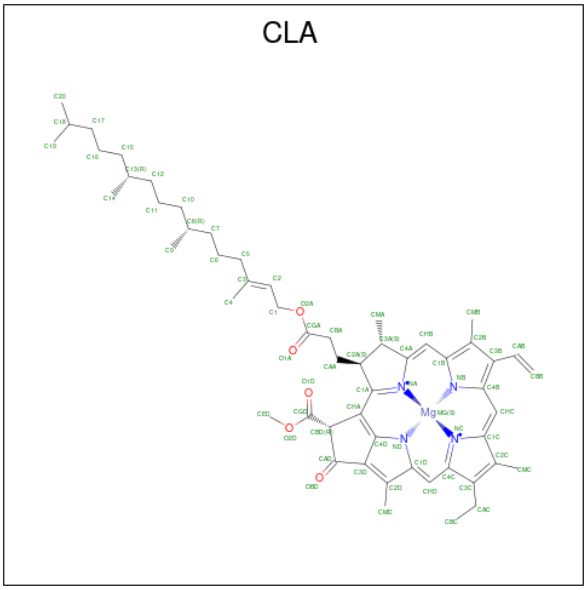
Mol	Chain	Residues	Atoms				AltConf	Trace
10	aM	29	Total	C	N	O	0	0
			190	127	30	33		
10	bM	29	Total	C	N	O	0	0
			190	127	30	33		
10	cM	29	Total	C	N	O	0	0
			190	127	30	33		

- Molecule 11 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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

- Molecule 12 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
12	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
12	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
12	aA	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
12	aB	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
12	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aB	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
12	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aF	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aL	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
12	aL	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	aL	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			53	43	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
12	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
12	bA	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
12	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
12	bB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bB	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
12	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bF	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bL	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
12	bL	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	bL	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
12	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
12	cA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
12	cA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
12	cB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cB	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
12	cF	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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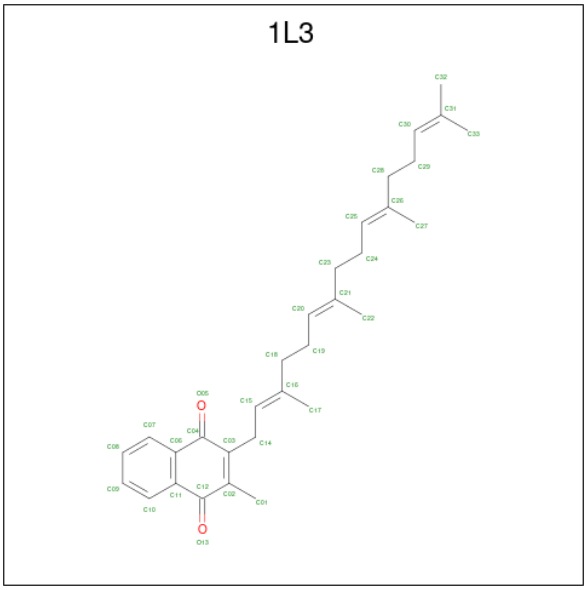
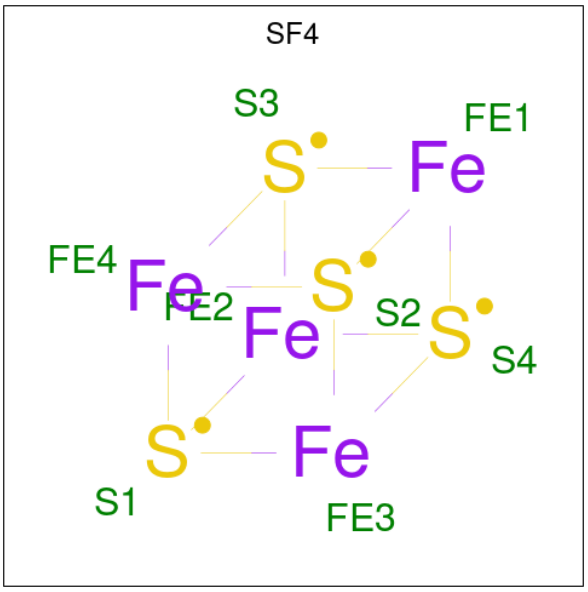
Mol	Chain	Residues	Atoms					AltConf
12	cL	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
12	cL	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	cL	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 13 is Menaquinone-4 (CCD ID: 1L3) (formula: $C_{31}H_{40}O_2$).



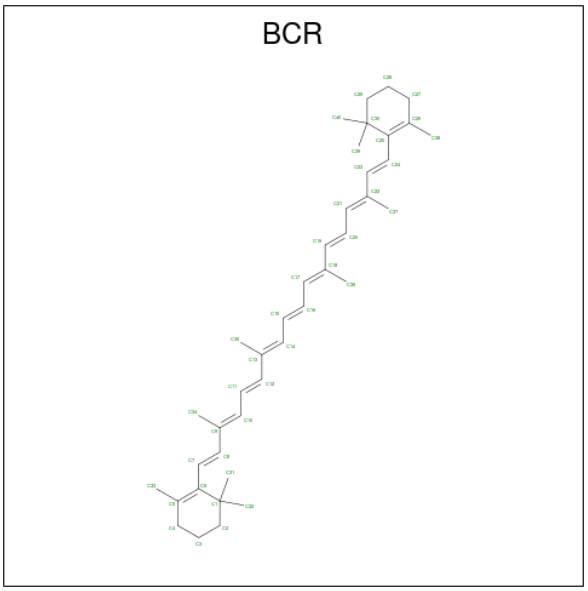
Mol	Chain	Residues	Atoms			AltConf
13	aA	1	Total	C	O	0
			33	31	2	
13	aB	1	Total	C	O	0
			33	31	2	
13	bA	1	Total	C	O	0
			33	31	2	
13	bB	1	Total	C	O	0
			33	31	2	
13	cA	1	Total	C	O	0
			33	31	2	
13	cB	1	Total	C	O	0
			33	31	2	

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



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

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



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

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

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

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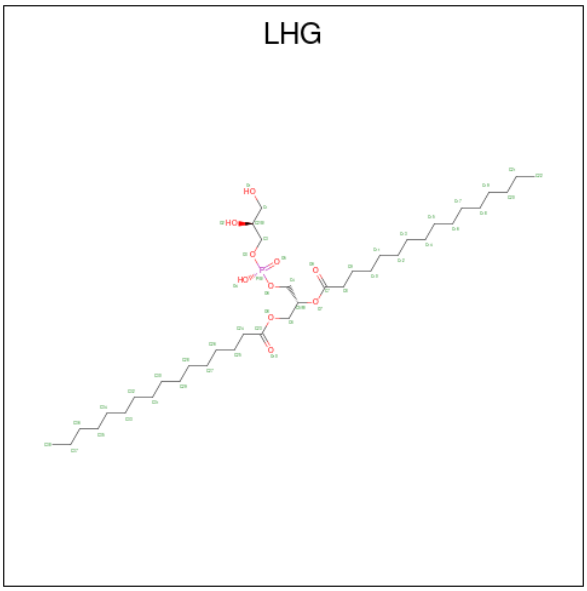
Mol	Chain	Residues	Atoms	AltConf
15	cL	1	Total C 40 40	0
15	cL	1	Total C 40 40	0
15	cL	1	Total C 40 40	0
15	cM	1	Total C 40 40	0

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



Mol	Chain	Residues	Atoms	AltConf
16	aA	1	Total C O P 49 38 10 1	0
16	aA	1	Total C O P 27 16 10 1	0
16	aB	1	Total C O P 23 12 10 1	0
16	bA	1	Total C O P 49 38 10 1	0
16	bA	1	Total C O P 27 16 10 1	0
16	bB	1	Total C O P 23 12 10 1	0
16	cA	1	Total C O P 49 38 10 1	0

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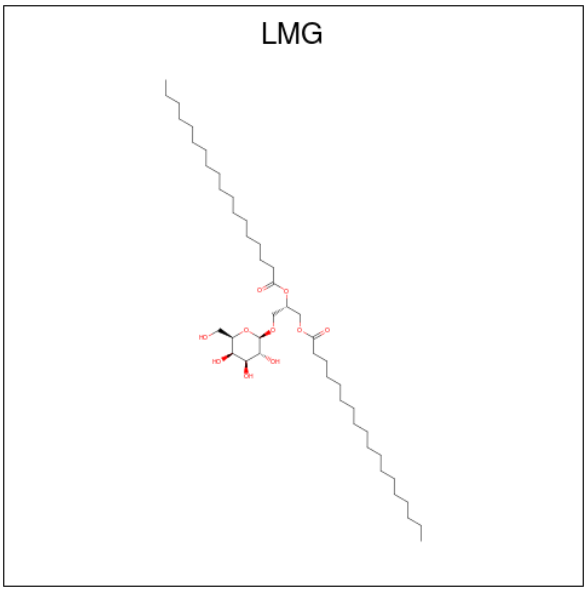
Mol	Chain	Residues	Atoms				AltConf
16	cA	1	Total	C	O	P	0
			27	16	10	1	
16	cB	1	Total	C	O	P	0
			23	12	10	1	

- Molecule 17 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
17	aB	1	Total	C	O	0
			43	33	10	
17	bB	1	Total	C	O	0
			43	33	10	
17	cB	1	Total	C	O	0
			43	33	10	

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		AltConf
18	aA	45	Total	O	0
			45	45	
18	aB	67	Total	O	0
			67	67	
18	aC	14	Total	O	0
			14	14	
18	aD	2	Total	O	0
			2	2	

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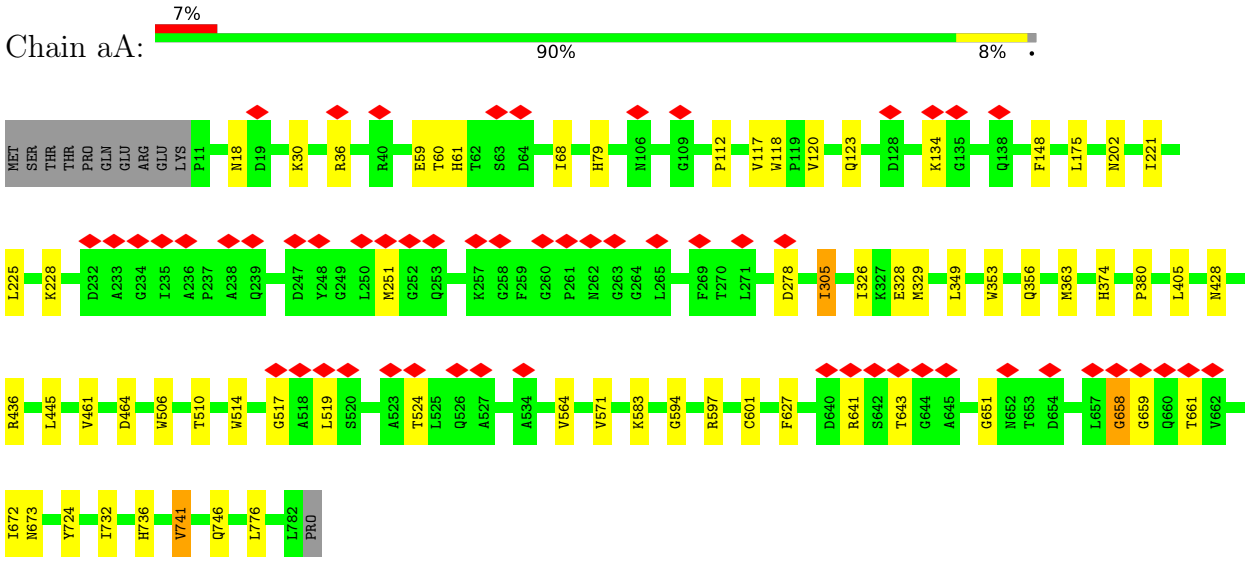
Mol	Chain	Residues	Atoms	AltConf
18	aE	3	Total O 3 3	0
18	aF	1	Total O 1 1	0
18	aJ	1	Total O 1 1	0
18	aL	1	Total O 1 1	0
18	bA	45	Total O 45 45	0
18	bB	67	Total O 67 67	0
18	bC	14	Total O 14 14	0
18	bD	2	Total O 2 2	0
18	bE	3	Total O 3 3	0
18	bF	1	Total O 1 1	0
18	bJ	1	Total O 1 1	0
18	bL	1	Total O 1 1	0
18	cA	45	Total O 45 45	0
18	cB	67	Total O 67 67	0
18	cC	14	Total O 14 14	0
18	cD	2	Total O 2 2	0
18	cE	3	Total O 3 3	0
18	cF	1	Total O 1 1	0
18	cJ	1	Total O 1 1	0
18	cL	1	Total O 1 1	0

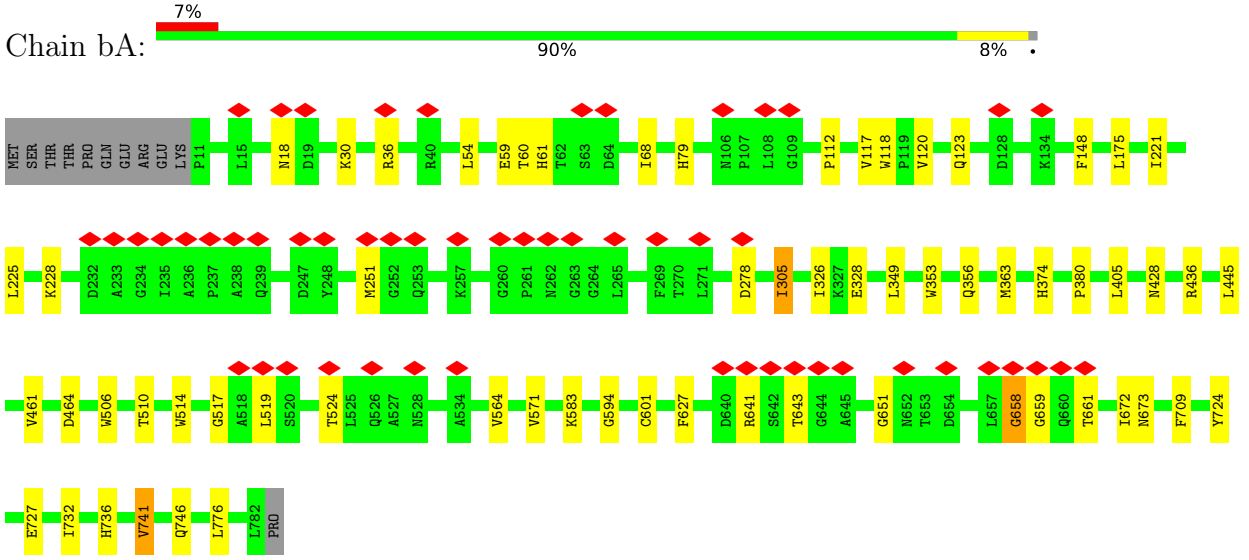
3 Residue-property plots (i)

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

• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

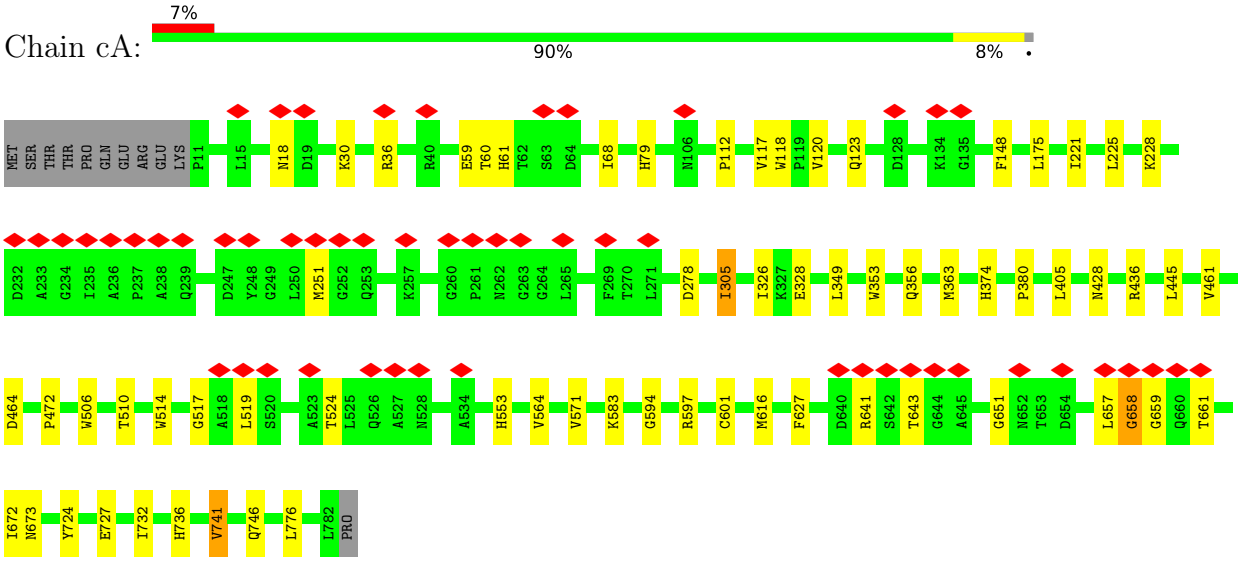


• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



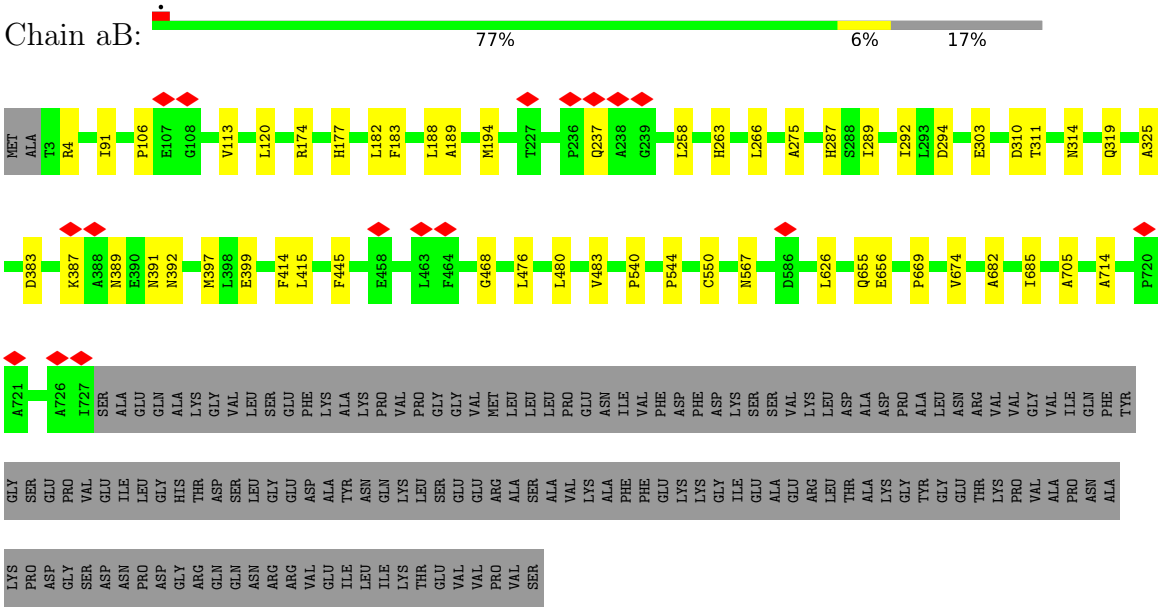
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain cA:



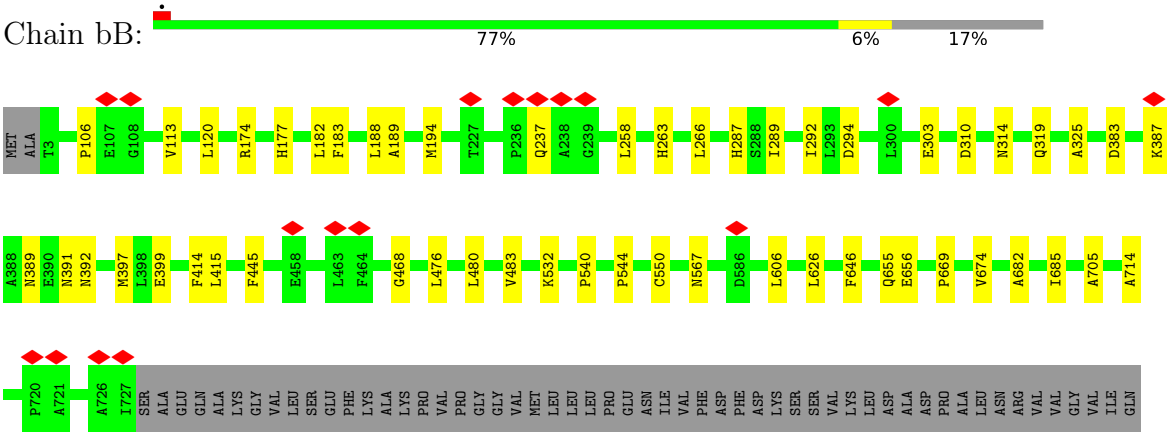
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

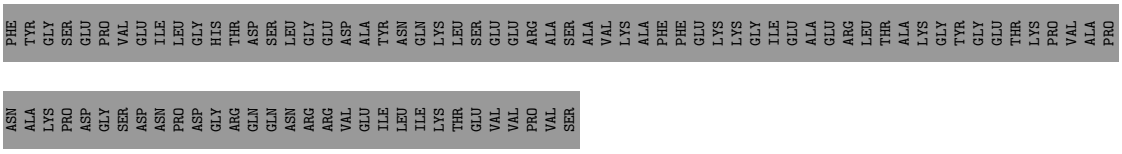
Chain aB:



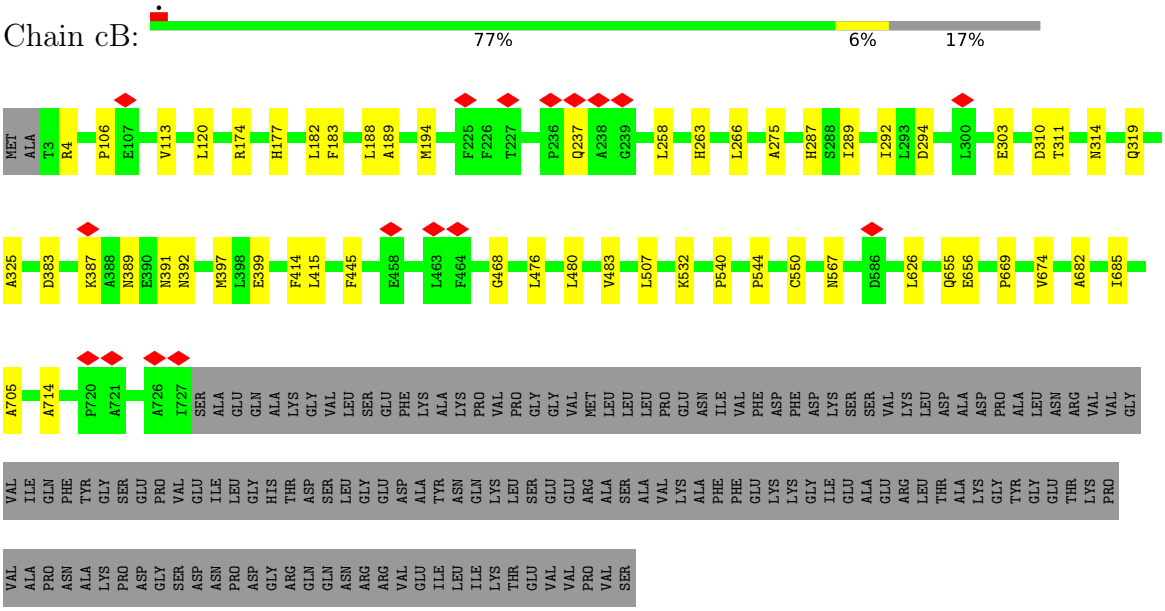
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain bB:

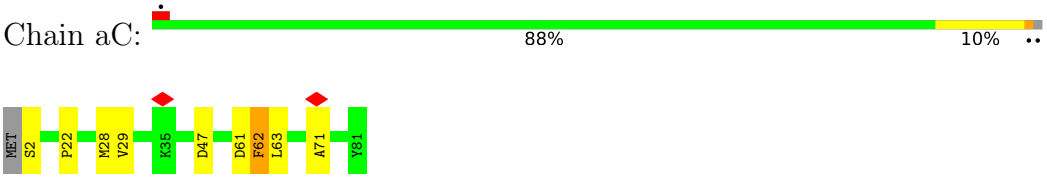




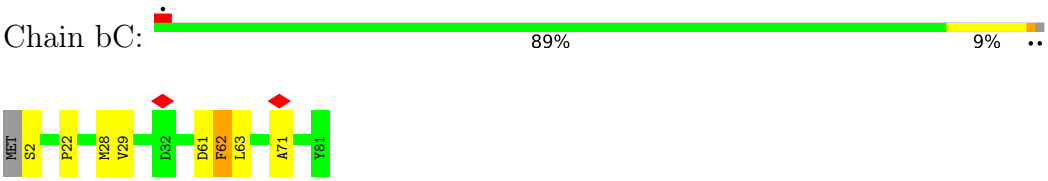
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



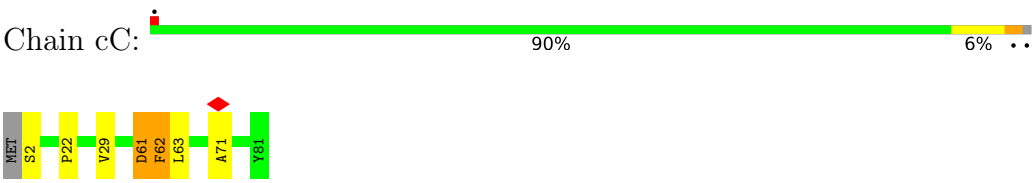
• Molecule 3: Photosystem I iron-sulfur center



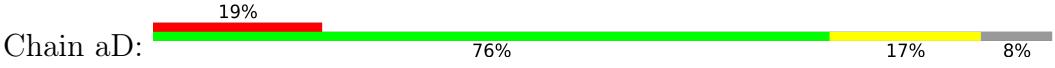
• Molecule 3: Photosystem I iron-sulfur center

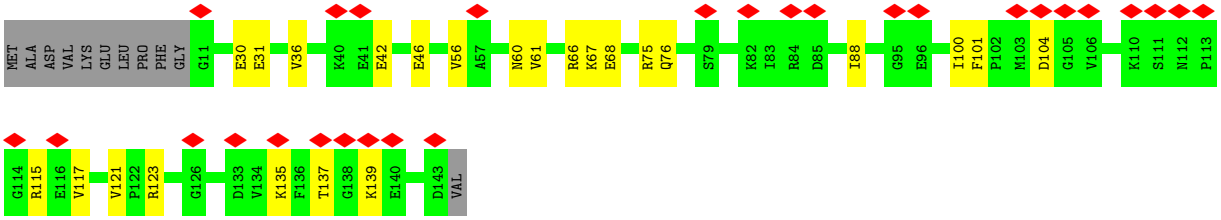


• Molecule 3: Photosystem I iron-sulfur center

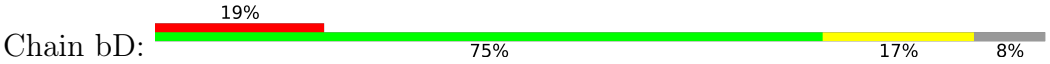


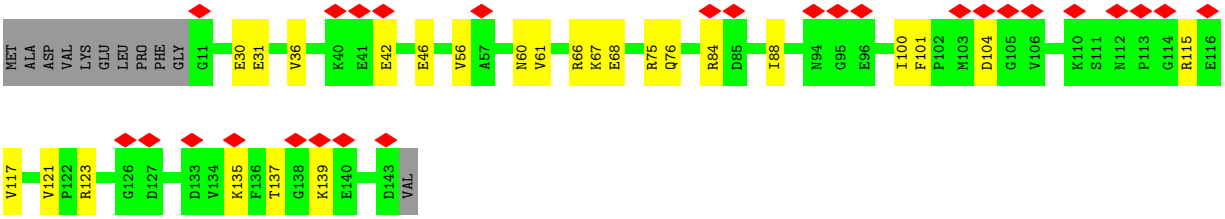
• Molecule 4: Photosystem I reaction center subunit II



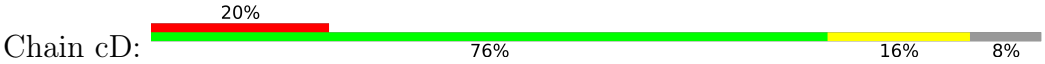


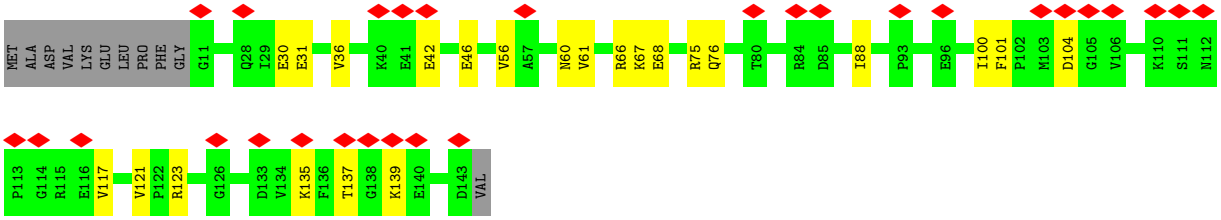
• Molecule 4: Photosystem I reaction center subunit II



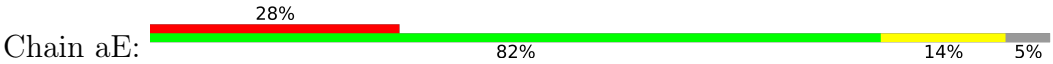


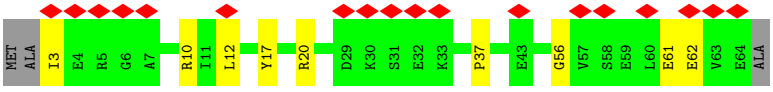
• Molecule 4: Photosystem I reaction center subunit II



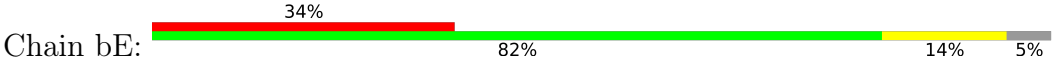


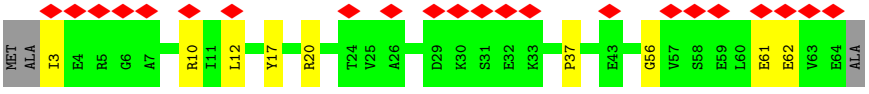
• Molecule 5: Photosystem I reaction center subunit IV



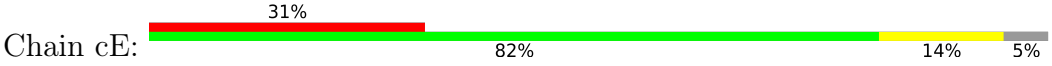


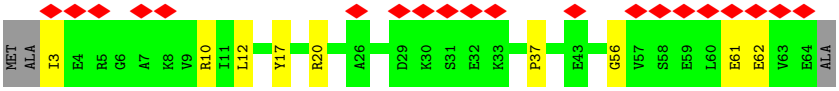
• Molecule 5: Photosystem I reaction center subunit IV





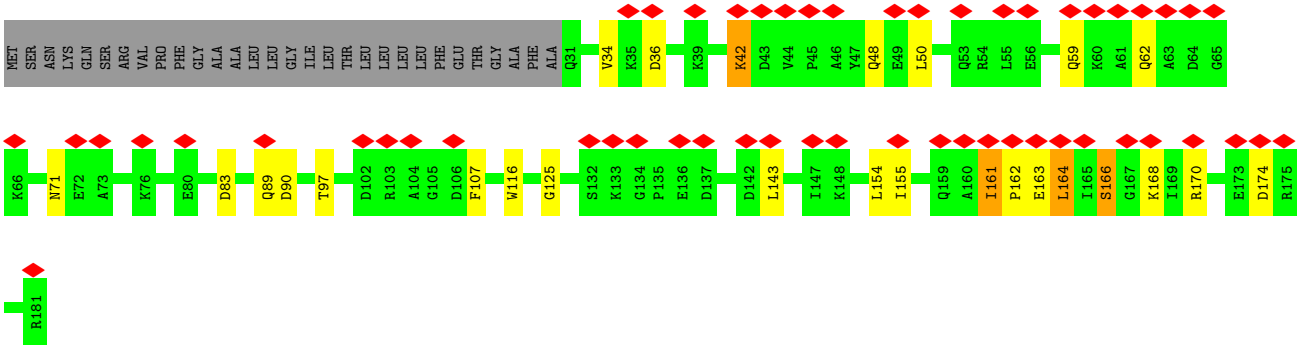
• Molecule 5: Photosystem I reaction center subunit IV





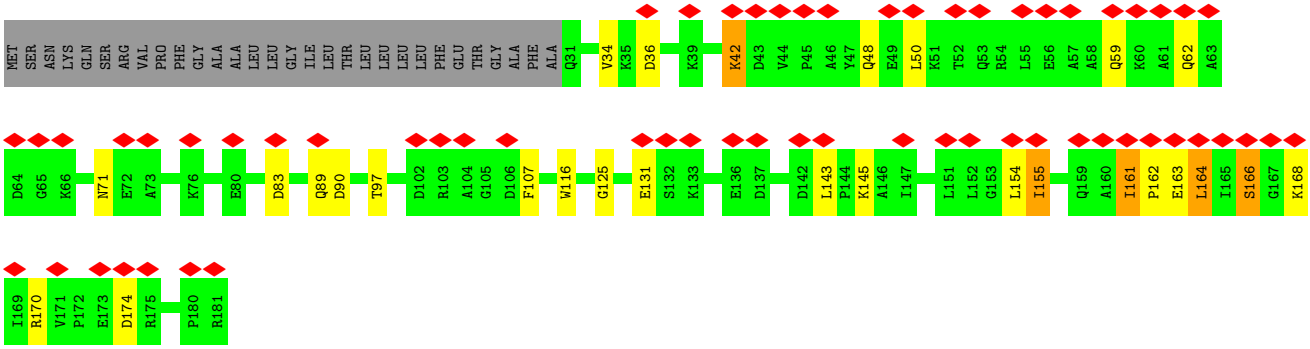
• Molecule 6: Photosystem I reaction center subunit III

Chain aF:



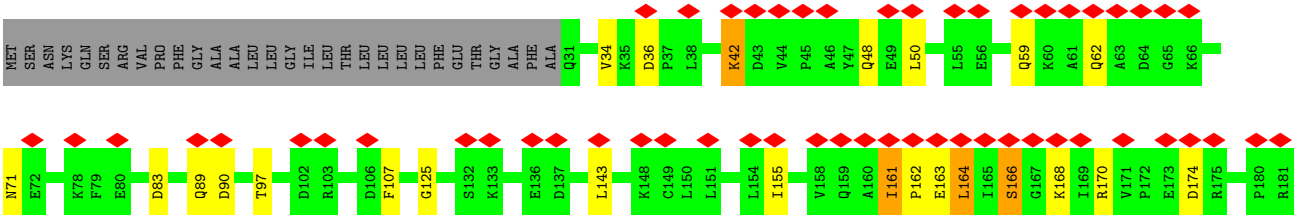
• Molecule 6: Photosystem I reaction center subunit III

Chain bF:



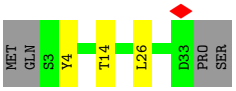
• Molecule 6: Photosystem I reaction center subunit III

Chain cF:



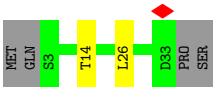
• Molecule 7: Photosystem I reaction center subunit Z

Chain aI:



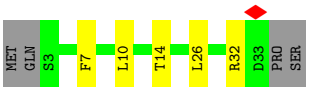
• Molecule 7: Photosystem I reaction center subunit Z

Chain bI:



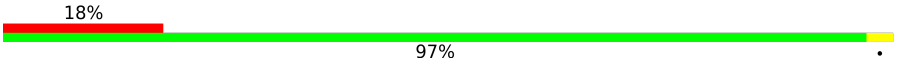
• Molecule 7: Photosystem I reaction center subunit Z

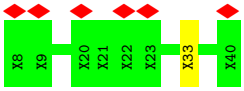
Chain cI:



• Molecule 8: Unknown protein

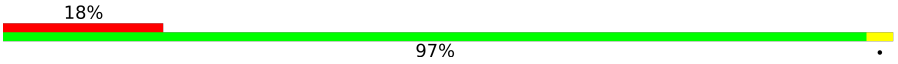
Chain aJ:

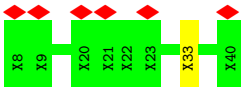




• Molecule 8: Unknown protein

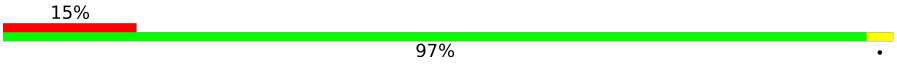
Chain bJ:

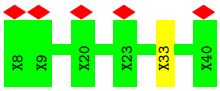




• Molecule 8: Unknown protein

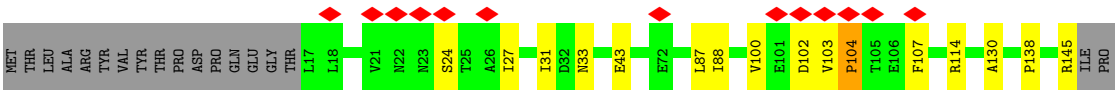
Chain cJ:





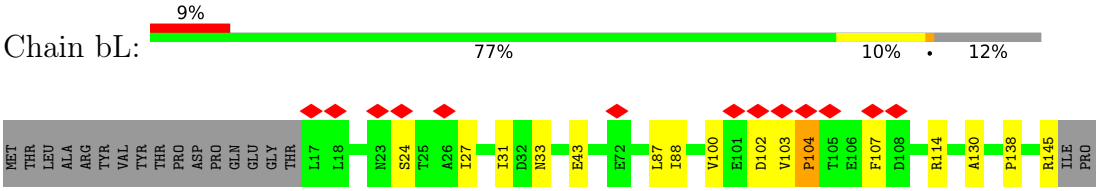
• Molecule 9: Photosystem I reaction center subunit XI

Chain aL:



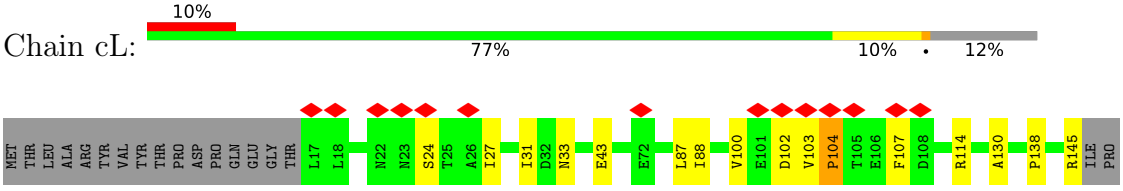
• Molecule 9: Photosystem I reaction center subunit XI

Chain bL:



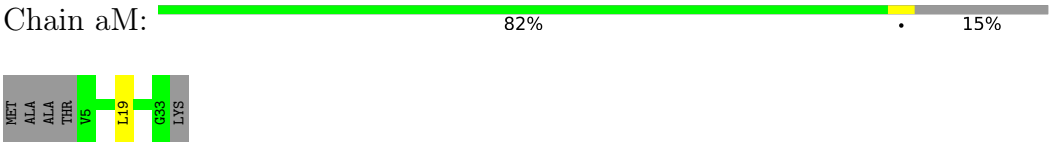
• Molecule 9: Photosystem I reaction center subunit XI

Chain cL:



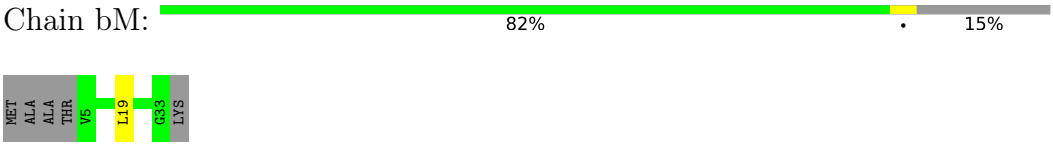
• Molecule 10: Photosystem I reaction center subunit XII

Chain aM:



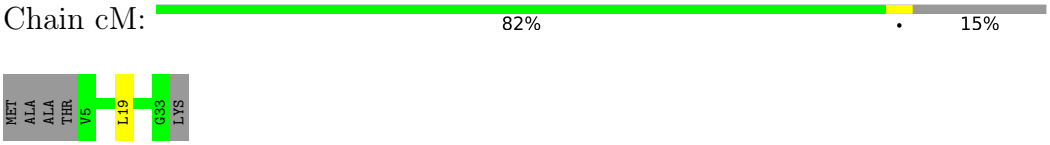
• Molecule 10: Photosystem I reaction center subunit XII

Chain bM:



• Molecule 10: Photosystem I reaction center subunit XII

Chain cM:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	261743	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 ($e^-/Å^2$)	70.22	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.465	Depositor
Minimum map value	-0.239	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	329.2, 329.2, 329.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.823, 0.823, 0.823	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMG, LHG, CL0, 1L3, SF4, CLA, BCR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	aA	0.31	0/6244	0.54	4/8520 (0.0%)
1	bA	0.31	0/6244	0.54	4/8520 (0.0%)
1	cA	0.31	0/6244	0.54	4/8520 (0.0%)
2	aB	0.32	0/5911	0.51	2/8084 (0.0%)
2	bB	0.32	0/5911	0.51	2/8084 (0.0%)
2	cB	0.32	0/5911	0.51	2/8084 (0.0%)
3	aC	0.30	0/609	0.61	2/825 (0.2%)
3	bC	0.31	0/609	0.61	2/825 (0.2%)
3	cC	0.30	0/609	0.61	2/825 (0.2%)
4	aD	0.26	0/1061	0.46	0/1434
4	bD	0.26	0/1061	0.46	0/1434
4	cD	0.26	0/1061	0.46	0/1434
5	aE	0.25	0/515	0.53	0/694
5	bE	0.26	0/515	0.53	0/694
5	cE	0.25	0/515	0.53	0/694
6	aF	0.26	0/1208	0.54	0/1638
6	bF	0.26	0/1208	0.53	0/1638
6	cF	0.26	0/1208	0.54	0/1638
7	aI	0.31	0/245	0.58	0/336
7	bI	0.32	0/245	0.58	0/336
7	cI	0.32	0/245	0.58	0/336
9	aL	0.32	0/997	0.63	0/1357
9	bL	0.32	0/997	0.63	0/1357
9	cL	0.32	0/997	0.63	0/1357
10	aM	0.29	0/190	0.43	0/260
10	bM	0.29	0/190	0.43	0/260
10	cM	0.28	0/190	0.44	0/260
All	All	0.31	0/50940	0.53	24/69444 (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	aC	0	1
3	bC	0	1
3	cC	0	1
8	aJ	0	1
8	bJ	0	1
8	cJ	0	1
9	aL	0	1
9	bL	0	1
9	cL	0	1
All	All	0	9

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	aA	517	GLY	CA-C-N	9.84	139.41	121.70
1	aA	517	GLY	C-N-CA	9.84	139.41	121.70
1	cA	517	GLY	CA-C-N	9.83	139.39	121.70
1	cA	517	GLY	C-N-CA	9.83	139.39	121.70
1	bA	517	GLY	CA-C-N	9.82	139.38	121.70
1	bA	517	GLY	C-N-CA	9.82	139.38	121.70
1	aA	658	GLY	N-CA-C	6.00	127.40	113.18
1	cA	658	GLY	N-CA-C	6.00	127.39	113.18
1	bA	658	GLY	N-CA-C	5.98	127.34	113.18
1	cA	651	GLY	N-CA-C	5.52	126.27	113.18
1	aA	651	GLY	N-CA-C	5.52	126.26	113.18
1	bA	651	GLY	N-CA-C	5.51	126.25	113.18
3	aC	62	PHE	CA-C-N	5.37	128.71	120.82
3	aC	62	PHE	C-N-CA	5.37	128.71	120.82
3	cC	62	PHE	CA-C-N	5.36	128.70	120.82
3	cC	62	PHE	C-N-CA	5.36	128.70	120.82
3	bC	62	PHE	CA-C-N	5.32	128.65	120.82
3	bC	62	PHE	C-N-CA	5.32	128.65	120.82
2	cB	669	PRO	CA-C-N	5.04	131.16	121.54
2	cB	669	PRO	C-N-CA	5.04	131.16	121.54
2	bB	669	PRO	CA-C-N	5.03	131.15	121.54
2	bB	669	PRO	C-N-CA	5.03	131.15	121.54
2	aB	669	PRO	CA-C-N	5.03	131.14	121.54
2	aB	669	PRO	C-N-CA	5.03	131.14	121.54

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	aC	61	ASP	Peptide
8	aJ	33	UNK	Peptide
9	aL	104	PRO	Peptide
3	bC	61	ASP	Peptide
8	bJ	33	UNK	Peptide
9	bL	104	PRO	Peptide
3	cC	61	ASP	Peptide
8	cJ	33	UNK	Peptide
9	cL	104	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	aA	6038	0	5897	35	0
1	bA	6038	0	5897	34	0
1	cA	6038	0	5897	36	0
2	aB	5701	0	5519	38	0
2	bB	5701	0	5519	37	0
2	cB	5701	0	5519	39	0
3	aC	599	0	579	5	0
3	bC	599	0	579	4	0
3	cC	599	0	579	4	0
4	aD	1038	0	1039	15	0
4	bD	1038	0	1039	14	0
4	cD	1038	0	1039	14	0
5	aE	507	0	504	4	0
5	bE	507	0	504	4	0
5	cE	507	0	504	5	0
6	aF	1182	0	1207	11	0
6	bF	1182	0	1207	13	0
6	cF	1182	0	1207	10	0
7	aI	240	0	255	3	0
7	bI	240	0	255	2	0
7	cI	240	0	255	4	0

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	aJ	164	0	35	0	0
8	bJ	164	0	35	0	0
8	cJ	164	0	35	0	0
9	aL	974	0	998	9	0
9	bL	974	0	998	9	0
9	cL	974	0	998	9	0
10	aM	190	0	215	0	0
10	bM	190	0	215	0	0
10	cM	190	0	215	0	0
11	aA	65	0	72	0	0
11	bA	65	0	72	0	0
11	cA	65	0	72	0	0
12	aA	2396	0	2199	54	0
12	aB	2144	0	1874	46	0
12	aF	45	0	33	0	0
12	aL	143	0	111	3	0
12	bA	2351	0	2166	55	0
12	bB	2144	0	1874	44	0
12	bF	45	0	33	0	0
12	bL	143	0	111	3	0
12	cA	2351	0	2166	61	0
12	cB	2099	0	1841	43	0
12	cF	45	0	33	0	0
12	cL	143	0	111	3	0
13	aA	33	0	0	0	0
13	aB	33	0	0	0	0
13	bA	33	0	0	0	0
13	bB	33	0	0	1	0
13	cA	33	0	0	0	0
13	cB	33	0	0	0	0
14	aA	8	0	0	0	0
14	aC	16	0	0	0	0
14	bA	8	0	0	0	0
14	bC	16	0	0	0	0
14	cA	8	0	0	0	0
14	cC	16	0	0	0	0
15	aA	200	0	280	8	0
15	aB	240	0	336	11	0
15	aF	120	0	168	7	0
15	aI	40	0	56	2	0
15	aJ	40	0	56	1	0
15	aL	120	0	168	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	aM	40	0	55	0	0
15	bA	200	0	280	10	0
15	bB	240	0	336	12	0
15	bF	120	0	168	5	0
15	bI	40	0	56	2	0
15	bJ	40	0	56	1	0
15	bL	120	0	168	4	0
15	bM	40	0	55	0	0
15	cA	200	0	280	12	0
15	cB	240	0	336	9	0
15	cF	120	0	168	7	0
15	cI	40	0	56	1	0
15	cJ	40	0	56	0	0
15	cL	120	0	168	6	0
15	cM	40	0	55	0	0
16	aA	76	0	98	1	0
16	aB	23	0	16	0	0
16	bA	76	0	98	2	0
16	bB	23	0	16	0	0
16	cA	76	0	98	2	0
16	cB	23	0	16	0	0
17	aB	43	0	56	0	0
17	bB	43	0	56	0	0
17	cB	43	0	56	0	0
18	aA	45	0	0	1	0
18	aB	67	0	0	1	0
18	aC	14	0	0	0	0
18	aD	2	0	0	0	0
18	aE	3	0	0	0	0
18	aF	1	0	0	0	0
18	aJ	1	0	0	0	0
18	aL	1	0	0	0	0
18	bA	45	0	0	1	0
18	bB	67	0	0	1	0
18	bC	14	0	0	0	0
18	bD	2	0	0	0	0
18	bE	3	0	0	0	0
18	bF	1	0	0	0	0
18	bJ	1	0	0	0	0
18	bL	1	0	0	0	0
18	cA	45	0	0	1	0
18	cB	67	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	cC	14	0	0	0	0
18	cD	2	0	0	0	0
18	cE	3	0	0	0	0
18	cF	1	0	0	0	0
18	cJ	1	0	0	0	0
18	cL	1	0	0	0	0
All	All	67641	0	65379	561	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 4.

All (561) 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)
12:cA:809:CLA:HBB2	12:cA:828:CLA:H171	1.71	0.72
12:bA:809:CLA:HBB2	12:bA:828:CLA:H171	1.71	0.72
12:aA:809:CLA:HBB2	12:aA:828:CLA:H171	1.71	0.71
12:bA:818:CLA:HBA2	12:bA:827:CLA:HBB2	1.73	0.71
12:aA:818:CLA:HBA2	12:aA:827:CLA:HBB2	1.73	0.69
12:cA:818:CLA:HBA2	12:cA:827:CLA:HBB2	1.73	0.69
4:cD:46:GLU:H	4:cD:76:GLN:HE22	1.41	0.67
4:bD:46:GLU:H	4:bD:76:GLN:HE22	1.41	0.67
4:aD:46:GLU:H	4:aD:76:GLN:HE22	1.41	0.66
12:aB:917:CLA:H8	12:aB:917:CLA:HAB	1.78	0.66
12:bB:917:CLA:HAB	12:bB:917:CLA:H8	1.78	0.65
12:cB:917:CLA:HAB	12:cB:917:CLA:H8	1.78	0.65
1:cA:380:PRO:HG3	12:cA:819:CLA:HBA2	1.78	0.65
1:bA:380:PRO:HG3	12:bA:819:CLA:HBA2	1.78	0.65
1:aA:380:PRO:HG3	12:aA:819:CLA:HBA2	1.78	0.63
2:aB:303:GLU:HG2	2:aB:391:ASN:HB3	1.81	0.62
12:aA:832:CLA:H42	9:aL:31:ILE:HD11	1.82	0.62
12:cA:832:CLA:H42	9:cL:31:ILE:HD11	1.82	0.61
4:aD:88:ILE:HB	4:aD:101:PHE:HB3	1.83	0.61
12:bA:832:CLA:H42	9:bL:31:ILE:HD11	1.82	0.61
2:cB:705:ALA:HB2	12:cB:926:CLA:HBB1	1.82	0.61
2:bB:303:GLU:HG2	2:bB:391:ASN:HB3	1.81	0.61
4:bD:88:ILE:HB	4:bD:101:PHE:HB3	1.83	0.61
2:cB:303:GLU:HG2	2:cB:391:ASN:HB3	1.81	0.61
12:cA:804:CLA:HED3	12:cA:841:CLA:HBA2	1.83	0.61
2:aB:705:ALA:HB2	12:aB:926:CLA:HBB1	1.82	0.61
1:bA:61:HIS:ND1	18:bA:901:HOH:O	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:cA:61:HIS:ND1	18:cA:901:HOH:O	2.31	0.60
2:bB:705:ALA:HB2	12:bB:926:CLA:HBB1	1.82	0.60
1:aA:428:ASN:OD1	1:aA:436:ARG:NH2	2.35	0.60
4:cD:88:ILE:HB	4:cD:101:PHE:HB3	1.83	0.60
6:aF:161:ILE:HA	6:aF:164:LEU:HB2	1.84	0.60
4:aD:56:VAL:H	4:aD:60:ASN:HD21	1.48	0.60
12:bA:804:CLA:HED3	12:bA:841:CLA:HBA2	1.83	0.60
6:bF:161:ILE:HA	6:bF:164:LEU:HB2	1.84	0.59
6:cF:161:ILE:HA	6:cF:164:LEU:HB2	1.84	0.59
1:cA:405:LEU:HD21	12:cA:807:CLA:H142	1.85	0.59
1:cA:428:ASN:OD1	1:cA:436:ARG:NH2	2.35	0.59
4:cD:56:VAL:H	4:cD:60:ASN:HD21	1.48	0.59
1:bA:428:ASN:OD1	1:bA:436:ARG:NH2	2.35	0.59
1:aA:405:LEU:HD21	12:aA:807:CLA:H142	1.85	0.59
12:aA:804:CLA:HED3	12:aA:841:CLA:HBA2	1.83	0.59
4:bD:56:VAL:H	4:bD:60:ASN:HD21	1.48	0.58
1:bA:405:LEU:HD21	12:bA:807:CLA:H142	1.85	0.58
1:aA:61:HIS:ND1	18:aA:901:HOH:O	2.31	0.57
1:bA:305:ILE:HD13	12:bA:819:CLA:HBB1	1.86	0.57
12:cB:930:CLA:O1A	6:cF:170:ARG:NH2	2.38	0.57
7:aI:14:THR:HB	15:aI:101:BCR:H333	1.87	0.57
2:bB:389:ASN:HD22	2:bB:392:ASN:HD21	1.53	0.57
7:bI:14:THR:HB	15:bI:101:BCR:H333	1.87	0.57
1:cA:305:ILE:HD13	12:cA:819:CLA:HBB1	1.86	0.57
1:aA:583:LYS:NZ	2:aB:656:GLU:OE1	2.35	0.57
2:aB:389:ASN:HD22	2:aB:392:ASN:HD21	1.53	0.57
12:aB:930:CLA:O1A	6:aF:170:ARG:NH2	2.38	0.56
12:bB:930:CLA:O1A	6:bF:170:ARG:NH2	2.38	0.56
6:bF:90:ASP:N	6:bF:90:ASP:OD1	2.37	0.56
6:cF:90:ASP:OD1	6:cF:90:ASP:N	2.38	0.56
6:aF:90:ASP:OD1	6:aF:90:ASP:N	2.37	0.56
2:cB:389:ASN:HD22	2:cB:392:ASN:HD21	1.53	0.56
7:cI:14:THR:HB	15:cI:101:BCR:H333	1.87	0.56
1:bA:221:ILE:HA	1:bA:225:LEU:HD12	1.87	0.56
1:bA:746:GLN:NE2	5:bE:17:TYR:OH	2.38	0.56
1:aA:305:ILE:HD13	12:aA:819:CLA:HBB1	1.86	0.56
1:cA:746:GLN:NE2	5:cE:17:TYR:OH	2.38	0.56
12:cA:838:CLA:HHC	12:cA:838:CLA:HBB1	1.89	0.55
12:aA:838:CLA:HHC	12:aA:838:CLA:HBB1	1.88	0.55
1:bA:583:LYS:NZ	2:bB:656:GLU:OE1	2.35	0.55
1:cA:221:ILE:HA	1:cA:225:LEU:HD12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:aA:746:GLN:NE2	5:aE:17:TYR:OH	2.38	0.55
1:aA:221:ILE:HA	1:aA:225:LEU:HD12	1.88	0.55
12:bB:922:CLA:HBA1	15:bB:944:BCR:H15C	1.89	0.55
9:aL:43:GLU:OE1	9:aL:114:ARG:NH1	2.39	0.54
12:cB:922:CLA:HBA1	15:cB:944:BCR:H15C	1.89	0.54
5:cE:37:PRO:HD2	5:cE:56:GLY:HA2	1.90	0.54
12:aB:911:CLA:HHC	12:aB:911:CLA:HBB1	1.89	0.54
12:bA:838:CLA:HHC	12:bA:838:CLA:HBB1	1.89	0.54
12:bB:911:CLA:HBB1	12:bB:911:CLA:HHC	1.89	0.54
4:bD:36:VAL:HG22	4:bD:61:VAL:HG12	1.90	0.54
5:bE:37:PRO:HD2	5:bE:56:GLY:HA2	1.90	0.54
12:aA:808:CLA:HMB3	12:aA:809:CLA:HHB	1.89	0.54
12:aA:843:CLA:H151	15:aL:205:BCR:H17C	1.90	0.54
1:cA:353:TRP:HB3	12:cA:806:CLA:HAC1	1.90	0.54
1:bA:353:TRP:HB3	12:bA:806:CLA:HAC1	1.90	0.53
12:aB:922:CLA:HBA1	15:aB:944:BCR:H15C	1.89	0.53
12:cB:911:CLA:HHC	12:cB:911:CLA:HBB1	1.90	0.53
4:aD:36:VAL:HG22	4:aD:61:VAL:HG12	1.90	0.53
12:bA:808:CLA:HMB3	12:bA:809:CLA:HHB	1.89	0.53
5:aE:37:PRO:HD2	5:aE:56:GLY:HA2	1.90	0.53
12:bA:843:CLA:H151	15:bL:205:BCR:H17C	1.90	0.53
12:cA:808:CLA:HMB3	12:cA:809:CLA:HHB	1.89	0.53
4:cD:36:VAL:HG22	4:cD:61:VAL:HG12	1.90	0.53
9:bL:43:GLU:OE1	9:bL:114:ARG:NH1	2.39	0.53
12:aB:906:CLA:H12	7:aI:14:THR:HG21	1.90	0.53
5:cE:10:ARG:NH1	5:cE:61:GLU:OE1	2.36	0.53
12:aA:833:CLA:HMA3	15:aI:101:BCR:H272	1.91	0.52
5:bE:10:ARG:NH1	5:bE:61:GLU:OE1	2.36	0.52
12:cA:843:CLA:H151	15:cL:205:BCR:H17C	1.90	0.52
1:aA:353:TRP:HB3	12:aA:806:CLA:HAC1	1.90	0.52
12:bB:906:CLA:H12	7:bI:14:THR:HG21	1.92	0.52
4:bD:30:GLU:HG2	4:bD:31:GLU:HG2	1.91	0.52
2:cB:626:LEU:HD11	2:cB:714:ALA:HB2	1.91	0.52
9:cL:43:GLU:OE1	9:cL:114:ARG:NH1	2.39	0.52
9:bL:102:ASP:OD1	9:bL:103:VAL:N	2.43	0.52
12:bA:829:CLA:H2	15:bA:847:BCR:H24C	1.92	0.52
4:aD:30:GLU:HG2	4:aD:31:GLU:HG2	1.91	0.51
9:cL:102:ASP:OD1	9:cL:103:VAL:N	2.43	0.51
1:aA:374:HIS:ND1	12:aA:818:CLA:OBD	2.42	0.51
12:cB:906:CLA:H12	7:cI:14:THR:HG21	1.92	0.51
1:aA:202:ASN:HB3	12:aA:820:CLA:HMD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:aA:461:VAL:HG12	12:aA:834:CLA:HBC2	1.93	0.51
1:cA:374:HIS:ND1	12:cA:818:CLA:OBD	2.42	0.51
2:aB:174:ARG:HB2	12:aB:912:CLA:HBC2	1.93	0.51
12:bA:840:CLA:H2	12:bB:931:CLA:H42	1.93	0.51
2:bB:626:LEU:HD11	2:bB:714:ALA:HB2	1.91	0.51
4:cD:30:GLU:HG2	4:cD:31:GLU:HG2	1.91	0.51
1:aA:658:GLY:H	1:aA:659:GLY:HA2	1.75	0.51
12:aA:821:CLA:HHC	12:aA:821:CLA:HBB1	1.93	0.51
12:bA:821:CLA:HHC	12:bA:821:CLA:HBB1	1.93	0.51
2:cB:177:HIS:HB3	12:cB:912:CLA:HBB1	1.93	0.51
2:aB:177:HIS:HB3	12:aB:912:CLA:HBB1	1.93	0.51
9:aL:102:ASP:OD1	9:aL:103:VAL:N	2.43	0.51
12:cA:829:CLA:H2	15:cA:847:BCR:H24C	1.92	0.51
12:cA:840:CLA:HBB2	6:cF:125:GLY:HA3	1.93	0.51
2:cB:174:ARG:HB2	12:cB:912:CLA:HBC2	1.93	0.50
2:aB:626:LEU:HD11	2:aB:714:ALA:HB2	1.91	0.50
1:cA:461:VAL:HG12	12:cA:834:CLA:HBC2	1.93	0.50
1:cA:658:GLY:H	1:cA:659:GLY:HA2	1.75	0.50
2:cB:468:GLY:HA2	2:cB:476:LEU:HD21	1.93	0.50
1:bA:374:HIS:ND1	12:bA:818:CLA:OBD	2.42	0.50
12:aA:840:CLA:H2	12:aB:931:CLA:H42	1.93	0.50
12:aA:840:CLA:HBB2	6:aF:125:GLY:HA3	1.93	0.50
1:bA:658:GLY:H	1:bA:659:GLY:HA2	1.75	0.50
12:aA:829:CLA:H2	15:aA:848:BCR:H24C	1.92	0.50
2:aB:468:GLY:HA2	2:aB:476:LEU:HD21	1.93	0.50
2:bB:174:ARG:HB2	12:bB:912:CLA:HBC2	1.93	0.50
2:bB:177:HIS:HB3	12:bB:912:CLA:HBB1	1.93	0.50
2:bB:397:MET:HE2	15:bB:944:BCR:H323	1.94	0.50
12:aA:806:CLA:H151	15:aA:848:BCR:H372	1.93	0.50
12:cA:840:CLA:H2	12:cB:931:CLA:H42	1.93	0.50
12:aA:834:CLA:H152	15:aL:201:BCR:H372	1.94	0.50
2:aB:397:MET:HE2	15:aB:944:BCR:H323	1.94	0.50
1:bA:461:VAL:HG12	12:bA:834:CLA:HBC2	1.93	0.50
15:bA:850:BCR:H362	12:bA:853:CLA:H2	1.94	0.50
12:cA:806:CLA:H151	15:cA:847:BCR:H372	1.93	0.50
3:cC:29:VAL:HG21	4:cD:117:VAL:HB	1.94	0.50
2:bB:415:LEU:HD11	12:bB:936:CLA:HMB2	1.94	0.49
3:bC:29:VAL:HG21	4:bD:117:VAL:HB	1.94	0.49
6:bF:162:PRO:O	6:bF:166:SER:OG	2.30	0.49
2:cB:397:MET:HE2	15:cB:944:BCR:H323	1.94	0.49
2:cB:415:LEU:HD11	12:cB:936:CLA:HMB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:aA:851:BCR:H362	12:aA:854:CLA:H2	1.94	0.49
12:bA:806:CLA:H151	15:bA:847:BCR:H372	1.93	0.49
5:aE:10:ARG:NH1	5:aE:61:GLU:OE1	2.36	0.49
12:cB:931:CLA:H61	15:cF:203:BCR:HC32	1.94	0.49
12:cB:936:CLA:HBC2	15:cF:204:BCR:HC7	1.94	0.49
12:bA:843:CLA:H71	12:bA:843:CLA:HBB1	1.94	0.49
12:bB:936:CLA:HBC2	15:bF:204:BCR:HC7	1.94	0.49
12:cA:821:CLA:HHC	12:cA:821:CLA:HBB1	1.93	0.49
9:cL:24:SER:HB2	9:cL:27:ILE:HB	1.94	0.49
12:bA:840:CLA:HBB2	6:bF:125:GLY:HA3	1.93	0.49
6:cF:162:PRO:O	6:cF:166:SER:OG	2.30	0.49
12:bA:834:CLA:H152	15:bL:201:BCR:H372	1.95	0.49
2:bB:468:GLY:HA2	2:bB:476:LEU:HD21	1.93	0.49
2:cB:182:LEU:HD11	12:cB:912:CLA:H12	1.95	0.49
2:aB:289:ILE:HG21	12:aB:923:CLA:HAC1	1.94	0.49
9:aL:24:SER:HB2	9:aL:27:ILE:HB	1.94	0.49
4:bD:121:VAL:HG12	4:bD:123:ARG:HG2	1.95	0.49
9:bL:24:SER:HB2	9:bL:27:ILE:HB	1.94	0.49
12:cA:843:CLA:H71	12:cA:843:CLA:HBB1	1.94	0.49
4:aD:121:VAL:HG12	4:aD:123:ARG:HG2	1.95	0.49
12:aA:802:CLA:H13	15:aB:946:BCR:H10C	1.95	0.48
12:aB:931:CLA:H61	15:aF:203:BCR:HC32	1.94	0.48
12:bA:802:CLA:H13	15:bB:946:BCR:H10C	1.95	0.48
2:bB:655:GLN:NE2	2:bB:682:ALA:H	2.11	0.48
2:bB:182:LEU:HD11	12:bB:912:CLA:H12	1.95	0.48
12:bB:931:CLA:H61	15:bF:203:BCR:HC32	1.95	0.48
15:cA:850:BCR:H362	12:cA:853:CLA:H2	1.94	0.48
12:aB:936:CLA:HBC2	15:aF:204:BCR:HC7	1.94	0.48
2:cB:289:ILE:HG21	12:cB:923:CLA:HAC1	1.94	0.48
3:aC:29:VAL:HG21	4:aD:117:VAL:HB	1.94	0.48
12:bA:817:CLA:H62	12:bA:817:CLA:H41	1.66	0.48
1:bA:326:ILE:HG21	12:bA:825:CLA:HAC1	1.96	0.48
2:bB:289:ILE:HG21	12:bB:923:CLA:HAC1	1.94	0.48
1:cA:583:LYS:NZ	2:cB:656:GLU:OE1	2.35	0.48
12:cB:933:CLA:HHC	12:cB:933:CLA:HBB1	1.96	0.48
2:aB:415:LEU:HD11	12:aB:936:CLA:HMB2	1.94	0.48
12:aB:933:CLA:HHC	12:aB:933:CLA:HBB1	1.96	0.48
6:aF:162:PRO:O	6:aF:166:SER:OG	2.30	0.48
12:cA:834:CLA:H152	15:cL:201:BCR:H372	1.95	0.48
2:cB:655:GLN:NE2	2:cB:682:ALA:H	2.11	0.48
12:cA:802:CLA:H13	15:cB:946:BCR:H10C	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:aA:843:CLA:H71	12:aA:843:CLA:HBB1	1.94	0.47
2:aB:182:LEU:HD11	12:aB:912:CLA:H12	1.95	0.47
12:cA:822:CLA:H3A	12:cA:822:CLA:HBA2	1.65	0.47
12:cA:825:CLA:HHC	12:cA:825:CLA:HBB1	1.96	0.47
4:cD:121:VAL:HG12	4:cD:123:ARG:HG2	1.95	0.47
4:aD:66:ARG:NH2	4:aD:68:GLU:OE2	2.48	0.47
9:bL:103:VAL:HB	9:bL:107:PHE:HB2	1.97	0.47
12:aA:819:CLA:H121	12:aA:827:CLA:H3A	1.97	0.47
6:aF:62:GLN:HE21	6:aF:71:ASN:HB2	1.80	0.47
12:bB:912:CLA:H112	12:bB:912:CLA:H142	1.78	0.47
1:cA:506:TRP:HB2	12:cA:836:CLA:HED2	1.97	0.47
12:cA:804:CLA:H43	12:cA:842:CLA:HBA2	1.97	0.47
12:cA:853:CLA:HBC2	2:cB:567:ASN:HB2	1.97	0.47
12:aA:825:CLA:HHC	12:aA:825:CLA:HBB1	1.96	0.47
6:bF:62:GLN:HE21	6:bF:71:ASN:HB2	1.80	0.47
1:cA:326:ILE:HG21	12:cA:825:CLA:HAC1	1.96	0.47
2:bB:263:HIS:HB3	12:bB:916:CLA:HMB2	1.97	0.47
12:bB:933:CLA:HHC	12:bB:933:CLA:HBB1	1.96	0.47
2:cB:445:PHE:HB3	12:cB:935:CLA:H42	1.97	0.47
2:aB:655:GLN:NE2	2:aB:682:ALA:H	2.11	0.47
12:bA:819:CLA:H121	12:bA:827:CLA:H3A	1.97	0.47
1:cA:597:ARG:NH2	4:cD:68:GLU:OE1	2.42	0.47
12:cB:919:CLA:HBA2	12:cB:919:CLA:H3A	1.65	0.47
1:aA:506:TRP:HB2	12:aA:836:CLA:HED2	1.97	0.46
12:bB:925:CLA:HHC	12:bB:925:CLA:HBB1	1.97	0.46
6:bF:97:THR:HG22	6:bF:107:PHE:HB2	1.96	0.46
15:cA:850:BCR:H20C	15:cA:850:BCR:H361	1.69	0.46
2:aB:263:HIS:HB3	12:aB:916:CLA:HMB2	1.97	0.46
2:aB:319:GLN:NE2	18:aB:1010:HOH:O	2.46	0.46
12:cB:927:CLA:H3A	12:cB:927:CLA:HBA2	1.66	0.46
6:cF:62:GLN:HE21	6:cF:71:ASN:HB2	1.80	0.46
1:aA:326:ILE:HG21	12:aA:825:CLA:HAC1	1.96	0.46
6:aF:97:THR:HG22	6:aF:107:PHE:HB2	1.96	0.46
2:cB:120:LEU:HD21	12:cB:927:CLA:HBA1	1.97	0.46
2:cB:319:GLN:NE2	18:cB:1010:HOH:O	2.46	0.46
12:cB:925:CLA:HBB1	12:cB:925:CLA:HHC	1.97	0.46
12:aA:830:CLA:H201	12:aA:842:CLA:H51	1.97	0.46
2:bB:445:PHE:HB3	12:bB:935:CLA:H42	1.97	0.46
15:aB:946:BCR:H20C	15:aB:946:BCR:H361	1.82	0.46
1:bA:506:TRP:HB2	12:bA:836:CLA:HED2	1.97	0.46
12:bB:919:CLA:HBA2	12:bB:919:CLA:H3A	1.65	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:bA:804:CLA:H43	12:bA:842:CLA:HBA2	1.97	0.46
1:cA:118:TRP:CD2	12:cA:810:CLA:HED3	2.51	0.46
12:cA:830:CLA:H201	12:cA:842:CLA:H51	1.97	0.46
2:aB:120:LEU:HD21	12:aB:927:CLA:HBA1	1.97	0.46
12:aB:926:CLA:H122	12:aB:926:CLA:HMD2	1.98	0.46
6:cF:97:THR:HG22	6:cF:107:PHE:HB2	1.97	0.46
1:aA:732:ILE:HD13	12:aA:840:CLA:HMD1	1.98	0.46
12:bA:825:CLA:HHC	12:bA:825:CLA:HBB1	1.96	0.46
1:cA:732:ILE:HD13	12:cA:840:CLA:HMD1	1.98	0.46
12:aA:804:CLA:H43	12:aA:842:CLA:HBA2	1.97	0.46
12:aA:854:CLA:HBC2	2:aB:567:ASN:HB2	1.97	0.46
12:cA:819:CLA:H121	12:cA:827:CLA:H3A	1.97	0.46
2:cB:325:ALA:HB2	15:cB:945:BCR:H372	1.98	0.46
2:aB:445:PHE:HB3	12:aB:935:CLA:H42	1.97	0.46
12:bA:826:CLA:HAB	15:bA:849:BCR:C8	2.46	0.46
4:cD:66:ARG:NH2	4:cD:68:GLU:OE2	2.48	0.46
2:aB:325:ALA:HB2	15:aB:945:BCR:H372	1.98	0.45
2:cB:263:HIS:HB3	12:cB:916:CLA:HMB2	1.97	0.45
1:bA:732:ILE:HD13	12:bA:840:CLA:HMD1	1.98	0.45
9:cL:33:ASN:HB3	12:cL:202:CLA:HAC1	1.98	0.45
1:bA:727:GLU:OE2	2:bB:532:LYS:NZ	2.48	0.45
2:bB:120:LEU:HD21	12:bB:927:CLA:HBA1	1.97	0.45
12:cB:929:CLA:H3A	12:cB:929:CLA:HBA2	1.70	0.45
12:aB:915:CLA:H41	12:aB:915:CLA:H61	1.65	0.45
1:bA:464:ASP:CG	1:bA:673:ASN:HB2	2.41	0.45
12:bA:812:CLA:H72	12:bA:812:CLA:H111	1.68	0.45
12:bA:853:CLA:HBC2	2:bB:567:ASN:HB2	1.97	0.45
2:bB:325:ALA:HB2	15:bB:945:BCR:H372	1.98	0.45
12:bB:905:CLA:H61	12:bB:905:CLA:H41	1.68	0.45
12:cB:926:CLA:HMD2	12:cB:926:CLA:H122	1.98	0.45
12:bA:832:CLA:H62	12:bA:832:CLA:H41	1.62	0.45
12:bB:915:CLA:H41	12:bB:915:CLA:H61	1.65	0.45
12:aA:814:CLA:HAA2	12:aA:825:CLA:H52	1.99	0.45
12:aB:925:CLA:HHC	12:aB:925:CLA:HBB1	1.97	0.45
9:aL:103:VAL:HB	9:aL:107:PHE:HB2	1.97	0.45
9:aL:138:PRO:O	9:aL:145:ARG:NH2	2.50	0.45
12:bB:926:CLA:H122	12:bB:926:CLA:HMD2	1.98	0.45
12:cA:820:CLA:HBA2	12:cA:820:CLA:H3A	1.71	0.45
15:cA:849:BCR:H15C	15:cA:849:BCR:H351	1.77	0.45
9:cL:103:VAL:HB	9:cL:107:PHE:HB2	1.97	0.45
1:aA:118:TRP:CD2	12:aA:810:CLA:HED3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:bL:33:ASN:HB3	12:bL:202:CLA:HAC1	1.98	0.45
9:aL:33:ASN:HB3	12:aL:202:CLA:HAC1	1.98	0.45
9:aL:87:LEU:HD11	12:bL:202:CLA:HAA1	1.99	0.45
2:bB:319:GLN:NE2	18:bB:1011:HOH:O	2.46	0.45
1:cA:445:LEU:HD21	1:cA:564:VAL:HG12	1.98	0.45
12:cA:814:CLA:HAA2	12:cA:825:CLA:H52	1.99	0.45
15:cL:201:BCR:H15C	15:cL:201:BCR:H351	1.88	0.45
1:aA:445:LEU:HD21	1:aA:564:VAL:HG12	1.98	0.45
12:aA:826:CLA:HAB	15:aA:850:BCR:C8	2.46	0.45
1:bA:118:TRP:CD2	12:bA:810:CLA:HED3	2.51	0.45
1:bA:445:LEU:HD21	1:bA:564:VAL:HG12	1.98	0.45
12:bA:814:CLA:HAA2	12:bA:825:CLA:H52	1.99	0.45
12:bA:830:CLA:H201	12:bA:842:CLA:H51	1.97	0.45
15:bB:943:BCR:H15C	15:bB:943:BCR:H351	1.89	0.45
9:bL:138:PRO:O	9:bL:145:ARG:NH2	2.50	0.45
1:cA:464:ASP:CG	1:cA:673:ASN:HB2	2.41	0.45
12:cA:842:CLA:H62	12:cA:842:CLA:H101	1.83	0.45
12:aB:925:CLA:H41	12:aB:925:CLA:H62	1.72	0.44
15:bA:847:BCR:H20C	15:bA:847:BCR:H361	1.80	0.44
15:bA:850:BCR:H361	15:bA:850:BCR:H20C	1.69	0.44
12:bB:931:CLA:H62	12:bB:931:CLA:H2	1.77	0.44
12:cA:826:CLA:HAB	15:cA:849:BCR:C8	2.46	0.44
12:cA:842:CLA:H152	12:cA:842:CLA:H111	1.69	0.44
12:cB:905:CLA:H41	12:cB:905:CLA:H61	1.68	0.44
15:cF:204:BCR:H15C	15:cF:204:BCR:H351	1.83	0.44
1:aA:464:ASP:CG	1:aA:673:ASN:HB2	2.41	0.44
12:aA:842:CLA:H62	12:aA:842:CLA:H101	1.83	0.44
12:bA:822:CLA:HBA2	12:bA:822:CLA:H3A	1.65	0.44
2:aB:4:ARG:HD2	2:aB:4:ARG:HA	1.82	0.44
12:aB:912:CLA:H112	12:aB:912:CLA:H142	1.78	0.44
12:aB:931:CLA:HHC	12:aB:931:CLA:HBB1	2.00	0.44
4:bD:66:ARG:NH2	4:bD:68:GLU:OE2	2.48	0.44
2:aB:183:PHE:HZ	12:aB:923:CLA:H12	1.83	0.44
5:cE:20:ARG:HE	6:cF:174:ASP:HA	1.83	0.44
12:aA:832:CLA:H62	12:aA:832:CLA:H41	1.62	0.44
15:cA:848:BCR:H20C	15:cA:848:BCR:H361	1.83	0.44
2:cB:106:PRO:HD3	2:cB:113:VAL:HG22	1.99	0.44
7:cI:32:ARG:HA	7:cI:32:ARG:HD3	1.83	0.44
12:aA:812:CLA:H111	12:aA:812:CLA:H72	1.68	0.44
15:aA:850:BCR:H15C	15:aA:850:BCR:H351	1.77	0.44
2:bB:183:PHE:HZ	12:bB:923:CLA:H12	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:aB:106:PRO:HD3	2:aB:113:VAL:HG22	1.99	0.44
12:aB:929:CLA:H3A	12:aB:929:CLA:HBA2	1.70	0.44
15:bA:848:BCR:H15C	15:bA:848:BCR:H351	1.86	0.44
4:bD:84:ARG:HE	4:bD:84:ARG:HB2	1.67	0.44
2:cB:183:PHE:HZ	12:cB:923:CLA:H12	1.83	0.44
12:aB:912:CLA:H111	12:aB:912:CLA:H71	1.72	0.43
12:aB:931:CLA:H2	12:aB:931:CLA:H62	1.77	0.43
12:bA:842:CLA:H62	12:bA:842:CLA:H101	1.83	0.43
9:cL:138:PRO:O	9:cL:145:ARG:NH2	2.50	0.43
2:aB:188:LEU:HD11	15:aB:941:BCR:HC7	2.00	0.43
15:aB:943:BCR:H15C	15:aB:943:BCR:H351	1.89	0.43
2:bB:287:HIS:HB3	2:bB:292:ILE:HD11	2.01	0.43
12:cB:931:CLA:HHC	12:cB:931:CLA:HBB1	2.00	0.43
2:aB:311:THR:OG1	2:aB:389:ASN:ND2	2.48	0.43
12:bB:904:CLA:HBA1	12:bB:904:CLA:H3A	1.83	0.43
15:cA:847:BCR:H20C	15:cA:847:BCR:H361	1.80	0.43
2:bB:106:PRO:HD3	2:bB:113:VAL:HG22	1.99	0.43
12:cB:916:CLA:H102	12:cB:916:CLA:H62	1.81	0.43
4:aD:67:LYS:HE3	4:aD:100:ILE:HD12	2.01	0.43
15:aL:205:BCR:H15C	15:aL:205:BCR:H351	1.89	0.43
5:bE:20:ARG:HE	6:bF:174:ASP:HA	1.83	0.43
12:cA:834:CLA:H92	12:cA:834:CLA:H61	1.86	0.43
12:aA:830:CLA:H122	12:aA:830:CLA:H161	1.82	0.43
2:aB:91:ILE:O	7:aI:4:TYR:OH	2.29	0.43
2:bB:646:PHE:HA	13:bB:940:1L3:O13	2.18	0.43
12:bB:909:CLA:HHC	12:bB:909:CLA:HBB1	2.01	0.43
12:cA:818:CLA:H61	12:cA:818:CLA:H41	1.75	0.43
15:cA:846:BCR:H15C	15:cA:846:BCR:H351	1.87	0.43
3:aC:2:SER:N	3:aC:71:ALA:O	2.52	0.43
1:bA:356:GLN:HG3	12:bA:825:CLA:H152	2.01	0.43
12:bB:931:CLA:HHC	12:bB:931:CLA:HBB1	2.00	0.43
4:bD:67:LYS:HE3	4:bD:100:ILE:HD12	2.01	0.43
12:cB:909:CLA:HHC	12:cB:909:CLA:HBB1	2.01	0.43
3:cC:22:PRO:HA	4:cD:75:ARG:HH12	1.84	0.43
2:bB:606:LEU:HD22	12:bB:901:CLA:HMD3	1.99	0.43
4:bD:104:ASP:OD1	4:bD:104:ASP:N	2.51	0.43
1:cA:363:MET:HG3	12:cA:825:CLA:HHB	2.01	0.43
4:cD:67:LYS:HE3	4:cD:100:ILE:HD12	2.01	0.43
4:cD:104:ASP:OD1	4:cD:104:ASP:N	2.51	0.43
2:aB:383:ASP:OD2	4:aD:135:LYS:NZ	2.52	0.43
4:aD:104:ASP:OD1	4:aD:104:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:bA:363:MET:HG3	12:bA:825:CLA:HHB	2.01	0.43
3:bC:28:MET:O	4:bD:115:ARG:NH1	2.47	0.43
2:cB:383:ASP:OD2	4:cD:135:LYS:NZ	2.52	0.43
15:cL:206:BCR:H20C	15:cL:206:BCR:H361	1.88	0.43
12:aB:902:CLA:H112	12:aB:902:CLA:H72	1.82	0.43
2:bB:383:ASP:OD2	4:bD:135:LYS:NZ	2.52	0.43
12:cA:806:CLA:HBA1	12:cA:806:CLA:H3A	1.82	0.43
12:cA:812:CLA:H111	12:cA:812:CLA:H72	1.67	0.43
12:cA:830:CLA:H161	12:cA:830:CLA:H122	1.83	0.43
2:aB:287:HIS:HB3	2:aB:292:ILE:HD11	2.00	0.42
12:aB:909:CLA:HHC	12:aB:909:CLA:HBB1	2.01	0.42
1:bA:59:GLU:HG3	1:bA:68:ILE:HD13	2.01	0.42
15:bF:204:BCR:H24C	15:bF:204:BCR:H371	1.80	0.42
1:cA:120:VAL:O	1:cA:123:GLN:HG2	2.19	0.42
3:cC:2:SER:N	3:cC:71:ALA:O	2.52	0.42
12:aA:840:CLA:HMB2	12:aB:931:CLA:H52	2.01	0.42
1:bA:627:PHE:HD1	12:bA:837:CLA:HAC1	1.84	0.42
12:bA:806:CLA:HBA1	12:bA:806:CLA:H3A	1.82	0.42
9:bL:87:LEU:HD11	12:cL:202:CLA:HAA1	2.02	0.42
9:bL:130:ALA:HB1	12:bL:204:CLA:HED1	2.01	0.42
12:cA:843:CLA:HAB	2:cB:674:VAL:HG11	2.02	0.42
2:cB:311:THR:OG1	2:cB:389:ASN:ND2	2.48	0.42
15:cB:945:BCR:H11C	15:cB:945:BCR:H341	1.89	0.42
5:aE:20:ARG:HE	6:aF:174:ASP:HA	1.83	0.42
12:bB:929:CLA:H3A	12:bB:929:CLA:HBA2	1.70	0.42
3:bC:2:SER:N	3:bC:71:ALA:O	2.52	0.42
2:cB:480:LEU:HA	2:cB:483:VAL:HG22	2.02	0.42
15:cB:945:BCR:H371	15:cB:945:BCR:H24C	1.84	0.42
12:aA:821:CLA:H42	15:aA:849:BCR:H352	2.01	0.42
12:bA:821:CLA:H42	15:bA:848:BCR:H352	2.01	0.42
2:cB:4:ARG:HD2	2:cB:4:ARG:HA	1.82	0.42
12:cB:913:CLA:H61	12:cB:913:CLA:H102	1.91	0.42
15:cL:205:BCR:H15C	15:cL:205:BCR:H351	1.89	0.42
12:bA:830:CLA:H122	12:bA:830:CLA:H161	1.82	0.42
1:cA:349:LEU:HD23	1:cA:349:LEU:HA	1.87	0.42
2:cB:188:LEU:HD11	15:cB:941:BCR:HC7	2.00	0.42
12:cB:925:CLA:H41	12:cB:925:CLA:H62	1.72	0.42
1:aA:627:PHE:HD1	12:aA:837:CLA:HAC1	1.84	0.42
3:aC:28:MET:O	4:aD:115:ARG:NH1	2.47	0.42
2:bB:189:ALA:HA	12:bB:914:CLA:HAB	2.02	0.42
2:bB:480:LEU:HA	2:bB:483:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:cA:727:GLU:OE2	2:cB:532:LYS:NZ	2.48	0.42
12:cA:809:CLA:HBB1	12:cA:810:CLA:C3D	2.50	0.42
12:cA:821:CLA:H42	15:cA:848:BCR:H352	2.01	0.42
12:cA:832:CLA:H62	12:cA:832:CLA:H41	1.62	0.42
12:aB:919:CLA:HBA2	12:aB:919:CLA:H3A	1.65	0.42
15:bL:201:BCR:H15C	15:bL:201:BCR:H351	1.89	0.42
2:cB:194:MET:HE1	2:cB:258:LEU:HD22	2.02	0.42
2:cB:287:HIS:HB3	2:cB:292:ILE:HD11	2.00	0.42
9:cL:130:ALA:HB1	12:cL:204:CLA:HED1	2.01	0.42
1:aA:363:MET:HG3	12:aA:825:CLA:HHB	2.01	0.42
12:aB:927:CLA:H51	15:aB:943:BCR:H392	2.02	0.42
12:aB:931:CLA:H112	12:aB:931:CLA:H152	1.84	0.42
12:aL:202:CLA:HAA1	9:cL:87:LEU:HD11	2.01	0.42
1:bA:736:HIS:HA	1:bA:741:VAL:HG23	2.02	0.42
12:bB:902:CLA:H112	12:bB:902:CLA:H72	1.82	0.42
12:bB:927:CLA:H51	15:bB:943:BCR:H392	2.02	0.42
12:cA:806:CLA:H111	12:cA:806:CLA:H93	1.85	0.42
2:cB:540:PRO:HB3	2:cB:685:ILE:HB	2.02	0.42
12:cB:927:CLA:H51	15:cB:943:BCR:H392	2.02	0.42
4:cD:56:VAL:N	4:cD:60:ASN:HD21	2.16	0.42
1:aA:571:VAL:HG21	15:aA:850:BCR:HC31	2.02	0.42
1:aA:736:HIS:HA	1:aA:741:VAL:HG23	2.02	0.42
12:aA:841:CLA:HMC1	15:aF:201:BCR:H381	2.02	0.42
12:aA:843:CLA:HAB	2:aB:674:VAL:HG11	2.01	0.42
2:bB:188:LEU:HD11	15:bB:941:BCR:HC7	2.00	0.42
3:bC:22:PRO:HA	4:bD:75:ARG:HH12	1.84	0.42
12:cA:807:CLA:H192	12:cA:807:CLA:H161	1.86	0.42
1:aA:510:THR:HG1	1:aA:514:TRP:CD1	2.38	0.42
12:aA:809:CLA:HBA2	12:aA:809:CLA:H3A	1.85	0.42
2:aB:194:MET:HE1	2:aB:258:LEU:HD22	2.02	0.42
12:bA:842:CLA:H111	12:bA:842:CLA:H152	1.69	0.42
2:bB:266:LEU:HD11	12:bB:915:CLA:HAB	2.02	0.42
12:cA:825:CLA:H143	12:cA:825:CLA:H111	1.92	0.42
12:cB:926:CLA:H112	12:cB:926:CLA:H152	1.95	0.42
1:aA:356:GLN:HG3	12:aA:825:CLA:H152	2.01	0.41
12:aA:809:CLA:HBB1	12:aA:810:CLA:C3D	2.50	0.41
2:aB:266:LEU:HD11	12:aB:915:CLA:HAB	2.02	0.41
12:aB:916:CLA:H62	12:aB:916:CLA:H102	1.81	0.41
1:bA:571:VAL:HG21	15:bA:849:BCR:HC31	2.02	0.41
2:cB:189:ALA:HA	12:cB:914:CLA:HAB	2.02	0.41
6:cF:163:GLU:HG2	6:cF:168:LYS:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:aL:206:BCR:H20C	15:aL:206:BCR:H361	1.88	0.41
1:bA:594:GLY:HA2	2:bB:544:PRO:HD3	2.03	0.41
12:bA:818:CLA:H61	12:bA:818:CLA:H41	1.75	0.41
12:bA:840:CLA:HMB2	12:bB:931:CLA:H52	2.01	0.41
12:bB:921:CLA:HBA2	12:bB:921:CLA:H3A	1.85	0.41
6:bF:116:TRP:NE1	6:bF:154:LEU:O	2.46	0.41
1:cA:59:GLU:HG3	1:cA:68:ILE:HD13	2.01	0.41
1:cA:736:HIS:HA	1:cA:741:VAL:HG23	2.02	0.41
16:cA:852:LHG:H242	16:cA:852:LHG:H112	2.02	0.41
1:aA:59:GLU:HG3	1:aA:68:ILE:HD13	2.01	0.41
2:aB:540:PRO:HB3	2:aB:685:ILE:HB	2.01	0.41
9:aL:130:ALA:HB1	12:aL:204:CLA:HED1	2.01	0.41
15:cL:201:BCR:H371	15:cL:201:BCR:H24C	1.86	0.41
1:aA:134:LYS:HE3	1:aA:134:LYS:HB3	1.92	0.41
1:aA:329:MET:HE2	1:aA:329:MET:HB3	1.86	0.41
6:aF:116:TRP:NE1	6:aF:154:LEU:O	2.46	0.41
15:aJ:101:BCR:H11C	15:aJ:101:BCR:H341	1.87	0.41
1:bA:120:VAL:O	1:bA:123:GLN:HG2	2.19	0.41
6:cF:42:LYS:O	6:cF:48:GLN:NE2	2.53	0.41
1:aA:349:LEU:HD23	1:aA:349:LEU:HA	1.87	0.41
16:aA:853:LHG:H242	16:aA:853:LHG:H112	2.02	0.41
12:aB:905:CLA:H152	12:aB:905:CLA:H111	1.84	0.41
6:aF:42:LYS:O	6:aF:48:GLN:NE2	2.53	0.41
1:bA:724:TYR:CE2	12:bA:803:CLA:HMD1	2.55	0.41
16:bA:852:LHG:H242	16:bA:852:LHG:H112	2.02	0.41
2:bB:540:PRO:HB3	2:bB:685:ILE:HB	2.02	0.41
12:bB:925:CLA:H62	12:bB:925:CLA:H41	1.72	0.41
1:cA:356:GLN:HG3	12:cA:825:CLA:H152	2.01	0.41
1:cA:571:VAL:HG21	15:cA:849:BCR:HC31	2.02	0.41
1:cA:627:PHE:HD1	12:cA:837:CLA:HAC1	1.84	0.41
12:cA:805:CLA:HBA2	12:cA:805:CLA:H3A	1.80	0.41
15:cA:849:BCR:H11C	15:cA:849:BCR:H341	1.90	0.41
15:cF:201:BCR:H20C	15:cF:201:BCR:H361	1.86	0.41
12:aB:904:CLA:HBA1	12:aB:904:CLA:H3A	1.83	0.41
15:aF:203:BCR:H20C	15:aF:203:BCR:H361	1.81	0.41
2:bB:414:PHE:CZ	15:bF:204:BCR:HC41	2.56	0.41
12:bB:926:CLA:H112	12:bB:926:CLA:H152	1.95	0.41
15:bB:944:BCR:H362	12:bB:949:CLA:HAB	2.02	0.41
1:cA:594:GLY:HA2	2:cB:544:PRO:HD3	2.03	0.41
1:aA:112:PRO:HB3	1:aA:148:PHE:CD1	2.56	0.41
1:aA:120:VAL:O	1:aA:123:GLN:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:bA:510:THR:HG1	1:bA:514:TRP:CD1	2.37	0.41
2:bB:399:GLU:HB3	12:bB:929:CLA:HED1	2.03	0.41
1:cA:79:HIS:CE1	12:cA:806:CLA:HMA3	2.55	0.41
12:cA:840:CLA:HMB2	12:cB:931:CLA:H52	2.01	0.41
12:cA:841:CLA:HMC1	15:cF:201:BCR:H381	2.02	0.41
1:aA:79:HIS:CE1	12:aA:806:CLA:HMA3	2.55	0.41
12:aA:817:CLA:H41	12:aA:817:CLA:H62	1.66	0.41
2:aB:399:GLU:HB3	12:aB:929:CLA:HED1	2.03	0.41
12:aB:927:CLA:H3A	12:aB:927:CLA:HBA2	1.66	0.41
1:bA:79:HIS:CE1	12:bA:806:CLA:HMA3	2.55	0.41
12:bA:843:CLA:HAB	2:bB:674:VAL:HG11	2.02	0.41
15:bB:943:BCR:H20C	15:bB:943:BCR:H361	1.90	0.41
1:cA:724:TYR:CE2	12:cA:803:CLA:HMD1	2.55	0.41
2:cB:266:LEU:HD11	12:cB:915:CLA:HAB	2.02	0.41
1:aA:594:GLY:HA2	2:aB:544:PRO:HD3	2.03	0.41
1:aA:724:TYR:CE2	12:aA:803:CLA:HMD1	2.55	0.41
12:aA:843:CLA:H192	12:aA:843:CLA:H162	1.90	0.41
2:aB:310:ASP:O	2:aB:314:ASN:ND2	2.54	0.41
15:aB:944:BCR:H362	12:aB:949:CLA:HAB	2.02	0.41
12:bA:809:CLA:HBB1	12:bA:810:CLA:C3D	2.50	0.41
12:bA:820:CLA:HBA2	12:bA:820:CLA:H3A	1.71	0.41
2:bB:310:ASP:O	2:bB:314:ASN:ND2	2.54	0.41
6:bF:42:LYS:O	6:bF:48:GLN:NE2	2.53	0.41
6:bF:163:GLU:HG2	6:bF:168:LYS:HD3	2.02	0.41
1:cA:553:HIS:CG	12:cA:838:CLA:HED3	2.56	0.41
2:cB:310:ASP:O	2:cB:314:ASN:ND2	2.54	0.41
12:cB:912:CLA:H111	12:cB:912:CLA:H71	1.72	0.41
12:cB:912:CLA:H142	12:cB:912:CLA:H112	1.78	0.41
15:cF:203:BCR:H20C	15:cF:203:BCR:H361	1.81	0.41
1:aA:597:ARG:NH2	4:aD:68:GLU:OE1	2.42	0.41
3:aC:22:PRO:HA	4:aD:75:ARG:HH12	1.84	0.41
1:bA:349:LEU:HA	1:bA:349:LEU:HD23	1.87	0.41
2:bB:194:MET:HE1	2:bB:258:LEU:HD22	2.02	0.41
12:bB:904:CLA:H61	12:bB:904:CLA:H102	1.91	0.41
15:bB:942:BCR:H20C	15:bB:942:BCR:H361	1.93	0.41
15:aA:851:BCR:H361	15:aA:851:BCR:H20C	1.69	0.40
15:aB:941:BCR:H15C	15:aB:941:BCR:H351	1.82	0.40
15:aB:943:BCR:H24C	15:aB:943:BCR:H371	1.86	0.40
6:aF:163:GLU:HG2	6:aF:168:LYS:HD3	2.02	0.40
15:bB:945:BCR:H371	15:bB:945:BCR:H24C	1.84	0.40
15:bB:946:BCR:H20C	15:bB:946:BCR:H361	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:bF:155:ILE:H	6:bF:155:ILE:HG13	1.46	0.40
15:bI:101:BCR:H15C	15:bI:101:BCR:H351	1.87	0.40
1:cA:616:MET:HE3	1:cA:616:MET:HB3	1.99	0.40
2:cB:399:GLU:HB3	12:cB:929:CLA:HED1	2.03	0.40
12:aA:837:CLA:H52	12:aA:837:CLA:H11	1.90	0.40
2:aB:480:LEU:HA	2:aB:483:VAL:HG22	2.01	0.40
12:aB:905:CLA:H61	12:aB:905:CLA:H41	1.68	0.40
12:aB:922:CLA:HMD3	12:aB:923:CLA:HHC	2.04	0.40
15:aF:201:BCR:H11C	15:aF:201:BCR:H341	1.97	0.40
16:cA:851:LHG:H282	16:cA:851:LHG:H311	1.70	0.40
12:cB:924:CLA:HED2	12:cB:925:CLA:HBD	2.03	0.40
2:aB:414:PHE:CZ	15:aF:204:BCR:HC41	2.56	0.40
1:bA:54:LEU:O	1:bA:61:HIS:NE2	2.42	0.40
1:bA:709:PHE:CG	15:bA:850:BCR:H363	2.57	0.40
12:bA:802:CLA:H171	12:bB:909:CLA:HMC2	2.04	0.40
12:bA:825:CLA:H203	12:bA:825:CLA:H161	1.94	0.40
12:bA:841:CLA:HMC1	15:bF:201:BCR:H381	2.02	0.40
1:cA:510:THR:HG1	1:cA:514:TRP:CD1	2.38	0.40
12:cA:843:CLA:H143	12:cA:843:CLA:H161	1.98	0.40
12:cA:853:CLA:HBB1	2:cB:507:LEU:HD21	2.04	0.40
12:cB:905:CLA:H93	12:cB:905:CLA:H111	1.98	0.40
12:cB:922:CLA:HMD3	12:cB:923:CLA:HHC	2.04	0.40
3:cC:61:ASP:OD2	5:cE:17:TYR:N	2.49	0.40
7:cI:7:PHE:HD2	7:cI:10:LEU:HD12	1.86	0.40
15:aF:204:BCR:H15C	15:aF:204:BCR:H351	1.82	0.40
12:bB:916:CLA:HBA2	12:bB:916:CLA:H3A	1.86	0.40
15:bJ:101:BCR:H11C	15:bJ:101:BCR:H341	1.87	0.40
1:cA:112:PRO:HB3	1:cA:148:PHE:CD1	2.56	0.40
2:cB:275:ALA:HB2	12:cB:918:CLA:HBC2	2.04	0.40
2:cB:414:PHE:CZ	15:cF:204:BCR:HC41	2.56	0.40
12:cB:915:CLA:H41	12:cB:915:CLA:H61	1.65	0.40
15:cB:943:BCR:H15C	15:cB:943:BCR:H351	1.89	0.40
12:aA:802:CLA:H171	12:aB:909:CLA:HMC2	2.04	0.40
2:aB:189:ALA:HA	12:aB:914:CLA:HAB	2.02	0.40
2:aB:275:ALA:HB2	12:aB:918:CLA:HBC2	2.04	0.40
3:aC:47:ASP:OD2	4:aD:67:LYS:NZ	2.48	0.40
1:bA:112:PRO:HB3	1:bA:148:PHE:CD1	2.56	0.40
16:bA:851:LHG:H311	16:bA:851:LHG:H282	1.70	0.40
6:bF:131:GLU:O	6:bF:145:LYS:NZ	2.45	0.40
15:bL:205:BCR:H20C	15:bL:205:BCR:H361	1.87	0.40
1:cA:472:PRO:HG2	1:cA:657:LEU:HD23	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:cA:817:CLA:H41	12:cA:817:CLA:H62	1.66	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	aA	770/783 (98%)	742 (96%)	28 (4%)	0	100	100
1	bA	770/783 (98%)	742 (96%)	28 (4%)	0	100	100
1	cA	770/783 (98%)	742 (96%)	28 (4%)	0	100	100
2	aB	723/872 (83%)	708 (98%)	15 (2%)	0	100	100
2	bB	723/872 (83%)	708 (98%)	15 (2%)	0	100	100
2	cB	723/872 (83%)	708 (98%)	15 (2%)	0	100	100
3	aC	78/81 (96%)	75 (96%)	2 (3%)	1 (1%)	9	3
3	bC	78/81 (96%)	75 (96%)	2 (3%)	1 (1%)	9	3
3	cC	78/81 (96%)	75 (96%)	2 (3%)	1 (1%)	9	3
4	aD	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
4	bD	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
4	cD	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
5	aE	60/65 (92%)	57 (95%)	3 (5%)	0	100	100
5	bE	60/65 (92%)	57 (95%)	3 (5%)	0	100	100
5	cE	60/65 (92%)	57 (95%)	3 (5%)	0	100	100
6	aF	149/181 (82%)	144 (97%)	5 (3%)	0	100	100
6	bF	149/181 (82%)	144 (97%)	5 (3%)	0	100	100
6	cF	149/181 (82%)	144 (97%)	5 (3%)	0	100	100
7	aI	29/35 (83%)	28 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	bI	29/35 (83%)	28 (97%)	1 (3%)	0	100	100
7	cI	29/35 (83%)	28 (97%)	1 (3%)	0	100	100
9	aL	127/147 (86%)	122 (96%)	4 (3%)	1 (1%)	16	9
9	bL	127/147 (86%)	122 (96%)	4 (3%)	1 (1%)	16	9
9	cL	127/147 (86%)	122 (96%)	4 (3%)	1 (1%)	16	9
10	aM	27/34 (79%)	27 (100%)	0	0	100	100
10	bM	27/34 (79%)	27 (100%)	0	0	100	100
10	cM	27/34 (79%)	27 (100%)	0	0	100	100
All	All	6282/7026 (89%)	6087 (97%)	189 (3%)	6 (0%)	49	43

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	aL	104	PRO
9	bL	104	PRO
9	cL	104	PRO
3	aC	62	PHE
3	bC	62	PHE
3	cC	62	PHE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	aA	612/623 (98%)	592 (97%)	20 (3%)	33	28
1	bA	612/623 (98%)	592 (97%)	20 (3%)	33	28
1	cA	612/623 (98%)	592 (97%)	20 (3%)	33	28
2	aB	573/694 (83%)	569 (99%)	4 (1%)	76	80
2	bB	573/694 (83%)	569 (99%)	4 (1%)	76	80
2	cB	573/694 (83%)	569 (99%)	4 (1%)	76	80
3	aC	68/69 (99%)	67 (98%)	1 (2%)	57	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	bC	68/69 (99%)	67 (98%)	1 (2%)	57 58
3	cC	68/69 (99%)	67 (98%)	1 (2%)	57 58
4	aD	113/122 (93%)	110 (97%)	3 (3%)	39 36
4	bD	113/122 (93%)	110 (97%)	3 (3%)	39 36
4	cD	113/122 (93%)	110 (97%)	3 (3%)	39 36
5	aE	56/57 (98%)	53 (95%)	3 (5%)	20 12
5	bE	56/57 (98%)	53 (95%)	3 (5%)	20 12
5	cE	56/57 (98%)	53 (95%)	3 (5%)	20 12
6	aF	125/148 (84%)	113 (90%)	12 (10%)	8 3
6	bF	125/148 (84%)	113 (90%)	12 (10%)	8 3
6	cF	125/148 (84%)	113 (90%)	12 (10%)	8 3
7	aI	26/30 (87%)	25 (96%)	1 (4%)	29 24
7	bI	26/30 (87%)	25 (96%)	1 (4%)	29 24
7	cI	26/30 (87%)	25 (96%)	1 (4%)	29 24
9	aL	100/116 (86%)	98 (98%)	2 (2%)	48 48
9	bL	100/116 (86%)	98 (98%)	2 (2%)	48 48
9	cL	100/116 (86%)	98 (98%)	2 (2%)	48 48
10	aM	18/21 (86%)	17 (94%)	1 (6%)	19 12
10	bM	18/21 (86%)	17 (94%)	1 (6%)	19 12
10	cM	18/21 (86%)	17 (94%)	1 (6%)	19 12
All	All	5073/5640 (90%)	4932 (97%)	141 (3%)	38 34

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	aA	18	ASN
1	aA	30	LYS
1	aA	36	ARG
1	aA	60	THR
1	aA	117	VAL
1	aA	175	LEU
1	aA	228	LYS
1	aA	251	MET
1	aA	278	ASP
1	aA	305	ILE

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Mol	Chain	Res	Type
1	aA	328	GLU
1	aA	519	LEU
1	aA	524	THR
1	aA	601	CYS
1	aA	641	ARG
1	aA	643	THR
1	aA	661	THR
1	aA	672	ILE
1	aA	741	VAL
1	aA	776	LEU
2	aB	237	GLN
2	aB	294	ASP
2	aB	387	LYS
2	aB	550	CYS
3	aC	63	LEU
4	aD	42	GLU
4	aD	137	THR
4	aD	139	LYS
5	aE	3	ILE
5	aE	12	LEU
5	aE	62	GLU
6	aF	34	VAL
6	aF	36	ASP
6	aF	42	LYS
6	aF	50	LEU
6	aF	59	GLN
6	aF	83	ASP
6	aF	89	GLN
6	aF	143	LEU
6	aF	155	ILE
6	aF	161	ILE
6	aF	164	LEU
6	aF	166	SER
7	aI	26	LEU
9	aL	88	ILE
9	aL	100	VAL
10	aM	19	LEU
1	bA	18	ASN
1	bA	30	LYS
1	bA	36	ARG
1	bA	60	THR
1	bA	117	VAL

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Mol	Chain	Res	Type
1	bA	175	LEU
1	bA	228	LYS
1	bA	251	MET
1	bA	278	ASP
1	bA	305	ILE
1	bA	328	GLU
1	bA	519	LEU
1	bA	524	THR
1	bA	601	CYS
1	bA	641	ARG
1	bA	643	THR
1	bA	661	THR
1	bA	672	ILE
1	bA	741	VAL
1	bA	776	LEU
2	bB	237	GLN
2	bB	294	ASP
2	bB	387	LYS
2	bB	550	CYS
3	bC	63	LEU
4	bD	42	GLU
4	bD	137	THR
4	bD	139	LYS
5	bE	3	ILE
5	bE	12	LEU
5	bE	62	GLU
6	bF	34	VAL
6	bF	36	ASP
6	bF	42	LYS
6	bF	50	LEU
6	bF	59	GLN
6	bF	83	ASP
6	bF	89	GLN
6	bF	143	LEU
6	bF	155	ILE
6	bF	161	ILE
6	bF	164	LEU
6	bF	166	SER
7	bI	26	LEU
9	bL	88	ILE
9	bL	100	VAL
10	bM	19	LEU

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Mol	Chain	Res	Type
1	cA	18	ASN
1	cA	30	LYS
1	cA	36	ARG
1	cA	60	THR
1	cA	117	VAL
1	cA	175	LEU
1	cA	228	LYS
1	cA	251	MET
1	cA	278	ASP
1	cA	305	ILE
1	cA	328	GLU
1	cA	519	LEU
1	cA	524	THR
1	cA	601	CYS
1	cA	641	ARG
1	cA	643	THR
1	cA	661	THR
1	cA	672	ILE
1	cA	741	VAL
1	cA	776	LEU
2	cB	237	GLN
2	cB	294	ASP
2	cB	387	LYS
2	cB	550	CYS
3	cC	63	LEU
4	cD	42	GLU
4	cD	137	THR
4	cD	139	LYS
5	cE	3	ILE
5	cE	12	LEU
5	cE	62	GLU
6	cF	34	VAL
6	cF	36	ASP
6	cF	42	LYS
6	cF	50	LEU
6	cF	59	GLN
6	cF	83	ASP
6	cF	89	GLN
6	cF	143	LEU
6	cF	155	ILE
6	cF	161	ILE
6	cF	164	LEU

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Mol	Chain	Res	Type
6	cF	166	SER
7	cI	26	LEU
9	cL	88	ILE
9	cL	100	VAL
10	cM	19	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	aA	18	ASN
1	aA	37	ASN
1	aA	195	GLN
1	aA	360	ASN
1	aA	446	ASN
1	aA	626	HIS
1	aA	746	GLN
2	aB	114	ASN
2	aB	214	ASN
2	aB	319	GLN
2	aB	349	GLN
2	aB	389	ASN
2	aB	487	ASN
2	aB	655	GLN
4	aD	60	ASN
4	aD	71	HIS
4	aD	76	GLN
6	aF	62	GLN
1	bA	18	ASN
1	bA	37	ASN
1	bA	195	GLN
1	bA	360	ASN
1	bA	446	ASN
1	bA	626	HIS
1	bA	746	GLN
2	bB	114	ASN
2	bB	214	ASN
2	bB	319	GLN
2	bB	349	GLN
2	bB	389	ASN
2	bB	487	ASN
2	bB	655	GLN
4	bD	60	ASN

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Mol	Chain	Res	Type
4	bD	71	HIS
4	bD	76	GLN
6	bF	62	GLN
1	cA	18	ASN
1	cA	37	ASN
1	cA	195	GLN
1	cA	360	ASN
1	cA	446	ASN
1	cA	544	HIS
1	cA	626	HIS
1	cA	648	HIS
1	cA	746	GLN
2	cB	114	ASN
2	cB	214	ASN
2	cB	319	GLN
2	cB	349	GLN
2	cB	389	ASN
2	cB	487	ASN
2	cB	655	GLN
4	cD	60	ASN
4	cD	71	HIS
4	cD	76	GLN
6	cF	62	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

354 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	CLA	bB	906	-	59,63,73	2.10	21 (35%)	70,101,113	2.77	31 (44%)
15	BCR	cM	101	-	41,41,41	1.06	3 (7%)	56,56,56	1.19	6 (10%)
12	CLA	bA	840	-	69,73,73	1.97	19 (27%)	82,113,113	2.52	30 (36%)
15	BCR	bB	945	-	41,41,41	1.04	2 (4%)	56,56,56	1.39	8 (14%)
12	CLA	aA	823	-	55,59,73	2.17	20 (36%)	64,96,113	2.98	31 (48%)
12	CLA	cF	202	6	49,53,73	2.35	21 (42%)	58,89,113	3.04	29 (50%)
12	CLA	aB	924	18	50,54,73	2.26	20 (40%)	59,90,113	3.06	27 (45%)
12	CLA	bB	949	16	45,49,73	2.47	19 (42%)	54,84,113	3.29	28 (51%)
12	CLA	bB	924	18	50,54,73	2.27	20 (40%)	59,90,113	3.06	27 (45%)
15	BCR	cB	946	-	41,41,41	1.07	3 (7%)	56,56,56	1.26	7 (12%)
12	CLA	aB	907	-	56,60,73	2.11	18 (32%)	65,97,113	2.92	32 (49%)
12	CLA	bB	923	18	58,62,73	2.06	19 (32%)	68,99,113	2.82	29 (42%)
12	CLA	bB	921	-	59,63,73	2.16	20 (33%)	70,101,113	2.87	28 (40%)
12	CLA	cB	921	-	59,63,73	2.15	20 (33%)	70,101,113	2.87	28 (40%)
12	CLA	aB	901	-	69,73,73	1.88	18 (26%)	82,113,113	2.67	31 (37%)
12	CLA	bA	811	-	49,53,73	2.35	18 (36%)	58,89,113	3.01	28 (48%)
16	LHG	cB	948	12	22,22,48	1.07	2 (9%)	25,28,54	1.14	1 (4%)
16	LHG	bA	852	12	26,26,48	0.97	1 (3%)	29,32,54	1.32	3 (10%)
11	CL0	aA	801	-	58,73,73	2.92	19 (32%)	60,113,113	2.73	19 (31%)
12	CLA	bB	938	18	55,59,73	2.18	19 (34%)	64,96,113	2.81	30 (46%)
12	CLA	cA	809	1	49,53,73	2.30	20 (40%)	58,89,113	3.08	30 (51%)
12	CLA	aA	805	-	57,61,73	2.16	22 (38%)	67,98,113	2.92	30 (44%)
15	BCR	cA	846	-	41,41,41	1.07	3 (7%)	56,56,56	1.28	8 (14%)
14	SF4	bC	101	3	0,12,12	-	-	-		
12	CLA	bA	817	-	58,62,73	2.17	19 (32%)	68,99,113	2.93	28 (41%)
15	BCR	cF	204	-	41,41,41	1.05	2 (4%)	56,56,56	1.31	10 (17%)
12	CLA	bB	929	-	49,53,73	2.32	19 (38%)	58,89,113	3.12	28 (48%)
14	SF4	cA	845	1,2	0,12,12	-	-	-		
12	CLA	aB	921	-	59,63,73	2.15	20 (33%)	70,101,113	2.87	28 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	cA	812	-	69,73,73	1.92	21 (30%)	82,113,113	2.62	32 (39%)
12	CLA	cB	926	-	69,73,73	1.90	20 (28%)	82,113,113	2.57	33 (40%)
12	CLA	cB	913	-	60,64,73	2.07	20 (33%)	71,102,113	2.80	33 (46%)
15	BCR	bB	943	-	41,41,41	1.08	2 (4%)	56,56,56	1.17	5 (8%)
12	CLA	cB	910	-	49,53,73	2.34	18 (36%)	58,89,113	2.99	29 (50%)
12	CLA	aA	829	-	64,68,73	1.99	19 (29%)	76,107,113	2.60	31 (40%)
12	CLA	aB	936	-	63,67,73	2.03	22 (34%)	74,105,113	2.77	32 (43%)
15	BCR	aB	944	-	41,41,41	1.09	3 (7%)	56,56,56	1.20	5 (8%)
12	CLA	bA	831	-	54,58,73	2.19	19 (35%)	64,95,113	2.88	34 (53%)
12	CLA	bB	911	-	49,53,73	2.31	19 (38%)	58,89,113	2.97	29 (50%)
12	CLA	aA	833	-	55,59,73	2.13	17 (30%)	64,96,113	2.90	34 (53%)
15	BCR	bB	944	-	41,41,41	1.10	3 (7%)	56,56,56	1.19	5 (8%)
12	CLA	aB	918	18	50,54,73	2.31	19 (38%)	59,90,113	2.84	28 (47%)
12	CLA	cA	813	-	49,53,73	2.39	21 (42%)	58,89,113	2.91	27 (46%)
12	CLA	cA	840	-	69,73,73	1.96	19 (27%)	82,113,113	2.52	30 (36%)
12	CLA	aA	837	-	55,59,73	2.17	21 (38%)	64,96,113	2.94	30 (46%)
16	LHG	bA	851	-	48,48,48	0.68	1 (2%)	51,54,54	1.29	6 (11%)
15	BCR	cB	944	-	41,41,41	1.10	3 (7%)	56,56,56	1.20	5 (8%)
12	CLA	cA	819	-	64,68,73	2.02	20 (31%)	76,107,113	2.89	36 (47%)
12	CLA	aA	827	-	50,54,73	2.25	18 (36%)	59,90,113	3.04	28 (47%)
12	CLA	bB	936	-	63,67,73	2.03	22 (34%)	74,105,113	2.77	32 (43%)
15	BCR	bJ	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.37	11 (19%)
12	CLA	cB	907	-	56,60,73	2.12	18 (32%)	65,97,113	2.93	31 (47%)
12	CLA	bB	901	-	69,73,73	1.87	18 (26%)	82,113,113	2.67	31 (37%)
12	CLA	bB	915	-	56,60,73	2.18	18 (32%)	65,97,113	2.99	28 (43%)
14	SF4	bA	845	1,2	0,12,12	-	-	-		
12	CLA	cB	936	-	63,67,73	2.03	22 (34%)	74,105,113	2.78	32 (43%)
12	CLA	cA	838	-	69,73,73	1.92	20 (28%)	82,113,113	2.65	29 (35%)
17	LMG	bB	947	-	43,43,55	0.95	2 (4%)	51,51,63	1.26	6 (11%)
13	1L3	aB	940	-	34,34,34	2.33	9 (26%)	43,45,45	1.46	7 (16%)
14	SF4	aA	846	1,2	0,12,12	-	-	-		
12	CLA	bB	903	-	55,59,73	2.17	20 (36%)	64,96,113	2.94	31 (48%)
12	CLA	cA	815	-	49,53,73	2.36	18 (36%)	58,89,113	3.00	28 (48%)
12	CLA	cB	930	-	53,57,73	2.25	20 (37%)	61,93,113	2.98	30 (49%)
12	CLA	bB	939	-	49,53,73	2.24	18 (36%)	58,89,113	3.13	27 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	cB	935	-	54,58,73	2.19	20 (37%)	64,95,113	2.99	33 (51%)
12	CLA	cA	837	-	55,59,73	2.16	21 (38%)	64,96,113	2.94	30 (46%)
12	CLA	bA	835	-	49,53,73	2.32	19 (38%)	58,89,113	2.84	29 (50%)
12	CLA	cA	839	-	49,53,73	2.26	19 (38%)	58,89,113	3.07	28 (48%)
15	BCR	bI	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.40	9 (16%)
12	CLA	bB	926	-	69,73,73	1.89	19 (27%)	82,113,113	2.57	33 (40%)
14	SF4	aC	101	3	0,12,12	-	-	-		
12	CLA	cB	928	-	54,58,73	2.20	18 (33%)	64,95,113	2.86	31 (48%)
12	CLA	cA	821	18	54,58,73	2.20	17 (31%)	64,95,113	2.78	30 (46%)
15	BCR	aM	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.19	6 (10%)
12	CLA	aB	916	-	63,67,73	2.03	18 (28%)	74,105,113	2.79	32 (43%)
12	CLA	cA	822	-	53,57,73	2.27	20 (37%)	61,93,113	3.07	27 (44%)
12	CLA	aA	828	-	69,73,73	1.96	20 (28%)	82,113,113	2.64	32 (39%)
12	CLA	cA	831	-	54,58,73	2.18	19 (35%)	64,95,113	2.88	34 (53%)
12	CLA	cB	915	-	56,60,73	2.17	18 (32%)	65,97,113	3.00	28 (43%)
12	CLA	cB	920	-	49,53,73	2.33	19 (38%)	58,89,113	3.11	25 (43%)
15	BCR	bA	846	-	41,41,41	1.07	2 (4%)	56,56,56	1.27	8 (14%)
12	CLA	aB	906	-	59,63,73	2.10	21 (35%)	70,101,113	2.76	31 (44%)
12	CLA	aB	932	-	49,53,73	2.31	17 (34%)	58,89,113	3.13	29 (50%)
16	LHG	cA	851	-	48,48,48	0.68	1 (2%)	51,54,54	1.29	6 (11%)
12	CLA	cA	834	-	69,73,73	1.94	19 (27%)	82,113,113	2.72	32 (39%)
12	CLA	bA	812	-	69,73,73	1.93	21 (30%)	82,113,113	2.62	32 (39%)
12	CLA	cB	927	-	69,73,73	1.95	19 (27%)	82,113,113	2.36	28 (34%)
12	CLA	aB	903	-	55,59,73	2.16	20 (36%)	64,96,113	2.94	31 (48%)
12	CLA	cB	905	-	69,73,73	1.92	19 (27%)	82,113,113	2.59	29 (35%)
12	CLA	aA	830	-	69,73,73	1.91	18 (26%)	82,113,113	2.57	29 (35%)
15	BCR	bB	946	-	41,41,41	1.07	3 (7%)	56,56,56	1.27	6 (10%)
12	CLA	aA	836	1	49,53,73	2.36	19 (38%)	58,89,113	2.92	29 (50%)
12	CLA	aB	920	-	49,53,73	2.33	19 (38%)	58,89,113	3.12	25 (43%)
12	CLA	bA	838	-	69,73,73	1.92	20 (28%)	82,113,113	2.65	29 (35%)
12	CLA	cA	826	18	59,63,73	2.07	20 (33%)	70,101,113	2.87	30 (42%)
12	CLA	bA	809	1	49,53,73	2.30	20 (40%)	58,89,113	3.08	30 (51%)
12	CLA	bA	825	18	69,73,73	1.98	20 (28%)	82,113,113	2.60	31 (37%)
15	BCR	aF	203	-	41,41,41	1.08	2 (4%)	56,56,56	1.34	8 (14%)
15	BCR	aF	201	-	41,41,41	1.05	2 (4%)	56,56,56	1.26	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	bA	834	-	69,73,73	1.93	19 (27%)	82,113,113	2.72	32 (39%)
12	CLA	aL	203	-	49,53,73	2.30	22 (44%)	58,89,113	3.04	26 (44%)
12	CLA	cB	918	18	50,54,73	2.31	19 (38%)	59,90,113	2.83	28 (47%)
12	CLA	bB	935	-	54,58,73	2.19	20 (37%)	64,95,113	2.98	33 (51%)
15	BCR	aL	205	-	41,41,41	1.05	4 (9%)	56,56,56	1.26	5 (8%)
12	CLA	cB	937	-	51,55,73	2.26	21 (41%)	60,91,113	3.04	28 (46%)
12	CLA	bA	821	18	54,58,73	2.20	17 (31%)	64,95,113	2.77	30 (46%)
15	BCR	cL	205	-	41,41,41	1.05	4 (9%)	56,56,56	1.26	5 (8%)
12	CLA	cA	806	-	69,73,73	1.92	20 (28%)	82,113,113	2.70	29 (35%)
12	CLA	bA	822	-	53,57,73	2.27	20 (37%)	61,93,113	3.07	27 (44%)
12	CLA	aA	818	-	58,62,73	2.09	19 (32%)	68,99,113	2.84	29 (42%)
12	CLA	aB	930	-	53,57,73	2.25	20 (37%)	61,93,113	2.98	30 (49%)
12	CLA	bA	826	18	59,63,73	2.07	20 (33%)	70,101,113	2.87	31 (44%)
12	CLA	aA	820	-	60,64,73	2.12	21 (35%)	71,102,113	2.79	33 (46%)
15	BCR	aA	847	-	41,41,41	1.08	2 (4%)	56,56,56	1.28	8 (14%)
12	CLA	bB	928	-	54,58,73	2.20	18 (33%)	64,95,113	2.86	31 (48%)
15	BCR	aB	942	-	41,41,41	1.07	3 (7%)	56,56,56	1.22	3 (5%)
15	BCR	aA	848	-	41,41,41	1.09	2 (4%)	56,56,56	1.53	14 (25%)
12	CLA	cA	827	-	50,54,73	2.25	18 (36%)	59,90,113	3.05	28 (47%)
16	LHG	aA	852	-	48,48,48	0.68	1 (2%)	51,54,54	1.29	6 (11%)
14	SF4	bC	102	3	0,12,12	-	-	-		
12	CLA	cB	933	18	49,53,73	2.25	19 (38%)	58,89,113	2.91	28 (48%)
12	CLA	bB	905	-	69,73,73	1.93	19 (27%)	82,113,113	2.59	29 (35%)
15	BCR	aB	943	-	41,41,41	1.08	2 (4%)	56,56,56	1.18	5 (8%)
12	CLA	aA	816	-	49,53,73	2.34	21 (42%)	58,89,113	2.99	26 (44%)
12	CLA	bA	843	18	69,73,73	1.91	20 (28%)	82,113,113	2.72	34 (41%)
12	CLA	bB	913	-	60,64,73	2.07	20 (33%)	71,102,113	2.79	33 (46%)
12	CLA	aB	911	-	49,53,73	2.31	18 (36%)	58,89,113	2.97	29 (50%)
12	CLA	aA	817	-	58,62,73	2.17	19 (32%)	68,99,113	2.93	28 (41%)
12	CLA	cA	835	-	49,53,73	2.32	19 (38%)	58,89,113	2.85	29 (50%)
17	LMG	cB	947	-	43,43,55	0.95	2 (4%)	51,51,63	1.26	6 (11%)
15	BCR	aA	850	-	41,41,41	1.15	3 (7%)	56,56,56	1.40	6 (10%)
12	CLA	aA	821	18	54,58,73	2.20	17 (31%)	64,95,113	2.78	30 (46%)
12	CLA	aA	841	18	55,59,73	2.20	22 (40%)	64,96,113	2.90	28 (43%)
12	CLA	cB	932	-	49,53,73	2.31	18 (36%)	58,89,113	3.12	29 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	aB	909	-	59,63,73	2.07	20 (33%)	70,101,113	2.69	32 (45%)
12	CLA	cB	911	-	49,53,73	2.31	18 (36%)	58,89,113	2.97	29 (50%)
12	CLA	aA	813	-	49,53,73	2.39	21 (42%)	58,89,113	2.91	27 (46%)
12	CLA	bA	815	-	49,53,73	2.37	18 (36%)	58,89,113	3.01	28 (48%)
12	CLA	bB	907	-	56,60,73	2.11	18 (32%)	65,97,113	2.92	31 (47%)
15	BCR	cB	941	-	41,41,41	1.08	3 (7%)	56,56,56	1.28	6 (10%)
12	CLA	aA	814	-	49,53,73	2.30	19 (38%)	58,89,113	2.93	27 (46%)
14	SF4	cC	101	3	0,12,12	-	-	-		
12	CLA	aA	844	16	49,53,73	2.31	19 (38%)	58,89,113	2.86	24 (41%)
12	CLA	aB	949	16	45,49,73	2.47	19 (42%)	54,84,113	3.28	28 (51%)
12	CLA	aA	803	-	69,73,73	1.91	20 (28%)	82,113,113	2.59	35 (42%)
12	CLA	aL	204	18	49,53,73	2.33	21 (42%)	58,89,113	3.04	27 (46%)
12	CLA	cB	912	-	69,73,73	1.90	22 (31%)	82,113,113	2.52	30 (36%)
12	CLA	cB	939	-	49,53,73	2.24	19 (38%)	58,89,113	3.12	27 (46%)
12	CLA	cA	816	-	49,53,73	2.33	20 (40%)	58,89,113	2.99	26 (44%)
12	CLA	cA	818	-	58,62,73	2.09	19 (32%)	68,99,113	2.85	29 (42%)
15	BCR	aB	945	-	41,41,41	1.05	2 (4%)	56,56,56	1.38	8 (14%)
12	CLA	aB	937	-	51,55,73	2.25	21 (41%)	60,91,113	3.03	27 (45%)
12	CLA	aB	922	-	49,53,73	2.30	19 (38%)	58,89,113	2.93	29 (50%)
12	CLA	cB	934	2	49,53,73	2.43	19 (38%)	58,89,113	2.88	25 (43%)
12	CLA	cB	949	16	45,49,73	2.47	18 (40%)	54,84,113	3.28	28 (51%)
12	CLA	cA	842	-	69,73,73	1.93	18 (26%)	82,113,113	2.64	31 (37%)
12	CLA	aB	928	-	54,58,73	2.20	18 (33%)	64,95,113	2.86	31 (48%)
15	BCR	cB	943	-	41,41,41	1.07	2 (4%)	56,56,56	1.17	5 (8%)
12	CLA	bB	917	-	59,63,73	2.07	18 (30%)	70,101,113	2.76	32 (45%)
15	BCR	aL	206	-	41,41,41	1.02	2 (4%)	56,56,56	1.22	5 (8%)
12	CLA	aB	935	-	54,58,73	2.19	20 (37%)	64,95,113	2.99	33 (51%)
12	CLA	bB	918	18	50,54,73	2.30	19 (38%)	59,90,113	2.83	28 (47%)
12	CLA	aA	824	-	51,55,73	2.27	20 (39%)	60,91,113	2.89	30 (50%)
15	BCR	aA	851	-	41,41,41	1.05	2 (4%)	56,56,56	1.32	8 (14%)
12	CLA	bB	912	-	69,73,73	1.89	21 (30%)	82,113,113	2.52	30 (36%)
12	CLA	bA	818	-	58,62,73	2.09	19 (32%)	68,99,113	2.84	29 (42%)
12	CLA	cL	203	-	49,53,73	2.30	22 (44%)	58,89,113	3.04	26 (44%)
15	BCR	aI	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.40	9 (16%)
15	BCR	cA	847	-	41,41,41	1.09	2 (4%)	56,56,56	1.53	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	aB	904	-	69,73,73	1.94	21 (30%)	82,113,113	2.72	34 (41%)
15	BCR	aB	941	-	41,41,41	1.08	3 (7%)	56,56,56	1.29	6 (10%)
12	CLA	bB	931	-	69,73,73	1.92	19 (27%)	82,113,113	2.77	32 (39%)
12	CLA	aB	933	18	49,53,73	2.25	19 (38%)	58,89,113	2.91	28 (48%)
12	CLA	bL	204	18	49,53,73	2.34	21 (42%)	58,89,113	3.05	27 (46%)
12	CLA	bA	807	-	69,73,73	1.96	21 (30%)	82,113,113	2.67	34 (41%)
12	CLA	bB	932	-	49,53,73	2.31	17 (34%)	58,89,113	3.11	29 (50%)
15	BCR	bL	201	-	41,41,41	1.20	3 (7%)	56,56,56	1.25	4 (7%)
12	CLA	cA	810	1	49,53,73	2.33	18 (36%)	58,89,113	3.11	30 (51%)
12	CLA	cA	830	-	69,73,73	1.92	18 (26%)	82,113,113	2.57	29 (35%)
12	CLA	bA	837	-	55,59,73	2.16	21 (38%)	64,96,113	2.94	30 (46%)
12	CLA	cB	929	-	49,53,73	2.32	18 (36%)	58,89,113	3.12	29 (50%)
12	CLA	cA	807	-	69,73,73	1.95	21 (30%)	82,113,113	2.67	34 (41%)
12	CLA	cA	814	-	49,53,73	2.30	19 (38%)	58,89,113	2.93	27 (46%)
12	CLA	aB	913	-	60,64,73	2.07	20 (33%)	71,102,113	2.80	33 (46%)
12	CLA	aF	202	6	49,53,73	2.35	20 (40%)	58,89,113	3.04	29 (50%)
15	BCR	aA	849	-	41,41,41	1.11	3 (7%)	56,56,56	1.20	4 (7%)
12	CLA	cB	917	-	59,63,73	2.07	18 (30%)	70,101,113	2.77	32 (45%)
12	CLA	aB	950	16	49,53,73	2.31	19 (38%)	58,89,113	2.85	24 (41%)
12	CLA	cB	902	-	65,69,73	1.94	18 (27%)	77,108,113	2.62	26 (33%)
12	CLA	aB	938	18	55,59,73	2.19	19 (34%)	64,96,113	2.82	30 (46%)
11	CL0	cA	801	-	58,73,73	2.92	19 (32%)	60,113,113	2.73	19 (31%)
12	CLA	bA	816	-	49,53,73	2.34	21 (42%)	58,89,113	2.98	26 (44%)
12	CLA	cB	909	-	59,63,73	2.07	20 (33%)	70,101,113	2.69	32 (45%)
12	CLA	bA	806	-	69,73,73	1.92	20 (28%)	82,113,113	2.70	29 (35%)
12	CLA	cB	906	-	59,63,73	2.11	21 (35%)	70,101,113	2.77	31 (44%)
13	1L3	aA	845	-	34,34,34	2.34	9 (26%)	43,45,45	1.64	9 (20%)
12	CLA	cA	832	-	59,63,73	2.12	19 (32%)	70,101,113	2.85	32 (45%)
16	LHG	aB	948	12	22,22,48	1.07	1 (4%)	25,28,54	1.14	1 (4%)
12	CLA	bA	810	1	49,53,73	2.33	18 (36%)	58,89,113	3.11	30 (51%)
12	CLA	aB	931	-	69,73,73	1.92	19 (27%)	82,113,113	2.78	32 (39%)
12	CLA	bA	827	-	50,54,73	2.25	18 (36%)	59,90,113	3.03	28 (47%)
12	CLA	bA	842	-	69,73,73	1.93	18 (26%)	82,113,113	2.63	31 (37%)
12	CLA	bA	830	-	69,73,73	1.91	18 (26%)	82,113,113	2.57	29 (35%)
12	CLA	bB	914	-	49,53,73	2.31	20 (40%)	58,89,113	3.14	26 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	cA	833	-	55,59,73	2.12	17 (30%)	64,96,113	2.89	34 (53%)
12	CLA	aB	939	-	49,53,73	2.24	19 (38%)	58,89,113	3.13	27 (46%)
12	CLA	bB	925	-	59,63,73	2.07	19 (32%)	70,101,113	2.94	33 (47%)
12	CLA	aA	854	18	60,64,73	2.03	21 (35%)	71,102,113	2.86	31 (43%)
12	CLA	bB	922	-	49,53,73	2.29	19 (38%)	58,89,113	2.92	29 (50%)
12	CLA	bA	814	-	49,53,73	2.30	20 (40%)	58,89,113	2.92	27 (46%)
12	CLA	cA	805	-	57,61,73	2.16	22 (38%)	67,98,113	2.92	30 (44%)
15	BCR	aL	201	-	41,41,41	1.20	4 (9%)	56,56,56	1.25	4 (7%)
12	CLA	bA	833	-	55,59,73	2.12	18 (32%)	64,96,113	2.90	34 (53%)
15	BCR	cA	848	-	41,41,41	1.11	3 (7%)	56,56,56	1.20	4 (7%)
12	CLA	aA	834	-	69,73,73	1.94	19 (27%)	82,113,113	2.72	32 (39%)
12	CLA	cA	803	-	69,73,73	1.91	20 (28%)	82,113,113	2.60	34 (41%)
12	CLA	aB	912	-	69,73,73	1.90	22 (31%)	82,113,113	2.52	30 (36%)
12	CLA	cA	824	-	51,55,73	2.27	20 (39%)	60,91,113	2.90	30 (50%)
12	CLA	aA	843	18	69,73,73	1.91	20 (28%)	82,113,113	2.73	34 (41%)
12	CLA	cB	923	18	58,62,73	2.06	19 (32%)	68,99,113	2.83	29 (42%)
12	CLA	bB	920	-	49,53,73	2.33	19 (38%)	58,89,113	3.12	25 (43%)
15	BCR	bM	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.19	6 (10%)
12	CLA	cB	904	-	69,73,73	1.94	21 (30%)	82,113,113	2.72	33 (40%)
12	CLA	bB	927	-	69,73,73	1.95	19 (27%)	82,113,113	2.35	27 (32%)
12	CLA	bA	841	18	55,59,73	2.21	22 (40%)	64,96,113	2.91	28 (43%)
12	CLA	cB	922	-	49,53,73	2.29	19 (38%)	58,89,113	2.92	29 (50%)
12	CLA	bA	813	-	49,53,73	2.39	21 (42%)	58,89,113	2.90	27 (46%)
12	CLA	aL	202	9	57,61,73	2.16	20 (35%)	67,98,113	2.93	30 (44%)
12	CLA	cA	829	-	64,68,73	1.99	19 (29%)	76,107,113	2.60	32 (42%)
12	CLA	bA	820	-	60,64,73	2.11	21 (35%)	71,102,113	2.79	33 (46%)
15	BCR	cA	849	-	41,41,41	1.16	2 (4%)	56,56,56	1.40	6 (10%)
15	BCR	cJ	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.37	10 (17%)
12	CLA	bL	202	9	57,61,73	2.15	20 (35%)	67,98,113	2.93	30 (44%)
12	CLA	bB	909	-	59,63,73	2.07	22 (37%)	70,101,113	2.69	32 (45%)
12	CLA	cB	901	-	69,73,73	1.87	18 (26%)	82,113,113	2.67	31 (37%)
12	CLA	bA	803	-	69,73,73	1.91	20 (28%)	82,113,113	2.60	35 (42%)
15	BCR	cB	942	-	41,41,41	1.07	3 (7%)	56,56,56	1.22	3 (5%)
12	CLA	bB	919	-	51,55,73	2.24	19 (37%)	60,91,113	2.97	29 (48%)
12	CLA	cB	916	-	63,67,73	2.03	18 (28%)	74,105,113	2.79	32 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	bA	853	18	60,64,73	2.03	21 (35%)	71,102,113	2.86	31 (43%)
12	CLA	cB	919	-	51,55,73	2.24	18 (35%)	60,91,113	2.98	29 (48%)
15	BCR	bF	201	-	41,41,41	1.05	2 (4%)	56,56,56	1.26	7 (12%)
12	CLA	cA	808	-	55,59,73	2.22	20 (36%)	64,96,113	2.92	32 (50%)
12	CLA	aA	806	-	69,73,73	1.92	20 (28%)	82,113,113	2.70	29 (35%)
12	CLA	bA	823	-	55,59,73	2.18	20 (36%)	64,96,113	2.97	31 (48%)
12	CLA	cA	843	18	69,73,73	1.91	20 (28%)	82,113,113	2.72	34 (41%)
15	BCR	bA	847	-	41,41,41	1.09	2 (4%)	56,56,56	1.53	14 (25%)
16	LHG	aA	853	12	26,26,48	0.97	2 (7%)	29,32,54	1.32	3 (10%)
12	CLA	cL	204	18	49,53,73	2.34	21 (42%)	58,89,113	3.05	27 (46%)
12	CLA	aB	927	-	69,73,73	1.95	19 (27%)	82,113,113	2.36	28 (34%)
12	CLA	aB	902	-	65,69,73	1.94	19 (29%)	77,108,113	2.61	26 (33%)
15	BCR	bA	848	-	41,41,41	1.11	3 (7%)	56,56,56	1.20	4 (7%)
12	CLA	cA	853	18	60,64,73	2.03	21 (35%)	71,102,113	2.86	32 (45%)
12	CLA	aA	842	-	69,73,73	1.94	18 (26%)	82,113,113	2.63	31 (37%)
12	CLA	cL	202	9	57,61,73	2.16	20 (35%)	67,98,113	2.93	30 (44%)
15	BCR	cL	201	-	41,41,41	1.18	3 (7%)	56,56,56	1.25	4 (7%)
15	BCR	bL	206	-	41,41,41	1.01	2 (4%)	56,56,56	1.22	6 (10%)
12	CLA	bB	937	-	51,55,73	2.26	22 (43%)	60,91,113	3.04	28 (46%)
12	CLA	aA	839	-	49,53,73	2.26	19 (38%)	58,89,113	3.07	27 (46%)
12	CLA	bL	203	-	49,53,73	2.29	22 (44%)	58,89,113	3.04	26 (44%)
12	CLA	cA	841	18	55,59,73	2.20	22 (40%)	64,96,113	2.91	27 (42%)
12	CLA	bB	950	16	49,53,73	2.32	19 (38%)	58,89,113	2.86	24 (41%)
12	CLA	bA	805	-	57,61,73	2.16	22 (38%)	67,98,113	2.92	30 (44%)
12	CLA	aB	905	-	69,73,73	1.93	19 (27%)	82,113,113	2.59	29 (35%)
15	BCR	bL	205	-	41,41,41	1.05	4 (9%)	56,56,56	1.26	5 (8%)
12	CLA	aA	811	-	49,53,73	2.35	18 (36%)	58,89,113	3.00	28 (48%)
15	BCR	cI	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.40	9 (16%)
12	CLA	bA	836	1	49,53,73	2.36	19 (38%)	58,89,113	2.92	29 (50%)
15	BCR	aF	204	-	41,41,41	1.05	2 (4%)	56,56,56	1.30	9 (16%)
14	SF4	aC	102	3	0,12,12	-	-	-		
12	CLA	aA	825	18	69,73,73	1.98	20 (28%)	82,113,113	2.59	31 (37%)
12	CLA	bF	202	6	49,53,73	2.35	20 (40%)	58,89,113	3.04	29 (50%)
12	CLA	aB	910	-	49,53,73	2.33	18 (36%)	58,89,113	2.98	29 (50%)
12	CLA	aB	923	18	58,62,73	2.06	19 (32%)	68,99,113	2.82	28 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	SF4	cC	102	3	0,12,12	-	-	-		
12	CLA	bB	933	18	49,53,73	2.26	19 (38%)	58,89,113	2.92	28 (48%)
12	CLA	bA	828	-	69,73,73	1.96	20 (28%)	82,113,113	2.64	32 (39%)
12	CLA	cA	811	-	49,53,73	2.35	18 (36%)	58,89,113	3.01	29 (50%)
12	CLA	cB	908	2	52,56,73	2.20	17 (32%)	61,92,113	2.73	28 (45%)
12	CLA	bA	802	18	69,73,73	1.91	19 (27%)	82,113,113	2.63	29 (35%)
13	1L3	bB	940	-	34,34,34	2.34	8 (23%)	43,45,45	1.46	7 (16%)
12	CLA	aA	835	-	49,53,73	2.31	19 (38%)	58,89,113	2.84	29 (50%)
12	CLA	cB	924	18	50,54,73	2.27	19 (38%)	59,90,113	3.07	27 (45%)
11	CL0	bA	801	-	58,73,73	2.93	19 (32%)	60,113,113	2.73	19 (31%)
12	CLA	aA	831	-	54,58,73	2.18	19 (35%)	64,95,113	2.88	34 (53%)
12	CLA	bA	832	-	59,63,73	2.11	18 (30%)	70,101,113	2.84	32 (45%)
12	CLA	aB	925	-	59,63,73	2.06	19 (32%)	70,101,113	2.94	33 (47%)
12	CLA	cA	828	-	69,73,73	1.95	20 (28%)	82,113,113	2.64	32 (39%)
12	CLA	aB	929	-	49,53,73	2.32	19 (38%)	58,89,113	3.13	28 (48%)
15	BCR	bB	941	-	41,41,41	1.09	3 (7%)	56,56,56	1.28	6 (10%)
12	CLA	cA	820	-	60,64,73	2.11	20 (33%)	71,102,113	2.78	32 (45%)
12	CLA	aA	810	1	49,53,73	2.34	18 (36%)	58,89,113	3.11	30 (51%)
12	CLA	aA	812	-	69,73,73	1.92	21 (30%)	82,113,113	2.63	32 (39%)
12	CLA	aB	926	-	69,73,73	1.90	20 (28%)	82,113,113	2.57	33 (40%)
17	LMG	aB	947	-	43,43,55	0.95	2 (4%)	51,51,63	1.26	6 (11%)
12	CLA	cB	931	-	69,73,73	1.92	21 (30%)	82,113,113	2.77	32 (39%)
12	CLA	bB	910	-	49,53,73	2.34	18 (36%)	58,89,113	2.99	29 (50%)
15	BCR	bA	850	-	41,41,41	1.05	2 (4%)	56,56,56	1.33	8 (14%)
12	CLA	cA	836	1	49,53,73	2.37	19 (38%)	58,89,113	2.93	29 (50%)
16	LHG	bB	948	12	22,22,48	1.07	2 (9%)	25,28,54	1.14	1 (4%)
12	CLA	aA	804	-	60,64,73	2.08	18 (30%)	71,102,113	2.81	29 (40%)
15	BCR	bF	203	-	41,41,41	1.09	2 (4%)	56,56,56	1.33	8 (14%)
12	CLA	aB	915	-	56,60,73	2.18	18 (32%)	65,97,113	3.00	28 (43%)
12	CLA	cB	914	-	49,53,73	2.30	20 (40%)	58,89,113	3.13	26 (44%)
12	CLA	bA	824	-	51,55,73	2.27	20 (39%)	60,91,113	2.90	30 (50%)
12	CLA	aA	819	-	64,68,73	2.02	20 (31%)	76,107,113	2.89	36 (47%)
12	CLA	aB	917	-	59,63,73	2.07	18 (30%)	70,101,113	2.76	32 (45%)
12	CLA	cA	802	18	69,73,73	1.92	19 (27%)	82,113,113	2.64	29 (35%)
12	CLA	cA	804	-	60,64,73	2.08	18 (30%)	71,102,113	2.81	29 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	cB	938	18	55,59,73	2.18	20 (36%)	64,96,113	2.80	30 (46%)
15	BCR	bF	204	-	41,41,41	1.05	2 (4%)	56,56,56	1.30	10 (17%)
13	1L3	bA	844	-	34,34,34	2.34	8 (23%)	43,45,45	1.64	9 (20%)
16	LHG	cA	852	12	26,26,48	0.97	1 (3%)	29,32,54	1.32	3 (10%)
12	CLA	bA	839	-	49,53,73	2.26	19 (38%)	58,89,113	3.07	28 (48%)
15	BCR	cL	206	-	41,41,41	1.01	2 (4%)	56,56,56	1.22	7 (12%)
12	CLA	cB	925	-	59,63,73	2.06	19 (32%)	70,101,113	2.93	33 (47%)
15	BCR	aB	946	-	41,41,41	1.07	3 (7%)	56,56,56	1.27	7 (12%)
12	CLA	bB	930	-	53,57,73	2.25	19 (35%)	61,93,113	2.97	30 (49%)
12	CLA	cB	903	-	55,59,73	2.17	20 (36%)	64,96,113	2.93	31 (48%)
12	CLA	cA	823	-	55,59,73	2.17	20 (36%)	64,96,113	2.97	31 (48%)
12	CLA	bA	829	-	64,68,73	1.99	19 (29%)	76,107,113	2.60	31 (40%)
15	BCR	aJ	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.37	11 (19%)
15	BCR	cB	945	-	41,41,41	1.05	2 (4%)	56,56,56	1.39	8 (14%)
12	CLA	aA	802	18	69,73,73	1.91	20 (28%)	82,113,113	2.63	29 (35%)
15	BCR	bA	849	-	41,41,41	1.15	3 (7%)	56,56,56	1.40	6 (10%)
12	CLA	bB	904	-	69,73,73	1.94	21 (30%)	82,113,113	2.72	33 (40%)
12	CLA	aA	840	-	69,73,73	1.97	19 (27%)	82,113,113	2.52	30 (36%)
12	CLA	aB	908	2	52,56,73	2.21	17 (32%)	61,92,113	2.73	28 (45%)
12	CLA	aB	919	-	51,55,73	2.24	19 (37%)	60,91,113	2.98	29 (48%)
15	BCR	cF	203	-	41,41,41	1.08	2 (4%)	56,56,56	1.34	8 (14%)
15	BCR	cA	850	-	41,41,41	1.05	2 (4%)	56,56,56	1.33	8 (14%)
15	BCR	bB	942	-	41,41,41	1.07	3 (7%)	56,56,56	1.21	4 (7%)
12	CLA	aA	838	-	69,73,73	1.92	20 (28%)	82,113,113	2.64	29 (35%)
12	CLA	bA	808	-	55,59,73	2.22	20 (36%)	64,96,113	2.92	32 (50%)
12	CLA	aA	809	1	49,53,73	2.30	19 (38%)	58,89,113	3.08	30 (51%)
12	CLA	aB	914	-	49,53,73	2.30	20 (40%)	58,89,113	3.13	26 (44%)
12	CLA	aA	815	-	49,53,73	2.37	18 (36%)	58,89,113	3.01	28 (48%)
12	CLA	aB	934	2	49,53,73	2.43	20 (40%)	58,89,113	2.88	25 (43%)
12	CLA	bB	934	2	49,53,73	2.43	19 (38%)	58,89,113	2.88	25 (43%)
12	CLA	aA	807	-	69,73,73	1.95	21 (30%)	82,113,113	2.67	34 (41%)
12	CLA	cA	817	-	58,62,73	2.17	19 (32%)	68,99,113	2.94	28 (41%)
13	1L3	cA	844	-	34,34,34	2.34	9 (26%)	43,45,45	1.64	9 (20%)
12	CLA	aA	826	18	59,63,73	2.08	20 (33%)	70,101,113	2.87	30 (42%)
12	CLA	bA	804	-	60,64,73	2.08	18 (30%)	71,102,113	2.81	29 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	aA	822	-	53,57,73	2.27	20 (37%)	61,93,113	3.08	27 (44%)
12	CLA	bB	908	2	52,56,73	2.20	18 (34%)	61,92,113	2.73	28 (45%)
12	CLA	bB	902	-	65,69,73	1.94	20 (30%)	77,108,113	2.61	26 (33%)
12	CLA	aA	832	-	59,63,73	2.12	19 (32%)	70,101,113	2.85	32 (45%)
13	1L3	cB	940	-	34,34,34	2.32	8 (23%)	43,45,45	1.46	7 (16%)
12	CLA	bB	916	-	63,67,73	2.03	19 (30%)	74,105,113	2.79	32 (43%)
12	CLA	cA	825	18	69,73,73	1.98	20 (28%)	82,113,113	2.59	32 (39%)
15	BCR	cF	201	-	41,41,41	1.05	2 (4%)	56,56,56	1.26	7 (12%)
12	CLA	aA	808	-	55,59,73	2.22	20 (36%)	64,96,113	2.91	32 (50%)
12	CLA	bA	819	-	64,68,73	2.01	20 (31%)	76,107,113	2.89	35 (46%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	bB	906	-	1/1/13/20	2/27/103/115	-
15	BCR	cM	101	-	-	18/29/63/63	0/2/2/2
12	CLA	bA	840	-	1/1/15/20	9/39/115/115	-
15	BCR	bB	945	-	-	10/29/63/63	0/2/2/2
12	CLA	aA	823	-	1/1/12/20	8/23/99/115	-
12	CLA	cF	202	6	1/1/11/20	9/15/91/115	-
12	CLA	aB	924	18	1/1/11/20	2/17/93/115	-
12	CLA	bB	949	16	1/1/10/20	2/10/86/115	-
12	CLA	bB	924	18	1/1/11/20	2/17/93/115	-
15	BCR	cB	946	-	-	3/29/63/63	0/2/2/2
12	CLA	aB	907	-	1/1/12/20	7/24/100/115	-
12	CLA	bB	923	18	1/1/12/20	11/26/102/115	-
12	CLA	bB	921	-	-	8/27/103/115	-
12	CLA	cB	921	-	-	8/27/103/115	-
12	CLA	aB	901	-	1/1/15/20	6/39/115/115	-
12	CLA	bA	811	-	1/1/11/20	3/15/91/115	-
16	LHG	cB	948	12	-	8/26/26/53	-
16	LHG	bA	852	12	-	11/31/31/53	-
11	CL0	aA	801	-	3/3/20/25	7/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	bB	938	18	1/1/12/20	1/23/99/115	-
12	CLA	cA	809	1	1/1/11/20	7/15/91/115	-
12	CLA	aA	805	-	1/1/12/20	5/25/101/115	-
15	BCR	cA	846	-	-	11/29/63/63	0/2/2/2
14	SF4	bC	101	3	-	-	0/6/5/5
12	CLA	bA	817	-	-	8/26/102/115	-
15	BCR	cF	204	-	-	6/29/63/63	0/2/2/2
12	CLA	bB	929	-	-	6/15/91/115	-
14	SF4	cA	845	1,2	-	-	0/6/5/5
12	CLA	aB	921	-	-	8/27/103/115	-
12	CLA	cA	812	-	1/1/15/20	10/39/115/115	-
12	CLA	cB	926	-	1/1/15/20	21/39/115/115	-
12	CLA	cB	913	-	1/1/13/20	5/29/105/115	-
15	BCR	bB	943	-	-	9/29/63/63	0/2/2/2
12	CLA	cB	910	-	1/1/11/20	3/15/91/115	-
12	CLA	aA	829	-	1/1/14/20	6/33/109/115	-
12	CLA	aB	936	-	1/1/13/20	9/32/108/115	-
15	BCR	aB	944	-	-	15/29/63/63	0/2/2/2
12	CLA	bA	831	-	-	5/21/97/115	-
12	CLA	bB	911	-	-	0/15/91/115	-
12	CLA	aA	833	-	1/1/12/20	5/23/99/115	-
15	BCR	bB	944	-	-	15/29/63/63	0/2/2/2
12	CLA	aB	918	18	1/1/11/20	3/17/93/115	-
12	CLA	cA	813	-	1/1/11/20	3/15/91/115	-
12	CLA	cA	840	-	1/1/15/20	9/39/115/115	-
12	CLA	aA	837	-	1/1/12/20	6/23/99/115	-
16	LHG	bA	851	-	-	22/53/53/53	-
15	BCR	cB	944	-	-	15/29/63/63	0/2/2/2
12	CLA	cA	819	-	1/1/14/20	6/33/109/115	-
12	CLA	aA	827	-	1/1/11/20	5/17/93/115	-
12	CLA	bB	936	-	1/1/13/20	9/32/108/115	-
15	BCR	bJ	101	-	-	13/29/63/63	0/2/2/2
12	CLA	cB	907	-	1/1/12/20	7/24/100/115	-
12	CLA	bB	901	-	1/1/15/20	6/39/115/115	-
12	CLA	bB	915	-	-	11/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	SF4	bA	845	1,2	-	-	0/6/5/5
12	CLA	cB	936	-	1/1/13/20	9/32/108/115	-
12	CLA	cA	838	-	1/1/15/20	8/39/115/115	-
17	LMG	bB	947	-	-	12/38/58/70	0/1/1/1
13	1L3	aB	940	-	-	1/23/43/43	0/2/2/2
14	SF4	aA	846	1,2	-	-	0/6/5/5
12	CLA	bB	903	-	1/1/12/20	5/23/99/115	-
12	CLA	cA	815	-	-	6/15/91/115	-
12	CLA	cB	930	-	1/1/11/20	4/20/96/115	-
12	CLA	bB	939	-	1/1/11/20	4/15/91/115	-
12	CLA	cB	935	-	1/1/12/20	6/21/97/115	-
12	CLA	cA	837	-	1/1/12/20	6/23/99/115	-
12	CLA	bA	835	-	1/1/11/20	2/15/91/115	-
12	CLA	cA	839	-	1/1/11/20	5/15/91/115	-
15	BCR	bI	101	-	-	9/29/63/63	0/2/2/2
12	CLA	bB	926	-	1/1/15/20	21/39/115/115	-
14	SF4	aC	101	3	-	-	0/6/5/5
12	CLA	cB	928	-	1/1/12/20	3/21/97/115	-
12	CLA	cA	821	18	1/1/12/20	4/21/97/115	-
15	BCR	aM	101	-	-	18/29/63/63	0/2/2/2
12	CLA	aB	916	-	-	9/32/108/115	-
12	CLA	cA	822	-	-	7/20/96/115	-
12	CLA	aA	828	-	1/1/15/20	3/39/115/115	-
12	CLA	cA	831	-	-	5/21/97/115	-
12	CLA	cB	915	-	-	11/24/100/115	-
12	CLA	cB	920	-	-	3/15/91/115	-
15	BCR	bA	846	-	-	11/29/63/63	0/2/2/2
12	CLA	aB	906	-	1/1/13/20	2/27/103/115	-
12	CLA	aB	932	-	-	4/15/91/115	-
16	LHG	cA	851	-	-	22/53/53/53	-
12	CLA	cA	834	-	1/1/15/20	13/39/115/115	-
12	CLA	bA	812	-	1/1/15/20	10/39/115/115	-
12	CLA	cB	927	-	1/1/15/20	8/39/115/115	-
12	CLA	aB	903	-	1/1/12/20	5/23/99/115	-
12	CLA	cB	905	-	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	aA	830	-	1/1/15/20	10/39/115/115	-
15	BCR	bB	946	-	-	3/29/63/63	0/2/2/2
12	CLA	aA	836	1	1/1/11/20	5/15/91/115	-
12	CLA	aB	920	-	-	3/15/91/115	-
12	CLA	bA	838	-	1/1/15/20	8/39/115/115	-
12	CLA	cA	826	18	1/1/13/20	7/27/103/115	-
12	CLA	bA	809	1	1/1/11/20	7/15/91/115	-
12	CLA	bA	825	18	1/1/15/20	9/39/115/115	-
15	BCR	aF	203	-	-	12/29/63/63	0/2/2/2
15	BCR	aF	201	-	-	8/29/63/63	0/2/2/2
12	CLA	bA	834	-	1/1/15/20	13/39/115/115	-
12	CLA	aL	203	-	-	5/15/91/115	-
12	CLA	cB	918	18	1/1/11/20	3/17/93/115	-
12	CLA	bB	935	-	1/1/12/20	6/21/97/115	-
15	BCR	aL	205	-	-	10/29/63/63	0/2/2/2
12	CLA	cB	937	-	1/1/11/20	1/18/94/115	-
12	CLA	bA	821	18	1/1/12/20	4/21/97/115	-
15	BCR	cL	205	-	-	10/29/63/63	0/2/2/2
12	CLA	cA	806	-	1/1/15/20	9/39/115/115	-
12	CLA	bA	822	-	-	7/20/96/115	-
12	CLA	aA	818	-	1/1/12/20	12/26/102/115	-
12	CLA	aB	930	-	1/1/11/20	4/20/96/115	-
12	CLA	bA	826	18	1/1/13/20	7/27/103/115	-
12	CLA	aA	820	-	1/1/13/20	11/29/105/115	-
15	BCR	aA	847	-	-	11/29/63/63	0/2/2/2
12	CLA	bB	928	-	1/1/12/20	3/21/97/115	-
15	BCR	aB	942	-	-	10/29/63/63	0/2/2/2
15	BCR	aA	848	-	-	6/29/63/63	0/2/2/2
12	CLA	cA	827	-	1/1/11/20	5/17/93/115	-
16	LHG	aA	852	-	-	22/53/53/53	-
14	SF4	bC	102	3	-	-	0/6/5/5
12	CLA	cB	933	18	1/1/11/20	3/15/91/115	-
12	CLA	bB	905	-	1/1/15/20	15/39/115/115	-
15	BCR	aB	943	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	aA	816	-	1/1/11/20	4/15/91/115	-
12	CLA	bA	843	18	1/1/15/20	10/39/115/115	-
12	CLA	bB	913	-	1/1/13/20	5/29/105/115	-
12	CLA	aB	911	-	-	0/15/91/115	-
12	CLA	aA	817	-	-	8/26/102/115	-
12	CLA	cA	835	-	1/1/11/20	2/15/91/115	-
17	LMG	cB	947	-	-	12/38/58/70	0/1/1/1
15	BCR	aA	850	-	-	10/29/63/63	0/2/2/2
12	CLA	aA	821	18	1/1/12/20	4/21/97/115	-
12	CLA	aA	841	18	1/1/12/20	5/23/99/115	-
12	CLA	cB	932	-	-	4/15/91/115	-
12	CLA	aB	909	-	1/1/13/20	8/27/103/115	-
12	CLA	cB	911	-	-	0/15/91/115	-
12	CLA	aA	813	-	1/1/11/20	3/15/91/115	-
12	CLA	bA	815	-	-	6/15/91/115	-
12	CLA	bB	907	-	1/1/12/20	7/24/100/115	-
15	BCR	cB	941	-	-	10/29/63/63	0/2/2/2
12	CLA	aA	814	-	1/1/11/20	7/15/91/115	-
14	SF4	cC	101	3	-	-	0/6/5/5
12	CLA	aA	844	16	-	6/15/91/115	-
12	CLA	aB	949	16	1/1/10/20	2/10/86/115	-
12	CLA	aA	803	-	1/1/15/20	5/39/115/115	-
12	CLA	aL	204	18	-	0/15/91/115	-
12	CLA	cB	912	-	1/1/15/20	15/39/115/115	-
12	CLA	cB	939	-	1/1/11/20	4/15/91/115	-
12	CLA	cA	816	-	1/1/11/20	4/15/91/115	-
12	CLA	cA	818	-	1/1/12/20	12/26/102/115	-
15	BCR	aB	945	-	-	10/29/63/63	0/2/2/2
12	CLA	aB	937	-	1/1/11/20	2/18/94/115	-
12	CLA	aB	922	-	1/1/11/20	5/15/91/115	-
12	CLA	cB	934	2	1/1/11/20	3/15/91/115	-
12	CLA	cB	949	16	1/1/10/20	2/10/86/115	-
12	CLA	cA	842	-	1/1/15/20	14/39/115/115	-
12	CLA	aB	928	-	1/1/12/20	3/21/97/115	-
15	BCR	cB	943	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	bB	917	-	1/1/13/20	9/27/103/115	-
15	BCR	aL	206	-	-	6/29/63/63	0/2/2/2
12	CLA	aB	935	-	1/1/12/20	6/21/97/115	-
12	CLA	bB	918	18	1/1/11/20	3/17/93/115	-
12	CLA	aA	824	-	-	5/18/94/115	-
15	BCR	aA	851	-	-	10/29/63/63	0/2/2/2
12	CLA	bB	912	-	1/1/15/20	15/39/115/115	-
12	CLA	bA	818	-	1/1/12/20	12/26/102/115	-
12	CLA	cL	203	-	-	5/15/91/115	-
15	BCR	aI	101	-	-	9/29/63/63	0/2/2/2
15	BCR	cA	847	-	-	6/29/63/63	0/2/2/2
12	CLA	aB	904	-	1/1/15/20	12/39/115/115	-
15	BCR	aB	941	-	-	10/29/63/63	0/2/2/2
12	CLA	bB	931	-	1/1/15/20	12/39/115/115	-
12	CLA	aB	933	18	1/1/11/20	3/15/91/115	-
12	CLA	bL	204	18	-	0/15/91/115	-
12	CLA	bA	807	-	1/1/15/20	13/39/115/115	-
12	CLA	bB	932	-	-	4/15/91/115	-
15	BCR	bL	201	-	-	7/29/63/63	0/2/2/2
12	CLA	cA	810	1	1/1/11/20	7/15/91/115	-
12	CLA	cA	830	-	1/1/15/20	10/39/115/115	-
12	CLA	bA	837	-	1/1/12/20	6/23/99/115	-
12	CLA	cB	929	-	-	6/15/91/115	-
12	CLA	cA	807	-	1/1/15/20	13/39/115/115	-
12	CLA	cA	814	-	1/1/11/20	7/15/91/115	-
12	CLA	aB	913	-	1/1/13/20	5/29/105/115	-
12	CLA	aF	202	6	1/1/11/20	9/15/91/115	-
15	BCR	aA	849	-	-	10/29/63/63	0/2/2/2
12	CLA	cB	917	-	1/1/13/20	9/27/103/115	-
12	CLA	aB	950	16	-	6/15/91/115	-
12	CLA	cB	902	-	1/1/14/20	9/35/111/115	-
12	CLA	aB	938	18	1/1/12/20	1/23/99/115	-
11	CL0	cA	801	-	3/3/20/25	7/37/135/135	-
12	CLA	bA	816	-	1/1/11/20	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	cB	909	-	1/1/13/20	8/27/103/115	-
12	CLA	bA	806	-	1/1/15/20	9/39/115/115	-
12	CLA	cB	906	-	1/1/13/20	2/27/103/115	-
13	1L3	aA	845	-	-	3/23/43/43	0/2/2/2
12	CLA	cA	832	-	1/1/13/20	9/27/103/115	-
16	LHG	aB	948	12	-	8/26/26/53	-
12	CLA	bA	810	1	1/1/11/20	7/15/91/115	-
12	CLA	aB	931	-	1/1/15/20	12/39/115/115	-
12	CLA	bA	827	-	1/1/11/20	5/17/93/115	-
12	CLA	bA	842	-	1/1/15/20	14/39/115/115	-
12	CLA	bA	830	-	1/1/15/20	10/39/115/115	-
12	CLA	bB	914	-	1/1/11/20	6/15/91/115	-
12	CLA	cA	833	-	1/1/12/20	5/23/99/115	-
12	CLA	aB	939	-	1/1/11/20	4/15/91/115	-
12	CLA	bB	925	-	1/1/13/20	5/27/103/115	-
12	CLA	aA	854	18	1/1/13/20	6/29/105/115	-
12	CLA	bB	922	-	1/1/11/20	5/15/91/115	-
12	CLA	bA	814	-	1/1/11/20	7/15/91/115	-
12	CLA	cA	805	-	1/1/12/20	5/25/101/115	-
15	BCR	aL	201	-	-	7/29/63/63	0/2/2/2
12	CLA	bA	833	-	1/1/12/20	5/23/99/115	-
15	BCR	cA	848	-	-	10/29/63/63	0/2/2/2
12	CLA	aA	834	-	1/1/15/20	13/39/115/115	-
12	CLA	cA	803	-	1/1/15/20	5/39/115/115	-
12	CLA	aB	912	-	1/1/15/20	15/39/115/115	-
12	CLA	cA	824	-	-	5/18/94/115	-
12	CLA	aA	843	18	1/1/15/20	10/39/115/115	-
12	CLA	cB	923	18	1/1/12/20	11/26/102/115	-
12	CLA	bB	920	-	-	3/15/91/115	-
15	BCR	bM	101	-	-	18/29/63/63	0/2/2/2
12	CLA	cB	904	-	1/1/15/20	12/39/115/115	-
12	CLA	bB	927	-	1/1/15/20	8/39/115/115	-
12	CLA	bA	841	18	1/1/12/20	5/23/99/115	-
12	CLA	cB	922	-	1/1/11/20	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	bA	813	-	1/1/11/20	3/15/91/115	-
12	CLA	aL	202	9	-	2/25/101/115	-
12	CLA	cA	829	-	1/1/14/20	6/33/109/115	-
12	CLA	bA	820	-	1/1/13/20	11/29/105/115	-
15	BCR	cA	849	-	-	10/29/63/63	0/2/2/2
15	BCR	cJ	101	-	-	13/29/63/63	0/2/2/2
12	CLA	bL	202	9	-	2/25/101/115	-
12	CLA	bB	909	-	1/1/13/20	8/27/103/115	-
12	CLA	cB	901	-	1/1/15/20	6/39/115/115	-
12	CLA	bA	803	-	1/1/15/20	5/39/115/115	-
15	BCR	cB	942	-	-	10/29/63/63	0/2/2/2
12	CLA	bB	919	-	1/1/11/20	7/18/94/115	-
12	CLA	cB	916	-	-	9/32/108/115	-
12	CLA	bA	853	18	1/1/13/20	6/29/105/115	-
12	CLA	cB	919	-	1/1/11/20	7/18/94/115	-
15	BCR	bF	201	-	-	8/29/63/63	0/2/2/2
12	CLA	cA	808	-	1/1/12/20	7/23/99/115	-
12	CLA	aA	806	-	1/1/15/20	9/39/115/115	-
12	CLA	bA	823	-	1/1/12/20	8/23/99/115	-
12	CLA	cA	843	18	1/1/15/20	10/39/115/115	-
15	BCR	bA	847	-	-	6/29/63/63	0/2/2/2
16	LHG	aA	853	12	-	11/31/31/53	-
12	CLA	cL	204	18	-	0/15/91/115	-
12	CLA	aB	927	-	1/1/15/20	9/39/115/115	-
12	CLA	aB	902	-	1/1/14/20	9/35/111/115	-
15	BCR	bA	848	-	-	10/29/63/63	0/2/2/2
12	CLA	cA	853	18	1/1/13/20	6/29/105/115	-
12	CLA	aA	842	-	1/1/15/20	14/39/115/115	-
12	CLA	cL	202	9	-	2/25/101/115	-
15	BCR	cL	201	-	-	7/29/63/63	0/2/2/2
15	BCR	bL	206	-	-	6/29/63/63	0/2/2/2
12	CLA	bB	937	-	1/1/11/20	2/18/94/115	-
12	CLA	aA	839	-	1/1/11/20	5/15/91/115	-
12	CLA	bL	203	-	-	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	cA	841	18	1/1/12/20	5/23/99/115	-
12	CLA	bB	950	16	-	6/15/91/115	-
12	CLA	bA	805	-	1/1/12/20	5/25/101/115	-
12	CLA	aB	905	-	1/1/15/20	15/39/115/115	-
15	BCR	bL	205	-	-	10/29/63/63	0/2/2/2
12	CLA	aA	811	-	1/1/11/20	3/15/91/115	-
15	BCR	cI	101	-	-	9/29/63/63	0/2/2/2
12	CLA	bA	836	1	1/1/11/20	5/15/91/115	-
15	BCR	aF	204	-	-	6/29/63/63	0/2/2/2
14	SF4	aC	102	3	-	-	0/6/5/5
12	CLA	aA	825	18	1/1/15/20	9/39/115/115	-
12	CLA	bF	202	6	1/1/11/20	9/15/91/115	-
12	CLA	aB	910	-	1/1/11/20	3/15/91/115	-
12	CLA	aB	923	18	1/1/12/20	11/26/102/115	-
14	SF4	cC	102	3	-	-	0/6/5/5
12	CLA	bB	933	18	1/1/11/20	3/15/91/115	-
12	CLA	bA	828	-	1/1/15/20	3/39/115/115	-
12	CLA	cA	811	-	1/1/11/20	3/15/91/115	-
12	CLA	cB	908	2	1/1/11/20	7/19/95/115	-
12	CLA	bA	802	18	1/1/15/20	5/39/115/115	-
13	1L3	bB	940	-	-	1/23/43/43	0/2/2/2
12	CLA	aA	835	-	1/1/11/20	2/15/91/115	-
12	CLA	cB	924	18	1/1/11/20	2/17/93/115	-
11	CL0	bA	801	-	3/3/20/25	7/37/135/135	-
12	CLA	aA	831	-	-	5/21/97/115	-
12	CLA	bA	832	-	1/1/13/20	9/27/103/115	-
12	CLA	aB	925	-	1/1/13/20	5/27/103/115	-
12	CLA	cA	828	-	1/1/15/20	3/39/115/115	-
12	CLA	aB	929	-	-	6/15/91/115	-
15	BCR	bB	941	-	-	10/29/63/63	0/2/2/2
12	CLA	cA	820	-	1/1/13/20	11/29/105/115	-
12	CLA	aA	810	1	1/1/11/20	7/15/91/115	-
12	CLA	aA	812	-	1/1/15/20	10/39/115/115	-
12	CLA	aB	926	-	1/1/15/20	21/39/115/115	-
17	LMG	aB	947	-	-	11/38/58/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	cB	931	-	1/1/15/20	12/39/115/115	-
12	CLA	bB	910	-	1/1/11/20	3/15/91/115	-
15	BCR	bA	850	-	-	9/29/63/63	0/2/2/2
12	CLA	cA	836	1	1/1/11/20	5/15/91/115	-
16	LHG	bB	948	12	-	8/26/26/53	-
12	CLA	aA	804	-	1/1/13/20	7/29/105/115	-
15	BCR	bF	203	-	-	12/29/63/63	0/2/2/2
12	CLA	aB	915	-	-	11/24/100/115	-
12	CLA	cB	914	-	1/1/11/20	6/15/91/115	-
12	CLA	bA	824	-	-	5/18/94/115	-
12	CLA	aA	819	-	1/1/14/20	6/33/109/115	-
12	CLA	aB	917	-	1/1/13/20	9/27/103/115	-
12	CLA	cA	802	18	1/1/15/20	5/39/115/115	-
12	CLA	cA	804	-	1/1/13/20	7/29/105/115	-
12	CLA	cB	938	18	1/1/12/20	1/23/99/115	-
15	BCR	bF	204	-	-	6/29/63/63	0/2/2/2
13	1L3	bA	844	-	-	3/23/43/43	0/2/2/2
16	LHG	cA	852	12	-	11/31/31/53	-
12	CLA	bA	839	-	1/1/11/20	5/15/91/115	-
15	BCR	cL	206	-	-	6/29/63/63	0/2/2/2
12	CLA	cB	925	-	1/1/13/20	5/27/103/115	-
15	BCR	aB	946	-	-	3/29/63/63	0/2/2/2
12	CLA	bB	930	-	1/1/11/20	4/20/96/115	-
12	CLA	cB	903	-	1/1/12/20	5/23/99/115	-
12	CLA	cA	823	-	1/1/12/20	8/23/99/115	-
12	CLA	bA	829	-	1/1/14/20	6/33/109/115	-
15	BCR	aJ	101	-	-	13/29/63/63	0/2/2/2
15	BCR	cB	945	-	-	10/29/63/63	0/2/2/2
12	CLA	aA	802	18	1/1/15/20	5/39/115/115	-
15	BCR	bA	849	-	-	11/29/63/63	0/2/2/2
12	CLA	bB	904	-	1/1/15/20	12/39/115/115	-
12	CLA	aA	840	-	1/1/15/20	9/39/115/115	-
12	CLA	aB	908	2	1/1/11/20	7/19/95/115	-
12	CLA	aB	919	-	1/1/11/20	7/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	cF	203	-	-	12/29/63/63	0/2/2/2
15	BCR	cA	850	-	-	10/29/63/63	0/2/2/2
15	BCR	bB	942	-	-	10/29/63/63	0/2/2/2
12	CLA	aA	838	-	1/1/15/20	8/39/115/115	-
12	CLA	bA	808	-	1/1/12/20	7/23/99/115	-
12	CLA	aA	809	1	1/1/11/20	7/15/91/115	-
12	CLA	aB	914	-	1/1/11/20	6/15/91/115	-
12	CLA	aA	815	-	-	6/15/91/115	-
12	CLA	aB	934	2	1/1/11/20	3/15/91/115	-
12	CLA	bB	934	2	1/1/11/20	3/15/91/115	-
12	CLA	aA	807	-	1/1/15/20	13/39/115/115	-
12	CLA	cA	817	-	-	8/26/102/115	-
13	1L3	cA	844	-	-	3/23/43/43	0/2/2/2
12	CLA	aA	826	18	1/1/13/20	7/27/103/115	-
12	CLA	bA	804	-	1/1/13/20	7/29/105/115	-
12	CLA	aA	822	-	-	7/20/96/115	-
12	CLA	bB	908	2	1/1/11/20	7/19/95/115	-
12	CLA	bB	902	-	1/1/14/20	9/35/111/115	-
12	CLA	aA	832	-	1/1/13/20	9/27/103/115	-
13	1L3	cB	940	-	-	1/23/43/43	0/2/2/2
12	CLA	bB	916	-	-	9/32/108/115	-
12	CLA	cA	825	18	1/1/15/20	9/39/115/115	-
15	BCR	cF	201	-	-	8/29/63/63	0/2/2/2
12	CLA	aA	808	-	1/1/12/20	7/23/99/115	-
12	CLA	bA	819	-	1/1/14/20	6/33/109/115	-

All (5408) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	bA	801	CL0	C1B-C2B	9.32	1.50	1.39
11	cA	801	CL0	C1B-C2B	9.22	1.50	1.39
11	aA	801	CL0	C1B-C2B	9.17	1.50	1.39
11	cA	801	CL0	C1A-CHA	8.59	1.49	1.40
11	bA	801	CL0	C1A-CHA	8.57	1.49	1.40
11	aA	801	CL0	C1A-CHA	8.56	1.49	1.40
13	bB	940	1L3	C03-C02	8.03	1.49	1.35
13	aB	940	1L3	C03-C02	8.00	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	cB	940	1L3	C03-C02	7.98	1.49	1.35
13	bA	844	1L3	C03-C02	7.91	1.49	1.35
13	cA	844	1L3	C03-C02	7.89	1.49	1.35
13	aA	845	1L3	C03-C02	7.89	1.49	1.35
11	bA	801	CL0	C3B-C4B	6.65	1.47	1.41
11	cA	801	CL0	C3B-C4B	6.55	1.47	1.41
11	aA	801	CL0	C3B-C4B	6.54	1.47	1.41
11	bA	801	CL0	C1D-C2D	5.82	1.46	1.39
11	cA	801	CL0	C1D-C2D	5.82	1.46	1.39
11	aA	801	CL0	C1D-C2D	5.75	1.46	1.39
11	aA	801	CL0	C3B-C2B	5.56	1.47	1.40
11	bA	801	CL0	C3B-C2B	5.54	1.47	1.40
11	cA	801	CL0	C3B-C2B	5.49	1.47	1.40
12	bA	813	CLA	C3C-C2C	5.37	1.48	1.36
12	bB	915	CLA	C3C-C2C	5.36	1.48	1.36
12	aB	949	CLA	C3C-C2C	5.34	1.48	1.36
12	cA	813	CLA	C3C-C2C	5.34	1.48	1.36
12	cB	915	CLA	C3C-C2C	5.34	1.48	1.36
12	cB	949	CLA	C3C-C2C	5.33	1.48	1.36
12	bB	931	CLA	C3C-C2C	5.33	1.48	1.36
12	aB	915	CLA	C3C-C2C	5.33	1.48	1.36
12	aA	813	CLA	C3C-C2C	5.32	1.48	1.36
12	aB	908	CLA	C1B-NB	-5.31	1.30	1.37
12	aB	931	CLA	C3C-C2C	5.31	1.48	1.36
12	bB	949	CLA	C3C-C2C	5.31	1.48	1.36
12	cB	931	CLA	C3C-C2C	5.30	1.48	1.36
12	aA	828	CLA	C3C-C2C	5.28	1.48	1.36
12	bB	908	CLA	C1B-NB	-5.28	1.30	1.37
12	aA	816	CLA	C3C-C2C	5.27	1.48	1.36
12	cA	816	CLA	C3C-C2C	5.27	1.48	1.36
12	bA	816	CLA	C3C-C2C	5.27	1.48	1.36
12	cA	828	CLA	C3C-C2C	5.24	1.48	1.36
12	bA	828	CLA	C3C-C2C	5.23	1.48	1.36
12	cB	908	CLA	C1B-NB	-5.23	1.31	1.37
12	aA	815	CLA	C3C-C2C	5.22	1.48	1.36
12	cB	929	CLA	C3C-C2C	5.22	1.48	1.36
12	cA	815	CLA	C3C-C2C	5.21	1.48	1.36
12	bA	815	CLA	C3C-C2C	5.20	1.48	1.36
12	cB	936	CLA	C3C-C2C	5.18	1.47	1.36
12	bB	927	CLA	C1B-NB	-5.18	1.31	1.37
12	aB	929	CLA	C3C-C2C	5.18	1.47	1.36
12	aB	927	CLA	C1B-NB	-5.17	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bB	929	CLA	C3C-C2C	5.16	1.47	1.36
12	aB	936	CLA	C3C-C2C	5.16	1.47	1.36
12	bB	930	CLA	C3C-C2C	5.16	1.47	1.36
12	cB	927	CLA	C1B-NB	-5.15	1.31	1.37
12	aB	930	CLA	C3C-C2C	5.14	1.47	1.36
12	bA	838	CLA	C3C-C2C	5.13	1.47	1.36
12	cB	930	CLA	C3C-C2C	5.13	1.47	1.36
12	bB	936	CLA	C3C-C2C	5.13	1.47	1.36
12	cB	910	CLA	C3C-C2C	5.13	1.47	1.36
12	cB	920	CLA	C3C-C2C	5.12	1.47	1.36
12	aB	934	CLA	C3C-C2C	5.12	1.47	1.36
12	aB	920	CLA	C3C-C2C	5.12	1.47	1.36
12	cB	934	CLA	C3C-C2C	5.11	1.47	1.36
12	bA	835	CLA	C3C-C2C	5.11	1.47	1.36
11	aA	801	CL0	C3A-C2A	-5.11	1.50	1.54
12	bA	804	CLA	C3C-C2C	5.10	1.47	1.36
12	bB	921	CLA	C3C-C2C	5.10	1.47	1.36
12	bB	920	CLA	C3C-C2C	5.10	1.47	1.36
12	aB	935	CLA	C3C-C2C	5.10	1.47	1.36
12	cA	838	CLA	C3C-C2C	5.10	1.47	1.36
12	cB	949	CLA	O2D-CGD	5.10	1.45	1.33
11	bA	801	CL0	C3A-C2A	-5.10	1.50	1.54
12	cB	918	CLA	C3C-C2C	5.09	1.47	1.36
12	bB	934	CLA	O2D-CGD	5.09	1.45	1.33
12	aA	838	CLA	C3C-C2C	5.09	1.47	1.36
12	aA	835	CLA	C3C-C2C	5.09	1.47	1.36
12	cA	803	CLA	C1B-NB	-5.09	1.31	1.37
12	cB	935	CLA	C3C-C2C	5.09	1.47	1.36
12	bA	827	CLA	C3C-C2C	5.08	1.47	1.36
12	bB	910	CLA	C3C-C2C	5.08	1.47	1.36
12	bB	934	CLA	C3C-C2C	5.08	1.47	1.36
12	aA	819	CLA	C3C-C2C	5.08	1.47	1.36
12	aB	921	CLA	C3C-C2C	5.07	1.47	1.36
12	aB	910	CLA	C3C-C2C	5.07	1.47	1.36
12	cA	835	CLA	C3C-C2C	5.07	1.47	1.36
12	cA	804	CLA	C3C-C2C	5.07	1.47	1.36
12	aA	803	CLA	C1B-NB	-5.07	1.31	1.37
12	bB	918	CLA	C3C-C2C	5.07	1.47	1.36
12	bB	935	CLA	C3C-C2C	5.07	1.47	1.36
12	cA	811	CLA	C3C-C2C	5.07	1.47	1.36
12	bA	803	CLA	C1B-NB	-5.07	1.31	1.37
12	aB	949	CLA	O2D-CGD	5.07	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bB	949	CLA	O2D-CGD	5.07	1.45	1.33
12	bA	825	CLA	C3C-C2C	5.07	1.47	1.36
12	cB	921	CLA	C3C-C2C	5.07	1.47	1.36
12	bA	822	CLA	C3C-C2C	5.07	1.47	1.36
12	cL	203	CLA	C3C-C2C	5.07	1.47	1.36
12	aA	837	CLA	C3C-C2C	5.06	1.47	1.36
12	aA	804	CLA	C3C-C2C	5.06	1.47	1.36
12	aB	928	CLA	C1B-NB	-5.06	1.31	1.37
12	cA	827	CLA	C3C-C2C	5.06	1.47	1.36
12	cA	837	CLA	C3C-C2C	5.06	1.47	1.36
12	cA	819	CLA	C3C-C2C	5.06	1.47	1.36
12	aA	827	CLA	C3C-C2C	5.05	1.47	1.36
12	cA	817	CLA	C3C-C2C	5.05	1.47	1.36
12	bL	203	CLA	C3C-C2C	5.05	1.47	1.36
12	bA	837	CLA	C3C-C2C	5.05	1.47	1.36
12	aA	811	CLA	C3C-C2C	5.04	1.47	1.36
12	aB	934	CLA	O2D-CGD	5.04	1.45	1.33
12	aA	832	CLA	C3C-C2C	5.04	1.47	1.36
12	bA	819	CLA	C3C-C2C	5.04	1.47	1.36
12	cB	934	CLA	O2D-CGD	5.04	1.45	1.33
12	aA	822	CLA	C3C-C2C	5.04	1.47	1.36
12	aB	918	CLA	C3C-C2C	5.04	1.47	1.36
12	aA	825	CLA	C3C-C2C	5.04	1.47	1.36
12	cA	825	CLA	C3C-C2C	5.04	1.47	1.36
12	bA	811	CLA	C3C-C2C	5.04	1.47	1.36
12	aB	931	CLA	CHC-C1C	5.03	1.48	1.38
12	cA	822	CLA	C3C-C2C	5.03	1.47	1.36
12	bA	834	CLA	C3C-C2C	5.03	1.47	1.36
12	aA	824	CLA	O2D-CGD	5.03	1.45	1.33
12	aL	203	CLA	C3C-C2C	5.02	1.47	1.36
12	cB	928	CLA	C1B-NB	-5.02	1.31	1.37
12	aB	905	CLA	O2D-CGD	5.02	1.45	1.33
12	aA	817	CLA	C3C-C2C	5.02	1.47	1.36
12	aA	833	CLA	C3C-C2C	5.02	1.47	1.36
12	bB	914	CLA	C3C-C2C	5.01	1.47	1.36
12	bB	905	CLA	O2D-CGD	5.01	1.45	1.33
12	cB	905	CLA	O2D-CGD	5.01	1.45	1.33
12	cA	824	CLA	O2D-CGD	5.01	1.45	1.33
12	bA	833	CLA	C3C-C2C	5.01	1.47	1.36
12	bB	931	CLA	CHC-C1C	5.01	1.48	1.38
12	bA	832	CLA	C3C-C2C	5.01	1.47	1.36
12	bB	928	CLA	C1B-NB	-5.01	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aA	809	CLA	C3C-C2C	5.01	1.47	1.36
12	cB	931	CLA	CHC-C1C	5.01	1.48	1.38
12	cA	834	CLA	C3C-C2C	5.00	1.47	1.36
12	cA	830	CLA	C3C-C2C	5.00	1.47	1.36
12	cA	836	CLA	O2D-CGD	5.00	1.45	1.33
12	cA	809	CLA	C3C-C2C	5.00	1.47	1.36
12	bA	824	CLA	O2D-CGD	5.00	1.45	1.33
12	aB	915	CLA	O2D-CGD	5.00	1.45	1.33
12	aA	821	CLA	C3C-C2C	5.00	1.47	1.36
12	bA	817	CLA	C3C-C2C	5.00	1.47	1.36
12	bB	938	CLA	O2D-CGD	5.00	1.45	1.33
12	cA	832	CLA	C3C-C2C	4.99	1.47	1.36
12	aA	836	CLA	O2D-CGD	4.99	1.45	1.33
12	bA	820	CLA	C3C-C2C	4.99	1.47	1.36
12	bA	830	CLA	C3C-C2C	4.99	1.47	1.36
12	bA	809	CLA	C3C-C2C	4.99	1.47	1.36
12	cA	821	CLA	C3C-C2C	4.99	1.47	1.36
12	bF	202	CLA	O2D-CGD	4.98	1.45	1.33
12	bA	821	CLA	C3C-C2C	4.98	1.47	1.36
12	aA	834	CLA	C3C-C2C	4.98	1.47	1.36
12	bA	839	CLA	C3C-C2C	4.98	1.47	1.36
12	cA	839	CLA	C3C-C2C	4.98	1.47	1.36
12	bA	831	CLA	C3C-C2C	4.98	1.47	1.36
12	aB	938	CLA	O2D-CGD	4.98	1.45	1.33
12	bA	836	CLA	O2D-CGD	4.98	1.45	1.33
12	cB	915	CLA	O2D-CGD	4.98	1.45	1.33
12	cF	202	CLA	O2D-CGD	4.98	1.45	1.33
12	cB	914	CLA	C3C-C2C	4.98	1.47	1.36
12	cB	937	CLA	C3C-C2C	4.98	1.47	1.36
12	aA	820	CLA	C3C-C2C	4.98	1.47	1.36
12	aA	842	CLA	C3C-C2C	4.97	1.47	1.36
12	cA	833	CLA	C3C-C2C	4.97	1.47	1.36
12	bB	915	CLA	O2D-CGD	4.97	1.45	1.33
12	aA	830	CLA	C3C-C2C	4.97	1.47	1.36
12	aB	914	CLA	C3C-C2C	4.97	1.47	1.36
12	cA	842	CLA	C3C-C2C	4.97	1.47	1.36
12	aA	805	CLA	C3C-C2C	4.97	1.47	1.36
12	aB	922	CLA	C3C-C2C	4.97	1.47	1.36
11	cA	801	CL0	C3A-C2A	-4.97	1.50	1.54
12	aA	831	CLA	C3C-C2C	4.97	1.47	1.36
12	bA	829	CLA	C3C-C2C	4.97	1.47	1.36
12	bB	937	CLA	C3C-C2C	4.97	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cB	910	CLA	O2D-CGD	4.97	1.45	1.33
12	bA	842	CLA	C3C-C2C	4.96	1.47	1.36
12	aF	202	CLA	O2D-CGD	4.96	1.45	1.33
12	bB	910	CLA	O2D-CGD	4.96	1.45	1.33
12	aA	839	CLA	C3C-C2C	4.96	1.47	1.36
12	aB	924	CLA	C3C-C2C	4.96	1.47	1.36
12	bA	810	CLA	C3C-C2C	4.96	1.47	1.36
12	aA	802	CLA	C3C-C2C	4.95	1.47	1.36
12	cA	820	CLA	C3C-C2C	4.95	1.47	1.36
12	cB	949	CLA	C1D-ND	4.95	1.44	1.37
12	cA	829	CLA	C3C-C2C	4.95	1.47	1.36
12	aA	829	CLA	C3C-C2C	4.95	1.47	1.36
12	cA	802	CLA	C3C-C2C	4.95	1.47	1.36
12	cA	805	CLA	C3C-C2C	4.95	1.47	1.36
12	aB	932	CLA	C3C-C2C	4.95	1.47	1.36
12	cB	938	CLA	O2D-CGD	4.95	1.45	1.33
12	cA	831	CLA	C3C-C2C	4.94	1.47	1.36
12	cB	924	CLA	C3C-C2C	4.94	1.47	1.36
12	cB	922	CLA	C3C-C2C	4.94	1.47	1.36
12	aB	929	CLA	O2D-CGD	4.94	1.45	1.33
12	bB	924	CLA	C3C-C2C	4.94	1.47	1.36
12	bB	929	CLA	O2D-CGD	4.94	1.45	1.33
12	cB	913	CLA	C3C-C2C	4.94	1.47	1.36
12	bA	802	CLA	C3C-C2C	4.94	1.47	1.36
12	aB	949	CLA	C1D-ND	4.93	1.44	1.37
12	bA	805	CLA	C3C-C2C	4.93	1.47	1.36
12	aB	937	CLA	C3C-C2C	4.93	1.47	1.36
12	cA	810	CLA	C3C-C2C	4.93	1.47	1.36
12	aA	810	CLA	C3C-C2C	4.93	1.47	1.36
12	cB	925	CLA	C3C-C2C	4.93	1.47	1.36
12	aB	913	CLA	C3C-C2C	4.93	1.47	1.36
12	bB	950	CLA	O2D-CGD	4.93	1.45	1.33
12	aB	910	CLA	O2D-CGD	4.93	1.45	1.33
12	aB	950	CLA	O2D-CGD	4.93	1.45	1.33
12	bB	922	CLA	C3C-C2C	4.92	1.47	1.36
12	bA	808	CLA	C3C-C2C	4.92	1.47	1.36
12	cB	932	CLA	C3C-C2C	4.92	1.47	1.36
12	cB	929	CLA	O2D-CGD	4.92	1.45	1.33
12	bB	912	CLA	C3C-C2C	4.92	1.47	1.36
12	bB	925	CLA	C3C-C2C	4.92	1.47	1.36
12	aB	912	CLA	C3C-C2C	4.92	1.47	1.36
12	aA	844	CLA	O2D-CGD	4.91	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aA	808	CLA	C3C-C2C	4.91	1.47	1.36
12	bB	932	CLA	C3C-C2C	4.91	1.47	1.36
12	cB	939	CLA	O2D-CGD	4.91	1.45	1.33
12	cA	808	CLA	C3C-C2C	4.91	1.47	1.36
12	cB	912	CLA	C3C-C2C	4.91	1.47	1.36
12	bA	840	CLA	C3C-C2C	4.91	1.47	1.36
12	cA	836	CLA	C3C-C2C	4.91	1.47	1.36
12	aB	939	CLA	O2D-CGD	4.91	1.45	1.33
12	aB	925	CLA	C3C-C2C	4.91	1.47	1.36
12	bB	913	CLA	C3C-C2C	4.90	1.47	1.36
12	bA	816	CLA	O2D-CGD	4.90	1.45	1.33
12	bA	853	CLA	C3C-C2C	4.90	1.47	1.36
12	bB	949	CLA	C1D-ND	4.90	1.44	1.37
12	cB	923	CLA	C3C-C2C	4.89	1.47	1.36
12	aB	938	CLA	C3C-C2C	4.89	1.47	1.36
12	aA	821	CLA	O2D-CGD	4.89	1.45	1.33
12	aA	840	CLA	C3C-C2C	4.89	1.47	1.36
12	cA	821	CLA	O2D-CGD	4.89	1.45	1.33
12	cA	840	CLA	C3C-C2C	4.88	1.47	1.36
12	cB	927	CLA	C3C-C2C	4.88	1.47	1.36
12	cL	202	CLA	C3C-C2C	4.88	1.47	1.36
12	bA	821	CLA	O2D-CGD	4.88	1.45	1.33
12	aB	923	CLA	C3C-C2C	4.88	1.47	1.36
12	cA	807	CLA	O2D-CGD	4.88	1.45	1.33
12	bB	927	CLA	C3C-C2C	4.88	1.47	1.36
12	aB	918	CLA	C1B-NB	-4.88	1.31	1.37
12	aA	816	CLA	O2D-CGD	4.87	1.45	1.33
12	aA	807	CLA	O2D-CGD	4.87	1.45	1.33
12	aB	927	CLA	C3C-C2C	4.87	1.47	1.36
12	cB	906	CLA	C3C-C2C	4.87	1.47	1.36
12	bB	938	CLA	C3C-C2C	4.87	1.47	1.36
12	bA	807	CLA	O2D-CGD	4.87	1.45	1.33
12	bB	923	CLA	C3C-C2C	4.86	1.47	1.36
12	bB	939	CLA	O2D-CGD	4.86	1.45	1.33
12	cB	938	CLA	C3C-C2C	4.86	1.47	1.36
12	aA	825	CLA	O2D-CGD	4.86	1.45	1.33
12	cA	823	CLA	C3C-C2C	4.86	1.47	1.36
12	aL	202	CLA	C3C-C2C	4.86	1.47	1.36
13	aB	940	1L3	C06-C04	4.86	1.57	1.48
12	bA	822	CLA	O2D-CGD	4.86	1.45	1.33
12	cA	853	CLA	C3C-C2C	4.85	1.47	1.36
12	bL	202	CLA	C3C-C2C	4.85	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aA	811	CLA	O2D-CGD	4.85	1.45	1.33
12	cA	816	CLA	O2D-CGD	4.85	1.45	1.33
11	bA	801	CL0	C3D-C2D	4.85	1.47	1.39
12	bB	939	CLA	C3C-C2C	4.85	1.47	1.36
12	bA	836	CLA	C3C-C2C	4.85	1.47	1.36
12	bA	840	CLA	O2D-CGD	4.85	1.45	1.33
12	bA	825	CLA	O2D-CGD	4.85	1.45	1.33
12	bB	906	CLA	C3C-C2C	4.85	1.47	1.36
12	bA	811	CLA	O2D-CGD	4.85	1.45	1.33
12	aA	854	CLA	C3C-C2C	4.85	1.47	1.36
12	aB	933	CLA	C3C-C2C	4.85	1.47	1.36
12	cA	840	CLA	O2D-CGD	4.85	1.45	1.33
11	aA	801	CL0	CHB-C1B	4.84	1.47	1.39
12	cB	933	CLA	C3C-C2C	4.84	1.47	1.36
12	aA	836	CLA	C3C-C2C	4.84	1.47	1.36
12	bA	824	CLA	C3C-C2C	4.84	1.47	1.36
13	bB	940	1L3	C06-C04	4.84	1.57	1.48
12	cA	825	CLA	O2D-CGD	4.84	1.45	1.33
12	cA	811	CLA	O2D-CGD	4.84	1.45	1.33
11	cA	801	CL0	CHB-C1B	4.84	1.47	1.39
12	bB	933	CLA	C3C-C2C	4.84	1.47	1.36
12	bA	808	CLA	O2D-CGD	4.84	1.45	1.33
12	aA	823	CLA	C3C-C2C	4.83	1.47	1.36
12	aA	840	CLA	O2D-CGD	4.83	1.45	1.33
11	cA	801	CL0	C3D-C2D	4.83	1.47	1.39
12	aA	822	CLA	O2D-CGD	4.83	1.45	1.33
12	bL	204	CLA	C3C-C2C	4.83	1.47	1.36
11	bA	801	CL0	CHB-C1B	4.83	1.47	1.39
12	aA	828	CLA	O2D-CGD	4.83	1.45	1.33
12	bA	828	CLA	O2D-CGD	4.83	1.45	1.33
12	bA	823	CLA	C3C-C2C	4.83	1.47	1.36
12	cL	204	CLA	C3C-C2C	4.83	1.47	1.36
12	cA	813	CLA	CHC-C1C	4.82	1.48	1.38
12	aA	826	CLA	C3C-C2C	4.82	1.47	1.36
12	cA	843	CLA	O2D-CGD	4.82	1.45	1.33
12	aA	843	CLA	O2D-CGD	4.82	1.45	1.33
12	aB	902	CLA	O2D-CGD	4.82	1.45	1.33
12	bA	835	CLA	O2D-CGD	4.82	1.45	1.33
13	cB	940	1L3	C06-C04	4.82	1.57	1.48
12	aA	813	CLA	CHC-C1C	4.82	1.48	1.38
12	cA	826	CLA	C3C-C2C	4.82	1.47	1.36
12	cA	841	CLA	C3C-C2C	4.82	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aB	906	CLA	C3C-C2C	4.82	1.47	1.36
12	cB	939	CLA	C3C-C2C	4.82	1.47	1.36
12	cF	202	CLA	C3C-C2C	4.82	1.47	1.36
12	bA	813	CLA	CHC-C1C	4.82	1.48	1.38
12	cA	824	CLA	C3C-C2C	4.82	1.47	1.36
12	aA	808	CLA	O2D-CGD	4.82	1.45	1.33
11	aA	801	CL0	C3D-C2D	4.82	1.47	1.39
12	bA	805	CLA	CHC-C1C	4.81	1.48	1.38
12	bA	843	CLA	O2D-CGD	4.81	1.45	1.33
12	bF	202	CLA	C3C-C2C	4.81	1.47	1.36
12	aF	202	CLA	C3C-C2C	4.81	1.47	1.36
12	cA	822	CLA	O2D-CGD	4.81	1.45	1.33
12	aA	844	CLA	C3C-C2C	4.81	1.47	1.36
12	cA	808	CLA	O2D-CGD	4.81	1.45	1.33
12	aB	928	CLA	C3C-C2C	4.80	1.47	1.36
12	cB	905	CLA	C3C-C2C	4.80	1.47	1.36
12	bB	907	CLA	C3C-C2C	4.80	1.47	1.36
12	cB	928	CLA	C3C-C2C	4.80	1.47	1.36
12	aL	204	CLA	C3C-C2C	4.80	1.47	1.36
12	aB	939	CLA	C3C-C2C	4.80	1.47	1.36
12	aA	841	CLA	O2D-CGD	4.80	1.45	1.33
12	bA	841	CLA	C3C-C2C	4.80	1.47	1.36
12	cB	906	CLA	O2D-CGD	4.80	1.45	1.33
12	aB	927	CLA	O2D-CGD	4.80	1.45	1.33
12	bB	919	CLA	C3C-C2C	4.80	1.47	1.36
12	aB	916	CLA	O2D-CGD	4.80	1.45	1.33
12	bB	927	CLA	O2D-CGD	4.80	1.45	1.33
12	bB	950	CLA	C3C-C2C	4.80	1.47	1.36
12	cA	818	CLA	C3C-C2C	4.80	1.47	1.36
12	cB	907	CLA	C3C-C2C	4.80	1.47	1.36
12	cA	828	CLA	O2D-CGD	4.79	1.45	1.33
12	aA	837	CLA	C1B-NB	-4.79	1.31	1.37
12	bA	806	CLA	O2D-CGD	4.79	1.45	1.33
13	cA	844	1L3	C06-C04	4.79	1.57	1.48
12	cA	806	CLA	O2D-CGD	4.79	1.45	1.33
12	aA	824	CLA	C3C-C2C	4.79	1.47	1.36
12	aB	906	CLA	O2D-CGD	4.79	1.45	1.33
12	bA	826	CLA	C3C-C2C	4.79	1.47	1.36
12	cA	841	CLA	O2D-CGD	4.79	1.45	1.33
12	cA	817	CLA	O2D-CGD	4.79	1.45	1.33
12	aA	841	CLA	C3C-C2C	4.79	1.47	1.36
12	cB	902	CLA	O2D-CGD	4.79	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cB	916	CLA	O2D-CGD	4.79	1.45	1.33
12	cB	922	CLA	O2D-CGD	4.79	1.45	1.33
12	aB	919	CLA	C3C-C2C	4.78	1.47	1.36
12	bB	922	CLA	O2D-CGD	4.78	1.45	1.33
12	bA	841	CLA	O2D-CGD	4.78	1.45	1.33
12	cB	920	CLA	O2D-CGD	4.78	1.45	1.33
12	bB	905	CLA	C3C-C2C	4.78	1.47	1.36
12	aA	842	CLA	O2D-CGD	4.78	1.45	1.33
12	cA	820	CLA	O2D-CGD	4.78	1.45	1.33
12	bA	818	CLA	C3C-C2C	4.78	1.47	1.36
12	bB	928	CLA	C3C-C2C	4.78	1.47	1.36
13	aA	845	1L3	C06-C04	4.78	1.57	1.48
12	aB	922	CLA	O2D-CGD	4.77	1.45	1.33
12	bA	817	CLA	O2D-CGD	4.77	1.45	1.33
12	cA	835	CLA	O2D-CGD	4.77	1.45	1.33
12	bB	916	CLA	O2D-CGD	4.77	1.45	1.33
12	bB	916	CLA	CHC-C1C	4.77	1.48	1.38
12	bB	906	CLA	O2D-CGD	4.77	1.45	1.33
12	cB	927	CLA	O2D-CGD	4.77	1.45	1.33
12	cA	842	CLA	O2D-CGD	4.77	1.45	1.33
12	aB	905	CLA	C3C-C2C	4.77	1.47	1.36
12	bA	822	CLA	CHC-C1C	4.77	1.48	1.38
12	aA	818	CLA	C3C-C2C	4.77	1.47	1.36
12	aA	832	CLA	O2D-CGD	4.77	1.45	1.33
12	bA	842	CLA	O2D-CGD	4.77	1.45	1.33
12	aB	907	CLA	C3C-C2C	4.77	1.47	1.36
12	cB	907	CLA	O2D-CGD	4.77	1.44	1.33
12	cA	825	CLA	CHC-C1C	4.77	1.48	1.38
12	aB	950	CLA	C3C-C2C	4.77	1.47	1.36
13	bA	844	1L3	C06-C04	4.76	1.57	1.48
12	aA	806	CLA	O2D-CGD	4.76	1.44	1.33
12	aA	820	CLA	O2D-CGD	4.76	1.44	1.33
12	bB	918	CLA	C1B-NB	-4.76	1.31	1.37
12	bA	820	CLA	O2D-CGD	4.76	1.44	1.33
12	bB	902	CLA	O2D-CGD	4.76	1.44	1.33
12	aA	835	CLA	O2D-CGD	4.76	1.44	1.33
12	cB	918	CLA	C1B-NB	-4.76	1.31	1.37
12	aA	825	CLA	CHC-C1C	4.76	1.48	1.38
12	aB	920	CLA	O2D-CGD	4.76	1.44	1.33
12	aA	803	CLA	C3C-C2C	4.76	1.47	1.36
12	bA	837	CLA	C1B-NB	-4.75	1.31	1.37
12	bB	920	CLA	O2D-CGD	4.75	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aA	805	CLA	CHC-C1C	4.75	1.48	1.38
12	cA	805	CLA	CHC-C1C	4.75	1.48	1.38
12	cB	919	CLA	C3C-C2C	4.75	1.47	1.36
12	aB	916	CLA	CHC-C1C	4.75	1.48	1.38
12	aB	916	CLA	C3C-C2C	4.75	1.47	1.36
12	aA	812	CLA	O2D-CGD	4.75	1.44	1.33
12	bB	907	CLA	O2D-CGD	4.75	1.44	1.33
12	aB	907	CLA	O2D-CGD	4.75	1.44	1.33
12	bA	817	CLA	CHC-C1C	4.75	1.48	1.38
12	bB	911	CLA	O2D-CGD	4.75	1.44	1.33
12	bA	823	CLA	O2D-CGD	4.74	1.44	1.33
12	cA	803	CLA	C3C-C2C	4.74	1.47	1.36
12	aA	810	CLA	O2D-CGD	4.74	1.44	1.33
12	bB	919	CLA	O2D-CGD	4.74	1.44	1.33
12	cB	916	CLA	C3C-C2C	4.74	1.47	1.36
12	aA	823	CLA	O2D-CGD	4.74	1.44	1.33
12	cA	812	CLA	C3C-C2C	4.74	1.47	1.36
12	aA	817	CLA	O2D-CGD	4.74	1.44	1.33
12	bA	803	CLA	C3C-C2C	4.74	1.47	1.36
12	bA	812	CLA	C3C-C2C	4.74	1.47	1.36
12	bB	916	CLA	C3C-C2C	4.74	1.47	1.36
12	aA	812	CLA	C3C-C2C	4.74	1.47	1.36
12	bA	810	CLA	O2D-CGD	4.73	1.44	1.33
12	bA	825	CLA	CHC-C1C	4.73	1.48	1.38
12	bA	812	CLA	O2D-CGD	4.73	1.44	1.33
12	cB	919	CLA	CHC-C1C	4.73	1.48	1.38
12	cB	916	CLA	CHC-C1C	4.73	1.48	1.38
12	aB	919	CLA	CHC-C1C	4.73	1.48	1.38
12	cA	823	CLA	O2D-CGD	4.72	1.44	1.33
12	cA	810	CLA	O2D-CGD	4.72	1.44	1.33
12	cA	832	CLA	O2D-CGD	4.72	1.44	1.33
12	aB	911	CLA	O2D-CGD	4.72	1.44	1.33
12	aB	919	CLA	O2D-CGD	4.72	1.44	1.33
12	bA	832	CLA	O2D-CGD	4.72	1.44	1.33
12	cB	919	CLA	O2D-CGD	4.72	1.44	1.33
12	bB	908	CLA	O2D-CGD	4.72	1.44	1.33
12	bB	903	CLA	C3C-C2C	4.71	1.46	1.36
12	aB	911	CLA	C3C-C2C	4.71	1.46	1.36
12	bB	923	CLA	CHC-C1C	4.71	1.47	1.38
12	aB	918	CLA	O2D-CGD	4.71	1.44	1.33
12	aA	814	CLA	C3C-C2C	4.71	1.46	1.36
12	bB	919	CLA	CHC-C1C	4.71	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cA	822	CLA	CHC-C1C	4.71	1.47	1.38
12	bA	826	CLA	O2D-CGD	4.71	1.44	1.33
12	aB	903	CLA	C3C-C2C	4.71	1.46	1.36
12	aA	820	CLA	O2A-CGA	4.71	1.47	1.33
12	cA	820	CLA	O2A-CGA	4.71	1.47	1.33
12	cB	908	CLA	O2D-CGD	4.71	1.44	1.33
12	cA	837	CLA	C1B-NB	-4.71	1.31	1.37
12	cB	903	CLA	C3C-C2C	4.71	1.46	1.36
12	aA	826	CLA	O2D-CGD	4.70	1.44	1.33
12	bA	805	CLA	O2D-CGD	4.70	1.44	1.33
12	bL	204	CLA	CHC-C1C	4.70	1.47	1.38
12	cB	911	CLA	O2D-CGD	4.70	1.44	1.33
12	cB	918	CLA	O2D-CGD	4.70	1.44	1.33
12	bB	911	CLA	C3C-C2C	4.70	1.46	1.36
12	aB	908	CLA	O2D-CGD	4.70	1.44	1.33
12	cB	923	CLA	CHC-C1C	4.70	1.47	1.38
12	bB	910	CLA	O2A-CGA	4.70	1.46	1.30
12	cB	911	CLA	C3C-C2C	4.70	1.46	1.36
12	aB	910	CLA	O2A-CGA	4.70	1.46	1.30
12	cA	817	CLA	CHC-C1C	4.70	1.47	1.38
12	bB	918	CLA	O2D-CGD	4.70	1.44	1.33
12	cA	812	CLA	O2D-CGD	4.70	1.44	1.33
12	aB	923	CLA	CHC-C1C	4.69	1.47	1.38
12	bB	934	CLA	CHC-C1C	4.69	1.47	1.38
12	cA	826	CLA	O2D-CGD	4.69	1.44	1.33
12	bA	814	CLA	C3C-C2C	4.69	1.46	1.36
12	aA	806	CLA	C3C-C2C	4.69	1.46	1.36
12	cL	204	CLA	CHC-C1C	4.69	1.47	1.38
12	cB	910	CLA	O2A-CGA	4.69	1.46	1.30
12	aA	805	CLA	O2D-CGD	4.69	1.44	1.33
12	bA	820	CLA	O2A-CGA	4.69	1.47	1.33
12	cB	934	CLA	CHC-C1C	4.69	1.47	1.38
12	aA	822	CLA	CHC-C1C	4.68	1.47	1.38
12	aB	934	CLA	CHC-C1C	4.68	1.47	1.38
12	aB	901	CLA	C3C-C2C	4.68	1.46	1.36
12	cB	926	CLA	O2D-CGD	4.68	1.44	1.33
12	aB	929	CLA	O2A-CGA	4.67	1.46	1.30
12	aA	817	CLA	O2A-CGA	4.67	1.47	1.33
12	cA	831	CLA	O2D-CGD	4.67	1.44	1.33
12	aA	813	CLA	O2D-CGD	4.67	1.44	1.33
12	bA	831	CLA	CHC-C1C	4.67	1.47	1.38
12	bA	831	CLA	O2D-CGD	4.67	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aA	817	CLA	CHC-C1C	4.67	1.47	1.38
12	cA	805	CLA	O2D-CGD	4.67	1.44	1.33
12	cB	923	CLA	O2D-CGD	4.67	1.44	1.33
12	cA	831	CLA	CHC-C1C	4.67	1.47	1.38
12	cB	929	CLA	O2A-CGA	4.67	1.46	1.30
12	cA	817	CLA	O2A-CGA	4.66	1.46	1.33
12	bB	926	CLA	C3C-C2C	4.66	1.46	1.36
12	bB	929	CLA	O2A-CGA	4.66	1.46	1.30
12	aL	204	CLA	CHC-C1C	4.66	1.47	1.38
12	cA	806	CLA	C3C-C2C	4.66	1.46	1.36
12	cB	901	CLA	C3C-C2C	4.65	1.46	1.36
12	cA	814	CLA	C3C-C2C	4.65	1.46	1.36
12	bB	909	CLA	C3C-C2C	4.65	1.46	1.36
12	bB	926	CLA	O2D-CGD	4.65	1.44	1.33
12	aA	804	CLA	O2D-CGD	4.65	1.44	1.33
12	cB	926	CLA	C3C-C2C	4.65	1.46	1.36
12	aA	831	CLA	O2D-CGD	4.65	1.44	1.33
12	aB	904	CLA	C3C-C2C	4.65	1.46	1.36
12	aA	804	CLA	O2A-CGA	4.65	1.46	1.33
12	cA	804	CLA	O2A-CGA	4.64	1.46	1.33
12	bB	949	CLA	CHC-C1C	4.64	1.47	1.38
12	aB	926	CLA	O2D-CGD	4.64	1.44	1.33
12	bA	817	CLA	O2A-CGA	4.64	1.46	1.33
12	aB	926	CLA	C3C-C2C	4.64	1.46	1.36
12	aB	923	CLA	O2D-CGD	4.64	1.44	1.33
12	cB	909	CLA	C3C-C2C	4.64	1.46	1.36
12	cA	804	CLA	O2D-CGD	4.64	1.44	1.33
12	bA	806	CLA	C3C-C2C	4.64	1.46	1.36
12	cA	841	CLA	CHC-C1C	4.64	1.47	1.38
12	cB	904	CLA	C3C-C2C	4.64	1.46	1.36
12	bB	921	CLA	O2D-CGD	4.64	1.44	1.33
12	bA	807	CLA	C1D-ND	4.64	1.44	1.37
12	bA	827	CLA	O2D-CGD	4.64	1.44	1.33
12	bA	841	CLA	CHC-C1C	4.63	1.47	1.38
12	bA	813	CLA	O2D-CGD	4.63	1.44	1.33
12	aA	827	CLA	O2D-CGD	4.63	1.44	1.33
12	bB	904	CLA	C3C-C2C	4.63	1.46	1.36
12	bB	920	CLA	O2A-CGA	4.63	1.46	1.30
12	aB	950	CLA	O2A-CGA	4.63	1.46	1.30
12	aB	909	CLA	C3C-C2C	4.62	1.46	1.36
12	aF	202	CLA	O2A-CGA	4.62	1.46	1.30
12	aA	821	CLA	CHC-C1C	4.62	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aA	831	CLA	CHC-C1C	4.62	1.47	1.38
12	bB	901	CLA	C3C-C2C	4.62	1.46	1.36
12	cB	932	CLA	O2D-CGD	4.62	1.44	1.33
12	aB	921	CLA	O2D-CGD	4.62	1.44	1.33
12	cA	821	CLA	CHC-C1C	4.62	1.47	1.38
12	cB	917	CLA	C3C-C2C	4.62	1.46	1.36
12	aA	844	CLA	O2A-CGA	4.62	1.46	1.30
12	bF	202	CLA	O2A-CGA	4.62	1.46	1.30
12	bA	804	CLA	O2A-CGA	4.62	1.46	1.33
12	cB	920	CLA	O2A-CGA	4.62	1.46	1.30
12	bA	836	CLA	O2A-CGA	4.61	1.46	1.30
12	cA	819	CLA	O2D-CGD	4.61	1.44	1.33
12	cB	939	CLA	O2A-CGA	4.61	1.46	1.30
12	cA	813	CLA	O2D-CGD	4.61	1.44	1.33
12	bB	923	CLA	O2D-CGD	4.61	1.44	1.33
12	bA	804	CLA	O2D-CGD	4.61	1.44	1.33
12	aB	939	CLA	O2A-CGA	4.61	1.46	1.30
12	bA	838	CLA	O2D-CGD	4.61	1.44	1.33
12	cB	921	CLA	O2D-CGD	4.61	1.44	1.33
12	cA	802	CLA	C1B-NB	-4.61	1.31	1.37
12	cA	810	CLA	O2A-CGA	4.61	1.46	1.30
12	bB	932	CLA	O2D-CGD	4.60	1.44	1.33
12	aB	922	CLA	CHC-C1C	4.60	1.47	1.38
12	bB	939	CLA	O2A-CGA	4.60	1.46	1.30
12	cF	202	CLA	O2A-CGA	4.60	1.46	1.30
12	cA	827	CLA	O2D-CGD	4.60	1.44	1.33
12	bB	950	CLA	O2A-CGA	4.60	1.46	1.30
12	bA	810	CLA	O2A-CGA	4.60	1.46	1.30
12	aB	920	CLA	O2A-CGA	4.60	1.46	1.30
12	cA	838	CLA	O2D-CGD	4.60	1.44	1.33
12	bB	917	CLA	C3C-C2C	4.60	1.46	1.36
12	cA	853	CLA	CHC-C1C	4.60	1.47	1.38
12	bA	819	CLA	O2D-CGD	4.60	1.44	1.33
12	cA	836	CLA	O2A-CGA	4.60	1.46	1.30
12	bB	934	CLA	C1D-ND	4.60	1.43	1.37
12	aB	917	CLA	C3C-C2C	4.60	1.46	1.36
12	aA	807	CLA	C1D-ND	4.60	1.43	1.37
12	aA	836	CLA	O2A-CGA	4.60	1.46	1.30
12	bA	821	CLA	CHC-C1C	4.59	1.47	1.38
12	bB	937	CLA	O2D-CGD	4.59	1.44	1.33
12	aA	810	CLA	O2A-CGA	4.59	1.46	1.30
12	aA	819	CLA	O2D-CGD	4.59	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aB	932	CLA	O2D-CGD	4.59	1.44	1.33
12	bA	811	CLA	O2A-CGA	4.59	1.46	1.30
12	aA	841	CLA	CHC-C1C	4.59	1.47	1.38
12	cB	922	CLA	CHC-C1C	4.59	1.47	1.38
12	aB	934	CLA	C1D-ND	4.59	1.43	1.37
12	aA	819	CLA	C1B-NB	-4.59	1.31	1.37
12	cA	819	CLA	C1B-NB	-4.59	1.31	1.37
12	aA	802	CLA	C1B-NB	-4.58	1.31	1.37
12	bB	930	CLA	O2D-CGD	4.58	1.44	1.33
12	cA	830	CLA	C1B-NB	-4.58	1.31	1.37
12	aA	834	CLA	O2D-CGD	4.58	1.44	1.33
12	cB	930	CLA	O2D-CGD	4.58	1.44	1.33
12	bA	815	CLA	O2A-CGA	4.58	1.46	1.30
12	bA	815	CLA	O2D-CGD	4.58	1.44	1.33
12	cL	204	CLA	O2A-CGA	4.58	1.46	1.30
12	aB	930	CLA	O2D-CGD	4.58	1.44	1.33
12	aA	815	CLA	O2A-CGA	4.58	1.45	1.30
12	aA	854	CLA	CHC-C1C	4.58	1.47	1.38
12	cB	949	CLA	CHC-C1C	4.57	1.47	1.38
12	aA	838	CLA	O2D-CGD	4.57	1.44	1.33
12	aA	827	CLA	CHC-C1C	4.57	1.47	1.38
12	cA	815	CLA	O2A-CGA	4.57	1.45	1.30
12	aA	815	CLA	O2D-CGD	4.57	1.44	1.33
12	cB	934	CLA	C1D-ND	4.56	1.43	1.37
12	bL	204	CLA	O2A-CGA	4.56	1.45	1.30
12	cA	811	CLA	O2A-CGA	4.56	1.45	1.30
12	aL	204	CLA	O2A-CGA	4.56	1.45	1.30
12	cB	937	CLA	O2D-CGD	4.56	1.44	1.33
12	aB	949	CLA	CHC-C1C	4.56	1.47	1.38
12	aB	937	CLA	O2D-CGD	4.56	1.44	1.33
12	cA	815	CLA	O2D-CGD	4.56	1.44	1.33
12	bB	921	CLA	CHC-C1C	4.56	1.47	1.38
12	aA	813	CLA	O2A-CGA	4.56	1.45	1.30
12	cA	813	CLA	O2A-CGA	4.56	1.45	1.30
12	bA	853	CLA	CHC-C1C	4.56	1.47	1.38
12	bA	802	CLA	C1B-NB	-4.56	1.31	1.37
12	bA	813	CLA	O2A-CGA	4.56	1.45	1.30
12	aB	930	CLA	CHC-C1C	4.56	1.47	1.38
12	bB	935	CLA	C1B-NB	-4.56	1.31	1.37
12	bB	937	CLA	CHC-C1C	4.56	1.47	1.38
12	bA	814	CLA	O2A-CGA	4.56	1.45	1.30
12	cA	834	CLA	O2D-CGD	4.55	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bB	922	CLA	CHC-C1C	4.55	1.47	1.38
12	aA	832	CLA	CHC-C1C	4.55	1.47	1.38
12	aA	808	CLA	C1D-ND	4.55	1.43	1.37
12	aB	921	CLA	CHC-C1C	4.55	1.47	1.38
12	aA	811	CLA	O2A-CGA	4.55	1.45	1.30
12	aB	904	CLA	O2D-CGD	4.55	1.44	1.33
12	cB	935	CLA	C1B-NB	-4.55	1.31	1.37
12	bA	815	CLA	CHC-C1C	4.55	1.47	1.38
12	cB	903	CLA	CHC-C1C	4.55	1.47	1.38
12	cA	807	CLA	C1D-ND	4.54	1.43	1.37
12	bA	832	CLA	CHC-C1C	4.54	1.47	1.38
12	aA	818	CLA	O2D-CGD	4.54	1.44	1.33
12	aA	803	CLA	O2D-CGD	4.54	1.44	1.33
12	bA	834	CLA	O2D-CGD	4.54	1.44	1.33
12	cB	930	CLA	CHC-C1C	4.54	1.47	1.38
12	bB	911	CLA	O2A-CGA	4.54	1.45	1.30
12	cL	202	CLA	CHC-C1C	4.54	1.47	1.38
12	aB	937	CLA	CHC-C1C	4.54	1.47	1.38
12	cB	937	CLA	CHC-C1C	4.54	1.47	1.38
12	cB	921	CLA	CHC-C1C	4.54	1.47	1.38
12	aA	814	CLA	O2A-CGA	4.54	1.45	1.30
12	aA	815	CLA	CHC-C1C	4.54	1.47	1.38
12	aA	807	CLA	C3C-C2C	4.54	1.46	1.36
12	cA	815	CLA	CHC-C1C	4.53	1.47	1.38
12	bL	202	CLA	CHC-C1C	4.53	1.47	1.38
12	cA	835	CLA	C1B-NB	-4.53	1.31	1.37
12	aB	914	CLA	O2A-CGA	4.53	1.45	1.30
12	cB	904	CLA	O2D-CGD	4.53	1.44	1.33
12	bB	930	CLA	CHC-C1C	4.53	1.47	1.38
12	cA	808	CLA	C1D-ND	4.53	1.43	1.37
12	cA	827	CLA	CHC-C1C	4.53	1.47	1.38
12	bA	803	CLA	O2D-CGD	4.53	1.44	1.33
12	bA	818	CLA	O2D-CGD	4.53	1.44	1.33
12	aL	203	CLA	CHC-C1C	4.52	1.47	1.38
12	cA	814	CLA	O2A-CGA	4.52	1.45	1.30
12	bA	827	CLA	CHC-C1C	4.52	1.47	1.38
12	bB	914	CLA	O2A-CGA	4.52	1.45	1.30
12	bB	934	CLA	O2A-CGA	4.52	1.45	1.30
12	cL	202	CLA	O2D-CGD	4.52	1.44	1.33
12	aL	202	CLA	CHC-C1C	4.52	1.47	1.38
12	cB	914	CLA	O2D-CGD	4.52	1.44	1.33
12	aB	911	CLA	O2A-CGA	4.52	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aL	202	CLA	O2D-CGD	4.52	1.44	1.33
12	cB	914	CLA	O2A-CGA	4.52	1.45	1.30
12	aA	835	CLA	C1B-NB	-4.52	1.31	1.37
12	cA	807	CLA	C3C-C2C	4.52	1.46	1.36
12	cA	832	CLA	CHC-C1C	4.52	1.47	1.38
12	aB	934	CLA	O2A-CGA	4.52	1.45	1.30
12	aB	935	CLA	C1B-NB	-4.52	1.31	1.37
12	bB	917	CLA	O2D-CGD	4.52	1.44	1.33
12	bA	830	CLA	C1B-NB	-4.51	1.31	1.37
12	bB	925	CLA	CHC-C1C	4.51	1.47	1.38
12	bA	807	CLA	C3C-C2C	4.51	1.46	1.36
12	bA	807	CLA	CHC-C1C	4.51	1.47	1.38
12	bB	904	CLA	O2D-CGD	4.51	1.44	1.33
12	cB	911	CLA	O2A-CGA	4.51	1.45	1.30
12	cA	803	CLA	O2D-CGD	4.51	1.44	1.33
12	bA	819	CLA	C1B-NB	-4.51	1.31	1.37
12	bB	908	CLA	C3C-C2C	4.51	1.46	1.36
12	bB	928	CLA	O2A-CGA	4.51	1.46	1.33
12	bA	808	CLA	C1D-ND	4.51	1.43	1.37
12	bL	202	CLA	O2D-CGD	4.51	1.44	1.33
12	cA	807	CLA	CHC-C1C	4.51	1.47	1.38
12	cB	928	CLA	O2A-CGA	4.51	1.46	1.33
12	cB	934	CLA	O2A-CGA	4.51	1.45	1.30
12	aB	925	CLA	CHC-C1C	4.51	1.47	1.38
12	aB	914	CLA	O2D-CGD	4.50	1.44	1.33
12	aB	904	CLA	C1B-NB	-4.50	1.31	1.37
12	aA	828	CLA	C1B-NB	-4.50	1.31	1.37
12	cB	909	CLA	O2D-CGD	4.50	1.44	1.33
12	aA	807	CLA	CHC-C1C	4.50	1.47	1.38
12	cA	818	CLA	O2D-CGD	4.50	1.44	1.33
12	bB	925	CLA	O2D-CGD	4.50	1.44	1.33
12	aB	909	CLA	O2D-CGD	4.50	1.44	1.33
12	cB	920	CLA	CHC-C1C	4.50	1.47	1.38
12	bA	828	CLA	C1B-NB	-4.50	1.32	1.37
12	bL	203	CLA	CHC-C1C	4.50	1.47	1.38
12	aB	925	CLA	O2D-CGD	4.50	1.44	1.33
12	bB	909	CLA	O2D-CGD	4.50	1.44	1.33
12	bB	914	CLA	O2D-CGD	4.49	1.44	1.33
12	cB	925	CLA	CHC-C1C	4.49	1.47	1.38
12	bB	922	CLA	O2A-CGA	4.49	1.45	1.30
12	bB	903	CLA	CHC-C1C	4.49	1.47	1.38
12	cB	908	CLA	C3C-C2C	4.49	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cB	933	CLA	O2A-CGA	4.49	1.45	1.30
12	cB	917	CLA	O2D-CGD	4.49	1.44	1.33
12	aB	926	CLA	C1B-NB	-4.49	1.32	1.37
12	bB	933	CLA	O2A-CGA	4.49	1.45	1.30
12	aF	202	CLA	CHC-C1C	4.49	1.47	1.38
12	cB	922	CLA	O2A-CGA	4.49	1.45	1.30
12	aB	903	CLA	CHC-C1C	4.49	1.47	1.38
12	aA	822	CLA	O2A-CGA	4.49	1.46	1.33
12	aB	908	CLA	C3C-C2C	4.49	1.46	1.36
12	aB	928	CLA	O2A-CGA	4.49	1.46	1.33
12	aB	934	CLA	CHD-C1D	4.49	1.47	1.38
12	aB	933	CLA	O2D-CGD	4.48	1.44	1.33
12	aB	906	CLA	CHC-C1C	4.48	1.47	1.38
12	bB	906	CLA	CHC-C1C	4.48	1.47	1.38
12	cL	203	CLA	CHC-C1C	4.48	1.47	1.38
12	bB	933	CLA	O2D-CGD	4.48	1.44	1.33
12	aL	203	CLA	O2D-CGD	4.48	1.44	1.33
12	aA	812	CLA	O2A-CGA	4.48	1.46	1.33
12	aB	936	CLA	O2D-CGD	4.48	1.44	1.33
12	bA	812	CLA	O2A-CGA	4.48	1.46	1.33
12	cA	822	CLA	O2A-CGA	4.48	1.46	1.33
12	aA	816	CLA	O2A-CGA	4.48	1.45	1.30
12	cB	906	CLA	CHC-C1C	4.47	1.47	1.38
12	aB	933	CLA	O2A-CGA	4.47	1.45	1.30
12	cB	904	CLA	C1B-NB	-4.47	1.32	1.37
12	aB	920	CLA	CHC-C1C	4.47	1.47	1.38
12	cA	812	CLA	O2A-CGA	4.47	1.46	1.33
12	bB	934	CLA	CHD-C1D	4.47	1.47	1.38
12	bL	203	CLA	O2D-CGD	4.47	1.44	1.33
12	bA	809	CLA	O2D-CGD	4.47	1.44	1.33
12	aB	922	CLA	O2A-CGA	4.47	1.45	1.30
12	aA	830	CLA	C1B-NB	-4.47	1.32	1.37
12	cF	202	CLA	CHC-C1C	4.46	1.47	1.38
12	aA	843	CLA	C3C-C2C	4.46	1.46	1.36
12	bL	203	CLA	O2A-CGA	4.46	1.45	1.30
12	aB	917	CLA	O2D-CGD	4.46	1.44	1.33
12	bA	835	CLA	C1B-NB	-4.46	1.32	1.37
12	aL	203	CLA	O2A-CGA	4.46	1.45	1.30
12	bA	822	CLA	O2A-CGA	4.46	1.46	1.33
12	bB	920	CLA	CHC-C1C	4.46	1.47	1.38
12	cB	936	CLA	O2D-CGD	4.46	1.44	1.33
12	bB	915	CLA	CHC-C1C	4.46	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cB	925	CLA	O2D-CGD	4.46	1.44	1.33
12	cA	816	CLA	O2A-CGA	4.46	1.45	1.30
12	cB	933	CLA	O2D-CGD	4.45	1.44	1.33
12	bB	904	CLA	C1B-NB	-4.45	1.32	1.37
12	bA	853	CLA	O2D-CGD	4.45	1.44	1.33
12	bB	924	CLA	O2D-CGD	4.45	1.44	1.33
12	bB	936	CLA	O2D-CGD	4.45	1.44	1.33
12	bA	835	CLA	O2A-CGA	4.45	1.45	1.30
12	cL	203	CLA	O2A-CGA	4.45	1.45	1.30
12	bF	202	CLA	CHC-C1C	4.45	1.47	1.38
12	bA	816	CLA	O2A-CGA	4.45	1.45	1.30
12	aB	924	CLA	O2D-CGD	4.45	1.44	1.33
12	bB	932	CLA	O2A-CGA	4.45	1.45	1.30
12	aB	932	CLA	O2A-CGA	4.45	1.45	1.30
12	aA	816	CLA	CHC-C1C	4.45	1.47	1.38
12	cA	805	CLA	O2A-CGA	4.44	1.46	1.33
12	cA	809	CLA	O2D-CGD	4.44	1.44	1.33
12	aA	805	CLA	O2A-CGA	4.44	1.46	1.33
12	cL	204	CLA	O2D-CGD	4.44	1.44	1.33
12	cA	835	CLA	O2A-CGA	4.44	1.45	1.30
12	bA	832	CLA	O2A-CGA	4.44	1.46	1.33
12	cA	835	CLA	CHC-C1C	4.44	1.47	1.38
12	aA	835	CLA	O2A-CGA	4.44	1.45	1.30
12	aA	854	CLA	O2D-CGD	4.44	1.44	1.33
12	cB	932	CLA	O2A-CGA	4.44	1.45	1.30
12	aA	815	CLA	C1D-ND	4.44	1.43	1.37
12	aA	832	CLA	O2A-CGA	4.44	1.46	1.33
12	cB	934	CLA	CHD-C1D	4.44	1.47	1.38
12	cA	832	CLA	O2A-CGA	4.44	1.46	1.33
12	bA	823	CLA	CHC-C1C	4.43	1.47	1.38
12	cA	828	CLA	C1B-NB	-4.43	1.32	1.37
12	aA	809	CLA	O2D-CGD	4.43	1.44	1.33
12	cA	814	CLA	O2D-CGD	4.43	1.44	1.33
12	aB	912	CLA	C1B-NB	-4.43	1.32	1.37
12	aL	204	CLA	O2D-CGD	4.43	1.44	1.33
12	aB	915	CLA	CHC-C1C	4.43	1.47	1.38
12	bA	816	CLA	CHC-C1C	4.43	1.47	1.38
12	cB	903	CLA	O2D-CGD	4.43	1.44	1.33
12	aA	823	CLA	CHC-C1C	4.43	1.47	1.38
12	cB	915	CLA	CHC-C1C	4.43	1.47	1.38
12	aA	814	CLA	O2D-CGD	4.43	1.44	1.33
12	bA	805	CLA	O2A-CGA	4.42	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aA	839	CLA	O2A-CGA	4.42	1.45	1.30
12	cB	924	CLA	O2D-CGD	4.42	1.44	1.33
12	aB	903	CLA	O2D-CGD	4.42	1.44	1.33
12	cL	203	CLA	O2D-CGD	4.42	1.44	1.33
12	cA	816	CLA	CHC-C1C	4.42	1.47	1.38
12	aA	836	CLA	C1D-ND	4.42	1.43	1.37
12	cA	853	CLA	O2D-CGD	4.42	1.44	1.33
12	bA	811	CLA	CHC-C1C	4.42	1.47	1.38
12	cB	912	CLA	C1B-NB	-4.42	1.32	1.37
12	bA	829	CLA	CHC-C1C	4.42	1.47	1.38
12	bA	835	CLA	CHC-C1C	4.42	1.47	1.38
12	bA	843	CLA	C3C-C2C	4.42	1.46	1.36
12	bA	814	CLA	O2D-CGD	4.41	1.44	1.33
12	cA	843	CLA	C3C-C2C	4.41	1.46	1.36
12	aA	820	CLA	CHC-C1C	4.41	1.47	1.38
12	bB	926	CLA	C1B-NB	-4.41	1.32	1.37
11	aA	801	CL0	O2D-CGD	4.41	1.44	1.33
12	aB	917	CLA	C1B-NB	-4.41	1.32	1.37
12	cB	905	CLA	CHC-C1C	4.41	1.47	1.38
12	cA	836	CLA	C1D-ND	4.41	1.43	1.37
13	bA	844	1L3	C11-C12	4.41	1.56	1.48
12	cB	926	CLA	CHC-C1C	4.41	1.47	1.38
12	cA	809	CLA	CHC-C1C	4.41	1.47	1.38
12	bB	905	CLA	CHC-C1C	4.41	1.47	1.38
11	bA	801	CL0	O2D-CGD	4.41	1.44	1.33
12	cA	839	CLA	O2A-CGA	4.40	1.45	1.30
12	bA	839	CLA	O2A-CGA	4.40	1.45	1.30
12	cB	914	CLA	CHC-C1C	4.40	1.47	1.38
12	cA	840	CLA	CHC-C1C	4.40	1.47	1.38
12	cA	811	CLA	CHC-C1C	4.40	1.47	1.38
12	bB	926	CLA	CHC-C1C	4.40	1.47	1.38
12	bA	809	CLA	CHC-C1C	4.40	1.47	1.38
12	cA	823	CLA	CHC-C1C	4.40	1.47	1.38
12	bA	840	CLA	CHC-C1C	4.40	1.47	1.38
12	aB	905	CLA	CHC-C1C	4.40	1.47	1.38
12	cA	829	CLA	CHC-C1C	4.40	1.47	1.38
12	bB	914	CLA	CHC-C1C	4.40	1.47	1.38
12	bB	912	CLA	C1B-NB	-4.40	1.32	1.37
12	bB	903	CLA	O2D-CGD	4.40	1.44	1.33
12	cB	926	CLA	C1B-NB	-4.40	1.32	1.37
12	aA	829	CLA	O2D-CGD	4.40	1.44	1.33
12	bL	204	CLA	O2D-CGD	4.40	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aA	829	CLA	CHC-C1C	4.40	1.47	1.38
12	cA	820	CLA	CHC-C1C	4.39	1.47	1.38
13	aA	845	1L3	C11-C12	4.39	1.56	1.48
12	cB	929	CLA	CHC-C1C	4.39	1.47	1.38
12	aA	840	CLA	CHC-C1C	4.39	1.47	1.38
12	aB	902	CLA	C3C-C2C	4.39	1.46	1.36
12	aA	817	CLA	C1D-ND	4.39	1.43	1.37
12	aA	839	CLA	O2D-CGD	4.39	1.44	1.33
12	bA	820	CLA	CHC-C1C	4.39	1.47	1.38
12	cA	802	CLA	O2D-CGD	4.39	1.44	1.33
12	aB	926	CLA	CHC-C1C	4.39	1.47	1.38
12	cA	810	CLA	CHC-C1C	4.39	1.47	1.38
12	cA	829	CLA	O2D-CGD	4.39	1.44	1.33
12	aA	809	CLA	CHC-C1C	4.39	1.47	1.38
12	cB	913	CLA	O2D-CGD	4.39	1.44	1.33
12	aA	835	CLA	CHC-C1C	4.39	1.47	1.38
12	cB	913	CLA	CHC-C1C	4.39	1.47	1.38
13	cA	844	1L3	C11-C12	4.39	1.56	1.48
12	bB	913	CLA	O2D-CGD	4.39	1.44	1.33
12	cB	910	CLA	C1B-NB	-4.39	1.32	1.37
11	cA	801	CL0	O2D-CGD	4.38	1.44	1.33
12	bA	836	CLA	C1D-ND	4.38	1.43	1.37
12	bB	932	CLA	CHC-C1C	4.38	1.47	1.38
12	aB	929	CLA	CHC-C1C	4.38	1.47	1.38
12	bA	815	CLA	C1D-ND	4.38	1.43	1.37
12	aA	810	CLA	CHC-C1C	4.38	1.47	1.38
12	aA	802	CLA	O2D-CGD	4.38	1.44	1.33
12	bA	810	CLA	CHC-C1C	4.38	1.47	1.38
12	bB	917	CLA	C1B-NB	-4.38	1.32	1.37
12	bB	929	CLA	CHC-C1C	4.37	1.47	1.38
12	cA	839	CLA	O2D-CGD	4.37	1.44	1.33
12	bA	836	CLA	CHD-C1D	4.37	1.46	1.38
12	bA	839	CLA	O2D-CGD	4.37	1.44	1.33
12	cB	902	CLA	C3C-C2C	4.37	1.46	1.36
12	cA	821	CLA	C1B-NB	-4.37	1.32	1.37
12	aA	838	CLA	CHC-C1C	4.37	1.47	1.38
12	aB	914	CLA	CHC-C1C	4.37	1.47	1.38
12	cB	917	CLA	C1B-NB	-4.37	1.32	1.37
12	cB	935	CLA	CHC-C1C	4.37	1.47	1.38
12	bB	935	CLA	CHC-C1C	4.37	1.47	1.38
12	bA	817	CLA	C1D-ND	4.36	1.43	1.37
12	bB	915	CLA	O2A-CGA	4.36	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bA	828	CLA	CHC-C1C	4.36	1.47	1.38
12	aA	811	CLA	CHC-C1C	4.36	1.47	1.38
12	cA	838	CLA	CHC-C1C	4.36	1.47	1.38
12	cB	938	CLA	O2A-CGA	4.36	1.46	1.33
12	aB	901	CLA	C1B-NB	-4.36	1.32	1.37
12	bB	936	CLA	CHC-C1C	4.36	1.47	1.38
12	bA	829	CLA	O2D-CGD	4.36	1.43	1.33
12	bB	924	CLA	C1B-NB	-4.36	1.32	1.37
12	bB	913	CLA	CHC-C1C	4.36	1.47	1.38
12	aB	913	CLA	O2D-CGD	4.36	1.43	1.33
12	aB	913	CLA	CHC-C1C	4.36	1.47	1.38
12	aB	938	CLA	O2A-CGA	4.36	1.46	1.33
12	aA	808	CLA	CHC-C1C	4.36	1.47	1.38
12	aB	932	CLA	CHC-C1C	4.36	1.47	1.38
12	cB	924	CLA	C1B-NB	-4.35	1.32	1.37
12	cB	915	CLA	O2A-CGA	4.35	1.46	1.33
12	bB	902	CLA	C3C-C2C	4.35	1.46	1.36
12	bA	802	CLA	O2D-CGD	4.35	1.43	1.33
12	aB	915	CLA	C1D-ND	4.35	1.43	1.37
12	aB	915	CLA	O2A-CGA	4.35	1.46	1.33
12	bB	938	CLA	O2A-CGA	4.34	1.46	1.33
12	cA	806	CLA	CHC-C1C	4.34	1.47	1.38
12	bA	808	CLA	CHC-C1C	4.34	1.47	1.38
12	cA	824	CLA	O2A-CGA	4.34	1.46	1.33
12	cA	815	CLA	C1D-ND	4.34	1.43	1.37
12	bB	910	CLA	C1B-NB	-4.34	1.32	1.37
12	aB	936	CLA	CHC-C1C	4.34	1.47	1.38
12	bA	824	CLA	O2A-CGA	4.34	1.46	1.33
12	bB	928	CLA	CHC-C1C	4.34	1.47	1.38
12	cB	936	CLA	CHC-C1C	4.34	1.47	1.38
12	bA	838	CLA	CHC-C1C	4.34	1.47	1.38
12	cA	828	CLA	CHC-C1C	4.34	1.47	1.38
12	cA	808	CLA	CHC-C1C	4.34	1.47	1.38
12	cA	802	CLA	CHC-C1C	4.33	1.47	1.38
12	cA	836	CLA	CHD-C1D	4.33	1.46	1.38
12	bA	821	CLA	C1B-NB	-4.33	1.32	1.37
12	bA	802	CLA	O2A-CGA	4.33	1.46	1.33
12	aB	928	CLA	CHC-C1C	4.33	1.47	1.38
12	aA	802	CLA	O2A-CGA	4.33	1.46	1.33
12	aA	802	CLA	CHC-C1C	4.33	1.47	1.38
12	aA	842	CLA	O2A-CGA	4.33	1.46	1.33
12	aA	824	CLA	O2A-CGA	4.33	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aB	930	CLA	O2A-CGA	4.33	1.46	1.33
12	cB	930	CLA	O2A-CGA	4.33	1.46	1.33
12	bA	826	CLA	CHC-C1C	4.33	1.47	1.38
12	aL	204	CLA	C1D-ND	4.33	1.43	1.37
12	cB	932	CLA	CHC-C1C	4.33	1.47	1.38
12	aB	935	CLA	CHC-C1C	4.32	1.47	1.38
12	cA	803	CLA	CHC-C1C	4.32	1.47	1.38
12	bB	930	CLA	O2A-CGA	4.32	1.46	1.33
12	aA	828	CLA	CHC-C1C	4.32	1.47	1.38
12	bA	833	CLA	O2D-CGD	4.32	1.43	1.33
12	cA	842	CLA	O2A-CGA	4.32	1.45	1.33
12	cA	819	CLA	CHC-C1C	4.32	1.47	1.38
12	cA	833	CLA	O2D-CGD	4.32	1.43	1.33
12	bB	915	CLA	C1D-ND	4.32	1.43	1.37
12	cL	204	CLA	C1D-ND	4.32	1.43	1.37
12	cA	826	CLA	CHC-C1C	4.31	1.47	1.38
12	cA	802	CLA	O2A-CGA	4.31	1.45	1.33
12	aA	821	CLA	C1B-NB	-4.31	1.32	1.37
12	cB	906	CLA	C1B-NB	-4.31	1.32	1.37
12	bB	921	CLA	O2A-CGA	4.31	1.45	1.33
12	bA	842	CLA	O2A-CGA	4.31	1.45	1.33
12	aA	826	CLA	CHC-C1C	4.31	1.47	1.38
12	bA	802	CLA	CHC-C1C	4.31	1.47	1.38
12	aA	833	CLA	O2D-CGD	4.31	1.43	1.33
12	cA	817	CLA	C1D-ND	4.31	1.43	1.37
12	aA	819	CLA	CHC-C1C	4.31	1.47	1.38
12	bA	803	CLA	CHC-C1C	4.31	1.47	1.38
12	cB	924	CLA	CHC-C1C	4.30	1.47	1.38
12	cA	809	CLA	O2A-CGA	4.30	1.45	1.30
12	bB	924	CLA	CHC-C1C	4.30	1.47	1.38
12	aB	906	CLA	C1B-NB	-4.30	1.32	1.37
12	cB	928	CLA	CHC-C1C	4.30	1.47	1.38
12	cB	915	CLA	C1D-ND	4.30	1.43	1.37
12	bA	809	CLA	O2A-CGA	4.30	1.45	1.30
12	cB	901	CLA	C1B-NB	-4.30	1.32	1.37
12	cA	815	CLA	CHD-C1D	4.29	1.46	1.38
12	cB	927	CLA	O2A-CGA	4.29	1.45	1.33
12	aB	924	CLA	C1B-NB	-4.29	1.32	1.37
12	bL	204	CLA	C1D-ND	4.29	1.43	1.37
12	bA	804	CLA	CHC-C1C	4.29	1.47	1.38
12	bB	918	CLA	CHC-C1C	4.29	1.47	1.38
12	aA	818	CLA	CHC-C1C	4.29	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cB	921	CLA	C1D-ND	4.29	1.43	1.37
12	bA	818	CLA	CHC-C1C	4.29	1.47	1.38
12	bB	906	CLA	C1B-NB	-4.29	1.32	1.37
12	bA	814	CLA	C1B-NB	-4.29	1.32	1.37
12	cB	921	CLA	O2A-CGA	4.28	1.45	1.33
12	aB	924	CLA	CHC-C1C	4.28	1.47	1.38
12	bA	825	CLA	C1B-NB	-4.28	1.32	1.37
12	aA	836	CLA	CHD-C1D	4.28	1.46	1.38
12	bB	927	CLA	O2A-CGA	4.28	1.45	1.33
12	aA	809	CLA	O2A-CGA	4.28	1.45	1.30
12	aA	806	CLA	CHC-C1C	4.28	1.47	1.38
12	bB	901	CLA	C1B-NB	-4.28	1.32	1.37
12	aB	927	CLA	O2A-CGA	4.28	1.45	1.33
12	cB	926	CLA	O2A-CGA	4.28	1.45	1.33
12	cA	814	CLA	C1B-NB	-4.28	1.32	1.37
12	cB	904	CLA	CHC-C1C	4.28	1.47	1.38
12	aB	906	CLA	O2A-CGA	4.27	1.45	1.33
12	cA	825	CLA	C1B-NB	-4.27	1.32	1.37
12	bB	921	CLA	C1D-ND	4.27	1.43	1.37
12	bB	910	CLA	CHC-C1C	4.27	1.47	1.38
12	aB	921	CLA	O2A-CGA	4.27	1.45	1.33
12	bA	806	CLA	CHC-C1C	4.27	1.47	1.38
12	cB	906	CLA	O2A-CGA	4.27	1.45	1.33
12	aA	814	CLA	C1B-NB	-4.27	1.32	1.37
12	aB	910	CLA	C1B-NB	-4.27	1.32	1.37
12	aB	926	CLA	O2A-CGA	4.26	1.45	1.33
12	cB	910	CLA	CHC-C1C	4.26	1.47	1.38
12	cA	804	CLA	CHC-C1C	4.26	1.47	1.38
12	cA	818	CLA	CHC-C1C	4.26	1.47	1.38
12	aA	804	CLA	CHC-C1C	4.26	1.47	1.38
12	bB	926	CLA	O2A-CGA	4.26	1.45	1.33
12	aB	921	CLA	C1D-ND	4.26	1.43	1.37
12	cA	841	CLA	O2A-CGA	4.26	1.45	1.33
12	bA	819	CLA	CHC-C1C	4.26	1.47	1.38
12	bB	904	CLA	CHC-C1C	4.26	1.47	1.38
12	aA	803	CLA	CHC-C1C	4.26	1.47	1.38
12	aA	825	CLA	C1B-NB	-4.26	1.32	1.37
12	bA	815	CLA	CHD-C1D	4.26	1.46	1.38
12	aA	815	CLA	CHD-C1D	4.25	1.46	1.38
12	aB	904	CLA	CHC-C1C	4.25	1.47	1.38
12	bB	903	CLA	O2A-CGA	4.25	1.45	1.33
12	bA	841	CLA	O2A-CGA	4.25	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aB	911	CLA	CHC-C1C	4.25	1.47	1.38
12	cB	903	CLA	O2A-CGA	4.25	1.45	1.33
12	cB	937	CLA	C1D-ND	4.25	1.43	1.37
12	cB	934	CLA	C1B-NB	-4.25	1.32	1.37
12	aB	901	CLA	CHC-C1C	4.24	1.47	1.38
12	cB	918	CLA	CHC-C1C	4.24	1.47	1.38
12	bB	908	CLA	O2A-CGA	4.24	1.45	1.33
12	aB	908	CLA	O2A-CGA	4.24	1.45	1.33
12	bB	906	CLA	O2A-CGA	4.24	1.45	1.33
12	aB	914	CLA	C1D-ND	4.24	1.43	1.37
12	aB	917	CLA	CHC-C1C	4.24	1.47	1.38
12	aB	910	CLA	CHC-C1C	4.24	1.47	1.38
12	bA	828	CLA	O2A-CGA	4.24	1.45	1.33
12	bB	911	CLA	CHC-C1C	4.24	1.47	1.38
12	aA	841	CLA	O2A-CGA	4.23	1.45	1.33
12	cB	913	CLA	O2A-CGA	4.23	1.45	1.33
12	aB	918	CLA	CHC-C1C	4.23	1.47	1.38
12	aA	828	CLA	O2A-CGA	4.23	1.45	1.33
12	aB	913	CLA	O2A-CGA	4.23	1.45	1.33
12	cB	908	CLA	O2A-CGA	4.22	1.45	1.33
12	cA	843	CLA	C1B-NB	-4.22	1.32	1.37
12	cB	914	CLA	C1D-ND	4.22	1.43	1.37
12	bA	811	CLA	C1D-ND	4.22	1.43	1.37
12	aA	823	CLA	O2A-CGA	4.22	1.45	1.33
12	bB	913	CLA	O2A-CGA	4.22	1.45	1.33
12	aB	934	CLA	C1B-NB	-4.22	1.32	1.37
12	bB	919	CLA	O2A-CGA	4.22	1.45	1.33
12	bB	937	CLA	C1D-ND	4.22	1.43	1.37
12	aB	912	CLA	O2D-CGD	4.22	1.43	1.33
12	aB	919	CLA	O2A-CGA	4.22	1.45	1.33
12	cB	919	CLA	O2A-CGA	4.22	1.45	1.33
12	cL	202	CLA	CHD-C1D	4.22	1.46	1.38
12	cA	828	CLA	O2A-CGA	4.22	1.45	1.33
12	cA	831	CLA	O2A-CGA	4.22	1.45	1.33
12	cB	912	CLA	O2D-CGD	4.22	1.43	1.33
12	aB	937	CLA	C1D-ND	4.22	1.43	1.37
12	aA	808	CLA	CHD-C1D	4.21	1.46	1.38
12	cA	806	CLA	O2A-CGA	4.21	1.45	1.33
12	bA	843	CLA	C1B-NB	-4.21	1.32	1.37
12	aB	903	CLA	O2A-CGA	4.21	1.45	1.33
12	bB	901	CLA	CHC-C1C	4.21	1.46	1.38
12	aA	844	CLA	CHC-C1C	4.21	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bB	950	CLA	CHC-C1C	4.21	1.46	1.38
12	aA	831	CLA	O2A-CGA	4.21	1.45	1.33
12	cB	911	CLA	CHC-C1C	4.21	1.46	1.38
12	aA	806	CLA	O2A-CGA	4.21	1.45	1.33
12	cA	823	CLA	O2A-CGA	4.21	1.45	1.33
12	bB	914	CLA	C1D-ND	4.20	1.43	1.37
12	aB	950	CLA	CHC-C1C	4.20	1.46	1.38
12	cA	821	CLA	O2A-CGA	4.20	1.45	1.33
12	cB	917	CLA	CHC-C1C	4.20	1.46	1.38
12	aA	834	CLA	O2A-CGA	4.20	1.45	1.33
12	bA	823	CLA	O2A-CGA	4.20	1.45	1.33
12	bB	917	CLA	CHC-C1C	4.20	1.46	1.38
12	bA	831	CLA	O2A-CGA	4.20	1.45	1.33
12	cA	808	CLA	CHD-C1D	4.20	1.46	1.38
12	bA	834	CLA	O2A-CGA	4.20	1.45	1.33
12	cB	901	CLA	CHC-C1C	4.20	1.46	1.38
12	cB	902	CLA	CHC-C1C	4.20	1.46	1.38
12	bB	902	CLA	CHC-C1C	4.19	1.46	1.38
12	bA	821	CLA	O2A-CGA	4.19	1.45	1.33
12	bA	834	CLA	C4B-NB	-4.19	1.32	1.37
12	cA	834	CLA	C4B-NB	-4.19	1.32	1.37
12	aA	821	CLA	O2A-CGA	4.19	1.45	1.33
12	bB	920	CLA	C1D-ND	4.19	1.43	1.37
12	bB	912	CLA	O2D-CGD	4.19	1.43	1.33
12	cA	811	CLA	C1B-NB	-4.19	1.32	1.37
12	cA	834	CLA	O2A-CGA	4.19	1.45	1.33
12	bB	931	CLA	C1B-NB	-4.19	1.32	1.37
12	aA	803	CLA	O2A-CGA	4.19	1.45	1.33
12	bA	806	CLA	O2A-CGA	4.19	1.45	1.33
12	cA	803	CLA	O2A-CGA	4.19	1.45	1.33
12	bA	839	CLA	C1B-NB	-4.18	1.32	1.37
12	aA	837	CLA	CHC-C1C	4.18	1.46	1.38
12	aA	811	CLA	C1B-NB	-4.18	1.32	1.37
12	aA	843	CLA	C1B-NB	-4.18	1.32	1.37
12	bA	830	CLA	O2D-CGD	4.18	1.43	1.33
12	aA	830	CLA	O2D-CGD	4.18	1.43	1.33
12	bA	803	CLA	O2A-CGA	4.18	1.45	1.33
12	bA	808	CLA	CHD-C1D	4.18	1.46	1.38
12	aB	930	CLA	C1D-ND	4.18	1.43	1.37
12	aB	902	CLA	CHC-C1C	4.18	1.46	1.38
12	cA	830	CLA	O2D-CGD	4.18	1.43	1.33
11	aA	801	CL0	CHC-C4B	4.17	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aA	830	CLA	CHC-C1C	4.17	1.46	1.38
12	bL	202	CLA	CHD-C1D	4.17	1.46	1.38
12	bB	921	CLA	CHD-C1D	4.17	1.46	1.38
12	aB	920	CLA	C1D-ND	4.17	1.43	1.37
12	aL	203	CLA	C1B-NB	-4.17	1.32	1.37
12	bB	927	CLA	CHC-C1C	4.17	1.46	1.38
12	cL	203	CLA	C1B-NB	-4.17	1.32	1.37
12	bB	934	CLA	C1B-NB	-4.17	1.32	1.37
11	bA	801	CL0	CHC-C4B	4.17	1.46	1.39
12	aA	833	CLA	C1B-NB	-4.17	1.32	1.37
12	aA	811	CLA	C1D-ND	4.17	1.43	1.37
12	cA	833	CLA	C1B-NB	-4.17	1.32	1.37
12	cA	811	CLA	C1D-ND	4.16	1.43	1.37
12	cB	937	CLA	O2A-CGA	4.16	1.45	1.33
12	cA	811	CLA	CHD-C1D	4.16	1.46	1.38
12	bA	830	CLA	CHC-C1C	4.16	1.46	1.38
12	aB	901	CLA	O2D-CGD	4.16	1.43	1.33
12	cA	826	CLA	O2A-CGA	4.16	1.45	1.33
12	cA	830	CLA	CHC-C1C	4.16	1.46	1.38
12	cA	837	CLA	CHC-C1C	4.16	1.46	1.38
12	bB	936	CLA	C1D-ND	4.16	1.43	1.37
12	aA	834	CLA	C4B-NB	-4.16	1.32	1.37
12	cB	920	CLA	C1D-ND	4.16	1.43	1.37
12	aB	902	CLA	O2A-CGA	4.15	1.45	1.33
11	cA	801	CL0	CHC-C4B	4.15	1.46	1.39
12	cB	921	CLA	CHD-C1D	4.15	1.46	1.38
12	cB	931	CLA	O2D-CGD	4.15	1.43	1.33
12	cB	927	CLA	C4B-NB	-4.15	1.32	1.37
12	bA	833	CLA	CHC-C1C	4.15	1.46	1.38
12	aB	936	CLA	C1D-ND	4.15	1.43	1.37
12	cB	931	CLA	C1B-NB	-4.15	1.32	1.37
12	aL	202	CLA	CHD-C1D	4.15	1.46	1.38
12	aA	826	CLA	O2A-CGA	4.15	1.45	1.33
12	bB	901	CLA	O2D-CGD	4.15	1.43	1.33
12	aA	839	CLA	C1B-NB	-4.15	1.32	1.37
12	aB	921	CLA	CHD-C1D	4.15	1.46	1.38
12	bB	930	CLA	C1D-ND	4.15	1.43	1.37
12	aB	927	CLA	CHC-C1C	4.15	1.46	1.38
12	bA	837	CLA	CHC-C1C	4.15	1.46	1.38
12	cB	902	CLA	O2A-CGA	4.15	1.45	1.33
12	aA	807	CLA	C1B-NB	-4.15	1.32	1.37
12	bA	827	CLA	O2A-CGA	4.14	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bB	937	CLA	O2A-CGA	4.14	1.45	1.33
12	aB	931	CLA	C1B-NB	-4.14	1.32	1.37
12	cB	901	CLA	O2D-CGD	4.14	1.43	1.33
12	aB	937	CLA	O2A-CGA	4.14	1.45	1.33
12	cL	202	CLA	O2A-CGA	4.14	1.45	1.33
12	bA	807	CLA	C1B-NB	-4.14	1.32	1.37
12	cA	827	CLA	O2A-CGA	4.14	1.45	1.33
12	cA	829	CLA	C1B-NB	-4.14	1.32	1.37
12	aB	931	CLA	O2D-CGD	4.13	1.43	1.33
12	bA	826	CLA	O2A-CGA	4.13	1.45	1.33
12	bB	902	CLA	O2A-CGA	4.13	1.45	1.33
12	cA	825	CLA	C1D-ND	4.13	1.43	1.37
12	cB	936	CLA	C1D-ND	4.13	1.43	1.37
12	bB	912	CLA	CHC-C1C	4.13	1.46	1.38
12	bA	831	CLA	C1B-NB	-4.13	1.32	1.37
12	bA	833	CLA	C1B-NB	-4.13	1.32	1.37
12	bL	203	CLA	C1B-NB	-4.13	1.32	1.37
12	bB	938	CLA	CHC-C1C	4.13	1.46	1.38
12	aA	827	CLA	O2A-CGA	4.13	1.45	1.33
12	bB	931	CLA	O2D-CGD	4.13	1.43	1.33
12	bA	811	CLA	C1B-NB	-4.12	1.32	1.37
12	aA	833	CLA	CHC-C1C	4.12	1.46	1.38
12	aB	927	CLA	C4B-NB	-4.12	1.32	1.37
12	aB	912	CLA	CHC-C1C	4.12	1.46	1.38
12	cB	931	CLA	O2A-CGA	4.12	1.45	1.33
12	cA	807	CLA	C1B-NB	-4.12	1.32	1.37
12	cA	818	CLA	O2A-CGA	4.12	1.45	1.33
12	bA	829	CLA	C1B-NB	-4.12	1.32	1.37
12	cB	927	CLA	CHC-C1C	4.12	1.46	1.38
12	bL	202	CLA	O2A-CGA	4.11	1.45	1.33
12	bB	925	CLA	C1B-NB	-4.11	1.32	1.37
12	cB	912	CLA	CHC-C1C	4.11	1.46	1.38
12	aB	938	CLA	CHC-C1C	4.11	1.46	1.38
12	cB	925	CLA	C1D-ND	4.11	1.43	1.37
12	aA	818	CLA	O2A-CGA	4.11	1.45	1.33
12	aB	910	CLA	CHD-C1D	4.11	1.46	1.38
12	cB	910	CLA	CHD-C1D	4.11	1.46	1.38
12	bB	930	CLA	C1B-NB	-4.11	1.32	1.37
12	aL	202	CLA	O2A-CGA	4.11	1.45	1.33
12	bB	927	CLA	C4B-NB	-4.11	1.32	1.37
12	cB	930	CLA	C1D-ND	4.10	1.43	1.37
12	bA	811	CLA	CHD-C1D	4.10	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bB	925	CLA	C1D-ND	4.10	1.43	1.37
12	cA	834	CLA	CHD-C1D	4.10	1.46	1.38
12	aB	931	CLA	O2A-CGA	4.10	1.45	1.33
12	aA	836	CLA	CHC-C1C	4.10	1.46	1.38
12	bA	840	CLA	C1D-ND	4.10	1.43	1.37
11	cA	801	CL0	O2A-CGA	4.10	1.45	1.33
12	cA	833	CLA	CHC-C1C	4.10	1.46	1.38
12	bB	931	CLA	O2A-CGA	4.10	1.45	1.33
12	aB	902	CLA	C1B-NB	-4.10	1.32	1.37
12	bA	836	CLA	CHC-C1C	4.09	1.46	1.38
12	cA	839	CLA	C1B-NB	-4.09	1.32	1.37
12	aB	911	CLA	CHD-C1D	4.09	1.46	1.38
12	aA	811	CLA	CHD-C1D	4.09	1.46	1.38
12	aA	840	CLA	CHD-C1D	4.09	1.46	1.38
12	bA	818	CLA	O2A-CGA	4.09	1.45	1.33
12	aA	842	CLA	C1D-ND	4.08	1.43	1.37
12	aB	925	CLA	C1B-NB	-4.08	1.32	1.37
12	cB	930	CLA	C1B-NB	-4.08	1.32	1.37
12	bB	910	CLA	CHD-C1D	4.08	1.46	1.38
12	bA	837	CLA	O2A-CGA	4.08	1.45	1.33
12	bA	843	CLA	CHC-C1C	4.08	1.46	1.38
12	aA	831	CLA	C1B-NB	-4.08	1.32	1.37
12	bB	913	CLA	C1B-NB	-4.08	1.32	1.37
12	cB	938	CLA	CHC-C1C	4.08	1.46	1.38
12	bA	840	CLA	CHD-C1D	4.08	1.46	1.38
12	cA	840	CLA	CHD-C1D	4.07	1.46	1.38
12	aA	825	CLA	C1D-ND	4.07	1.43	1.37
12	cA	836	CLA	CHC-C1C	4.07	1.46	1.38
12	cB	925	CLA	O2A-CGA	4.07	1.45	1.33
11	aA	801	CL0	O2A-CGA	4.07	1.45	1.33
12	bA	808	CLA	O2A-CGA	4.07	1.45	1.33
12	aB	918	CLA	O2A-CGA	4.07	1.45	1.33
12	aA	840	CLA	C1D-ND	4.07	1.43	1.37
12	cA	823	CLA	C1D-ND	4.07	1.43	1.37
12	cB	918	CLA	O2A-CGA	4.07	1.45	1.33
12	cB	929	CLA	C1D-ND	4.07	1.43	1.37
12	cB	913	CLA	C1B-NB	-4.06	1.32	1.37
12	aA	808	CLA	O2A-CGA	4.06	1.45	1.33
12	bB	925	CLA	O2A-CGA	4.06	1.45	1.33
12	cA	831	CLA	C1B-NB	-4.06	1.32	1.37
12	bA	807	CLA	O2A-CGA	4.06	1.45	1.33
12	aA	823	CLA	C1D-ND	4.06	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cA	816	CLA	C1D-ND	4.06	1.43	1.37
11	bA	801	CL0	O2A-CGA	4.06	1.45	1.33
12	aA	834	CLA	C1B-NB	-4.06	1.32	1.37
12	aA	838	CLA	O2A-CGA	4.06	1.45	1.33
12	cA	838	CLA	O2A-CGA	4.06	1.45	1.33
12	bB	911	CLA	CHD-C1D	4.06	1.46	1.38
12	aA	816	CLA	C1D-ND	4.06	1.43	1.37
12	aB	930	CLA	C1B-NB	-4.06	1.32	1.37
12	bB	950	CLA	C1B-NB	-4.06	1.32	1.37
12	aA	837	CLA	O2A-CGA	4.06	1.45	1.33
12	bA	822	CLA	C1B-NB	-4.05	1.32	1.37
12	bA	823	CLA	C1D-ND	4.05	1.43	1.37
12	bB	902	CLA	C1B-NB	-4.05	1.32	1.37
12	cA	843	CLA	CHC-C1C	4.05	1.46	1.38
12	cA	853	CLA	C1B-NB	-4.05	1.32	1.37
12	aF	202	CLA	CHD-C1D	4.05	1.46	1.38
12	aB	925	CLA	C1D-ND	4.05	1.43	1.37
12	cA	822	CLA	C1B-NB	-4.05	1.32	1.37
12	aA	829	CLA	C1B-NB	-4.05	1.32	1.37
12	aB	925	CLA	O2A-CGA	4.05	1.45	1.33
12	aB	909	CLA	C1B-NB	-4.05	1.32	1.37
12	aB	950	CLA	C1B-NB	-4.04	1.32	1.37
12	bA	838	CLA	O2A-CGA	4.04	1.45	1.33
12	cB	902	CLA	C1B-NB	-4.04	1.32	1.37
12	aB	938	CLA	C1B-NB	-4.04	1.32	1.37
12	cB	922	CLA	C1B-NB	-4.04	1.32	1.37
12	bA	825	CLA	C1D-ND	4.04	1.43	1.37
12	bA	840	CLA	O2A-CGA	4.04	1.45	1.33
12	cB	911	CLA	CHD-C1D	4.04	1.46	1.38
12	bA	814	CLA	CHD-C1D	4.04	1.46	1.38
12	bB	918	CLA	O2A-CGA	4.04	1.45	1.33
12	aA	822	CLA	C1B-NB	-4.04	1.32	1.37
12	bB	917	CLA	O2A-CGA	4.04	1.45	1.33
12	cA	814	CLA	CHD-C1D	4.04	1.46	1.38
12	cA	808	CLA	O2A-CGA	4.04	1.45	1.33
12	aA	813	CLA	CHD-C1D	4.04	1.46	1.38
12	bF	202	CLA	CHD-C1D	4.04	1.46	1.38
12	cF	202	CLA	CHD-C1D	4.04	1.46	1.38
12	cA	840	CLA	C1D-ND	4.03	1.43	1.37
12	aA	840	CLA	O2A-CGA	4.03	1.45	1.33
12	bB	909	CLA	C1B-NB	-4.03	1.32	1.37
12	bA	834	CLA	CHD-C1D	4.03	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cB	938	CLA	CHD-C1D	4.03	1.46	1.38
12	aB	922	CLA	C1B-NB	-4.03	1.32	1.37
12	bB	929	CLA	C1D-ND	4.03	1.43	1.37
12	aA	843	CLA	CHC-C1C	4.03	1.46	1.38
12	aB	938	CLA	CHD-C1D	4.03	1.46	1.38
12	cA	813	CLA	CHD-C1D	4.03	1.46	1.38
12	cA	840	CLA	O2A-CGA	4.03	1.45	1.33
12	bB	938	CLA	CHD-C1D	4.03	1.46	1.38
12	aA	842	CLA	CHC-C1C	4.03	1.46	1.38
12	aB	917	CLA	O2A-CGA	4.02	1.45	1.33
12	aA	834	CLA	CHD-C1D	4.02	1.46	1.38
12	bB	935	CLA	O2D-CGD	4.02	1.43	1.33
12	cB	917	CLA	O2A-CGA	4.02	1.45	1.33
12	cB	932	CLA	CHD-C1D	4.02	1.46	1.38
12	bA	834	CLA	C1B-NB	-4.02	1.32	1.37
12	bB	934	CLA	CHD-C4C	4.02	1.48	1.39
12	cA	838	CLA	C1D-ND	4.02	1.43	1.37
12	cA	842	CLA	C1D-ND	4.02	1.43	1.37
12	cB	925	CLA	C1B-NB	-4.02	1.32	1.37
12	cA	837	CLA	O2A-CGA	4.02	1.45	1.33
12	aB	929	CLA	C1D-ND	4.02	1.43	1.37
12	cB	924	CLA	O2A-CGA	4.02	1.45	1.33
12	bA	812	CLA	CHC-C1C	4.02	1.46	1.38
12	aA	824	CLA	C1D-ND	4.02	1.43	1.37
12	bA	842	CLA	C1D-ND	4.02	1.43	1.37
12	aA	810	CLA	C1D-ND	4.02	1.43	1.37
12	aA	838	CLA	C1B-NB	-4.02	1.32	1.37
12	aA	812	CLA	CHC-C1C	4.02	1.46	1.38
12	bA	813	CLA	CHD-C1D	4.02	1.46	1.38
12	bA	816	CLA	C1D-ND	4.02	1.43	1.37
12	aA	844	CLA	C1B-NB	-4.01	1.32	1.37
12	cB	935	CLA	O2D-CGD	4.01	1.43	1.33
12	cA	822	CLA	C1D-ND	4.01	1.43	1.37
12	cA	824	CLA	CHC-C1C	4.01	1.46	1.38
12	aB	934	CLA	CHD-C4C	4.01	1.48	1.39
12	cA	807	CLA	O2A-CGA	4.01	1.45	1.33
12	aA	814	CLA	CHD-C1D	4.01	1.46	1.38
12	aA	834	CLA	CHC-C1C	4.01	1.46	1.38
12	aA	854	CLA	C1B-NB	-4.01	1.32	1.37
12	aB	935	CLA	O2D-CGD	4.01	1.43	1.33
12	bA	853	CLA	C1B-NB	-4.01	1.32	1.37
12	aA	822	CLA	C1D-ND	4.01	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cL	202	CLA	C1D-ND	4.01	1.43	1.37
12	cA	809	CLA	C1D-ND	4.01	1.43	1.37
12	cB	909	CLA	C1B-NB	-4.00	1.32	1.37
12	bB	932	CLA	CHD-C1D	4.00	1.46	1.38
12	aA	829	CLA	O2A-CGA	4.00	1.45	1.33
12	aB	932	CLA	CHD-C1D	4.00	1.46	1.38
12	bB	924	CLA	O2A-CGA	4.00	1.45	1.33
12	aA	838	CLA	C1D-ND	4.00	1.43	1.37
12	cA	824	CLA	C1D-ND	4.00	1.43	1.37
12	aA	807	CLA	O2A-CGA	4.00	1.45	1.33
12	cA	842	CLA	CHC-C1C	4.00	1.46	1.38
12	aB	924	CLA	O2A-CGA	4.00	1.45	1.33
12	aF	202	CLA	C1D-ND	4.00	1.43	1.37
12	cB	919	CLA	C1D-ND	4.00	1.43	1.37
12	aL	202	CLA	C1D-ND	4.00	1.43	1.37
12	bB	932	CLA	C1D-ND	4.00	1.43	1.37
12	bA	842	CLA	CHC-C1C	4.00	1.46	1.38
12	bB	915	CLA	CHD-C1D	3.99	1.46	1.38
12	aB	932	CLA	C1D-ND	3.99	1.43	1.37
12	cB	933	CLA	C1B-NB	-3.99	1.32	1.37
12	bF	202	CLA	C1D-ND	3.99	1.43	1.37
12	bA	834	CLA	CHC-C1C	3.99	1.46	1.38
12	cA	829	CLA	O2A-CGA	3.99	1.45	1.33
12	cA	834	CLA	CHC-C1C	3.99	1.46	1.38
12	cB	907	CLA	C1D-ND	3.99	1.43	1.37
12	aB	913	CLA	C1B-NB	-3.99	1.32	1.37
12	aB	908	CLA	CHD-C1D	3.99	1.46	1.38
12	cA	810	CLA	C1D-ND	3.99	1.43	1.37
12	bB	938	CLA	C1B-NB	-3.99	1.32	1.37
12	bL	204	CLA	CHD-C1D	3.99	1.46	1.38
12	bB	933	CLA	C1B-NB	-3.99	1.32	1.37
12	bA	824	CLA	C1D-ND	3.99	1.43	1.37
12	cA	813	CLA	C1B-NB	-3.99	1.32	1.37
12	cB	915	CLA	CHD-C1D	3.98	1.46	1.38
12	bA	813	CLA	C1B-NB	-3.98	1.32	1.37
12	cA	812	CLA	CHC-C1C	3.98	1.46	1.38
12	cA	833	CLA	O2A-CGA	3.98	1.45	1.33
12	cA	814	CLA	CHC-C1C	3.98	1.46	1.38
12	aB	935	CLA	O2A-CGA	3.98	1.44	1.33
12	cB	935	CLA	O2A-CGA	3.98	1.44	1.33
12	aB	919	CLA	C1D-ND	3.98	1.43	1.37
12	bB	919	CLA	C1D-ND	3.98	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bB	937	CLA	C1B-NB	-3.98	1.32	1.37
12	cB	934	CLA	CHD-C4C	3.98	1.48	1.39
12	aB	937	CLA	C1B-NB	-3.98	1.32	1.37
12	cA	820	CLA	C1D-ND	3.98	1.43	1.37
12	bA	809	CLA	C1D-ND	3.98	1.43	1.37
12	cB	932	CLA	C1D-ND	3.98	1.43	1.37
12	aB	905	CLA	O2A-CGA	3.98	1.44	1.33
12	cA	834	CLA	C1B-NB	-3.98	1.32	1.37
12	cB	937	CLA	C1B-NB	-3.98	1.32	1.37
12	cB	938	CLA	C1B-NB	-3.98	1.32	1.37
12	cB	905	CLA	O2A-CGA	3.97	1.44	1.33
12	bA	838	CLA	C1B-NB	-3.97	1.32	1.37
12	cF	202	CLA	C1D-ND	3.97	1.43	1.37
12	aA	824	CLA	CHC-C1C	3.97	1.46	1.38
12	cA	838	CLA	C1B-NB	-3.97	1.32	1.37
13	bB	940	1L3	C11-C12	3.97	1.55	1.48
12	aA	825	CLA	O2A-CGA	3.97	1.44	1.33
12	bB	935	CLA	O2A-CGA	3.97	1.44	1.33
12	cL	204	CLA	CHD-C1D	3.97	1.46	1.38
12	bB	928	CLA	O2D-CGD	3.97	1.43	1.33
12	aB	907	CLA	O2A-CGA	3.97	1.44	1.33
12	cA	832	CLA	CHD-C1D	3.97	1.46	1.38
12	bA	822	CLA	C1D-ND	3.97	1.43	1.37
12	bA	825	CLA	O2A-CGA	3.97	1.44	1.33
12	bA	824	CLA	C1B-NB	-3.97	1.32	1.37
12	bA	824	CLA	CHC-C1C	3.96	1.46	1.38
12	bA	829	CLA	O2A-CGA	3.96	1.44	1.33
12	bB	905	CLA	O2A-CGA	3.96	1.44	1.33
12	aB	915	CLA	CHD-C1D	3.96	1.46	1.38
12	bA	810	CLA	C1D-ND	3.96	1.43	1.37
12	aA	829	CLA	C4B-NB	-3.96	1.32	1.37
12	bB	922	CLA	C1B-NB	-3.96	1.32	1.37
12	aA	832	CLA	CHD-C1D	3.96	1.46	1.38
12	bA	832	CLA	C1D-ND	3.96	1.43	1.37
12	bL	202	CLA	C1D-ND	3.96	1.43	1.37
12	cB	912	CLA	CHD-C1D	3.96	1.46	1.38
12	cA	840	CLA	CHD-C4C	3.96	1.48	1.39
12	aB	901	CLA	O2A-CGA	3.96	1.44	1.33
12	cB	907	CLA	O2A-CGA	3.96	1.44	1.33
12	cA	813	CLA	C1D-ND	3.96	1.43	1.37
12	aB	936	CLA	O2A-CGA	3.96	1.44	1.33
12	aA	813	CLA	C1B-NB	-3.96	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bB	935	CLA	C1D-ND	3.96	1.43	1.37
12	cA	825	CLA	O2A-CGA	3.96	1.44	1.33
12	aA	832	CLA	C1D-ND	3.96	1.43	1.37
12	bA	832	CLA	CHD-C1D	3.96	1.46	1.38
12	cA	832	CLA	C1D-ND	3.96	1.43	1.37
12	aA	833	CLA	O2A-CGA	3.96	1.44	1.33
12	bA	814	CLA	CHC-C1C	3.96	1.46	1.38
12	bB	908	CLA	CHD-C1D	3.96	1.46	1.38
12	bA	836	CLA	CHD-C4C	3.95	1.48	1.39
12	bB	936	CLA	O2A-CGA	3.95	1.44	1.33
12	bB	907	CLA	O2A-CGA	3.95	1.44	1.33
12	cB	901	CLA	O2A-CGA	3.95	1.44	1.33
12	cA	853	CLA	O2A-CGA	3.95	1.44	1.33
12	cB	933	CLA	CHC-C1C	3.95	1.46	1.38
12	cA	836	CLA	CHD-C4C	3.95	1.48	1.39
12	bA	837	CLA	O2D-CGD	3.95	1.42	1.33
12	aA	836	CLA	CHD-C4C	3.95	1.48	1.39
12	aB	928	CLA	O2D-CGD	3.95	1.42	1.33
12	aA	843	CLA	CHD-C1D	3.95	1.46	1.38
12	aL	202	CLA	C1B-NB	-3.95	1.32	1.37
12	cB	932	CLA	CHD-C4C	3.95	1.48	1.39
12	cA	820	CLA	C1B-NB	-3.95	1.32	1.37
12	bB	901	CLA	O2A-CGA	3.95	1.44	1.33
12	aL	204	CLA	CHD-C1D	3.94	1.46	1.38
12	bB	937	CLA	CHD-C1D	3.94	1.46	1.38
12	cB	909	CLA	O2A-CGA	3.94	1.44	1.33
12	bA	833	CLA	O2A-CGA	3.94	1.44	1.33
12	cB	908	CLA	CHD-C1D	3.94	1.46	1.38
12	aA	808	CLA	CHD-C4C	3.94	1.48	1.39
12	bB	907	CLA	C1D-ND	3.94	1.43	1.37
12	aA	854	CLA	O2A-CGA	3.94	1.44	1.33
12	cB	928	CLA	O2D-CGD	3.94	1.42	1.33
12	aA	814	CLA	CHC-C1C	3.94	1.46	1.38
12	cA	837	CLA	O2D-CGD	3.94	1.42	1.33
12	aA	809	CLA	C1D-ND	3.94	1.43	1.37
12	cB	935	CLA	C1D-ND	3.94	1.43	1.37
12	cB	919	CLA	CHD-C1D	3.94	1.46	1.38
12	bA	840	CLA	CHD-C4C	3.94	1.48	1.39
12	aB	932	CLA	CHD-C4C	3.94	1.48	1.39
12	cB	930	CLA	CHD-C1D	3.94	1.46	1.38
13	aB	940	1L3	C11-C12	3.94	1.55	1.48
12	bA	838	CLA	C1D-ND	3.94	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bA	820	CLA	C1B-NB	-3.93	1.32	1.37
12	bB	909	CLA	O2A-CGA	3.93	1.44	1.33
12	bA	813	CLA	C1D-ND	3.93	1.43	1.37
12	cB	936	CLA	O2A-CGA	3.93	1.44	1.33
12	bA	853	CLA	O2A-CGA	3.93	1.44	1.33
12	bA	808	CLA	CHD-C4C	3.93	1.48	1.39
12	bB	936	CLA	CHD-C4C	3.93	1.48	1.39
12	bA	820	CLA	C1D-ND	3.93	1.43	1.37
12	cB	936	CLA	CHD-C4C	3.93	1.48	1.39
12	aB	936	CLA	CHD-C4C	3.93	1.48	1.39
12	bB	932	CLA	CHD-C4C	3.93	1.48	1.39
12	cL	202	CLA	C1B-NB	-3.93	1.32	1.37
12	bL	202	CLA	C1B-NB	-3.93	1.32	1.37
12	aB	912	CLA	CHD-C1D	3.92	1.46	1.38
12	bB	912	CLA	CHD-C1D	3.92	1.46	1.38
12	aB	916	CLA	C1B-NB	-3.92	1.32	1.37
13	cB	940	1L3	C11-C12	3.92	1.55	1.48
12	bB	904	CLA	C4B-NB	-3.92	1.32	1.37
12	aA	840	CLA	CHD-C4C	3.92	1.48	1.39
12	aA	837	CLA	O2D-CGD	3.92	1.42	1.33
12	aA	820	CLA	C1D-ND	3.92	1.43	1.37
12	bL	204	CLA	C1B-NB	-3.92	1.32	1.37
12	bB	939	CLA	C1B-NB	-3.92	1.32	1.37
12	cA	843	CLA	CHD-C1D	3.92	1.46	1.38
12	aA	813	CLA	C1D-ND	3.92	1.43	1.37
12	aB	933	CLA	C1B-NB	-3.92	1.32	1.37
12	aB	904	CLA	C4B-NB	-3.91	1.32	1.37
12	bB	933	CLA	CHC-C1C	3.91	1.46	1.38
12	bB	916	CLA	C1B-NB	-3.91	1.32	1.37
12	bA	819	CLA	O2A-CGA	3.91	1.44	1.33
12	aB	909	CLA	O2A-CGA	3.91	1.44	1.33
12	aA	823	CLA	CHD-C1D	3.91	1.46	1.38
12	cA	808	CLA	CHD-C4C	3.91	1.48	1.39
12	aB	935	CLA	C1D-ND	3.91	1.43	1.37
12	aA	824	CLA	C1B-NB	-3.91	1.32	1.37
12	cA	843	CLA	C3D-C2D	3.90	1.49	1.39
12	cA	824	CLA	C1B-NB	-3.90	1.32	1.37
12	bA	823	CLA	CHD-C1D	3.90	1.46	1.38
12	cB	904	CLA	C4B-NB	-3.90	1.32	1.37
12	aA	815	CLA	CHD-C4C	3.90	1.48	1.39
12	aB	933	CLA	CHC-C1C	3.90	1.46	1.38
12	bB	930	CLA	CHD-C1D	3.90	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bB	949	CLA	CHD-C1D	3.90	1.46	1.38
12	cA	818	CLA	C1D-ND	3.90	1.43	1.37
12	cA	824	CLA	CHD-C1D	3.90	1.46	1.38
12	cA	842	CLA	C1B-NB	-3.90	1.32	1.37
12	bB	909	CLA	CHC-C1C	3.89	1.46	1.38
12	cA	815	CLA	CHD-C4C	3.89	1.48	1.39
12	bA	829	CLA	C4B-NB	-3.89	1.32	1.37
12	bB	911	CLA	C1B-NB	-3.89	1.32	1.37
12	bB	905	CLA	C1B-NB	-3.89	1.32	1.37
12	cB	939	CLA	C1B-NB	-3.89	1.32	1.37
12	bA	815	CLA	CHD-C4C	3.89	1.48	1.39
12	cB	911	CLA	C1B-NB	-3.89	1.32	1.37
12	aA	824	CLA	CHD-C1D	3.89	1.46	1.38
12	aB	930	CLA	CHD-C1D	3.89	1.46	1.38
12	aB	905	CLA	C1B-NB	-3.89	1.32	1.37
12	bA	843	CLA	CHD-C1D	3.89	1.46	1.38
12	aB	903	CLA	C1B-NB	-3.89	1.32	1.37
12	aB	909	CLA	CHC-C1C	3.89	1.46	1.38
12	bA	824	CLA	CHD-C1D	3.89	1.46	1.38
12	cA	810	CLA	C4B-NB	-3.89	1.32	1.37
12	cA	827	CLA	C1B-NB	-3.89	1.32	1.37
12	cB	909	CLA	CHC-C1C	3.89	1.46	1.38
12	bB	936	CLA	CHD-C1D	3.88	1.46	1.38
12	cA	841	CLA	C1D-ND	3.88	1.43	1.37
12	bA	827	CLA	C1B-NB	-3.88	1.32	1.37
12	aA	819	CLA	O2A-CGA	3.88	1.44	1.33
12	bB	916	CLA	C1D-ND	3.88	1.43	1.37
12	cB	921	CLA	C1B-NB	-3.88	1.32	1.37
12	aB	937	CLA	CHD-C1D	3.88	1.46	1.38
12	cB	905	CLA	C1B-NB	-3.88	1.32	1.37
11	aA	801	CL0	CHC-C1C	3.88	1.46	1.39
12	aB	949	CLA	CHD-C1D	3.88	1.46	1.38
12	cB	949	CLA	CHD-C1D	3.88	1.46	1.38
12	aA	827	CLA	C1B-NB	-3.88	1.32	1.37
12	bA	841	CLA	C1D-ND	3.88	1.43	1.37
12	cA	828	CLA	C4B-NB	-3.88	1.32	1.37
12	aA	810	CLA	C4B-NB	-3.88	1.32	1.37
12	bB	903	CLA	C1B-NB	-3.88	1.32	1.37
12	cA	819	CLA	O2A-CGA	3.88	1.44	1.33
12	bB	919	CLA	CHD-C1D	3.88	1.46	1.38
12	cB	916	CLA	C1B-NB	-3.88	1.32	1.37
12	bB	918	CLA	CHD-C1D	3.88	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aB	907	CLA	C1D-ND	3.87	1.43	1.37
12	aA	828	CLA	C4B-NB	-3.87	1.32	1.37
12	aA	818	CLA	C1D-ND	3.87	1.42	1.37
12	aB	905	CLA	C1D-ND	3.87	1.42	1.37
12	aA	839	CLA	CHC-C1C	3.87	1.46	1.38
12	cA	812	CLA	C1D-ND	3.87	1.42	1.37
12	aA	820	CLA	CHD-C1D	3.87	1.46	1.38
12	aA	820	CLA	C1B-NB	-3.87	1.32	1.37
12	bB	921	CLA	C1B-NB	-3.87	1.32	1.37
12	cB	903	CLA	C1B-NB	-3.87	1.32	1.37
12	bA	810	CLA	C4B-NB	-3.87	1.32	1.37
12	bB	920	CLA	CHD-C4C	3.87	1.48	1.39
12	aB	921	CLA	CHD-C4C	3.87	1.48	1.39
12	aA	843	CLA	C3D-C2D	3.87	1.49	1.39
12	aB	919	CLA	CHD-C1D	3.87	1.46	1.38
12	bA	843	CLA	C3D-C2D	3.87	1.49	1.39
12	bA	820	CLA	CHD-C1D	3.87	1.46	1.38
12	bA	802	CLA	CHD-C1D	3.87	1.46	1.38
12	cB	918	CLA	CHD-C1D	3.87	1.46	1.38
12	bA	812	CLA	C1D-ND	3.87	1.42	1.37
12	cA	829	CLA	C4B-NB	-3.87	1.32	1.37
12	cA	837	CLA	C4B-NB	-3.87	1.32	1.37
12	bB	911	CLA	C1D-ND	3.86	1.42	1.37
12	bA	839	CLA	CHC-C1C	3.86	1.46	1.38
12	aB	911	CLA	C1B-NB	-3.86	1.32	1.37
12	cB	936	CLA	CHD-C1D	3.86	1.45	1.38
12	aA	837	CLA	C4B-NB	-3.86	1.32	1.37
12	cB	937	CLA	CHD-C1D	3.86	1.45	1.38
12	aB	911	CLA	C1D-ND	3.86	1.42	1.37
12	aB	916	CLA	C1D-ND	3.86	1.42	1.37
12	aB	921	CLA	C1B-NB	-3.86	1.32	1.37
12	cA	802	CLA	CHD-C1D	3.85	1.45	1.38
12	cA	839	CLA	CHC-C1C	3.85	1.46	1.38
12	bA	810	CLA	CHD-C1D	3.85	1.45	1.38
12	cB	911	CLA	C1D-ND	3.85	1.42	1.37
12	bB	921	CLA	CHD-C4C	3.85	1.48	1.39
11	cA	801	CL0	CHC-C1C	3.85	1.46	1.39
12	aA	810	CLA	C1B-NB	-3.85	1.32	1.37
12	cB	920	CLA	CHD-C4C	3.85	1.48	1.39
12	bB	925	CLA	CHC-C4B	3.85	1.48	1.39
12	cA	823	CLA	CHD-C1D	3.85	1.45	1.38
12	cA	832	CLA	C4B-NB	-3.85	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cB	907	CLA	C1B-NB	-3.85	1.32	1.37
12	cB	921	CLA	CHD-C4C	3.84	1.48	1.39
12	cA	825	CLA	CHC-C4B	3.84	1.48	1.39
12	bA	806	CLA	C4B-NB	-3.84	1.32	1.37
12	aA	810	CLA	CHD-C1D	3.84	1.45	1.38
12	aB	927	CLA	CHD-C1D	3.84	1.45	1.38
12	cA	827	CLA	C4B-NB	-3.84	1.32	1.37
12	cB	916	CLA	C1D-ND	3.84	1.42	1.37
12	aA	841	CLA	C1D-ND	3.84	1.42	1.37
12	aA	842	CLA	C1B-NB	-3.84	1.32	1.37
12	cA	820	CLA	CHD-C1D	3.84	1.45	1.38
12	bA	818	CLA	C1D-ND	3.84	1.42	1.37
12	bA	837	CLA	C4B-NB	-3.84	1.32	1.37
12	bA	826	CLA	C1B-NB	-3.84	1.32	1.37
12	aB	939	CLA	C1B-NB	-3.84	1.32	1.37
12	aB	925	CLA	CHC-C4B	3.84	1.48	1.39
11	bA	801	CL0	CHC-C1C	3.84	1.46	1.39
12	bA	840	CLA	C1B-NB	-3.83	1.32	1.37
12	bA	823	CLA	C1B-NB	-3.83	1.32	1.37
12	bA	825	CLA	CHD-C1D	3.83	1.45	1.38
12	aA	827	CLA	C4B-NB	-3.83	1.32	1.37
12	bA	828	CLA	C4B-NB	-3.83	1.32	1.37
12	aB	933	CLA	CHD-C1D	3.83	1.45	1.38
12	bA	825	CLA	CHC-C4B	3.83	1.48	1.39
12	aB	936	CLA	C1B-NB	-3.83	1.32	1.37
12	bA	827	CLA	C4B-NB	-3.83	1.32	1.37
12	cB	929	CLA	C1B-NB	-3.83	1.32	1.37
12	cA	810	CLA	CHD-C1D	3.83	1.45	1.38
12	bA	818	CLA	C1B-NB	-3.83	1.32	1.37
12	aA	822	CLA	CHD-C4C	3.83	1.47	1.39
12	bA	810	CLA	C1B-NB	-3.83	1.32	1.37
12	bA	842	CLA	C1B-NB	-3.83	1.32	1.37
12	bB	907	CLA	CHC-C1C	3.83	1.46	1.38
12	aA	806	CLA	C4B-NB	-3.83	1.32	1.37
12	cA	823	CLA	C1B-NB	-3.83	1.32	1.37
12	aB	929	CLA	C1B-NB	-3.83	1.32	1.37
12	bA	805	CLA	CHD-C1D	3.82	1.45	1.38
12	bB	933	CLA	CHD-C1D	3.82	1.45	1.38
12	bB	923	CLA	C1B-NB	-3.82	1.32	1.37
12	aB	916	CLA	O2A-CGA	3.82	1.44	1.33
12	bB	908	CLA	C3D-C2D	3.82	1.49	1.39
12	cB	920	CLA	C3D-C2D	3.82	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aL	204	CLA	C1B-NB	-3.82	1.32	1.37
12	cB	927	CLA	CHD-C1D	3.82	1.45	1.38
12	aB	904	CLA	C1D-ND	3.82	1.42	1.37
12	bB	905	CLA	C1D-ND	3.82	1.42	1.37
12	bB	907	CLA	C1B-NB	-3.82	1.32	1.37
12	aA	816	CLA	CHD-C1D	3.82	1.45	1.38
12	bB	910	CLA	CHD-C4C	3.82	1.47	1.39
12	cB	907	CLA	CHC-C1C	3.82	1.46	1.38
12	bA	811	CLA	CHD-C4C	3.82	1.47	1.39
12	cB	936	CLA	C1B-NB	-3.82	1.32	1.37
12	cL	204	CLA	C1B-NB	-3.82	1.32	1.37
12	cB	908	CLA	C3D-C2D	3.82	1.49	1.39
12	aA	805	CLA	CHD-C1D	3.82	1.45	1.38
12	aB	936	CLA	CHD-C1D	3.82	1.45	1.38
12	bA	830	CLA	O2A-CGA	3.82	1.44	1.33
12	aB	918	CLA	CHD-C1D	3.82	1.45	1.38
12	cB	916	CLA	O2A-CGA	3.82	1.44	1.33
12	bB	910	CLA	C1D-ND	3.82	1.42	1.37
12	aA	825	CLA	CHD-C1D	3.82	1.45	1.38
12	aA	818	CLA	C1B-NB	-3.82	1.32	1.37
12	aA	854	CLA	C3D-C2D	3.82	1.49	1.39
12	bB	903	CLA	CHD-C1D	3.81	1.45	1.38
12	bA	806	CLA	CHD-C4C	3.81	1.47	1.39
12	aA	840	CLA	C1B-NB	-3.81	1.32	1.37
12	aB	920	CLA	CHD-C4C	3.81	1.47	1.39
12	aB	923	CLA	C1B-NB	-3.81	1.32	1.37
12	bB	920	CLA	C3D-C2D	3.81	1.49	1.39
12	cA	833	CLA	CHD-C1D	3.81	1.45	1.38
12	bA	812	CLA	C1B-NB	-3.81	1.32	1.37
12	cA	816	CLA	CHD-C1D	3.81	1.45	1.38
12	aB	920	CLA	C3D-C2D	3.81	1.49	1.39
12	aB	907	CLA	CHC-C1C	3.81	1.46	1.38
12	cA	828	CLA	CHD-C1D	3.81	1.45	1.38
12	cB	907	CLA	CHD-C1D	3.81	1.45	1.38
12	cA	830	CLA	O2A-CGA	3.81	1.44	1.33
12	aA	825	CLA	CHC-C4B	3.81	1.48	1.39
12	bB	949	CLA	OBD-CAD	3.81	1.29	1.22
12	aB	910	CLA	C1D-ND	3.81	1.42	1.37
12	cA	817	CLA	CHD-C1D	3.81	1.45	1.38
12	bA	822	CLA	CHD-C4C	3.81	1.47	1.39
12	bA	830	CLA	C3D-C2D	3.81	1.49	1.39
12	bB	916	CLA	O2A-CGA	3.81	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aB	903	CLA	CHD-C1D	3.80	1.45	1.38
12	aB	908	CLA	C3D-C2D	3.80	1.49	1.39
12	cB	916	CLA	CHD-C4C	3.80	1.47	1.39
12	cA	810	CLA	C1B-NB	-3.80	1.32	1.37
12	aA	833	CLA	CHD-C1D	3.80	1.45	1.38
12	aA	832	CLA	CHD-C4C	3.80	1.47	1.39
12	aA	802	CLA	CHD-C1D	3.80	1.45	1.38
12	cA	818	CLA	C1B-NB	-3.80	1.32	1.37
12	cA	818	CLA	C4B-NB	-3.80	1.32	1.37
12	cB	935	CLA	C4B-NB	-3.80	1.32	1.37
12	cA	825	CLA	CHD-C1D	3.80	1.45	1.38
12	bA	832	CLA	CHD-C4C	3.80	1.47	1.39
12	cA	835	CLA	C3D-C2D	3.80	1.49	1.39
12	aB	913	CLA	C4B-NB	-3.80	1.32	1.37
12	cB	904	CLA	C1D-ND	3.80	1.42	1.37
12	cA	853	CLA	C3D-C2D	3.80	1.49	1.39
12	aA	812	CLA	C1D-ND	3.80	1.42	1.37
12	bA	833	CLA	CHD-C1D	3.80	1.45	1.38
12	bB	927	CLA	CHD-C1D	3.80	1.45	1.38
12	aA	831	CLA	CHD-C1D	3.80	1.45	1.38
12	aA	830	CLA	C3D-C2D	3.80	1.49	1.39
12	aB	949	CLA	OBD-CAD	3.80	1.29	1.22
12	cA	826	CLA	C1B-NB	-3.80	1.32	1.37
12	bA	816	CLA	CHD-C1D	3.80	1.45	1.38
12	bA	805	CLA	C3D-C2D	3.80	1.49	1.39
12	aA	828	CLA	CHD-C1D	3.80	1.45	1.38
12	aB	923	CLA	O2A-CGA	3.79	1.44	1.33
12	cA	834	CLA	CHD-C4C	3.79	1.47	1.39
12	aF	202	CLA	CHD-C4C	3.79	1.47	1.39
12	bB	907	CLA	CHD-C1D	3.79	1.45	1.38
12	cA	805	CLA	CHD-C1D	3.79	1.45	1.38
12	aA	835	CLA	C3D-C2D	3.79	1.49	1.39
12	bA	853	CLA	C3D-C2D	3.79	1.49	1.39
12	cA	821	CLA	CHD-C1D	3.79	1.45	1.38
12	cB	905	CLA	C1D-ND	3.79	1.42	1.37
12	bF	202	CLA	CHD-C4C	3.79	1.47	1.39
12	cB	910	CLA	CHD-C4C	3.79	1.47	1.39
12	aA	830	CLA	O2A-CGA	3.79	1.44	1.33
12	cB	918	CLA	CHD-C4C	3.79	1.47	1.39
12	aA	818	CLA	C4B-NB	-3.79	1.32	1.37
12	aA	812	CLA	C1B-NB	-3.79	1.32	1.37
12	cB	903	CLA	CHD-C1D	3.79	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bB	918	CLA	CHD-C4C	3.79	1.47	1.39
12	aB	903	CLA	C1D-ND	3.79	1.42	1.37
12	bA	835	CLA	C3D-C2D	3.79	1.49	1.39
12	cB	933	CLA	CHD-C1D	3.79	1.45	1.38
12	cB	925	CLA	CHC-C4B	3.79	1.47	1.39
12	cA	822	CLA	CHD-C4C	3.79	1.47	1.39
12	aB	950	CLA	C3D-C2D	3.79	1.49	1.39
12	cB	949	CLA	OBD-CAD	3.79	1.29	1.22
12	bA	810	CLA	C3D-C2D	3.79	1.49	1.39
12	bB	916	CLA	CHD-C4C	3.79	1.47	1.39
12	cA	802	CLA	CHD-C4C	3.79	1.47	1.39
12	cA	832	CLA	CHD-C4C	3.79	1.47	1.39
12	bA	832	CLA	C4B-NB	-3.79	1.32	1.37
12	cA	830	CLA	C3D-C2D	3.78	1.49	1.39
12	bA	831	CLA	CHD-C1D	3.78	1.45	1.38
12	bB	929	CLA	C1B-NB	-3.78	1.32	1.37
12	bB	936	CLA	C1B-NB	-3.78	1.32	1.37
12	aB	910	CLA	CHD-C4C	3.78	1.47	1.39
12	cA	812	CLA	C1B-NB	-3.78	1.32	1.37
12	bA	828	CLA	CHD-C1D	3.78	1.45	1.38
12	bA	843	CLA	O2A-CGA	3.78	1.44	1.33
12	aA	806	CLA	CHD-C4C	3.78	1.47	1.39
12	cA	826	CLA	CHD-C1D	3.78	1.45	1.38
12	aA	834	CLA	CHD-C4C	3.78	1.47	1.39
12	aB	949	CLA	C1B-NB	-3.78	1.32	1.37
12	aA	811	CLA	CHD-C4C	3.78	1.47	1.39
12	cF	202	CLA	CHD-C4C	3.78	1.47	1.39
12	bB	950	CLA	C3D-C2D	3.78	1.49	1.39
12	cA	843	CLA	O2A-CGA	3.78	1.44	1.33
12	cA	804	CLA	C1B-NB	-3.78	1.32	1.37
12	cA	806	CLA	C4B-NB	-3.78	1.32	1.37
12	cB	923	CLA	C1B-NB	-3.78	1.32	1.37
12	aB	937	CLA	CHD-C4C	3.78	1.47	1.39
12	cA	831	CLA	CHD-C1D	3.78	1.45	1.38
12	bA	841	CLA	C1B-NB	-3.78	1.32	1.37
12	cA	811	CLA	CHD-C4C	3.78	1.47	1.39
12	bB	923	CLA	O2A-CGA	3.78	1.44	1.33
12	aA	826	CLA	CHD-C1D	3.78	1.45	1.38
12	cA	836	CLA	C1B-NB	-3.78	1.32	1.37
12	aA	817	CLA	CHD-C1D	3.78	1.45	1.38
12	cA	835	CLA	CHD-C1D	3.77	1.45	1.38
12	bB	933	CLA	C3D-C2D	3.77	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aB	907	CLA	C1B-NB	-3.77	1.32	1.37
12	aA	810	CLA	C3D-C2D	3.77	1.49	1.39
12	cA	810	CLA	C3D-C2D	3.77	1.49	1.39
12	aB	909	CLA	C1D-ND	3.77	1.42	1.37
12	aB	935	CLA	C4B-NB	-3.77	1.32	1.37
12	aA	805	CLA	C3D-C2D	3.77	1.49	1.39
12	cB	924	CLA	CHD-C1D	3.77	1.45	1.38
12	cB	937	CLA	CHD-C4C	3.77	1.47	1.39
12	aA	804	CLA	C1D-ND	3.77	1.42	1.37
12	cA	839	CLA	C1D-ND	3.77	1.42	1.37
12	aA	823	CLA	C1B-NB	-3.77	1.32	1.37
12	aA	841	CLA	C1B-NB	-3.77	1.32	1.37
12	aA	843	CLA	O2A-CGA	3.77	1.44	1.33
12	bA	835	CLA	CHD-C1D	3.77	1.45	1.38
12	cB	949	CLA	CHD-C4C	3.77	1.47	1.39
12	aB	907	CLA	CHD-C1D	3.77	1.45	1.38
12	bF	202	CLA	CHC-C4B	3.77	1.47	1.39
12	bB	913	CLA	C4B-NB	-3.77	1.32	1.37
12	cB	913	CLA	C4B-NB	-3.77	1.32	1.37
12	cB	923	CLA	O2A-CGA	3.77	1.44	1.33
12	aA	804	CLA	C1B-NB	-3.77	1.32	1.37
12	bA	839	CLA	C1D-ND	3.77	1.42	1.37
12	bA	834	CLA	CHD-C4C	3.77	1.47	1.39
12	bA	821	CLA	CHD-C1D	3.77	1.45	1.38
12	aB	918	CLA	CHD-C4C	3.77	1.47	1.39
12	aA	826	CLA	C1B-NB	-3.77	1.32	1.37
12	aB	914	CLA	C1B-NB	-3.77	1.32	1.37
12	cA	815	CLA	C1B-NB	-3.77	1.32	1.37
12	cA	806	CLA	CHD-C4C	3.77	1.47	1.39
12	bA	830	CLA	CHD-C1D	3.77	1.45	1.38
12	bA	826	CLA	CHD-C1D	3.76	1.45	1.38
12	cL	203	CLA	C3D-C2D	3.76	1.49	1.39
12	cB	933	CLA	C3D-C2D	3.76	1.49	1.39
12	bA	817	CLA	C3D-C2D	3.76	1.49	1.39
12	bL	203	CLA	C3D-C2D	3.76	1.49	1.39
12	aB	929	CLA	CHD-C1D	3.76	1.45	1.38
12	aA	826	CLA	C3D-C2D	3.76	1.49	1.39
12	aA	844	CLA	C3D-C2D	3.76	1.49	1.39
12	aA	839	CLA	C1D-ND	3.76	1.42	1.37
11	cA	801	CL0	OBD-CAD	3.76	1.27	1.22
12	cF	202	CLA	CHC-C4B	3.76	1.47	1.39
12	aA	821	CLA	CHD-C1D	3.76	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bB	929	CLA	CHD-C1D	3.76	1.45	1.38
12	cA	805	CLA	C3D-C2D	3.76	1.49	1.39
12	aF	202	CLA	CHC-C4B	3.76	1.47	1.39
11	aA	801	CL0	CHB-C4A	-3.76	1.34	1.38
12	aL	203	CLA	C3D-C2D	3.76	1.49	1.39
12	bA	804	CLA	C1B-NB	-3.76	1.32	1.37
11	cA	801	CL0	CHB-C4A	-3.75	1.34	1.38
12	cB	903	CLA	C1D-ND	3.75	1.42	1.37
11	bA	801	CL0	OBD-CAD	3.75	1.27	1.22
12	aA	802	CLA	CHD-C4C	3.75	1.47	1.39
12	aA	832	CLA	C4B-NB	-3.75	1.32	1.37
12	aB	949	CLA	CHD-C4C	3.75	1.47	1.39
12	aA	816	CLA	C1B-NB	-3.75	1.32	1.37
12	aB	918	CLA	C4B-NB	-3.75	1.32	1.37
12	cB	918	CLA	C4B-NB	-3.75	1.32	1.37
12	cA	830	CLA	CHD-C1D	3.75	1.45	1.38
12	bA	818	CLA	C4B-NB	-3.75	1.32	1.37
12	cA	806	CLA	C1B-NB	-3.75	1.32	1.37
12	cA	840	CLA	C1B-NB	-3.75	1.32	1.37
12	bA	826	CLA	C3D-C2D	3.75	1.49	1.39
11	bA	801	CL0	CHB-C4A	-3.75	1.34	1.38
12	cA	817	CLA	C3D-C2D	3.75	1.49	1.39
12	cA	813	CLA	CHC-C4B	3.75	1.47	1.39
12	bB	930	CLA	C3D-C2D	3.74	1.49	1.39
12	cA	804	CLA	C1D-ND	3.74	1.42	1.37
12	aB	930	CLA	C3D-C2D	3.74	1.49	1.39
12	bA	836	CLA	C1B-NB	-3.74	1.32	1.37
12	aA	841	CLA	CHC-C4B	3.74	1.47	1.39
12	aB	916	CLA	CHD-C4C	3.74	1.47	1.39
12	aB	906	CLA	C1D-ND	3.74	1.42	1.37
12	bA	824	CLA	CHD-C4C	3.74	1.47	1.39
12	bB	903	CLA	C1D-ND	3.74	1.42	1.37
12	aA	817	CLA	C3D-C2D	3.74	1.49	1.39
11	aA	801	CL0	CHD-C1D	3.74	1.45	1.39
12	aA	813	CLA	CHC-C4B	3.74	1.47	1.39
12	cB	909	CLA	C1D-ND	3.74	1.42	1.37
12	bB	905	CLA	C4B-NB	-3.74	1.33	1.37
12	aA	806	CLA	C1B-NB	-3.74	1.33	1.37
12	bA	815	CLA	C1B-NB	-3.74	1.33	1.37
12	bA	839	CLA	C4B-NB	-3.74	1.33	1.37
12	cB	930	CLA	C3D-C2D	3.74	1.49	1.39
12	aB	924	CLA	CHD-C1D	3.73	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cB	902	CLA	C3D-C2D	3.73	1.49	1.39
12	bA	813	CLA	CHC-C4B	3.73	1.47	1.39
12	aA	822	CLA	C3D-C2D	3.73	1.49	1.39
12	bA	822	CLA	C3D-C2D	3.73	1.49	1.39
12	aA	835	CLA	CHD-C1D	3.73	1.45	1.38
12	bA	831	CLA	C1D-ND	3.73	1.42	1.37
12	bB	949	CLA	CHD-C4C	3.73	1.47	1.39
12	cA	819	CLA	CHD-C1D	3.73	1.45	1.38
12	aA	822	CLA	CHC-C4B	3.73	1.47	1.39
12	cA	822	CLA	CHC-C4B	3.73	1.47	1.39
12	aB	902	CLA	C3D-C2D	3.73	1.49	1.39
12	cB	905	CLA	C4B-NB	-3.73	1.33	1.37
12	bB	917	CLA	C3D-C2D	3.73	1.49	1.39
12	aB	938	CLA	C1D-ND	3.73	1.42	1.37
12	aB	914	CLA	C3D-C2D	3.73	1.49	1.39
12	aB	934	CLA	C3D-C2D	3.73	1.49	1.39
12	bB	935	CLA	C4B-NB	-3.73	1.33	1.37
12	bB	934	CLA	C3D-C2D	3.73	1.49	1.39
12	aA	814	CLA	C1D-ND	3.73	1.42	1.37
12	cB	910	CLA	C1D-ND	3.73	1.42	1.37
11	aA	801	CL0	OBD-CAD	3.73	1.27	1.22
12	cA	822	CLA	C3D-C2D	3.73	1.49	1.39
12	aB	904	CLA	O2A-CGA	3.73	1.44	1.33
12	bB	917	CLA	C1D-ND	3.73	1.42	1.37
12	bA	817	CLA	CHD-C1D	3.73	1.45	1.38
12	bB	904	CLA	O2A-CGA	3.73	1.44	1.33
12	aA	824	CLA	CHD-C4C	3.73	1.47	1.39
12	bA	816	CLA	CHD-C4C	3.73	1.47	1.39
12	bB	914	CLA	C3D-C2D	3.73	1.49	1.39
12	bA	813	CLA	C4B-NB	-3.73	1.33	1.37
12	cB	914	CLA	C1B-NB	-3.73	1.33	1.37
12	bA	819	CLA	CHD-C1D	3.73	1.45	1.38
15	cB	944	BCR	C1-C6	-3.73	1.49	1.53
12	bA	806	CLA	C1B-NB	-3.73	1.33	1.37
12	aB	933	CLA	C3D-C2D	3.72	1.49	1.39
12	aB	905	CLA	C4B-NB	-3.72	1.33	1.37
11	bA	801	CL0	CHD-C4C	3.72	1.46	1.39
11	cA	801	CL0	CHD-C4C	3.72	1.46	1.39
12	cA	813	CLA	C3D-C2D	3.72	1.49	1.39
12	cA	814	CLA	C1D-ND	3.72	1.42	1.37
12	cA	831	CLA	C1D-ND	3.72	1.42	1.37
12	bB	949	CLA	C1B-NB	-3.72	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cA	826	CLA	C3D-C2D	3.72	1.49	1.39
12	aA	813	CLA	C4B-NB	-3.72	1.33	1.37
12	bB	924	CLA	CHD-C1D	3.72	1.45	1.38
12	bA	809	CLA	C1B-NB	-3.72	1.33	1.37
12	cB	903	CLA	C4B-NB	-3.72	1.33	1.37
12	bA	802	CLA	CHD-C4C	3.72	1.47	1.39
12	bA	815	CLA	C3D-C2D	3.72	1.49	1.39
12	cB	917	CLA	C3D-C2D	3.72	1.49	1.39
12	bA	814	CLA	C1D-ND	3.72	1.42	1.37
12	bB	904	CLA	C1D-ND	3.72	1.42	1.37
12	bB	937	CLA	CHD-C4C	3.72	1.47	1.39
12	cB	929	CLA	CHD-C1D	3.72	1.45	1.38
12	cB	914	CLA	C3D-C2D	3.72	1.49	1.39
12	cB	949	CLA	C1B-NB	-3.72	1.33	1.37
12	aB	931	CLA	CHC-C4B	3.72	1.47	1.39
12	aB	917	CLA	C3D-C2D	3.71	1.49	1.39
12	bB	902	CLA	C3D-C2D	3.71	1.49	1.39
12	bA	837	CLA	CHD-C4C	3.71	1.47	1.39
12	aA	815	CLA	C3D-C2D	3.71	1.49	1.39
12	aB	950	CLA	C4B-NB	-3.71	1.33	1.37
12	bA	822	CLA	CHC-C4B	3.71	1.47	1.39
12	bB	949	CLA	C3D-C2D	3.71	1.49	1.39
12	cA	815	CLA	C3D-C2D	3.71	1.49	1.39
12	cA	841	CLA	CHC-C4B	3.71	1.47	1.39
12	cA	813	CLA	C4B-NB	-3.71	1.33	1.37
12	bB	924	CLA	C4B-NB	-3.71	1.33	1.37
12	cB	928	CLA	CHD-C1D	3.71	1.45	1.38
12	aA	837	CLA	C1D-ND	3.71	1.42	1.37
12	cA	839	CLA	CHD-C1D	3.71	1.45	1.38
12	cB	934	CLA	CHC-C4B	3.71	1.47	1.39
12	aA	819	CLA	C1D-ND	3.71	1.42	1.37
12	bA	809	CLA	CHD-C4C	3.71	1.47	1.39
12	cA	832	CLA	C1B-NB	-3.71	1.33	1.37
12	aA	816	CLA	CHD-C4C	3.71	1.47	1.39
12	cB	931	CLA	CHC-C4B	3.71	1.47	1.39
12	aA	836	CLA	C1B-NB	-3.71	1.33	1.37
12	bA	819	CLA	C1D-ND	3.71	1.42	1.37
12	bA	832	CLA	C1B-NB	-3.71	1.33	1.37
12	bB	931	CLA	CHC-C4B	3.71	1.47	1.39
12	aA	813	CLA	C3D-C2D	3.71	1.49	1.39
12	cA	837	CLA	C1D-ND	3.71	1.42	1.37
12	bB	914	CLA	C1B-NB	-3.71	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bA	804	CLA	C3D-C2D	3.70	1.49	1.39
12	bA	813	CLA	C3D-C2D	3.70	1.49	1.39
12	cB	934	CLA	C3D-C2D	3.70	1.49	1.39
12	aB	916	CLA	CHD-C1D	3.70	1.45	1.38
12	aA	832	CLA	C1B-NB	-3.70	1.33	1.37
12	cA	839	CLA	C4B-NB	-3.70	1.33	1.37
12	aA	844	CLA	C4B-NB	-3.70	1.33	1.37
11	aA	801	CL0	CHD-C4C	3.70	1.46	1.39
12	aA	819	CLA	CHD-C1D	3.70	1.45	1.38
12	aA	831	CLA	C1D-ND	3.70	1.42	1.37
12	bB	918	CLA	C4B-NB	-3.70	1.33	1.37
12	aA	815	CLA	C1B-NB	-3.70	1.33	1.37
12	aA	839	CLA	C4B-NB	-3.70	1.33	1.37
12	bB	931	CLA	CHD-C4C	3.70	1.47	1.39
12	bB	903	CLA	C4B-NB	-3.70	1.33	1.37
12	bB	950	CLA	C4B-NB	-3.70	1.33	1.37
12	bA	820	CLA	C3D-C2D	3.70	1.49	1.39
12	aA	839	CLA	CHD-C1D	3.70	1.45	1.38
12	aA	809	CLA	CHD-C4C	3.70	1.47	1.39
12	aA	809	CLA	CHD-C1D	3.70	1.45	1.38
12	bA	809	CLA	CHD-C1D	3.70	1.45	1.38
12	aL	202	CLA	C3D-C2D	3.70	1.49	1.39
12	cA	833	CLA	C1D-ND	3.70	1.42	1.37
11	cA	801	CL0	CHD-C1D	3.70	1.45	1.39
12	aB	918	CLA	C1D-ND	3.70	1.42	1.37
12	aA	830	CLA	CHD-C1D	3.70	1.45	1.38
12	aA	820	CLA	C3D-C2D	3.69	1.49	1.39
12	bB	928	CLA	CHD-C1D	3.69	1.45	1.38
12	bA	804	CLA	C1D-ND	3.69	1.42	1.37
12	bB	909	CLA	C1D-ND	3.69	1.42	1.37
12	bL	202	CLA	C3D-C2D	3.69	1.49	1.39
12	bB	934	CLA	CHC-C4B	3.69	1.47	1.39
12	aB	915	CLA	CHD-C4C	3.69	1.47	1.39
12	aA	843	CLA	C1D-ND	3.69	1.42	1.37
12	cA	824	CLA	CHD-C4C	3.69	1.47	1.39
12	cA	816	CLA	CHD-C4C	3.69	1.47	1.39
12	cB	917	CLA	C1D-ND	3.69	1.42	1.37
12	aB	917	CLA	C1D-ND	3.69	1.42	1.37
12	cB	904	CLA	O2A-CGA	3.69	1.44	1.33
12	aA	804	CLA	C3D-C2D	3.69	1.49	1.39
12	aA	840	CLA	C3D-C2D	3.69	1.49	1.39
12	cB	924	CLA	C4B-NB	-3.69	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cA	809	CLA	CHD-C1D	3.69	1.45	1.38
12	cB	917	CLA	CHD-C1D	3.69	1.45	1.38
12	bA	816	CLA	C1B-NB	-3.69	1.33	1.37
12	cA	816	CLA	C1B-NB	-3.69	1.33	1.37
12	bA	824	CLA	C3D-C2D	3.69	1.49	1.39
12	aB	914	CLA	CHC-C4B	3.69	1.47	1.39
12	bA	840	CLA	C3D-C2D	3.69	1.49	1.39
12	bA	808	CLA	C1B-NB	-3.69	1.33	1.37
12	aA	837	CLA	CHD-C4C	3.69	1.47	1.39
12	aA	824	CLA	C3D-C2D	3.68	1.49	1.39
12	cL	202	CLA	C3D-C2D	3.68	1.49	1.39
12	cB	938	CLA	C1D-ND	3.68	1.42	1.37
12	aA	842	CLA	C3D-C2D	3.68	1.49	1.39
12	bA	839	CLA	CHD-C1D	3.68	1.45	1.38
12	cA	840	CLA	C3D-C2D	3.68	1.49	1.39
12	aB	931	CLA	CHD-C4C	3.68	1.47	1.39
12	bB	938	CLA	C1D-ND	3.68	1.42	1.37
12	bA	841	CLA	CHC-C4B	3.68	1.47	1.39
12	cB	949	CLA	C3D-C2D	3.68	1.49	1.39
12	cA	820	CLA	C3D-C2D	3.68	1.49	1.39
12	bB	914	CLA	CHC-C4B	3.68	1.47	1.39
12	cA	805	CLA	C1D-ND	3.68	1.42	1.37
15	bB	944	BCR	C1-C6	-3.68	1.49	1.53
11	bA	801	CL0	CHD-C1D	3.68	1.45	1.39
12	cB	909	CLA	CHD-C1D	3.68	1.45	1.38
12	cA	819	CLA	C1D-ND	3.68	1.42	1.37
12	bB	938	CLA	CHD-C4C	3.68	1.47	1.39
12	bB	910	CLA	C3D-C2D	3.67	1.49	1.39
12	cA	824	CLA	C3D-C2D	3.67	1.49	1.39
12	bB	938	CLA	C4B-NB	-3.67	1.33	1.37
12	aB	929	CLA	C3D-C2D	3.67	1.49	1.39
12	cB	916	CLA	CHD-C1D	3.67	1.45	1.38
12	aA	854	CLA	CHC-C4B	3.67	1.47	1.39
12	aA	818	CLA	CHD-C4C	3.67	1.47	1.39
12	cA	836	CLA	C3D-C2D	3.67	1.49	1.39
12	aB	928	CLA	CHD-C1D	3.67	1.45	1.38
12	cB	939	CLA	CHC-C1C	3.67	1.45	1.38
12	bA	837	CLA	C1D-ND	3.67	1.42	1.37
12	aB	924	CLA	C4B-NB	-3.67	1.33	1.37
12	bB	912	CLA	O2A-CGA	3.67	1.44	1.33
12	aB	938	CLA	CHD-C4C	3.67	1.47	1.39
12	bA	827	CLA	CHD-C4C	3.67	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aA	808	CLA	C1B-NB	-3.67	1.33	1.37
12	cA	805	CLA	C1B-NB	-3.67	1.33	1.37
12	aB	939	CLA	CHC-C1C	3.67	1.45	1.38
12	cB	906	CLA	C1D-ND	3.67	1.42	1.37
12	aB	904	CLA	CHD-C1D	3.67	1.45	1.38
12	aA	807	CLA	CHC-C4B	3.67	1.47	1.39
12	cB	929	CLA	C3D-C2D	3.67	1.49	1.39
12	aA	833	CLA	C1D-ND	3.67	1.42	1.37
12	cB	918	CLA	C1D-ND	3.67	1.42	1.37
12	cA	841	CLA	C1B-NB	-3.67	1.33	1.37
12	aA	831	CLA	C3D-C2D	3.67	1.49	1.39
12	aB	910	CLA	C3D-C2D	3.67	1.49	1.39
12	aB	913	CLA	CHD-C1D	3.67	1.45	1.38
12	cB	931	CLA	CHD-C4C	3.67	1.47	1.39
12	aB	949	CLA	C3D-C2D	3.67	1.49	1.39
12	aB	903	CLA	C4B-NB	-3.67	1.33	1.37
12	aB	938	CLA	C4B-NB	-3.67	1.33	1.37
12	bB	916	CLA	CHD-C1D	3.67	1.45	1.38
12	cB	919	CLA	CHC-C4B	3.67	1.47	1.39
12	bA	831	CLA	C3D-C2D	3.67	1.49	1.39
12	bB	939	CLA	CHC-C1C	3.67	1.45	1.38
12	cA	807	CLA	CHC-C4B	3.67	1.47	1.39
12	aA	817	CLA	CHC-C4B	3.67	1.47	1.39
12	aL	202	CLA	CHD-C4C	3.67	1.47	1.39
12	cA	809	CLA	CHD-C4C	3.67	1.47	1.39
12	cA	827	CLA	CHD-C4C	3.67	1.47	1.39
12	bB	906	CLA	C1D-ND	3.66	1.42	1.37
12	cA	834	CLA	C1D-ND	3.66	1.42	1.37
12	bB	929	CLA	C3D-C2D	3.66	1.49	1.39
12	cB	915	CLA	CHD-C4C	3.66	1.47	1.39
12	aA	827	CLA	CHD-C4C	3.66	1.47	1.39
12	bA	842	CLA	C3D-C2D	3.66	1.49	1.39
12	aB	934	CLA	CHC-C4B	3.66	1.47	1.39
12	cA	804	CLA	C3D-C2D	3.66	1.49	1.39
12	aB	909	CLA	CHD-C1D	3.66	1.45	1.38
12	bB	904	CLA	CHD-C1D	3.66	1.45	1.38
12	bA	807	CLA	CHC-C4B	3.66	1.47	1.39
12	bB	915	CLA	CHD-C4C	3.66	1.47	1.39
12	aA	814	CLA	C3D-C2D	3.66	1.49	1.39
12	cB	912	CLA	O2A-CGA	3.66	1.44	1.33
12	aB	920	CLA	CHD-C1D	3.66	1.45	1.38
12	cA	837	CLA	CHD-C4C	3.66	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aA	805	CLA	C1B-NB	-3.66	1.33	1.37
12	cB	904	CLA	CHD-C1D	3.66	1.45	1.38
12	bF	202	CLA	C3D-C2D	3.66	1.49	1.39
12	aB	919	CLA	CHC-C4B	3.66	1.47	1.39
12	cB	938	CLA	C4B-NB	-3.66	1.33	1.37
12	aA	829	CLA	CHD-C1D	3.66	1.45	1.38
12	cB	914	CLA	CHC-C4B	3.66	1.47	1.39
12	cB	910	CLA	C3D-C2D	3.66	1.49	1.39
12	bB	903	CLA	CHC-C4B	3.66	1.47	1.39
12	bA	843	CLA	C1D-ND	3.66	1.42	1.37
12	aB	917	CLA	CHD-C1D	3.66	1.45	1.38
15	aB	944	BCR	C1-C6	-3.65	1.49	1.53
12	aB	912	CLA	O2A-CGA	3.65	1.44	1.33
12	bL	202	CLA	CHD-C4C	3.65	1.47	1.39
12	aA	809	CLA	C1B-NB	-3.65	1.33	1.37
12	cA	809	CLA	C1B-NB	-3.65	1.33	1.37
12	bA	817	CLA	CHC-C4B	3.65	1.47	1.39
12	bA	805	CLA	C1B-NB	-3.65	1.33	1.37
12	bB	939	CLA	C1D-ND	3.65	1.42	1.37
12	cA	817	CLA	CHC-C4B	3.65	1.47	1.39
12	aA	836	CLA	C3D-C2D	3.65	1.48	1.39
12	aB	923	CLA	CHC-C4B	3.65	1.47	1.39
12	aA	834	CLA	C1D-ND	3.65	1.42	1.37
12	bB	924	CLA	CHD-C4C	3.65	1.47	1.39
12	bA	836	CLA	C3D-C2D	3.65	1.48	1.39
12	cB	918	CLA	C3D-C2D	3.65	1.48	1.39
12	cL	202	CLA	CHD-C4C	3.65	1.47	1.39
12	bB	919	CLA	CHC-C4B	3.65	1.47	1.39
12	bB	914	CLA	CHD-C1D	3.65	1.45	1.38
12	cB	933	CLA	C1D-ND	3.65	1.42	1.37
12	cB	920	CLA	CHD-C1D	3.64	1.45	1.38
12	aF	202	CLA	C3D-C2D	3.64	1.48	1.39
12	bA	814	CLA	C3D-C2D	3.64	1.48	1.39
12	cA	831	CLA	C3D-C2D	3.64	1.48	1.39
12	aL	203	CLA	CHC-C4B	3.64	1.47	1.39
12	cA	821	CLA	CHC-C4B	3.64	1.47	1.39
12	bA	841	CLA	CHD-C1D	3.64	1.45	1.38
12	bB	920	CLA	CHD-C1D	3.64	1.45	1.38
12	aA	814	CLA	CHD-C4C	3.64	1.47	1.39
12	bA	817	CLA	CHD-C4C	3.64	1.47	1.39
12	cA	805	CLA	CHC-C4B	3.64	1.47	1.39
12	aB	918	CLA	C3D-C2D	3.64	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cB	936	CLA	C3D-C2D	3.64	1.48	1.39
12	bB	917	CLA	CHD-C1D	3.64	1.45	1.38
12	bA	807	CLA	CHD-C4C	3.64	1.47	1.39
12	cA	814	CLA	C3D-C2D	3.64	1.48	1.39
12	bA	818	CLA	CHD-C4C	3.64	1.47	1.39
12	bA	833	CLA	C1D-ND	3.64	1.42	1.37
12	bB	909	CLA	CHD-C1D	3.64	1.45	1.38
12	aB	903	CLA	CHC-C4B	3.64	1.47	1.39
12	cA	853	CLA	CHC-C4B	3.64	1.47	1.39
12	aA	813	CLA	CHD-C4C	3.64	1.47	1.39
12	aB	922	CLA	C4B-NB	-3.64	1.33	1.37
12	cA	807	CLA	CHD-C4C	3.64	1.47	1.39
12	aA	805	CLA	C1D-ND	3.64	1.42	1.37
12	bB	918	CLA	C3D-C2D	3.64	1.48	1.39
12	cB	913	CLA	CHD-C1D	3.64	1.45	1.38
12	aA	817	CLA	CHD-C4C	3.64	1.47	1.39
12	cA	818	CLA	CHD-C4C	3.64	1.47	1.39
12	aB	939	CLA	CHB-C1B	3.63	1.47	1.39
12	cA	803	CLA	C3D-C2D	3.63	1.48	1.39
12	cL	203	CLA	CHC-C4B	3.63	1.47	1.39
12	cA	842	CLA	C3D-C2D	3.63	1.48	1.39
12	cA	808	CLA	C1B-NB	-3.63	1.33	1.37
12	bB	936	CLA	C3D-C2D	3.63	1.48	1.39
12	bB	913	CLA	CHD-C1D	3.63	1.45	1.38
12	bA	834	CLA	C3D-C2D	3.63	1.48	1.39
12	cF	202	CLA	C3D-C2D	3.63	1.48	1.39
12	cB	939	CLA	C1D-ND	3.63	1.42	1.37
12	cA	804	CLA	C4B-NB	-3.63	1.33	1.37
12	bB	923	CLA	CHC-C4B	3.63	1.47	1.39
12	aA	825	CLA	C3D-C2D	3.63	1.48	1.39
12	aA	805	CLA	CHD-C4C	3.63	1.47	1.39
12	bA	834	CLA	C1D-ND	3.63	1.42	1.37
12	bA	853	CLA	CHC-C4B	3.63	1.47	1.39
12	aA	807	CLA	CHD-C4C	3.63	1.47	1.39
12	cA	817	CLA	CHD-C4C	3.63	1.47	1.39
12	bA	808	CLA	C3D-C2D	3.63	1.48	1.39
12	cB	939	CLA	CHB-C1B	3.63	1.47	1.39
12	aA	821	CLA	C1D-ND	3.63	1.42	1.37
12	bL	203	CLA	CHD-C4C	3.62	1.47	1.39
12	aB	932	CLA	C3D-C2D	3.62	1.48	1.39
12	aA	808	CLA	C3D-C2D	3.62	1.48	1.39
12	cB	908	CLA	CHD-C4C	3.62	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aA	821	CLA	CHC-C4B	3.62	1.47	1.39
12	aA	834	CLA	C3D-C2D	3.62	1.48	1.39
12	cA	814	CLA	CHD-C4C	3.62	1.47	1.39
12	cB	938	CLA	CHD-C4C	3.62	1.47	1.39
12	aB	924	CLA	CHD-C4C	3.62	1.47	1.39
12	cB	916	CLA	CHC-C4B	3.62	1.47	1.39
12	cA	808	CLA	C3D-C2D	3.62	1.48	1.39
12	aB	916	CLA	C3D-C2D	3.62	1.48	1.39
12	bA	813	CLA	CHD-C4C	3.62	1.47	1.39
12	aB	913	CLA	C3D-C2D	3.62	1.48	1.39
12	cA	825	CLA	C3D-C2D	3.62	1.48	1.39
12	cA	806	CLA	CHD-C1D	3.62	1.45	1.38
12	cB	923	CLA	CHD-C1D	3.62	1.45	1.38
12	bL	203	CLA	CHC-C4B	3.62	1.47	1.39
12	aA	841	CLA	CHD-C1D	3.62	1.45	1.38
12	bA	825	CLA	C3D-C2D	3.62	1.48	1.39
12	cA	834	CLA	C3D-C2D	3.61	1.48	1.39
12	bA	810	CLA	CHD-C4C	3.61	1.47	1.39
12	bA	821	CLA	CHC-C4B	3.61	1.47	1.39
12	cB	914	CLA	CHD-C1D	3.61	1.45	1.38
12	cB	916	CLA	C3D-C2D	3.61	1.48	1.39
12	cA	813	CLA	CHD-C4C	3.61	1.47	1.39
12	bB	933	CLA	C1D-ND	3.61	1.42	1.37
12	cB	903	CLA	CHC-C4B	3.61	1.47	1.39
15	bB	941	BCR	C1-C6	-3.61	1.49	1.53
12	cL	203	CLA	CHD-C4C	3.61	1.47	1.39
12	cA	821	CLA	C1D-ND	3.61	1.42	1.37
12	bA	803	CLA	C3D-C2D	3.61	1.48	1.39
12	aB	904	CLA	CHD-C4C	3.61	1.47	1.39
12	cB	913	CLA	C3D-C2D	3.61	1.48	1.39
12	aA	803	CLA	C3D-C2D	3.61	1.48	1.39
12	bB	916	CLA	C3D-C2D	3.61	1.48	1.39
12	bB	904	CLA	CHD-C4C	3.61	1.47	1.39
12	bB	908	CLA	CHD-C4C	3.61	1.47	1.39
12	aB	936	CLA	C3D-C2D	3.61	1.48	1.39
12	aA	838	CLA	CHD-C1D	3.61	1.45	1.38
12	aB	919	CLA	CHD-C4C	3.61	1.47	1.39
12	bB	939	CLA	CHB-C1B	3.61	1.47	1.39
12	aA	818	CLA	CHD-C1D	3.61	1.45	1.38
12	aB	923	CLA	CHD-C1D	3.61	1.45	1.38
12	cA	829	CLA	CHD-C1D	3.61	1.45	1.38
12	bA	805	CLA	CHD-C4C	3.61	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cA	816	CLA	C3D-C2D	3.61	1.48	1.39
12	aA	806	CLA	CHD-C1D	3.60	1.45	1.38
12	bA	806	CLA	CHD-C1D	3.60	1.45	1.38
12	cA	822	CLA	CHD-C1D	3.60	1.45	1.38
12	cA	838	CLA	CHC-C4B	3.60	1.47	1.39
12	bA	818	CLA	CHD-C1D	3.60	1.45	1.38
12	cA	843	CLA	C1D-ND	3.60	1.42	1.37
12	bA	814	CLA	CHD-C4C	3.60	1.47	1.39
12	cB	904	CLA	CHD-C4C	3.60	1.47	1.39
12	cA	818	CLA	CHD-C1D	3.60	1.45	1.38
12	cB	932	CLA	C3D-C2D	3.60	1.48	1.39
12	cB	911	CLA	CHC-C4B	3.60	1.47	1.39
12	aB	926	CLA	C3D-C2D	3.60	1.48	1.39
13	bB	940	1L3	C28-C26	3.60	1.58	1.51
12	bA	805	CLA	CHC-C4B	3.60	1.47	1.39
12	bB	911	CLA	CHC-C4B	3.60	1.47	1.39
12	bA	805	CLA	C1D-ND	3.60	1.42	1.37
12	cB	924	CLA	CHD-C4C	3.60	1.47	1.39
12	bA	822	CLA	CHD-C1D	3.60	1.45	1.38
12	cA	841	CLA	CHD-C1D	3.60	1.45	1.38
12	bB	913	CLA	C3D-C2D	3.60	1.48	1.39
12	bB	913	CLA	C1D-ND	3.60	1.42	1.37
12	bB	918	CLA	C1D-ND	3.60	1.42	1.37
12	cB	922	CLA	C4B-NB	-3.60	1.33	1.37
12	bB	932	CLA	C3D-C2D	3.60	1.48	1.39
12	bA	829	CLA	CHD-C1D	3.60	1.45	1.38
12	bA	812	CLA	CHD-C4C	3.60	1.47	1.39
12	bB	926	CLA	C3D-C2D	3.60	1.48	1.39
12	aL	203	CLA	CHD-C4C	3.60	1.47	1.39
12	aB	914	CLA	CHD-C1D	3.60	1.45	1.38
12	bA	816	CLA	C3D-C2D	3.60	1.48	1.39
12	cB	929	CLA	CHD-C4C	3.59	1.47	1.39
12	aB	901	CLA	C4B-NB	-3.59	1.33	1.37
12	cB	930	CLA	CHD-C4C	3.59	1.47	1.39
12	bB	916	CLA	CHC-C4B	3.59	1.47	1.39
12	aA	822	CLA	CHD-C1D	3.59	1.45	1.38
12	bB	950	CLA	C1D-ND	3.59	1.42	1.37
12	aA	805	CLA	CHC-C4B	3.59	1.47	1.39
12	bB	950	CLA	CHD-C1D	3.59	1.45	1.38
12	cB	935	CLA	CHD-C1D	3.59	1.45	1.38
12	cB	913	CLA	C1D-ND	3.59	1.42	1.37
12	aB	935	CLA	CHD-C1D	3.59	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cB	923	CLA	CHC-C4B	3.59	1.47	1.39
12	cB	921	CLA	C3D-C2D	3.59	1.48	1.39
12	aA	811	CLA	C4B-NB	-3.59	1.33	1.37
12	aA	816	CLA	C3D-C2D	3.59	1.48	1.39
12	bA	838	CLA	CHD-C1D	3.59	1.45	1.38
12	aA	844	CLA	C1D-ND	3.59	1.42	1.37
12	aA	819	CLA	CHD-C4C	3.59	1.47	1.39
12	bB	933	CLA	CHC-C4B	3.59	1.47	1.39
12	bA	824	CLA	C4B-NB	-3.59	1.33	1.37
12	bA	841	CLA	C3D-C2D	3.59	1.48	1.39
13	aB	940	1L3	C28-C26	3.59	1.58	1.51
12	aA	812	CLA	CHD-C1D	3.59	1.45	1.38
12	aA	803	CLA	CHD-C4C	3.59	1.47	1.39
12	cL	202	CLA	C4B-NB	-3.59	1.33	1.37
12	bB	919	CLA	CHD-C4C	3.59	1.47	1.39
12	bB	902	CLA	C4B-NB	-3.58	1.33	1.37
12	bB	920	CLA	C1B-NB	-3.58	1.33	1.37
12	bB	923	CLA	CHD-C1D	3.58	1.45	1.38
12	aA	804	CLA	CHD-C4C	3.58	1.47	1.39
12	aB	950	CLA	C1D-ND	3.58	1.42	1.37
12	bA	811	CLA	C3D-C2D	3.58	1.48	1.39
12	cA	811	CLA	C3D-C2D	3.58	1.48	1.39
12	aA	802	CLA	C1D-ND	3.58	1.42	1.37
12	aA	831	CLA	C4B-NB	-3.58	1.33	1.37
12	cA	820	CLA	CHD-C4C	3.58	1.47	1.39
12	bB	925	CLA	CHD-C1D	3.58	1.45	1.38
12	aA	820	CLA	CHD-C4C	3.58	1.47	1.39
12	bB	930	CLA	CHD-C4C	3.58	1.47	1.39
12	aA	811	CLA	C3D-C2D	3.58	1.48	1.39
12	cB	933	CLA	CHC-C4B	3.58	1.47	1.39
12	cB	926	CLA	C3D-C2D	3.58	1.48	1.39
12	aA	841	CLA	C3D-C2D	3.58	1.48	1.39
13	cB	940	1L3	C28-C26	3.58	1.58	1.51
12	cA	831	CLA	C4B-NB	-3.58	1.33	1.37
12	cB	920	CLA	C1B-NB	-3.58	1.33	1.37
12	aA	838	CLA	CHC-C4B	3.58	1.47	1.39
12	aA	821	CLA	C3D-C2D	3.58	1.48	1.39
12	aB	916	CLA	CHC-C4B	3.58	1.47	1.39
12	cA	803	CLA	CHD-C4C	3.58	1.47	1.39
12	cA	805	CLA	CHD-C4C	3.58	1.47	1.39
12	aB	913	CLA	C1D-ND	3.58	1.42	1.37
12	aA	824	CLA	C4B-NB	-3.58	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bB	929	CLA	CHC-C4B	3.57	1.47	1.39
12	aA	807	CLA	CHD-C1D	3.57	1.45	1.38
12	aB	925	CLA	CHD-C1D	3.57	1.45	1.38
12	cA	812	CLA	CHC-C4B	3.57	1.47	1.39
12	cF	202	CLA	C1B-NB	-3.57	1.33	1.37
12	aB	902	CLA	C4B-NB	-3.57	1.33	1.37
12	bA	803	CLA	CHD-C4C	3.57	1.47	1.39
12	bA	831	CLA	C4B-NB	-3.57	1.33	1.37
12	bA	829	CLA	CHD-C4C	3.57	1.47	1.39
12	cF	202	CLA	OBD-CAD	3.57	1.28	1.22
12	bA	814	CLA	CHB-C1B	3.57	1.47	1.39
12	aB	921	CLA	C3D-C2D	3.57	1.48	1.39
12	bA	820	CLA	CHD-C4C	3.57	1.47	1.39
12	cB	911	CLA	C3D-C2D	3.57	1.48	1.39
12	bB	922	CLA	C4B-NB	-3.57	1.33	1.37
12	cA	810	CLA	CHD-C4C	3.57	1.47	1.39
12	aA	806	CLA	C1D-ND	3.57	1.42	1.37
12	cA	809	CLA	C4B-NB	-3.57	1.33	1.37
12	cA	821	CLA	C3D-C2D	3.57	1.48	1.39
12	aB	930	CLA	CHD-C4C	3.57	1.47	1.39
12	aB	933	CLA	C1D-ND	3.57	1.42	1.37
12	bB	927	CLA	CHD-C4C	3.57	1.47	1.39
12	cA	838	CLA	CHD-C1D	3.57	1.45	1.38
12	aB	933	CLA	CHC-C4B	3.57	1.47	1.39
12	bA	821	CLA	C1D-ND	3.57	1.42	1.37
12	cA	812	CLA	CHD-C1D	3.57	1.45	1.38
12	cA	807	CLA	CHD-C1D	3.57	1.45	1.38
12	aA	810	CLA	CHD-C4C	3.57	1.47	1.39
12	bB	921	CLA	C3D-C2D	3.56	1.48	1.39
12	aB	913	CLA	CHD-C4C	3.56	1.47	1.39
12	bA	811	CLA	C4B-NB	-3.56	1.33	1.37
12	bB	935	CLA	CHD-C1D	3.56	1.45	1.38
12	aB	911	CLA	C3D-C2D	3.56	1.48	1.39
12	aB	911	CLA	CHC-C4B	3.56	1.47	1.39
12	aA	809	CLA	C3D-C2D	3.56	1.48	1.39
12	cA	841	CLA	C3D-C2D	3.56	1.48	1.39
12	bA	809	CLA	C3D-C2D	3.56	1.48	1.39
12	bL	202	CLA	C4B-NB	-3.56	1.33	1.37
12	cA	809	CLA	C3D-C2D	3.56	1.48	1.39
12	bA	838	CLA	CHC-C4B	3.56	1.47	1.39
12	bA	843	CLA	CHB-C1B	3.56	1.47	1.39
12	bA	819	CLA	CHD-C4C	3.56	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cB	935	CLA	CHC-C4B	3.56	1.47	1.39
15	cB	941	BCR	C1-C6	-3.56	1.49	1.53
12	bA	821	CLA	C3D-C2D	3.56	1.48	1.39
12	aA	843	CLA	CHB-C1B	3.56	1.47	1.39
12	aB	950	CLA	CHD-C1D	3.56	1.45	1.38
12	aB	920	CLA	C1B-NB	-3.56	1.33	1.37
12	aB	939	CLA	C1D-ND	3.56	1.42	1.37
12	cB	924	CLA	C3D-C2D	3.56	1.48	1.39
12	bA	804	CLA	CHD-C4C	3.56	1.47	1.39
12	cB	919	CLA	CHD-C4C	3.56	1.47	1.39
12	cA	804	CLA	CHD-C4C	3.56	1.47	1.39
12	aB	920	CLA	CHC-C4B	3.56	1.47	1.39
12	aA	812	CLA	CHC-C4B	3.56	1.47	1.39
12	cA	811	CLA	C4B-NB	-3.56	1.33	1.37
12	cB	920	CLA	CHC-C4B	3.55	1.47	1.39
12	bL	204	CLA	CHD-C4C	3.55	1.47	1.39
12	aA	804	CLA	CHB-C1B	3.55	1.47	1.39
12	bB	911	CLA	C3D-C2D	3.55	1.48	1.39
12	cB	927	CLA	CHD-C4C	3.55	1.47	1.39
12	bA	812	CLA	CHD-C1D	3.55	1.45	1.38
12	aA	835	CLA	CHD-C4C	3.55	1.47	1.39
12	bA	835	CLA	CHD-C4C	3.55	1.47	1.39
12	cA	819	CLA	CHD-C4C	3.55	1.47	1.39
12	aB	908	CLA	CHD-C4C	3.55	1.47	1.39
12	aB	908	CLA	C4B-NB	-3.55	1.33	1.37
12	bB	906	CLA	C4B-NB	-3.55	1.33	1.37
12	cA	829	CLA	CHD-C4C	3.55	1.47	1.39
12	bB	901	CLA	C4B-NB	-3.55	1.33	1.37
12	aA	814	CLA	CHB-C1B	3.55	1.47	1.39
12	aA	812	CLA	C3D-C2D	3.55	1.48	1.39
12	cL	204	CLA	CHB-C1B	3.55	1.47	1.39
15	aB	941	BCR	C1-C6	-3.55	1.49	1.53
12	aB	924	CLA	C3D-C2D	3.55	1.48	1.39
12	aB	929	CLA	CHC-C4B	3.55	1.47	1.39
12	aL	204	CLA	CHB-C1B	3.55	1.47	1.39
12	bA	828	CLA	C3D-C2D	3.54	1.48	1.39
12	cA	843	CLA	CHB-C1B	3.54	1.47	1.39
12	aA	827	CLA	C1D-ND	3.54	1.42	1.37
12	bA	806	CLA	C1D-ND	3.54	1.42	1.37
12	aA	828	CLA	C3D-C2D	3.54	1.48	1.39
12	aA	829	CLA	C3D-C2D	3.54	1.48	1.39
12	bB	937	CLA	CHC-C4B	3.54	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cA	814	CLA	CHB-C1B	3.54	1.47	1.39
12	aA	825	CLA	CHD-C4C	3.54	1.47	1.39
12	aB	927	CLA	CHD-C4C	3.54	1.47	1.39
12	aB	905	CLA	CHD-C1D	3.54	1.45	1.38
12	cB	902	CLA	C4B-NB	-3.54	1.33	1.37
12	bA	838	CLA	CHD-C4C	3.54	1.47	1.39
12	bB	913	CLA	CHD-C4C	3.54	1.47	1.39
12	bB	934	CLA	OBD-CAD	3.54	1.28	1.22
12	bA	832	CLA	C3D-C2D	3.54	1.48	1.39
12	bB	924	CLA	C3D-C2D	3.54	1.48	1.39
12	bA	842	CLA	C4B-NB	-3.54	1.33	1.37
12	cB	936	CLA	C4B-NB	-3.54	1.33	1.37
12	aB	935	CLA	CHC-C4B	3.54	1.47	1.39
12	cA	825	CLA	CHD-C4C	3.54	1.47	1.39
12	bB	935	CLA	CHC-C4B	3.54	1.47	1.39
12	cA	824	CLA	C4B-NB	-3.54	1.33	1.37
12	cA	835	CLA	CHD-C4C	3.54	1.47	1.39
12	aA	832	CLA	C3D-C2D	3.54	1.48	1.39
12	aA	844	CLA	CHD-C1D	3.54	1.45	1.38
12	bA	804	CLA	C4B-NB	-3.54	1.33	1.37
12	cA	853	CLA	C4B-NB	-3.54	1.33	1.37
12	cB	901	CLA	C4B-NB	-3.54	1.33	1.37
12	bA	807	CLA	CHD-C1D	3.54	1.45	1.38
12	bB	920	CLA	CHC-C4B	3.54	1.47	1.39
12	cA	802	CLA	C1D-ND	3.54	1.42	1.37
12	cB	929	CLA	CHC-C4B	3.54	1.47	1.39
12	cA	812	CLA	CHD-C4C	3.54	1.47	1.39
12	bF	202	CLA	C1B-NB	-3.53	1.33	1.37
12	bA	802	CLA	C3D-C2D	3.53	1.48	1.39
12	aA	829	CLA	CHD-C4C	3.53	1.47	1.39
12	cA	832	CLA	C3D-C2D	3.53	1.48	1.39
12	bA	827	CLA	C1D-ND	3.53	1.42	1.37
12	cA	812	CLA	C3D-C2D	3.53	1.48	1.39
12	aB	934	CLA	OBD-CAD	3.53	1.28	1.22
12	cA	836	CLA	OBD-CAD	3.53	1.28	1.22
12	aL	204	CLA	CHD-C4C	3.53	1.47	1.39
12	aL	202	CLA	C4B-NB	-3.53	1.33	1.37
12	bA	833	CLA	CHD-C4C	3.53	1.47	1.39
12	aA	812	CLA	CHD-C4C	3.53	1.47	1.39
12	aA	826	CLA	CHC-C4B	3.53	1.47	1.39
12	bA	812	CLA	C3D-C2D	3.53	1.48	1.39
12	bA	804	CLA	CHB-C1B	3.53	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bB	930	CLA	C4B-NB	-3.53	1.33	1.37
12	cL	204	CLA	CHD-C4C	3.53	1.47	1.39
12	bA	829	CLA	C3D-C2D	3.53	1.48	1.39
12	bB	931	CLA	C1D-ND	3.53	1.42	1.37
12	aA	833	CLA	CHD-C4C	3.53	1.47	1.39
12	cB	925	CLA	CHD-C1D	3.53	1.45	1.38
12	bA	827	CLA	CHC-C4B	3.53	1.47	1.39
12	aB	937	CLA	CHC-C4B	3.53	1.47	1.39
12	bB	905	CLA	CHD-C1D	3.53	1.45	1.38
12	bA	842	CLA	CHD-C1D	3.53	1.45	1.38
12	aA	838	CLA	C3D-C2D	3.53	1.48	1.39
12	bL	204	CLA	CHB-C1B	3.53	1.47	1.39
12	cB	908	CLA	CHC-C1C	3.53	1.45	1.38
12	aB	915	CLA	C3D-C2D	3.52	1.48	1.39
12	cA	842	CLA	CHD-C1D	3.52	1.45	1.38
12	cA	829	CLA	C3D-C2D	3.52	1.48	1.39
12	aB	929	CLA	CHD-C4C	3.52	1.47	1.39
12	cA	827	CLA	CHC-C4B	3.52	1.47	1.39
12	cB	906	CLA	CHD-C1D	3.52	1.45	1.38
12	bA	820	CLA	CHC-C4B	3.52	1.47	1.39
12	cA	819	CLA	C3D-C2D	3.52	1.48	1.39
12	bB	906	CLA	CHC-C4B	3.52	1.47	1.39
12	bA	819	CLA	C3D-C2D	3.52	1.48	1.39
12	bB	917	CLA	C4B-NB	-3.52	1.33	1.37
12	bA	825	CLA	CHD-C4C	3.52	1.47	1.39
12	bB	909	CLA	C3D-C2D	3.52	1.48	1.39
12	bF	202	CLA	OBD-CAD	3.52	1.28	1.22
12	aA	804	CLA	C4B-NB	-3.52	1.33	1.37
12	cA	827	CLA	C1D-ND	3.52	1.42	1.37
12	cA	827	CLA	CHD-C1D	3.52	1.45	1.38
12	cA	828	CLA	C3D-C2D	3.52	1.48	1.39
12	aA	826	CLA	C4B-NB	-3.52	1.33	1.37
12	cA	842	CLA	C4B-NB	-3.52	1.33	1.37
12	cA	804	CLA	CHB-C1B	3.52	1.47	1.39
12	bA	812	CLA	CHC-C4B	3.52	1.47	1.39
12	aB	930	CLA	C4B-NB	-3.52	1.33	1.37
12	cA	838	CLA	CHD-C4C	3.52	1.47	1.39
12	cB	931	CLA	C1D-ND	3.52	1.42	1.37
12	bB	909	CLA	CHB-C1B	3.52	1.47	1.39
12	aA	827	CLA	CHD-C1D	3.52	1.45	1.38
12	cA	817	CLA	C1B-NB	-3.52	1.33	1.37
12	cB	906	CLA	C3D-C2D	3.52	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bB	929	CLA	CHD-C4C	3.52	1.47	1.39
12	cB	905	CLA	CHD-C1D	3.51	1.45	1.38
12	aL	202	CLA	CHC-C4B	3.51	1.47	1.39
12	cB	937	CLA	CHC-C4B	3.51	1.47	1.39
12	bA	808	CLA	CHC-C4B	3.51	1.47	1.39
12	bB	908	CLA	C4B-NB	-3.51	1.33	1.37
12	bB	906	CLA	C3D-C2D	3.51	1.48	1.39
12	aB	906	CLA	CHD-C1D	3.51	1.45	1.38
12	aB	931	CLA	C1D-ND	3.51	1.42	1.37
12	cB	928	CLA	CHB-C1B	3.51	1.47	1.39
12	aA	802	CLA	C3D-C2D	3.51	1.48	1.39
12	aB	928	CLA	CHD-C4C	3.51	1.47	1.39
12	aF	202	CLA	OBD-CAD	3.51	1.28	1.22
12	cA	809	CLA	CHC-C4B	3.51	1.47	1.39
12	aA	803	CLA	C4B-NB	-3.51	1.33	1.37
12	aA	842	CLA	C4B-NB	-3.51	1.33	1.37
12	bL	204	CLA	C4B-NB	-3.51	1.33	1.37
12	aB	905	CLA	CHC-C4B	3.51	1.47	1.39
12	cB	906	CLA	CHC-C4B	3.51	1.47	1.39
12	cB	917	CLA	C4B-NB	-3.51	1.33	1.37
12	aA	819	CLA	C3D-C2D	3.51	1.48	1.39
12	cB	908	CLA	C4B-NB	-3.51	1.33	1.37
12	cB	930	CLA	C4B-NB	-3.51	1.33	1.37
12	aA	815	CLA	CHC-C4B	3.51	1.47	1.39
12	bB	906	CLA	CHD-C1D	3.51	1.45	1.38
12	bB	908	CLA	CHC-C1C	3.51	1.45	1.38
12	bA	838	CLA	C3D-C2D	3.51	1.48	1.39
12	cA	806	CLA	C1D-ND	3.51	1.42	1.37
12	aA	854	CLA	C4B-NB	-3.51	1.33	1.37
12	bB	915	CLA	C3D-C2D	3.50	1.48	1.39
12	cA	820	CLA	CHC-C4B	3.50	1.47	1.39
12	aB	906	CLA	C3D-C2D	3.50	1.48	1.39
12	aA	820	CLA	CHC-C4B	3.50	1.47	1.39
12	cA	838	CLA	C3D-C2D	3.50	1.48	1.39
12	cB	934	CLA	OBD-CAD	3.50	1.28	1.22
12	cA	808	CLA	CHC-C4B	3.50	1.47	1.39
12	cA	802	CLA	C3D-C2D	3.50	1.48	1.39
12	cB	913	CLA	CHD-C4C	3.50	1.47	1.39
12	aA	836	CLA	OBD-CAD	3.50	1.28	1.22
12	aB	909	CLA	CHB-C1B	3.50	1.47	1.39
12	aB	909	CLA	C3D-C2D	3.50	1.48	1.39
12	aA	827	CLA	CHC-C4B	3.50	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cA	842	CLA	CHC-C4B	3.50	1.47	1.39
12	aA	836	CLA	CHB-C1B	3.50	1.47	1.39
12	cA	833	CLA	CHD-C4C	3.50	1.47	1.39
12	bB	923	CLA	CHD-C4C	3.50	1.47	1.39
12	cB	905	CLA	CHC-C4B	3.50	1.47	1.39
12	bA	815	CLA	CHC-C4B	3.50	1.47	1.39
12	aB	937	CLA	C3D-C2D	3.50	1.48	1.39
12	bB	949	CLA	CHB-C1B	3.50	1.47	1.39
12	bA	826	CLA	CHC-C4B	3.50	1.47	1.39
12	cB	937	CLA	C3D-C2D	3.50	1.48	1.39
12	bL	204	CLA	CHC-C4B	3.50	1.47	1.39
12	cB	923	CLA	CHD-C4C	3.50	1.47	1.39
12	cA	815	CLA	CHC-C4B	3.49	1.47	1.39
12	bB	928	CLA	CHB-C1B	3.49	1.47	1.39
12	aA	809	CLA	CHC-C4B	3.49	1.47	1.39
12	aA	844	CLA	CHD-C4C	3.49	1.47	1.39
12	aA	842	CLA	CHD-C1D	3.49	1.45	1.38
12	cB	917	CLA	CHD-C4C	3.49	1.47	1.39
12	cB	915	CLA	C3D-C2D	3.49	1.48	1.39
12	aB	906	CLA	C4B-NB	-3.49	1.33	1.37
12	cB	909	CLA	C3D-C2D	3.49	1.48	1.39
12	bA	827	CLA	CHD-C1D	3.49	1.45	1.38
12	bB	905	CLA	CHC-C4B	3.49	1.47	1.39
12	cA	826	CLA	CHC-C4B	3.49	1.47	1.39
12	bB	950	CLA	CHD-C4C	3.49	1.47	1.39
12	aB	949	CLA	CHC-C4B	3.49	1.47	1.39
12	aA	838	CLA	CHD-C4C	3.49	1.47	1.39
12	bB	928	CLA	CHD-C4C	3.49	1.47	1.39
12	cA	829	CLA	C1D-ND	3.49	1.42	1.37
12	bA	809	CLA	C4B-NB	-3.49	1.33	1.37
12	bB	903	CLA	C3D-C2D	3.49	1.48	1.39
12	cA	836	CLA	CHB-C1B	3.49	1.47	1.39
12	cL	202	CLA	CHC-C4B	3.49	1.47	1.39
12	bA	809	CLA	CHC-C4B	3.49	1.47	1.39
12	cB	914	CLA	CHD-C4C	3.49	1.47	1.39
12	bL	202	CLA	CHC-C4B	3.49	1.47	1.39
12	aB	950	CLA	CHD-C4C	3.49	1.47	1.39
12	aA	844	CLA	CHB-C1B	3.49	1.47	1.39
12	cB	928	CLA	CHD-C4C	3.49	1.47	1.39
12	bA	836	CLA	OBD-CAD	3.49	1.28	1.22
12	cB	909	CLA	CHB-C1B	3.49	1.47	1.39
12	cB	903	CLA	C3D-C2D	3.49	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cA	812	CLA	C4B-NB	-3.49	1.33	1.37
12	bA	817	CLA	C1B-NB	-3.49	1.33	1.37
12	cB	906	CLA	C4B-NB	-3.48	1.33	1.37
12	bB	906	CLA	CHD-C4C	3.48	1.47	1.39
12	aB	908	CLA	CHC-C1C	3.48	1.45	1.38
12	bB	914	CLA	CHD-C4C	3.48	1.47	1.39
12	bB	905	CLA	CHD-C4C	3.48	1.47	1.39
12	aA	812	CLA	C4B-NB	-3.48	1.33	1.37
12	aB	921	CLA	CHC-C4B	3.48	1.47	1.39
12	bB	950	CLA	CHB-C1B	3.48	1.47	1.39
12	bB	937	CLA	C3D-C2D	3.48	1.48	1.39
12	aA	808	CLA	CHC-C4B	3.48	1.47	1.39
12	aB	915	CLA	C1B-NB	-3.48	1.33	1.37
12	aB	903	CLA	C3D-C2D	3.48	1.48	1.39
12	aB	914	CLA	CHD-C4C	3.48	1.47	1.39
12	bB	936	CLA	C4B-NB	-3.48	1.33	1.37
12	cA	833	CLA	C3D-C2D	3.48	1.48	1.39
12	aB	932	CLA	C4B-NB	-3.48	1.33	1.37
12	cA	803	CLA	C4B-NB	-3.48	1.33	1.37
12	aB	917	CLA	C4B-NB	-3.48	1.33	1.37
12	bA	803	CLA	C4B-NB	-3.48	1.33	1.37
12	aB	917	CLA	CHD-C4C	3.48	1.47	1.39
12	aA	816	CLA	CHB-C1B	3.47	1.47	1.39
12	aA	842	CLA	CHC-C4B	3.47	1.47	1.39
12	aF	202	CLA	C1B-NB	-3.47	1.33	1.37
12	cA	823	CLA	C3D-C2D	3.47	1.48	1.39
12	aA	809	CLA	C4B-NB	-3.47	1.33	1.37
12	cB	925	CLA	CHD-C4C	3.47	1.47	1.39
12	cA	820	CLA	CHB-C1B	3.47	1.47	1.39
12	cA	837	CLA	CHD-C1D	3.47	1.45	1.38
12	aB	919	CLA	C3D-C2D	3.47	1.48	1.39
12	aB	919	CLA	C1B-NB	-3.47	1.33	1.37
12	aB	906	CLA	CHC-C4B	3.47	1.47	1.39
12	bA	820	CLA	CHB-C1B	3.47	1.47	1.39
12	bB	915	CLA	CHC-C4B	3.47	1.47	1.39
12	aA	823	CLA	C3D-C2D	3.47	1.48	1.39
12	aB	922	CLA	CHD-C1D	3.47	1.45	1.38
12	aA	817	CLA	C1B-NB	-3.47	1.33	1.37
12	bA	802	CLA	C1D-ND	3.47	1.42	1.37
12	cB	906	CLA	CHD-C4C	3.47	1.47	1.39
12	aA	823	CLA	CHC-C4B	3.47	1.47	1.39
12	bA	842	CLA	CHC-C4B	3.47	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aB	949	CLA	CHB-C1B	3.47	1.47	1.39
12	bA	826	CLA	C4B-NB	-3.47	1.33	1.37
12	aA	840	CLA	C4B-NB	-3.47	1.33	1.37
12	aL	204	CLA	C4B-NB	-3.47	1.33	1.37
12	cB	919	CLA	C3D-C2D	3.47	1.48	1.39
12	cB	915	CLA	CHC-C4B	3.47	1.47	1.39
12	cA	840	CLA	C4B-NB	-3.47	1.33	1.37
12	cB	921	CLA	CHC-C4B	3.47	1.47	1.39
12	bB	917	CLA	CHD-C4C	3.47	1.47	1.39
12	bB	919	CLA	C3D-C2D	3.47	1.48	1.39
12	aB	928	CLA	CHB-C1B	3.46	1.47	1.39
12	cB	949	CLA	CHB-C1B	3.46	1.47	1.39
12	aB	923	CLA	CHD-C4C	3.46	1.47	1.39
12	bA	853	CLA	C4B-NB	-3.46	1.33	1.37
12	aB	925	CLA	CHD-C4C	3.46	1.47	1.39
12	aB	915	CLA	CHC-C4B	3.46	1.47	1.39
12	cB	949	CLA	CHC-C4B	3.46	1.47	1.39
12	bA	837	CLA	CHD-C1D	3.46	1.45	1.38
12	aB	922	CLA	C1D-ND	3.46	1.42	1.37
12	bA	823	CLA	CHC-C4B	3.46	1.47	1.39
12	bB	922	CLA	CHD-C1D	3.46	1.45	1.38
12	bA	836	CLA	CHB-C1B	3.46	1.47	1.39
12	bB	925	CLA	CHD-C4C	3.46	1.47	1.39
12	bB	921	CLA	CHC-C4B	3.46	1.47	1.39
12	cB	905	CLA	CHD-C4C	3.46	1.47	1.39
12	aA	840	CLA	CHC-C4B	3.46	1.47	1.39
12	cB	930	CLA	CHC-C4B	3.46	1.47	1.39
12	bA	823	CLA	C3D-C2D	3.46	1.48	1.39
12	bL	204	CLA	C3D-C2D	3.46	1.48	1.39
12	bB	905	CLA	CHB-C1B	3.46	1.47	1.39
12	aB	906	CLA	CHD-C4C	3.45	1.47	1.39
12	bA	831	CLA	CHD-C4C	3.45	1.47	1.39
12	cL	204	CLA	C4B-NB	-3.45	1.33	1.37
12	aB	936	CLA	C4B-NB	-3.45	1.33	1.37
12	bB	909	CLA	CHC-C4B	3.45	1.47	1.39
12	bA	812	CLA	C4B-NB	-3.45	1.33	1.37
12	bA	833	CLA	C4B-NB	-3.45	1.33	1.37
12	bA	833	CLA	C3D-C2D	3.45	1.48	1.39
12	aB	938	CLA	CHC-C4B	3.45	1.47	1.39
12	bB	929	CLA	C4B-NB	-3.45	1.33	1.37
12	cB	915	CLA	C1B-NB	-3.45	1.33	1.37
12	aB	950	CLA	CHB-C1B	3.45	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aA	833	CLA	C3D-C2D	3.45	1.48	1.39
12	bA	826	CLA	C1D-ND	3.45	1.42	1.37
15	bB	943	BCR	C1-C6	-3.45	1.49	1.53
12	aB	909	CLA	CHD-C4C	3.45	1.47	1.39
12	aA	829	CLA	C1D-ND	3.45	1.42	1.37
12	bA	813	CLA	OBD-CAD	3.45	1.28	1.22
12	cA	823	CLA	CHC-C4B	3.45	1.47	1.39
12	aL	204	CLA	CHC-C4B	3.44	1.47	1.39
12	bB	949	CLA	CHC-C4B	3.44	1.47	1.39
12	aA	831	CLA	CHD-C4C	3.44	1.47	1.39
12	cB	902	CLA	CHC-C4B	3.44	1.47	1.39
12	bA	814	CLA	C4B-NB	-3.44	1.33	1.37
12	cB	928	CLA	C1D-ND	3.44	1.42	1.37
12	aB	929	CLA	C4B-NB	-3.44	1.33	1.37
12	aB	930	CLA	CHC-C4B	3.44	1.47	1.39
12	cL	204	CLA	CHC-C4B	3.44	1.47	1.39
12	cA	814	CLA	C4B-NB	-3.44	1.33	1.37
12	cA	826	CLA	C4B-NB	-3.44	1.33	1.37
12	aA	837	CLA	CHD-C1D	3.44	1.45	1.38
12	cL	204	CLA	C3D-C2D	3.44	1.48	1.39
12	aA	820	CLA	CHB-C1B	3.44	1.47	1.39
12	aA	833	CLA	C4B-NB	-3.44	1.33	1.37
12	bA	840	CLA	CHC-C4B	3.44	1.47	1.39
12	aL	203	CLA	C1D-ND	3.44	1.42	1.37
12	bB	930	CLA	CHC-C4B	3.44	1.47	1.39
12	cB	929	CLA	C4B-NB	-3.43	1.33	1.37
12	bB	938	CLA	CHC-C4B	3.43	1.47	1.39
12	cB	909	CLA	CHC-C4B	3.43	1.47	1.39
12	aL	204	CLA	C3D-C2D	3.43	1.48	1.39
12	aB	905	CLA	CHD-C4C	3.43	1.47	1.39
12	bB	904	CLA	C3D-C2D	3.43	1.48	1.39
12	aB	904	CLA	C3D-C2D	3.43	1.48	1.39
12	cL	203	CLA	C1D-ND	3.43	1.42	1.37
12	bB	915	CLA	C1B-NB	-3.43	1.33	1.37
12	bB	932	CLA	C4B-NB	-3.43	1.33	1.37
12	bB	911	CLA	CHD-C4C	3.43	1.47	1.39
12	cB	909	CLA	CHD-C4C	3.43	1.47	1.39
12	aA	826	CLA	C1D-ND	3.43	1.42	1.37
12	cA	819	CLA	C4B-NB	-3.43	1.33	1.37
12	aA	819	CLA	C4B-NB	-3.43	1.33	1.37
12	cB	905	CLA	CHB-C1B	3.43	1.47	1.39
12	bL	203	CLA	C1D-ND	3.43	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bA	816	CLA	C4B-NB	-3.43	1.33	1.37
12	bB	919	CLA	C1B-NB	-3.43	1.33	1.37
12	aB	912	CLA	CHD-C4C	3.43	1.47	1.39
12	cA	832	CLA	CHC-C4B	3.42	1.47	1.39
12	aA	807	CLA	C3D-C2D	3.42	1.48	1.39
12	cA	840	CLA	CHC-C4B	3.42	1.47	1.39
12	cA	826	CLA	C1D-ND	3.42	1.42	1.37
12	cB	932	CLA	C4B-NB	-3.42	1.33	1.37
12	cB	938	CLA	CHC-C4B	3.42	1.47	1.39
12	bA	835	CLA	CHC-C4B	3.42	1.47	1.39
12	cA	813	CLA	OBD-CAD	3.42	1.28	1.22
12	cB	922	CLA	CHD-C1D	3.42	1.45	1.38
12	bA	826	CLA	CHD-C4C	3.42	1.47	1.39
12	aB	937	CLA	C4B-NB	-3.42	1.33	1.37
12	cB	919	CLA	C1B-NB	-3.42	1.33	1.37
12	cB	933	CLA	CHD-C4C	3.42	1.47	1.39
12	cB	904	CLA	C3D-C2D	3.42	1.48	1.39
12	cB	911	CLA	CHD-C4C	3.42	1.47	1.39
12	aA	828	CLA	CHD-C4C	3.42	1.47	1.39
12	aB	911	CLA	CHD-C4C	3.42	1.47	1.39
12	cA	823	CLA	CHB-C1B	3.42	1.47	1.39
12	cA	835	CLA	CHC-C4B	3.42	1.47	1.39
12	cA	816	CLA	CHB-C1B	3.42	1.47	1.39
12	bA	807	CLA	C4B-NB	-3.42	1.33	1.37
12	bA	829	CLA	C1D-ND	3.42	1.42	1.37
12	aA	835	CLA	CHC-C4B	3.42	1.47	1.39
12	aB	939	CLA	C4B-NB	-3.42	1.33	1.37
12	aA	813	CLA	OBD-CAD	3.41	1.28	1.22
12	bB	902	CLA	CHD-C4C	3.41	1.47	1.39
12	aB	909	CLA	CHC-C4B	3.41	1.47	1.39
12	bA	817	CLA	C4B-NB	-3.41	1.33	1.37
12	bA	816	CLA	CHB-C1B	3.41	1.47	1.39
12	cA	831	CLA	CHD-C4C	3.41	1.47	1.39
15	cB	943	BCR	C1-C6	-3.41	1.49	1.53
12	aA	821	CLA	CHD-C4C	3.41	1.47	1.39
12	aA	839	CLA	CHC-C4B	3.41	1.47	1.39
12	aB	903	CLA	CHD-C4C	3.41	1.47	1.39
12	cA	833	CLA	C4B-NB	-3.41	1.33	1.37
12	cA	821	CLA	CHD-C4C	3.41	1.47	1.39
12	aA	823	CLA	CHB-C1B	3.41	1.47	1.39
12	aB	928	CLA	C1D-ND	3.41	1.42	1.37
12	aB	901	CLA	CHB-C1B	3.41	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bA	807	CLA	C3D-C2D	3.41	1.48	1.39
12	cA	807	CLA	C3D-C2D	3.41	1.48	1.39
12	aA	804	CLA	CHD-C1D	3.41	1.45	1.38
12	cA	807	CLA	C4B-NB	-3.41	1.33	1.37
12	cL	203	CLA	C4B-NB	-3.41	1.33	1.37
12	cA	818	CLA	CHB-C1B	3.41	1.47	1.39
12	bB	909	CLA	CHD-C4C	3.41	1.47	1.39
12	bB	933	CLA	CHD-C4C	3.41	1.47	1.39
12	aA	822	CLA	CHB-C1B	3.41	1.47	1.39
12	aA	830	CLA	C4B-NB	-3.41	1.33	1.37
12	bA	821	CLA	CHD-C4C	3.41	1.47	1.39
12	bB	903	CLA	CHD-C4C	3.41	1.47	1.39
12	aA	807	CLA	C4B-NB	-3.41	1.33	1.37
12	bA	840	CLA	C4B-NB	-3.41	1.33	1.37
12	bB	922	CLA	C1D-ND	3.41	1.42	1.37
12	bA	823	CLA	CHB-C1B	3.41	1.47	1.39
12	aB	905	CLA	CHB-C1B	3.41	1.47	1.39
12	bA	805	CLA	C4B-NB	-3.41	1.33	1.37
12	bB	913	CLA	CHB-C1B	3.40	1.47	1.39
12	bB	901	CLA	CHB-C1B	3.40	1.47	1.39
12	bA	819	CLA	C4B-NB	-3.40	1.33	1.37
12	aB	916	CLA	C4B-NB	-3.40	1.33	1.37
12	cL	203	CLA	CHD-C1D	3.40	1.45	1.38
12	bA	839	CLA	CHC-C4B	3.40	1.47	1.39
12	cA	804	CLA	CHD-C1D	3.40	1.45	1.38
12	aA	814	CLA	C4B-NB	-3.40	1.33	1.37
12	cA	826	CLA	CHD-C4C	3.40	1.46	1.39
12	bA	804	CLA	CHD-C1D	3.40	1.45	1.38
12	cB	913	CLA	CHB-C1B	3.40	1.47	1.39
13	bA	844	1L3	C28-C26	3.40	1.58	1.51
12	bB	902	CLA	CHC-C4B	3.40	1.47	1.39
12	bA	853	CLA	CHD-C4C	3.40	1.46	1.39
12	cB	903	CLA	CHD-C4C	3.40	1.46	1.39
12	aL	203	CLA	C4B-NB	-3.40	1.33	1.37
12	cB	902	CLA	CHD-C4C	3.40	1.46	1.39
12	aA	826	CLA	CHD-C4C	3.39	1.46	1.39
12	cB	901	CLA	CHB-C1B	3.39	1.47	1.39
12	cB	912	CLA	CHD-C4C	3.39	1.46	1.39
12	aB	902	CLA	CHC-C4B	3.39	1.47	1.39
12	aB	902	CLA	CHD-C4C	3.39	1.46	1.39
12	bB	926	CLA	CHD-C4C	3.39	1.46	1.39
12	aB	932	CLA	CHC-C4B	3.39	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aL	203	CLA	CHD-C1D	3.39	1.45	1.38
12	cB	911	CLA	OBD-CAD	3.39	1.28	1.22
12	cA	841	CLA	OBD-CAD	3.39	1.28	1.22
12	cA	836	CLA	CHC-C4B	3.39	1.47	1.39
12	bB	912	CLA	CHD-C4C	3.39	1.46	1.39
12	cA	839	CLA	CHC-C4B	3.39	1.47	1.39
12	bB	937	CLA	C4B-NB	-3.39	1.33	1.37
12	cB	907	CLA	C4B-NB	-3.39	1.33	1.37
12	aB	933	CLA	CHD-C4C	3.39	1.46	1.39
12	bA	822	CLA	CHB-C1B	3.39	1.47	1.39
12	cA	842	CLA	CHD-C4C	3.39	1.46	1.39
12	cB	922	CLA	C1D-ND	3.39	1.42	1.37
12	bA	815	CLA	C4B-NB	-3.39	1.33	1.37
12	bA	818	CLA	CHB-C1B	3.39	1.47	1.39
12	cA	822	CLA	CHB-C1B	3.39	1.47	1.39
12	aB	926	CLA	CHB-C1B	3.39	1.47	1.39
12	bA	830	CLA	C1D-ND	3.38	1.42	1.37
12	bB	920	CLA	CHB-C1B	3.38	1.47	1.39
12	bA	828	CLA	CHD-C4C	3.38	1.46	1.39
13	aA	845	1L3	C28-C26	3.38	1.58	1.51
12	aB	939	CLA	CHD-C1D	3.38	1.45	1.38
12	bA	823	CLA	C4B-NB	-3.38	1.33	1.37
12	aA	830	CLA	CHD-C4C	3.38	1.46	1.39
12	aA	842	CLA	CHD-C4C	3.38	1.46	1.39
12	bB	939	CLA	C4B-NB	-3.38	1.33	1.37
13	cA	844	1L3	C28-C26	3.38	1.58	1.51
12	aB	920	CLA	CHB-C1B	3.38	1.47	1.39
12	bB	912	CLA	C4B-NB	-3.38	1.33	1.37
12	cB	901	CLA	CHD-C1D	3.38	1.45	1.38
15	aB	943	BCR	C1-C6	-3.38	1.49	1.53
12	aA	832	CLA	CHC-C4B	3.37	1.47	1.39
12	cB	920	CLA	CHB-C1B	3.37	1.47	1.39
12	aB	913	CLA	CHB-C1B	3.37	1.47	1.39
12	bA	804	CLA	CHC-C4B	3.37	1.47	1.39
12	cB	932	CLA	CHC-C4B	3.37	1.47	1.39
12	cA	853	CLA	CHD-C4C	3.37	1.46	1.39
12	cA	805	CLA	C4B-NB	-3.37	1.33	1.37
12	aB	911	CLA	OBD-CAD	3.37	1.28	1.22
12	aA	841	CLA	OBD-CAD	3.37	1.28	1.22
12	cB	926	CLA	CHB-C1B	3.37	1.47	1.39
12	cA	830	CLA	C4B-NB	-3.37	1.33	1.37
12	bA	841	CLA	CHD-C4C	3.37	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bA	841	CLA	CHB-C1B	3.37	1.47	1.39
12	cA	815	CLA	C4B-NB	-3.37	1.33	1.37
12	aA	816	CLA	C4B-NB	-3.37	1.33	1.37
12	bL	203	CLA	C4B-NB	-3.37	1.33	1.37
12	cA	823	CLA	C4B-NB	-3.37	1.33	1.37
12	cB	901	CLA	C1D-ND	3.36	1.42	1.37
12	aA	836	CLA	CHC-C4B	3.36	1.47	1.39
12	cA	841	CLA	CHD-C4C	3.36	1.46	1.39
12	bB	926	CLA	CHB-C1B	3.36	1.47	1.39
12	cA	804	CLA	CHC-C4B	3.36	1.47	1.39
12	aA	841	CLA	CHD-C4C	3.36	1.46	1.39
12	cB	939	CLA	C4B-NB	-3.36	1.33	1.37
12	bA	830	CLA	C4B-NB	-3.36	1.33	1.37
12	aB	926	CLA	CHD-C4C	3.36	1.46	1.39
12	bA	832	CLA	CHC-C4B	3.36	1.47	1.39
12	bB	901	CLA	CHD-C1D	3.36	1.45	1.38
12	bB	901	CLA	C1D-ND	3.36	1.42	1.37
12	aA	818	CLA	CHB-C1B	3.36	1.47	1.39
12	bB	922	CLA	CHD-C4C	3.36	1.46	1.39
12	cA	828	CLA	C1D-ND	3.36	1.42	1.37
12	aB	927	CLA	C3D-C2D	3.36	1.48	1.39
12	cA	828	CLA	CHD-C4C	3.36	1.46	1.39
12	bB	932	CLA	CHC-C4B	3.36	1.46	1.39
12	cB	939	CLA	CHD-C1D	3.36	1.45	1.38
12	aA	805	CLA	C4B-NB	-3.36	1.33	1.37
12	cB	922	CLA	CHB-C1B	3.35	1.46	1.39
12	bB	907	CLA	C4B-NB	-3.35	1.33	1.37
12	aA	802	CLA	CHB-C1B	3.35	1.46	1.39
12	bA	842	CLA	CHD-C4C	3.35	1.46	1.39
12	bB	923	CLA	CHB-C1B	3.35	1.46	1.39
12	aB	935	CLA	C3D-C2D	3.35	1.48	1.39
12	aB	923	CLA	CHB-C1B	3.35	1.46	1.39
12	aA	828	CLA	C1D-ND	3.35	1.42	1.37
12	aA	829	CLA	CHC-C4B	3.35	1.46	1.39
12	cB	926	CLA	CHD-C4C	3.35	1.46	1.39
12	bA	830	CLA	CHD-C4C	3.35	1.46	1.39
12	cA	830	CLA	CHD-C4C	3.35	1.46	1.39
12	cB	922	CLA	CHD-C4C	3.35	1.46	1.39
12	bL	203	CLA	CHD-C1D	3.35	1.44	1.38
12	bB	924	CLA	C1D-ND	3.35	1.42	1.37
12	aA	811	CLA	CHC-C4B	3.35	1.46	1.39
12	aA	815	CLA	C4B-NB	-3.35	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cB	936	CLA	CHC-C4B	3.35	1.46	1.39
12	aA	854	CLA	CHD-C1D	3.35	1.44	1.38
12	aB	901	CLA	CHD-C1D	3.34	1.44	1.38
12	bA	810	CLA	CHB-C1B	3.34	1.46	1.39
12	aA	854	CLA	CHD-C4C	3.34	1.46	1.39
12	aA	828	CLA	CHC-C4B	3.34	1.46	1.39
12	aA	817	CLA	C4B-NB	-3.34	1.33	1.37
12	cB	937	CLA	C4B-NB	-3.34	1.33	1.37
12	bB	927	CLA	C3D-C2D	3.34	1.48	1.39
12	bA	836	CLA	CHC-C4B	3.34	1.46	1.39
12	bB	939	CLA	CHD-C1D	3.34	1.44	1.38
12	cB	926	CLA	CHD-C1D	3.34	1.44	1.38
12	cB	949	CLA	C3A-C2A	-3.34	1.51	1.54
12	bA	841	CLA	OBD-CAD	3.34	1.28	1.22
12	cB	916	CLA	CHB-C1B	3.34	1.46	1.39
12	bB	922	CLA	CHC-C4B	3.34	1.46	1.39
12	aB	912	CLA	C4B-NB	-3.34	1.33	1.37
12	aA	814	CLA	OBD-CAD	3.34	1.28	1.22
12	aA	806	CLA	C3D-C2D	3.34	1.48	1.39
12	cB	912	CLA	C4B-NB	-3.34	1.33	1.37
12	aB	935	CLA	CHD-C4C	3.34	1.46	1.39
12	cA	805	CLA	OBD-CAD	3.34	1.28	1.22
12	bA	828	CLA	CHC-C4B	3.34	1.46	1.39
12	cA	815	CLA	CHB-C1B	3.34	1.46	1.39
12	cB	923	CLA	CHB-C1B	3.34	1.46	1.39
12	bB	911	CLA	OBD-CAD	3.33	1.28	1.22
12	aB	915	CLA	CHB-C1B	3.33	1.46	1.39
12	cA	839	CLA	C3D-C2D	3.33	1.48	1.39
12	aA	804	CLA	CHC-C4B	3.33	1.46	1.39
12	bB	928	CLA	C1D-ND	3.33	1.42	1.37
12	aA	843	CLA	CHD-C4C	3.33	1.46	1.39
12	bA	843	CLA	CHD-C4C	3.33	1.46	1.39
12	bA	806	CLA	C3D-C2D	3.33	1.48	1.39
12	aB	916	CLA	CHB-C1B	3.33	1.46	1.39
12	aB	912	CLA	C3D-C2D	3.33	1.48	1.39
12	cA	817	CLA	OBD-CAD	3.33	1.28	1.22
12	cA	843	CLA	CHD-C4C	3.33	1.46	1.39
12	aB	914	CLA	CHB-C1B	3.33	1.46	1.39
12	cB	924	CLA	C1D-ND	3.33	1.42	1.37
12	aA	841	CLA	CHB-C1B	3.33	1.46	1.39
12	cA	802	CLA	CHB-C1B	3.33	1.46	1.39
12	bA	814	CLA	OBD-CAD	3.33	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bA	817	CLA	OBD-CAD	3.33	1.28	1.22
12	aA	815	CLA	CHB-C1B	3.33	1.46	1.39
12	aB	936	CLA	CHC-C4B	3.33	1.46	1.39
12	bA	802	CLA	CHB-C1B	3.33	1.46	1.39
12	bA	815	CLA	CHB-C1B	3.33	1.46	1.39
12	cA	817	CLA	C4B-NB	-3.33	1.33	1.37
12	bB	936	CLA	CHC-C4B	3.33	1.46	1.39
12	bA	811	CLA	CHC-C4B	3.32	1.46	1.39
12	aA	825	CLA	C4B-NB	-3.32	1.33	1.37
12	bB	931	CLA	C3D-C2D	3.32	1.48	1.39
12	cB	927	CLA	C3D-C2D	3.32	1.48	1.39
12	aA	837	CLA	CHC-C4B	3.32	1.46	1.39
12	bB	935	CLA	C3D-C2D	3.32	1.48	1.39
12	bB	949	CLA	C3A-C2A	-3.32	1.51	1.54
12	cA	830	CLA	CHB-C1B	3.32	1.46	1.39
12	aB	922	CLA	CHD-C4C	3.32	1.46	1.39
12	aB	912	CLA	C1D-ND	3.32	1.42	1.37
12	cB	912	CLA	C1D-ND	3.32	1.42	1.37
12	aB	907	CLA	C4B-NB	-3.32	1.33	1.37
12	cA	853	CLA	CHD-C1D	3.32	1.44	1.38
12	aA	839	CLA	C3D-C2D	3.32	1.48	1.39
12	bB	922	CLA	CHB-C1B	3.32	1.46	1.39
12	cB	908	CLA	CHB-C1B	3.32	1.46	1.39
12	bB	915	CLA	C4B-NB	-3.32	1.33	1.37
12	cA	816	CLA	C4B-NB	-3.32	1.33	1.37
12	bB	912	CLA	C3D-C2D	3.32	1.48	1.39
12	cA	814	CLA	OBD-CAD	3.32	1.28	1.22
12	aB	922	CLA	CHB-C1B	3.32	1.46	1.39
12	aA	824	CLA	CHC-C4B	3.32	1.46	1.39
12	aA	823	CLA	C4B-NB	-3.32	1.33	1.37
12	cA	835	CLA	C1D-ND	3.32	1.42	1.37
12	bB	932	CLA	OBD-CAD	3.32	1.28	1.22
12	bB	905	CLA	C3D-C2D	3.32	1.48	1.39
12	aA	817	CLA	OBD-CAD	3.31	1.28	1.22
12	aB	915	CLA	C4B-NB	-3.31	1.33	1.37
12	cB	916	CLA	C4B-NB	-3.31	1.33	1.37
12	cA	837	CLA	CHC-C4B	3.31	1.46	1.39
12	cB	935	CLA	CHD-C4C	3.31	1.46	1.39
12	cB	907	CLA	CHB-C1B	3.31	1.46	1.39
12	cB	935	CLA	C3D-C2D	3.31	1.48	1.39
12	bB	916	CLA	C4B-NB	-3.31	1.33	1.37
12	cB	931	CLA	C3D-C2D	3.31	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aB	907	CLA	CHB-C1B	3.31	1.46	1.39
12	aA	810	CLA	CHB-C1B	3.31	1.46	1.39
12	cB	936	CLA	CHB-C1B	3.31	1.46	1.39
12	cA	839	CLA	CHD-C4C	3.31	1.46	1.39
12	cB	922	CLA	CHC-C4B	3.31	1.46	1.39
12	bB	907	CLA	CHB-C1B	3.31	1.46	1.39
12	cA	828	CLA	CHC-C4B	3.31	1.46	1.39
12	aA	830	CLA	C1D-ND	3.31	1.42	1.37
12	cB	907	CLA	C3D-C2D	3.31	1.48	1.39
12	cA	810	CLA	CHB-C1B	3.31	1.46	1.39
12	aB	908	CLA	CHB-C1B	3.31	1.46	1.39
12	bB	914	CLA	CHB-C1B	3.31	1.46	1.39
12	cA	841	CLA	CHB-C1B	3.31	1.46	1.39
12	bB	926	CLA	CHD-C1D	3.31	1.44	1.38
12	bB	925	CLA	C3D-C2D	3.31	1.48	1.39
12	aB	907	CLA	C3D-C2D	3.31	1.48	1.39
12	aA	835	CLA	C1D-ND	3.31	1.42	1.37
12	aB	932	CLA	OBD-CAD	3.31	1.28	1.22
12	cB	931	CLA	OBD-CAD	3.31	1.28	1.22
12	aB	931	CLA	C3D-C2D	3.30	1.48	1.39
12	bA	828	CLA	C1D-ND	3.30	1.42	1.37
12	cA	830	CLA	C1D-ND	3.30	1.42	1.37
12	aB	922	CLA	OBD-CAD	3.30	1.28	1.22
12	aA	818	CLA	C3D-C2D	3.30	1.48	1.39
12	cA	806	CLA	C3D-C2D	3.30	1.48	1.39
12	aB	926	CLA	CHD-C1D	3.30	1.44	1.38
12	cB	914	CLA	CHB-C1B	3.30	1.46	1.39
15	cA	849	BCR	C1-C6	-3.30	1.49	1.53
12	aA	805	CLA	OBD-CAD	3.30	1.28	1.22
12	aA	830	CLA	CHB-C1B	3.30	1.46	1.39
12	cA	811	CLA	CHC-C4B	3.30	1.46	1.39
12	cB	915	CLA	C4B-NB	-3.30	1.33	1.37
12	cB	912	CLA	C3D-C2D	3.30	1.48	1.39
12	aB	949	CLA	C3A-C2A	-3.30	1.51	1.54
15	bL	201	BCR	C1-C6	-3.30	1.49	1.53
12	bB	907	CLA	C3D-C2D	3.30	1.48	1.39
12	aB	910	CLA	CHC-C4B	3.30	1.46	1.39
12	bB	916	CLA	CHB-C1B	3.30	1.46	1.39
12	bA	839	CLA	CHD-C4C	3.30	1.46	1.39
15	aL	201	BCR	C1-C6	-3.30	1.49	1.53
12	aB	924	CLA	C1D-ND	3.30	1.42	1.37
12	cB	932	CLA	C1B-NB	-3.30	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aB	925	CLA	C3D-C2D	3.30	1.48	1.39
12	bA	818	CLA	C3D-C2D	3.30	1.48	1.39
12	bA	824	CLA	CHC-C4B	3.30	1.46	1.39
12	bB	910	CLA	CHC-C4B	3.30	1.46	1.39
12	bA	839	CLA	C3D-C2D	3.30	1.48	1.39
12	cA	829	CLA	CHC-C4B	3.30	1.46	1.39
12	cB	905	CLA	C3D-C2D	3.30	1.48	1.39
12	aB	905	CLA	C3D-C2D	3.30	1.48	1.39
12	cB	910	CLA	CHC-C4B	3.30	1.46	1.39
12	cA	803	CLA	CHC-C4B	3.30	1.46	1.39
12	aB	922	CLA	CHC-C4B	3.29	1.46	1.39
12	bA	820	CLA	OBD-CAD	3.29	1.28	1.22
12	bA	837	CLA	CHC-C4B	3.29	1.46	1.39
12	cB	922	CLA	OBD-CAD	3.29	1.28	1.22
12	bA	829	CLA	CHC-C4B	3.29	1.46	1.39
12	cA	818	CLA	C3D-C2D	3.29	1.48	1.39
12	cA	810	CLA	OBD-CAD	3.29	1.28	1.22
12	cB	925	CLA	C3D-C2D	3.29	1.48	1.39
12	aA	838	CLA	CHB-C1B	3.29	1.46	1.39
12	bB	908	CLA	CHB-C1B	3.29	1.46	1.39
12	bB	935	CLA	CHD-C4C	3.29	1.46	1.39
12	cA	824	CLA	CHC-C4B	3.29	1.46	1.39
12	bA	805	CLA	OBD-CAD	3.29	1.28	1.22
12	bB	907	CLA	CHD-C4C	3.29	1.46	1.39
12	cB	939	CLA	OBD-CAD	3.29	1.28	1.22
12	bA	816	CLA	CHC-C4B	3.29	1.46	1.39
12	aB	901	CLA	C1D-ND	3.29	1.42	1.37
12	cA	827	CLA	C3D-C2D	3.29	1.48	1.39
12	bB	931	CLA	OBD-CAD	3.28	1.28	1.22
12	bA	830	CLA	CHB-C1B	3.28	1.46	1.39
12	cA	838	CLA	CHB-C1B	3.28	1.46	1.39
12	aA	839	CLA	CHD-C4C	3.28	1.46	1.39
12	bB	915	CLA	CHB-C1B	3.28	1.46	1.39
12	cB	915	CLA	CHB-C1B	3.28	1.46	1.39
12	bB	932	CLA	C1B-NB	-3.28	1.33	1.37
12	aL	202	CLA	CHB-C1B	3.28	1.46	1.39
12	bB	922	CLA	OBD-CAD	3.28	1.28	1.22
12	aB	907	CLA	CHD-C4C	3.28	1.46	1.39
12	bA	835	CLA	C1D-ND	3.28	1.42	1.37
12	bB	902	CLA	C1D-ND	3.28	1.42	1.37
12	bL	202	CLA	CHB-C1B	3.28	1.46	1.39
12	bA	812	CLA	OBD-CAD	3.28	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cA	812	CLA	OBD-CAD	3.28	1.28	1.22
12	cA	823	CLA	CHD-C4C	3.28	1.46	1.39
12	bA	803	CLA	CHC-C4B	3.28	1.46	1.39
12	bB	911	CLA	CHB-C1B	3.28	1.46	1.39
12	aB	911	CLA	CHB-C1B	3.28	1.46	1.39
12	aB	904	CLA	CHC-C4B	3.28	1.46	1.39
12	aA	837	CLA	C3D-C2D	3.28	1.47	1.39
12	cA	816	CLA	CHC-C4B	3.28	1.46	1.39
12	aB	931	CLA	OBD-CAD	3.28	1.28	1.22
12	aA	818	CLA	CHC-C4B	3.28	1.46	1.39
12	cB	911	CLA	CHB-C1B	3.27	1.46	1.39
12	cA	820	CLA	OBD-CAD	3.27	1.28	1.22
12	bB	921	CLA	C4B-NB	-3.27	1.33	1.37
12	aA	810	CLA	OBD-CAD	3.27	1.28	1.22
12	cB	932	CLA	OBD-CAD	3.27	1.28	1.22
15	bA	849	BCR	C1-C6	-3.27	1.49	1.53
12	aB	932	CLA	C1B-NB	-3.27	1.33	1.37
12	bA	838	CLA	CHB-C1B	3.27	1.46	1.39
12	aA	823	CLA	CHD-C4C	3.27	1.46	1.39
12	cB	907	CLA	CHD-C4C	3.27	1.46	1.39
12	cB	904	CLA	CHC-C4B	3.27	1.46	1.39
12	cB	911	CLA	C4B-NB	-3.27	1.33	1.37
12	aA	816	CLA	CHC-C4B	3.27	1.46	1.39
12	cA	818	CLA	CHC-C4B	3.27	1.46	1.39
12	aB	902	CLA	C1D-ND	3.27	1.42	1.37
12	aB	926	CLA	C4B-NB	-3.27	1.33	1.37
12	aA	806	CLA	CHC-C4B	3.27	1.46	1.39
12	aA	820	CLA	OBD-CAD	3.27	1.28	1.22
12	bB	910	CLA	OBD-CAD	3.27	1.28	1.22
12	bA	853	CLA	CHD-C1D	3.27	1.44	1.38
12	aA	827	CLA	C3D-C2D	3.26	1.47	1.39
12	cL	202	CLA	CHB-C1B	3.26	1.46	1.39
12	cB	910	CLA	OBD-CAD	3.26	1.28	1.22
12	aB	913	CLA	CHC-C4B	3.26	1.46	1.39
12	cB	923	CLA	C3D-C2D	3.26	1.47	1.39
12	aA	803	CLA	CHC-C4B	3.26	1.46	1.39
12	aB	923	CLA	C3D-C2D	3.26	1.47	1.39
12	bB	936	CLA	CHB-C1B	3.26	1.46	1.39
12	aA	831	CLA	CHC-C4B	3.26	1.46	1.39
12	aB	926	CLA	CHC-C4B	3.26	1.46	1.39
12	bB	911	CLA	C4B-NB	-3.26	1.33	1.37
12	cA	825	CLA	C4B-NB	-3.26	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bA	806	CLA	CHC-C4B	3.26	1.46	1.39
12	bB	923	CLA	C3D-C2D	3.26	1.47	1.39
12	bA	825	CLA	C4B-NB	-3.26	1.33	1.37
12	aB	936	CLA	CHB-C1B	3.26	1.46	1.39
12	bA	818	CLA	CHC-C4B	3.26	1.46	1.39
12	cB	913	CLA	CHC-C4B	3.26	1.46	1.39
12	bB	904	CLA	CHC-C4B	3.25	1.46	1.39
12	cB	919	CLA	C4B-NB	-3.25	1.33	1.37
12	bA	827	CLA	C3D-C2D	3.25	1.47	1.39
12	aA	828	CLA	CHB-C1B	3.25	1.46	1.39
12	aB	928	CLA	C4B-NB	-3.25	1.33	1.37
12	aB	918	CLA	CHC-C4B	3.25	1.46	1.39
12	aB	932	CLA	CHB-C1B	3.25	1.46	1.39
12	bB	912	CLA	C1D-ND	3.25	1.42	1.37
12	bB	913	CLA	CHC-C4B	3.25	1.46	1.39
12	cA	828	CLA	CHB-C1B	3.25	1.46	1.39
12	bB	939	CLA	OBD-CAD	3.25	1.28	1.22
12	cB	902	CLA	CHD-C1D	3.25	1.44	1.38
12	aB	910	CLA	OBD-CAD	3.24	1.28	1.22
12	aB	939	CLA	OBD-CAD	3.24	1.28	1.22
12	bA	823	CLA	CHD-C4C	3.24	1.46	1.39
12	cB	908	CLA	C1D-ND	3.24	1.42	1.37
12	cB	918	CLA	CHC-C4B	3.24	1.46	1.39
12	bL	204	CLA	OBD-CAD	3.24	1.28	1.22
12	aB	911	CLA	C4B-NB	-3.24	1.33	1.37
12	aB	920	CLA	OBD-CAD	3.24	1.28	1.22
12	bB	920	CLA	OBD-CAD	3.24	1.28	1.22
12	aB	938	CLA	C3D-C2D	3.24	1.47	1.39
12	cA	822	CLA	OBD-CAD	3.24	1.28	1.22
15	aA	847	BCR	C1-C6	-3.24	1.49	1.53
12	bB	912	CLA	CHC-C4B	3.24	1.46	1.39
12	cB	912	CLA	CHC-C4B	3.24	1.46	1.39
12	aA	822	CLA	OBD-CAD	3.24	1.28	1.22
12	aB	908	CLA	C1D-ND	3.24	1.42	1.37
12	aL	204	CLA	OBD-CAD	3.24	1.28	1.22
12	bA	822	CLA	OBD-CAD	3.24	1.28	1.22
12	aA	844	CLA	CHC-C4B	3.24	1.46	1.39
12	cA	841	CLA	C4B-NB	-3.24	1.33	1.37
12	bA	831	CLA	CHC-C4B	3.24	1.46	1.39
12	bB	939	CLA	C3D-C2D	3.23	1.47	1.39
12	bA	828	CLA	CHB-C1B	3.23	1.46	1.39
12	aA	812	CLA	OBD-CAD	3.23	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bA	810	CLA	OBD-CAD	3.23	1.28	1.22
12	cB	928	CLA	C4B-NB	-3.23	1.33	1.37
12	aB	921	CLA	C4B-NB	-3.23	1.33	1.37
15	aA	850	BCR	C1-C6	-3.23	1.49	1.53
15	cL	201	BCR	C1-C6	-3.23	1.49	1.53
12	aB	903	CLA	CHB-C1B	3.23	1.46	1.39
12	cA	837	CLA	C3D-C2D	3.23	1.47	1.39
12	bB	917	CLA	CHB-C1B	3.23	1.46	1.39
12	aB	919	CLA	C4B-NB	-3.23	1.33	1.37
12	bB	903	CLA	CHB-C1B	3.23	1.46	1.39
12	cB	927	CLA	OBD-CAD	3.22	1.28	1.22
12	aB	918	CLA	OBD-CAD	3.22	1.28	1.22
12	bB	932	CLA	CHB-C1B	3.22	1.46	1.39
15	bA	846	BCR	C1-C6	-3.22	1.49	1.53
12	aB	909	CLA	C4B-NB	-3.22	1.33	1.37
12	cB	938	CLA	C3D-C2D	3.22	1.47	1.39
12	cB	921	CLA	C4B-NB	-3.22	1.33	1.37
12	bB	938	CLA	C3D-C2D	3.22	1.47	1.39
12	aB	917	CLA	CHB-C1B	3.22	1.46	1.39
12	cA	806	CLA	CHC-C4B	3.22	1.46	1.39
12	cB	903	CLA	CHB-C1B	3.22	1.46	1.39
12	cB	928	CLA	CHC-C4B	3.22	1.46	1.39
12	bB	919	CLA	C4B-NB	-3.22	1.33	1.37
15	cA	846	BCR	C1-C6	-3.22	1.49	1.53
12	aB	928	CLA	CHC-C4B	3.22	1.46	1.39
12	cB	920	CLA	OBD-CAD	3.22	1.28	1.22
12	bA	822	CLA	C4B-NB	-3.22	1.33	1.37
12	cA	831	CLA	CHC-C4B	3.22	1.46	1.39
12	cB	932	CLA	CHB-C1B	3.22	1.46	1.39
12	bA	837	CLA	C3D-C2D	3.22	1.47	1.39
12	bB	926	CLA	C4B-NB	-3.21	1.33	1.37
12	bB	950	CLA	CHC-C4B	3.21	1.46	1.39
12	aB	939	CLA	C3D-C2D	3.21	1.47	1.39
12	bB	926	CLA	CHC-C4B	3.21	1.46	1.39
12	aB	927	CLA	OBD-CAD	3.21	1.28	1.22
12	bA	835	CLA	C4B-NB	-3.21	1.33	1.37
12	bA	843	CLA	CHC-C4B	3.21	1.46	1.39
15	cA	849	BCR	C30-C25	-3.21	1.49	1.53
12	bA	841	CLA	C4B-NB	-3.21	1.33	1.37
12	aB	902	CLA	CHD-C1D	3.21	1.44	1.38
12	cB	917	CLA	CHB-C1B	3.21	1.46	1.39
12	bB	902	CLA	CHD-C1D	3.21	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aA	833	CLA	CHC-C4B	3.21	1.46	1.39
12	cB	926	CLA	C4B-NB	-3.21	1.33	1.37
12	aB	910	CLA	C4B-NB	-3.21	1.33	1.37
12	bB	928	CLA	C4B-NB	-3.21	1.33	1.37
12	cB	926	CLA	CHC-C4B	3.21	1.46	1.39
12	aA	843	CLA	CHC-C4B	3.21	1.46	1.39
12	cB	902	CLA	C1D-ND	3.21	1.42	1.37
15	cJ	101	BCR	C1-C6	-3.20	1.49	1.53
12	aA	841	CLA	C4B-NB	-3.20	1.33	1.37
12	aB	931	CLA	CHB-C1B	3.20	1.46	1.39
12	cA	843	CLA	CHC-C4B	3.20	1.46	1.39
12	aB	950	CLA	CHC-C4B	3.20	1.46	1.39
12	cL	204	CLA	OBD-CAD	3.20	1.28	1.22
12	aA	832	CLA	CHB-C1B	3.20	1.46	1.39
12	bA	810	CLA	CHC-C4B	3.20	1.46	1.39
12	bB	918	CLA	CHC-C4B	3.20	1.46	1.39
12	cB	921	CLA	CHB-C1B	3.20	1.46	1.39
12	cB	915	CLA	OBD-CAD	3.20	1.28	1.22
12	cA	813	CLA	CHB-C1B	3.20	1.46	1.39
12	cA	817	CLA	CHB-C1B	3.20	1.46	1.39
12	cA	842	CLA	CHB-C1B	3.20	1.46	1.39
12	aB	912	CLA	CHC-C4B	3.20	1.46	1.39
12	bB	933	CLA	CHB-C1B	3.20	1.46	1.39
12	bB	909	CLA	C4B-NB	-3.20	1.33	1.37
12	bA	832	CLA	CHB-C1B	3.20	1.46	1.39
12	cA	833	CLA	CHC-C4B	3.20	1.46	1.39
12	aA	813	CLA	CHB-C1B	3.20	1.46	1.39
12	aB	921	CLA	CHB-C1B	3.19	1.46	1.39
12	aB	933	CLA	CHB-C1B	3.19	1.46	1.39
12	cA	822	CLA	C4B-NB	-3.19	1.33	1.37
12	cB	918	CLA	OBD-CAD	3.19	1.28	1.22
12	bA	817	CLA	CHB-C1B	3.19	1.46	1.39
12	cA	838	CLA	C4B-NB	-3.19	1.33	1.37
15	bA	848	BCR	C1-C6	-3.19	1.49	1.53
12	aA	810	CLA	CHC-C4B	3.19	1.46	1.39
12	aA	829	CLA	CHB-C1B	3.19	1.46	1.39
12	bA	842	CLA	CHB-C1B	3.19	1.46	1.39
12	cB	933	CLA	CHB-C1B	3.19	1.46	1.39
12	aB	923	CLA	C4B-NB	-3.19	1.33	1.37
12	bA	813	CLA	CHB-C1B	3.19	1.46	1.39
12	cA	827	CLA	CHB-C1B	3.19	1.46	1.39
12	cB	909	CLA	C4B-NB	-3.19	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bB	924	CLA	OBD-CAD	3.19	1.28	1.22
12	aA	817	CLA	CHB-C1B	3.19	1.46	1.39
12	cA	811	CLA	OBD-CAD	3.18	1.28	1.22
12	bB	928	CLA	CHC-C4B	3.18	1.46	1.39
12	aB	922	CLA	C3D-C2D	3.18	1.47	1.39
12	bA	829	CLA	CHB-C1B	3.18	1.46	1.39
12	cB	939	CLA	C3D-C2D	3.18	1.47	1.39
12	bB	931	CLA	CHB-C1B	3.18	1.46	1.39
12	cB	939	CLA	CHD-C4C	3.18	1.46	1.39
12	cA	835	CLA	C4B-NB	-3.18	1.33	1.37
12	bB	908	CLA	C1D-ND	3.18	1.42	1.37
12	bB	927	CLA	OBD-CAD	3.18	1.28	1.22
12	aA	827	CLA	CHB-C1B	3.18	1.46	1.39
12	bA	811	CLA	OBD-CAD	3.18	1.28	1.22
12	cA	816	CLA	OBD-CAD	3.18	1.28	1.22
12	cA	819	CLA	CHC-C4B	3.18	1.46	1.39
12	cB	910	CLA	C4B-NB	-3.18	1.33	1.37
12	aA	842	CLA	CHB-C1B	3.18	1.46	1.39
12	aA	808	CLA	CHB-C1B	3.18	1.46	1.39
12	cB	931	CLA	CHB-C1B	3.17	1.46	1.39
12	bB	918	CLA	OBD-CAD	3.17	1.27	1.22
12	bB	906	CLA	CHB-C1B	3.17	1.46	1.39
12	aA	811	CLA	OBD-CAD	3.17	1.27	1.22
12	aA	838	CLA	C4B-NB	-3.17	1.33	1.37
12	cA	810	CLA	CHC-C4B	3.17	1.46	1.39
12	bB	914	CLA	C4B-NB	-3.17	1.33	1.37
12	bA	827	CLA	CHB-C1B	3.17	1.46	1.39
12	bA	838	CLA	C4B-NB	-3.17	1.33	1.37
12	aA	819	CLA	CHC-C4B	3.17	1.46	1.39
12	aB	912	CLA	CHB-C1B	3.17	1.46	1.39
12	bB	921	CLA	CHB-C1B	3.17	1.46	1.39
12	aB	915	CLA	OBD-CAD	3.17	1.27	1.22
12	cB	922	CLA	C3D-C2D	3.17	1.47	1.39
12	cB	924	CLA	CHB-C1B	3.17	1.46	1.39
12	cB	924	CLA	OBD-CAD	3.17	1.27	1.22
12	cB	926	CLA	C1D-ND	3.16	1.42	1.37
12	bB	922	CLA	C3D-C2D	3.16	1.47	1.39
12	aB	926	CLA	C1D-ND	3.16	1.42	1.37
15	aA	850	BCR	C30-C25	-3.16	1.49	1.53
12	aF	202	CLA	CHB-C1B	3.16	1.46	1.39
12	bB	915	CLA	OBD-CAD	3.16	1.27	1.22
12	cA	832	CLA	CHB-C1B	3.16	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cB	906	CLA	CHB-C1B	3.16	1.46	1.39
12	aB	924	CLA	OBD-CAD	3.16	1.27	1.22
15	bJ	101	BCR	C1-C6	-3.16	1.49	1.53
12	bA	808	CLA	CHB-C1B	3.16	1.46	1.39
12	cA	803	CLA	CHD-C1D	3.16	1.44	1.38
12	bB	939	CLA	CHD-C4C	3.16	1.46	1.39
12	bA	803	CLA	CHD-C1D	3.15	1.44	1.38
12	aB	923	CLA	C1D-ND	3.15	1.42	1.37
12	bA	802	CLA	C4B-NB	-3.15	1.33	1.37
12	cB	914	CLA	C4B-NB	-3.15	1.33	1.37
12	aB	924	CLA	CHB-C1B	3.15	1.46	1.39
12	cA	839	CLA	CHB-C1B	3.15	1.46	1.39
12	bA	839	CLA	CHB-C1B	3.15	1.46	1.39
12	bB	917	CLA	CHC-C4B	3.15	1.46	1.39
12	bA	816	CLA	OBD-CAD	3.15	1.27	1.22
12	bA	819	CLA	CHC-C4B	3.15	1.46	1.39
12	bA	833	CLA	CHC-C4B	3.15	1.46	1.39
12	bA	808	CLA	OBD-CAD	3.15	1.27	1.22
12	bB	950	CLA	OBD-CAD	3.15	1.27	1.22
12	cA	829	CLA	CHB-C1B	3.15	1.46	1.39
12	aA	843	CLA	C4B-NB	-3.15	1.33	1.37
12	cA	808	CLA	CHB-C1B	3.15	1.46	1.39
12	aA	803	CLA	CHD-C1D	3.15	1.44	1.38
12	aB	939	CLA	CHD-C4C	3.15	1.46	1.39
12	aB	917	CLA	CHC-C4B	3.15	1.46	1.39
12	cB	912	CLA	CHB-C1B	3.15	1.46	1.39
12	aB	914	CLA	C4B-NB	-3.15	1.33	1.37
12	cA	808	CLA	OBD-CAD	3.15	1.27	1.22
12	cF	202	CLA	CHB-C1B	3.15	1.46	1.39
12	cB	907	CLA	CHC-C4B	3.15	1.46	1.39
12	bB	923	CLA	C1D-ND	3.15	1.42	1.37
12	bA	840	CLA	OBD-CAD	3.15	1.27	1.22
15	bA	849	BCR	C30-C25	-3.14	1.49	1.53
12	cB	930	CLA	OBD-CAD	3.14	1.27	1.22
12	aA	816	CLA	OBD-CAD	3.14	1.27	1.22
12	bL	203	CLA	OBD-CAD	3.14	1.27	1.22
12	aA	835	CLA	OBD-CAD	3.14	1.27	1.22
12	cB	923	CLA	C4B-NB	-3.14	1.33	1.37
12	cA	833	CLA	CHB-C1B	3.14	1.46	1.39
12	bA	835	CLA	OBD-CAD	3.14	1.27	1.22
12	aA	806	CLA	CHB-C1B	3.14	1.46	1.39
12	bA	806	CLA	CHB-C1B	3.14	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aA	822	CLA	C4B-NB	-3.14	1.33	1.37
15	aJ	101	BCR	C1-C6	-3.14	1.49	1.53
12	aB	907	CLA	CHC-C4B	3.14	1.46	1.39
12	cB	917	CLA	CHC-C4B	3.14	1.46	1.39
12	aB	906	CLA	CHB-C1B	3.14	1.46	1.39
12	aA	826	CLA	CHB-C1B	3.13	1.46	1.39
12	bB	912	CLA	CHB-C1B	3.13	1.46	1.39
12	cB	923	CLA	C1D-ND	3.13	1.42	1.37
12	aA	833	CLA	CHB-C1B	3.13	1.46	1.39
12	cA	806	CLA	CHB-C1B	3.13	1.46	1.39
12	bB	903	CLA	OBD-CAD	3.13	1.27	1.22
12	aA	834	CLA	CHC-C4B	3.13	1.46	1.39
12	aB	929	CLA	CHB-C1B	3.13	1.46	1.39
12	aA	815	CLA	OBD-CAD	3.13	1.27	1.22
12	cB	903	CLA	OBD-CAD	3.13	1.27	1.22
12	aA	839	CLA	CHB-C1B	3.13	1.46	1.39
12	bB	924	CLA	CHB-C1B	3.13	1.46	1.39
12	cL	203	CLA	OBD-CAD	3.13	1.27	1.22
12	bB	914	CLA	OBD-CAD	3.13	1.27	1.22
12	cA	802	CLA	C4B-NB	-3.13	1.33	1.37
12	bB	928	CLA	C3D-C2D	3.13	1.47	1.39
12	aA	812	CLA	CHB-C1B	3.13	1.46	1.39
12	aA	802	CLA	C4B-NB	-3.13	1.33	1.37
12	cB	919	CLA	CHB-C1B	3.13	1.46	1.39
12	bB	907	CLA	CHC-C4B	3.13	1.46	1.39
12	bB	906	CLA	OBD-CAD	3.13	1.27	1.22
12	cA	835	CLA	OBD-CAD	3.13	1.27	1.22
12	bB	926	CLA	C1D-ND	3.13	1.42	1.37
12	aL	203	CLA	OBD-CAD	3.12	1.27	1.22
12	cA	821	CLA	CHB-C1B	3.12	1.46	1.39
12	cB	929	CLA	CHB-C1B	3.12	1.46	1.39
12	bA	815	CLA	OBD-CAD	3.12	1.27	1.22
12	bB	930	CLA	OBD-CAD	3.12	1.27	1.22
12	aA	808	CLA	OBD-CAD	3.12	1.27	1.22
12	cA	808	CLA	C4B-NB	-3.12	1.33	1.37
12	bA	821	CLA	OBD-CAD	3.12	1.27	1.22
12	cA	809	CLA	OBD-CAD	3.12	1.27	1.22
12	cA	840	CLA	CHB-C1B	3.12	1.46	1.39
12	bA	811	CLA	CHB-C1B	3.12	1.46	1.39
12	cA	811	CLA	CHB-C1B	3.12	1.46	1.39
12	cB	920	CLA	C4B-NB	-3.12	1.33	1.37
12	bB	935	CLA	CHB-C1B	3.12	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bB	939	CLA	CHC-C4B	3.12	1.46	1.39
12	bB	925	CLA	C4B-NB	-3.12	1.33	1.37
12	bA	833	CLA	CHB-C1B	3.12	1.46	1.39
12	aB	903	CLA	OBD-CAD	3.12	1.27	1.22
12	aA	835	CLA	C4B-NB	-3.12	1.33	1.37
15	cA	848	BCR	C1-C6	-3.12	1.49	1.53
12	aB	935	CLA	CHB-C1B	3.12	1.46	1.39
12	aB	930	CLA	OBD-CAD	3.12	1.27	1.22
12	aB	939	CLA	CHC-C4B	3.12	1.46	1.39
15	cM	101	BCR	C1-C6	-3.12	1.49	1.53
12	cL	203	CLA	CHB-C1B	3.11	1.46	1.39
12	aA	842	CLA	OBD-CAD	3.11	1.27	1.22
12	cB	935	CLA	CHB-C1B	3.11	1.46	1.39
12	cA	826	CLA	CHB-C1B	3.11	1.46	1.39
12	cA	843	CLA	C4B-NB	-3.11	1.33	1.37
12	bB	929	CLA	CHB-C1B	3.11	1.46	1.39
12	bB	923	CLA	C4B-NB	-3.11	1.33	1.37
12	aA	840	CLA	OBD-CAD	3.11	1.27	1.22
15	aM	101	BCR	C1-C6	-3.11	1.49	1.53
12	bA	853	CLA	C1D-ND	3.11	1.41	1.37
12	cB	928	CLA	C3D-C2D	3.11	1.47	1.39
12	bB	910	CLA	C4B-NB	-3.11	1.33	1.37
12	bF	202	CLA	CHB-C1B	3.11	1.46	1.39
13	aB	940	1L3	O13-C12	-3.11	1.16	1.23
12	cA	812	CLA	CHB-C1B	3.11	1.46	1.39
12	cA	815	CLA	OBD-CAD	3.11	1.27	1.22
12	bA	812	CLA	CHB-C1B	3.11	1.46	1.39
15	bF	203	BCR	C1-C6	-3.11	1.49	1.53
12	aA	808	CLA	C4B-NB	-3.11	1.33	1.37
12	aB	931	CLA	CHD-C1D	3.10	1.44	1.38
12	aB	928	CLA	C3D-C2D	3.10	1.47	1.39
12	aA	811	CLA	CHB-C1B	3.10	1.46	1.39
12	bA	853	CLA	CHB-C1B	3.10	1.46	1.39
12	bA	840	CLA	CHB-C1B	3.10	1.46	1.39
12	cB	906	CLA	OBD-CAD	3.10	1.27	1.22
12	aA	836	CLA	C4B-NB	-3.10	1.33	1.37
12	cA	821	CLA	OBD-CAD	3.10	1.27	1.22
12	aA	840	CLA	CHB-C1B	3.10	1.46	1.39
12	bA	834	CLA	CHC-C4B	3.10	1.46	1.39
12	cB	914	CLA	OBD-CAD	3.10	1.27	1.22
12	aL	203	CLA	CHB-C1B	3.09	1.46	1.39
12	cA	834	CLA	CHC-C4B	3.09	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cA	842	CLA	OBD-CAD	3.09	1.27	1.22
15	aF	203	BCR	C1-C6	-3.09	1.49	1.53
12	aB	914	CLA	OBD-CAD	3.09	1.27	1.22
12	aB	906	CLA	OBD-CAD	3.09	1.27	1.22
12	bL	203	CLA	CHB-C1B	3.09	1.46	1.39
12	cB	901	CLA	CHC-C4B	3.09	1.46	1.39
12	aB	950	CLA	OBD-CAD	3.09	1.27	1.22
12	cB	939	CLA	CHC-C4B	3.09	1.46	1.39
12	bB	924	CLA	CHC-C4B	3.09	1.46	1.39
12	aB	925	CLA	C4B-NB	-3.09	1.33	1.37
12	bA	826	CLA	CHB-C1B	3.09	1.46	1.39
12	bA	809	CLA	OBD-CAD	3.09	1.27	1.22
12	bB	919	CLA	CHB-C1B	3.09	1.46	1.39
12	aA	844	CLA	OBD-CAD	3.09	1.27	1.22
12	aB	938	CLA	CHB-C1B	3.09	1.46	1.39
12	aB	901	CLA	CHC-C4B	3.08	1.46	1.39
12	bB	901	CLA	CHC-C4B	3.08	1.46	1.39
15	aA	849	BCR	C1-C6	-3.08	1.49	1.53
12	cA	840	CLA	OBD-CAD	3.08	1.27	1.22
12	cA	830	CLA	CHC-C4B	3.08	1.46	1.39
12	aA	821	CLA	OBD-CAD	3.08	1.27	1.22
12	aB	933	CLA	OBD-CAD	3.08	1.27	1.22
12	aA	854	CLA	C1D-ND	3.08	1.41	1.37
12	bB	929	CLA	OBD-CAD	3.08	1.27	1.22
13	bB	940	1L3	O13-C12	-3.08	1.16	1.23
12	bA	842	CLA	OBD-CAD	3.08	1.27	1.22
12	bA	843	CLA	C4B-NB	-3.08	1.33	1.37
12	bB	933	CLA	OBD-CAD	3.08	1.27	1.22
12	cB	902	CLA	OBD-CAD	3.08	1.27	1.22
12	bB	904	CLA	CHB-C1B	3.08	1.46	1.39
12	aB	949	CLA	C4B-NB	-3.08	1.33	1.37
12	aB	924	CLA	CHC-C4B	3.08	1.46	1.39
12	cB	931	CLA	CHD-C1D	3.07	1.44	1.38
12	aA	826	CLA	OBD-CAD	3.07	1.27	1.22
12	bB	931	CLA	CHD-C1D	3.07	1.44	1.38
12	aB	904	CLA	CHB-C1B	3.07	1.46	1.39
12	aA	835	CLA	CHB-C1B	3.07	1.46	1.39
12	aB	919	CLA	CHB-C1B	3.07	1.46	1.39
12	aA	825	CLA	OBD-CAD	3.07	1.27	1.22
12	cA	835	CLA	CHB-C1B	3.07	1.46	1.39
12	aA	804	CLA	OBD-CAD	3.07	1.27	1.22
12	cB	901	CLA	C3D-C2D	3.07	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cA	825	CLA	OBD-CAD	3.07	1.27	1.22
12	cB	933	CLA	OBD-CAD	3.07	1.27	1.22
12	aB	929	CLA	OBD-CAD	3.07	1.27	1.22
12	bB	901	CLA	C3D-C2D	3.07	1.47	1.39
12	cA	853	CLA	CHB-C1B	3.06	1.46	1.39
13	cB	940	1L3	O13-C12	-3.06	1.16	1.23
12	bA	826	CLA	OBD-CAD	3.06	1.27	1.22
12	cB	929	CLA	OBD-CAD	3.06	1.27	1.22
12	bA	825	CLA	OBD-CAD	3.06	1.27	1.22
12	bA	808	CLA	C4B-NB	-3.06	1.33	1.37
12	cB	904	CLA	CHB-C1B	3.06	1.46	1.39
12	aB	920	CLA	C4B-NB	-3.06	1.33	1.37
12	bB	920	CLA	C4B-NB	-3.06	1.33	1.37
12	cA	826	CLA	OBD-CAD	3.06	1.27	1.22
12	bA	830	CLA	CHC-C4B	3.06	1.46	1.39
12	cB	924	CLA	CHC-C4B	3.06	1.46	1.39
12	cB	938	CLA	CHB-C1B	3.06	1.46	1.39
12	bA	836	CLA	C4B-NB	-3.06	1.33	1.37
12	aB	901	CLA	C3D-C2D	3.06	1.47	1.39
12	cA	853	CLA	C1D-ND	3.05	1.41	1.37
12	bA	821	CLA	CHB-C1B	3.05	1.46	1.39
12	aA	809	CLA	OBD-CAD	3.05	1.27	1.22
12	aA	821	CLA	CHB-C1B	3.05	1.46	1.39
12	aA	830	CLA	CHC-C4B	3.05	1.46	1.39
12	cA	804	CLA	OBD-CAD	3.05	1.27	1.22
12	aF	202	CLA	C4B-NB	-3.05	1.33	1.37
12	cB	925	CLA	C4B-NB	-3.05	1.33	1.37
12	bB	938	CLA	CHB-C1B	3.05	1.46	1.39
12	aB	902	CLA	OBD-CAD	3.04	1.27	1.22
15	cF	203	BCR	C1-C6	-3.04	1.49	1.53
12	bA	804	CLA	OBD-CAD	3.04	1.27	1.22
12	aA	854	CLA	CHB-C1B	3.04	1.46	1.39
12	bA	835	CLA	CHB-C1B	3.04	1.46	1.39
12	bA	837	CLA	CHB-C1B	3.04	1.46	1.39
12	aA	837	CLA	CHB-C1B	3.04	1.46	1.39
12	cA	837	CLA	CHB-C1B	3.04	1.46	1.39
12	aA	818	CLA	OBD-CAD	3.03	1.27	1.22
12	aB	901	CLA	CHD-C4C	3.03	1.46	1.39
12	aA	803	CLA	OBD-CAD	3.03	1.27	1.22
15	bM	101	BCR	C1-C6	-3.03	1.49	1.53
12	cA	802	CLA	CHC-C4B	3.02	1.46	1.39
12	cB	949	CLA	C4B-NB	-3.02	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bB	902	CLA	OBD-CAD	3.02	1.27	1.22
12	bA	803	CLA	OBD-CAD	3.02	1.27	1.22
15	cA	848	BCR	C30-C25	-3.02	1.49	1.53
12	bB	933	CLA	C4B-NB	-3.02	1.33	1.37
12	cB	921	CLA	OBD-CAD	3.01	1.27	1.22
12	bB	910	CLA	CHB-C1B	3.01	1.46	1.39
12	bA	823	CLA	OBD-CAD	3.01	1.27	1.22
12	cA	803	CLA	OBD-CAD	3.01	1.27	1.22
12	bA	809	CLA	CHB-C1B	3.01	1.46	1.39
12	cB	901	CLA	CHD-C4C	3.01	1.46	1.39
12	cB	910	CLA	CHB-C1B	3.01	1.46	1.39
12	bB	937	CLA	CHB-C1B	3.01	1.46	1.39
12	aB	928	CLA	OBD-CAD	3.01	1.27	1.22
12	aB	921	CLA	OBD-CAD	3.01	1.27	1.22
12	aB	930	CLA	CHB-C1B	3.01	1.46	1.39
12	cA	824	CLA	OBD-CAD	3.01	1.27	1.22
12	bA	818	CLA	OBD-CAD	3.00	1.27	1.22
12	bB	919	CLA	OBD-CAD	3.00	1.27	1.22
12	aA	824	CLA	CHB-C1B	3.00	1.46	1.39
12	cB	930	CLA	CHB-C1B	3.00	1.46	1.39
12	cA	809	CLA	CHB-C1B	3.00	1.46	1.39
15	aA	849	BCR	C30-C25	-3.00	1.49	1.53
12	aA	809	CLA	CHB-C1B	3.00	1.46	1.39
12	bB	921	CLA	OBD-CAD	3.00	1.27	1.22
12	bB	928	CLA	OBD-CAD	3.00	1.27	1.22
12	bB	949	CLA	C4B-NB	-2.99	1.33	1.37
12	cB	937	CLA	CHB-C1B	2.99	1.46	1.39
13	bB	940	1L3	C22-C21	2.99	1.58	1.50
12	aB	933	CLA	C4B-NB	-2.99	1.33	1.37
12	cA	814	CLA	CHC-C4B	2.99	1.46	1.39
12	aA	814	CLA	CHC-C4B	2.99	1.46	1.39
13	aB	940	1L3	C22-C21	2.99	1.58	1.50
12	bA	824	CLA	OBD-CAD	2.99	1.27	1.22
12	bA	802	CLA	CHC-C4B	2.99	1.46	1.39
12	cB	927	CLA	CHB-C1B	2.99	1.46	1.39
12	aB	910	CLA	CHB-C1B	2.99	1.46	1.39
12	bB	916	CLA	OBD-CAD	2.98	1.27	1.22
12	cA	818	CLA	OBD-CAD	2.98	1.27	1.22
12	aB	919	CLA	OBD-CAD	2.98	1.27	1.22
12	cA	836	CLA	C4B-NB	-2.98	1.33	1.37
12	bF	202	CLA	C4B-NB	-2.98	1.33	1.37
12	bB	901	CLA	CHD-C4C	2.98	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aA	802	CLA	CHC-C4B	2.98	1.46	1.39
12	bA	824	CLA	CHB-C1B	2.98	1.46	1.39
12	cA	824	CLA	CHB-C1B	2.98	1.46	1.39
12	aA	806	CLA	OBD-CAD	2.98	1.27	1.22
12	aB	937	CLA	CHB-C1B	2.98	1.46	1.39
12	cA	823	CLA	OBD-CAD	2.98	1.27	1.22
12	bA	814	CLA	CHC-C4B	2.98	1.46	1.39
12	aA	831	CLA	CHB-C1B	2.98	1.46	1.39
12	bA	825	CLA	CHB-C1B	2.98	1.46	1.39
15	aL	201	BCR	C30-C25	-2.98	1.50	1.53
12	cB	933	CLA	C4B-NB	-2.98	1.34	1.37
12	cF	202	CLA	C4B-NB	-2.98	1.34	1.37
12	cB	928	CLA	OBD-CAD	2.98	1.27	1.22
12	cB	919	CLA	OBD-CAD	2.97	1.27	1.22
12	bA	831	CLA	CHB-C1B	2.97	1.46	1.39
15	cL	201	BCR	C30-C25	-2.97	1.50	1.53
12	cA	805	CLA	CHB-C1B	2.97	1.46	1.39
12	bB	930	CLA	CHB-C1B	2.97	1.46	1.39
12	aA	823	CLA	OBD-CAD	2.97	1.27	1.22
12	aA	824	CLA	OBD-CAD	2.97	1.27	1.22
12	bB	927	CLA	CHC-C4B	2.97	1.46	1.39
12	aA	805	CLA	CHB-C1B	2.96	1.46	1.39
12	bB	925	CLA	CHB-C1B	2.96	1.46	1.39
12	aB	925	CLA	CHB-C1B	2.96	1.46	1.39
15	bA	848	BCR	C30-C25	-2.96	1.50	1.53
12	cA	831	CLA	CHB-C1B	2.96	1.46	1.39
12	cB	927	CLA	CHC-C4B	2.96	1.46	1.39
12	cB	925	CLA	CHB-C1B	2.95	1.46	1.39
12	aB	934	CLA	CHB-C1B	2.95	1.46	1.39
12	aB	938	CLA	OBD-CAD	2.95	1.27	1.22
15	bL	201	BCR	C30-C25	-2.95	1.50	1.53
12	aB	927	CLA	CHC-C4B	2.95	1.46	1.39
12	bA	805	CLA	CHB-C1B	2.95	1.46	1.39
12	aB	916	CLA	OBD-CAD	2.95	1.27	1.22
13	cB	940	1L3	C22-C21	2.95	1.57	1.50
12	cB	934	CLA	CHB-C1B	2.95	1.46	1.39
12	bB	934	CLA	CHB-C1B	2.94	1.46	1.39
12	bB	938	CLA	OBD-CAD	2.94	1.27	1.22
12	aB	927	CLA	CHB-C1B	2.94	1.46	1.39
12	cB	916	CLA	OBD-CAD	2.94	1.27	1.22
12	aA	825	CLA	CHB-C1B	2.94	1.46	1.39
12	cA	825	CLA	CHB-C1B	2.94	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cB	938	CLA	OBD-CAD	2.93	1.27	1.22
12	bB	901	CLA	OBD-CAD	2.93	1.27	1.22
12	bA	830	CLA	OBD-CAD	2.93	1.27	1.22
12	aA	820	CLA	C4B-NB	-2.93	1.34	1.37
12	bB	927	CLA	CHB-C1B	2.92	1.46	1.39
15	bA	847	BCR	C30-C25	-2.92	1.50	1.53
12	aA	807	CLA	CHB-C1B	2.91	1.46	1.39
12	cA	830	CLA	OBD-CAD	2.91	1.27	1.22
12	bA	806	CLA	OBD-CAD	2.90	1.27	1.22
12	cB	912	CLA	OBD-CAD	2.90	1.27	1.22
12	cA	819	CLA	CHB-C1B	2.90	1.45	1.39
12	bB	917	CLA	OBD-CAD	2.90	1.27	1.22
12	cA	806	CLA	OBD-CAD	2.90	1.27	1.22
12	bA	807	CLA	CHB-C1B	2.90	1.45	1.39
12	cB	917	CLA	OBD-CAD	2.90	1.27	1.22
12	cA	807	CLA	CHB-C1B	2.90	1.45	1.39
12	bA	819	CLA	CHB-C1B	2.90	1.45	1.39
12	aB	901	CLA	OBD-CAD	2.89	1.27	1.22
15	cA	847	BCR	C30-C25	-2.89	1.50	1.53
12	aA	830	CLA	OBD-CAD	2.89	1.27	1.22
12	cB	901	CLA	C1B-C2B	2.88	1.49	1.43
12	aB	917	CLA	OBD-CAD	2.88	1.27	1.22
12	cB	901	CLA	OBD-CAD	2.88	1.27	1.22
15	aA	848	BCR	C30-C25	-2.87	1.50	1.53
12	aB	935	CLA	C3D-C4D	-2.87	1.37	1.44
12	aA	819	CLA	CHB-C1B	2.87	1.45	1.39
12	bB	925	CLA	C3D-C4D	-2.87	1.37	1.44
12	aB	912	CLA	OBD-CAD	2.86	1.27	1.22
12	bA	807	CLA	C4D-CHA	2.86	1.48	1.38
15	bB	942	BCR	C1-C6	-2.86	1.50	1.53
12	aB	913	CLA	C1B-C2B	2.86	1.49	1.43
12	bA	820	CLA	C4B-NB	-2.86	1.34	1.37
12	bB	935	CLA	C3D-C4D	-2.86	1.37	1.44
12	bB	913	CLA	C1B-C2B	2.86	1.49	1.43
12	bB	912	CLA	OBD-CAD	2.85	1.27	1.22
12	aB	925	CLA	C3D-C4D	-2.85	1.37	1.44
12	cA	807	CLA	C4D-CHA	2.85	1.48	1.38
12	cB	913	CLA	C1B-C2B	2.85	1.49	1.43
12	cB	935	CLA	C3D-C4D	-2.85	1.37	1.44
12	bB	901	CLA	C1B-C2B	2.85	1.49	1.43
12	cA	820	CLA	C4B-NB	-2.85	1.34	1.37
12	cB	927	CLA	C1D-ND	2.85	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aA	807	CLA	C4D-CHA	2.85	1.48	1.38
12	aB	902	CLA	CHB-C1B	2.84	1.45	1.39
12	aB	901	CLA	C1B-C2B	2.84	1.49	1.43
12	aB	902	CLA	C1C-NC	-2.84	1.33	1.37
15	cF	204	BCR	C30-C25	-2.83	1.50	1.53
12	aB	934	CLA	C4D-CHA	2.83	1.48	1.38
12	bB	904	CLA	OBD-CAD	2.83	1.27	1.22
12	cB	925	CLA	C3D-C4D	-2.83	1.37	1.44
12	bB	902	CLA	C1C-NC	-2.83	1.33	1.37
12	aA	834	CLA	OBD-CAD	2.83	1.27	1.22
12	cB	902	CLA	C1C-NC	-2.82	1.33	1.37
12	bB	902	CLA	CHB-C1B	2.82	1.45	1.39
12	aA	821	CLA	C4B-NB	-2.82	1.34	1.37
12	bB	934	CLA	C4D-CHA	2.82	1.48	1.38
12	cB	934	CLA	C4D-CHA	2.82	1.48	1.38
15	bF	204	BCR	C30-C25	-2.82	1.50	1.53
16	bA	852	LHG	O7-C5	-2.82	1.40	1.46
12	aB	904	CLA	OBD-CAD	2.82	1.27	1.22
15	cB	942	BCR	C1-C6	-2.82	1.50	1.53
13	aA	845	1L3	C22-C21	2.82	1.57	1.50
12	bB	907	CLA	OBD-CAD	2.82	1.27	1.22
16	cA	852	LHG	O7-C5	-2.81	1.40	1.46
12	aB	907	CLA	OBD-CAD	2.81	1.27	1.22
13	cA	844	1L3	C22-C21	2.81	1.57	1.50
15	aB	942	BCR	C1-C6	-2.81	1.50	1.53
13	bA	844	1L3	C22-C21	2.81	1.57	1.50
12	bB	919	CLA	C4D-CHA	2.81	1.48	1.38
12	cB	907	CLA	OBD-CAD	2.81	1.27	1.22
12	cB	902	CLA	CHB-C1B	2.81	1.45	1.39
12	aB	919	CLA	C4D-CHA	2.81	1.48	1.38
12	cA	834	CLA	OBD-CAD	2.80	1.27	1.22
12	cB	919	CLA	C4D-CHA	2.80	1.48	1.38
12	bB	926	CLA	OBD-CAD	2.80	1.27	1.22
12	cB	926	CLA	OBD-CAD	2.80	1.27	1.22
12	cB	904	CLA	OBD-CAD	2.80	1.27	1.22
12	aA	834	CLA	CHB-C1B	2.79	1.45	1.39
16	aA	853	LHG	O7-C5	-2.79	1.40	1.46
12	bA	821	CLA	C4B-NB	-2.78	1.34	1.37
12	aB	926	CLA	OBD-CAD	2.78	1.27	1.22
12	bA	820	CLA	C1B-C2B	2.78	1.49	1.43
12	aA	820	CLA	C1B-C2B	2.78	1.49	1.43
12	cA	834	CLA	CHB-C1B	2.78	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aB	927	CLA	C1D-ND	2.78	1.41	1.37
15	bM	101	BCR	C30-C25	-2.78	1.50	1.53
12	bB	927	CLA	C1D-ND	2.77	1.41	1.37
12	bA	834	CLA	CHB-C1B	2.77	1.45	1.39
12	bA	834	CLA	OBD-CAD	2.77	1.27	1.22
12	cA	820	CLA	C1B-C2B	2.77	1.49	1.43
15	aF	204	BCR	C30-C25	-2.77	1.50	1.53
12	cB	949	CLA	C4D-CHA	2.77	1.47	1.38
12	aA	825	CLA	C3B-C4B	2.76	1.50	1.42
12	bB	911	CLA	C3B-C4B	2.76	1.50	1.42
12	cB	911	CLA	C3B-C4B	2.76	1.50	1.42
12	bB	949	CLA	C4D-CHA	2.76	1.47	1.38
15	bI	101	BCR	C30-C25	-2.76	1.50	1.53
12	bB	939	CLA	C1B-C2B	2.76	1.49	1.43
12	bA	808	CLA	C4D-CHA	2.76	1.47	1.38
12	bA	824	CLA	C4D-CHA	2.76	1.47	1.38
12	cA	821	CLA	C4B-NB	-2.76	1.34	1.37
12	cB	917	CLA	C4D-CHA	2.76	1.47	1.38
12	cB	939	CLA	C1B-C2B	2.75	1.49	1.43
12	cA	808	CLA	C4D-CHA	2.75	1.47	1.38
12	aB	949	CLA	C4D-CHA	2.75	1.47	1.38
12	bB	914	CLA	C4D-CHA	2.75	1.47	1.38
12	bB	917	CLA	C4D-CHA	2.75	1.47	1.38
12	bB	921	CLA	C3D-C4D	-2.75	1.38	1.44
12	aB	928	CLA	C3D-C4D	-2.75	1.38	1.44
12	bA	831	CLA	C3D-C4D	-2.75	1.38	1.44
12	aB	939	CLA	C1B-C2B	2.75	1.49	1.43
12	aB	911	CLA	C3B-C4B	2.75	1.50	1.42
15	cI	101	BCR	C30-C25	-2.75	1.50	1.53
12	cA	831	CLA	OBD-CAD	2.75	1.27	1.22
12	cB	913	CLA	OBD-CAD	2.75	1.27	1.22
12	cA	827	CLA	C3D-C4D	-2.74	1.38	1.44
15	cF	201	BCR	C1-C6	-2.74	1.50	1.53
12	cA	831	CLA	C3D-C4D	-2.74	1.38	1.44
12	aB	914	CLA	C4D-CHA	2.74	1.47	1.38
12	bB	913	CLA	OBD-CAD	2.74	1.27	1.22
12	cA	824	CLA	C4D-CHA	2.74	1.47	1.38
12	aB	917	CLA	C4D-CHA	2.74	1.47	1.38
12	bA	825	CLA	C3B-C4B	2.74	1.50	1.42
12	cA	819	CLA	C3D-C4D	-2.74	1.38	1.44
12	aA	828	CLA	OBD-CAD	2.74	1.27	1.22
12	cA	828	CLA	OBD-CAD	2.73	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aA	831	CLA	C3D-C4D	-2.73	1.38	1.44
12	bA	843	CLA	OBD-CAD	2.73	1.27	1.22
12	cB	921	CLA	C3D-C4D	-2.73	1.38	1.44
12	aA	827	CLA	C3D-C4D	-2.73	1.38	1.44
12	aA	808	CLA	C4D-CHA	2.73	1.47	1.38
15	cA	850	BCR	C30-C25	-2.73	1.50	1.53
12	bA	804	CLA	C1B-C2B	2.73	1.49	1.43
12	bB	928	CLA	C3D-C4D	-2.72	1.38	1.44
12	bA	828	CLA	OBD-CAD	2.72	1.27	1.22
12	cA	843	CLA	OBD-CAD	2.72	1.27	1.22
15	cF	203	BCR	C30-C25	-2.72	1.50	1.53
12	cA	815	CLA	C4D-CHA	2.72	1.47	1.38
12	cB	934	CLA	C4B-NB	-2.72	1.34	1.37
12	aB	921	CLA	C3D-C4D	-2.72	1.38	1.44
12	cA	804	CLA	C1B-C2B	2.72	1.49	1.43
12	aB	905	CLA	C4D-CHA	2.72	1.47	1.38
12	bA	819	CLA	C3D-C4D	-2.72	1.38	1.44
12	cA	825	CLA	C3B-C4B	2.72	1.50	1.42
12	bA	827	CLA	C3D-C4D	-2.72	1.38	1.44
12	aA	843	CLA	OBD-CAD	2.72	1.27	1.22
12	aA	824	CLA	C4D-CHA	2.72	1.47	1.38
12	bB	935	CLA	OBD-CAD	2.71	1.27	1.22
12	aB	938	CLA	C3D-C4D	-2.71	1.38	1.44
12	aA	819	CLA	C3D-C4D	-2.71	1.38	1.44
12	cB	905	CLA	C4D-CHA	2.71	1.47	1.38
12	cB	914	CLA	C4D-CHA	2.71	1.47	1.38
12	bA	815	CLA	C4D-CHA	2.71	1.47	1.38
12	cB	924	CLA	C3D-C4D	-2.71	1.38	1.44
12	aA	815	CLA	C4D-CHA	2.71	1.47	1.38
12	bB	938	CLA	C3D-C4D	-2.71	1.38	1.44
12	bB	924	CLA	C3D-C4D	-2.71	1.38	1.44
12	aA	833	CLA	OBD-CAD	2.71	1.27	1.22
15	aM	101	BCR	C30-C25	-2.71	1.50	1.53
12	bB	925	CLA	C4D-CHA	2.71	1.47	1.38
12	bA	827	CLA	OBD-CAD	2.70	1.27	1.22
12	bB	934	CLA	C4B-NB	-2.70	1.34	1.37
15	aI	101	BCR	C30-C25	-2.70	1.50	1.53
12	cB	928	CLA	C3D-C4D	-2.70	1.38	1.44
12	bA	835	CLA	C4D-CHA	2.70	1.47	1.38
12	aB	934	CLA	C3B-C4B	2.70	1.50	1.42
12	aA	836	CLA	C4D-CHA	2.70	1.47	1.38
12	aA	804	CLA	C1B-C2B	2.70	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aB	909	CLA	C4D-CHA	2.70	1.47	1.38
12	bA	813	CLA	C4D-CHA	2.70	1.47	1.38
12	cB	925	CLA	C4D-CHA	2.70	1.47	1.38
12	aA	831	CLA	OBD-CAD	2.70	1.27	1.22
12	cB	938	CLA	C3D-C4D	-2.70	1.38	1.44
12	bB	905	CLA	C4D-CHA	2.70	1.47	1.38
15	cM	101	BCR	C30-C25	-2.70	1.50	1.53
12	cA	813	CLA	C4D-CHA	2.70	1.47	1.38
12	bA	831	CLA	OBD-CAD	2.70	1.27	1.22
12	cB	909	CLA	C4D-CHA	2.70	1.47	1.38
12	cA	831	CLA	C4D-CHA	2.70	1.47	1.38
12	aA	813	CLA	C4D-CHA	2.70	1.47	1.38
15	bF	203	BCR	C30-C25	-2.70	1.50	1.53
12	aB	908	CLA	C4D-CHA	2.69	1.47	1.38
12	aB	913	CLA	OBD-CAD	2.69	1.27	1.22
12	cB	934	CLA	C3B-C4B	2.69	1.50	1.42
12	bA	840	CLA	C4D-CHA	2.69	1.47	1.38
12	bA	836	CLA	C4D-CHA	2.69	1.47	1.38
12	cA	836	CLA	C4D-CHA	2.69	1.47	1.38
12	aB	924	CLA	C3D-C4D	-2.69	1.38	1.44
12	aB	925	CLA	C4D-CHA	2.69	1.47	1.38
12	bB	909	CLA	C4D-CHA	2.69	1.47	1.38
12	bB	901	CLA	C1C-NC	-2.69	1.33	1.37
12	bB	920	CLA	C4D-CHA	2.69	1.47	1.38
12	cB	921	CLA	C4D-CHA	2.69	1.47	1.38
12	aA	820	CLA	C4D-CHA	2.68	1.47	1.38
15	aF	203	BCR	C30-C25	-2.68	1.50	1.53
12	aB	918	CLA	CHB-C1B	2.68	1.45	1.39
12	aA	840	CLA	C4D-CHA	2.68	1.47	1.38
12	aA	805	CLA	C4D-CHA	2.68	1.47	1.38
12	cA	835	CLA	C4D-CHA	2.68	1.47	1.38
12	bB	931	CLA	C3B-C4B	2.68	1.50	1.42
15	bB	942	BCR	C30-C25	-2.68	1.50	1.53
12	bA	831	CLA	C4D-CHA	2.68	1.47	1.38
12	bA	820	CLA	C4D-CHA	2.68	1.47	1.38
15	aB	942	BCR	C30-C25	-2.68	1.50	1.53
15	aF	201	BCR	C1-C6	-2.68	1.50	1.53
12	aB	922	CLA	C3D-C4D	-2.68	1.38	1.44
12	bB	908	CLA	C4D-CHA	2.68	1.47	1.38
12	bB	934	CLA	C3B-C4B	2.68	1.50	1.42
12	aB	921	CLA	C4D-CHA	2.68	1.47	1.38
12	cB	935	CLA	OBD-CAD	2.68	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aA	831	CLA	C4D-CHA	2.67	1.47	1.38
12	cB	908	CLA	C4D-CHA	2.67	1.47	1.38
12	aA	835	CLA	C4D-CHA	2.67	1.47	1.38
12	aB	935	CLA	OBD-CAD	2.67	1.27	1.22
12	aB	901	CLA	C1C-NC	-2.67	1.33	1.37
12	cA	820	CLA	C4D-CHA	2.67	1.47	1.38
12	cB	901	CLA	C1C-NC	-2.67	1.33	1.37
12	bL	204	CLA	C1B-C2B	2.67	1.49	1.43
12	aB	920	CLA	C4D-CHA	2.67	1.47	1.38
12	bB	921	CLA	C4D-CHA	2.67	1.47	1.38
12	aB	931	CLA	C3B-C4B	2.67	1.50	1.42
12	bB	909	CLA	C3D-C4D	-2.67	1.38	1.44
15	bI	101	BCR	C1-C6	-2.67	1.50	1.53
12	cA	819	CLA	OBD-CAD	2.67	1.27	1.22
12	bA	841	CLA	C3B-C4B	2.67	1.50	1.42
12	cA	841	CLA	C3B-C4B	2.67	1.50	1.42
12	cA	832	CLA	C3D-C4D	-2.67	1.38	1.44
12	aA	841	CLA	C3B-C4B	2.66	1.50	1.42
15	bA	850	BCR	C1-C6	-2.66	1.50	1.53
12	cA	805	CLA	C4D-CHA	2.66	1.47	1.38
12	cA	833	CLA	OBD-CAD	2.66	1.27	1.22
12	aA	822	CLA	C4D-CHA	2.66	1.47	1.38
12	cA	840	CLA	C4D-CHA	2.66	1.47	1.38
12	cB	918	CLA	CHB-C1B	2.66	1.45	1.39
12	cB	931	CLA	C3B-C4B	2.66	1.50	1.42
12	cA	827	CLA	OBD-CAD	2.66	1.27	1.22
12	bA	805	CLA	C4D-CHA	2.66	1.47	1.38
12	bA	822	CLA	C4D-CHA	2.66	1.47	1.38
12	aB	909	CLA	C3D-C4D	-2.66	1.38	1.44
12	aB	939	CLA	C3D-C4D	-2.65	1.38	1.44
15	aA	851	BCR	C30-C25	-2.65	1.50	1.53
12	aA	819	CLA	OBD-CAD	2.65	1.27	1.22
12	cB	939	CLA	C3D-C4D	-2.65	1.38	1.44
12	cB	920	CLA	C4D-CHA	2.65	1.47	1.38
12	cB	909	CLA	C3D-C4D	-2.65	1.38	1.44
12	bB	939	CLA	C3D-C4D	-2.65	1.38	1.44
12	bB	918	CLA	CHB-C1B	2.65	1.45	1.39
12	aA	837	CLA	C3D-C4D	-2.65	1.38	1.44
12	aB	923	CLA	OBD-CAD	2.65	1.27	1.22
12	cA	839	CLA	OBD-CAD	2.65	1.27	1.22
12	cA	811	CLA	C4D-CHA	2.65	1.47	1.38
12	bA	837	CLA	C3D-C4D	-2.65	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aA	827	CLA	OBD-CAD	2.65	1.27	1.22
12	cB	929	CLA	C4D-CHA	2.64	1.47	1.38
15	bA	850	BCR	C30-C25	-2.64	1.50	1.53
12	cB	909	CLA	C1C-NC	-2.64	1.33	1.37
12	bA	829	CLA	C4D-CHA	2.64	1.47	1.38
12	cB	903	CLA	C4D-CHA	2.64	1.47	1.38
12	bA	839	CLA	OBD-CAD	2.64	1.27	1.22
12	cB	904	CLA	C3D-C4D	-2.64	1.38	1.44
15	bF	201	BCR	C1-C6	-2.64	1.50	1.53
12	aB	907	CLA	C1B-C2B	2.64	1.49	1.43
12	cA	822	CLA	C4D-CHA	2.64	1.47	1.38
12	aA	832	CLA	C3D-C4D	-2.64	1.38	1.44
12	bB	907	CLA	C1B-C2B	2.64	1.49	1.43
12	bA	811	CLA	C4D-CHA	2.64	1.47	1.38
12	bA	803	CLA	CHB-C1B	2.64	1.45	1.39
12	bF	202	CLA	C4D-CHA	2.64	1.47	1.38
15	aF	204	BCR	C1-C6	-2.64	1.50	1.53
12	cA	803	CLA	CHB-C1B	2.64	1.45	1.39
12	aA	842	CLA	C4D-CHA	2.64	1.47	1.38
12	cB	935	CLA	C4D-CHA	2.64	1.47	1.38
12	cB	923	CLA	C3D-C4D	-2.64	1.38	1.44
12	bA	823	CLA	C1B-C2B	2.64	1.49	1.43
12	aB	904	CLA	C3D-C4D	-2.64	1.38	1.44
12	cA	837	CLA	C3D-C4D	-2.64	1.38	1.44
12	cL	204	CLA	C1B-C2B	2.63	1.49	1.43
12	aA	839	CLA	OBD-CAD	2.63	1.27	1.22
15	cA	850	BCR	C1-C6	-2.63	1.50	1.53
12	cB	922	CLA	C3D-C4D	-2.63	1.38	1.44
12	bB	929	CLA	C4D-CHA	2.63	1.47	1.38
12	aB	903	CLA	C4D-CHA	2.63	1.47	1.38
12	aB	908	CLA	C3D-C4D	-2.63	1.38	1.44
12	aB	929	CLA	C4D-CHA	2.63	1.47	1.38
12	aB	935	CLA	C4D-CHA	2.63	1.47	1.38
12	bB	904	CLA	C3D-C4D	-2.63	1.38	1.44
12	bB	925	CLA	C3B-C4B	2.63	1.50	1.42
12	cB	925	CLA	C3B-C4B	2.63	1.50	1.42
12	bB	923	CLA	OBD-CAD	2.63	1.27	1.22
12	aA	839	CLA	C1C-NC	-2.63	1.33	1.37
13	bA	844	1L3	O13-C12	-2.63	1.17	1.23
12	cA	842	CLA	C4D-CHA	2.63	1.47	1.38
12	aA	843	CLA	C4D-CHA	2.63	1.47	1.38
12	cA	832	CLA	OBD-CAD	2.63	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	cB	942	BCR	C30-C25	-2.63	1.50	1.53
12	bB	911	CLA	C4D-CHA	2.63	1.47	1.38
12	cB	911	CLA	C4D-CHA	2.63	1.47	1.38
12	bA	833	CLA	OBD-CAD	2.63	1.27	1.22
12	cB	907	CLA	C1B-C2B	2.63	1.49	1.43
12	bB	923	CLA	C3D-C4D	-2.63	1.38	1.44
12	bB	903	CLA	C4D-CHA	2.63	1.47	1.38
12	cA	829	CLA	OBD-CAD	2.62	1.27	1.22
12	aF	202	CLA	C4D-CHA	2.62	1.47	1.38
12	aL	204	CLA	C1B-C2B	2.62	1.49	1.43
15	cI	101	BCR	C1-C6	-2.62	1.50	1.53
12	aB	934	CLA	C4B-NB	-2.62	1.34	1.37
12	cA	818	CLA	C1B-C2B	2.62	1.49	1.43
12	cF	202	CLA	C4D-CHA	2.62	1.47	1.38
12	aB	909	CLA	C1C-NC	-2.62	1.33	1.37
12	bB	909	CLA	C1C-NC	-2.62	1.33	1.37
13	aA	845	1L3	O13-C12	-2.62	1.17	1.23
12	bB	922	CLA	C3D-C4D	-2.62	1.38	1.44
12	bA	819	CLA	OBD-CAD	2.62	1.27	1.22
12	bB	935	CLA	C4D-CHA	2.62	1.47	1.38
12	cA	823	CLA	C1B-C2B	2.62	1.49	1.43
12	bA	832	CLA	C3D-C4D	-2.62	1.38	1.44
15	cF	204	BCR	C1-C6	-2.62	1.50	1.53
12	bA	818	CLA	C1B-C2B	2.62	1.49	1.43
12	bB	933	CLA	C4D-CHA	2.62	1.47	1.38
12	aA	814	CLA	C1B-C2B	2.62	1.49	1.43
12	aA	818	CLA	C1B-C2B	2.62	1.49	1.43
12	aB	923	CLA	C3D-C4D	-2.62	1.38	1.44
13	cA	844	1L3	O13-C12	-2.62	1.17	1.23
12	aB	932	CLA	C4D-CHA	2.62	1.47	1.38
12	aA	842	CLA	C3B-C4B	2.61	1.50	1.42
12	aA	817	CLA	C3D-C4D	-2.61	1.38	1.44
12	bB	950	CLA	C4D-CHA	2.61	1.47	1.38
12	aA	829	CLA	C4D-CHA	2.61	1.47	1.38
12	cA	810	CLA	C4D-CHA	2.61	1.47	1.38
12	aA	829	CLA	OBD-CAD	2.61	1.27	1.22
12	bA	832	CLA	OBD-CAD	2.61	1.27	1.22
12	aA	830	CLA	C4D-CHA	2.61	1.47	1.38
12	cA	839	CLA	C1C-NC	-2.61	1.33	1.37
12	bB	932	CLA	C4D-CHA	2.61	1.47	1.38
12	cA	830	CLA	C4D-CHA	2.61	1.47	1.38
12	cA	816	CLA	C4D-CHA	2.61	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bL	202	CLA	OBD-CAD	2.61	1.27	1.22
12	bB	932	CLA	C3D-C4D	-2.61	1.38	1.44
12	bA	839	CLA	C1C-NC	-2.61	1.33	1.37
12	cA	829	CLA	C4D-CHA	2.61	1.47	1.38
12	aA	811	CLA	C4D-CHA	2.61	1.47	1.38
12	aB	939	CLA	C4D-CHA	2.61	1.47	1.38
12	cB	915	CLA	C4D-CHA	2.61	1.47	1.38
12	bA	810	CLA	C4D-CHA	2.61	1.47	1.38
12	aL	202	CLA	OBD-CAD	2.61	1.27	1.22
12	aB	950	CLA	C4D-CHA	2.61	1.47	1.38
12	aA	832	CLA	OBD-CAD	2.61	1.27	1.22
12	cA	843	CLA	C4D-CHA	2.61	1.47	1.38
12	aA	837	CLA	C4D-CHA	2.61	1.47	1.38
12	bA	842	CLA	C3B-C4B	2.60	1.50	1.42
12	cB	933	CLA	C4D-CHA	2.60	1.47	1.38
12	cB	923	CLA	OBD-CAD	2.60	1.27	1.22
12	aA	821	CLA	C3B-C4B	2.60	1.50	1.42
12	bB	939	CLA	C4D-CHA	2.60	1.47	1.38
12	cA	817	CLA	C3D-C4D	-2.60	1.38	1.44
12	bA	843	CLA	C4D-CHA	2.60	1.47	1.38
12	aA	803	CLA	CHB-C1B	2.60	1.45	1.39
12	bB	924	CLA	C4D-CHA	2.60	1.47	1.38
12	bA	830	CLA	C4D-CHA	2.60	1.47	1.38
12	aB	933	CLA	C4D-CHA	2.60	1.47	1.38
12	aB	911	CLA	C4D-CHA	2.60	1.47	1.38
15	aB	946	BCR	C1-C6	-2.60	1.50	1.53
12	cA	814	CLA	C1B-C2B	2.60	1.49	1.43
12	cB	924	CLA	C4D-CHA	2.60	1.47	1.38
12	aB	907	CLA	C3D-C4D	-2.60	1.38	1.44
12	aA	810	CLA	C4D-CHA	2.60	1.47	1.38
12	bB	908	CLA	C3D-C4D	-2.60	1.38	1.44
12	cA	842	CLA	C3B-C4B	2.60	1.50	1.42
12	bA	843	CLA	C1B-C2B	2.60	1.49	1.43
12	cB	908	CLA	C3D-C4D	-2.60	1.38	1.44
15	aI	101	BCR	C1-C6	-2.60	1.50	1.53
12	bA	842	CLA	C4D-CHA	2.60	1.47	1.38
12	bB	930	CLA	C4D-CHA	2.59	1.47	1.38
12	bA	829	CLA	OBD-CAD	2.59	1.27	1.22
12	cA	837	CLA	C4D-CHA	2.59	1.47	1.38
12	aB	925	CLA	C3B-C4B	2.59	1.50	1.42
12	aB	949	CLA	C1B-C2B	2.59	1.49	1.43
12	cA	812	CLA	C4D-CHA	2.59	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bB	907	CLA	C3D-C4D	-2.59	1.38	1.44
12	aA	816	CLA	C4D-CHA	2.59	1.47	1.38
12	bB	915	CLA	C4D-CHA	2.59	1.47	1.38
12	bA	812	CLA	C4D-CHA	2.59	1.47	1.38
12	aB	930	CLA	C4D-CHA	2.59	1.47	1.38
15	bB	946	BCR	C1-C6	-2.59	1.50	1.53
12	aA	844	CLA	C4D-CHA	2.59	1.47	1.38
12	aA	823	CLA	C1B-C2B	2.59	1.49	1.43
12	bA	842	CLA	C3D-C4D	-2.59	1.38	1.44
12	aB	918	CLA	C4D-CHA	2.59	1.47	1.38
12	bA	837	CLA	C4D-CHA	2.59	1.47	1.38
12	bA	809	CLA	C3D-C4D	-2.59	1.38	1.44
12	aB	915	CLA	C4D-CHA	2.58	1.47	1.38
12	aA	842	CLA	C3D-C4D	-2.58	1.38	1.44
12	aB	936	CLA	C4D-CHA	2.58	1.47	1.38
12	cB	949	CLA	C1B-C2B	2.58	1.49	1.43
12	aA	821	CLA	C3D-C4D	-2.58	1.38	1.44
15	bA	846	BCR	C30-C25	-2.58	1.50	1.53
12	aA	825	CLA	C1C-C2C	2.58	1.49	1.44
12	bA	814	CLA	C1B-C2B	2.58	1.49	1.43
12	bA	825	CLA	C4D-CHA	2.58	1.47	1.38
15	bF	204	BCR	C1-C6	-2.58	1.50	1.53
12	aA	806	CLA	C3D-C4D	-2.58	1.38	1.44
12	bA	816	CLA	C4D-CHA	2.58	1.47	1.38
12	cB	939	CLA	C4D-CHA	2.58	1.47	1.38
12	aB	924	CLA	C4D-CHA	2.58	1.47	1.38
12	cA	809	CLA	C3D-C4D	-2.58	1.38	1.44
12	aB	922	CLA	C4D-CHA	2.58	1.47	1.38
12	aL	202	CLA	C4D-CHA	2.58	1.47	1.38
12	cB	930	CLA	C4D-CHA	2.58	1.47	1.38
12	cB	918	CLA	C4D-CHA	2.58	1.47	1.38
12	aB	950	CLA	C4C-C3C	2.58	1.49	1.45
12	cA	827	CLA	C4D-CHA	2.58	1.47	1.38
12	cA	830	CLA	C1C-NC	-2.58	1.33	1.37
12	aA	821	CLA	C4D-CHA	2.58	1.47	1.38
12	bB	950	CLA	C4C-C3C	2.58	1.49	1.45
12	cB	932	CLA	C4D-CHA	2.58	1.47	1.38
12	cA	843	CLA	C1B-C2B	2.58	1.49	1.43
12	cA	825	CLA	C4D-CHA	2.58	1.47	1.38
12	cA	821	CLA	C3B-C4B	2.57	1.50	1.42
12	cA	839	CLA	C3D-C4D	-2.57	1.38	1.44
12	cB	907	CLA	C3D-C4D	-2.57	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cL	202	CLA	C4D-CHA	2.57	1.47	1.38
12	aA	818	CLA	C1C-NC	-2.57	1.33	1.37
12	aB	908	CLA	C1C-NC	-2.57	1.33	1.37
12	aB	932	CLA	C3D-C4D	-2.57	1.38	1.44
12	bA	817	CLA	C3D-C4D	-2.57	1.38	1.44
12	aA	812	CLA	C4D-CHA	2.57	1.47	1.38
12	aA	809	CLA	C3D-C4D	-2.57	1.38	1.44
12	aA	828	CLA	C1B-C2B	2.57	1.49	1.43
12	bA	806	CLA	C3D-C4D	-2.57	1.38	1.44
12	bA	828	CLA	C1B-C2B	2.57	1.49	1.43
12	cB	922	CLA	C4D-CHA	2.57	1.47	1.38
12	aA	825	CLA	C4D-CHA	2.57	1.47	1.38
12	bA	833	CLA	C1B-C2B	2.57	1.49	1.43
12	bA	827	CLA	C4D-CHA	2.57	1.47	1.38
12	aB	949	CLA	C3B-C4B	2.57	1.50	1.42
12	cB	949	CLA	C3B-C4B	2.57	1.50	1.42
12	bA	821	CLA	C3B-C4B	2.57	1.50	1.42
12	cB	932	CLA	C3D-C4D	-2.57	1.38	1.44
12	aA	843	CLA	C1B-C2B	2.57	1.49	1.43
12	aA	814	CLA	C3D-C4D	-2.57	1.38	1.44
12	bB	918	CLA	C4D-CHA	2.57	1.47	1.38
12	bA	805	CLA	C3B-C4B	2.57	1.50	1.42
12	aB	909	CLA	C1B-C2B	2.56	1.49	1.43
12	aA	844	CLA	C4C-C3C	2.56	1.49	1.45
12	bA	840	CLA	C4C-C3C	2.56	1.49	1.45
12	bA	821	CLA	C3D-C4D	-2.56	1.38	1.44
12	aA	833	CLA	C1B-C2B	2.56	1.49	1.43
12	cB	936	CLA	C4D-CHA	2.56	1.47	1.38
12	cL	202	CLA	OBD-CAD	2.56	1.26	1.22
12	bB	949	CLA	C1B-C2B	2.56	1.49	1.43
12	bB	913	CLA	C4D-CHA	2.56	1.47	1.38
12	aA	827	CLA	C4D-CHA	2.56	1.47	1.38
12	bB	936	CLA	C4D-CHA	2.56	1.47	1.38
12	cB	909	CLA	C1B-C2B	2.56	1.49	1.43
12	aB	913	CLA	C4D-CHA	2.56	1.47	1.38
12	bA	825	CLA	C1C-C2C	2.55	1.49	1.44
12	bA	818	CLA	C1C-NC	-2.55	1.33	1.37
12	bL	202	CLA	C4D-CHA	2.55	1.47	1.38
12	bA	836	CLA	C4C-C3C	2.55	1.49	1.45
12	bA	821	CLA	C4D-CHA	2.55	1.47	1.38
12	cB	936	CLA	C3D-C4D	-2.55	1.38	1.44
12	bA	817	CLA	C4D-CHA	2.55	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cA	825	CLA	C1C-C2C	2.55	1.49	1.44
12	cA	821	CLA	C3D-C4D	-2.55	1.38	1.44
12	cA	821	CLA	C4D-CHA	2.55	1.47	1.38
12	aA	817	CLA	C4D-CHA	2.55	1.47	1.38
12	cB	920	CLA	C1B-C2B	2.55	1.49	1.43
12	bA	839	CLA	C3D-C4D	-2.55	1.38	1.44
12	bB	909	CLA	C1B-C2B	2.55	1.49	1.43
15	aA	851	BCR	C1-C6	-2.55	1.50	1.53
12	cA	817	CLA	C4D-CHA	2.55	1.47	1.38
12	bB	905	CLA	OBD-CAD	2.55	1.26	1.22
12	cB	926	CLA	C1C-NC	-2.55	1.33	1.37
12	cB	908	CLA	C1C-NC	-2.55	1.33	1.37
12	cA	806	CLA	C3D-C4D	-2.55	1.38	1.44
12	cA	828	CLA	C1B-C2B	2.54	1.49	1.43
12	bB	922	CLA	C4D-CHA	2.54	1.47	1.38
12	bB	949	CLA	C3B-C4B	2.54	1.50	1.42
12	cA	828	CLA	C3D-C4D	-2.54	1.38	1.44
12	aA	805	CLA	C3B-C4B	2.54	1.50	1.42
12	aA	839	CLA	C3D-C4D	-2.54	1.38	1.44
12	aB	914	CLA	C1C-C2C	2.54	1.49	1.44
12	aA	817	CLA	C1B-C2B	2.54	1.49	1.43
12	bA	830	CLA	C1C-NC	-2.54	1.33	1.37
12	aB	913	CLA	C3D-C4D	-2.54	1.38	1.44
12	cA	814	CLA	C3D-C4D	-2.54	1.38	1.44
12	cA	817	CLA	C1B-C2B	2.54	1.49	1.43
12	cA	804	CLA	C4D-CHA	2.54	1.47	1.38
12	cA	842	CLA	C3D-C4D	-2.54	1.38	1.44
12	cB	914	CLA	C1C-C2C	2.54	1.49	1.44
12	bB	939	CLA	C1C-NC	-2.54	1.33	1.37
12	aB	915	CLA	C3D-C4D	-2.54	1.38	1.44
12	cA	822	CLA	C1B-C2B	2.54	1.49	1.43
12	aB	936	CLA	C3D-C4D	-2.53	1.38	1.44
12	cB	913	CLA	C4D-CHA	2.53	1.47	1.38
12	aB	939	CLA	C1C-NC	-2.53	1.33	1.37
12	cA	833	CLA	C1B-C2B	2.53	1.49	1.43
12	aA	840	CLA	C4C-C3C	2.53	1.49	1.45
12	cB	939	CLA	C1C-NC	-2.53	1.33	1.37
12	bA	828	CLA	C3D-C4D	-2.53	1.38	1.44
12	cB	905	CLA	C1B-C2B	2.53	1.49	1.43
12	aA	808	CLA	C3B-C4B	2.53	1.50	1.42
12	aA	804	CLA	C4D-CHA	2.53	1.47	1.38
12	cB	932	CLA	C1C-NC	-2.53	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aA	823	CLA	C4D-CHA	2.53	1.47	1.38
12	bA	808	CLA	C3B-C4B	2.53	1.50	1.42
12	cB	915	CLA	C3D-C4D	-2.53	1.38	1.44
12	aB	922	CLA	C1B-C2B	2.53	1.49	1.43
12	bA	817	CLA	C1B-C2B	2.52	1.49	1.43
12	cA	826	CLA	C4D-CHA	2.52	1.47	1.38
12	bA	809	CLA	C4D-CHA	2.52	1.47	1.38
12	cL	204	CLA	C4D-CHA	2.52	1.47	1.38
12	aB	905	CLA	C3D-C4D	-2.52	1.38	1.44
12	aB	904	CLA	C1B-C2B	2.52	1.49	1.43
12	cA	805	CLA	C3B-C4B	2.52	1.50	1.42
12	bA	838	CLA	C3D-C4D	-2.52	1.38	1.44
12	aA	810	CLA	C1B-C2B	2.52	1.49	1.43
12	cB	924	CLA	C1B-C2B	2.52	1.49	1.43
12	bA	824	CLA	C3D-C4D	-2.52	1.38	1.44
12	bA	823	CLA	C4D-CHA	2.52	1.47	1.38
12	bB	936	CLA	C3D-C4D	-2.52	1.38	1.44
15	cB	946	BCR	C1-C6	-2.52	1.50	1.53
12	cA	808	CLA	C3B-C4B	2.52	1.50	1.42
12	aB	904	CLA	C4D-CHA	2.52	1.47	1.38
12	cB	938	CLA	C4D-CHA	2.52	1.47	1.38
12	aA	834	CLA	C3D-C4D	-2.52	1.38	1.44
12	aB	932	CLA	C1C-NC	-2.52	1.33	1.37
12	bA	836	CLA	C1B-C2B	2.52	1.49	1.43
12	aB	926	CLA	C1C-NC	-2.52	1.33	1.37
12	bB	920	CLA	C1B-C2B	2.52	1.49	1.43
12	bB	910	CLA	C4D-CHA	2.52	1.47	1.38
12	bB	914	CLA	C1C-C2C	2.52	1.49	1.44
12	cA	806	CLA	C1B-C2B	2.52	1.49	1.43
12	aA	814	CLA	C4D-CHA	2.52	1.47	1.38
12	bB	938	CLA	C4D-CHA	2.52	1.47	1.38
12	bB	908	CLA	C1C-NC	-2.51	1.33	1.37
12	bB	905	CLA	C1B-C2B	2.51	1.49	1.43
12	cB	907	CLA	C4D-CHA	2.51	1.47	1.38
12	aA	836	CLA	C4C-C3C	2.51	1.49	1.45
15	bF	201	BCR	C30-C25	-2.51	1.50	1.53
12	aA	833	CLA	C3D-C4D	-2.51	1.38	1.44
12	bA	804	CLA	C4D-CHA	2.51	1.47	1.38
12	aA	809	CLA	C4D-CHA	2.51	1.47	1.38
12	cA	843	CLA	C3D-C4D	-2.51	1.38	1.44
12	bA	833	CLA	C3D-C4D	-2.51	1.38	1.44
12	bF	202	CLA	C3B-C4B	2.51	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cA	833	CLA	C3D-C4D	-2.51	1.38	1.44
12	cA	840	CLA	C4C-C3C	2.51	1.49	1.45
12	cB	911	CLA	C3D-C4D	-2.51	1.38	1.44
12	aB	938	CLA	C4D-CHA	2.51	1.47	1.38
12	bA	807	CLA	C3B-C4B	2.51	1.50	1.42
12	bB	922	CLA	C1B-C2B	2.51	1.49	1.43
12	aA	826	CLA	C4D-CHA	2.51	1.47	1.38
12	bA	829	CLA	C1B-C2B	2.51	1.49	1.43
15	aB	946	BCR	C30-C25	-2.51	1.50	1.53
12	aL	204	CLA	C4D-CHA	2.51	1.47	1.38
12	cA	834	CLA	C3D-C4D	-2.51	1.38	1.44
12	aB	907	CLA	C4D-CHA	2.51	1.47	1.38
12	cB	904	CLA	C4D-CHA	2.51	1.47	1.38
12	aA	830	CLA	C1C-NC	-2.51	1.34	1.37
12	bB	932	CLA	C1C-NC	-2.51	1.34	1.37
12	bB	915	CLA	C3D-C4D	-2.51	1.38	1.44
12	aA	829	CLA	C1B-C2B	2.51	1.49	1.43
12	bA	810	CLA	C1B-C2B	2.51	1.49	1.43
12	cA	836	CLA	C1B-C2B	2.51	1.49	1.43
12	cA	823	CLA	C4D-CHA	2.51	1.47	1.38
12	aA	843	CLA	C3D-C4D	-2.50	1.38	1.44
12	bB	924	CLA	C1B-C2B	2.50	1.49	1.43
15	bL	206	BCR	C1-C6	-2.50	1.50	1.53
15	cF	201	BCR	C30-C25	-2.50	1.50	1.53
12	bA	814	CLA	C4D-CHA	2.50	1.47	1.38
12	cA	830	CLA	C3D-C4D	-2.50	1.38	1.44
12	cB	905	CLA	OBD-CAD	2.50	1.26	1.22
12	bL	204	CLA	C4D-CHA	2.50	1.47	1.38
12	aB	905	CLA	OBD-CAD	2.50	1.26	1.22
15	aF	201	BCR	C30-C25	-2.50	1.50	1.53
12	aB	905	CLA	C1B-C2B	2.50	1.49	1.43
12	aA	828	CLA	C3D-C4D	-2.50	1.38	1.44
12	cA	838	CLA	C4D-CHA	2.50	1.47	1.38
12	bA	814	CLA	C3D-C4D	-2.50	1.38	1.44
12	aB	910	CLA	C4D-CHA	2.50	1.47	1.38
12	cB	904	CLA	C1B-C2B	2.50	1.49	1.43
15	cL	205	BCR	C1-C6	-2.50	1.50	1.53
12	cB	924	CLA	C1C-NC	-2.50	1.34	1.37
12	cA	832	CLA	C4D-CHA	2.50	1.47	1.38
12	bB	906	CLA	C4D-CHA	2.50	1.47	1.38
15	aA	847	BCR	C30-C25	-2.50	1.50	1.53
12	bB	904	CLA	C1B-C2B	2.50	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bA	832	CLA	C4D-CHA	2.50	1.47	1.38
12	cB	910	CLA	C4D-CHA	2.50	1.47	1.38
15	cL	206	BCR	C1-C6	-2.50	1.50	1.53
12	cF	202	CLA	C3B-C4B	2.50	1.50	1.42
12	bA	806	CLA	C1B-C2B	2.50	1.49	1.43
12	aA	807	CLA	C3D-C4D	-2.50	1.38	1.44
12	bA	822	CLA	C1B-C2B	2.50	1.49	1.43
12	cA	818	CLA	C4D-CHA	2.50	1.47	1.38
12	bA	826	CLA	C4D-CHA	2.50	1.47	1.38
12	aF	202	CLA	C3B-C4B	2.50	1.50	1.42
12	aB	937	CLA	C4D-CHA	2.50	1.47	1.38
12	bB	907	CLA	C4D-CHA	2.49	1.47	1.38
12	aB	920	CLA	C1B-C2B	2.49	1.49	1.43
12	aA	832	CLA	C4D-CHA	2.49	1.47	1.38
12	cB	905	CLA	C3D-C4D	-2.49	1.38	1.44
12	aA	806	CLA	C1B-C2B	2.49	1.49	1.43
12	aA	822	CLA	C1B-C2B	2.49	1.49	1.43
12	bA	841	CLA	C4D-CHA	2.49	1.47	1.38
12	cA	841	CLA	C1C-NC	-2.49	1.34	1.37
12	aA	836	CLA	C1B-C2B	2.49	1.49	1.43
12	cB	921	CLA	C1B-C2B	2.49	1.49	1.43
12	bB	921	CLA	C1B-C2B	2.49	1.49	1.43
12	cA	829	CLA	C1B-C2B	2.49	1.49	1.43
12	bB	905	CLA	C3D-C4D	-2.49	1.38	1.44
12	bA	838	CLA	C4D-CHA	2.49	1.46	1.38
12	cA	841	CLA	C4D-CHA	2.49	1.46	1.38
12	bB	928	CLA	C4D-CHA	2.49	1.46	1.38
12	cA	814	CLA	C4D-CHA	2.49	1.46	1.38
12	cA	807	CLA	C3B-C4B	2.49	1.50	1.42
12	bB	904	CLA	C4D-CHA	2.49	1.46	1.38
12	aA	807	CLA	C3B-C4B	2.49	1.50	1.42
12	bA	843	CLA	C3D-C4D	-2.49	1.38	1.44
12	bB	913	CLA	C3D-C4D	-2.49	1.38	1.44
12	cB	906	CLA	C4D-CHA	2.49	1.46	1.38
12	cB	913	CLA	C3D-C4D	-2.49	1.38	1.44
12	cB	922	CLA	C1B-C2B	2.49	1.49	1.43
12	cA	824	CLA	C3D-C4D	-2.49	1.38	1.44
15	aL	206	BCR	C1-C6	-2.49	1.50	1.53
12	aA	838	CLA	C3D-C4D	-2.49	1.38	1.44
15	bB	944	BCR	C30-C25	-2.49	1.50	1.53
12	cB	937	CLA	C4D-CHA	2.49	1.46	1.38
12	cA	809	CLA	C4D-CHA	2.49	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aA	841	CLA	C4D-CHA	2.49	1.46	1.38
12	bA	807	CLA	C3D-C4D	-2.48	1.38	1.44
12	cA	839	CLA	C4D-CHA	2.48	1.46	1.38
15	aL	205	BCR	C1-C6	-2.48	1.50	1.53
12	cA	818	CLA	C1C-NC	-2.48	1.34	1.37
15	cA	846	BCR	C30-C25	-2.48	1.50	1.53
12	aB	924	CLA	C1C-NC	-2.48	1.34	1.37
12	bA	834	CLA	C3D-C4D	-2.48	1.38	1.44
12	cA	838	CLA	C3D-C4D	-2.48	1.38	1.44
12	cB	909	CLA	C3B-C4B	2.48	1.50	1.42
12	cA	836	CLA	C4C-C3C	2.48	1.49	1.45
12	aA	824	CLA	C3D-C4D	-2.48	1.38	1.44
15	bL	205	BCR	C1-C6	-2.48	1.50	1.53
12	cB	910	CLA	C1B-C2B	2.48	1.48	1.43
12	bB	937	CLA	C4D-CHA	2.48	1.46	1.38
12	cA	853	CLA	C4D-CHA	2.48	1.46	1.38
12	aB	906	CLA	C4D-CHA	2.48	1.46	1.38
12	cB	928	CLA	C4D-CHA	2.48	1.46	1.38
12	aA	833	CLA	C4D-CHA	2.48	1.46	1.38
12	aA	818	CLA	C4D-CHA	2.48	1.46	1.38
12	bA	838	CLA	C3B-C4B	2.48	1.49	1.42
12	cA	833	CLA	C4D-CHA	2.47	1.46	1.38
12	bB	916	CLA	C3D-C4D	-2.47	1.38	1.44
12	bA	830	CLA	C3D-C4D	-2.47	1.38	1.44
12	aB	928	CLA	C4D-CHA	2.47	1.46	1.38
17	aB	947	LMG	O1-C7	-2.47	1.39	1.43
12	cL	203	CLA	C4D-CHA	2.47	1.46	1.38
15	cB	946	BCR	C30-C25	-2.47	1.50	1.53
12	aB	924	CLA	C1B-C2B	2.47	1.48	1.43
12	bL	203	CLA	C4D-CHA	2.47	1.46	1.38
12	aA	837	CLA	OBD-CAD	2.47	1.26	1.22
12	cB	930	CLA	C3D-C4D	-2.47	1.38	1.44
12	aA	830	CLA	C3D-C4D	-2.47	1.38	1.44
12	aB	911	CLA	C3D-C4D	-2.47	1.38	1.44
12	bA	806	CLA	C4D-CHA	2.47	1.46	1.38
12	bA	853	CLA	C4D-CHA	2.47	1.46	1.38
12	aA	838	CLA	C3B-C4B	2.47	1.49	1.42
12	bA	818	CLA	C4D-CHA	2.47	1.46	1.38
12	bB	926	CLA	C1C-NC	-2.47	1.34	1.37
12	aB	916	CLA	C3D-C4D	-2.47	1.38	1.44
12	bB	911	CLA	C3D-C4D	-2.47	1.38	1.44
12	aA	838	CLA	C4D-CHA	2.47	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aA	854	CLA	C4D-CHA	2.47	1.46	1.38
12	aA	807	CLA	C1C-NC	-2.47	1.34	1.37
12	bA	839	CLA	C4D-CHA	2.47	1.46	1.38
12	cB	916	CLA	C3D-C4D	-2.47	1.38	1.44
12	aA	834	CLA	C4D-CHA	2.47	1.46	1.38
12	bB	931	CLA	C4B-NB	-2.47	1.34	1.37
12	aB	909	CLA	C3B-C4B	2.47	1.49	1.42
12	cA	810	CLA	C1B-C2B	2.47	1.48	1.43
12	bA	813	CLA	C3B-C2B	2.46	1.49	1.41
12	cA	807	CLA	C1C-NC	-2.46	1.34	1.37
17	bB	947	LMG	O1-C7	-2.46	1.39	1.43
12	aA	819	CLA	C4D-CHA	2.46	1.46	1.38
12	cB	927	CLA	C4D-CHA	2.46	1.46	1.38
12	cB	907	CLA	C1C-NC	-2.46	1.34	1.37
12	cA	807	CLA	C3D-C4D	-2.46	1.38	1.44
12	bB	910	CLA	C1B-C2B	2.46	1.48	1.43
12	bF	202	CLA	C3D-C4D	-2.46	1.38	1.44
12	bA	833	CLA	C4D-CHA	2.46	1.46	1.38
12	bA	807	CLA	C1C-NC	-2.46	1.34	1.37
12	cA	802	CLA	OBD-CAD	2.46	1.26	1.22
12	aB	921	CLA	C1B-C2B	2.46	1.48	1.43
12	bB	909	CLA	C3B-C4B	2.46	1.49	1.42
12	aB	927	CLA	C4D-CHA	2.46	1.46	1.38
15	bB	946	BCR	C30-C25	-2.46	1.50	1.53
12	bA	841	CLA	C1C-NC	-2.46	1.34	1.37
12	cB	906	CLA	C3D-C4D	-2.46	1.38	1.44
12	aA	842	CLA	C1C-NC	-2.46	1.34	1.37
12	bA	819	CLA	C4D-CHA	2.45	1.46	1.38
12	aA	839	CLA	C4D-CHA	2.45	1.46	1.38
12	aL	203	CLA	C4D-CHA	2.45	1.46	1.38
12	aB	907	CLA	C1C-NC	-2.45	1.34	1.37
12	cA	806	CLA	C4D-CHA	2.45	1.46	1.38
12	aB	910	CLA	C1B-C2B	2.45	1.48	1.43
12	cA	819	CLA	C4D-CHA	2.45	1.46	1.38
12	cB	928	CLA	C1C-NC	-2.45	1.34	1.37
12	bA	834	CLA	C4D-CHA	2.45	1.46	1.38
15	aB	944	BCR	C30-C25	-2.45	1.50	1.53
12	aA	806	CLA	C4D-CHA	2.45	1.46	1.38
12	bB	901	CLA	C3D-C4D	-2.45	1.38	1.44
12	cB	918	CLA	C3D-C4D	-2.45	1.38	1.44
12	cA	813	CLA	C3B-C2B	2.45	1.49	1.41
12	bA	808	CLA	C1B-C2B	2.45	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aB	930	CLA	C3D-C4D	-2.45	1.38	1.44
12	bA	837	CLA	OBD-CAD	2.45	1.26	1.22
12	cA	837	CLA	C4C-C3C	2.45	1.49	1.45
12	bB	906	CLA	C3B-C4B	2.45	1.49	1.42
12	cB	931	CLA	C4B-NB	-2.45	1.34	1.37
12	aA	813	CLA	C3B-C2B	2.45	1.49	1.41
12	cL	203	CLA	C3D-C4D	-2.45	1.38	1.44
12	bB	906	CLA	C3D-C4D	-2.45	1.38	1.44
17	cB	947	LMG	O1-C7	-2.44	1.39	1.43
12	aB	931	CLA	C4B-NB	-2.44	1.34	1.37
12	bL	203	CLA	C3D-C4D	-2.44	1.38	1.44
11	bA	801	CL0	CMD-C2D	-2.44	1.46	1.51
12	bF	202	CLA	C4C-C3C	2.44	1.49	1.45
12	cA	838	CLA	C3B-C4B	2.44	1.49	1.42
12	aB	918	CLA	C3D-C4D	-2.44	1.38	1.44
12	cA	842	CLA	C1C-NC	-2.44	1.34	1.37
12	bB	927	CLA	C4D-CHA	2.44	1.46	1.38
12	aA	837	CLA	C4C-C3C	2.44	1.49	1.45
12	cA	834	CLA	C4D-CHA	2.44	1.46	1.38
12	aB	906	CLA	C3B-C4B	2.44	1.49	1.42
12	aA	824	CLA	C1C-NC	-2.44	1.34	1.37
12	bB	903	CLA	C1C-NC	-2.44	1.34	1.37
12	aB	923	CLA	C1C-C2C	2.44	1.49	1.44
12	cB	906	CLA	C3B-C4B	2.44	1.49	1.42
12	bA	842	CLA	C1C-NC	-2.43	1.34	1.37
15	cB	943	BCR	C30-C25	-2.43	1.50	1.53
12	bA	803	CLA	C1D-ND	2.43	1.41	1.37
12	aB	902	CLA	C4D-CHA	2.43	1.46	1.38
12	bB	928	CLA	C1C-NC	-2.43	1.34	1.37
12	cA	831	CLA	C1C-NC	-2.43	1.34	1.37
12	bA	807	CLA	OBD-CAD	2.43	1.26	1.22
12	bB	902	CLA	C4D-CHA	2.43	1.46	1.38
12	cA	853	CLA	C1B-C2B	2.43	1.48	1.43
12	bB	920	CLA	C1C-C2C	2.43	1.49	1.44
12	cB	923	CLA	C1C-C2C	2.43	1.49	1.44
12	cB	902	CLA	C4D-CHA	2.43	1.46	1.38
12	aF	202	CLA	C3D-C4D	-2.43	1.38	1.44
12	aA	841	CLA	C1C-NC	-2.43	1.34	1.37
12	aL	203	CLA	C3D-C4D	-2.43	1.38	1.44
12	aF	202	CLA	C4C-C3C	2.43	1.49	1.45
11	cA	801	CL0	CMD-C2D	-2.43	1.46	1.51
12	cA	803	CLA	C4D-CHA	2.43	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aA	823	CLA	C3D-C4D	-2.43	1.38	1.44
12	bB	918	CLA	C3D-C4D	-2.43	1.38	1.44
12	cB	903	CLA	C1C-NC	-2.43	1.34	1.37
12	bB	908	CLA	OBD-CAD	2.43	1.26	1.22
12	cA	807	CLA	OBD-CAD	2.43	1.26	1.22
12	cF	202	CLA	C4C-C3C	2.43	1.49	1.45
12	cA	837	CLA	OBD-CAD	2.43	1.26	1.22
12	bB	903	CLA	C1B-C2B	2.43	1.48	1.43
12	aB	920	CLA	C1C-C2C	2.43	1.49	1.44
12	aA	837	CLA	C1C-NC	-2.42	1.34	1.37
12	bB	924	CLA	C1C-NC	-2.42	1.34	1.37
12	cA	816	CLA	C1B-C2B	2.42	1.48	1.43
12	bA	816	CLA	C3D-C4D	-2.42	1.38	1.44
12	aB	928	CLA	C1C-NC	-2.42	1.34	1.37
12	bA	814	CLA	C1C-NC	-2.42	1.34	1.37
12	cA	823	CLA	C3D-C4D	-2.42	1.38	1.44
12	bA	828	CLA	C1C-NC	-2.42	1.34	1.37
12	bA	831	CLA	C1C-NC	-2.42	1.34	1.37
12	cB	938	CLA	C1B-C2B	2.42	1.48	1.43
12	aB	908	CLA	CHC-C4B	2.42	1.44	1.39
12	cB	932	CLA	C1B-C2B	2.42	1.48	1.43
12	aB	901	CLA	C3D-C4D	-2.42	1.38	1.44
12	bB	908	CLA	CHC-C4B	2.42	1.44	1.39
12	bA	802	CLA	OBD-CAD	2.42	1.26	1.22
15	bB	943	BCR	C30-C25	-2.42	1.50	1.53
12	bA	803	CLA	C4D-CHA	2.42	1.46	1.38
12	aB	933	CLA	C3B-C4B	2.42	1.49	1.42
12	bA	823	CLA	C3D-C4D	-2.42	1.38	1.44
12	bA	853	CLA	C1B-C2B	2.42	1.48	1.43
12	bB	907	CLA	C1C-NC	-2.42	1.34	1.37
12	bA	812	CLA	C3D-C4D	-2.42	1.38	1.44
12	bB	933	CLA	C3B-C4B	2.42	1.49	1.42
12	cA	816	CLA	C3D-C4D	-2.42	1.38	1.44
12	aA	803	CLA	C4D-CHA	2.42	1.46	1.38
12	cB	903	CLA	C1B-C2B	2.42	1.48	1.43
12	aA	854	CLA	C1B-C2B	2.41	1.48	1.43
12	aB	932	CLA	C1B-C2B	2.41	1.48	1.43
12	bB	930	CLA	C3D-C4D	-2.41	1.38	1.44
15	aB	943	BCR	C30-C25	-2.41	1.50	1.53
12	aA	808	CLA	C1B-C2B	2.41	1.48	1.43
12	cA	803	CLA	C1D-ND	2.41	1.41	1.37
12	bA	837	CLA	C1C-NC	-2.41	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bA	843	CLA	C1C-NC	-2.41	1.34	1.37
12	cB	908	CLA	CHC-C4B	2.41	1.44	1.39
12	cB	931	CLA	C3D-C4D	-2.41	1.38	1.44
12	bB	909	CLA	OBD-CAD	2.41	1.26	1.22
12	cA	837	CLA	C1C-NC	-2.41	1.34	1.37
12	aA	807	CLA	OBD-CAD	2.40	1.26	1.22
12	cA	814	CLA	C1C-NC	-2.40	1.34	1.37
12	cB	937	CLA	C4C-C3C	2.40	1.49	1.45
12	aB	938	CLA	C1B-C2B	2.40	1.48	1.43
15	cB	944	BCR	C30-C25	-2.40	1.50	1.53
12	aB	906	CLA	C3D-C4D	-2.40	1.38	1.44
12	aA	812	CLA	C3D-C4D	-2.40	1.38	1.44
12	bB	932	CLA	C1B-C2B	2.40	1.48	1.43
12	aB	931	CLA	C3D-C4D	-2.40	1.38	1.44
11	aA	801	CL0	CMD-C2D	-2.40	1.46	1.51
12	cB	910	CLA	C3D-C4D	-2.40	1.38	1.44
12	aB	912	CLA	C3D-C4D	-2.40	1.38	1.44
12	cF	202	CLA	C3D-C4D	-2.40	1.38	1.44
12	aB	937	CLA	C3D-C4D	-2.40	1.38	1.44
12	cA	808	CLA	C1B-C2B	2.40	1.48	1.43
12	cB	901	CLA	C3D-C4D	-2.40	1.38	1.44
12	cB	920	CLA	C1C-C2C	2.40	1.49	1.44
12	bA	853	CLA	C1C-NC	-2.40	1.34	1.37
12	aA	803	CLA	C1D-ND	2.40	1.41	1.37
12	aB	916	CLA	C4D-CHA	2.40	1.46	1.38
12	aA	810	CLA	C1C-NC	-2.40	1.34	1.37
12	aA	802	CLA	OBD-CAD	2.40	1.26	1.22
12	aA	816	CLA	C1B-C2B	2.40	1.48	1.43
12	aB	903	CLA	C1C-NC	-2.40	1.34	1.37
12	cA	826	CLA	C3D-C4D	-2.40	1.38	1.44
12	bB	930	CLA	C1B-C2B	2.40	1.48	1.43
12	aA	815	CLA	C3D-C4D	-2.40	1.38	1.44
13	aB	940	1L3	O05-C04	-2.40	1.18	1.23
12	bA	837	CLA	C4C-C3C	2.39	1.49	1.45
12	aB	912	CLA	C4D-CHA	2.39	1.46	1.38
12	bA	834	CLA	C4C-C3C	2.39	1.49	1.45
12	cB	912	CLA	C4D-CHA	2.39	1.46	1.38
12	bB	923	CLA	C1C-C2C	2.39	1.49	1.44
12	aB	926	CLA	C1B-C2B	2.39	1.48	1.43
12	aA	804	CLA	C3D-C4D	-2.39	1.38	1.44
12	aA	825	CLA	C3D-C4D	-2.39	1.38	1.44
12	cA	812	CLA	C3D-C4D	-2.39	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cA	815	CLA	C3D-C4D	-2.39	1.38	1.44
12	cB	912	CLA	C3D-C4D	-2.39	1.38	1.44
12	cB	908	CLA	OBD-CAD	2.39	1.26	1.22
12	cB	933	CLA	C3B-C4B	2.39	1.49	1.42
13	bB	940	1L3	O05-C04	-2.39	1.18	1.23
12	bB	910	CLA	C3D-C4D	-2.39	1.38	1.44
15	bL	201	BCR	C33-C5	-2.39	1.47	1.50
12	aA	813	CLA	C3D-C4D	-2.39	1.38	1.44
12	bB	937	CLA	C3D-C4D	-2.39	1.38	1.44
12	aA	831	CLA	C1C-NC	-2.39	1.34	1.37
12	cB	937	CLA	OBD-CAD	2.39	1.26	1.22
12	bB	937	CLA	C4C-C3C	2.39	1.49	1.45
12	cA	804	CLA	C3D-C4D	-2.39	1.38	1.44
12	bB	916	CLA	C4D-CHA	2.39	1.46	1.38
15	cA	847	BCR	C1-C6	-2.39	1.50	1.53
12	bA	809	CLA	C3B-C4B	2.38	1.49	1.42
12	cA	853	CLA	C1C-NC	-2.38	1.34	1.37
12	cB	937	CLA	C3D-C4D	-2.38	1.38	1.44
12	aA	814	CLA	C1C-NC	-2.38	1.34	1.37
12	bA	833	CLA	C1C-NC	-2.38	1.34	1.37
12	bA	815	CLA	C3D-C4D	-2.38	1.38	1.44
12	bB	912	CLA	C4D-CHA	2.38	1.46	1.38
12	bB	931	CLA	C3D-C4D	-2.38	1.38	1.44
12	aB	910	CLA	C3D-C4D	-2.38	1.38	1.44
12	bB	938	CLA	C1B-C2B	2.38	1.48	1.43
12	aA	809	CLA	C3B-C4B	2.38	1.49	1.42
12	bB	937	CLA	OBD-CAD	2.38	1.26	1.22
12	cA	828	CLA	C4D-CHA	2.38	1.46	1.38
12	bB	903	CLA	C3D-C4D	-2.38	1.38	1.44
12	cA	823	CLA	C1C-NC	-2.38	1.34	1.37
12	aA	844	CLA	C1C-NC	-2.38	1.34	1.37
12	bB	949	CLA	C1C-NC	-2.38	1.34	1.37
12	aA	854	CLA	C1C-NC	-2.38	1.34	1.37
12	cA	824	CLA	C1C-NC	-2.38	1.34	1.37
12	cB	909	CLA	OBD-CAD	2.38	1.26	1.22
12	aA	831	CLA	C1B-C2B	2.38	1.48	1.43
12	bA	831	CLA	C1B-C2B	2.38	1.48	1.43
12	cA	831	CLA	C1B-C2B	2.38	1.48	1.43
12	aA	844	CLA	C3D-C4D	-2.38	1.38	1.44
12	aA	844	CLA	C3B-C2B	2.38	1.49	1.41
12	aB	950	CLA	C1C-NC	-2.38	1.34	1.37
12	bA	810	CLA	C1C-NC	-2.38	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aB	950	CLA	C3B-C2B	2.38	1.49	1.41
12	aB	930	CLA	C1B-C2B	2.37	1.48	1.43
12	aA	838	CLA	C1C-NC	-2.37	1.34	1.37
12	cA	838	CLA	C1C-NC	-2.37	1.34	1.37
12	bA	816	CLA	C1B-C2B	2.37	1.48	1.43
12	cA	824	CLA	C1B-C2B	2.37	1.48	1.43
12	cB	926	CLA	C1B-C2B	2.37	1.48	1.43
12	bA	825	CLA	C3D-C4D	-2.37	1.38	1.44
12	cA	834	CLA	C4C-C3C	2.37	1.49	1.45
12	aA	826	CLA	C3D-C4D	-2.37	1.38	1.44
12	cL	203	CLA	C3B-C4B	2.37	1.49	1.42
12	aA	828	CLA	C4D-CHA	2.37	1.46	1.38
12	cB	916	CLA	C4D-CHA	2.37	1.46	1.38
12	cA	843	CLA	C1C-NC	-2.37	1.34	1.37
12	aA	828	CLA	C1C-NC	-2.37	1.34	1.37
12	cL	204	CLA	C3D-C4D	-2.37	1.38	1.44
12	bA	824	CLA	C1B-C2B	2.37	1.48	1.43
12	aB	908	CLA	OBD-CAD	2.37	1.26	1.22
12	aA	843	CLA	C1C-NC	-2.37	1.34	1.37
12	cB	922	CLA	C3B-C2B	2.37	1.49	1.41
15	aL	201	BCR	C33-C5	-2.37	1.47	1.50
12	bB	926	CLA	C4D-CHA	2.37	1.46	1.38
12	bL	203	CLA	C3B-C4B	2.37	1.49	1.42
12	bB	912	CLA	C3D-C4D	-2.37	1.38	1.44
12	cB	903	CLA	C3D-C4D	-2.37	1.38	1.44
12	aA	812	CLA	C1C-NC	-2.37	1.34	1.37
12	aB	903	CLA	C3D-C4D	-2.37	1.38	1.44
12	cA	815	CLA	C1B-C2B	2.37	1.48	1.43
12	bL	204	CLA	C3D-C4D	-2.37	1.38	1.44
12	aB	922	CLA	C3B-C2B	2.37	1.49	1.41
12	bA	815	CLA	C1B-C2B	2.36	1.48	1.43
12	aA	823	CLA	C1C-NC	-2.36	1.34	1.37
12	bB	949	CLA	C3D-C4D	-2.36	1.38	1.44
12	bA	828	CLA	C4D-CHA	2.36	1.46	1.38
12	bB	950	CLA	C1C-NC	-2.36	1.34	1.37
12	cA	809	CLA	C3B-C4B	2.36	1.49	1.42
12	cB	930	CLA	C1B-C2B	2.36	1.48	1.43
16	bB	948	LHG	P-O6	2.36	1.68	1.59
12	cB	926	CLA	C4D-CHA	2.36	1.46	1.38
12	bB	950	CLA	C3B-C2B	2.36	1.49	1.41
12	bB	914	CLA	C1B-C2B	2.36	1.48	1.43
12	bA	804	CLA	C3D-C4D	-2.36	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aA	834	CLA	C4C-C3C	2.36	1.49	1.45
12	bA	808	CLA	C4C-C3C	2.36	1.49	1.45
12	cA	814	CLA	C4C-C3C	2.36	1.49	1.45
12	bB	901	CLA	C4D-CHA	2.36	1.46	1.38
12	aA	818	CLA	C3D-C4D	-2.36	1.38	1.44
12	bA	827	CLA	C1C-NC	-2.36	1.34	1.37
12	cB	934	CLA	C4C-C3C	2.36	1.49	1.45
12	aB	922	CLA	C1C-NC	-2.36	1.34	1.37
12	bA	812	CLA	C1C-NC	-2.36	1.34	1.37
12	bA	818	CLA	C3D-C4D	-2.36	1.38	1.44
12	aB	909	CLA	OBD-CAD	2.36	1.26	1.22
12	bA	813	CLA	C3D-C4D	-2.36	1.38	1.44
12	cA	828	CLA	C1C-NC	-2.36	1.34	1.37
16	aB	948	LHG	P-O6	2.36	1.68	1.59
12	aA	827	CLA	C1C-NC	-2.36	1.34	1.37
12	aA	816	CLA	C3D-C4D	-2.36	1.38	1.44
13	cB	940	1L3	O05-C04	-2.36	1.18	1.23
12	cB	938	CLA	C1C-NC	-2.36	1.34	1.37
12	bB	922	CLA	C3B-C2B	2.36	1.49	1.41
12	aB	901	CLA	C4D-CHA	2.35	1.46	1.38
12	bB	926	CLA	C1B-C2B	2.35	1.48	1.43
12	cA	810	CLA	C3D-C4D	-2.35	1.38	1.44
12	bA	840	CLA	C1B-C2B	2.35	1.48	1.43
12	cA	835	CLA	C3D-C4D	-2.35	1.38	1.44
12	cL	202	CLA	C3D-C4D	-2.35	1.38	1.44
12	aB	923	CLA	C4D-CHA	2.35	1.46	1.38
12	aB	950	CLA	C3D-C4D	-2.35	1.38	1.44
12	aB	950	CLA	C1B-C2B	2.35	1.48	1.43
12	aA	810	CLA	C3D-C4D	-2.35	1.38	1.44
12	aL	204	CLA	C3D-C4D	-2.35	1.38	1.44
12	bB	950	CLA	C3D-C4D	-2.35	1.38	1.44
12	cA	818	CLA	C3D-C4D	-2.35	1.38	1.44
12	cA	825	CLA	C3D-C4D	-2.35	1.38	1.44
12	aA	815	CLA	C1B-C2B	2.35	1.48	1.43
12	bA	823	CLA	C1C-NC	-2.35	1.34	1.37
12	aB	903	CLA	C1B-C2B	2.35	1.48	1.43
12	aA	833	CLA	C1C-NC	-2.35	1.34	1.37
12	cA	813	CLA	C3D-C4D	-2.35	1.38	1.44
12	cA	822	CLA	C3B-C2B	2.35	1.49	1.41
12	cA	841	CLA	C1B-C2B	2.35	1.48	1.43
12	bB	950	CLA	C1B-C2B	2.35	1.48	1.43
12	bA	826	CLA	C3D-C4D	-2.35	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aA	844	CLA	C1B-C2B	2.35	1.48	1.43
12	cB	923	CLA	C4D-CHA	2.35	1.46	1.38
12	cA	827	CLA	C1C-NC	-2.35	1.34	1.37
12	cB	919	CLA	C1B-C2B	2.35	1.48	1.43
12	cL	202	CLA	C1C-NC	-2.35	1.34	1.37
12	aA	835	CLA	C3D-C4D	-2.35	1.38	1.44
12	cA	810	CLA	C1C-NC	-2.35	1.34	1.37
12	cA	833	CLA	C1C-NC	-2.35	1.34	1.37
12	aB	937	CLA	OBD-CAD	2.34	1.26	1.22
12	aA	803	CLA	C1C-NC	-2.34	1.34	1.37
12	aA	841	CLA	C1B-C2B	2.34	1.48	1.43
12	aL	202	CLA	C1C-NC	-2.34	1.34	1.37
12	aB	926	CLA	C4D-CHA	2.34	1.46	1.38
12	aL	203	CLA	C3B-C4B	2.34	1.49	1.42
12	bB	938	CLA	C1C-NC	-2.34	1.34	1.37
12	bA	835	CLA	C3D-C4D	-2.34	1.38	1.44
12	cB	901	CLA	C4D-CHA	2.34	1.46	1.38
15	cL	201	BCR	C33-C5	-2.34	1.47	1.50
12	cB	914	CLA	C1B-C2B	2.34	1.48	1.43
12	cL	204	CLA	C1C-NC	-2.34	1.34	1.37
15	aB	945	BCR	C30-C25	-2.34	1.50	1.53
12	cA	805	CLA	C1C-C2C	2.34	1.49	1.44
15	aA	848	BCR	C1-C6	-2.34	1.50	1.53
12	bB	923	CLA	C4D-CHA	2.34	1.46	1.38
12	cA	803	CLA	C1C-NC	-2.34	1.34	1.37
12	aB	937	CLA	C1B-C2B	2.34	1.48	1.43
12	aB	906	CLA	C1B-C2B	2.33	1.48	1.43
12	aB	937	CLA	C4C-C3C	2.33	1.49	1.45
12	bB	919	CLA	C1B-C2B	2.33	1.48	1.43
12	bA	841	CLA	C1B-C2B	2.33	1.48	1.43
12	bL	202	CLA	C3D-C4D	-2.33	1.38	1.44
12	bL	202	CLA	C1C-NC	-2.33	1.34	1.37
12	aB	929	CLA	C3D-C4D	-2.33	1.38	1.44
12	aB	919	CLA	C1B-C2B	2.33	1.48	1.43
12	cA	802	CLA	C3D-C4D	-2.33	1.38	1.44
12	aA	814	CLA	C4C-C3C	2.33	1.49	1.45
12	bA	802	CLA	C3D-C4D	-2.33	1.38	1.44
12	aB	914	CLA	C1B-C2B	2.33	1.48	1.43
12	bL	204	CLA	C1C-NC	-2.33	1.34	1.37
12	cA	811	CLA	C3D-C4D	-2.33	1.38	1.44
12	bB	921	CLA	C4C-C3C	2.33	1.49	1.45
12	cA	808	CLA	C4C-C3C	2.33	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bA	810	CLA	C3D-C4D	-2.33	1.38	1.44
12	aL	202	CLA	C3D-C4D	-2.33	1.39	1.44
12	aB	915	CLA	C1B-C2B	2.33	1.48	1.43
12	bB	937	CLA	C1B-C2B	2.33	1.48	1.43
12	aB	924	CLA	C3B-C2B	2.33	1.49	1.41
12	cA	840	CLA	C1B-C2B	2.33	1.48	1.43
12	bA	803	CLA	C1C-NC	-2.33	1.34	1.37
12	cA	823	CLA	C3B-C4B	2.33	1.49	1.42
11	bA	801	CL0	C3D-C4D	-2.33	1.38	1.41
12	bA	809	CLA	C1B-C2B	2.33	1.48	1.43
12	aB	949	CLA	C1C-NC	-2.33	1.34	1.37
12	bA	838	CLA	C1C-NC	-2.33	1.34	1.37
12	aA	824	CLA	C1B-C2B	2.33	1.48	1.43
12	aA	842	CLA	C1B-C2B	2.33	1.48	1.43
12	bA	839	CLA	C1B-C2B	2.33	1.48	1.43
12	bA	824	CLA	C1C-NC	-2.32	1.34	1.37
12	bA	811	CLA	C3D-C4D	-2.32	1.39	1.44
12	bB	929	CLA	C3D-C4D	-2.32	1.39	1.44
12	cA	840	CLA	C3D-C4D	-2.32	1.39	1.44
12	cB	922	CLA	C1C-NC	-2.32	1.34	1.37
12	bB	924	CLA	C3B-C2B	2.32	1.49	1.41
12	aB	904	CLA	C3B-C2B	2.32	1.49	1.41
12	cA	839	CLA	C1B-C2B	2.32	1.48	1.43
16	cB	948	LHG	P-O6	2.32	1.68	1.59
12	bA	823	CLA	C3B-C4B	2.32	1.49	1.42
12	aB	912	CLA	C4C-C3C	2.32	1.49	1.45
12	bA	811	CLA	C1B-C2B	2.32	1.48	1.43
12	cA	812	CLA	C1C-NC	-2.32	1.34	1.37
12	aA	822	CLA	C3B-C2B	2.32	1.49	1.41
12	cB	949	CLA	C3D-C4D	-2.32	1.39	1.44
12	aA	840	CLA	C1B-C2B	2.32	1.48	1.43
12	bA	812	CLA	C3B-C4B	2.32	1.49	1.42
12	cB	949	CLA	C1C-NC	-2.32	1.34	1.37
12	aA	805	CLA	C1C-C2C	2.32	1.49	1.44
12	cB	925	CLA	C1C-NC	-2.32	1.34	1.37
12	bB	904	CLA	C3B-C2B	2.32	1.49	1.41
12	aB	921	CLA	C4C-C3C	2.32	1.49	1.45
12	cB	921	CLA	C4C-C3C	2.32	1.49	1.45
12	bB	915	CLA	C1B-C2B	2.32	1.48	1.43
12	bA	822	CLA	C3B-C2B	2.32	1.49	1.41
12	bA	840	CLA	C3D-C4D	-2.32	1.39	1.44
13	bA	844	1L3	O05-C04	-2.31	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bA	847	BCR	C1-C6	-2.31	1.50	1.53
12	bB	919	CLA	C3B-C4B	2.31	1.49	1.42
12	bB	906	CLA	C1B-C2B	2.31	1.48	1.43
12	aA	839	CLA	C1B-C2B	2.31	1.48	1.43
12	aA	808	CLA	C3D-C4D	-2.31	1.39	1.44
12	cA	836	CLA	C3D-C4D	-2.31	1.39	1.44
12	cA	811	CLA	C1B-C2B	2.31	1.48	1.43
12	cA	809	CLA	C1B-C2B	2.31	1.48	1.43
12	bA	814	CLA	C4C-C3C	2.31	1.49	1.45
12	cA	806	CLA	C4C-C3C	2.31	1.49	1.45
12	cB	904	CLA	C3B-C2B	2.31	1.49	1.41
12	aB	920	CLA	C3D-C4D	-2.31	1.39	1.44
12	aA	823	CLA	C3B-C4B	2.31	1.49	1.42
12	bB	934	CLA	C4C-C3C	2.31	1.49	1.45
12	bB	929	CLA	C1B-C2B	2.31	1.48	1.43
12	cB	915	CLA	C1B-C2B	2.31	1.48	1.43
12	aB	949	CLA	C3D-C4D	-2.31	1.39	1.44
15	cB	945	BCR	C1-C6	-2.31	1.50	1.53
12	aB	929	CLA	C1B-C2B	2.31	1.48	1.43
12	bB	920	CLA	C3D-C4D	-2.31	1.39	1.44
12	aA	811	CLA	C1B-C2B	2.30	1.48	1.43
12	cA	806	CLA	C1C-NC	-2.30	1.34	1.37
12	bA	824	CLA	C3B-C4B	2.30	1.49	1.42
12	aL	202	CLA	C4C-C3C	2.30	1.48	1.45
12	aB	938	CLA	C1C-NC	-2.30	1.34	1.37
12	aA	806	CLA	C4C-C3C	2.30	1.48	1.45
12	bB	917	CLA	C3D-C4D	-2.30	1.39	1.44
12	cA	803	CLA	CHB-C4A	-2.30	1.31	1.37
12	aA	809	CLA	C1B-C2B	2.30	1.48	1.43
12	cB	906	CLA	C1C-C2C	2.30	1.49	1.44
12	bB	912	CLA	C4C-C3C	2.30	1.48	1.45
12	bA	805	CLA	C1C-C2C	2.30	1.49	1.44
12	cB	906	CLA	C1B-C2B	2.30	1.48	1.43
12	cB	919	CLA	C3B-C4B	2.30	1.49	1.42
12	cA	812	CLA	C3B-C4B	2.30	1.49	1.42
12	aB	912	CLA	C1C-NC	-2.30	1.34	1.37
12	aA	802	CLA	C3D-C4D	-2.30	1.39	1.44
12	bA	806	CLA	C3B-C2B	2.30	1.48	1.41
12	cL	203	CLA	C1C-C2C	2.30	1.49	1.44
12	aB	917	CLA	C3D-C4D	-2.30	1.39	1.44
12	cB	924	CLA	C3B-C2B	2.30	1.48	1.41
12	bA	836	CLA	C3B-C4B	2.30	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bB	923	CLA	C1B-C2B	2.30	1.48	1.43
11	cA	801	CL0	C3D-C4D	-2.30	1.38	1.41
12	aB	909	CLA	C4C-C3C	2.30	1.48	1.45
12	aA	854	CLA	C3D-C4D	-2.30	1.39	1.44
12	cA	842	CLA	C1B-C2B	2.30	1.48	1.43
12	aB	920	CLA	C3B-C2B	2.30	1.48	1.41
12	aB	919	CLA	C3B-C4B	2.30	1.49	1.42
12	aA	840	CLA	C3D-C4D	-2.30	1.39	1.44
12	aA	808	CLA	C4C-C3C	2.30	1.48	1.45
12	cB	917	CLA	C3D-C4D	-2.30	1.39	1.44
12	cA	837	CLA	C3B-C2B	2.30	1.48	1.41
12	bA	816	CLA	C1C-C2C	2.30	1.49	1.44
12	cB	937	CLA	C1B-C2B	2.29	1.48	1.43
15	bB	941	BCR	C30-C25	-2.29	1.50	1.53
12	cA	809	CLA	C1C-NC	-2.29	1.34	1.37
12	cB	912	CLA	C1C-NC	-2.29	1.34	1.37
12	aA	812	CLA	C3B-C4B	2.29	1.49	1.42
12	bA	817	CLA	C3B-C2B	2.29	1.48	1.41
12	bA	837	CLA	C3B-C2B	2.29	1.48	1.41
12	bA	808	CLA	C3D-C4D	-2.29	1.39	1.44
12	aB	936	CLA	C1B-C2B	2.29	1.48	1.43
12	cA	808	CLA	C3D-C4D	-2.29	1.39	1.44
12	aB	923	CLA	C1B-C2B	2.29	1.48	1.43
12	bA	842	CLA	C1B-C2B	2.29	1.48	1.43
12	aA	836	CLA	C3D-C4D	-2.29	1.39	1.44
12	cB	929	CLA	C3D-C4D	-2.29	1.39	1.44
12	bB	938	CLA	C3B-C4B	2.29	1.49	1.42
12	cB	929	CLA	C1B-C2B	2.29	1.48	1.43
12	cB	928	CLA	C4C-C3C	2.29	1.48	1.45
12	cB	911	CLA	C1B-C2B	2.29	1.48	1.43
12	cB	926	CLA	C3D-C4D	-2.29	1.39	1.44
12	bB	911	CLA	C1B-C2B	2.29	1.48	1.43
12	bB	922	CLA	C1C-NC	-2.29	1.34	1.37
12	aB	934	CLA	C4C-C3C	2.29	1.48	1.45
12	aA	817	CLA	C3B-C2B	2.29	1.48	1.41
15	aL	205	BCR	C30-C25	-2.29	1.50	1.53
15	cB	945	BCR	C30-C25	-2.29	1.50	1.53
12	aB	911	CLA	C1B-C2B	2.29	1.48	1.43
15	cL	205	BCR	C30-C25	-2.29	1.50	1.53
12	bB	926	CLA	C3D-C4D	-2.28	1.39	1.44
12	bB	925	CLA	C1C-NC	-2.28	1.34	1.37
12	aB	906	CLA	C1C-C2C	2.28	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cB	912	CLA	C4C-C3C	2.28	1.48	1.45
12	aA	836	CLA	C3B-C4B	2.28	1.49	1.42
12	aL	204	CLA	C1C-NC	-2.28	1.34	1.37
12	bA	806	CLA	C1C-NC	-2.28	1.34	1.37
12	bB	912	CLA	C1C-NC	-2.28	1.34	1.37
12	aB	927	CLA	C3D-C4D	-2.28	1.39	1.44
12	cA	853	CLA	C3D-C4D	-2.28	1.39	1.44
12	bB	913	CLA	C3B-C2B	2.28	1.48	1.41
13	cA	844	1L3	O05-C04	-2.28	1.18	1.23
13	aA	845	1L3	O05-C04	-2.28	1.18	1.23
12	cA	817	CLA	C3B-C2B	2.28	1.48	1.41
12	cL	204	CLA	C3B-C2B	2.28	1.48	1.41
12	aA	824	CLA	C3B-C4B	2.28	1.49	1.42
13	aA	845	1L3	C23-C21	2.28	1.56	1.51
12	aB	933	CLA	C3D-C4D	-2.28	1.39	1.44
12	cA	806	CLA	C3B-C2B	2.28	1.48	1.41
12	aA	837	CLA	C3B-C2B	2.28	1.48	1.41
12	bA	803	CLA	CHB-C4A	-2.28	1.32	1.37
12	cB	927	CLA	C3D-C4D	-2.28	1.39	1.44
12	aB	931	CLA	C4D-CHA	2.28	1.46	1.38
15	bL	205	BCR	C30-C25	-2.28	1.50	1.53
12	bB	933	CLA	C3D-C4D	-2.28	1.39	1.44
12	cB	923	CLA	C1B-C2B	2.28	1.48	1.43
12	cB	933	CLA	C3D-C4D	-2.28	1.39	1.44
12	aA	803	CLA	CHB-C4A	-2.28	1.32	1.37
12	cB	913	CLA	C3B-C2B	2.28	1.48	1.41
12	aB	925	CLA	C1C-NC	-2.28	1.34	1.37
12	aB	928	CLA	C4C-C3C	2.28	1.48	1.45
12	cB	920	CLA	C3D-C4D	-2.28	1.39	1.44
12	bB	936	CLA	C1B-C2B	2.28	1.48	1.43
12	aA	811	CLA	C3D-C4D	-2.28	1.39	1.44
12	bB	903	CLA	C1C-C2C	2.28	1.49	1.44
12	cB	931	CLA	C4D-CHA	2.28	1.46	1.38
12	bB	920	CLA	C3B-C2B	2.28	1.48	1.41
12	aA	835	CLA	C1C-C2C	2.27	1.49	1.44
12	aA	829	CLA	C1C-NC	-2.27	1.34	1.37
12	cB	914	CLA	C3D-C4D	-2.27	1.39	1.44
12	cB	920	CLA	C3B-C2B	2.27	1.48	1.41
12	bB	931	CLA	C4D-CHA	2.27	1.46	1.38
12	aA	806	CLA	C3B-C2B	2.27	1.48	1.41
12	cB	936	CLA	C1B-C2B	2.27	1.48	1.43
12	cB	938	CLA	C3B-C4B	2.27	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aL	203	CLA	C1C-C2C	2.27	1.49	1.44
12	bL	203	CLA	C1C-C2C	2.27	1.49	1.44
12	bA	836	CLA	C3D-C4D	-2.27	1.39	1.44
12	bB	935	CLA	C1C-C2C	2.27	1.49	1.44
12	bA	809	CLA	C1C-NC	-2.27	1.34	1.37
12	aA	839	CLA	C3B-C4B	2.27	1.49	1.42
12	cA	835	CLA	C1C-NC	-2.27	1.34	1.37
12	cB	904	CLA	C1C-NC	-2.27	1.34	1.37
12	aB	913	CLA	C3B-C2B	2.27	1.48	1.41
12	aB	926	CLA	C3D-C4D	-2.27	1.39	1.44
12	cA	841	CLA	C3D-C4D	-2.27	1.39	1.44
12	cA	824	CLA	C3B-C4B	2.27	1.49	1.42
12	bA	835	CLA	C1C-NC	-2.27	1.34	1.37
12	cA	836	CLA	C3B-C4B	2.27	1.49	1.42
12	bB	904	CLA	C1C-NC	-2.27	1.34	1.37
12	bA	804	CLA	C3B-C2B	2.27	1.48	1.41
12	bL	204	CLA	C3B-C2B	2.26	1.48	1.41
12	bA	841	CLA	C3D-C4D	-2.26	1.39	1.44
12	bA	826	CLA	C1B-C2B	2.26	1.48	1.43
12	bL	202	CLA	C4C-C3C	2.26	1.48	1.45
12	cB	935	CLA	C1C-C2C	2.26	1.49	1.44
12	aB	931	CLA	C1C-C2C	2.26	1.49	1.44
12	cB	931	CLA	C1C-C2C	2.26	1.49	1.44
12	aB	904	CLA	C1C-NC	-2.26	1.34	1.37
12	bA	835	CLA	C3B-C4B	2.26	1.49	1.42
12	aB	935	CLA	C1C-C2C	2.26	1.49	1.44
11	aA	801	CL0	C3D-C4D	-2.26	1.38	1.41
12	aL	204	CLA	C3B-C2B	2.26	1.48	1.41
12	cA	835	CLA	C3B-C4B	2.26	1.49	1.42
12	aA	806	CLA	C1C-NC	-2.26	1.34	1.37
12	bA	829	CLA	C1C-NC	-2.26	1.34	1.37
12	aB	929	CLA	C1C-C2C	2.26	1.49	1.44
12	bA	835	CLA	C1C-C2C	2.26	1.49	1.44
12	aA	805	CLA	C3D-C4D	-2.26	1.39	1.44
12	aB	938	CLA	C3B-C4B	2.26	1.49	1.42
12	bB	906	CLA	C1C-C2C	2.26	1.49	1.44
12	aA	826	CLA	C1B-C2B	2.26	1.48	1.43
12	bA	806	CLA	C4C-C3C	2.26	1.48	1.45
12	bB	928	CLA	C4C-C3C	2.26	1.48	1.45
12	bB	929	CLA	C1C-C2C	2.26	1.49	1.44
12	bA	805	CLA	C3D-C4D	-2.25	1.39	1.44
12	cA	839	CLA	C3B-C4B	2.25	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cB	912	CLA	C1B-C2B	2.25	1.48	1.43
12	bA	841	CLA	C1C-C2C	2.25	1.49	1.44
12	cA	816	CLA	C1C-C2C	2.25	1.49	1.44
12	bA	839	CLA	C3B-C4B	2.25	1.49	1.42
12	aA	826	CLA	C1C-C2C	2.25	1.49	1.44
12	cA	832	CLA	C1B-C2B	2.25	1.48	1.43
12	aA	809	CLA	C1C-NC	-2.25	1.34	1.37
12	aB	915	CLA	C3B-C4B	2.25	1.49	1.42
12	bA	822	CLA	C3B-C4B	2.25	1.49	1.42
12	bA	817	CLA	C3B-C4B	2.25	1.49	1.42
12	aB	918	CLA	CHB-C4A	-2.25	1.32	1.37
12	bB	927	CLA	C3D-C4D	-2.25	1.39	1.44
15	aB	945	BCR	C1-C6	-2.25	1.50	1.53
12	cA	805	CLA	C3D-C4D	-2.25	1.39	1.44
12	cL	202	CLA	C4C-C3C	2.25	1.48	1.45
12	aA	829	CLA	C3D-C4D	-2.25	1.39	1.44
12	bB	909	CLA	C4C-C3C	2.25	1.48	1.45
12	bA	829	CLA	C3D-C4D	-2.25	1.39	1.44
12	cA	820	CLA	C3B-C4B	2.25	1.49	1.42
13	bA	844	1L3	C23-C21	2.25	1.55	1.51
12	aA	841	CLA	C3D-C4D	-2.25	1.39	1.44
12	aA	835	CLA	C3B-C4B	2.25	1.49	1.42
12	aB	903	CLA	C1C-C2C	2.25	1.49	1.44
12	cA	835	CLA	C1C-C2C	2.25	1.49	1.44
12	aA	816	CLA	C1C-C2C	2.24	1.49	1.44
12	bL	202	CLA	C1B-C2B	2.24	1.48	1.43
12	cA	832	CLA	C1C-C2C	2.24	1.49	1.44
12	bB	911	CLA	C1C-NC	-2.24	1.34	1.37
12	aA	841	CLA	C1C-C2C	2.24	1.49	1.44
12	aB	936	CLA	C4C-C3C	2.24	1.48	1.45
12	aA	822	CLA	C3B-C4B	2.24	1.49	1.42
12	aB	902	CLA	C1B-C2B	2.24	1.48	1.43
15	bB	945	BCR	C1-C6	-2.24	1.50	1.53
12	cA	853	CLA	C1C-C2C	2.24	1.49	1.44
12	aA	854	CLA	C1C-C2C	2.24	1.49	1.44
12	cA	804	CLA	C3B-C2B	2.24	1.48	1.41
12	aB	930	CLA	C3B-C2B	2.24	1.48	1.41
12	aB	903	CLA	C3B-C2B	2.24	1.48	1.41
12	bA	820	CLA	C3B-C2B	2.24	1.48	1.41
12	cA	820	CLA	C3B-C2B	2.24	1.48	1.41
12	aA	820	CLA	C3B-C4B	2.24	1.49	1.42
12	cB	915	CLA	C3B-C4B	2.24	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bA	812	CLA	C1B-C2B	2.24	1.48	1.43
15	cB	941	BCR	C30-C25	-2.24	1.50	1.53
12	bB	916	CLA	C1C-NC	-2.24	1.34	1.37
12	aB	935	CLA	C3B-C2B	2.24	1.48	1.41
12	cB	929	CLA	C1C-C2C	2.24	1.49	1.44
12	bA	853	CLA	C3D-C4D	-2.24	1.39	1.44
12	cA	826	CLA	C1B-C2B	2.24	1.48	1.43
12	cA	821	CLA	C1C-NC	-2.24	1.34	1.37
12	cA	802	CLA	C1B-C2B	2.24	1.48	1.43
12	cL	202	CLA	C1B-C2B	2.23	1.48	1.43
12	aB	914	CLA	C3D-C4D	-2.23	1.39	1.44
12	cB	903	CLA	C3B-C2B	2.23	1.48	1.41
12	bA	853	CLA	C1C-C2C	2.23	1.49	1.44
12	cB	935	CLA	C1B-C2B	2.23	1.48	1.43
12	aA	820	CLA	C3B-C2B	2.23	1.48	1.41
12	bB	930	CLA	C3B-C2B	2.23	1.48	1.41
12	bA	853	CLA	OBD-CAD	2.23	1.26	1.22
12	bA	822	CLA	C3D-C4D	-2.23	1.39	1.44
12	cB	935	CLA	C3B-C2B	2.23	1.48	1.41
12	cB	903	CLA	C1C-C2C	2.23	1.49	1.44
12	bB	935	CLA	C3B-C2B	2.23	1.48	1.41
12	cB	918	CLA	CHB-C4A	-2.23	1.32	1.37
12	cB	909	CLA	C4C-C3C	2.23	1.48	1.45
12	bA	819	CLA	C1C-NC	-2.23	1.34	1.37
12	bA	826	CLA	C1C-C2C	2.23	1.49	1.44
12	aA	804	CLA	C3B-C2B	2.23	1.48	1.41
12	bB	931	CLA	C1C-C2C	2.23	1.49	1.44
12	bA	837	CLA	C1B-C2B	2.23	1.48	1.43
12	aB	919	CLA	C3D-C4D	-2.23	1.39	1.44
12	cB	927	CLA	C1C-NC	-2.23	1.34	1.37
12	aA	817	CLA	C3B-C4B	2.23	1.49	1.42
12	bB	915	CLA	C3B-C4B	2.23	1.49	1.42
13	cA	844	1L3	C23-C21	2.23	1.55	1.51
12	aA	822	CLA	C3D-C4D	-2.22	1.39	1.44
12	bB	936	CLA	C4C-C3C	2.22	1.48	1.45
12	cA	837	CLA	C1B-C2B	2.22	1.48	1.43
12	bB	903	CLA	C3B-C2B	2.22	1.48	1.41
12	aB	934	CLA	CHB-C4A	-2.22	1.32	1.37
12	aA	802	CLA	C4D-CHA	2.22	1.46	1.38
12	aA	840	CLA	C3B-C4B	2.22	1.49	1.42
12	cB	930	CLA	C3B-C2B	2.22	1.48	1.41
12	bB	927	CLA	C1C-NC	-2.22	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cB	904	CLA	C1C-C2C	2.22	1.49	1.44
12	bA	805	CLA	C1B-C2B	2.22	1.48	1.43
12	cA	812	CLA	C1B-C2B	2.22	1.48	1.43
12	cB	902	CLA	C1B-C2B	2.22	1.48	1.43
12	bA	843	CLA	C4C-C3C	2.22	1.48	1.45
12	cA	822	CLA	C3B-C4B	2.22	1.49	1.42
12	bA	820	CLA	C3B-C4B	2.22	1.49	1.42
12	bB	912	CLA	C1B-C2B	2.22	1.48	1.43
12	aA	834	CLA	C1C-NC	-2.22	1.34	1.37
12	aL	202	CLA	C1B-C2B	2.22	1.48	1.43
12	bA	832	CLA	C1B-C2B	2.22	1.48	1.43
15	cL	206	BCR	C30-C25	-2.22	1.50	1.53
12	cB	919	CLA	C3D-C4D	-2.22	1.39	1.44
12	bA	827	CLA	C3B-C2B	2.22	1.48	1.41
12	cA	829	CLA	C3B-C2B	2.22	1.48	1.41
12	bB	935	CLA	C1B-C2B	2.22	1.48	1.43
12	cB	913	CLA	C1C-C2C	2.22	1.49	1.44
12	bA	829	CLA	C3B-C2B	2.22	1.48	1.41
12	bB	914	CLA	C3D-C4D	-2.22	1.39	1.44
12	bB	918	CLA	CHB-C4A	-2.21	1.32	1.37
12	cA	853	CLA	OBD-CAD	2.21	1.26	1.22
12	aA	819	CLA	C1C-NC	-2.21	1.34	1.37
12	aA	854	CLA	OBD-CAD	2.21	1.26	1.22
12	aA	802	CLA	C1B-C2B	2.21	1.48	1.43
12	cA	838	CLA	C1C-C2C	2.21	1.49	1.44
12	aA	832	CLA	C1B-C2B	2.21	1.48	1.43
12	cA	817	CLA	C3B-C4B	2.21	1.49	1.42
12	bA	818	CLA	C3B-C2B	2.21	1.48	1.41
12	cA	818	CLA	C3B-C2B	2.21	1.48	1.41
12	aA	822	CLA	C1C-C2C	2.21	1.49	1.44
12	cA	827	CLA	C3B-C2B	2.21	1.48	1.41
12	bA	840	CLA	C3B-C4B	2.21	1.49	1.42
12	aA	805	CLA	C1B-C2B	2.21	1.48	1.43
12	bA	838	CLA	C1C-C2C	2.21	1.49	1.44
15	aL	206	BCR	C30-C25	-2.21	1.51	1.53
15	bB	945	BCR	C30-C25	-2.21	1.51	1.53
12	cA	834	CLA	C1C-NC	-2.21	1.34	1.37
12	cA	840	CLA	C3B-C4B	2.21	1.49	1.42
12	cA	822	CLA	C1C-C2C	2.21	1.49	1.44
12	aA	821	CLA	C1C-NC	-2.21	1.34	1.37
12	bA	802	CLA	C1B-C2B	2.21	1.48	1.43
12	bB	902	CLA	C1B-C2B	2.21	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aA	820	CLA	C3D-C4D	-2.21	1.39	1.44
12	bB	904	CLA	C3B-C4B	2.21	1.49	1.42
12	bB	934	CLA	CHB-C4A	-2.21	1.32	1.37
12	aB	913	CLA	C1C-NC	-2.21	1.34	1.37
12	aA	832	CLA	C3B-C2B	2.21	1.48	1.41
12	aA	835	CLA	C1C-NC	-2.21	1.34	1.37
12	cB	918	CLA	C1C-NC	-2.20	1.34	1.37
15	aB	941	BCR	C30-C25	-2.20	1.51	1.53
12	aB	912	CLA	C1B-C2B	2.20	1.48	1.43
12	bA	813	CLA	C1B-C2B	2.20	1.48	1.43
12	bB	904	CLA	C1C-C2C	2.20	1.49	1.44
12	cA	829	CLA	C3D-C4D	-2.20	1.39	1.44
12	cB	934	CLA	C3D-C4D	-2.20	1.39	1.44
12	aB	904	CLA	C3B-C4B	2.20	1.49	1.42
12	cA	802	CLA	C4D-CHA	2.20	1.46	1.38
12	aA	812	CLA	C1B-C2B	2.20	1.48	1.43
12	aA	837	CLA	C1B-C2B	2.20	1.48	1.43
12	aB	935	CLA	C1B-C2B	2.20	1.48	1.43
12	bA	832	CLA	C3B-C2B	2.20	1.48	1.41
12	aB	934	CLA	C3D-C4D	-2.20	1.39	1.44
12	aA	829	CLA	C3B-C2B	2.20	1.48	1.41
12	cB	924	CLA	C4C-C3C	2.20	1.48	1.45
12	aB	916	CLA	C1C-NC	-2.20	1.34	1.37
12	aA	818	CLA	C3B-C2B	2.20	1.48	1.41
12	cA	813	CLA	C1C-NC	-2.20	1.34	1.37
12	cA	819	CLA	C1C-NC	-2.20	1.34	1.37
12	cA	841	CLA	C1C-C2C	2.20	1.49	1.44
12	bA	802	CLA	C4D-CHA	2.20	1.46	1.38
12	bB	919	CLA	C3D-C4D	-2.20	1.39	1.44
12	aA	803	CLA	C3B-C2B	2.20	1.48	1.41
12	aA	813	CLA	C1C-C2C	2.20	1.49	1.44
12	cA	827	CLA	C1B-C2B	2.20	1.48	1.43
12	cA	803	CLA	C3B-C2B	2.20	1.48	1.41
12	bA	803	CLA	C3B-C2B	2.20	1.48	1.41
12	cA	826	CLA	C1C-C2C	2.20	1.49	1.44
12	cA	824	CLA	C4C-C3C	2.20	1.48	1.45
12	cA	832	CLA	C3B-C2B	2.20	1.48	1.41
12	aA	838	CLA	C1C-C2C	2.20	1.49	1.44
12	aB	925	CLA	C1C-C2C	2.20	1.49	1.44
12	aA	826	CLA	C3B-C4B	2.20	1.49	1.42
12	aA	827	CLA	C3B-C2B	2.20	1.48	1.41
12	bA	822	CLA	C1C-C2C	2.20	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cA	830	CLA	C4C-C3C	2.20	1.48	1.45
12	aA	830	CLA	C4C-C3C	2.19	1.48	1.45
12	aB	927	CLA	C1C-NC	-2.19	1.34	1.37
12	aB	904	CLA	C1C-C2C	2.19	1.49	1.44
15	cB	946	BCR	C38-C26	-2.19	1.47	1.50
12	aB	911	CLA	C1C-NC	-2.19	1.34	1.37
12	bB	918	CLA	C1C-NC	-2.19	1.34	1.37
12	bB	935	CLA	C1C-NC	-2.19	1.34	1.37
12	bB	927	CLA	C1C-C2C	2.19	1.49	1.44
12	aA	827	CLA	C1B-C2B	2.19	1.48	1.43
12	cB	904	CLA	C3B-C4B	2.19	1.49	1.42
12	aB	916	CLA	C3B-C4B	2.19	1.49	1.42
12	bA	813	CLA	C1C-NC	-2.19	1.34	1.37
12	bA	832	CLA	C1C-C2C	2.19	1.49	1.44
15	aB	946	BCR	C38-C26	-2.19	1.47	1.50
12	cA	828	CLA	C1C-C2C	2.19	1.49	1.44
12	bA	821	CLA	C1C-NC	-2.19	1.34	1.37
12	cA	822	CLA	C3D-C4D	-2.19	1.39	1.44
12	aF	202	CLA	C1C-C2C	2.19	1.49	1.44
12	bA	834	CLA	C1C-NC	-2.19	1.34	1.37
12	cA	805	CLA	C1B-C2B	2.19	1.48	1.43
12	bB	906	CLA	C1C-NC	-2.18	1.34	1.37
12	cA	829	CLA	C1C-NC	-2.18	1.34	1.37
12	bB	934	CLA	C3D-C4D	-2.18	1.39	1.44
12	bA	828	CLA	C3B-C2B	2.18	1.48	1.41
12	cB	903	CLA	C3B-C4B	2.18	1.49	1.42
12	bA	802	CLA	CBD-CAD	-2.18	1.46	1.56
12	aB	918	CLA	C1C-NC	-2.18	1.34	1.37
12	bA	838	CLA	CBD-CAD	-2.18	1.46	1.56
12	cB	934	CLA	CHB-C4A	-2.18	1.32	1.37
12	aA	828	CLA	C1C-C2C	2.18	1.48	1.44
12	cB	927	CLA	C1C-C2C	2.18	1.48	1.44
12	cF	202	CLA	C1C-C2C	2.18	1.48	1.44
12	aA	813	CLA	C1B-C2B	2.18	1.48	1.43
12	bA	828	CLA	C1C-C2C	2.18	1.48	1.44
12	cA	813	CLA	C1B-C2B	2.18	1.48	1.43
12	bA	825	CLA	C4C-C3C	2.18	1.48	1.45
12	aA	834	CLA	C1B-C2B	2.18	1.48	1.43
12	cA	828	CLA	C3B-C2B	2.18	1.48	1.41
12	bB	913	CLA	C1C-C2C	2.18	1.48	1.44
12	cB	906	CLA	C1C-NC	-2.18	1.34	1.37
12	cB	925	CLA	C1C-C2C	2.18	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cA	834	CLA	CHB-C4A	-2.18	1.32	1.37
12	bB	914	CLA	C1C-NC	-2.18	1.34	1.37
12	cB	916	CLA	C1C-NC	-2.18	1.34	1.37
12	cB	921	CLA	C3B-C2B	2.17	1.48	1.41
12	aA	819	CLA	CHB-C4A	-2.17	1.32	1.37
12	cA	820	CLA	C3D-C4D	-2.17	1.39	1.44
12	cA	802	CLA	CBD-CAD	-2.17	1.46	1.56
12	aB	910	CLA	C1C-C2C	2.17	1.48	1.44
12	cB	936	CLA	C4C-C3C	2.17	1.48	1.45
12	cA	838	CLA	CBD-CAD	-2.17	1.46	1.56
12	aA	832	CLA	C1C-C2C	2.17	1.48	1.44
12	aB	913	CLA	C1C-C2C	2.17	1.48	1.44
12	aL	203	CLA	C3B-C2B	2.17	1.48	1.41
12	cB	923	CLA	C1C-NC	-2.17	1.34	1.37
12	cA	819	CLA	CHB-C4A	-2.17	1.32	1.37
12	cA	843	CLA	C4C-C3C	2.17	1.48	1.45
12	aA	834	CLA	CHB-C4A	-2.17	1.32	1.37
12	cA	803	CLA	C3D-C4D	-2.17	1.39	1.44
12	cB	916	CLA	C3B-C4B	2.17	1.49	1.42
12	bA	813	CLA	C3B-C4B	2.17	1.49	1.42
12	aA	813	CLA	C1C-NC	-2.17	1.34	1.37
12	aB	921	CLA	C3B-C2B	2.17	1.48	1.41
12	cA	813	CLA	C3B-C4B	2.17	1.49	1.42
12	aA	826	CLA	C4C-C3C	2.17	1.48	1.45
12	aA	805	CLA	C3B-C2B	2.17	1.48	1.41
12	bA	826	CLA	C3B-C4B	2.17	1.49	1.42
12	bA	810	CLA	C3B-C2B	2.17	1.48	1.41
12	cB	935	CLA	C1C-NC	-2.17	1.34	1.37
12	cA	826	CLA	C4C-C3C	2.17	1.48	1.45
12	aB	908	CLA	C4C-C3C	2.17	1.48	1.45
12	aA	838	CLA	CBD-CAD	-2.17	1.46	1.56
12	aB	935	CLA	C1C-NC	-2.17	1.34	1.37
12	bB	921	CLA	C3B-C2B	2.17	1.48	1.41
12	aA	802	CLA	CBD-CAD	-2.17	1.46	1.56
12	bA	815	CLA	C4C-C3C	2.17	1.48	1.45
12	aA	828	CLA	C3B-C2B	2.16	1.48	1.41
12	bL	203	CLA	C3B-C2B	2.16	1.48	1.41
12	cA	834	CLA	C1B-C2B	2.16	1.48	1.43
12	cA	816	CLA	C3B-C2B	2.16	1.48	1.41
12	aB	923	CLA	C1C-NC	-2.16	1.34	1.37
12	cA	826	CLA	C3B-C4B	2.16	1.49	1.42
12	bB	924	CLA	C4C-C3C	2.16	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	bA	848	BCR	C33-C5	-2.16	1.47	1.50
12	bA	813	CLA	C1C-C2C	2.16	1.48	1.44
12	aA	810	CLA	C3B-C2B	2.16	1.48	1.41
12	aB	906	CLA	C1C-NC	-2.16	1.34	1.37
12	cB	909	CLA	C1C-C2C	2.16	1.48	1.44
12	aA	835	CLA	C4C-C3C	2.16	1.48	1.45
12	bA	807	CLA	C1B-C2B	2.16	1.48	1.43
12	bA	827	CLA	C1B-C2B	2.16	1.48	1.43
12	aA	811	CLA	C1C-NC	-2.16	1.34	1.37
12	cB	928	CLA	C3B-C2B	2.16	1.48	1.41
12	bA	834	CLA	CHB-C4A	-2.16	1.32	1.37
12	aB	927	CLA	C1C-C2C	2.16	1.48	1.44
12	bA	820	CLA	C3D-C4D	-2.16	1.39	1.44
12	aB	925	CLA	OBD-CAD	2.16	1.26	1.22
12	bB	916	CLA	C3B-C4B	2.16	1.49	1.42
12	bB	909	CLA	C1C-C2C	2.16	1.48	1.44
12	bB	925	CLA	C1C-C2C	2.16	1.48	1.44
12	bF	202	CLA	C1C-C2C	2.16	1.48	1.44
12	cL	203	CLA	C3B-C2B	2.16	1.48	1.41
12	cL	204	CLA	C3B-C4B	2.16	1.49	1.42
15	cA	848	BCR	C33-C5	-2.16	1.47	1.50
12	cB	914	CLA	C1C-NC	-2.16	1.34	1.37
12	bB	903	CLA	C3B-C4B	2.16	1.49	1.42
12	cA	819	CLA	C3B-C4B	2.16	1.49	1.42
12	aB	909	CLA	C1C-C2C	2.16	1.48	1.44
12	bA	834	CLA	C1B-C2B	2.16	1.48	1.43
12	aB	903	CLA	C3B-C4B	2.16	1.49	1.42
12	aL	204	CLA	C3B-C4B	2.16	1.49	1.42
12	bA	825	CLA	CHB-C4A	-2.16	1.32	1.37
12	aA	816	CLA	C3B-C2B	2.16	1.48	1.41
12	bA	835	CLA	C4C-C3C	2.16	1.48	1.45
12	cA	825	CLA	CHB-C4A	-2.16	1.32	1.37
12	cB	911	CLA	C1C-NC	-2.16	1.34	1.37
12	cL	202	CLA	C3B-C2B	2.15	1.48	1.41
12	aA	813	CLA	C3B-C4B	2.15	1.49	1.42
12	aA	815	CLA	C4C-C3C	2.15	1.48	1.45
12	aB	928	CLA	C3B-C2B	2.15	1.48	1.41
12	cA	807	CLA	C1B-C2B	2.15	1.48	1.43
15	bL	206	BCR	C30-C25	-2.15	1.51	1.53
12	bB	936	CLA	OBD-CAD	2.15	1.26	1.22
12	aL	202	CLA	C3B-C2B	2.15	1.48	1.41
12	cA	805	CLA	C3B-C2B	2.15	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aB	917	CLA	C1C-NC	-2.15	1.34	1.37
12	cB	917	CLA	C1C-NC	-2.15	1.34	1.37
12	cA	813	CLA	C1C-C2C	2.15	1.48	1.44
12	aA	817	CLA	C1C-C2C	2.15	1.48	1.44
12	cB	938	CLA	C1C-C2C	2.15	1.48	1.44
12	bA	830	CLA	C4C-C3C	2.15	1.48	1.45
12	bB	936	CLA	C1C-NC	-2.15	1.34	1.37
12	cB	913	CLA	C1C-NC	-2.15	1.34	1.37
12	cA	825	CLA	C4C-C3C	2.15	1.48	1.45
12	bB	928	CLA	C3B-C2B	2.15	1.48	1.41
12	aB	912	CLA	C3B-C4B	2.15	1.49	1.42
12	aA	812	CLA	C4C-C3C	2.15	1.48	1.45
12	cA	835	CLA	C4C-C3C	2.15	1.48	1.45
12	bA	853	CLA	C3B-C4B	2.15	1.49	1.42
12	cA	806	CLA	C3B-C4B	2.15	1.49	1.42
12	cA	843	CLA	C3B-C4B	2.15	1.49	1.42
15	bB	946	BCR	C38-C26	-2.15	1.47	1.50
12	cB	936	CLA	C1C-C2C	2.14	1.48	1.44
12	bL	202	CLA	C3B-C2B	2.14	1.48	1.41
12	cA	810	CLA	C3B-C2B	2.14	1.48	1.41
12	bA	819	CLA	C3B-C4B	2.14	1.49	1.42
15	aJ	101	BCR	C33-C5	-2.14	1.47	1.50
12	bA	811	CLA	C1C-NC	-2.14	1.34	1.37
12	bA	816	CLA	C1C-NC	-2.14	1.34	1.37
12	bB	912	CLA	C3B-C4B	2.14	1.49	1.42
12	bA	816	CLA	C3B-C2B	2.14	1.48	1.41
12	aA	843	CLA	C3B-C4B	2.14	1.49	1.42
16	cA	851	LHG	O7-C5	-2.14	1.41	1.46
12	bB	936	CLA	C1C-C2C	2.14	1.48	1.44
12	bA	825	CLA	C1C-NC	-2.14	1.34	1.37
12	cA	853	CLA	C3B-C2B	2.14	1.48	1.41
12	bA	819	CLA	CHB-C4A	-2.14	1.32	1.37
11	bA	801	CL0	CBD-CGD	-2.14	1.49	1.52
12	cA	811	CLA	C1C-NC	-2.14	1.34	1.37
12	bA	802	CLA	C1C-C2C	2.14	1.48	1.44
12	aA	806	CLA	C3B-C4B	2.14	1.49	1.42
12	aA	815	CLA	C3B-C2B	2.14	1.48	1.41
12	aA	819	CLA	C3B-C4B	2.14	1.49	1.42
13	bB	940	1L3	C18-C16	2.13	1.55	1.51
12	bA	805	CLA	C3B-C2B	2.13	1.48	1.41
12	cA	853	CLA	C3B-C4B	2.13	1.49	1.42
12	cB	918	CLA	C3B-C4B	2.13	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	bA	851	LHG	O7-C5	-2.13	1.41	1.46
12	aB	924	CLA	C4C-C3C	2.13	1.48	1.45
12	cA	853	CLA	CBD-CAD	-2.13	1.46	1.56
12	aA	825	CLA	CHB-C4A	-2.13	1.32	1.37
12	bA	802	CLA	C3B-C4B	2.13	1.49	1.42
12	cA	802	CLA	C1C-C2C	2.13	1.48	1.44
12	aB	914	CLA	C1C-NC	-2.13	1.34	1.37
12	cB	936	CLA	C1C-NC	-2.13	1.34	1.37
12	aB	918	CLA	C4C-C3C	2.13	1.48	1.45
12	aA	802	CLA	C1C-C2C	2.13	1.48	1.44
16	aA	852	LHG	O7-C5	-2.13	1.41	1.46
12	aA	825	CLA	C4C-C3C	2.13	1.48	1.45
12	bL	204	CLA	C3B-C4B	2.13	1.49	1.42
12	aA	826	CLA	C1C-NC	-2.13	1.34	1.37
12	bA	843	CLA	C3B-C4B	2.13	1.48	1.42
12	aA	854	CLA	C3B-C2B	2.13	1.48	1.41
12	cB	910	CLA	C1C-C2C	2.13	1.48	1.44
12	bA	803	CLA	C3D-C4D	-2.13	1.39	1.44
12	bB	917	CLA	C1C-NC	-2.13	1.34	1.37
12	bA	824	CLA	C4C-C3C	2.13	1.48	1.45
15	cJ	101	BCR	C33-C5	-2.13	1.47	1.50
12	bA	840	CLA	C1C-NC	-2.13	1.34	1.37
12	bB	913	CLA	C1C-NC	-2.13	1.34	1.37
12	bA	826	CLA	C4C-C3C	2.13	1.48	1.45
13	cB	940	1L3	C18-C16	2.13	1.55	1.51
12	bA	820	CLA	C4C-C3C	2.13	1.48	1.45
12	aA	802	CLA	C3B-C4B	2.12	1.48	1.42
12	cA	805	CLA	C1A-CHA	2.12	1.51	1.43
12	cF	202	CLA	C1B-C2B	2.12	1.48	1.43
12	aA	854	CLA	C3B-C4B	2.12	1.48	1.42
12	aB	936	CLA	C1C-C2C	2.12	1.48	1.44
12	bA	815	CLA	C3B-C2B	2.12	1.48	1.41
15	aA	849	BCR	C33-C5	-2.12	1.47	1.50
12	cB	907	CLA	C4C-C3C	2.12	1.48	1.45
12	bB	918	CLA	C3B-C4B	2.12	1.48	1.42
12	aA	820	CLA	C1C-NC	-2.12	1.34	1.37
12	cB	931	CLA	CHB-C4A	-2.12	1.32	1.37
12	aA	824	CLA	C4C-C3C	2.12	1.48	1.45
12	cA	820	CLA	C4C-C3C	2.12	1.48	1.45
12	cB	912	CLA	C3B-C4B	2.12	1.48	1.42
12	aA	805	CLA	C1A-CHA	2.12	1.51	1.43
12	aA	824	CLA	C3B-C2B	2.12	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cA	813	CLA	C4C-C3C	2.12	1.48	1.45
12	cB	908	CLA	C4C-C3C	2.12	1.48	1.45
12	bB	902	CLA	C3B-C2B	2.12	1.48	1.41
12	aA	807	CLA	C1B-C2B	2.12	1.48	1.43
12	bA	806	CLA	C3B-C4B	2.12	1.48	1.42
12	aB	927	CLA	C4C-C3C	2.12	1.48	1.45
12	cA	815	CLA	C4C-C3C	2.12	1.48	1.45
12	aB	912	CLA	O2D-CED	-2.12	1.40	1.45
11	aA	801	CL0	CBD-CGD	-2.12	1.49	1.52
15	bJ	101	BCR	C33-C5	-2.12	1.47	1.50
12	aB	936	CLA	OBD-CAD	2.12	1.26	1.22
12	bB	910	CLA	C1C-C2C	2.12	1.48	1.44
12	bB	914	CLA	C3B-C2B	2.12	1.48	1.41
12	bA	811	CLA	C3B-C2B	2.12	1.48	1.41
12	cA	807	CLA	CHB-C4A	-2.12	1.32	1.37
12	aA	854	CLA	CBD-CAD	-2.12	1.47	1.56
12	bA	804	CLA	C1C-NC	-2.12	1.34	1.37
12	bA	853	CLA	C3B-C2B	2.12	1.48	1.41
12	bF	202	CLA	C1B-C2B	2.12	1.48	1.43
12	aA	803	CLA	C3D-C4D	-2.12	1.39	1.44
12	bA	853	CLA	CBD-CAD	-2.12	1.47	1.56
12	aA	823	CLA	C1C-C2C	2.11	1.48	1.44
15	cB	941	BCR	C33-C5	-2.11	1.47	1.50
12	aA	843	CLA	C4C-C3C	2.11	1.48	1.45
12	bB	923	CLA	C1C-NC	-2.11	1.34	1.37
12	cB	918	CLA	C4C-C3C	2.11	1.48	1.45
12	bB	912	CLA	O2D-CED	-2.11	1.40	1.45
12	bB	926	CLA	C3B-C2B	2.11	1.48	1.41
15	bB	941	BCR	C33-C5	-2.11	1.47	1.50
12	aB	914	CLA	C3B-C2B	2.11	1.48	1.41
12	aL	204	CLA	C4C-C3C	2.11	1.48	1.45
12	bA	816	CLA	C4C-C3C	2.11	1.48	1.45
12	cA	838	CLA	C1B-C2B	2.11	1.48	1.43
12	bB	930	CLA	C3B-C4B	2.11	1.48	1.42
12	bA	805	CLA	C1A-CHA	2.11	1.51	1.43
12	cB	925	CLA	OBD-CAD	2.11	1.26	1.22
12	bA	805	CLA	C1C-NC	-2.11	1.34	1.37
12	cB	936	CLA	C3B-C4B	2.11	1.48	1.42
12	cB	926	CLA	C3B-C2B	2.11	1.48	1.41
12	bB	925	CLA	OBD-CAD	2.11	1.26	1.22
12	cA	824	CLA	C3B-C2B	2.11	1.48	1.41
12	aA	840	CLA	C1C-NC	-2.11	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bB	930	CLA	C1C-NC	-2.11	1.34	1.37
12	bA	824	CLA	C3B-C2B	2.11	1.48	1.41
12	bB	929	CLA	C4C-C3C	2.11	1.48	1.45
12	cB	906	CLA	C4C-C3C	2.11	1.48	1.45
12	bA	838	CLA	C1B-C2B	2.11	1.48	1.43
12	cA	812	CLA	C4C-C3C	2.10	1.48	1.45
12	cL	204	CLA	C4C-C3C	2.10	1.48	1.45
12	cA	826	CLA	C1C-NC	-2.10	1.34	1.37
12	cA	823	CLA	C1C-C2C	2.10	1.48	1.44
12	aA	838	CLA	C1B-C2B	2.10	1.48	1.43
12	aA	820	CLA	C4C-C3C	2.10	1.48	1.45
12	aF	202	CLA	C1B-C2B	2.10	1.48	1.43
11	cA	801	CL0	CBD-CGD	-2.10	1.49	1.52
12	bB	905	CLA	C3B-C2B	2.10	1.48	1.41
12	cB	923	CLA	C3B-C4B	2.10	1.48	1.42
12	bB	937	CLA	CHB-C4A	-2.10	1.32	1.37
12	cB	937	CLA	CHB-C4A	-2.10	1.32	1.37
12	aA	807	CLA	CHB-C4A	-2.10	1.32	1.37
12	cB	912	CLA	O2D-CED	-2.10	1.40	1.45
12	aB	918	CLA	C3B-C4B	2.10	1.48	1.42
12	bA	817	CLA	C1C-C2C	2.10	1.48	1.44
12	bA	807	CLA	CHB-C4A	-2.10	1.32	1.37
12	aB	923	CLA	C3B-C4B	2.10	1.48	1.42
13	aB	940	1L3	C18-C16	2.10	1.55	1.51
12	cA	802	CLA	C3B-C4B	2.10	1.48	1.42
12	aB	936	CLA	C1C-NC	-2.10	1.34	1.37
12	bB	917	CLA	CHB-C4A	-2.10	1.32	1.37
12	cA	816	CLA	C1C-NC	-2.10	1.34	1.37
12	aB	926	CLA	C3B-C2B	2.10	1.48	1.41
12	bF	202	CLA	C3B-C2B	2.10	1.48	1.41
12	bB	927	CLA	C4C-C3C	2.10	1.48	1.45
12	cB	902	CLA	C3B-C2B	2.10	1.48	1.41
12	aB	917	CLA	CHB-C4A	-2.10	1.32	1.37
12	bB	936	CLA	C3B-C4B	2.10	1.48	1.42
12	cB	914	CLA	C3B-C2B	2.10	1.48	1.41
12	cB	912	CLA	CBD-CAD	-2.10	1.47	1.56
12	bB	931	CLA	CHB-C4A	-2.10	1.32	1.37
12	bA	823	CLA	C1C-C2C	2.09	1.48	1.44
12	aB	912	CLA	CBD-CAD	-2.09	1.47	1.56
12	aB	931	CLA	C1C-NC	-2.09	1.34	1.37
12	bB	921	CLA	C1C-C2C	2.09	1.48	1.44
12	bB	923	CLA	C3B-C4B	2.09	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aB	902	CLA	C3B-C2B	2.09	1.48	1.41
12	aB	934	CLA	C1C-C2C	2.09	1.48	1.44
17	cB	947	LMG	O7-C8	-2.09	1.41	1.46
12	aB	937	CLA	CHB-C4A	-2.09	1.32	1.37
12	cA	817	CLA	C1C-C2C	2.09	1.48	1.44
12	bB	906	CLA	C4C-C3C	2.09	1.48	1.45
12	aB	905	CLA	C3B-C2B	2.09	1.48	1.41
12	cA	811	CLA	C3B-C2B	2.09	1.48	1.41
12	bB	912	CLA	CBD-CAD	-2.09	1.47	1.56
12	cB	905	CLA	C3B-C2B	2.09	1.48	1.41
12	cB	933	CLA	C1B-C2B	2.09	1.48	1.43
12	aB	906	CLA	C4C-C3C	2.09	1.48	1.45
12	bA	813	CLA	C4C-C3C	2.09	1.48	1.45
12	bL	203	CLA	C1C-NC	-2.09	1.34	1.37
12	cA	815	CLA	C3B-C2B	2.09	1.48	1.41
12	bB	908	CLA	C4C-C3C	2.09	1.48	1.45
12	cA	804	CLA	C1C-NC	-2.09	1.34	1.37
12	aA	803	CLA	C3B-C4B	2.09	1.48	1.42
12	aB	931	CLA	CHB-C4A	-2.09	1.32	1.37
12	cA	808	CLA	C3B-C2B	2.09	1.48	1.41
12	bB	936	CLA	CBD-CAD	-2.09	1.47	1.56
12	bA	812	CLA	C4C-C3C	2.09	1.48	1.45
12	bA	837	CLA	O2D-CED	-2.09	1.40	1.45
12	aB	904	CLA	CHB-C4A	-2.09	1.32	1.37
12	bB	905	CLA	C1C-C2C	2.09	1.48	1.44
12	aB	936	CLA	C3B-C2B	2.09	1.48	1.41
12	cB	931	CLA	C1C-NC	-2.09	1.34	1.37
12	aA	808	CLA	C3B-C2B	2.09	1.48	1.41
12	bA	808	CLA	C3B-C2B	2.09	1.48	1.41
12	aB	935	CLA	C3B-C4B	2.08	1.48	1.42
12	aB	905	CLA	C1C-C2C	2.08	1.48	1.44
12	bB	934	CLA	C1C-C2C	2.08	1.48	1.44
12	cF	202	CLA	C3B-C2B	2.08	1.48	1.41
12	aB	936	CLA	CBD-CAD	-2.08	1.47	1.56
12	bB	936	CLA	C3B-C2B	2.08	1.48	1.41
12	cB	935	CLA	C3B-C4B	2.08	1.48	1.42
12	bA	838	CLA	OBD-CAD	2.08	1.26	1.22
12	aA	837	CLA	O2D-CED	-2.08	1.40	1.45
12	aF	202	CLA	C3B-C2B	2.08	1.48	1.41
15	aB	941	BCR	C33-C5	-2.08	1.47	1.50
12	cB	926	CLA	CBD-CAD	-2.08	1.47	1.56
12	aB	936	CLA	C3B-C4B	2.08	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aA	830	CLA	C3B-C2B	2.08	1.48	1.41
12	cA	830	CLA	C3B-C2B	2.08	1.48	1.41
12	aL	203	CLA	C1B-C2B	2.08	1.48	1.43
12	cB	933	CLA	C1C-NC	-2.08	1.34	1.37
12	aA	841	CLA	C4C-C3C	2.08	1.48	1.45
12	bB	938	CLA	C1C-C2C	2.08	1.48	1.44
12	bA	826	CLA	C1C-NC	-2.08	1.34	1.37
12	cB	930	CLA	C1C-NC	-2.08	1.34	1.37
12	bA	830	CLA	C3B-C2B	2.08	1.48	1.41
12	aB	907	CLA	C4C-C3C	2.08	1.48	1.45
12	cB	936	CLA	OBD-CAD	2.08	1.26	1.22
12	aB	926	CLA	CBD-CAD	-2.08	1.47	1.56
12	cA	805	CLA	C1C-NC	-2.08	1.34	1.37
12	bB	913	CLA	CBD-CAD	-2.08	1.47	1.56
12	bB	937	CLA	C3B-C4B	2.08	1.48	1.42
12	aB	938	CLA	C1C-C2C	2.08	1.48	1.44
12	cB	917	CLA	CHB-C4A	-2.08	1.32	1.37
17	bB	947	LMG	O7-C8	-2.07	1.41	1.46
12	aL	203	CLA	C1C-NC	-2.07	1.34	1.37
12	cA	838	CLA	OBD-CAD	2.07	1.26	1.22
12	cB	913	CLA	CBD-CAD	-2.07	1.47	1.56
12	aA	805	CLA	C1C-NC	-2.07	1.34	1.37
12	bA	803	CLA	C3B-C4B	2.07	1.48	1.42
12	bB	917	CLA	C1A-CHA	2.07	1.51	1.43
12	aB	917	CLA	C1A-CHA	2.07	1.51	1.43
12	aB	910	CLA	C4C-C3C	2.07	1.48	1.45
12	bA	803	CLA	C4C-C3C	2.07	1.48	1.45
12	cB	936	CLA	CBD-CAD	-2.07	1.47	1.56
12	aB	930	CLA	C3B-C4B	2.07	1.48	1.42
12	aA	804	CLA	C1C-NC	-2.07	1.34	1.37
12	cB	936	CLA	C3B-C2B	2.07	1.48	1.41
12	aB	930	CLA	C1C-NC	-2.07	1.34	1.37
12	aA	811	CLA	C3B-C2B	2.07	1.48	1.41
12	bB	935	CLA	C3B-C4B	2.07	1.48	1.42
12	bB	926	CLA	CBD-CAD	-2.07	1.47	1.56
12	cA	841	CLA	C4C-C3C	2.07	1.48	1.45
12	cB	905	CLA	C1C-C2C	2.07	1.48	1.44
12	cL	204	CLA	C1C-C2C	2.07	1.48	1.44
12	aB	929	CLA	C4C-C3C	2.07	1.48	1.45
12	bB	918	CLA	C4C-C3C	2.07	1.48	1.45
12	aB	913	CLA	CBD-CAD	-2.07	1.47	1.56
12	bB	916	CLA	C1C-C2C	2.07	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bA	807	CLA	CBD-CAD	-2.07	1.47	1.56
12	aB	933	CLA	C1B-C2B	2.07	1.48	1.43
12	cA	809	CLA	C1C-C2C	2.07	1.48	1.44
12	cB	930	CLA	C3B-C4B	2.07	1.48	1.42
12	cB	925	CLA	C1B-C2B	2.07	1.48	1.43
12	cL	203	CLA	C1B-C2B	2.07	1.48	1.43
12	cB	934	CLA	C1C-C2C	2.07	1.48	1.44
12	bB	939	CLA	C3B-C4B	2.06	1.48	1.42
12	bB	904	CLA	CHB-C4A	-2.06	1.32	1.37
12	cB	939	CLA	C3B-C4B	2.06	1.48	1.42
12	aL	202	CLA	C1C-C2C	2.06	1.48	1.44
12	bB	901	CLA	CBD-CAD	-2.06	1.47	1.56
12	aL	204	CLA	C1C-C2C	2.06	1.48	1.44
12	aA	816	CLA	C1C-NC	-2.06	1.34	1.37
12	cB	905	CLA	C1C-NC	-2.06	1.34	1.37
12	aA	813	CLA	C4C-C3C	2.06	1.48	1.45
12	aA	816	CLA	C4C-C3C	2.06	1.48	1.45
12	bA	820	CLA	C1C-NC	-2.06	1.34	1.37
12	cB	916	CLA	C1C-C2C	2.06	1.48	1.44
12	cB	921	CLA	C1C-C2C	2.06	1.48	1.44
12	cB	917	CLA	C1A-CHA	2.06	1.51	1.43
12	aB	905	CLA	C1C-NC	-2.06	1.34	1.37
12	cA	819	CLA	CBD-CAD	-2.06	1.47	1.56
12	cA	840	CLA	C1C-NC	-2.06	1.34	1.37
12	aA	819	CLA	CBD-CAD	-2.06	1.47	1.56
12	bB	933	CLA	C4C-C3C	2.06	1.48	1.45
12	cB	927	CLA	C4C-C3C	2.06	1.48	1.45
12	aB	937	CLA	C3B-C4B	2.06	1.48	1.42
12	aB	939	CLA	C3B-C4B	2.06	1.48	1.42
12	cB	901	CLA	CBD-CAD	-2.06	1.47	1.56
12	cA	837	CLA	O2D-CED	-2.06	1.40	1.45
15	cM	101	BCR	C33-C5	-2.06	1.47	1.50
12	aA	809	CLA	C1C-C2C	2.06	1.48	1.44
17	aB	947	LMG	O7-C8	-2.06	1.41	1.46
12	aB	914	CLA	C3B-C4B	2.06	1.48	1.42
12	cA	803	CLA	C3B-C4B	2.06	1.48	1.42
12	bB	933	CLA	C1B-C2B	2.06	1.48	1.43
12	bB	933	CLA	C1C-NC	-2.06	1.34	1.37
12	cA	825	CLA	C1C-NC	-2.06	1.34	1.37
12	aA	838	CLA	OBD-CAD	2.06	1.26	1.22
12	bA	819	CLA	CBD-CAD	-2.06	1.47	1.56
12	cL	203	CLA	C4C-C3C	2.06	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bA	829	CLA	CBD-CAD	-2.05	1.47	1.56
12	bA	841	CLA	CBD-CAD	-2.05	1.47	1.56
12	aA	836	CLA	C1A-CHA	2.05	1.51	1.43
15	cB	944	BCR	C33-C5	-2.05	1.47	1.50
12	bL	204	CLA	C4C-C3C	2.05	1.48	1.45
12	bL	203	CLA	C1B-C2B	2.05	1.47	1.43
12	bA	841	CLA	C4C-C3C	2.05	1.48	1.45
16	bB	948	LHG	O7-C5	-2.05	1.41	1.46
12	aB	901	CLA	CBD-CAD	-2.05	1.47	1.56
12	cB	912	CLA	C1C-C2C	2.05	1.48	1.44
12	aA	808	CLA	C1C-NC	-2.05	1.34	1.37
12	cA	820	CLA	C1C-NC	-2.05	1.34	1.37
15	aB	944	BCR	C33-C5	-2.05	1.47	1.50
12	aA	831	CLA	C1C-C2C	2.05	1.48	1.44
12	aB	921	CLA	C1C-C2C	2.05	1.48	1.44
12	bA	839	CLA	C3B-C2B	2.05	1.48	1.41
12	bA	836	CLA	C1A-CHA	2.05	1.51	1.43
12	bL	203	CLA	CHB-C4A	-2.05	1.32	1.37
12	cA	807	CLA	CBD-CAD	-2.05	1.47	1.56
12	bA	809	CLA	C1C-C2C	2.05	1.48	1.44
12	aA	825	CLA	C1C-NC	-2.05	1.34	1.37
12	bB	907	CLA	C4C-C3C	2.05	1.48	1.45
12	cB	922	CLA	C3B-C4B	2.05	1.48	1.42
12	aA	807	CLA	C3B-C2B	2.05	1.48	1.41
15	cL	205	BCR	C38-C26	-2.05	1.47	1.50
12	bB	905	CLA	C1C-NC	-2.05	1.34	1.37
12	aA	805	CLA	CHB-C4A	-2.05	1.32	1.37
12	cA	836	CLA	C1A-CHA	2.05	1.51	1.43
12	aL	203	CLA	CHB-C4A	-2.05	1.32	1.37
12	cA	816	CLA	C4C-C3C	2.05	1.48	1.45
12	aB	937	CLA	C3B-C2B	2.05	1.48	1.41
12	cB	927	CLA	C3B-C2B	2.05	1.48	1.41
15	aL	205	BCR	C33-C5	-2.05	1.47	1.50
12	cB	937	CLA	C3B-C4B	2.05	1.48	1.42
12	cA	843	CLA	C3B-C2B	2.04	1.48	1.41
15	bL	205	BCR	C38-C26	-2.04	1.47	1.50
12	bB	920	CLA	C3B-C4B	2.04	1.48	1.42
12	aB	933	CLA	C1C-NC	-2.04	1.34	1.37
12	cL	203	CLA	CHB-C4A	-2.04	1.32	1.37
12	cB	933	CLA	C4C-C3C	2.04	1.48	1.45
12	aB	920	CLA	C3B-C4B	2.04	1.48	1.42
15	aL	205	BCR	C38-C26	-2.04	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	cA	807	CLA	C3B-C2B	2.04	1.48	1.41
12	aA	807	CLA	CBD-CAD	-2.04	1.47	1.56
12	cL	202	CLA	C1C-C2C	2.04	1.48	1.44
12	cA	841	CLA	C3B-C2B	2.04	1.48	1.41
12	bA	841	CLA	C3B-C2B	2.04	1.48	1.41
12	aA	803	CLA	C4C-C3C	2.04	1.48	1.45
12	cB	937	CLA	C3B-C2B	2.04	1.48	1.41
12	cB	902	CLA	C3D-C4D	-2.04	1.39	1.44
12	cA	841	CLA	CBD-CAD	-2.04	1.47	1.56
12	aB	922	CLA	C3B-C4B	2.04	1.48	1.42
12	cB	920	CLA	C3B-C4B	2.04	1.48	1.42
12	bL	204	CLA	C1C-C2C	2.04	1.48	1.44
12	cB	914	CLA	C3B-C4B	2.04	1.48	1.42
12	aA	812	CLA	C3B-C2B	2.04	1.48	1.41
12	aB	916	CLA	C1C-C2C	2.04	1.48	1.44
12	bB	949	CLA	C4C-C3C	2.04	1.48	1.45
12	cA	803	CLA	C4C-C3C	2.04	1.48	1.45
12	bA	807	CLA	C3B-C2B	2.04	1.48	1.41
12	aA	839	CLA	C3B-C2B	2.04	1.48	1.41
12	cB	906	CLA	C3B-C2B	2.04	1.48	1.41
12	aB	926	CLA	C1C-C2C	2.04	1.48	1.44
12	bB	910	CLA	C4C-C3C	2.03	1.48	1.45
12	aB	915	CLA	C3B-C2B	2.03	1.48	1.41
12	bB	914	CLA	C3B-C4B	2.03	1.48	1.42
13	aA	845	1L3	C09-C08	2.03	1.42	1.38
12	cA	832	CLA	C1C-NC	-2.03	1.34	1.37
12	bB	937	CLA	C3B-C2B	2.03	1.48	1.41
15	cB	942	BCR	C33-C5	-2.03	1.47	1.50
12	aA	832	CLA	C1C-NC	-2.03	1.34	1.37
12	bB	902	CLA	C4C-C3C	2.03	1.48	1.45
12	bB	921	CLA	CBD-CAD	-2.03	1.47	1.56
12	bA	808	CLA	C1C-NC	-2.03	1.34	1.37
12	bB	937	CLA	C1C-NC	-2.03	1.34	1.37
12	cL	203	CLA	C1C-NC	-2.03	1.34	1.37
12	bB	919	CLA	C4C-C3C	2.03	1.48	1.45
12	cB	929	CLA	C4C-C3C	2.03	1.48	1.45
12	cA	828	CLA	CBD-CAD	-2.03	1.47	1.56
12	cA	823	CLA	C3B-C2B	2.03	1.48	1.41
12	aA	837	CLA	CBD-CAD	-2.03	1.47	1.56
12	cB	921	CLA	CBD-CAD	-2.03	1.47	1.56
12	bB	931	CLA	C1C-NC	-2.03	1.34	1.37
12	aA	841	CLA	CBD-CAD	-2.03	1.47	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aA	818	CLA	CBD-CAD	-2.03	1.47	1.56
12	bB	902	CLA	C3B-C4B	2.03	1.48	1.42
12	cB	926	CLA	C1C-C2C	2.03	1.48	1.44
12	bB	925	CLA	C1B-C2B	2.03	1.47	1.43
12	cA	812	CLA	C3B-C2B	2.03	1.48	1.41
12	aA	812	CLA	C1A-CHA	2.03	1.51	1.43
12	aA	816	CLA	C3B-C4B	2.03	1.48	1.42
12	cA	808	CLA	C1C-NC	-2.03	1.34	1.37
12	bB	902	CLA	C3D-C4D	-2.03	1.39	1.44
15	bA	849	BCR	C33-C5	-2.03	1.47	1.50
12	bB	937	CLA	CBD-CAD	-2.03	1.47	1.56
12	cB	910	CLA	C4C-C3C	2.03	1.48	1.45
12	bA	812	CLA	C1A-CHA	2.03	1.51	1.43
12	cB	937	CLA	CBD-CAD	-2.03	1.47	1.56
12	aA	841	CLA	C3B-C2B	2.03	1.48	1.41
12	aB	930	CLA	C4C-C3C	2.03	1.48	1.45
12	bB	915	CLA	C3B-C2B	2.03	1.48	1.41
12	cA	831	CLA	C3B-C4B	2.03	1.48	1.42
12	aB	949	CLA	C4C-C3C	2.02	1.48	1.45
12	bL	203	CLA	C4C-C3C	2.02	1.48	1.45
12	bA	818	CLA	CBD-CAD	-2.02	1.47	1.56
12	aB	921	CLA	CBD-CAD	-2.02	1.47	1.56
13	cA	844	1L3	C09-C08	2.02	1.42	1.38
12	aL	203	CLA	C4C-C3C	2.02	1.48	1.45
12	cB	919	CLA	C3B-C2B	2.02	1.48	1.41
12	cA	805	CLA	CHB-C4A	-2.02	1.32	1.37
12	cB	904	CLA	CHB-C4A	-2.02	1.32	1.37
12	cA	831	CLA	C1C-C2C	2.02	1.48	1.44
12	aA	831	CLA	C3B-C4B	2.02	1.48	1.42
12	cA	829	CLA	CBD-CAD	-2.02	1.47	1.56
12	bA	805	CLA	CHB-C4A	-2.02	1.32	1.37
12	bA	812	CLA	C3B-C2B	2.02	1.48	1.41
12	bA	819	CLA	C1C-C2C	2.02	1.48	1.44
12	aB	919	CLA	C3B-C2B	2.02	1.48	1.41
12	bB	906	CLA	C3B-C2B	2.02	1.48	1.41
16	aA	853	LHG	O8-C6	-2.02	1.40	1.45
12	bA	828	CLA	CBD-CAD	-2.02	1.47	1.56
12	cA	818	CLA	CBD-CAD	-2.02	1.47	1.56
12	aB	902	CLA	C3D-C4D	-2.02	1.39	1.44
12	cB	915	CLA	C3B-C2B	2.02	1.48	1.41
15	aB	942	BCR	C33-C5	-2.02	1.47	1.50
12	aB	924	CLA	C1C-C2C	2.02	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	bA	837	CLA	CBD-CAD	-2.02	1.47	1.56
12	aA	820	CLA	C1C-C2C	2.02	1.48	1.44
12	bA	831	CLA	C1C-C2C	2.02	1.48	1.44
12	cB	930	CLA	C1C-C2C	2.02	1.48	1.44
12	bA	823	CLA	C3B-C2B	2.02	1.48	1.41
12	bB	927	CLA	C3B-C2B	2.02	1.48	1.41
12	cB	931	CLA	C1B-C2B	2.02	1.47	1.43
12	cA	814	CLA	C3B-C2B	2.02	1.48	1.41
12	cB	938	CLA	CBD-CAD	-2.02	1.47	1.56
12	aB	912	CLA	C1C-C2C	2.01	1.48	1.44
12	aA	843	CLA	C3B-C2B	2.01	1.48	1.41
12	bA	831	CLA	C3B-C4B	2.01	1.48	1.42
12	bA	843	CLA	C3B-C2B	2.01	1.48	1.41
12	cB	931	CLA	C4C-C3C	2.01	1.48	1.45
12	aB	933	CLA	C4C-C3C	2.01	1.48	1.45
12	bB	919	CLA	C3B-C2B	2.01	1.48	1.41
12	aA	828	CLA	CBD-CAD	-2.01	1.47	1.56
12	aB	929	CLA	CHB-C4A	-2.01	1.32	1.37
12	cA	839	CLA	C3B-C2B	2.01	1.48	1.41
12	aA	829	CLA	CBD-CAD	-2.01	1.47	1.56
12	bA	816	CLA	C3B-C4B	2.01	1.48	1.42
12	aB	937	CLA	CBD-CAD	-2.01	1.47	1.56
12	bB	909	CLA	C3B-C2B	2.01	1.48	1.41
16	cB	948	LHG	O7-C5	-2.01	1.41	1.46
12	cA	809	CLA	C3B-C2B	2.01	1.47	1.41
12	aB	906	CLA	C3B-C2B	2.01	1.47	1.41
12	aB	925	CLA	C1B-C2B	2.01	1.47	1.43
12	cA	837	CLA	CBD-CAD	-2.01	1.47	1.56
12	aB	939	CLA	C1A-CHA	2.01	1.51	1.43
12	cB	932	CLA	C3B-C4B	2.01	1.48	1.42
12	cB	939	CLA	C1A-CHA	2.01	1.51	1.43
12	aA	802	CLA	C1C-NC	-2.01	1.34	1.37
15	cL	205	BCR	C33-C5	-2.01	1.47	1.50
12	aB	934	CLA	C3B-C2B	2.01	1.47	1.41
12	cA	822	CLA	C1C-NC	-2.01	1.34	1.37
12	bA	809	CLA	C3B-C2B	2.01	1.47	1.41
12	cA	812	CLA	C1A-CHA	2.01	1.51	1.43
12	bA	814	CLA	C3B-C2B	2.01	1.47	1.41
12	bB	929	CLA	CHB-C4A	-2.01	1.32	1.37
12	bB	922	CLA	C3B-C4B	2.01	1.48	1.42
15	bB	942	BCR	C33-C5	-2.01	1.47	1.50
12	aA	823	CLA	C3B-C2B	2.01	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	aA	819	CLA	C1C-C2C	2.01	1.48	1.44
12	bA	820	CLA	C1A-CHA	2.01	1.51	1.43
12	aA	814	CLA	C3B-C2B	2.01	1.47	1.41
12	bB	908	CLA	CMB-C2B	-2.01	1.46	1.50
15	bL	205	BCR	C33-C5	-2.00	1.47	1.50
12	aB	902	CLA	C3B-C4B	2.00	1.48	1.42
12	aB	927	CLA	C3B-C2B	2.00	1.47	1.41
12	bA	833	CLA	C4C-C3C	2.00	1.48	1.45
15	aA	850	BCR	C33-C5	-2.00	1.47	1.50
12	aA	822	CLA	C1C-NC	-2.00	1.34	1.37
12	bL	202	CLA	C1C-C2C	2.00	1.48	1.44
12	bB	916	CLA	CBD-CAD	-2.00	1.47	1.56
12	cA	819	CLA	C1C-C2C	2.00	1.48	1.44
12	bB	911	CLA	C4C-C3C	2.00	1.48	1.45
12	bA	822	CLA	C1C-NC	-2.00	1.34	1.37
15	aL	201	BCR	C38-C26	-2.00	1.47	1.50
15	bB	944	BCR	C33-C5	-2.00	1.47	1.50
15	cA	846	BCR	C33-C5	-2.00	1.47	1.50
12	bA	814	CLA	O2D-CED	-2.00	1.40	1.45
12	aB	919	CLA	C4C-C3C	2.00	1.48	1.45
12	cF	202	CLA	C1C-NC	-2.00	1.34	1.37
12	bB	909	CLA	O2D-CED	-2.00	1.40	1.45
12	bB	924	CLA	C1C-C2C	2.00	1.48	1.44
13	aB	940	1L3	C09-C08	2.00	1.42	1.38

All (8428) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aB	931	CLA	C1D-ND-C4D	-10.74	98.77	106.31
12	cB	931	CLA	C1D-ND-C4D	-10.70	98.81	106.31
12	bB	931	CLA	C1D-ND-C4D	-10.68	98.82	106.31
11	cA	801	CL0	C1B-CHB-C4A	10.34	127.97	121.32
11	aA	801	CL0	C1B-CHB-C4A	10.29	127.94	121.32
11	bA	801	CL0	C1B-CHB-C4A	10.26	127.92	121.32
12	aL	203	CLA	C1D-ND-C4D	-9.99	99.30	106.31
12	cL	203	CLA	C1D-ND-C4D	-9.99	99.30	106.31
12	aB	920	CLA	C1D-ND-C4D	-9.98	99.31	106.31
12	bB	920	CLA	C1D-ND-C4D	-9.97	99.32	106.31
12	aB	939	CLA	C1D-ND-C4D	-9.96	99.32	106.31
12	bB	939	CLA	C1D-ND-C4D	-9.95	99.33	106.31
12	bL	203	CLA	C1D-ND-C4D	-9.94	99.34	106.31
12	cB	920	CLA	C1D-ND-C4D	-9.93	99.34	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cB	939	CLA	C1D-ND-C4D	-9.91	99.36	106.31
12	aA	822	CLA	C1D-ND-C4D	-9.75	99.47	106.31
12	bA	822	CLA	C1D-ND-C4D	-9.72	99.49	106.31
12	aB	915	CLA	C1D-ND-C4D	-9.69	99.51	106.31
12	cA	822	CLA	C1D-ND-C4D	-9.69	99.51	106.31
12	cB	915	CLA	C1D-ND-C4D	-9.67	99.53	106.31
12	aB	932	CLA	C1D-ND-C4D	-9.64	99.55	106.31
12	aB	916	CLA	C1D-ND-C4D	-9.63	99.55	106.31
12	bB	916	CLA	C1D-ND-C4D	-9.63	99.55	106.31
12	aA	806	CLA	C1D-ND-C4D	-9.62	99.56	106.31
12	bB	932	CLA	C1D-ND-C4D	-9.62	99.56	106.31
12	cB	932	CLA	C1D-ND-C4D	-9.61	99.57	106.31
12	bA	806	CLA	C1D-ND-C4D	-9.60	99.58	106.31
12	bB	915	CLA	C1D-ND-C4D	-9.59	99.58	106.31
12	bA	838	CLA	C1D-ND-C4D	-9.58	99.59	106.31
12	cA	806	CLA	C1D-ND-C4D	-9.58	99.59	106.31
12	cB	916	CLA	C1D-ND-C4D	-9.57	99.60	106.31
12	cL	204	CLA	C1D-ND-C4D	-9.56	99.60	106.31
12	cA	817	CLA	C1D-ND-C4D	-9.54	99.62	106.31
12	cA	838	CLA	C1D-ND-C4D	-9.53	99.62	106.31
12	aL	204	CLA	C1D-ND-C4D	-9.53	99.63	106.31
12	bL	204	CLA	C1D-ND-C4D	-9.53	99.63	106.31
12	aA	838	CLA	C1D-ND-C4D	-9.52	99.63	106.31
12	aA	817	CLA	C1D-ND-C4D	-9.50	99.64	106.31
12	cA	804	CLA	C1D-ND-C4D	-9.49	99.65	106.31
12	bA	817	CLA	C1D-ND-C4D	-9.46	99.68	106.31
12	aA	804	CLA	C1D-ND-C4D	-9.45	99.68	106.31
12	cA	803	CLA	C1D-ND-C4D	-9.43	99.69	106.31
12	bA	803	CLA	C1D-ND-C4D	-9.41	99.71	106.31
12	bB	949	CLA	C1D-ND-C4D	-9.41	99.71	106.31
12	bA	804	CLA	C1D-ND-C4D	-9.39	99.72	106.31
12	cB	949	CLA	C1D-ND-C4D	-9.38	99.73	106.31
12	bB	929	CLA	C1D-ND-C4D	-9.37	99.74	106.31
12	aB	929	CLA	C1D-ND-C4D	-9.36	99.75	106.31
12	aB	906	CLA	C1D-ND-C4D	-9.36	99.75	106.31
12	aA	803	CLA	C1D-ND-C4D	-9.35	99.75	106.31
12	cB	929	CLA	C1D-ND-C4D	-9.34	99.76	106.31
12	aB	949	CLA	C1D-ND-C4D	-9.34	99.76	106.31
12	bB	906	CLA	C1D-ND-C4D	-9.33	99.77	106.31
12	bA	841	CLA	C1D-ND-C4D	-9.32	99.77	106.31
12	cB	906	CLA	C1D-ND-C4D	-9.31	99.78	106.31
12	bB	914	CLA	C1D-ND-C4D	-9.31	99.78	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	841	CLA	C1D-ND-C4D	-9.29	99.79	106.31
12	cB	914	CLA	C1D-ND-C4D	-9.28	99.80	106.31
12	cB	937	CLA	C1D-ND-C4D	-9.27	99.81	106.31
12	aB	914	CLA	C1D-ND-C4D	-9.26	99.81	106.31
12	bB	937	CLA	C1D-ND-C4D	-9.26	99.82	106.31
12	aA	841	CLA	C1D-ND-C4D	-9.25	99.82	106.31
12	aB	937	CLA	C1D-ND-C4D	-9.24	99.83	106.31
12	aL	202	CLA	C1D-ND-C4D	-9.23	99.84	106.31
12	cL	202	CLA	C1D-ND-C4D	-9.22	99.84	106.31
12	cA	810	CLA	C1D-ND-C4D	-9.19	99.86	106.31
12	aA	810	CLA	C1D-ND-C4D	-9.18	99.87	106.31
12	cA	839	CLA	C1D-ND-C4D	-9.18	99.87	106.31
12	bA	823	CLA	C1D-ND-C4D	-9.18	99.87	106.31
12	bA	839	CLA	C1D-ND-C4D	-9.18	99.87	106.31
12	bA	810	CLA	C1D-ND-C4D	-9.18	99.87	106.31
12	aA	823	CLA	C1D-ND-C4D	-9.15	99.89	106.31
12	bL	202	CLA	C1D-ND-C4D	-9.15	99.89	106.31
12	aA	839	CLA	C1D-ND-C4D	-9.14	99.90	106.31
12	cA	823	CLA	C1D-ND-C4D	-9.13	99.90	106.31
12	aA	809	CLA	C1D-ND-C4D	-9.12	99.91	106.31
12	cA	826	CLA	C1D-ND-C4D	-9.11	99.92	106.31
12	cA	809	CLA	C1D-ND-C4D	-9.10	99.93	106.31
12	bB	902	CLA	C1D-ND-C4D	-9.09	99.93	106.31
12	bA	826	CLA	C1D-ND-C4D	-9.09	99.94	106.31
12	bA	809	CLA	C1D-ND-C4D	-9.09	99.94	106.31
12	aB	902	CLA	C1D-ND-C4D	-9.08	99.94	106.31
12	cB	902	CLA	C1D-ND-C4D	-9.07	99.94	106.31
12	bB	936	CLA	C1D-ND-C4D	-9.06	99.95	106.31
12	aA	826	CLA	C1D-ND-C4D	-9.06	99.95	106.31
12	aA	820	CLA	C1D-ND-C4D	-9.04	99.97	106.31
12	cB	936	CLA	C1D-ND-C4D	-9.03	99.97	106.31
12	cA	808	CLA	C1D-ND-C4D	-9.03	99.98	106.31
12	aB	936	CLA	C1D-ND-C4D	-9.01	99.99	106.31
12	bA	820	CLA	C1D-ND-C4D	-9.00	100.00	106.31
12	aA	808	CLA	C1D-ND-C4D	-8.98	100.01	106.31
12	bF	202	CLA	C1D-ND-C4D	-8.98	100.01	106.31
12	aB	913	CLA	C1D-ND-C4D	-8.98	100.01	106.31
12	aF	202	CLA	C1D-ND-C4D	-8.98	100.01	106.31
12	cA	820	CLA	C1D-ND-C4D	-8.97	100.02	106.31
12	aB	930	CLA	C1D-ND-C4D	-8.97	100.02	106.31
12	bB	925	CLA	C1D-ND-C4D	-8.96	100.03	106.31
12	bA	808	CLA	C1D-ND-C4D	-8.95	100.03	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bB	901	CLA	C1D-ND-C4D	-8.95	100.03	106.31
12	cB	901	CLA	C1D-ND-C4D	-8.95	100.03	106.31
12	aB	904	CLA	C1D-ND-C4D	-8.94	100.04	106.31
12	cB	911	CLA	C1D-ND-C4D	-8.93	100.05	106.31
12	bB	930	CLA	C1D-ND-C4D	-8.93	100.05	106.31
12	cF	202	CLA	C1D-ND-C4D	-8.93	100.05	106.31
12	bB	904	CLA	C1D-ND-C4D	-8.92	100.06	106.31
12	cB	930	CLA	C1D-ND-C4D	-8.91	100.06	106.31
12	aB	911	CLA	C1D-ND-C4D	-8.91	100.06	106.31
12	aB	925	CLA	C1D-ND-C4D	-8.91	100.06	106.31
12	aB	901	CLA	C1D-ND-C4D	-8.89	100.07	106.31
12	cB	904	CLA	C1D-ND-C4D	-8.89	100.08	106.31
12	bA	816	CLA	C1D-ND-C4D	-8.88	100.08	106.31
12	cB	923	CLA	C1D-ND-C4D	-8.87	100.09	106.31
12	bA	840	CLA	C1D-ND-C4D	-8.87	100.09	106.31
12	bB	911	CLA	C1D-ND-C4D	-8.87	100.09	106.31
12	cA	816	CLA	C1D-ND-C4D	-8.86	100.09	106.31
12	cA	842	CLA	C1D-ND-C4D	-8.86	100.10	106.31
12	cB	925	CLA	C1D-ND-C4D	-8.85	100.10	106.31
12	cA	832	CLA	C1D-ND-C4D	-8.85	100.10	106.31
12	bB	913	CLA	C1D-ND-C4D	-8.85	100.11	106.31
12	bA	842	CLA	C1D-ND-C4D	-8.84	100.11	106.31
12	aA	854	CLA	C1D-ND-C4D	-8.84	100.11	106.31
12	aA	842	CLA	C1D-ND-C4D	-8.84	100.11	106.31
12	bA	807	CLA	C1D-ND-C4D	-8.83	100.11	106.31
12	cB	913	CLA	C1D-ND-C4D	-8.83	100.11	106.31
12	aB	923	CLA	C1D-ND-C4D	-8.83	100.12	106.31
12	aA	805	CLA	C1D-ND-C4D	-8.83	100.12	106.31
12	aA	840	CLA	C1D-ND-C4D	-8.83	100.12	106.31
12	bA	853	CLA	C1D-ND-C4D	-8.82	100.12	106.31
12	cA	805	CLA	C1D-ND-C4D	-8.82	100.12	106.31
12	cA	853	CLA	C1D-ND-C4D	-8.82	100.13	106.31
12	aA	816	CLA	C1D-ND-C4D	-8.81	100.13	106.31
12	cA	807	CLA	C1D-ND-C4D	-8.81	100.13	106.31
12	aB	905	CLA	C1D-ND-C4D	-8.80	100.14	106.31
12	bA	836	CLA	C1D-ND-C4D	-8.80	100.14	106.31
12	bB	923	CLA	C1D-ND-C4D	-8.80	100.14	106.31
12	bA	805	CLA	C1D-ND-C4D	-8.80	100.14	106.31
12	aA	832	CLA	C1D-ND-C4D	-8.79	100.14	106.31
12	aA	836	CLA	C1D-ND-C4D	-8.79	100.15	106.31
12	bA	832	CLA	C1D-ND-C4D	-8.78	100.16	106.31
12	cA	836	CLA	C1D-ND-C4D	-8.78	100.16	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	807	CLA	C1D-ND-C4D	-8.77	100.16	106.31
12	cA	840	CLA	C1D-ND-C4D	-8.76	100.17	106.31
12	cA	828	CLA	C1D-ND-C4D	-8.76	100.17	106.31
12	bA	812	CLA	C1D-ND-C4D	-8.73	100.19	106.31
12	cA	812	CLA	C1D-ND-C4D	-8.72	100.20	106.31
12	aA	843	CLA	C1D-ND-C4D	-8.72	100.20	106.31
12	bA	828	CLA	C1D-ND-C4D	-8.72	100.20	106.31
12	bB	905	CLA	C1D-ND-C4D	-8.71	100.20	106.31
12	aA	828	CLA	C1D-ND-C4D	-8.71	100.20	106.31
12	aA	812	CLA	C1D-ND-C4D	-8.70	100.21	106.31
12	cB	921	CLA	C1D-ND-C4D	-8.67	100.23	106.31
12	cB	905	CLA	C1D-ND-C4D	-8.66	100.23	106.31
12	cA	802	CLA	C1D-ND-C4D	-8.65	100.24	106.31
12	bB	933	CLA	C1D-ND-C4D	-8.65	100.25	106.31
12	cA	843	CLA	C1D-ND-C4D	-8.65	100.25	106.31
12	cA	827	CLA	C1D-ND-C4D	-8.64	100.25	106.31
12	bB	921	CLA	C1D-ND-C4D	-8.64	100.25	106.31
12	aA	827	CLA	C1D-ND-C4D	-8.62	100.26	106.31
12	aB	933	CLA	C1D-ND-C4D	-8.61	100.27	106.31
12	aA	802	CLA	C1D-ND-C4D	-8.61	100.27	106.31
12	aA	815	CLA	C1D-ND-C4D	-8.60	100.28	106.31
12	bA	843	CLA	C1D-ND-C4D	-8.60	100.28	106.31
12	cB	933	CLA	C1D-ND-C4D	-8.60	100.28	106.31
12	bA	815	CLA	C1D-ND-C4D	-8.59	100.28	106.31
12	cA	815	CLA	C1D-ND-C4D	-8.58	100.29	106.31
12	aB	922	CLA	C1D-ND-C4D	-8.58	100.29	106.31
12	aB	921	CLA	C1D-ND-C4D	-8.58	100.30	106.31
12	cA	818	CLA	C1D-ND-C4D	-8.56	100.31	106.31
12	cA	811	CLA	C1D-ND-C4D	-8.55	100.31	106.31
12	bA	811	CLA	C1D-ND-C4D	-8.55	100.31	106.31
12	bA	827	CLA	C1D-ND-C4D	-8.54	100.32	106.31
12	bB	922	CLA	C1D-ND-C4D	-8.54	100.32	106.31
12	bA	802	CLA	C1D-ND-C4D	-8.54	100.32	106.31
12	bA	825	CLA	C1D-ND-C4D	-8.53	100.33	106.31
12	bA	818	CLA	C1D-ND-C4D	-8.53	100.33	106.31
12	aA	818	CLA	C1D-ND-C4D	-8.51	100.34	106.31
12	bB	950	CLA	C1D-ND-C4D	-8.51	100.34	106.31
12	cA	825	CLA	C1D-ND-C4D	-8.50	100.34	106.31
12	cB	924	CLA	C1D-ND-C4D	-8.49	100.35	106.31
12	aA	825	CLA	C1D-ND-C4D	-8.49	100.35	106.31
12	cB	922	CLA	C1D-ND-C4D	-8.47	100.37	106.31
12	aA	844	CLA	C1D-ND-C4D	-8.46	100.37	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aB	938	CLA	C1D-ND-C4D	-8.46	100.38	106.31
12	bB	938	CLA	C1D-ND-C4D	-8.46	100.38	106.31
12	bB	926	CLA	C1D-ND-C4D	-8.45	100.38	106.31
12	aB	926	CLA	C1D-ND-C4D	-8.45	100.39	106.31
12	aA	811	CLA	C1D-ND-C4D	-8.45	100.39	106.31
12	aB	950	CLA	C1D-ND-C4D	-8.44	100.39	106.31
12	cB	912	CLA	C1D-ND-C4D	-8.44	100.39	106.31
12	bB	924	CLA	C1D-ND-C4D	-8.44	100.39	106.31
12	aB	918	CLA	C1D-ND-C4D	-8.43	100.39	106.31
12	cB	926	CLA	C1D-ND-C4D	-8.43	100.40	106.31
12	cB	938	CLA	C1D-ND-C4D	-8.43	100.40	106.31
12	cA	814	CLA	C1D-ND-C4D	-8.43	100.40	106.31
12	aB	912	CLA	C1D-ND-C4D	-8.41	100.41	106.31
12	bA	819	CLA	C1D-ND-C4D	-8.41	100.41	106.31
12	cB	918	CLA	C1D-ND-C4D	-8.41	100.41	106.31
12	bB	912	CLA	C1D-ND-C4D	-8.40	100.42	106.31
12	aB	924	CLA	C1D-ND-C4D	-8.40	100.42	106.31
12	cB	909	CLA	C1D-ND-C4D	-8.39	100.42	106.31
12	aA	814	CLA	C1D-ND-C4D	-8.39	100.43	106.31
12	cA	819	CLA	C1D-ND-C4D	-8.38	100.43	106.31
12	aA	819	CLA	C1D-ND-C4D	-8.37	100.44	106.31
12	aA	837	CLA	C1D-ND-C4D	-8.36	100.44	106.31
12	aA	821	CLA	C1D-ND-C4D	-8.36	100.45	106.31
12	cA	833	CLA	C1D-ND-C4D	-8.36	100.45	106.31
12	aB	909	CLA	C1D-ND-C4D	-8.35	100.45	106.31
12	cA	837	CLA	C1D-ND-C4D	-8.34	100.46	106.31
12	aA	833	CLA	C1D-ND-C4D	-8.34	100.46	106.31
12	bA	814	CLA	C1D-ND-C4D	-8.34	100.46	106.31
12	bB	918	CLA	C1D-ND-C4D	-8.33	100.46	106.31
12	cA	821	CLA	C1D-ND-C4D	-8.33	100.47	106.31
12	bA	833	CLA	C1D-ND-C4D	-8.31	100.48	106.31
12	aB	903	CLA	C1D-ND-C4D	-8.31	100.48	106.31
12	bA	821	CLA	C1D-ND-C4D	-8.30	100.48	106.31
12	bA	837	CLA	C1D-ND-C4D	-8.30	100.49	106.31
12	bB	909	CLA	C1D-ND-C4D	-8.29	100.49	106.31
12	cB	907	CLA	C1D-ND-C4D	-8.29	100.49	106.31
12	aB	934	CLA	C1D-ND-C4D	-8.28	100.50	106.31
12	bB	934	CLA	C1D-ND-C4D	-8.28	100.50	106.31
12	cA	834	CLA	C1D-ND-C4D	-8.26	100.52	106.31
12	cA	835	CLA	C1D-ND-C4D	-8.25	100.53	106.31
12	bB	907	CLA	C1D-ND-C4D	-8.24	100.53	106.31
12	cB	903	CLA	C1D-ND-C4D	-8.24	100.53	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	834	CLA	C1D-ND-C4D	-8.23	100.53	106.31
12	bB	903	CLA	C1D-ND-C4D	-8.23	100.54	106.31
12	bA	835	CLA	C1D-ND-C4D	-8.23	100.54	106.31
12	cB	934	CLA	C1D-ND-C4D	-8.21	100.55	106.31
12	bB	910	CLA	C1D-ND-C4D	-8.20	100.56	106.31
12	aA	835	CLA	C1D-ND-C4D	-8.20	100.56	106.31
12	bA	834	CLA	C1D-ND-C4D	-8.19	100.57	106.31
12	aB	910	CLA	C1D-ND-C4D	-8.18	100.57	106.31
12	aB	907	CLA	C1D-ND-C4D	-8.18	100.57	106.31
12	aA	813	CLA	C1D-ND-C4D	-8.17	100.58	106.31
12	cA	813	CLA	C1D-ND-C4D	-8.16	100.58	106.31
12	cB	910	CLA	C1D-ND-C4D	-8.15	100.60	106.31
12	bA	813	CLA	C1D-ND-C4D	-8.14	100.60	106.31
12	bA	824	CLA	C1D-ND-C4D	-8.14	100.60	106.31
12	aA	829	CLA	C1D-ND-C4D	-8.14	100.60	106.31
12	cA	824	CLA	C1D-ND-C4D	-8.14	100.60	106.31
12	cB	919	CLA	C1D-ND-C4D	-8.14	100.60	106.31
12	cA	829	CLA	C1D-ND-C4D	-8.13	100.61	106.31
12	aA	824	CLA	C1D-ND-C4D	-8.13	100.61	106.31
12	aB	935	CLA	C1D-ND-C4D	-8.12	100.62	106.31
12	aB	919	CLA	C1D-ND-C4D	-8.11	100.62	106.31
12	bA	829	CLA	C1D-ND-C4D	-8.10	100.63	106.31
12	cB	935	CLA	C1D-ND-C4D	-8.10	100.63	106.31
12	bB	919	CLA	C1D-ND-C4D	-8.08	100.64	106.31
12	bB	935	CLA	C1D-ND-C4D	-8.06	100.65	106.31
12	cB	917	CLA	C1D-ND-C4D	-8.04	100.67	106.31
12	aB	917	CLA	C1D-ND-C4D	-8.04	100.67	106.31
12	bB	917	CLA	C1D-ND-C4D	-8.04	100.67	106.31
12	cA	831	CLA	C1D-ND-C4D	-7.89	100.78	106.31
12	aA	831	CLA	C1D-ND-C4D	-7.85	100.80	106.31
12	bA	830	CLA	C1D-ND-C4D	-7.85	100.80	106.31
12	bA	831	CLA	C1D-ND-C4D	-7.85	100.81	106.31
12	aA	830	CLA	C1D-ND-C4D	-7.78	100.85	106.31
12	cA	830	CLA	C1D-ND-C4D	-7.78	100.86	106.31
12	bA	843	CLA	CAA-C2A-C3A	-7.74	92.09	113.00
12	cA	843	CLA	CAA-C2A-C3A	-7.74	92.09	113.00
12	aA	843	CLA	CAA-C2A-C3A	-7.74	92.09	113.00
11	aA	801	CL0	O2D-CGD-CBD	7.65	119.35	110.95
11	cA	801	CL0	O2D-CGD-CBD	7.64	119.34	110.95
12	cB	927	CLA	C1D-ND-C4D	-7.61	100.97	106.31
11	bA	801	CL0	O2D-CGD-CBD	7.60	119.30	110.95
12	aB	927	CLA	C1D-ND-C4D	-7.54	101.02	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aB	931	CLA	C2D-C1D-ND	7.54	117.58	110.13
12	aB	928	CLA	C1D-ND-C4D	-7.51	101.04	106.31
12	cA	834	CLA	O2D-CGD-CBD	7.50	124.34	111.23
12	cB	931	CLA	C2D-C1D-ND	7.50	117.55	110.13
12	aA	834	CLA	O2D-CGD-CBD	7.50	124.33	111.23
12	bA	834	CLA	O2D-CGD-CBD	7.50	124.33	111.23
12	bB	931	CLA	C2D-C1D-ND	7.49	117.54	110.13
12	cB	928	CLA	C1D-ND-C4D	-7.48	101.06	106.31
12	bB	927	CLA	C1D-ND-C4D	-7.46	101.08	106.31
12	bB	928	CLA	C1D-ND-C4D	-7.45	101.09	106.31
12	aB	938	CLA	CMD-C2D-C1D	7.30	137.57	124.73
12	cB	938	CLA	CMD-C2D-C1D	7.28	137.55	124.73
12	bB	938	CLA	CMD-C2D-C1D	7.28	137.54	124.73
12	aL	203	CLA	C2D-C1D-ND	7.12	117.17	110.13
12	bA	818	CLA	CMD-C2D-C1D	7.11	137.25	124.73
12	cL	203	CLA	C2D-C1D-ND	7.11	117.16	110.13
12	aA	818	CLA	CMD-C2D-C1D	7.11	137.24	124.73
12	cA	818	CLA	CMD-C2D-C1D	7.09	137.22	124.73
12	bL	203	CLA	C2D-C1D-ND	7.08	117.14	110.13
12	bA	803	CLA	C2D-C1D-ND	7.03	117.09	110.13
12	cA	803	CLA	C2D-C1D-ND	7.03	117.09	110.13
12	aA	803	CLA	C2D-C1D-ND	7.00	117.05	110.13
12	bB	928	CLA	CMD-C2D-C1D	6.99	137.04	124.73
12	aB	928	CLA	CMD-C2D-C1D	6.99	137.04	124.73
12	cB	928	CLA	CMD-C2D-C1D	6.99	137.04	124.73
12	cB	920	CLA	C2D-C1D-ND	6.95	117.01	110.13
12	bA	807	CLA	CMD-C2D-C1D	6.94	136.96	124.73
12	cA	807	CLA	CMD-C2D-C1D	6.94	136.95	124.73
12	aB	920	CLA	C2D-C1D-ND	6.94	116.99	110.13
12	aA	807	CLA	CMD-C2D-C1D	6.93	136.93	124.73
12	cB	925	CLA	O2D-CGD-CBD	6.93	123.34	111.23
12	bB	920	CLA	C2D-C1D-ND	6.93	116.98	110.13
12	cB	902	CLA	C2D-C1D-ND	6.92	116.98	110.13
12	bB	925	CLA	O2D-CGD-CBD	6.92	123.33	111.23
12	aA	822	CLA	C2D-C1D-ND	6.91	116.96	110.13
12	aB	902	CLA	C2D-C1D-ND	6.91	116.96	110.13
12	aB	925	CLA	O2D-CGD-CBD	6.90	123.30	111.23
12	cA	822	CLA	C2D-C1D-ND	6.89	116.94	110.13
12	aB	919	CLA	O2D-CGD-CBD	6.89	123.27	111.23
12	bA	822	CLA	C2D-C1D-ND	6.89	116.94	110.13
12	cB	919	CLA	O2D-CGD-CBD	6.87	123.25	111.23
12	bB	902	CLA	C2D-C1D-ND	6.87	116.93	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bB	919	CLA	O2D-CGD-CBD	6.87	123.23	111.23
12	cB	921	CLA	CMD-C2D-C1D	6.85	136.79	124.73
12	aB	921	CLA	CMD-C2D-C1D	6.85	136.79	124.73
12	bB	921	CLA	CMD-C2D-C1D	6.84	136.77	124.73
12	bA	819	CLA	CAA-C2A-C1A	-6.80	89.70	111.97
12	aB	935	CLA	CMD-C2D-C1D	6.79	136.69	124.73
12	cA	853	CLA	C2D-C1D-ND	6.79	116.85	110.13
12	cA	819	CLA	CAA-C2A-C1A	-6.79	89.72	111.97
12	aA	819	CLA	CAA-C2A-C1A	-6.79	89.72	111.97
12	aB	935	CLA	CHD-C4C-C3C	-6.78	114.89	124.77
12	bA	853	CLA	C2D-C1D-ND	6.77	116.83	110.13
12	aA	854	CLA	C2D-C1D-ND	6.77	116.83	110.13
12	cB	935	CLA	CMD-C2D-C1D	6.77	136.65	124.73
12	bB	935	CLA	CMD-C2D-C1D	6.76	136.63	124.73
12	aB	908	CLA	C1D-ND-C4D	-6.75	101.57	106.31
12	bB	935	CLA	CHD-C4C-C3C	-6.75	114.93	124.77
12	cB	935	CLA	CHD-C4C-C3C	-6.74	114.95	124.77
12	bA	833	CLA	CMD-C2D-C1D	6.73	136.58	124.73
12	cA	833	CLA	CMD-C2D-C1D	6.72	136.56	124.73
12	cB	908	CLA	C1D-ND-C4D	-6.71	101.61	106.31
12	aA	833	CLA	CMD-C2D-C1D	6.70	136.53	124.73
12	aA	811	CLA	CMD-C2D-C1D	6.70	136.52	124.73
12	bB	908	CLA	C1D-ND-C4D	-6.69	101.62	106.31
12	cA	811	CLA	CMD-C2D-C1D	6.68	136.49	124.73
12	aB	937	CLA	CMD-C2D-C1D	6.67	136.48	124.73
12	cB	937	CLA	CMD-C2D-C1D	6.67	136.47	124.73
12	bB	937	CLA	CMD-C2D-C1D	6.66	136.47	124.73
12	bA	811	CLA	CMD-C2D-C1D	6.66	136.46	124.73
12	aB	915	CLA	CMD-C2D-C1D	6.65	136.44	124.73
12	bA	808	CLA	CMD-C2D-C1D	6.65	136.43	124.73
12	bB	931	CLA	CMD-C2D-C1D	6.65	136.43	124.73
12	cB	915	CLA	CMD-C2D-C1D	6.64	136.42	124.73
12	bB	915	CLA	CMD-C2D-C1D	6.64	136.42	124.73
12	aA	826	CLA	C2D-C1D-ND	6.64	116.69	110.13
12	bA	826	CLA	C2D-C1D-ND	6.63	116.69	110.13
12	cA	808	CLA	CMD-C2D-C1D	6.63	136.41	124.73
12	bL	204	CLA	CMD-C2D-C1D	6.63	136.41	124.73
12	cA	826	CLA	C2D-C1D-ND	6.62	116.68	110.13
12	aA	808	CLA	CMD-C2D-C1D	6.62	136.39	124.73
12	aB	931	CLA	CMD-C2D-C1D	6.62	136.39	124.73
12	aL	204	CLA	CMD-C2D-C1D	6.61	136.38	124.73
12	cL	204	CLA	CMD-C2D-C1D	6.61	136.37	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cB	931	CLA	CMD-C2D-C1D	6.61	136.37	124.73
12	aB	932	CLA	CMD-C2D-C1D	6.61	136.37	124.73
12	bB	925	CLA	CMD-C2D-C1D	6.61	136.36	124.73
12	bB	932	CLA	CMD-C2D-C1D	6.60	136.35	124.73
12	aB	925	CLA	CMD-C2D-C1D	6.60	136.34	124.73
12	cB	932	CLA	CMD-C2D-C1D	6.59	136.33	124.73
12	bB	914	CLA	C2D-C1D-ND	6.59	116.64	110.13
12	cB	924	CLA	CMD-C2D-C1D	6.58	136.32	124.73
12	bL	202	CLA	CMD-C2D-C1D	6.58	136.32	124.73
12	bA	804	CLA	O2D-CGD-CBD	6.58	122.73	111.23
12	cB	925	CLA	CMD-C2D-C1D	6.57	136.30	124.73
12	bB	936	CLA	CMD-C2D-C1D	6.57	136.30	124.73
12	bB	915	CLA	CHD-C4C-C3C	-6.57	115.20	124.77
12	cB	901	CLA	CHD-C4C-C3C	-6.57	115.20	124.77
12	aL	202	CLA	CMD-C2D-C1D	6.56	136.29	124.73
12	cB	915	CLA	CHD-C4C-C3C	-6.56	115.21	124.77
12	cB	936	CLA	CMD-C2D-C1D	6.56	136.28	124.73
12	bB	949	CLA	CMD-C2D-C1D	6.56	136.28	124.73
12	bB	923	CLA	O2D-CGD-CBD	6.56	122.69	111.23
12	bB	924	CLA	CMD-C2D-C1D	6.55	136.27	124.73
12	cL	202	CLA	CMD-C2D-C1D	6.55	136.26	124.73
12	aB	923	CLA	O2D-CGD-CBD	6.55	122.68	111.23
12	aB	915	CLA	CHD-C4C-C3C	-6.55	115.22	124.77
12	aB	924	CLA	CMD-C2D-C1D	6.55	136.26	124.73
12	cB	923	CLA	O2D-CGD-CBD	6.55	122.67	111.23
12	aA	804	CLA	O2D-CGD-CBD	6.55	122.67	111.23
12	aB	901	CLA	CHD-C4C-C3C	-6.54	115.23	124.77
12	bB	914	CLA	CHD-C4C-C3C	-6.54	115.23	124.77
12	bB	901	CLA	CHD-C4C-C3C	-6.54	115.24	124.77
12	cA	804	CLA	O2D-CGD-CBD	6.54	122.66	111.23
12	cB	914	CLA	C2D-C1D-ND	6.53	116.59	110.13
12	bA	838	CLA	C2D-C1D-ND	6.53	116.59	110.13
12	cA	815	CLA	CMD-C2D-C1D	6.53	136.22	124.73
12	aB	936	CLA	CMD-C2D-C1D	6.53	136.22	124.73
12	aB	914	CLA	CHD-C4C-C3C	-6.53	115.26	124.77
12	cA	805	CLA	O2D-CGD-CBD	6.53	122.64	111.23
12	cB	914	CLA	CHD-C4C-C3C	-6.53	115.26	124.77
12	aA	838	CLA	C2D-C1D-ND	6.52	116.57	110.13
12	aB	939	CLA	C2D-C1D-ND	6.52	116.57	110.13
12	cB	949	CLA	CMD-C2D-C1D	6.51	136.19	124.73
12	bB	914	CLA	O2D-CGD-CBD	6.51	122.61	111.23
12	aB	949	CLA	CMD-C2D-C1D	6.51	136.19	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aB	914	CLA	C2D-C1D-ND	6.51	116.57	110.13
12	bA	806	CLA	CMD-C2D-C1D	6.51	136.18	124.73
12	aB	925	CLA	CHD-C4C-C3C	-6.50	115.29	124.77
12	aA	815	CLA	CMD-C2D-C1D	6.50	136.18	124.73
12	bA	805	CLA	O2D-CGD-CBD	6.50	122.60	111.23
12	bA	815	CLA	CMD-C2D-C1D	6.50	136.18	124.73
12	cA	806	CLA	CMD-C2D-C1D	6.50	136.18	124.73
12	aA	805	CLA	O2D-CGD-CBD	6.50	122.59	111.23
12	cB	914	CLA	O2D-CGD-CBD	6.50	122.59	111.23
12	aB	914	CLA	O2D-CGD-CBD	6.50	122.59	111.23
12	aB	934	CLA	CMD-C2D-C1D	6.50	136.17	124.73
12	bB	925	CLA	CHD-C4C-C3C	-6.49	115.30	124.77
12	aA	806	CLA	CMD-C2D-C1D	6.49	136.16	124.73
12	cB	925	CLA	CHD-C4C-C3C	-6.49	115.31	124.77
12	cA	838	CLA	C2D-C1D-ND	6.48	116.54	110.13
12	cB	934	CLA	CMD-C2D-C1D	6.48	136.14	124.73
12	bB	934	CLA	CMD-C2D-C1D	6.47	136.12	124.73
12	bB	939	CLA	C2D-C1D-ND	6.46	116.52	110.13
12	cB	922	CLA	CMD-C2D-C1D	6.46	136.11	124.73
12	aA	823	CLA	CMD-C2D-C1D	6.46	136.11	124.73
12	bA	810	CLA	C2D-C1D-ND	6.46	116.52	110.13
12	bB	922	CLA	CMD-C2D-C1D	6.46	136.10	124.73
12	bB	929	CLA	O2D-CGD-CBD	6.46	122.52	111.23
12	aA	810	CLA	C2D-C1D-ND	6.45	116.51	110.13
12	aB	929	CLA	O2D-CGD-CBD	6.45	122.51	111.23
12	cA	809	CLA	CMD-C2D-C1D	6.45	136.09	124.73
12	aA	837	CLA	CMD-C2D-C1D	6.45	136.09	124.73
12	cA	810	CLA	C2D-C1D-ND	6.45	116.51	110.13
12	cB	929	CLA	O2D-CGD-CBD	6.45	122.50	111.23
12	bA	809	CLA	CMD-C2D-C1D	6.44	136.08	124.73
12	bB	924	CLA	O2D-CGD-CBD	6.44	122.49	111.23
12	aB	922	CLA	CMD-C2D-C1D	6.44	136.07	124.73
12	aB	929	CLA	C2D-C1D-ND	6.44	116.50	110.13
12	cA	823	CLA	CMD-C2D-C1D	6.44	136.06	124.73
12	aB	924	CLA	O2D-CGD-CBD	6.44	122.48	111.23
12	aA	809	CLA	CMD-C2D-C1D	6.43	136.06	124.73
12	cB	924	CLA	O2D-CGD-CBD	6.43	122.48	111.23
12	cA	837	CLA	CMD-C2D-C1D	6.43	136.05	124.73
12	bB	929	CLA	C2D-C1D-ND	6.43	116.49	110.13
12	cB	939	CLA	C2D-C1D-ND	6.43	116.49	110.13
12	bA	823	CLA	CMD-C2D-C1D	6.42	136.03	124.73
12	bA	804	CLA	C2D-C1D-ND	6.41	116.47	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	837	CLA	CMD-C2D-C1D	6.40	136.00	124.73
12	cB	929	CLA	C2D-C1D-ND	6.39	116.45	110.13
12	bA	822	CLA	CMD-C2D-C1D	6.39	135.98	124.73
12	cA	804	CLA	C2D-C1D-ND	6.38	116.44	110.13
12	cA	822	CLA	CMD-C2D-C1D	6.38	135.96	124.73
12	cB	926	CLA	CHD-C4C-C3C	-6.37	115.48	124.77
12	aA	822	CLA	CMD-C2D-C1D	6.37	135.95	124.73
12	cA	839	CLA	C2D-C1D-ND	6.37	116.43	110.13
12	aA	804	CLA	C2D-C1D-ND	6.36	116.42	110.13
12	aB	920	CLA	CMD-C2D-C1D	6.36	135.93	124.73
12	aB	939	CLA	CMD-C2D-C1D	6.36	135.93	124.73
12	aB	906	CLA	C2D-C1D-ND	6.36	116.42	110.13
12	aB	925	CLA	C2D-C1D-ND	6.36	116.42	110.13
12	bB	926	CLA	CHD-C4C-C3C	-6.36	115.50	124.77
12	aA	830	CLA	O2D-CGD-CBD	6.36	122.34	111.23
12	aB	916	CLA	C2D-C1D-ND	6.35	116.42	110.13
12	cB	908	CLA	C2C-C1C-NC	6.35	116.66	109.98
12	bB	905	CLA	CMD-C2D-C1D	6.35	135.92	124.73
12	aA	839	CLA	C2D-C1D-ND	6.35	116.41	110.13
12	bB	920	CLA	CMD-C2D-C1D	6.35	135.91	124.73
12	bA	830	CLA	O2D-CGD-CBD	6.35	122.33	111.23
12	bB	916	CLA	C2D-C1D-ND	6.35	116.41	110.13
12	bB	939	CLA	CMD-C2D-C1D	6.35	135.91	124.73
12	cA	830	CLA	O2D-CGD-CBD	6.35	122.33	111.23
12	cB	920	CLA	CMD-C2D-C1D	6.35	135.91	124.73
12	bA	839	CLA	C2D-C1D-ND	6.35	116.41	110.13
12	bB	925	CLA	C2D-C1D-ND	6.35	116.41	110.13
12	cB	905	CLA	CMD-C2D-C1D	6.35	135.91	124.73
12	cA	821	CLA	CMD-C2D-C1D	6.34	135.90	124.73
12	bB	906	CLA	C2D-C1D-ND	6.34	116.40	110.13
12	cB	916	CLA	C2D-C1D-ND	6.33	116.39	110.13
12	cA	853	CLA	O2D-CGD-CBD	6.33	122.30	111.23
12	bA	805	CLA	C2D-C1D-ND	6.33	116.39	110.13
12	cB	906	CLA	C2D-C1D-ND	6.33	116.39	110.13
12	aA	821	CLA	CMD-C2D-C1D	6.33	135.87	124.73
12	aB	905	CLA	CMD-C2D-C1D	6.33	135.87	124.73
12	bA	821	CLA	CMD-C2D-C1D	6.33	135.87	124.73
12	cB	919	CLA	CMD-C2D-C1D	6.33	135.87	124.73
12	aB	926	CLA	CHD-C4C-C3C	-6.32	115.55	124.77
12	aB	915	CLA	C2D-C1D-ND	6.32	116.38	110.13
12	aA	854	CLA	O2D-CGD-CBD	6.32	122.28	111.23
12	aB	926	CLA	C2D-C1D-ND	6.31	116.37	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	841	CLA	C2D-C1D-ND	6.31	116.37	110.13
12	bB	926	CLA	C2D-C1D-ND	6.31	116.37	110.13
12	cB	939	CLA	CMD-C2D-C1D	6.31	135.84	124.73
12	bB	908	CLA	C2C-C1C-NC	6.31	116.61	109.98
12	aA	805	CLA	C2D-C1D-ND	6.31	116.37	110.13
12	aB	905	CLA	C2D-C1D-ND	6.31	116.37	110.13
12	aB	919	CLA	CMD-C2D-C1D	6.31	135.83	124.73
12	bA	838	CLA	CMD-C2D-C1D	6.30	135.83	124.73
12	cA	827	CLA	C2D-C1D-ND	6.30	116.36	110.13
12	aA	838	CLA	CMD-C2D-C1D	6.30	135.82	124.73
12	bB	905	CLA	C2D-C1D-ND	6.30	116.36	110.13
12	cA	838	CLA	CMD-C2D-C1D	6.30	135.81	124.73
12	bA	853	CLA	O2D-CGD-CBD	6.30	122.23	111.23
12	aA	841	CLA	C2D-C1D-ND	6.29	116.36	110.13
12	cB	925	CLA	C2D-C1D-ND	6.29	116.36	110.13
12	aB	908	CLA	C2C-C1C-NC	6.29	116.59	109.98
11	aA	801	CL0	CMA-C3A-C4A	-6.29	101.05	114.61
12	bB	919	CLA	CMD-C2D-C1D	6.29	135.81	124.73
11	bA	801	CL0	CMA-C3A-C4A	-6.29	101.06	114.61
12	bB	915	CLA	C2D-C1D-ND	6.29	116.35	110.13
12	aA	842	CLA	CMD-C2D-C1D	6.28	135.80	124.73
12	cB	915	CLA	C2D-C1D-ND	6.28	116.35	110.13
12	cB	923	CLA	CHD-C4C-C3C	-6.28	115.61	124.77
12	aA	827	CLA	C2D-C1D-ND	6.28	116.34	110.13
12	cA	805	CLA	C2D-C1D-ND	6.28	116.34	110.13
12	bA	842	CLA	CMD-C2D-C1D	6.28	135.78	124.73
11	cA	801	CL0	CMA-C3A-C4A	-6.27	101.09	114.61
12	cB	905	CLA	C2D-C1D-ND	6.27	116.33	110.13
12	cB	926	CLA	C2D-C1D-ND	6.27	116.33	110.13
12	cA	827	CLA	CHD-C4C-C3C	-6.27	115.64	124.77
12	bA	827	CLA	CHD-C4C-C3C	-6.27	115.64	124.77
12	cB	907	CLA	O2D-CGD-CBD	6.26	122.18	111.23
12	aB	907	CLA	O2D-CGD-CBD	6.26	122.18	111.23
12	cA	842	CLA	CMD-C2D-C1D	6.26	135.75	124.73
12	aA	809	CLA	C2D-C1D-ND	6.26	116.32	110.13
12	aA	827	CLA	CHD-C4C-C3C	-6.26	115.65	124.77
12	cB	929	CLA	CHD-C4C-C3C	-6.25	115.66	124.77
12	cA	841	CLA	C2D-C1D-ND	6.25	116.31	110.13
12	bA	802	CLA	CMD-C2D-C1D	6.24	135.72	124.73
12	bB	907	CLA	O2D-CGD-CBD	6.24	122.13	111.23
12	aB	923	CLA	CHD-C4C-C3C	-6.23	115.68	124.77
12	bA	809	CLA	C2D-C1D-ND	6.23	116.29	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bB	929	CLA	CHD-C4C-C3C	-6.23	115.70	124.77
12	bB	929	CLA	CMD-C2D-C1D	6.23	135.69	124.73
12	cA	802	CLA	CMD-C2D-C1D	6.22	135.68	124.73
12	aA	806	CLA	C2D-C1D-ND	6.22	116.28	110.13
12	bA	827	CLA	C2D-C1D-ND	6.22	116.28	110.13
12	cA	807	CLA	C2D-C1D-ND	6.22	116.28	110.13
12	cA	842	CLA	C2D-C1D-ND	6.22	116.28	110.13
12	bB	923	CLA	CHD-C4C-C3C	-6.22	115.71	124.77
12	aB	929	CLA	CHD-C4C-C3C	-6.22	115.71	124.77
12	cB	903	CLA	O2D-CGD-CBD	6.21	122.09	111.23
12	cA	809	CLA	C2D-C1D-ND	6.21	116.28	110.13
12	bA	842	CLA	C2D-C1D-ND	6.21	116.27	110.13
12	bB	903	CLA	O2D-CGD-CBD	6.21	122.08	111.23
12	bA	820	CLA	C2D-C1D-ND	6.20	116.27	110.13
12	aB	929	CLA	CMD-C2D-C1D	6.20	135.65	124.73
12	cA	806	CLA	C2D-C1D-ND	6.20	116.27	110.13
12	bB	912	CLA	CMD-C2D-C1D	6.20	135.65	124.73
12	aA	820	CLA	C2D-C1D-ND	6.20	116.26	110.13
12	aB	903	CLA	O2D-CGD-CBD	6.20	122.07	111.23
12	aB	912	CLA	CMD-C2D-C1D	6.20	135.65	124.73
12	cB	929	CLA	CMD-C2D-C1D	6.20	135.64	124.73
12	aA	842	CLA	C2D-C1D-ND	6.20	116.26	110.13
12	bA	806	CLA	C2D-C1D-ND	6.19	116.25	110.13
12	aA	802	CLA	CMD-C2D-C1D	6.19	135.63	124.73
11	aA	801	CL0	CBC-CAC-C3C	-6.19	104.01	112.87
12	bB	920	CLA	O2D-CGD-CBD	6.19	122.04	111.23
12	bB	905	CLA	CHD-C4C-C3C	-6.18	115.76	124.77
12	bL	204	CLA	C2D-C1D-ND	6.18	116.24	110.13
12	cL	204	CLA	C2D-C1D-ND	6.18	116.24	110.13
12	bB	937	CLA	C2D-C1D-ND	6.18	116.24	110.13
12	aB	937	CLA	C2D-C1D-ND	6.17	116.24	110.13
12	aA	828	CLA	CHD-C4C-C3C	-6.17	115.77	124.77
12	cB	907	CLA	CMD-C2D-C1D	6.17	135.60	124.73
12	aB	920	CLA	O2D-CGD-CBD	6.17	122.02	111.23
12	bB	907	CLA	CMD-C2D-C1D	6.17	135.60	124.73
12	aB	907	CLA	CMD-C2D-C1D	6.17	135.59	124.73
12	cB	912	CLA	CMD-C2D-C1D	6.17	135.59	124.73
12	bB	933	CLA	C2D-C1D-ND	6.17	116.23	110.13
12	aF	202	CLA	CMD-C2D-C1D	6.17	135.59	124.73
12	aA	831	CLA	O2D-CGD-CBD	6.17	122.01	111.23
12	aA	822	CLA	O2D-CGD-CBD	6.17	122.01	111.23
12	bA	807	CLA	C2D-C1D-ND	6.17	116.23	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aB	903	CLA	CMD-C2D-C1D	6.17	135.59	124.73
12	cB	920	CLA	O2D-CGD-CBD	6.17	122.01	111.23
12	cA	810	CLA	CAA-C2A-C3A	-6.17	96.34	113.00
12	bB	903	CLA	CMD-C2D-C1D	6.17	135.59	124.73
12	cB	916	CLA	CHD-C4C-C3C	-6.17	115.78	124.77
12	bF	202	CLA	CMD-C2D-C1D	6.16	135.58	124.73
12	cA	839	CLA	CHD-C4C-C3C	-6.16	115.79	124.77
12	cB	905	CLA	CHD-C4C-C3C	-6.16	115.79	124.77
12	bA	817	CLA	CMD-C2D-C1D	6.16	135.58	124.73
12	cB	903	CLA	CMD-C2D-C1D	6.16	135.58	124.73
12	bA	810	CLA	CAA-C2A-C3A	-6.16	96.35	113.00
12	bA	831	CLA	O2D-CGD-CBD	6.16	122.00	111.23
12	aA	810	CLA	CAA-C2A-C3A	-6.16	96.35	113.00
12	cA	817	CLA	CMD-C2D-C1D	6.16	135.57	124.73
12	cF	202	CLA	CMD-C2D-C1D	6.16	135.57	124.73
12	aL	204	CLA	C2D-C1D-ND	6.16	116.22	110.13
12	cB	937	CLA	C2D-C1D-ND	6.16	116.22	110.13
11	cA	801	CL0	CBC-CAC-C3C	-6.16	104.06	112.87
12	aA	817	CLA	CMD-C2D-C1D	6.16	135.57	124.73
11	bA	801	CL0	CBC-CAC-C3C	-6.15	104.06	112.87
12	cA	831	CLA	O2D-CGD-CBD	6.15	121.99	111.23
12	cA	817	CLA	CHD-C4C-C3C	-6.15	115.80	124.77
12	aA	812	CLA	CMD-C2D-C1D	6.15	135.56	124.73
12	cA	828	CLA	CHD-C4C-C3C	-6.15	115.80	124.77
12	aA	817	CLA	CHD-C4C-C3C	-6.15	115.81	124.77
12	cA	817	CLA	C2D-C1D-ND	6.15	116.21	110.13
12	bB	916	CLA	CHD-C4C-C3C	-6.15	115.81	124.77
12	aB	933	CLA	C2D-C1D-ND	6.15	116.21	110.13
12	cA	827	CLA	CMD-C2D-C1D	6.14	135.55	124.73
12	cA	822	CLA	O2D-CGD-CBD	6.14	121.97	111.23
12	bA	828	CLA	CHD-C4C-C3C	-6.14	115.82	124.77
12	aB	905	CLA	CHD-C4C-C3C	-6.14	115.82	124.77
12	aA	807	CLA	C2D-C1D-ND	6.14	116.20	110.13
12	aA	807	CLA	CHD-C4C-C3C	-6.14	115.83	124.77
12	aB	949	CLA	CHD-C4C-C3C	-6.13	115.83	124.77
12	cA	834	CLA	CMD-C2D-C1D	6.13	135.53	124.73
12	bL	202	CLA	O2D-CGD-CBD	6.13	121.95	111.23
12	aA	839	CLA	CHD-C4C-C3C	-6.13	115.83	124.77
12	aA	827	CLA	CMD-C2D-C1D	6.13	135.52	124.73
12	bA	839	CLA	CHD-C4C-C3C	-6.13	115.84	124.77
12	bB	939	CLA	CHD-C4C-C3C	-6.13	115.84	124.77
12	aA	841	CLA	CMD-C2D-C1D	6.13	135.52	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	820	CLA	C2D-C1D-ND	6.13	116.19	110.13
12	cA	812	CLA	CMD-C2D-C1D	6.13	135.52	124.73
12	bA	834	CLA	CMD-C2D-C1D	6.12	135.51	124.73
12	bA	812	CLA	CMD-C2D-C1D	6.12	135.51	124.73
12	bB	949	CLA	C2D-C1D-ND	6.12	116.19	110.13
12	bA	807	CLA	CHD-C4C-C3C	-6.12	115.85	124.77
12	cB	904	CLA	C2B-C1B-NB	6.12	116.67	110.33
12	aB	939	CLA	CHD-C4C-C3C	-6.12	115.85	124.77
12	bA	841	CLA	CMD-C2D-C1D	6.12	135.50	124.73
12	cL	202	CLA	O2D-CGD-CBD	6.12	121.92	111.23
12	aA	834	CLA	CMD-C2D-C1D	6.12	135.50	124.73
12	aB	916	CLA	CHD-C4C-C3C	-6.12	115.86	124.77
12	cA	841	CLA	CMD-C2D-C1D	6.11	135.50	124.73
12	cB	939	CLA	CHD-C4C-C3C	-6.11	115.86	124.77
12	aA	812	CLA	C2D-C1D-ND	6.11	116.18	110.13
12	bA	822	CLA	O2D-CGD-CBD	6.11	121.92	111.23
12	cA	842	CLA	CHD-C4C-C3C	-6.11	115.86	124.77
12	aB	904	CLA	C2B-C1B-NB	6.11	116.66	110.33
12	cB	933	CLA	C2D-C1D-ND	6.11	116.17	110.13
12	bA	817	CLA	CHD-C4C-C3C	-6.11	115.87	124.77
12	cA	807	CLA	CHD-C4C-C3C	-6.11	115.87	124.77
12	bB	913	CLA	O2D-CGD-CBD	6.10	121.90	111.23
12	cA	814	CLA	CMD-C2D-C1D	6.10	135.48	124.73
12	cB	949	CLA	CHD-C4C-C3C	-6.10	115.88	124.77
12	bB	904	CLA	C2B-C1B-NB	6.10	116.65	110.33
12	aL	202	CLA	O2D-CGD-CBD	6.10	121.89	111.23
12	cB	913	CLA	O2D-CGD-CBD	6.10	121.89	111.23
12	bA	827	CLA	CMD-C2D-C1D	6.10	135.47	124.73
12	bB	949	CLA	CHD-C4C-C3C	-6.10	115.89	124.77
12	aA	814	CLA	CMD-C2D-C1D	6.09	135.46	124.73
12	bA	814	CLA	CMD-C2D-C1D	6.09	135.45	124.73
12	aB	913	CLA	O2D-CGD-CBD	6.09	121.87	111.23
12	cA	812	CLA	C2D-C1D-ND	6.09	116.15	110.13
12	aA	842	CLA	CHD-C4C-C3C	-6.09	115.90	124.77
12	aA	823	CLA	CHD-C4C-C3C	-6.08	115.90	124.77
12	bA	825	CLA	CHD-C4C-C3C	-6.08	115.91	124.77
12	bB	917	CLA	CMD-C2D-C1D	6.08	135.43	124.73
12	cB	917	CLA	CMD-C2D-C1D	6.08	135.43	124.73
12	cA	832	CLA	CMD-C2D-C1D	6.07	135.42	124.73
12	cB	949	CLA	C2D-C1D-ND	6.07	116.14	110.13
12	cA	823	CLA	CHD-C4C-C3C	-6.07	115.92	124.77
12	cB	923	CLA	CMD-C2D-C1D	6.07	135.42	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	817	CLA	C2D-C1D-ND	6.07	116.13	110.13
12	bA	812	CLA	C2D-C1D-ND	6.07	116.13	110.13
12	aA	832	CLA	CMD-C2D-C1D	6.07	135.41	124.73
12	bA	842	CLA	CHD-C4C-C3C	-6.07	115.93	124.77
12	aB	923	CLA	CMD-C2D-C1D	6.06	135.40	124.73
12	aB	949	CLA	C2D-C1D-ND	6.06	116.12	110.13
12	bB	923	CLA	CMD-C2D-C1D	6.06	135.40	124.73
12	bA	828	CLA	C2D-C1D-ND	6.06	116.12	110.13
12	aA	825	CLA	CHD-C4C-C3C	-6.06	115.94	124.77
12	aA	817	CLA	C2D-C1D-ND	6.06	116.12	110.13
12	aA	827	CLA	O2D-CGD-CBD	6.06	121.82	111.23
12	aB	917	CLA	CMD-C2D-C1D	6.06	135.39	124.73
12	aA	828	CLA	C2D-C1D-ND	6.06	116.12	110.13
12	cB	901	CLA	C2D-C1D-ND	6.06	116.12	110.13
12	cL	202	CLA	C2D-C1D-ND	6.06	116.12	110.13
12	bA	823	CLA	CHD-C4C-C3C	-6.05	115.95	124.77
12	cA	828	CLA	C2D-C1D-ND	6.05	116.12	110.13
12	bA	832	CLA	CMD-C2D-C1D	6.05	135.38	124.73
12	bA	831	CLA	CHD-C4C-C3C	-6.05	115.95	124.77
12	cA	825	CLA	CHD-C4C-C3C	-6.05	115.95	124.77
12	aA	831	CLA	CHD-C4C-C3C	-6.05	115.96	124.77
12	cA	827	CLA	O2D-CGD-CBD	6.04	121.80	111.23
12	cB	901	CLA	CMD-C2D-C1D	6.04	135.37	124.73
12	aB	903	CLA	C2D-C1D-ND	6.04	116.10	110.13
12	cA	818	CLA	CHD-C4C-C3C	-6.04	115.97	124.77
12	aL	202	CLA	C2D-C1D-ND	6.04	116.10	110.13
12	bL	202	CLA	C2D-C1D-ND	6.04	116.10	110.13
12	cB	916	CLA	CMD-C2D-C1D	6.03	135.34	124.73
12	bB	928	CLA	O2D-CGD-CBD	6.03	121.77	111.23
12	aB	901	CLA	CMD-C2D-C1D	6.03	135.34	124.73
12	bB	901	CLA	CMD-C2D-C1D	6.03	135.34	124.73
12	aA	818	CLA	CHD-C4C-C3C	-6.03	115.99	124.77
12	cB	903	CLA	C2D-C1D-ND	6.02	116.09	110.13
12	bB	903	CLA	C2D-C1D-ND	6.02	116.08	110.13
12	bA	827	CLA	O2D-CGD-CBD	6.02	121.75	111.23
12	aB	932	CLA	C2D-C1D-ND	6.02	116.08	110.13
12	bB	901	CLA	C2D-C1D-ND	6.02	116.08	110.13
12	cA	819	CLA	CMD-C2D-C1D	6.01	135.32	124.73
12	aB	901	CLA	C2D-C1D-ND	6.01	116.08	110.13
12	cB	932	CLA	C2D-C1D-ND	6.01	116.08	110.13
12	bB	933	CLA	CHD-C4C-C3C	-6.01	116.01	124.77
12	cA	831	CLA	CHD-C4C-C3C	-6.01	116.01	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bB	916	CLA	CMD-C2D-C1D	6.01	135.31	124.73
12	aB	917	CLA	C2D-C1D-ND	6.00	116.07	110.13
12	cB	917	CLA	C2D-C1D-ND	6.00	116.07	110.13
12	aB	916	CLA	CMD-C2D-C1D	6.00	135.30	124.73
12	bA	819	CLA	CMD-C2D-C1D	6.00	135.30	124.73
12	cA	839	CLA	CMD-C2D-C1D	6.00	135.29	124.73
12	cA	840	CLA	CMD-C2D-C1D	6.00	135.29	124.73
12	aA	839	CLA	CMD-C2D-C1D	6.00	135.29	124.73
12	aA	840	CLA	CMD-C2D-C1D	6.00	135.29	124.73
12	bA	823	CLA	C2D-C1D-ND	6.00	116.06	110.13
12	bB	950	CLA	C2D-C1D-ND	6.00	116.06	110.13
12	cA	834	CLA	C2D-C1D-ND	5.99	116.06	110.13
12	aA	819	CLA	CMD-C2D-C1D	5.99	135.28	124.73
12	bA	840	CLA	CMD-C2D-C1D	5.99	135.28	124.73
12	aB	928	CLA	O2D-CGD-CBD	5.99	121.70	111.23
12	bA	818	CLA	CHD-C4C-C3C	-5.99	116.04	124.77
12	cB	928	CLA	O2D-CGD-CBD	5.99	121.70	111.23
12	cB	933	CLA	CHD-C4C-C3C	-5.99	116.04	124.77
12	cA	826	CLA	O2D-CGD-CBD	5.99	121.70	111.23
12	bA	816	CLA	C2D-C1D-ND	5.99	116.05	110.13
12	bB	903	CLA	CHD-C4C-C3C	-5.99	116.04	124.77
12	aB	933	CLA	CHD-C4C-C3C	-5.98	116.05	124.77
12	aA	837	CLA	C2D-C1D-ND	5.98	116.05	110.13
12	bA	839	CLA	CMD-C2D-C1D	5.98	135.26	124.73
12	cB	904	CLA	CMD-C2D-C1D	5.98	135.26	124.73
12	cA	837	CLA	C2D-C1D-ND	5.98	116.04	110.13
12	bA	817	CLA	O2D-CGD-CBD	5.98	121.68	111.23
12	bB	932	CLA	C2D-C1D-ND	5.98	116.04	110.13
12	bA	826	CLA	O2D-CGD-CBD	5.98	121.68	111.23
12	cB	903	CLA	CHD-C4C-C3C	-5.98	116.06	124.77
12	bB	904	CLA	C2D-C1D-ND	5.97	116.04	110.13
12	bA	834	CLA	C2D-C1D-ND	5.97	116.04	110.13
12	bB	904	CLA	CMD-C2D-C1D	5.97	135.24	124.73
12	aB	903	CLA	CHD-C4C-C3C	-5.97	116.07	124.77
12	aB	904	CLA	CMD-C2D-C1D	5.97	135.24	124.73
12	aA	823	CLA	C2D-C1D-ND	5.97	116.03	110.13
12	bB	917	CLA	C2D-C1D-ND	5.97	116.03	110.13
12	aA	817	CLA	O2D-CGD-CBD	5.97	121.66	111.23
12	aA	826	CLA	O2D-CGD-CBD	5.97	121.66	111.23
12	cA	816	CLA	C2D-C1D-ND	5.96	116.03	110.13
12	cA	823	CLA	C2D-C1D-ND	5.96	116.03	110.13
12	cA	817	CLA	O2D-CGD-CBD	5.96	121.65	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	834	CLA	C2D-C1D-ND	5.96	116.02	110.13
12	bB	922	CLA	CHD-C4C-C3C	-5.95	116.09	124.77
12	aA	816	CLA	C2D-C1D-ND	5.95	116.02	110.13
12	bA	825	CLA	C2D-C1D-ND	5.95	116.02	110.13
12	bA	837	CLA	C2D-C1D-ND	5.95	116.02	110.13
12	bB	920	CLA	CHD-C4C-C3C	-5.95	116.10	124.77
12	aA	824	CLA	CMD-C2D-C1D	5.94	135.20	124.73
12	bA	824	CLA	CMD-C2D-C1D	5.94	135.20	124.73
12	cB	922	CLA	CHD-C4C-C3C	-5.94	116.11	124.77
12	aB	904	CLA	C2D-C1D-ND	5.93	116.00	110.13
12	aB	920	CLA	CHD-C4C-C3C	-5.93	116.12	124.77
12	bB	936	CLA	C2D-C1D-ND	5.93	116.00	110.13
12	aB	950	CLA	C2D-C1D-ND	5.93	115.99	110.13
12	aB	922	CLA	CHD-C4C-C3C	-5.93	116.13	124.77
12	aB	910	CLA	CMD-C2D-C1D	5.93	135.16	124.73
12	aB	930	CLA	CMD-C2D-C1D	5.92	135.16	124.73
12	cA	824	CLA	CMD-C2D-C1D	5.92	135.15	124.73
12	aA	844	CLA	C2D-C1D-ND	5.92	115.98	110.13
12	aA	805	CLA	CHD-C4C-C3C	-5.92	116.14	124.77
12	bB	910	CLA	CMD-C2D-C1D	5.92	135.15	124.73
12	cB	930	CLA	CMD-C2D-C1D	5.92	135.15	124.73
12	bF	202	CLA	O2D-CGD-CBD	5.92	121.57	111.23
12	bA	802	CLA	C2D-C1D-ND	5.92	115.98	110.13
12	cA	802	CLA	C2D-C1D-ND	5.91	115.98	110.13
12	cB	911	CLA	CMD-C2D-C1D	5.91	135.14	124.73
12	bB	911	CLA	CMD-C2D-C1D	5.91	135.14	124.73
12	cB	920	CLA	CHD-C4C-C3C	-5.91	116.15	124.77
12	aF	202	CLA	O2D-CGD-CBD	5.91	121.56	111.23
12	cB	904	CLA	C2D-C1D-ND	5.91	115.97	110.13
12	cF	202	CLA	O2D-CGD-CBD	5.91	121.56	111.23
12	bB	930	CLA	CMD-C2D-C1D	5.91	135.13	124.73
12	aA	825	CLA	C2D-C1D-ND	5.91	115.97	110.13
12	aB	911	CLA	CMD-C2D-C1D	5.91	135.13	124.73
12	cB	910	CLA	CMD-C2D-C1D	5.91	135.13	124.73
12	cA	805	CLA	CHD-C4C-C3C	-5.90	116.17	124.77
12	cB	936	CLA	C2D-C1D-ND	5.90	115.97	110.13
12	cA	836	CLA	CMD-C2D-C1D	5.90	135.12	124.73
12	aA	836	CLA	CMD-C2D-C1D	5.89	135.11	124.73
12	bA	805	CLA	CHD-C4C-C3C	-5.89	116.18	124.77
12	cA	843	CLA	C2D-C1D-ND	5.89	115.96	110.13
12	aA	802	CLA	C2D-C1D-ND	5.89	115.95	110.13
12	cL	203	CLA	O2D-CGD-CBD	5.89	121.52	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	825	CLA	C2D-C1D-ND	5.89	115.95	110.13
12	aB	937	CLA	O2D-CGD-CBD	5.89	121.52	111.23
12	aA	843	CLA	C2D-C1D-ND	5.89	115.95	110.13
12	bA	836	CLA	CMD-C2D-C1D	5.88	135.09	124.73
12	cB	937	CLA	O2D-CGD-CBD	5.88	121.51	111.23
12	aA	825	CLA	CMD-C2D-C1D	5.88	135.08	124.73
12	aA	829	CLA	C2D-C1D-ND	5.88	115.94	110.13
12	cB	923	CLA	C2D-C1D-ND	5.88	115.94	110.13
12	aL	203	CLA	O2D-CGD-CBD	5.88	121.50	111.23
12	bA	825	CLA	CMD-C2D-C1D	5.87	135.07	124.73
12	bA	809	CLA	O2D-CGD-CBD	5.87	121.50	111.23
12	bA	820	CLA	O2D-CGD-CBD	5.87	121.50	111.23
12	bA	806	CLA	O2D-CGD-CBD	5.87	121.50	111.23
12	aA	809	CLA	O2D-CGD-CBD	5.87	121.49	111.23
12	aA	820	CLA	O2D-CGD-CBD	5.87	121.49	111.23
12	bL	203	CLA	O2D-CGD-CBD	5.87	121.48	111.23
12	cA	806	CLA	O2D-CGD-CBD	5.86	121.48	111.23
12	bB	930	CLA	C2D-C1D-ND	5.86	115.93	110.13
12	cB	930	CLA	C2D-C1D-ND	5.86	115.93	110.13
12	aA	806	CLA	O2D-CGD-CBD	5.86	121.47	111.23
12	bB	937	CLA	O2D-CGD-CBD	5.86	121.47	111.23
12	cA	825	CLA	CMD-C2D-C1D	5.85	135.04	124.73
12	cA	829	CLA	C2D-C1D-ND	5.85	115.92	110.13
12	aB	930	CLA	C2D-C1D-ND	5.85	115.92	110.13
12	cB	919	CLA	C2D-C1D-ND	5.84	115.91	110.13
12	cA	820	CLA	O2D-CGD-CBD	5.84	121.44	111.23
12	aB	923	CLA	C2D-C1D-ND	5.84	115.91	110.13
12	aB	936	CLA	C2D-C1D-ND	5.84	115.91	110.13
12	aB	913	CLA	C2D-C1D-ND	5.84	115.91	110.13
12	bA	829	CLA	C2D-C1D-ND	5.84	115.91	110.13
12	bB	923	CLA	C2D-C1D-ND	5.84	115.91	110.13
12	cA	809	CLA	O2D-CGD-CBD	5.84	121.44	111.23
12	bL	204	CLA	O2D-CGD-CBD	5.84	121.44	111.23
12	bB	912	CLA	C2D-C1D-ND	5.84	115.90	110.13
12	aB	921	CLA	C4A-NA-C1A	-5.84	104.02	106.68
12	bA	802	CLA	O2D-CGD-CBD	5.83	121.42	111.23
12	aL	204	CLA	O2D-CGD-CBD	5.83	121.42	111.23
12	cB	912	CLA	C2D-C1D-ND	5.82	115.89	110.13
12	bA	843	CLA	C2D-C1D-ND	5.82	115.89	110.13
12	aA	805	CLA	C2B-C1B-NB	5.82	116.36	110.33
12	bB	919	CLA	C2D-C1D-ND	5.82	115.88	110.13
12	cB	912	CLA	CHD-C4C-C3C	-5.82	116.29	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cB	935	CLA	O2D-CGD-CBD	5.82	121.40	111.23
12	aA	822	CLA	CHD-C4C-C3C	-5.81	116.30	124.77
12	cA	832	CLA	C2D-C1D-ND	5.81	115.88	110.13
12	bB	935	CLA	O2D-CGD-CBD	5.81	121.39	111.23
12	aA	826	CLA	CMD-C2D-C1D	5.81	134.96	124.73
12	cA	822	CLA	CHD-C4C-C3C	-5.81	116.30	124.77
12	aB	919	CLA	C2D-C1D-ND	5.81	115.88	110.13
12	bA	826	CLA	CMD-C2D-C1D	5.81	134.96	124.73
12	aA	802	CLA	O2D-CGD-CBD	5.81	121.38	111.23
12	aB	935	CLA	O2D-CGD-CBD	5.81	121.38	111.23
12	bA	853	CLA	CHD-C4C-C3C	-5.81	116.31	124.77
12	cA	826	CLA	CMD-C2D-C1D	5.80	134.95	124.73
12	aA	816	CLA	CHD-C4C-C3C	-5.80	116.31	124.77
12	bA	816	CLA	CHD-C4C-C3C	-5.80	116.31	124.77
12	aB	912	CLA	C2D-C1D-ND	5.80	115.87	110.13
12	aB	912	CLA	CHD-C4C-C3C	-5.80	116.31	124.77
12	bB	909	CLA	CMD-C2D-C1D	5.80	134.95	124.73
12	aA	804	CLA	CHD-C4C-C3C	-5.80	116.31	124.77
12	bA	822	CLA	CHD-C4C-C3C	-5.80	116.32	124.77
12	cA	802	CLA	O2D-CGD-CBD	5.80	121.36	111.23
12	aA	832	CLA	C2D-C1D-ND	5.80	115.86	110.13
12	aA	854	CLA	CHD-C4C-C3C	-5.79	116.33	124.77
12	bB	912	CLA	CHD-C4C-C3C	-5.79	116.33	124.77
12	cL	204	CLA	O2D-CGD-CBD	5.79	121.35	111.23
12	cB	909	CLA	CMD-C2D-C1D	5.79	134.92	124.73
12	aF	202	CLA	C2D-C1D-ND	5.79	115.85	110.13
12	cA	816	CLA	CHD-C4C-C3C	-5.79	116.33	124.77
12	bA	830	CLA	C2D-C1D-ND	5.79	115.85	110.13
12	bB	913	CLA	C2D-C1D-ND	5.79	115.85	110.13
12	cA	805	CLA	C2B-C1B-NB	5.78	116.33	110.33
12	cA	833	CLA	C2D-C1D-ND	5.78	115.85	110.13
12	bF	202	CLA	C2D-C1D-ND	5.78	115.85	110.13
12	cB	913	CLA	C2D-C1D-ND	5.78	115.85	110.13
12	cF	202	CLA	C2D-C1D-ND	5.78	115.85	110.13
12	cB	907	CLA	CHD-C4C-C3C	-5.78	116.34	124.77
12	bA	839	CLA	O2D-CGD-CBD	5.78	121.33	111.23
12	bB	918	CLA	CMD-C2D-C1D	5.78	134.91	124.73
12	aA	831	CLA	CMD-C2D-C1D	5.78	134.91	124.73
12	aB	909	CLA	CMD-C2D-C1D	5.78	134.91	124.73
12	bA	833	CLA	C2D-C1D-ND	5.78	115.84	110.13
12	cB	918	CLA	CMD-C2D-C1D	5.78	134.90	124.73
12	cA	853	CLA	CHD-C4C-C3C	-5.77	116.36	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	833	CLA	C2D-C1D-ND	5.77	115.84	110.13
12	bA	832	CLA	C2D-C1D-ND	5.77	115.84	110.13
12	cA	804	CLA	CHD-C4C-C3C	-5.77	116.36	124.77
12	cA	831	CLA	CMD-C2D-C1D	5.77	134.88	124.73
12	aA	830	CLA	C2D-C1D-ND	5.77	115.83	110.13
12	aB	918	CLA	CMD-C2D-C1D	5.76	134.88	124.73
12	aB	913	CLA	CHD-C4C-C3C	-5.76	116.37	124.77
12	aB	911	CLA	C2D-C1D-ND	5.76	115.83	110.13
12	cB	913	CLA	CHD-C4C-C3C	-5.76	116.37	124.77
12	bA	804	CLA	CHD-C4C-C3C	-5.76	116.37	124.77
12	bA	818	CLA	C2D-C1D-ND	5.76	115.83	110.13
12	aA	838	CLA	CHD-C4C-C3C	-5.76	116.38	124.77
12	bA	838	CLA	CHD-C4C-C3C	-5.76	116.38	124.77
12	cA	838	CLA	CHD-C4C-C3C	-5.76	116.38	124.77
12	bB	921	CLA	C4A-NA-C1A	-5.76	104.05	106.68
12	bA	831	CLA	CMD-C2D-C1D	5.76	134.86	124.73
12	cB	904	CLA	C3B-C2B-C1B	-5.75	100.39	107.17
12	aA	839	CLA	O2D-CGD-CBD	5.75	121.29	111.23
12	bA	805	CLA	C2B-C1B-NB	5.75	116.29	110.33
12	cB	906	CLA	CHD-C4C-C3C	-5.75	116.39	124.77
12	aB	949	CLA	CAA-C2A-C3A	-5.75	103.05	116.23
12	cB	909	CLA	C2D-C1D-ND	5.75	115.82	110.13
12	aA	818	CLA	C2D-C1D-ND	5.75	115.81	110.13
12	cB	911	CLA	C2D-C1D-ND	5.75	115.81	110.13
12	bB	907	CLA	CHD-C4C-C3C	-5.75	116.39	124.77
12	aB	904	CLA	C3B-C2B-C1B	-5.74	100.40	107.17
12	cA	839	CLA	O2D-CGD-CBD	5.74	121.27	111.23
12	bB	949	CLA	CAA-C2A-C3A	-5.74	103.06	116.23
12	bB	913	CLA	CHD-C4C-C3C	-5.74	116.40	124.77
12	bB	909	CLA	C2D-C1D-ND	5.74	115.80	110.13
12	bB	904	CLA	C3B-C2B-C1B	-5.74	100.41	107.17
12	bA	805	CLA	CMD-C2D-C1D	5.74	134.83	124.73
12	bB	906	CLA	CHD-C4C-C3C	-5.74	116.41	124.77
12	cA	818	CLA	C2D-C1D-ND	5.73	115.80	110.13
12	cA	809	CLA	CHD-C4C-C3C	-5.73	116.41	124.77
12	cA	830	CLA	C2D-C1D-ND	5.73	115.80	110.13
12	aB	949	CLA	O2D-CGD-CBD	5.73	121.25	111.23
12	aB	907	CLA	CHD-C4C-C3C	-5.73	116.42	124.77
12	cB	949	CLA	CAA-C2A-C3A	-5.73	103.09	116.23
12	cA	816	CLA	O2D-CGD-CBD	5.73	121.24	111.23
12	aA	816	CLA	O2D-CGD-CBD	5.73	121.24	111.23
12	bB	949	CLA	O2D-CGD-CBD	5.72	121.24	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bB	914	CLA	CMD-C2D-C1D	5.72	134.81	124.73
12	aA	805	CLA	CMD-C2D-C1D	5.72	134.81	124.73
12	cB	914	CLA	CMD-C2D-C1D	5.72	134.81	124.73
12	cB	936	CLA	O2D-CGD-CBD	5.72	121.23	111.23
12	aB	909	CLA	C2D-C1D-ND	5.72	115.79	110.13
12	cA	813	CLA	CHD-C4C-C3C	-5.72	116.43	124.77
12	aA	813	CLA	CHD-C4C-C3C	-5.72	116.43	124.77
12	cB	921	CLA	C4A-NA-C1A	-5.72	104.07	106.68
12	aA	810	CLA	C3B-C2B-C1B	-5.72	100.43	107.17
12	cB	913	CLA	CMD-C2D-C1D	5.72	134.80	124.73
12	bA	810	CLA	C3B-C2B-C1B	-5.72	100.43	107.17
12	cB	949	CLA	O2D-CGD-CBD	5.71	121.21	111.23
12	aA	835	CLA	CHD-C4C-C3C	-5.71	116.45	124.77
12	bA	835	CLA	CHD-C4C-C3C	-5.71	116.45	124.77
12	bA	816	CLA	O2D-CGD-CBD	5.71	121.21	111.23
12	bB	913	CLA	CMD-C2D-C1D	5.71	134.78	124.73
12	aB	913	CLA	CMD-C2D-C1D	5.71	134.78	124.73
12	bA	813	CLA	CHD-C4C-C3C	-5.71	116.45	124.77
12	aB	909	CLA	CHD-C4C-C3C	-5.70	116.46	124.77
12	aA	809	CLA	CHD-C4C-C3C	-5.70	116.46	124.77
12	aB	906	CLA	CHD-C4C-C3C	-5.70	116.46	124.77
12	cA	805	CLA	CMD-C2D-C1D	5.70	134.76	124.73
12	aB	936	CLA	O2D-CGD-CBD	5.70	121.19	111.23
12	aB	939	CLA	C2C-C1C-NC	5.70	115.96	109.98
12	bA	809	CLA	CHD-C4C-C3C	-5.69	116.47	124.77
12	bB	911	CLA	C2D-C1D-ND	5.69	115.76	110.13
12	aB	914	CLA	CMD-C2D-C1D	5.69	134.75	124.73
12	bB	939	CLA	C2C-C1C-NC	5.69	115.96	109.98
12	cA	810	CLA	CMD-C2D-C1D	5.69	134.75	124.73
12	cA	812	CLA	O2D-CGD-CBD	5.69	121.18	111.23
12	aA	812	CLA	O2D-CGD-CBD	5.68	121.17	111.23
12	cA	835	CLA	CHD-C4C-C3C	-5.68	116.49	124.77
12	cA	814	CLA	C2D-C1D-ND	5.68	115.75	110.13
12	aA	810	CLA	CHD-C4C-C3C	-5.68	116.50	124.77
12	bB	909	CLA	CHD-C4C-C3C	-5.68	116.50	124.77
12	bA	810	CLA	CMD-C2D-C1D	5.68	134.72	124.73
12	bA	812	CLA	O2D-CGD-CBD	5.68	121.15	111.23
12	cA	810	CLA	C3B-C2B-C1B	-5.67	100.48	107.17
12	cB	909	CLA	CHD-C4C-C3C	-5.67	116.50	124.77
12	aA	810	CLA	CMD-C2D-C1D	5.67	134.72	124.73
12	bA	836	CLA	C2D-C1D-ND	5.67	115.74	110.13
12	bA	840	CLA	C2D-C1D-ND	5.67	115.74	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bB	936	CLA	O2D-CGD-CBD	5.67	121.14	111.23
12	aA	840	CLA	C2D-C1D-ND	5.67	115.73	110.13
12	bA	806	CLA	C2B-C1B-NB	5.66	116.20	110.33
12	cA	840	CLA	C2D-C1D-ND	5.66	115.73	110.13
12	bA	810	CLA	CHD-C4C-C3C	-5.66	116.52	124.77
12	cA	806	CLA	C2B-C1B-NB	5.66	116.19	110.33
12	bA	820	CLA	CHD-C4C-C3C	-5.66	116.53	124.77
12	cA	814	CLA	CHD-C4C-C3C	-5.66	116.53	124.77
12	aA	814	CLA	CHD-C4C-C3C	-5.65	116.53	124.77
12	cB	939	CLA	C2C-C1C-NC	5.65	115.92	109.98
12	aA	814	CLA	C2D-C1D-ND	5.65	115.72	110.13
12	cB	924	CLA	C2D-C1D-ND	5.65	115.72	110.13
12	cA	821	CLA	CHD-C4C-C3C	-5.65	116.54	124.77
12	cA	836	CLA	C2D-C1D-ND	5.65	115.72	110.13
12	bA	819	CLA	CHD-C4C-C3C	-5.65	116.54	124.77
12	cA	820	CLA	CHD-C4C-C3C	-5.65	116.54	124.77
12	bA	814	CLA	C2D-C1D-ND	5.65	115.72	110.13
12	cB	926	CLA	O2D-CGD-CBD	5.65	121.10	111.23
12	aA	806	CLA	C2B-C1B-NB	5.65	116.18	110.33
12	bB	926	CLA	O2D-CGD-CBD	5.65	121.10	111.23
12	aA	819	CLA	CHD-C4C-C3C	-5.65	116.54	124.77
12	cA	810	CLA	CHD-C4C-C3C	-5.65	116.54	124.77
12	aA	821	CLA	CHD-C4C-C3C	-5.64	116.54	124.77
12	aA	820	CLA	CHD-C4C-C3C	-5.64	116.55	124.77
12	cA	819	CLA	CHD-C4C-C3C	-5.64	116.55	124.77
12	aB	938	CLA	CHD-C4C-C3C	-5.64	116.56	124.77
12	bB	938	CLA	CHD-C4C-C3C	-5.64	116.56	124.77
12	aA	836	CLA	C2D-C1D-ND	5.63	115.70	110.13
12	cB	931	CLA	O2D-CGD-CBD	5.63	121.08	111.23
12	bA	811	CLA	CHD-C4C-C3C	-5.63	116.56	124.77
12	bA	814	CLA	CHD-C4C-C3C	-5.63	116.56	124.77
12	bA	828	CLA	CMD-C2D-C1D	5.63	134.65	124.73
12	aA	824	CLA	C2D-C1D-ND	5.63	115.70	110.13
12	aA	828	CLA	CMD-C2D-C1D	5.63	134.64	124.73
12	bA	824	CLA	C2D-C1D-ND	5.63	115.70	110.13
12	cA	828	CLA	CMD-C2D-C1D	5.63	134.64	124.73
12	bA	821	CLA	CHD-C4C-C3C	-5.63	116.57	124.77
12	aB	919	CLA	CHD-C4C-C3C	-5.63	116.57	124.77
12	bB	931	CLA	O2D-CGD-CBD	5.63	121.06	111.23
12	cA	824	CLA	C2D-C1D-ND	5.62	115.69	110.13
12	cA	811	CLA	CHD-C4C-C3C	-5.62	116.58	124.77
12	aB	902	CLA	CAC-C3C-C4C	5.62	132.10	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aB	926	CLA	O2D-CGD-CBD	5.62	121.05	111.23
12	bB	919	CLA	CHD-C4C-C3C	-5.62	116.58	124.77
12	bB	902	CLA	CAC-C3C-C4C	5.62	132.10	124.79
12	aA	811	CLA	CHD-C4C-C3C	-5.62	116.58	124.77
12	cB	938	CLA	CHD-C4C-C3C	-5.62	116.59	124.77
12	aA	829	CLA	CHD-C4C-C3C	-5.61	116.59	124.77
12	aB	931	CLA	O2D-CGD-CBD	5.61	121.04	111.23
12	cA	829	CLA	CHD-C4C-C3C	-5.60	116.61	124.77
12	cA	835	CLA	C2D-C1D-ND	5.60	115.67	110.13
12	cB	932	CLA	CHD-C4C-C3C	-5.60	116.61	124.77
12	cB	902	CLA	CAC-C3C-C4C	5.60	132.07	124.79
12	aB	932	CLA	CHD-C4C-C3C	-5.60	116.61	124.77
12	bA	833	CLA	CHD-C4C-C3C	-5.60	116.61	124.77
12	bA	829	CLA	CHD-C4C-C3C	-5.60	116.61	124.77
12	cL	203	CLA	CHD-C4C-C3C	-5.60	116.61	124.77
12	aA	823	CLA	O2D-CGD-CBD	5.60	121.01	111.23
12	aA	834	CLA	C3B-C2B-C1B	-5.60	100.57	107.17
12	cB	930	CLA	CHD-C4C-C3C	-5.59	116.62	124.77
12	aA	833	CLA	CHD-C4C-C3C	-5.59	116.62	124.77
12	cB	919	CLA	CHD-C4C-C3C	-5.59	116.63	124.77
12	aB	904	CLA	CHD-C4C-C3C	-5.59	116.63	124.77
12	cA	813	CLA	C2D-C1D-ND	5.58	115.65	110.13
12	aB	924	CLA	C2D-C1D-ND	5.58	115.65	110.13
12	bL	203	CLA	CHD-C4C-C3C	-5.58	116.64	124.77
12	cA	834	CLA	C3B-C2B-C1B	-5.58	100.59	107.17
12	aA	813	CLA	C2D-C1D-ND	5.58	115.65	110.13
12	bB	930	CLA	CHD-C4C-C3C	-5.58	116.64	124.77
12	bB	932	CLA	CHD-C4C-C3C	-5.58	116.64	124.77
12	cB	904	CLA	CHD-C4C-C3C	-5.58	116.64	124.77
12	bA	835	CLA	C2D-C1D-ND	5.58	115.64	110.13
12	bB	924	CLA	C2D-C1D-ND	5.57	115.64	110.13
12	cA	823	CLA	O2D-CGD-CBD	5.57	120.97	111.23
12	aB	921	CLA	CHD-C4C-C3C	-5.57	116.65	124.77
12	bB	921	CLA	CHD-C4C-C3C	-5.57	116.65	124.77
12	bA	819	CLA	C2D-C1D-ND	5.57	115.64	110.13
12	bB	909	CLA	C2C-C1C-NC	5.57	115.83	109.98
12	aL	203	CLA	CHD-C4C-C3C	-5.57	116.66	124.77
12	cA	833	CLA	CHD-C4C-C3C	-5.57	116.66	124.77
12	aB	930	CLA	CHD-C4C-C3C	-5.57	116.66	124.77
12	bA	823	CLA	O2D-CGD-CBD	5.56	120.95	111.23
12	bB	911	CLA	CHD-C4C-C3C	-5.56	116.67	124.77
12	aB	911	CLA	CHD-C4C-C3C	-5.56	116.67	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cB	918	CLA	C2D-C1D-ND	5.55	115.62	110.13
12	bA	834	CLA	C3B-C2B-C1B	-5.55	100.62	107.17
12	bB	904	CLA	CHD-C4C-C3C	-5.55	116.68	124.77
12	cA	828	CLA	O2D-CGD-CBD	5.55	120.94	111.23
12	bB	918	CLA	C2D-C1D-ND	5.55	115.62	110.13
12	aB	918	CLA	C2D-C1D-ND	5.55	115.62	110.13
12	cA	819	CLA	C2D-C1D-ND	5.55	115.61	110.13
12	cA	824	CLA	C2C-C1C-NC	5.55	115.81	109.98
12	cA	841	CLA	CHD-C4C-C3C	-5.54	116.69	124.77
11	cA	801	CL0	CHA-C1A-C2A	-5.54	120.30	133.31
12	bA	813	CLA	C2D-C1D-ND	5.54	115.61	110.13
12	aA	835	CLA	C2D-C1D-ND	5.54	115.61	110.13
12	aB	931	CLA	CHD-C4C-C3C	-5.54	116.70	124.77
12	aB	930	CLA	C2B-C1B-NB	5.54	116.07	110.33
12	aA	819	CLA	C2D-C1D-ND	5.54	115.61	110.13
12	bA	828	CLA	O2D-CGD-CBD	5.53	120.91	111.23
12	aA	841	CLA	CHD-C4C-C3C	-5.53	116.70	124.77
12	aA	828	CLA	O2D-CGD-CBD	5.53	120.90	111.23
12	bB	927	CLA	CHD-C4C-C3C	-5.53	116.71	124.77
12	bA	820	CLA	CMD-C2D-C1D	5.53	134.47	124.73
12	bA	841	CLA	CHD-C4C-C3C	-5.53	116.71	124.77
12	aB	927	CLA	CHD-C4C-C3C	-5.53	116.71	124.77
12	aA	820	CLA	CMD-C2D-C1D	5.53	134.46	124.73
12	cB	921	CLA	CHD-C4C-C3C	-5.53	116.71	124.77
11	aA	801	CL0	CHA-C1A-C2A	-5.53	120.33	133.31
12	cA	821	CLA	C2D-C1D-ND	5.52	115.59	110.13
12	aB	936	CLA	CHD-C4C-C3C	-5.52	116.72	124.77
12	aA	824	CLA	C2C-C1C-NC	5.52	115.78	109.98
12	cA	825	CLA	O2D-CGD-CBD	5.52	120.88	111.23
12	cB	930	CLA	C2B-C1B-NB	5.52	116.05	110.33
12	bB	936	CLA	CHD-C4C-C3C	-5.52	116.72	124.77
12	aA	825	CLA	O2D-CGD-CBD	5.52	120.88	111.23
12	aA	838	CLA	O2D-CGD-CBD	5.52	120.88	111.23
12	bB	933	CLA	C2C-C1C-NC	5.52	115.78	109.98
12	bA	806	CLA	C3B-C2B-C1B	-5.52	100.67	107.17
12	cB	933	CLA	C2C-C1C-NC	5.52	115.78	109.98
12	bB	931	CLA	CHD-C4C-C3C	-5.52	116.73	124.77
12	cB	911	CLA	CHD-C4C-C3C	-5.52	116.73	124.77
12	cB	931	CLA	CHD-C4C-C3C	-5.51	116.73	124.77
12	bB	922	CLA	C2D-C1D-ND	5.51	115.58	110.13
12	cB	909	CLA	C2C-C1C-NC	5.51	115.77	109.98
12	cA	838	CLA	O2D-CGD-CBD	5.51	120.87	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	bA	801	CL0	CHA-C1A-C2A	-5.51	120.36	133.31
12	cB	927	CLA	CHD-C4C-C3C	-5.51	116.74	124.77
12	cA	820	CLA	CMD-C2D-C1D	5.51	134.43	124.73
12	bA	838	CLA	O2D-CGD-CBD	5.51	120.86	111.23
12	bA	825	CLA	O2D-CGD-CBD	5.51	120.86	111.23
12	cB	936	CLA	CHD-C4C-C3C	-5.51	116.74	124.77
12	aA	837	CLA	O2D-CGD-CBD	5.50	120.85	111.23
12	cA	837	CLA	O2D-CGD-CBD	5.50	120.85	111.23
12	cA	827	CLA	C3B-C2B-C1B	-5.50	100.69	107.17
12	bA	824	CLA	C2C-C1C-NC	5.50	115.75	109.98
12	aB	909	CLA	C2C-C1C-NC	5.49	115.75	109.98
12	bA	837	CLA	O2D-CGD-CBD	5.49	120.83	111.23
12	aA	821	CLA	C2D-C1D-ND	5.49	115.56	110.13
12	cA	826	CLA	CHD-C4C-C3C	-5.49	116.77	124.77
12	bA	821	CLA	C2D-C1D-ND	5.49	115.56	110.13
12	bB	930	CLA	C2B-C1B-NB	5.49	116.02	110.33
12	aB	933	CLA	C2C-C1C-NC	5.49	115.75	109.98
12	cA	806	CLA	C3B-C2B-C1B	-5.49	100.70	107.17
12	cB	922	CLA	C2D-C1D-ND	5.48	115.55	110.13
12	cA	802	CLA	CHD-C4C-C3C	-5.48	116.78	124.77
12	aA	806	CLA	C3B-C2B-C1B	-5.48	100.71	107.17
12	aB	922	CLA	C2D-C1D-ND	5.48	115.55	110.13
12	aA	805	CLA	C3B-C2B-C1B	-5.47	100.72	107.17
12	cB	917	CLA	CHD-C4C-C3C	-5.47	116.79	124.77
12	bA	827	CLA	C3B-C2B-C1B	-5.47	100.72	107.17
12	bA	802	CLA	CHD-C4C-C3C	-5.46	116.81	124.77
12	aA	826	CLA	CHD-C4C-C3C	-5.46	116.81	124.77
12	aB	917	CLA	CHD-C4C-C3C	-5.46	116.81	124.77
12	aA	827	CLA	C3B-C2B-C1B	-5.46	100.73	107.17
12	bA	826	CLA	CHD-C4C-C3C	-5.46	116.81	124.77
12	aA	836	CLA	C2C-C1C-NC	5.46	115.72	109.98
12	cA	808	CLA	C2D-C1D-ND	5.46	115.53	110.13
12	bB	917	CLA	CHD-C4C-C3C	-5.46	116.82	124.77
12	cA	836	CLA	C2C-C1C-NC	5.45	115.71	109.98
12	bA	836	CLA	C2C-C1C-NC	5.45	115.70	109.98
12	aA	802	CLA	CHD-C4C-C3C	-5.44	116.84	124.77
12	bL	204	CLA	CHD-C4C-C3C	-5.44	116.84	124.77
12	cB	931	CLA	C3D-C2D-C1D	-5.44	98.41	105.83
12	cB	904	CLA	O2D-CGD-CBD	5.44	120.73	111.23
12	aA	808	CLA	C2D-C1D-ND	5.43	115.50	110.13
12	bB	910	CLA	CHD-C4C-C3C	-5.43	116.85	124.77
12	aB	931	CLA	C3D-C2D-C1D	-5.43	98.42	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	805	CLA	C3B-C2B-C1B	-5.43	100.77	107.17
12	aA	807	CLA	C4A-NA-C1A	-5.43	104.20	106.68
12	aB	910	CLA	CHD-C4C-C3C	-5.43	116.85	124.77
12	aB	904	CLA	O2D-CGD-CBD	5.43	120.72	111.23
12	aB	928	CLA	C2C-C1C-NC	5.42	115.68	109.98
12	bB	928	CLA	C2C-C1C-NC	5.42	115.68	109.98
12	cA	815	CLA	C2D-C1D-ND	5.42	115.49	110.13
12	cB	910	CLA	CHD-C4C-C3C	-5.42	116.87	124.77
12	bA	805	CLA	C3B-C2B-C1B	-5.42	100.78	107.17
12	bB	904	CLA	O2D-CGD-CBD	5.42	120.70	111.23
12	aB	925	CLA	C3D-C2D-C1D	-5.42	98.44	105.83
12	cB	925	CLA	C3D-C2D-C1D	-5.42	98.44	105.83
12	aA	815	CLA	C2B-C1B-NB	5.42	115.94	110.33
12	bA	832	CLA	CHD-C4C-C3C	-5.42	116.88	124.77
12	bB	925	CLA	C3D-C2D-C1D	-5.42	98.44	105.83
12	bA	808	CLA	C2D-C1D-ND	5.41	115.48	110.13
12	bA	815	CLA	C2D-C1D-ND	5.41	115.48	110.13
12	aL	204	CLA	CHD-C4C-C3C	-5.41	116.89	124.77
12	aA	832	CLA	CHD-C4C-C3C	-5.41	116.89	124.77
12	bB	931	CLA	C3D-C2D-C1D	-5.41	98.45	105.83
12	bA	807	CLA	C4A-NA-C1A	-5.40	104.21	106.68
12	cA	832	CLA	CHD-C4C-C3C	-5.40	116.90	124.77
12	aA	815	CLA	CHD-C4C-C3C	-5.40	116.90	124.77
12	cA	811	CLA	C2D-C1D-ND	5.40	115.47	110.13
12	aA	829	CLA	C3B-C2B-C1B	-5.40	100.81	107.17
12	aB	935	CLA	C2D-C1D-ND	5.39	115.47	110.13
12	cL	204	CLA	CHD-C4C-C3C	-5.39	116.91	124.77
12	cB	928	CLA	C2C-C1C-NC	5.39	115.65	109.98
12	cA	829	CLA	C3B-C2B-C1B	-5.39	100.81	107.17
12	bA	815	CLA	C2B-C1B-NB	5.39	115.92	110.33
12	cA	815	CLA	CHD-C4C-C3C	-5.39	116.92	124.77
12	aA	829	CLA	CMD-C2D-C1D	5.39	134.21	124.73
12	bA	829	CLA	CMD-C2D-C1D	5.38	134.21	124.73
12	aA	815	CLA	C2D-C1D-ND	5.38	115.45	110.13
12	bA	829	CLA	C3B-C2B-C1B	-5.38	100.83	107.17
12	aB	929	CLA	C3B-C2B-C1B	-5.38	100.83	107.17
12	bB	907	CLA	C2D-C1D-ND	5.37	115.44	110.13
12	bA	815	CLA	CHD-C4C-C3C	-5.37	116.94	124.77
12	cA	829	CLA	CMD-C2D-C1D	5.37	134.19	124.73
12	aB	910	CLA	C2D-C1D-ND	5.37	115.44	110.13
12	bA	808	CLA	CHD-C4C-C3C	-5.37	116.94	124.77
12	cB	937	CLA	C3B-C2B-C1B	-5.37	100.84	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bB	910	CLA	C2D-C1D-ND	5.36	115.43	110.13
12	aA	811	CLA	C2D-C1D-ND	5.36	115.43	110.13
12	aB	930	CLA	C3B-C2B-C1B	-5.36	100.85	107.17
12	cB	907	CLA	C2D-C1D-ND	5.36	115.43	110.13
12	bA	811	CLA	C2D-C1D-ND	5.36	115.43	110.13
12	bB	937	CLA	C3B-C2B-C1B	-5.36	100.85	107.17
12	aB	917	CLA	C2C-C1C-NC	5.36	115.61	109.98
12	cA	807	CLA	C3D-C2D-C1D	-5.36	98.52	105.83
12	cB	930	CLA	C3B-C2B-C1B	-5.35	100.86	107.17
11	aA	801	CL0	C4D-ND-C1D	-5.35	101.16	105.22
12	bB	930	CLA	C3B-C2B-C1B	-5.35	100.86	107.17
12	cB	910	CLA	C2D-C1D-ND	5.35	115.42	110.13
12	bB	917	CLA	C2C-C1C-NC	5.35	115.60	109.98
12	aB	937	CLA	C3B-C2B-C1B	-5.35	100.86	107.17
12	cA	818	CLA	C3B-C2B-C1B	-5.35	100.86	107.17
12	bA	818	CLA	C3B-C2B-C1B	-5.35	100.87	107.17
12	aA	808	CLA	CHD-C4C-C3C	-5.35	116.98	124.77
12	bB	929	CLA	C3B-C2B-C1B	-5.35	100.87	107.17
12	cB	906	CLA	CMD-C2D-C1D	5.34	134.14	124.73
12	aB	906	CLA	CMD-C2D-C1D	5.34	134.14	124.73
12	cA	807	CLA	C4A-NA-C1A	-5.34	104.24	106.68
12	aB	907	CLA	C2D-C1D-ND	5.34	115.41	110.13
12	cB	935	CLA	C2D-C1D-ND	5.34	115.41	110.13
12	bA	826	CLA	C3B-C2B-C1B	-5.34	100.88	107.17
12	bB	906	CLA	CMD-C2D-C1D	5.34	134.13	124.73
12	aA	826	CLA	C3B-C2B-C1B	-5.34	100.88	107.17
12	cA	815	CLA	C2B-C1B-NB	5.34	115.86	110.33
12	bA	813	CLA	C3B-C2B-C1B	-5.34	100.88	107.17
12	cB	929	CLA	C3B-C2B-C1B	-5.34	100.88	107.17
12	aA	818	CLA	C3B-C2B-C1B	-5.34	100.88	107.17
12	cB	917	CLA	C2C-C1C-NC	5.33	115.58	109.98
12	cA	808	CLA	CHD-C4C-C3C	-5.33	117.00	124.77
12	bA	825	CLA	C2B-C1B-NB	5.33	115.85	110.33
12	cB	907	CLA	C2C-C1C-NC	5.33	115.58	109.98
12	cA	803	CLA	C2B-C1B-NB	5.33	115.85	110.33
12	bA	803	CLA	C2B-C1B-NB	5.32	115.85	110.33
12	bB	935	CLA	C2D-C1D-ND	5.32	115.39	110.13
12	aA	807	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
12	cA	813	CLA	C3B-C2B-C1B	-5.32	100.90	107.17
12	cA	813	CLA	C2B-C1B-NB	5.32	115.84	110.33
12	cA	826	CLA	C3B-C2B-C1B	-5.32	100.90	107.17
12	cA	839	CLA	C2C-C1C-NC	5.31	115.56	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	813	CLA	C2B-C1B-NB	5.31	115.84	110.33
12	bA	843	CLA	C2C-C1C-NC	5.31	115.56	109.98
12	aB	907	CLA	C2C-C1C-NC	5.31	115.56	109.98
12	bB	907	CLA	C2C-C1C-NC	5.31	115.56	109.98
12	aA	803	CLA	C2B-C1B-NB	5.31	115.83	110.33
12	bA	807	CLA	C3D-C2D-C1D	-5.31	98.59	105.83
11	bA	801	CL0	C4D-ND-C1D	-5.31	101.19	105.22
12	aA	839	CLA	C2C-C1C-NC	5.31	115.56	109.98
12	aB	911	CLA	O2D-CGD-CBD	5.31	120.50	111.23
12	aA	813	CLA	C3B-C2B-C1B	-5.30	100.92	107.17
12	aB	930	CLA	O2D-CGD-CBD	5.30	120.50	111.23
12	aA	828	CLA	C2B-C1B-NB	5.30	115.82	110.33
12	bA	828	CLA	C2B-C1B-NB	5.30	115.82	110.33
11	cA	801	CL0	C4D-ND-C1D	-5.30	101.20	105.22
12	cL	202	CLA	CHD-C4C-C3C	-5.30	117.05	124.77
12	aL	202	CLA	CHD-C4C-C3C	-5.30	117.05	124.77
12	bA	828	CLA	C3B-C2B-C1B	-5.30	100.93	107.17
12	aA	813	CLA	C2B-C1B-NB	5.29	115.82	110.33
12	bB	930	CLA	O2D-CGD-CBD	5.29	120.49	111.23
12	bB	911	CLA	O2D-CGD-CBD	5.29	120.48	111.23
12	bA	837	CLA	CHD-C4C-C3C	-5.29	117.06	124.77
12	aA	837	CLA	CHD-C4C-C3C	-5.28	117.07	124.77
12	cA	843	CLA	C2C-C1C-NC	5.28	115.53	109.98
12	cB	911	CLA	O2D-CGD-CBD	5.28	120.46	111.23
12	aA	825	CLA	C2B-C1B-NB	5.28	115.80	110.33
12	cA	837	CLA	CHD-C4C-C3C	-5.28	117.08	124.77
12	aA	822	CLA	C3D-C2D-C1D	-5.27	98.63	105.83
12	cB	921	CLA	C2D-C1D-ND	5.27	115.34	110.13
12	cB	930	CLA	O2D-CGD-CBD	5.27	120.45	111.23
12	cA	828	CLA	C2B-C1B-NB	5.27	115.79	110.33
12	cA	827	CLA	C3D-C2D-C1D	-5.27	98.64	105.83
12	bL	202	CLA	CHD-C4C-C3C	-5.27	117.09	124.77
12	aA	843	CLA	C2C-C1C-NC	5.27	115.52	109.98
12	cA	825	CLA	C2B-C1B-NB	5.27	115.79	110.33
12	aA	828	CLA	C3B-C2B-C1B	-5.27	100.96	107.17
12	cB	934	CLA	CHD-C4C-C3C	-5.26	117.11	124.77
12	aA	854	CLA	C3B-C2B-C1B	-5.26	100.97	107.17
12	aA	834	CLA	C2B-C1B-NB	5.26	115.78	110.33
12	aA	819	CLA	O2D-CGD-CBD	5.26	120.42	111.23
12	bA	853	CLA	C3B-C2B-C1B	-5.26	100.97	107.17
12	bB	934	CLA	CHD-C4C-C3C	-5.26	117.11	124.77
12	aA	827	CLA	C3D-C2D-C1D	-5.25	98.66	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	839	CLA	C2C-C1C-NC	5.25	115.50	109.98
12	cA	828	CLA	C3B-C2B-C1B	-5.25	100.98	107.17
12	cA	822	CLA	C3D-C2D-C1D	-5.25	98.66	105.83
12	aB	934	CLA	CHD-C4C-C3C	-5.25	117.12	124.77
12	aA	822	CLA	C2B-C1B-NB	5.25	115.77	110.33
12	bA	827	CLA	C3D-C2D-C1D	-5.25	98.67	105.83
12	cB	937	CLA	C2B-C1B-NB	5.25	115.77	110.33
12	bA	822	CLA	C3D-C2D-C1D	-5.25	98.67	105.83
12	aB	934	CLA	C2D-C1D-ND	5.25	115.32	110.13
12	bA	815	CLA	C3B-C2B-C1B	-5.24	100.99	107.17
12	cF	202	CLA	CHD-C4C-C3C	-5.24	117.13	124.77
12	bB	937	CLA	C2B-C1B-NB	5.24	115.76	110.33
12	cA	853	CLA	C3B-C2B-C1B	-5.24	100.99	107.17
12	cA	819	CLA	O2D-CGD-CBD	5.24	120.39	111.23
12	bA	843	CLA	CHD-C4C-C3C	-5.24	117.14	124.77
12	aF	202	CLA	CHD-C4C-C3C	-5.24	117.14	124.77
12	aA	815	CLA	C3B-C2B-C1B	-5.24	101.00	107.17
12	bF	202	CLA	CHD-C4C-C3C	-5.24	117.14	124.77
12	aA	843	CLA	CHD-C4C-C3C	-5.23	117.14	124.77
12	bB	921	CLA	C2D-C1D-ND	5.23	115.31	110.13
12	cA	843	CLA	CHD-C4C-C3C	-5.23	117.15	124.77
12	cA	834	CLA	C2B-C1B-NB	5.23	115.75	110.33
12	cA	829	CLA	C2B-C1B-NB	5.23	115.75	110.33
12	bA	819	CLA	O2D-CGD-CBD	5.23	120.37	111.23
12	cA	824	CLA	C2B-C1B-NB	5.23	115.75	110.33
12	aB	921	CLA	C2D-C1D-ND	5.22	115.30	110.13
12	bB	927	CLA	C2C-C1C-NC	5.22	115.47	109.98
12	aA	834	CLA	C2C-C1C-NC	5.22	115.46	109.98
12	cA	811	CLA	O2D-CGD-CBD	5.21	120.34	111.23
12	cA	834	CLA	C2C-C1C-NC	5.21	115.45	109.98
12	aA	824	CLA	C2B-C1B-NB	5.21	115.73	110.33
12	bA	834	CLA	C2C-C1C-NC	5.21	115.45	109.98
12	bA	829	CLA	C2B-C1B-NB	5.21	115.73	110.33
12	cA	817	CLA	C3B-C2B-C1B	-5.21	101.03	107.17
12	bA	822	CLA	C2B-C1B-NB	5.20	115.72	110.33
12	aA	829	CLA	C2B-C1B-NB	5.20	115.72	110.33
12	bB	934	CLA	C2D-C1D-ND	5.20	115.27	110.13
12	bA	811	CLA	O2D-CGD-CBD	5.20	120.31	111.23
12	cB	932	CLA	O2D-CGD-CBD	5.20	120.31	111.23
12	aB	927	CLA	C2C-C1C-NC	5.19	115.44	109.98
12	aA	831	CLA	C2D-C1D-ND	5.19	115.27	110.13
12	bA	853	CLA	C2B-C1B-NB	5.19	115.71	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	815	CLA	C3B-C2B-C1B	-5.19	101.05	107.17
12	bB	905	CLA	C3B-C2B-C1B	-5.19	101.05	107.17
12	cB	924	CLA	CHD-C4C-C3C	-5.19	117.21	124.77
12	aB	920	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
12	aA	812	CLA	C2C-C1C-NC	5.19	115.43	109.98
12	cA	816	CLA	CMD-C2D-C1D	5.19	133.86	124.73
12	cB	924	CLA	C3B-C2B-C1B	-5.19	101.06	107.17
12	cA	822	CLA	C2B-C1B-NB	5.19	115.70	110.33
12	aB	932	CLA	O2D-CGD-CBD	5.19	120.30	111.23
12	bA	834	CLA	C2B-C1B-NB	5.19	115.70	110.33
12	bB	915	CLA	C2C-C1C-NC	5.19	115.43	109.98
12	aA	842	CLA	C2C-C1C-NC	5.18	115.43	109.98
12	aB	937	CLA	C2B-C1B-NB	5.18	115.70	110.33
12	aA	817	CLA	C3B-C2B-C1B	-5.18	101.06	107.17
12	bA	824	CLA	C2B-C1B-NB	5.18	115.70	110.33
12	aA	811	CLA	O2D-CGD-CBD	5.18	120.29	111.23
12	aA	816	CLA	CMD-C2D-C1D	5.18	133.85	124.73
12	cB	920	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
12	bB	924	CLA	CHD-C4C-C3C	-5.18	117.22	124.77
12	aB	924	CLA	C3B-C2B-C1B	-5.18	101.06	107.17
12	bA	817	CLA	C3B-C2B-C1B	-5.18	101.06	107.17
12	bB	932	CLA	O2D-CGD-CBD	5.18	120.29	111.23
12	bA	832	CLA	O2D-CGD-CBD	5.18	120.28	111.23
12	bB	920	CLA	C3D-C2D-C1D	-5.18	98.77	105.83
12	bA	842	CLA	C2C-C1C-NC	5.18	115.42	109.98
12	cA	831	CLA	C2D-C1D-ND	5.18	115.25	110.13
12	cA	832	CLA	O2D-CGD-CBD	5.18	120.28	111.23
12	cA	842	CLA	C2C-C1C-NC	5.18	115.42	109.98
12	aA	832	CLA	O2D-CGD-CBD	5.18	120.28	111.23
12	cA	809	CLA	C3B-C2B-C1B	-5.18	101.07	107.17
12	bA	816	CLA	CMD-C2D-C1D	5.18	133.84	124.73
12	cA	832	CLA	C3B-C2B-C1B	-5.18	101.07	107.17
12	aA	832	CLA	C3B-C2B-C1B	-5.17	101.07	107.17
12	bA	809	CLA	C3B-C2B-C1B	-5.17	101.07	107.17
12	bA	831	CLA	C2D-C1D-ND	5.17	115.25	110.13
12	aB	924	CLA	CHD-C4C-C3C	-5.17	117.23	124.77
12	cB	927	CLA	C2C-C1C-NC	5.17	115.42	109.98
12	bB	933	CLA	O2D-CGD-CBD	5.17	120.27	111.23
12	bB	903	CLA	C3B-C2B-C1B	-5.17	101.07	107.17
12	cB	902	CLA	C3B-C2B-C1B	-5.17	101.08	107.17
12	cB	934	CLA	C2D-C1D-ND	5.17	115.24	110.13
12	bL	203	CLA	C2B-C1B-NB	5.17	115.69	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aL	203	CLA	C3B-C2B-C1B	-5.17	101.08	107.17
12	aB	933	CLA	O2D-CGD-CBD	5.16	120.26	111.23
12	bA	834	CLA	C3D-C2D-C1D	-5.16	98.78	105.83
12	aB	925	CLA	C2B-C1B-NB	5.16	115.68	110.33
12	cB	905	CLA	C3B-C2B-C1B	-5.16	101.08	107.17
12	bB	924	CLA	C3B-C2B-C1B	-5.16	101.08	107.17
12	aL	203	CLA	C2B-C1B-NB	5.16	115.68	110.33
12	cB	915	CLA	C2C-C1C-NC	5.16	115.40	109.98
12	aB	902	CLA	CMD-C2D-C1D	5.16	133.81	124.73
12	cB	902	CLA	CMD-C2D-C1D	5.16	133.81	124.73
12	cA	815	CLA	O2D-CGD-CBD	5.16	120.25	111.23
12	cL	203	CLA	C3B-C2B-C1B	-5.16	101.09	107.17
12	cL	203	CLA	C2B-C1B-NB	5.16	115.67	110.33
12	cB	933	CLA	O2D-CGD-CBD	5.16	120.24	111.23
12	bA	832	CLA	C3B-C2B-C1B	-5.15	101.09	107.17
12	bB	918	CLA	CHD-C4C-C3C	-5.15	117.26	124.77
12	cA	834	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
12	aB	905	CLA	C3B-C2B-C1B	-5.15	101.10	107.17
12	bA	815	CLA	O2D-CGD-CBD	5.15	120.24	111.23
12	cB	910	CLA	O2D-CGD-CBD	5.15	120.23	111.23
12	cB	919	CLA	C3B-C2B-C1B	-5.15	101.10	107.17
12	aA	854	CLA	C2B-C1B-NB	5.15	115.67	110.33
12	cA	822	CLA	C3B-C2B-C1B	-5.15	101.10	107.17
12	aA	834	CLA	C3D-C2D-C1D	-5.15	98.81	105.83
12	bB	906	CLA	C2B-C1B-NB	5.15	115.66	110.33
12	cB	918	CLA	CHD-C4C-C3C	-5.15	117.27	124.77
12	aB	931	CLA	C2B-C1B-NB	5.14	115.66	110.33
12	aA	815	CLA	O2D-CGD-CBD	5.14	120.22	111.23
12	aB	915	CLA	C2C-C1C-NC	5.14	115.39	109.98
12	aB	902	CLA	C3B-C2B-C1B	-5.14	101.11	107.17
12	cA	813	CLA	CMD-C2D-C1D	5.14	133.78	124.73
12	bA	812	CLA	C2C-C1C-NC	5.14	115.38	109.98
12	bB	938	CLA	C2D-C1D-ND	5.14	115.21	110.13
12	aB	919	CLA	C3B-C2B-C1B	-5.14	101.11	107.17
12	cB	937	CLA	CHD-C4C-C3C	-5.14	117.28	124.77
12	aA	822	CLA	C3B-C2B-C1B	-5.14	101.11	107.17
12	cB	903	CLA	C3B-C2B-C1B	-5.14	101.11	107.17
12	aB	918	CLA	CHD-C4C-C3C	-5.14	117.28	124.77
12	cA	812	CLA	C2C-C1C-NC	5.14	115.38	109.98
12	aB	903	CLA	C3B-C2B-C1B	-5.14	101.12	107.17
12	aB	938	CLA	C2D-C1D-ND	5.13	115.21	110.13
12	aB	924	CLA	C2B-C1B-NB	5.13	115.65	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	813	CLA	CMD-C2D-C1D	5.13	133.77	124.73
12	cB	906	CLA	C2B-C1B-NB	5.13	115.65	110.33
12	aB	921	CLA	C2B-C1B-NB	5.13	115.65	110.33
12	aA	809	CLA	C3B-C2B-C1B	-5.13	101.12	107.17
12	bA	822	CLA	C3B-C2B-C1B	-5.13	101.12	107.17
12	bB	902	CLA	C3B-C2B-C1B	-5.13	101.12	107.17
12	cB	938	CLA	C2D-C1D-ND	5.13	115.20	110.13
12	cA	853	CLA	C2B-C1B-NB	5.13	115.64	110.33
12	aB	901	CLA	C3B-C2B-C1B	-5.13	101.13	107.17
12	bL	203	CLA	C3B-C2B-C1B	-5.13	101.13	107.17
12	aB	910	CLA	O2D-CGD-CBD	5.13	120.19	111.23
12	bB	902	CLA	CMD-C2D-C1D	5.12	133.75	124.73
12	cB	924	CLA	C2B-C1B-NB	5.12	115.64	110.33
12	cB	925	CLA	C2B-C1B-NB	5.12	115.64	110.33
12	aB	935	CLA	C2B-C1B-NB	5.12	115.64	110.33
12	bB	937	CLA	CHD-C4C-C3C	-5.12	117.31	124.77
12	aA	816	CLA	C3B-C2B-C1B	-5.12	101.13	107.17
12	bB	921	CLA	C3B-C2B-C1B	-5.12	101.13	107.17
12	cA	816	CLA	C3B-C2B-C1B	-5.12	101.13	107.17
12	bB	931	CLA	C2B-C1B-NB	5.12	115.64	110.33
12	aA	844	CLA	O2D-CGD-CBD	5.12	120.18	111.23
12	bB	921	CLA	C2B-C1B-NB	5.12	115.63	110.33
12	aB	921	CLA	C2C-C1C-NC	5.12	115.36	109.98
12	bB	910	CLA	O2D-CGD-CBD	5.12	120.17	111.23
12	aB	937	CLA	CHD-C4C-C3C	-5.11	117.32	124.77
12	bB	935	CLA	C2B-C1B-NB	5.11	115.63	110.33
12	bB	925	CLA	C2B-C1B-NB	5.11	115.63	110.33
12	bA	808	CLA	C2C-C1C-NC	5.11	115.35	109.98
12	cB	901	CLA	C3B-C2B-C1B	-5.11	101.15	107.17
12	aA	816	CLA	C2B-C1B-NB	5.11	115.62	110.33
12	bB	935	CLA	C3B-C2B-C1B	-5.11	101.15	107.17
12	aB	905	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
12	aB	935	CLA	C3B-C2B-C1B	-5.11	101.15	107.17
12	bB	901	CLA	C3B-C2B-C1B	-5.11	101.15	107.17
12	bB	914	CLA	C3B-C2B-C1B	-5.11	101.15	107.17
12	aA	838	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
12	cA	808	CLA	C2C-C1C-NC	5.11	115.34	109.98
12	aA	808	CLA	C2C-C1C-NC	5.10	115.34	109.98
12	cB	905	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
12	bB	919	CLA	C3B-C2B-C1B	-5.10	101.16	107.17
12	bB	905	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
12	cA	837	CLA	C3D-C2D-C1D	-5.10	98.87	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	837	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
12	bA	813	CLA	CMD-C2D-C1D	5.10	133.70	124.73
12	bA	838	CLA	C3D-C2D-C1D	-5.10	98.88	105.83
12	bB	921	CLA	C2C-C1C-NC	5.10	115.33	109.98
12	cB	935	CLA	C3B-C2B-C1B	-5.10	101.16	107.17
12	aB	921	CLA	C3B-C2B-C1B	-5.10	101.16	107.17
12	bB	924	CLA	CAA-C2A-C3A	-5.09	99.23	113.00
12	aA	830	CLA	C2C-C1C-NC	5.09	115.33	109.98
12	aA	837	CLA	C3D-C2D-C1D	-5.09	98.88	105.83
12	cA	826	CLA	C3D-C2D-C1D	-5.09	98.88	105.83
12	cB	910	CLA	C2C-C1C-NC	5.09	115.33	109.98
12	cB	935	CLA	C2B-C1B-NB	5.09	115.61	110.33
12	cA	853	CLA	C3D-C2D-C1D	-5.09	98.88	105.83
12	cB	921	CLA	C2B-C1B-NB	5.09	115.61	110.33
12	cB	924	CLA	CAA-C2A-C3A	-5.09	99.24	113.00
12	bB	914	CLA	C2B-C1B-NB	5.09	115.61	110.33
12	cB	913	CLA	C3B-C2B-C1B	-5.09	101.17	107.17
12	cB	921	CLA	C3B-C2B-C1B	-5.09	101.17	107.17
12	aB	913	CLA	C3B-C2B-C1B	-5.09	101.17	107.17
12	cB	928	CLA	CHD-C4C-C3C	-5.09	117.35	124.77
12	bB	950	CLA	O2D-CGD-CBD	5.09	120.12	111.23
12	cA	830	CLA	C2C-C1C-NC	5.09	115.32	109.98
12	aA	826	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
12	aB	950	CLA	O2D-CGD-CBD	5.09	120.12	111.23
12	aB	924	CLA	CAA-C2A-C3A	-5.09	99.26	113.00
12	bA	830	CLA	C2C-C1C-NC	5.08	115.32	109.98
12	cB	931	CLA	C2B-C1B-NB	5.08	115.60	110.33
12	cB	914	CLA	C3B-C2B-C1B	-5.08	101.18	107.17
12	aA	844	CLA	C2C-C1C-NC	5.08	115.32	109.98
12	bA	826	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
12	cB	914	CLA	C2B-C1B-NB	5.08	115.60	110.33
12	bB	910	CLA	C2C-C1C-NC	5.08	115.32	109.98
12	cA	827	CLA	C2B-C1B-NB	5.08	115.59	110.33
12	aB	950	CLA	C2C-C1C-NC	5.08	115.32	109.98
12	cA	838	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
12	bA	827	CLA	C2B-C1B-NB	5.08	115.59	110.33
12	bA	831	CLA	C3B-C2B-C1B	-5.08	101.18	107.17
12	cA	819	CLA	CAA-C2A-C3A	-5.08	99.28	113.00
12	bA	826	CLA	C2B-C1B-NB	5.08	115.59	110.33
12	bB	911	CLA	C2C-C1C-NC	5.08	115.31	109.98
12	aB	906	CLA	C2B-C1B-NB	5.08	115.59	110.33
12	aA	819	CLA	CAA-C2A-C3A	-5.08	99.28	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	826	CLA	C2B-C1B-NB	5.07	115.59	110.33
12	cB	921	CLA	C2C-C1C-NC	5.07	115.31	109.98
12	aB	922	CLA	C3B-C2B-C1B	-5.07	101.19	107.17
12	bB	913	CLA	C3B-C2B-C1B	-5.07	101.19	107.17
12	cB	902	CLA	C3D-C2D-C1D	-5.07	98.92	105.83
12	bB	924	CLA	C2B-C1B-NB	5.07	115.58	110.33
12	aA	831	CLA	C3B-C2B-C1B	-5.07	101.20	107.17
12	bB	950	CLA	CHD-C4C-C3C	-5.07	117.39	124.77
12	bA	816	CLA	C3B-C2B-C1B	-5.06	101.20	107.17
12	cA	817	CLA	C2B-C1B-NB	5.06	115.58	110.33
12	aA	803	CLA	CHD-C4C-C3C	-5.06	117.39	124.77
12	aB	914	CLA	C2B-C1B-NB	5.06	115.58	110.33
12	bA	809	CLA	C2B-C1B-NB	5.06	115.58	110.33
12	bA	819	CLA	CAA-C2A-C3A	-5.06	99.32	113.00
12	bA	817	CLA	C2B-C1B-NB	5.06	115.57	110.33
12	bA	853	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
12	cA	816	CLA	C2B-C1B-NB	5.06	115.57	110.33
12	cB	919	CLA	C2B-C1B-NB	5.06	115.57	110.33
12	bB	950	CLA	C2C-C1C-NC	5.06	115.29	109.98
12	aA	809	CLA	C2B-C1B-NB	5.05	115.57	110.33
12	aF	202	CLA	C2B-C1B-NB	5.05	115.57	110.33
12	aB	928	CLA	CHD-C4C-C3C	-5.05	117.41	124.77
12	cA	813	CLA	O2D-CGD-CBD	5.05	120.06	111.23
12	aB	950	CLA	CHD-C4C-C3C	-5.05	117.41	124.77
12	aA	854	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
12	cA	812	CLA	CHD-C4C-C3C	-5.05	117.41	124.77
12	cA	826	CLA	C2B-C1B-NB	5.05	115.56	110.33
12	aA	810	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
12	bA	812	CLA	CHD-C4C-C3C	-5.05	117.42	124.77
12	aA	817	CLA	C2B-C1B-NB	5.04	115.56	110.33
12	aA	812	CLA	CHD-C4C-C3C	-5.04	117.42	124.77
12	aA	844	CLA	CHD-C4C-C3C	-5.04	117.42	124.77
12	aB	902	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
12	bA	842	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
12	aA	813	CLA	O2D-CGD-CBD	5.04	120.04	111.23
12	aB	914	CLA	C3B-C2B-C1B	-5.04	101.23	107.17
12	cA	831	CLA	C3B-C2B-C1B	-5.04	101.23	107.17
12	cB	922	CLA	C3B-C2B-C1B	-5.04	101.23	107.17
12	aA	842	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
12	cA	840	CLA	CHD-C4C-C3C	-5.04	117.43	124.77
12	aB	911	CLA	C2C-C1C-NC	5.04	115.27	109.98
12	cA	809	CLA	C2B-C1B-NB	5.04	115.55	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	833	CLA	C3B-C2B-C1B	-5.04	101.23	107.17
12	aA	827	CLA	C2B-C1B-NB	5.04	115.55	110.33
12	bA	840	CLA	CHD-C4C-C3C	-5.03	117.44	124.77
12	bB	902	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
12	bF	202	CLA	C2B-C1B-NB	5.03	115.54	110.33
12	bB	928	CLA	CHD-C4C-C3C	-5.03	117.44	124.77
12	bA	803	CLA	CHD-C4C-C3C	-5.03	117.44	124.77
12	cF	202	CLA	C2B-C1B-NB	5.02	115.54	110.33
12	aB	919	CLA	C2B-C1B-NB	5.02	115.54	110.33
12	cA	842	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
12	bB	916	CLA	C2B-C1B-NB	5.02	115.53	110.33
12	bB	949	CLA	C2B-C1B-NB	5.02	115.53	110.33
12	aB	908	CLA	CHD-C4C-C3C	-5.02	117.46	124.77
12	cB	908	CLA	CHD-C4C-C3C	-5.02	117.46	124.77
12	bA	813	CLA	O2D-CGD-CBD	5.02	120.00	111.23
12	cB	916	CLA	C2B-C1B-NB	5.02	115.53	110.33
12	bB	922	CLA	C3B-C2B-C1B	-5.02	101.26	107.17
12	cA	839	CLA	C3D-C2D-C1D	-5.02	98.99	105.83
12	bA	810	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
12	cA	810	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
12	cA	803	CLA	CHD-C4C-C3C	-5.01	117.47	124.77
12	bA	816	CLA	C2B-C1B-NB	5.01	115.52	110.33
12	aA	823	CLA	C2C-C1C-NC	5.01	115.24	109.98
12	aA	833	CLA	C3B-C2B-C1B	-5.01	101.27	107.17
12	cB	911	CLA	C2C-C1C-NC	5.01	115.24	109.98
12	aB	912	CLA	O2D-CGD-CBD	5.01	119.98	111.23
12	cB	912	CLA	O2D-CGD-CBD	5.01	119.98	111.23
12	cA	823	CLA	C2C-C1C-NC	5.01	115.24	109.98
12	cA	824	CLA	C3B-C2B-C1B	-5.00	101.27	107.17
12	aB	910	CLA	C2C-C1C-NC	5.00	115.24	109.98
12	bA	833	CLA	C2C-C1C-NC	5.00	115.24	109.98
12	bB	908	CLA	CHD-C4C-C3C	-5.00	117.48	124.77
12	aB	949	CLA	C2B-C1B-NB	5.00	115.52	110.33
12	bB	912	CLA	O2D-CGD-CBD	5.00	119.98	111.23
12	aA	840	CLA	CHD-C4C-C3C	-5.00	117.48	124.77
12	cB	908	CLA	C1C-C2C-C3C	-5.00	101.72	106.98
12	aB	916	CLA	C2B-C1B-NB	5.00	115.51	110.33
12	cA	833	CLA	C3B-C2B-C1B	-5.00	101.28	107.17
12	bB	919	CLA	C2B-C1B-NB	5.00	115.51	110.33
12	bA	842	CLA	O2D-CGD-CBD	5.00	119.97	111.23
12	cB	914	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
12	cA	842	CLA	O2D-CGD-CBD	4.99	119.96	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bB	914	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
12	aB	911	CLA	C2B-C1B-NB	4.99	115.50	110.33
12	cB	911	CLA	C2B-C1B-NB	4.99	115.50	110.33
12	cA	835	CLA	CMD-C2D-C1D	4.99	133.51	124.73
12	aA	839	CLA	C3D-C2D-C1D	-4.99	99.03	105.83
12	bB	911	CLA	C2B-C1B-NB	4.98	115.50	110.33
12	bB	916	CLA	C3B-C2B-C1B	-4.98	101.29	107.17
12	bL	204	CLA	C3B-C2B-C1B	-4.98	101.29	107.17
12	bA	831	CLA	C2B-C1B-NB	4.98	115.49	110.33
12	cB	902	CLA	C2B-C1B-NB	4.98	115.49	110.33
12	aB	917	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
12	aA	808	CLA	C2B-C1B-NB	4.98	115.49	110.33
12	aA	833	CLA	C2C-C1C-NC	4.98	115.21	109.98
12	bA	823	CLA	C2C-C1C-NC	4.98	115.21	109.98
12	cB	929	CLA	C2C-C1C-NC	4.98	115.21	109.98
12	bA	839	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
12	cB	949	CLA	C2B-C1B-NB	4.97	115.48	110.33
12	cL	204	CLA	C3B-C2B-C1B	-4.97	101.31	107.17
12	aA	842	CLA	O2D-CGD-CBD	4.97	119.92	111.23
12	aA	835	CLA	CMD-C2D-C1D	4.97	133.48	124.73
12	bB	908	CLA	CMD-C2D-C1D	4.97	133.48	124.73
12	bA	824	CLA	C3B-C2B-C1B	-4.97	101.31	107.17
12	aB	914	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
12	aB	929	CLA	C2C-C1C-NC	4.97	115.20	109.98
12	aA	824	CLA	C3B-C2B-C1B	-4.97	101.32	107.17
12	aA	831	CLA	C2B-C1B-NB	4.96	115.47	110.33
12	aA	814	CLA	O2D-CGD-CBD	4.96	119.91	111.23
12	bB	908	CLA	C1C-C2C-C3C	-4.96	101.76	106.98
12	bA	835	CLA	CMD-C2D-C1D	4.96	133.47	124.73
12	bA	808	CLA	C2B-C1B-NB	4.96	115.47	110.33
12	cB	917	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
12	cA	825	CLA	C4A-NA-C1A	-4.96	104.42	106.68
12	bL	203	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
12	bA	825	CLA	C3B-C2B-C1B	-4.96	101.32	107.17
12	bB	903	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
12	aB	908	CLA	C1C-C2C-C3C	-4.95	101.77	106.98
12	cB	903	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
12	bB	902	CLA	C2B-C1B-NB	4.95	115.46	110.33
12	bB	906	CLA	C3B-C2B-C1B	-4.95	101.33	107.17
12	bB	917	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
12	cA	808	CLA	C2B-C1B-NB	4.95	115.46	110.33
12	bA	814	CLA	O2D-CGD-CBD	4.95	119.88	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	802	CLA	CAA-C2A-C3A	-4.95	99.63	113.00
12	aB	903	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
12	cL	203	CLA	C3D-C2D-C1D	-4.94	99.08	105.83
12	bA	837	CLA	C2B-C1B-NB	4.94	115.45	110.33
12	aL	203	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
12	cA	837	CLA	C2C-C1C-NC	4.94	115.17	109.98
12	aB	916	CLA	C3B-C2B-C1B	-4.94	101.35	107.17
12	bB	908	CLA	C2D-C1D-ND	4.94	115.01	110.13
12	aA	837	CLA	C2C-C1C-NC	4.94	115.17	109.98
12	bA	840	CLA	C2C-C1C-NC	4.94	115.17	109.98
12	aA	830	CLA	CMD-C2D-C1D	4.93	133.42	124.73
12	aL	204	CLA	C3B-C2B-C1B	-4.93	101.35	107.17
12	cA	814	CLA	O2D-CGD-CBD	4.93	119.85	111.23
12	cB	908	CLA	CMD-C2D-C1D	4.93	133.41	124.73
12	aB	908	CLA	CMD-C2D-C1D	4.93	133.41	124.73
12	cA	833	CLA	C2C-C1C-NC	4.93	115.16	109.98
12	aA	837	CLA	C2B-C1B-NB	4.93	115.44	110.33
11	bA	801	CL0	CAA-C2A-C3A	-4.93	99.68	113.00
12	aL	202	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
12	bL	202	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
12	aB	902	CLA	C2B-C1B-NB	4.93	115.44	110.33
12	bA	802	CLA	CAA-C2A-C3A	-4.93	99.69	113.00
12	bB	929	CLA	C2C-C1C-NC	4.93	115.16	109.98
12	aA	825	CLA	C3B-C2B-C1B	-4.92	101.36	107.17
12	cB	916	CLA	C3B-C2B-C1B	-4.92	101.36	107.17
12	cA	830	CLA	CMD-C2D-C1D	4.92	133.40	124.73
12	cA	831	CLA	C2B-C1B-NB	4.92	115.43	110.33
12	bA	825	CLA	C4A-NA-C1A	-4.92	104.43	106.68
12	cA	802	CLA	CAA-C2A-C3A	-4.92	99.70	113.00
11	cA	801	CL0	CAA-C2A-C3A	-4.92	99.70	113.00
12	aB	929	CLA	C3D-C2D-C1D	-4.92	99.12	105.83
11	aA	801	CL0	CAA-C2A-C3A	-4.92	99.71	113.00
12	bA	830	CLA	CMD-C2D-C1D	4.92	133.38	124.73
12	aB	915	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
12	cL	202	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
12	cA	837	CLA	C2B-C1B-NB	4.91	115.42	110.33
12	bA	837	CLA	C2C-C1C-NC	4.91	115.14	109.98
12	cA	834	CLA	CHD-C4C-C3C	-4.91	117.61	124.77
12	bA	809	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
12	aB	906	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
12	cB	906	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
12	bB	915	CLA	C3D-C2D-C1D	-4.91	99.14	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	809	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
12	aA	825	CLA	C4A-NA-C1A	-4.90	104.44	106.68
12	aB	903	CLA	C2B-C1B-NB	4.90	115.41	110.33
12	cB	915	CLA	C3B-C2B-C1B	-4.90	101.39	107.17
12	aB	915	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
12	bA	808	CLA	O2D-CGD-CBD	4.90	119.80	111.23
12	aB	935	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
12	aB	937	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
12	aB	908	CLA	C2D-C1D-ND	4.90	114.97	110.13
12	bA	834	CLA	CHD-C4C-C3C	-4.90	117.63	124.77
12	cA	809	CLA	C3D-C2D-C1D	-4.90	99.15	105.83
12	aB	930	CLA	C2C-C1C-NC	4.90	115.13	109.98
12	bB	937	CLA	C3D-C2D-C1D	-4.90	99.15	105.83
12	cL	202	CLA	C3D-C2D-C1D	-4.89	99.15	105.83
12	cA	825	CLA	C3B-C2B-C1B	-4.89	101.40	107.17
12	cF	202	CLA	C2C-C1C-NC	4.89	115.12	109.98
12	bB	903	CLA	C2B-C1B-NB	4.89	115.40	110.33
12	cB	908	CLA	C2D-C1D-ND	4.89	114.97	110.13
12	bB	930	CLA	C2C-C1C-NC	4.89	115.11	109.98
12	bL	202	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
12	cA	840	CLA	C2C-C1C-NC	4.89	115.11	109.98
12	bB	915	CLA	C3B-C2B-C1B	-4.89	101.41	107.17
12	cA	837	CLA	C3B-C2B-C1B	-4.88	101.41	107.17
12	cB	915	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
12	cA	808	CLA	O2D-CGD-CBD	4.88	119.77	111.23
12	aA	840	CLA	C2C-C1C-NC	4.88	115.11	109.98
12	cA	835	CLA	C2C-C1C-NC	4.88	115.11	109.98
12	aA	829	CLA	C2C-C1C-NC	4.88	115.11	109.98
12	bA	818	CLA	C2C-C1C-NC	4.88	115.11	109.98
12	bB	929	CLA	C3D-C2D-C1D	-4.88	99.18	105.83
12	cB	937	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
12	bA	837	CLA	C3B-C2B-C1B	-4.87	101.43	107.17
12	cB	929	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
12	cB	930	CLA	C2C-C1C-NC	4.87	115.10	109.98
12	aA	830	CLA	CHD-C4C-C3C	-4.87	117.68	124.77
12	bA	830	CLA	CHD-C4C-C3C	-4.86	117.68	124.77
12	cA	811	CLA	C2C-C1C-NC	4.86	115.09	109.98
12	cA	830	CLA	CHD-C4C-C3C	-4.86	117.68	124.77
12	cB	920	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
12	cB	935	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
12	bA	835	CLA	C2C-C1C-NC	4.86	115.08	109.98
12	bB	935	CLA	C3D-C2D-C1D	-4.86	99.20	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	814	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
12	bA	829	CLA	C2C-C1C-NC	4.86	115.08	109.98
12	aA	820	CLA	C2C-C1C-NC	4.85	115.08	109.98
12	aA	834	CLA	CHD-C4C-C3C	-4.85	117.69	124.77
12	aA	840	CLA	C2B-C1B-NB	4.85	115.36	110.33
12	bA	811	CLA	C2C-C1C-NC	4.85	115.08	109.98
12	aA	808	CLA	O2D-CGD-CBD	4.85	119.72	111.23
12	aF	202	CLA	C2C-C1C-NC	4.85	115.08	109.98
12	bL	202	CLA	C2C-C1C-NC	4.85	115.08	109.98
12	cB	903	CLA	C2B-C1B-NB	4.85	115.36	110.33
12	cL	202	CLA	C2C-C1C-NC	4.85	115.08	109.98
12	aL	202	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
12	cA	840	CLA	C2B-C1B-NB	4.85	115.35	110.33
12	bA	840	CLA	C2B-C1B-NB	4.85	115.35	110.33
12	aB	931	CLA	CHD-C1D-ND	-4.85	117.98	124.80
12	bA	840	CLA	C3B-C2B-C1B	-4.85	101.46	107.17
12	cA	840	CLA	C3B-C2B-C1B	-4.85	101.46	107.17
12	aL	202	CLA	C2C-C1C-NC	4.85	115.07	109.98
12	aB	916	CLA	C3D-C2D-C1D	-4.84	99.22	105.83
12	bB	938	CLA	C2C-C1C-NC	4.84	115.07	109.98
12	bA	836	CLA	CHD-C4C-C3C	-4.84	117.71	124.77
12	cA	829	CLA	C2C-C1C-NC	4.84	115.07	109.98
12	bA	814	CLA	C3B-C2B-C1B	-4.84	101.46	107.17
12	aA	837	CLA	C3B-C2B-C1B	-4.84	101.47	107.17
12	aA	811	CLA	C2C-C1C-NC	4.84	115.06	109.98
12	bF	202	CLA	C2C-C1C-NC	4.83	115.06	109.98
12	cA	820	CLA	C2C-C1C-NC	4.83	115.06	109.98
12	cA	806	CLA	C2C-C1C-NC	4.83	115.06	109.98
12	bB	920	CLA	C3B-C2B-C1B	-4.83	101.47	107.17
12	aA	835	CLA	C2B-C1B-NB	4.83	115.34	110.33
12	aB	927	CLA	C2D-C1D-ND	4.83	114.91	110.13
12	aB	938	CLA	C2C-C1C-NC	4.83	115.06	109.98
12	bB	916	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
12	aB	901	CLA	C2C-C1C-NC	4.83	115.05	109.98
12	cB	915	CLA	O2D-CGD-CBD	4.83	119.67	111.23
12	cB	936	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
12	bB	936	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
12	aA	840	CLA	C3B-C2B-C1B	-4.82	101.48	107.17
12	aA	807	CLA	C2B-C1B-NB	4.82	115.33	110.33
12	aB	915	CLA	C2B-C1B-NB	4.82	115.33	110.33
12	bA	833	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
12	aB	920	CLA	C3B-C2B-C1B	-4.82	101.49	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	835	CLA	C2C-C1C-NC	4.82	115.05	109.98
12	bB	949	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
12	bB	915	CLA	O2D-CGD-CBD	4.82	119.66	111.23
12	aA	844	CLA	C3B-C2B-C1B	-4.82	101.49	107.17
12	cA	814	CLA	C3B-C2B-C1B	-4.82	101.49	107.17
12	aA	819	CLA	CBA-CAA-C2A	4.82	128.13	113.79
12	aA	812	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
12	bA	819	CLA	CBA-CAA-C2A	4.82	128.12	113.79
12	bA	814	CLA	C2B-C1B-NB	4.82	115.32	110.33
12	cB	916	CLA	C3D-C2D-C1D	-4.81	99.26	105.83
12	bB	906	CLA	C2C-C1C-NC	4.81	115.04	109.98
12	aB	936	CLA	C3D-C2D-C1D	-4.81	99.26	105.83
12	aB	915	CLA	O2D-CGD-CBD	4.81	119.64	111.23
12	bB	933	CLA	CMD-C2D-C1D	4.81	133.20	124.73
12	cA	836	CLA	CHD-C4C-C3C	-4.81	117.76	124.77
12	bA	820	CLA	C2C-C1C-NC	4.81	115.03	109.98
12	cB	906	CLA	C2C-C1C-NC	4.81	115.03	109.98
12	bA	841	CLA	C2B-C1B-NB	4.81	115.31	110.33
12	cA	832	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
12	cA	833	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
12	cB	931	CLA	CHD-C1D-ND	-4.81	118.04	124.80
12	cB	915	CLA	C2B-C1B-NB	4.81	115.31	110.33
12	aL	204	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
12	cB	927	CLA	C2D-C1D-ND	4.81	114.88	110.13
12	aA	841	CLA	C2B-C1B-NB	4.81	115.31	110.33
12	cA	807	CLA	C2B-C1B-NB	4.81	115.31	110.33
12	cA	819	CLA	CBA-CAA-C2A	4.80	128.09	113.79
12	cA	818	CLA	C2C-C1C-NC	4.80	115.03	109.98
12	aB	928	CLA	C4B-C3B-C2B	-4.80	101.33	107.30
12	aA	814	CLA	C2B-C1B-NB	4.80	115.31	110.33
12	bA	824	CLA	CHD-C4C-C3C	-4.80	117.77	124.77
12	bA	804	CLA	C3B-C2B-C1B	-4.80	101.51	107.17
12	aB	950	CLA	C3B-C2B-C1B	-4.80	101.51	107.17
12	bB	923	CLA	C3B-C2B-C1B	-4.80	101.51	107.17
12	cA	824	CLA	CHD-C4C-C3C	-4.80	117.78	124.77
12	bA	807	CLA	C2B-C1B-NB	4.80	115.30	110.33
12	cB	936	CLA	C2C-C1C-NC	4.80	115.02	109.98
12	aB	912	CLA	C2B-C1B-NB	4.80	115.30	110.33
12	bA	825	CLA	C3D-C2D-C1D	-4.80	99.29	105.83
12	aA	807	CLA	CAA-C2A-C3A	-4.80	100.04	113.00
12	cB	949	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
12	cA	807	CLA	CAA-C2A-C3A	-4.79	100.04	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	833	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
12	aB	906	CLA	C2C-C1C-NC	4.79	115.02	109.98
12	aB	938	CLA	C3B-C2B-C1B	-4.79	101.52	107.17
12	bB	950	CLA	C3B-C2B-C1B	-4.79	101.52	107.17
12	cA	835	CLA	C2B-C1B-NB	4.79	115.29	110.33
12	cA	812	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
12	aA	806	CLA	C2C-C1C-NC	4.79	115.01	109.98
12	aA	818	CLA	C2C-C1C-NC	4.79	115.01	109.98
12	cB	928	CLA	C4B-C3B-C2B	-4.79	101.35	107.30
12	cB	938	CLA	C2C-C1C-NC	4.79	115.01	109.98
12	aA	804	CLA	C3B-C2B-C1B	-4.78	101.53	107.17
12	bB	931	CLA	CHD-C1D-ND	-4.78	118.07	124.80
12	cL	204	CLA	C3D-C2D-C1D	-4.78	99.30	105.83
12	cL	203	CLA	CMD-C2D-C1D	4.78	133.15	124.73
12	aA	832	CLA	C3D-C2D-C1D	-4.78	99.30	105.83
12	cB	934	CLA	C4A-NA-C1A	-4.78	104.50	106.68
12	cB	908	CLA	C4B-C3B-C2B	-4.78	101.36	107.30
12	bA	812	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
12	aL	203	CLA	CMD-C2D-C1D	4.78	133.15	124.73
12	cA	804	CLA	C3B-C2B-C1B	-4.78	101.53	107.17
12	cB	935	CLA	C2C-C1C-NC	4.78	115.00	109.98
12	bL	204	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
12	aA	825	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
12	bB	927	CLA	C2D-C1D-ND	4.78	114.86	110.13
12	cB	938	CLA	C3B-C2B-C1B	-4.78	101.54	107.17
12	bB	935	CLA	C2C-C1C-NC	4.78	115.00	109.98
12	aB	935	CLA	C2C-C1C-NC	4.78	115.00	109.98
12	aA	836	CLA	CHD-C4C-C3C	-4.78	117.81	124.77
12	aB	949	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
12	aA	832	CLA	C2B-C1B-NB	4.78	115.28	110.33
12	bA	807	CLA	CAA-C2A-C3A	-4.77	100.10	113.00
12	aB	923	CLA	C3B-C2B-C1B	-4.77	101.54	107.17
12	aB	934	CLA	C2B-C1B-NB	4.77	115.28	110.33
12	bA	832	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
12	aA	844	CLA	C2B-C1B-NB	4.77	115.27	110.33
12	aA	824	CLA	CHD-C4C-C3C	-4.77	117.82	124.77
12	cB	923	CLA	C3B-C2B-C1B	-4.77	101.55	107.17
12	cA	825	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
12	aB	933	CLA	CMD-C2D-C1D	4.76	133.12	124.73
12	bB	915	CLA	C2B-C1B-NB	4.76	115.27	110.33
12	aB	939	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
12	bB	928	CLA	C4B-C3B-C2B	-4.76	101.38	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bB	901	CLA	C2C-C1C-NC	4.76	114.98	109.98
12	bL	203	CLA	CMD-C2D-C1D	4.76	133.11	124.73
12	cA	841	CLA	C2B-C1B-NB	4.76	115.26	110.33
12	cB	933	CLA	CMD-C2D-C1D	4.76	133.11	124.73
12	bB	939	CLA	C1C-C2C-C3C	-4.76	101.97	106.98
12	aA	839	CLA	C2B-C1B-NB	4.76	115.26	110.33
12	bB	939	CLA	C3D-C2D-C1D	-4.76	99.34	105.83
12	aA	805	CLA	C3D-C2D-C1D	-4.76	99.34	105.83
12	bA	802	CLA	C3D-C2D-C1D	-4.76	99.34	105.83
12	cA	805	CLA	C3D-C2D-C1D	-4.76	99.34	105.83
12	bA	810	CLA	C2B-C1B-NB	4.75	115.26	110.33
12	bA	805	CLA	C3D-C2D-C1D	-4.75	99.34	105.83
12	aA	802	CLA	CHD-C1D-ND	-4.75	118.11	124.80
12	aB	936	CLA	C2C-C1C-NC	4.75	114.97	109.98
12	aB	932	CLA	C3B-C2B-C1B	-4.75	101.57	107.17
12	bB	912	CLA	C2B-C1B-NB	4.75	115.25	110.33
12	cA	814	CLA	C2B-C1B-NB	4.75	115.25	110.33
12	aA	814	CLA	C2C-C1C-NC	4.75	114.97	109.98
12	cA	826	CLA	C2C-C1C-NC	4.75	114.97	109.98
12	cB	934	CLA	C2B-C1B-NB	4.75	115.25	110.33
12	cB	919	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
12	cB	939	CLA	C1C-C2C-C3C	-4.75	101.99	106.98
12	bA	814	CLA	C2C-C1C-NC	4.75	114.97	109.98
12	cA	819	CLA	C2C-C1C-NC	4.75	114.97	109.98
12	aB	939	CLA	C1C-C2C-C3C	-4.75	101.99	106.98
12	cA	842	CLA	C2B-C1B-NB	4.75	115.25	110.33
12	aA	826	CLA	C2C-C1C-NC	4.75	114.97	109.98
12	cA	814	CLA	C2C-C1C-NC	4.74	114.97	109.98
12	cA	817	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
12	aB	912	CLA	C3B-C2B-C1B	-4.74	101.58	107.17
12	cB	912	CLA	C2B-C1B-NB	4.74	115.24	110.33
12	cB	901	CLA	C2C-C1C-NC	4.74	114.96	109.98
12	bB	908	CLA	C4B-C3B-C2B	-4.74	101.41	107.30
12	cB	912	CLA	C3B-C2B-C1B	-4.74	101.58	107.17
12	bA	842	CLA	C2B-C1B-NB	4.74	115.24	110.33
12	aA	807	CLA	C3B-C2B-C1B	-4.74	101.58	107.17
12	aB	908	CLA	C4B-C3B-C2B	-4.74	101.41	107.30
12	bA	806	CLA	C2C-C1C-NC	4.73	114.95	109.98
12	cB	939	CLA	C3D-C2D-C1D	-4.73	99.37	105.83
12	bB	934	CLA	C2B-C1B-NB	4.73	115.23	110.33
12	bA	818	CLA	C3D-C2D-C1D	-4.73	99.37	105.83
12	bA	832	CLA	C2B-C1B-NB	4.73	115.23	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cL	204	CLA	C2B-C1B-NB	4.73	115.23	110.33
12	bB	950	CLA	C2B-C1B-NB	4.73	115.23	110.33
12	bA	802	CLA	CHD-C1D-ND	-4.73	118.14	124.80
12	cA	802	CLA	CHD-C1D-ND	-4.73	118.14	124.80
12	bB	936	CLA	C2C-C1C-NC	4.73	114.95	109.98
12	bB	912	CLA	C3B-C2B-C1B	-4.73	101.59	107.17
12	bA	826	CLA	C2C-C1C-NC	4.73	114.95	109.98
12	cA	802	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
12	cB	932	CLA	C3B-C2B-C1B	-4.73	101.60	107.17
12	aA	802	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
12	aB	950	CLA	C2B-C1B-NB	4.73	115.23	110.33
12	bB	938	CLA	C3B-C2B-C1B	-4.72	101.60	107.17
12	bB	919	CLA	C3D-C2D-C1D	-4.72	99.38	105.83
12	cA	838	CLA	C2C-C1C-NC	4.72	114.94	109.98
12	cA	818	CLA	C3D-C2D-C1D	-4.72	99.38	105.83
12	bA	841	CLA	C3B-C2B-C1B	-4.72	101.60	107.17
12	cA	807	CLA	C3B-C2B-C1B	-4.72	101.60	107.17
12	cA	839	CLA	C2B-C1B-NB	4.72	115.22	110.33
12	aB	919	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
12	bA	839	CLA	C2B-C1B-NB	4.72	115.22	110.33
12	bB	932	CLA	C3B-C2B-C1B	-4.72	101.61	107.17
12	bA	807	CLA	C3B-C2B-C1B	-4.72	101.61	107.17
12	cA	822	CLA	CHD-C1D-ND	-4.71	118.17	124.80
12	aA	818	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
12	aB	938	CLA	C2B-C1B-NB	4.71	115.21	110.33
12	aA	815	CLA	C2C-C1C-NC	4.71	114.93	109.98
12	cA	841	CLA	C2C-C1C-NC	4.71	114.93	109.98
12	bA	835	CLA	C2B-C1B-NB	4.71	115.21	110.33
12	aA	841	CLA	C3B-C2B-C1B	-4.71	101.62	107.17
12	bB	904	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
12	cA	821	CLA	C2C-C1C-NC	4.71	114.93	109.98
12	aB	929	CLA	C2B-C1B-NB	4.71	115.21	110.33
12	bB	906	CLA	O2D-CGD-CBD	4.71	119.46	111.23
12	bA	823	CLA	C3B-C2B-C1B	-4.71	101.62	107.17
12	bB	934	CLA	C4A-NA-C1A	-4.71	104.53	106.68
12	cA	843	CLA	CMD-C2D-C1D	4.71	133.01	124.73
12	cA	813	CLA	C2C-C1C-NC	4.71	114.92	109.98
12	cA	832	CLA	C2B-C1B-NB	4.70	115.20	110.33
12	aB	913	CLA	C2C-C1C-NC	4.70	114.92	109.98
12	bA	813	CLA	C2C-C1C-NC	4.70	114.92	109.98
12	cA	810	CLA	C2B-C1B-NB	4.70	115.20	110.33
12	aA	817	CLA	C3D-C2D-C1D	-4.70	99.41	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	810	CLA	C2B-C1B-NB	4.70	115.20	110.33
12	aA	822	CLA	CHD-C1D-ND	-4.70	118.19	124.80
12	cL	202	CLA	CHD-C1D-ND	-4.70	118.19	124.80
12	aA	813	CLA	C2C-C1C-NC	4.70	114.92	109.98
12	bA	822	CLA	CHD-C1D-ND	-4.70	118.19	124.80
12	bA	815	CLA	C2C-C1C-NC	4.70	114.92	109.98
12	bA	821	CLA	C2C-C1C-NC	4.70	114.92	109.98
12	cA	841	CLA	C3B-C2B-C1B	-4.70	101.63	107.17
12	aA	806	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
12	bA	824	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
12	cB	929	CLA	C2B-C1B-NB	4.69	115.19	110.33
12	aA	803	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
12	aA	826	CLA	CAA-C2A-C3A	-4.69	100.32	113.00
12	aB	904	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
12	aA	819	CLA	C2C-C1C-NC	4.69	114.91	109.98
12	aA	843	CLA	CMD-C2D-C1D	4.69	132.99	124.73
12	aL	202	CLA	C2B-C1B-NB	4.69	115.19	110.33
12	aA	838	CLA	C2C-C1C-NC	4.69	114.91	109.98
12	aA	816	CLA	C2C-C1C-NC	4.69	114.91	109.98
12	cA	826	CLA	CAA-C2A-C3A	-4.69	100.33	113.00
12	cB	904	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
12	aL	202	CLA	CHD-C1D-ND	-4.69	118.20	124.80
12	cA	823	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
12	bL	204	CLA	C2B-C1B-NB	4.69	115.19	110.33
12	aB	917	CLA	O2D-CGD-CBD	4.69	119.42	111.23
12	bA	826	CLA	CAA-C2A-C3A	-4.69	100.34	113.00
12	aA	833	CLA	C2B-C1B-NB	4.68	115.18	110.33
12	aA	842	CLA	C2B-C1B-NB	4.68	115.18	110.33
12	aL	204	CLA	C2B-C1B-NB	4.68	115.18	110.33
12	aA	821	CLA	C2C-C1C-NC	4.68	114.90	109.98
12	cA	806	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
12	bA	841	CLA	C2C-C1C-NC	4.68	114.90	109.98
12	cB	906	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
12	cA	803	CLA	C3B-C2B-C1B	-4.68	101.65	107.17
12	cB	906	CLA	O2D-CGD-CBD	4.68	119.41	111.23
12	aB	906	CLA	O2D-CGD-CBD	4.68	119.41	111.23
12	cB	938	CLA	C2B-C1B-NB	4.68	115.18	110.33
12	cA	833	CLA	C2B-C1B-NB	4.68	115.18	110.33
12	bB	913	CLA	C2C-C1C-NC	4.68	114.90	109.98
12	bA	806	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
12	bA	834	CLA	C4A-NA-C1A	-4.68	104.55	106.68
12	cB	917	CLA	O2D-CGD-CBD	4.68	119.41	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	803	CLA	C3B-C2B-C1B	-4.68	101.66	107.17
12	bB	938	CLA	C2B-C1B-NB	4.67	115.17	110.33
12	bB	906	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
12	aA	824	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
12	bA	819	CLA	C2C-C1C-NC	4.67	114.89	109.98
12	bA	817	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
12	cA	824	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
12	bA	833	CLA	C2B-C1B-NB	4.67	115.17	110.33
12	bA	816	CLA	C2C-C1C-NC	4.67	114.89	109.98
12	cB	913	CLA	C2C-C1C-NC	4.67	114.89	109.98
12	aB	906	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
12	bA	843	CLA	CMD-C2D-C1D	4.67	132.95	124.73
12	cB	919	CLA	C2C-C1C-NC	4.67	114.88	109.98
12	bB	910	CLA	C4A-NA-C1A	-4.67	104.55	106.68
12	aB	936	CLA	C3B-C2B-C1B	-4.66	101.67	107.17
12	bB	920	CLA	C2B-C1B-NB	4.66	115.16	110.33
12	aB	949	CLA	C3B-C2B-C1B	-4.66	101.67	107.17
12	bL	202	CLA	CHD-C1D-ND	-4.66	118.24	124.80
12	aA	828	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
12	bA	838	CLA	C2C-C1C-NC	4.66	114.88	109.98
12	bB	917	CLA	O2D-CGD-CBD	4.66	119.38	111.23
12	cA	828	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
12	aB	920	CLA	C2B-C1B-NB	4.66	115.16	110.33
12	bL	202	CLA	C2B-C1B-NB	4.66	115.16	110.33
12	bB	929	CLA	C2B-C1B-NB	4.66	115.16	110.33
12	cB	922	CLA	C2B-C1B-NB	4.65	115.15	110.33
12	aA	823	CLA	C3B-C2B-C1B	-4.65	101.68	107.17
12	bA	823	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
12	bA	804	CLA	C2C-C1C-NC	4.65	114.87	109.98
12	cB	936	CLA	C3B-C2B-C1B	-4.65	101.69	107.17
12	aB	919	CLA	C2C-C1C-NC	4.65	114.86	109.98
12	bB	919	CLA	C2C-C1C-NC	4.65	114.86	109.98
12	cB	920	CLA	C2B-C1B-NB	4.65	115.15	110.33
12	aF	202	CLA	C3B-C2B-C1B	-4.65	101.69	107.17
12	cA	816	CLA	C2C-C1C-NC	4.65	114.86	109.98
12	aA	823	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
12	bB	949	CLA	C3B-C2B-C1B	-4.64	101.69	107.17
12	cB	937	CLA	C2C-C1C-NC	4.64	114.86	109.98
12	aA	819	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
12	aB	922	CLA	C2B-C1B-NB	4.64	115.14	110.33
12	bA	828	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
12	aA	830	CLA	C3D-C2D-C1D	-4.64	99.50	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aB	932	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
12	bB	909	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
12	aB	934	CLA	C4A-NA-C1A	-4.64	104.56	106.68
12	cB	932	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
12	bA	819	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
12	aA	841	CLA	C2C-C1C-NC	4.64	114.85	109.98
12	aB	932	CLA	C3D-C4D-ND	4.63	117.52	109.99
12	bB	937	CLA	C2C-C1C-NC	4.63	114.85	109.98
12	aB	910	CLA	C4A-NA-C1A	-4.63	104.56	106.68
12	bB	936	CLA	C3B-C2B-C1B	-4.63	101.71	107.17
12	cL	202	CLA	C2B-C1B-NB	4.63	115.13	110.33
12	cA	823	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
12	bB	932	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
12	cA	830	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
12	bA	811	CLA	C3B-C2B-C1B	-4.63	101.71	107.17
12	bA	839	CLA	C3B-C2B-C1B	-4.63	101.71	107.17
12	bF	202	CLA	C3B-C2B-C1B	-4.63	101.71	107.17
12	cB	926	CLA	C3B-C2B-C1B	-4.63	101.72	107.17
12	bB	932	CLA	C3D-C4D-ND	4.62	117.50	109.99
12	cA	839	CLA	C3B-C2B-C1B	-4.62	101.72	107.17
12	cB	913	CLA	C2B-C1B-NB	4.62	115.12	110.33
12	bA	814	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
12	cA	815	CLA	C2C-C1C-NC	4.62	114.84	109.98
12	aA	839	CLA	C3B-C2B-C1B	-4.62	101.72	107.17
12	cA	813	CLA	C4A-NA-C1A	-4.62	104.57	106.68
12	cF	202	CLA	C3B-C2B-C1B	-4.62	101.72	107.17
12	bB	926	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
12	aA	814	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
12	aA	811	CLA	C3B-C2B-C1B	-4.62	101.72	107.17
12	cA	804	CLA	C2C-C1C-NC	4.62	114.83	109.98
12	cA	819	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
12	cB	930	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
12	cB	949	CLA	C3B-C2B-C1B	-4.61	101.73	107.17
12	aB	927	CLA	CMD-C2D-C1D	4.61	132.85	124.73
12	cB	936	CLA	C2B-C1B-NB	4.61	115.11	110.33
12	aA	834	CLA	C4A-NA-C1A	-4.61	104.57	106.68
12	bA	841	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
12	cB	925	CLA	C3B-C2B-C1B	-4.61	101.73	107.17
12	bA	830	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
12	cA	814	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
12	aB	925	CLA	C3B-C2B-C1B	-4.61	101.74	107.17
12	bB	913	CLA	C2B-C1B-NB	4.61	115.10	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	802	CLA	C2C-C1C-NC	4.61	114.82	109.98
12	aA	813	CLA	C4A-NA-C1A	-4.61	104.58	106.68
12	cA	811	CLA	C3B-C2B-C1B	-4.61	101.74	107.17
12	cB	926	CLA	C2B-C1B-NB	4.60	115.10	110.33
12	aB	926	CLA	C3B-C2B-C1B	-4.60	101.74	107.17
12	bB	912	CLA	C2C-C1C-NC	4.60	114.82	109.98
12	cB	932	CLA	C3D-C4D-ND	4.60	117.47	109.99
12	bB	926	CLA	C2B-C1B-NB	4.60	115.10	110.33
12	aB	926	CLA	C2B-C1B-NB	4.60	115.10	110.33
12	aB	936	CLA	C2B-C1B-NB	4.60	115.10	110.33
12	cB	926	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
12	aB	913	CLA	C2B-C1B-NB	4.60	115.09	110.33
12	aB	937	CLA	C2C-C1C-NC	4.60	114.81	109.98
12	aB	926	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
12	aA	841	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
12	bB	922	CLA	C2B-C1B-NB	4.59	115.09	110.33
12	cA	834	CLA	C4A-NA-C1A	-4.59	104.58	106.68
12	aB	902	CLA	CHD-C1D-ND	-4.59	118.34	124.80
12	bB	936	CLA	C2B-C1B-NB	4.59	115.09	110.33
12	cB	927	CLA	CMD-C2D-C1D	4.59	132.81	124.73
12	cB	909	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
12	cB	910	CLA	C4A-NA-C1A	-4.59	104.58	106.68
12	aB	909	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
12	aA	812	CLA	C2B-C1B-NB	4.59	115.09	110.33
12	bA	831	CLA	C2C-C1C-NC	4.59	114.80	109.98
12	cB	927	CLA	C2B-C1B-NB	4.59	115.08	110.33
12	bB	927	CLA	CMD-C2D-C1D	4.59	132.81	124.73
12	bL	204	CLA	C2C-C1C-NC	4.58	114.80	109.98
12	bA	810	CLA	C2C-C1C-NC	4.58	114.80	109.98
12	aB	927	CLA	C2B-C1B-NB	4.58	115.08	110.33
12	cA	818	CLA	C2B-C1B-NB	4.58	115.08	110.33
12	bB	930	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
12	aL	202	CLA	C3D-C4D-ND	4.58	117.43	109.99
12	aA	831	CLA	C2C-C1C-NC	4.58	114.79	109.98
12	cA	812	CLA	C2B-C1B-NB	4.58	115.07	110.33
12	cA	841	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
12	cB	902	CLA	CHD-C1D-ND	-4.58	118.36	124.80
12	bB	926	CLA	C3B-C2B-C1B	-4.58	101.78	107.17
12	bB	916	CLA	O2D-CGD-CBD	4.58	119.23	111.23
12	cA	836	CLA	C1C-C2C-C3C	-4.58	102.17	106.98
12	cA	831	CLA	C2C-C1C-NC	4.57	114.79	109.98
12	cB	912	CLA	C2C-C1C-NC	4.57	114.79	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aB	930	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
12	bB	902	CLA	CHD-C1D-ND	-4.57	118.36	124.80
12	aB	912	CLA	C2C-C1C-NC	4.57	114.78	109.98
12	aA	812	CLA	C3B-C2B-C1B	-4.57	101.78	107.17
12	bA	818	CLA	C2B-C1B-NB	4.57	115.07	110.33
12	bB	925	CLA	C3B-C2B-C1B	-4.57	101.78	107.17
12	cA	812	CLA	C3B-C2B-C1B	-4.57	101.79	107.17
12	bF	202	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
12	aA	829	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
12	aB	934	CLA	C2C-C1C-NC	4.57	114.78	109.98
12	cB	904	CLA	C2C-C1C-NC	4.57	114.78	109.98
12	aA	810	CLA	C2C-C1C-NC	4.56	114.78	109.98
12	cB	917	CLA	C1C-C2C-C3C	-4.56	102.18	106.98
12	aB	904	CLA	C2C-C1C-NC	4.56	114.77	109.98
12	bB	904	CLA	C2C-C1C-NC	4.56	114.77	109.98
12	aA	804	CLA	C2C-C1C-NC	4.56	114.77	109.98
12	aA	818	CLA	C2B-C1B-NB	4.56	115.06	110.33
12	bA	813	CLA	C4A-NA-C1A	-4.56	104.60	106.68
12	cB	924	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
12	cL	204	CLA	C2C-C1C-NC	4.56	114.77	109.98
12	aA	802	CLA	C2C-C1C-NC	4.55	114.77	109.98
12	cB	912	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
12	cB	928	CLA	C4A-NA-C1A	-4.55	104.60	106.68
12	bA	829	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
12	bA	812	CLA	C2B-C1B-NB	4.55	115.05	110.33
12	aB	916	CLA	O2D-CGD-CBD	4.55	119.18	111.23
12	bB	934	CLA	C2C-C1C-NC	4.55	114.76	109.98
12	aF	202	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
12	bA	812	CLA	C3B-C2B-C1B	-4.55	101.81	107.17
12	cB	934	CLA	C2C-C1C-NC	4.55	114.76	109.98
12	cA	829	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
12	cL	202	CLA	C3D-C4D-ND	4.55	117.38	109.99
12	aB	912	CLA	C3D-C2D-C1D	-4.55	99.63	105.83
12	bB	912	CLA	C3D-C2D-C1D	-4.55	99.63	105.83
12	cF	202	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
12	cA	810	CLA	C2C-C1C-NC	4.54	114.75	109.98
12	cA	820	CLA	C3B-C2B-C1B	-4.54	101.82	107.17
12	cB	916	CLA	O2D-CGD-CBD	4.54	119.17	111.23
12	bA	819	CLA	C2B-C1B-NB	4.54	115.03	110.33
12	bA	830	CLA	C4B-C3B-C2B	-4.54	101.66	107.30
12	aB	917	CLA	C1C-C2C-C3C	-4.54	102.20	106.98
12	aA	817	CLA	C3D-C4D-ND	4.54	117.37	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bB	931	CLA	C3D-C4D-ND	4.54	117.36	109.99
12	bB	905	CLA	C2B-C1B-NB	4.54	115.03	110.33
12	bB	924	CLA	C3D-C2D-C1D	-4.53	99.64	105.83
12	aA	820	CLA	C3B-C2B-C1B	-4.53	101.82	107.17
12	aB	924	CLA	C3D-C2D-C1D	-4.53	99.64	105.83
12	bL	202	CLA	C3D-C4D-ND	4.53	117.36	109.99
12	bA	820	CLA	C3B-C2B-C1B	-4.53	101.83	107.17
12	bB	917	CLA	C1C-C2C-C3C	-4.53	102.21	106.98
12	aB	931	CLA	C3D-C4D-ND	4.53	117.35	109.99
12	cA	830	CLA	C4B-C3B-C2B	-4.53	101.67	107.30
12	cB	931	CLA	C3D-C4D-ND	4.53	117.35	109.99
12	bB	927	CLA	C2B-C1B-NB	4.53	115.02	110.33
12	cA	819	CLA	C2B-C1B-NB	4.53	115.02	110.33
12	bA	802	CLA	C2C-C1C-NC	4.53	114.74	109.98
12	cB	905	CLA	C2B-C1B-NB	4.53	115.02	110.33
12	aA	825	CLA	C2C-C1C-NC	4.52	114.73	109.98
12	cL	203	CLA	C3D-C4D-ND	4.52	117.34	109.99
12	aA	806	CLA	CHD-C1D-ND	-4.52	118.44	124.80
12	bB	923	CLA	C2C-C1C-NC	4.52	114.73	109.98
12	bA	817	CLA	C3D-C4D-ND	4.52	117.33	109.99
12	aB	911	CLA	C3B-C2B-C1B	-4.52	101.84	107.17
12	bA	836	CLA	C1C-C2C-C3C	-4.52	102.23	106.98
12	bB	918	CLA	C2C-C1C-NC	4.52	114.73	109.98
12	aA	808	CLA	C3B-C2B-C1B	-4.52	101.85	107.17
12	cA	817	CLA	C3D-C4D-ND	4.51	117.32	109.99
12	cB	918	CLA	C2C-C1C-NC	4.51	114.72	109.98
12	aA	821	CLA	C4A-NA-C1A	-4.51	104.62	106.68
12	cA	827	CLA	C4A-NA-C1A	-4.51	104.62	106.68
12	aL	203	CLA	C3D-C4D-ND	4.51	117.32	109.99
12	bA	803	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
12	aB	905	CLA	C2B-C1B-NB	4.51	115.00	110.33
12	aB	921	CLA	O2D-CGD-CBD	4.51	119.11	111.23
12	aA	830	CLA	C4B-C3B-C2B	-4.51	101.70	107.30
12	cA	825	CLA	C2C-C1C-NC	4.51	114.72	109.98
12	bB	911	CLA	C3B-C2B-C1B	-4.51	101.86	107.17
12	aB	916	CLA	C3D-C4D-ND	4.51	117.31	109.99
12	cB	903	CLA	C2C-C1C-NC	4.50	114.71	109.98
12	bA	808	CLA	C3B-C2B-C1B	-4.50	101.86	107.17
12	aA	836	CLA	C1C-C2C-C3C	-4.50	102.24	106.98
12	bL	203	CLA	C3D-C4D-ND	4.50	117.31	109.99
12	cB	920	CLA	CHD-C1D-ND	-4.50	118.47	124.80
12	cB	911	CLA	C3B-C2B-C1B	-4.50	101.86	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aB	922	CLA	C2C-C1C-NC	4.50	114.71	109.98
12	aB	908	CLA	O2D-CGD-CBD	4.50	119.10	111.23
12	bB	908	CLA	O2D-CGD-CBD	4.50	119.10	111.23
12	cB	921	CLA	O2D-CGD-CBD	4.50	119.09	111.23
12	cB	908	CLA	C3B-C4B-NB	4.50	114.55	110.53
12	cB	901	CLA	C1D-CHD-C4C	-4.50	116.46	126.02
12	cA	808	CLA	C3B-C2B-C1B	-4.50	101.87	107.17
12	bB	920	CLA	CHD-C1D-ND	-4.50	118.47	124.80
12	bB	933	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
12	aB	926	CLA	CMD-C2D-C1D	4.50	132.64	124.73
12	bB	914	CLA	C2C-C1C-NC	4.49	114.70	109.98
12	bB	901	CLA	C1D-CHD-C4C	-4.49	116.47	126.02
12	aA	827	CLA	C4A-NA-C1A	-4.49	104.63	106.68
12	cA	821	CLA	C4A-NA-C1A	-4.49	104.63	106.68
12	aB	901	CLA	C1D-CHD-C4C	-4.49	116.47	126.02
12	aB	920	CLA	CHD-C1D-ND	-4.49	118.48	124.80
12	bB	928	CLA	C4A-NA-C1A	-4.49	104.63	106.68
12	bB	908	CLA	C3B-C4B-NB	4.49	114.54	110.53
12	cA	803	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
12	cA	842	CLA	C3B-C2B-C1B	-4.49	101.88	107.17
12	aA	820	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
12	bB	939	CLA	C3D-C4D-ND	4.49	117.28	109.99
12	cB	923	CLA	C2C-C1C-NC	4.49	114.69	109.98
12	bB	921	CLA	O2D-CGD-CBD	4.49	119.07	111.23
12	aA	803	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
12	aB	933	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
12	aB	934	CLA	O2D-CGD-CBD	4.48	119.07	111.23
12	bA	843	CLA	O2D-CGD-CBD	4.48	119.07	111.23
12	aL	204	CLA	C2C-C1C-NC	4.48	114.69	109.98
12	bA	820	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
12	cB	910	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
12	aA	854	CLA	CAA-C2A-C3A	-4.48	100.89	113.00
12	cA	836	CLA	C2B-C1B-NB	4.48	114.97	110.33
12	aB	910	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
12	bA	828	CLA	C2C-C1C-NC	4.48	114.69	109.98
12	bB	926	CLA	CMD-C2D-C1D	4.48	132.61	124.73
12	bA	817	CLA	C2C-C1C-NC	4.48	114.68	109.98
12	cB	908	CLA	O2D-CGD-CBD	4.48	119.06	111.23
12	bB	916	CLA	C3D-C4D-ND	4.48	117.26	109.99
12	cA	843	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
12	aA	819	CLA	C2B-C1B-NB	4.48	114.97	110.33
12	cA	843	CLA	O2D-CGD-CBD	4.48	119.06	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	825	CLA	C2C-C1C-NC	4.48	114.68	109.98
12	bA	806	CLA	C3D-C4D-ND	4.47	117.26	109.99
12	aB	923	CLA	C2C-C1C-NC	4.47	114.68	109.98
12	cB	922	CLA	C2C-C1C-NC	4.47	114.68	109.98
12	bB	903	CLA	C2C-C1C-NC	4.47	114.68	109.98
12	cA	817	CLA	C2C-C1C-NC	4.47	114.68	109.98
12	cA	806	CLA	CHD-C1D-ND	-4.47	118.51	124.80
12	cB	933	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
12	cA	853	CLA	CAA-C2A-C3A	-4.47	100.92	113.00
12	bA	806	CLA	CHD-C1D-ND	-4.47	118.51	124.80
12	cB	934	CLA	O2D-CGD-CBD	4.47	119.04	111.23
12	aA	806	CLA	C3D-C4D-ND	4.47	117.25	109.99
12	aB	939	CLA	C3D-C4D-ND	4.46	117.24	109.99
12	bA	842	CLA	C3B-C2B-C1B	-4.46	101.91	107.17
12	aA	828	CLA	C2C-C1C-NC	4.46	114.67	109.98
12	aA	843	CLA	CAC-C3C-C4C	4.46	130.59	124.79
12	aB	914	CLA	C2C-C1C-NC	4.46	114.67	109.98
12	bA	853	CLA	CAA-C2A-C3A	-4.46	100.95	113.00
12	bA	827	CLA	C4A-NA-C1A	-4.46	104.64	106.68
12	bB	910	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
12	aA	817	CLA	C2C-C1C-NC	4.46	114.66	109.98
12	aA	843	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
12	bA	816	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
12	aA	823	CLA	C2B-C1B-NB	4.46	114.95	110.33
12	cA	806	CLA	C3D-C4D-ND	4.45	117.23	109.99
12	cB	916	CLA	C3D-C4D-ND	4.45	117.23	109.99
12	bB	934	CLA	O2D-CGD-CBD	4.45	119.01	111.23
12	bB	922	CLA	C2C-C1C-NC	4.45	114.66	109.98
12	aB	920	CLA	C2C-C1C-NC	4.45	114.66	109.98
12	cB	926	CLA	CMD-C2D-C1D	4.45	132.57	124.73
12	cA	828	CLA	C2C-C1C-NC	4.45	114.66	109.98
12	cB	914	CLA	C2C-C1C-NC	4.45	114.66	109.98
12	cA	841	CLA	C4A-NA-C1A	-4.45	104.65	106.68
12	cA	823	CLA	C2B-C1B-NB	4.45	114.94	110.33
12	aB	908	CLA	C3B-C4B-NB	4.45	114.50	110.53
12	cB	939	CLA	C3D-C4D-ND	4.45	117.21	109.99
12	aA	832	CLA	C2C-C1C-NC	4.45	114.65	109.98
12	bA	841	CLA	C4A-NA-C1A	-4.45	104.65	106.68
12	aB	918	CLA	C2C-C1C-NC	4.44	114.65	109.98
12	aA	842	CLA	C3B-C2B-C1B	-4.44	101.93	107.17
12	bA	811	CLA	C2B-C1B-NB	4.44	114.93	110.33
12	bA	823	CLA	C2B-C1B-NB	4.44	114.93	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aB	903	CLA	C2C-C1C-NC	4.44	114.65	109.98
12	aA	816	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
12	cF	202	CLA	C4A-NA-C1A	-4.44	104.65	106.68
12	bA	843	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
12	cA	820	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
12	bA	843	CLA	CAC-C3C-C4C	4.44	130.57	124.79
12	aA	843	CLA	O2D-CGD-CBD	4.44	118.99	111.23
12	cA	843	CLA	CAC-C3C-C4C	4.44	130.56	124.79
12	aB	928	CLA	C4A-NA-C1A	-4.44	104.66	106.68
12	bA	821	CLA	C4A-NA-C1A	-4.43	104.66	106.68
12	cB	901	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
12	aA	802	CLA	C4A-NA-C1A	-4.43	104.66	106.68
12	bA	833	CLA	O2D-CGD-CBD	4.43	118.98	111.23
12	aA	811	CLA	C2B-C1B-NB	4.43	114.92	110.33
12	aA	836	CLA	C2B-C1B-NB	4.43	114.92	110.33
12	bB	931	CLA	C4A-NA-C1A	-4.43	104.66	106.68
12	cA	816	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
16	bA	852	LHG	O4-P-O5	4.43	133.04	112.44
12	bA	804	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
12	aB	901	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
12	bA	853	CLA	C3C-C4C-NC	4.43	116.10	110.43
12	cA	808	CLA	C3D-C4D-ND	4.42	117.18	109.99
12	aB	935	CLA	C3C-C4C-NC	4.42	116.10	110.43
12	cA	811	CLA	C2B-C1B-NB	4.42	114.91	110.33
16	cA	852	LHG	O4-P-O5	4.42	133.03	112.44
12	cA	815	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
12	bA	815	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
12	aA	854	CLA	CMD-C2D-C1D	4.42	132.51	124.73
12	cA	853	CLA	CMD-C2D-C1D	4.42	132.51	124.73
12	aB	913	CLA	C3D-C4D-ND	4.42	117.17	109.99
12	bB	907	CLA	C3B-C2B-C1B	-4.42	101.96	107.17
12	bA	832	CLA	C2C-C1C-NC	4.42	114.62	109.98
12	cA	821	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
12	aA	804	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
16	aA	853	LHG	O4-P-O5	4.42	133.00	112.44
12	bB	928	CLA	C2D-C1D-ND	4.42	114.50	110.13
12	aB	932	CLA	C2B-C1B-NB	4.42	114.91	110.33
12	cA	830	CLA	C3B-C4B-NB	4.42	114.47	110.53
12	bB	902	CLA	CHD-C4C-C3C	-4.42	118.33	124.77
12	aA	830	CLA	C3B-C4B-NB	4.42	114.47	110.53
12	bA	808	CLA	C3D-C4D-ND	4.42	117.16	109.99
12	bB	920	CLA	C2C-C1C-NC	4.41	114.62	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cB	920	CLA	C2C-C1C-NC	4.41	114.62	109.98
12	cB	932	CLA	C2B-C1B-NB	4.41	114.90	110.33
16	aA	852	LHG	O4-P-O5	4.41	132.97	112.44
12	bA	821	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
12	cA	833	CLA	O2D-CGD-CBD	4.41	118.94	111.23
16	cA	851	LHG	O4-P-O5	4.41	132.97	112.44
12	aA	854	CLA	C2C-C1C-NC	4.41	114.61	109.98
12	bA	836	CLA	C2B-C1B-NB	4.41	114.90	110.33
12	cB	923	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
12	bB	901	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
12	aA	821	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
12	aB	907	CLA	C3B-C2B-C1B	-4.41	101.97	107.17
12	aA	854	CLA	C3C-C4C-NC	4.41	116.08	110.43
12	bB	936	CLA	CHD-C1D-ND	-4.41	118.60	124.80
12	cA	804	CLA	C3D-C2D-C1D	-4.41	99.82	105.83
12	aA	815	CLA	C3D-C2D-C1D	-4.41	99.82	105.83
12	cB	907	CLA	C3B-C2B-C1B	-4.41	101.97	107.17
12	cB	928	CLA	C2D-C1D-ND	4.41	114.49	110.13
12	aB	917	CLA	C2B-C1B-NB	4.41	114.90	110.33
12	bA	853	CLA	C2C-C1C-NC	4.41	114.61	109.98
12	bB	932	CLA	C2B-C1B-NB	4.41	114.89	110.33
16	bA	851	LHG	O4-P-O5	4.41	132.94	112.44
12	bB	926	CLA	C3C-C4C-NC	4.41	116.07	110.43
12	aA	833	CLA	O2D-CGD-CBD	4.40	118.93	111.23
12	aA	813	CLA	C3D-C2D-C1D	-4.40	99.82	105.83
12	aB	928	CLA	C2D-C1D-ND	4.40	114.48	110.13
12	bB	917	CLA	C2B-C1B-NB	4.40	114.89	110.33
12	cB	924	CLA	C2C-C1C-NC	4.40	114.60	109.98
12	bA	853	CLA	CMD-C2D-C1D	4.40	132.47	124.73
12	aB	918	CLA	C2B-C1B-NB	4.40	114.89	110.33
12	bB	923	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
12	aB	924	CLA	C2C-C1C-NC	4.39	114.60	109.98
12	bB	924	CLA	C2C-C1C-NC	4.39	114.60	109.98
12	cL	204	CLA	C3D-C4D-ND	4.39	117.13	109.99
12	cA	840	CLA	C3D-C2D-C1D	-4.39	99.83	105.83
12	aL	204	CLA	C3D-C4D-ND	4.39	117.12	109.99
12	cA	804	CLA	C3D-C4D-ND	4.39	117.12	109.99
12	aB	925	CLA	C2C-C1C-NC	4.39	114.59	109.98
12	cA	853	CLA	C2C-C1C-NC	4.39	114.59	109.98
12	aA	841	CLA	C4A-NA-C1A	-4.39	104.68	106.68
12	aA	808	CLA	C3D-C4D-ND	4.39	117.12	109.99
12	bB	918	CLA	C2B-C1B-NB	4.38	114.87	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aB	923	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
12	aA	804	CLA	C3D-C4D-ND	4.38	117.11	109.99
12	bB	920	CLA	C3D-C4D-ND	4.38	117.11	109.99
12	cA	853	CLA	C3C-C4C-NC	4.38	116.05	110.43
12	cA	811	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
12	aA	806	CLA	CAC-C3C-C4C	4.38	130.49	124.79
12	cB	925	CLA	C2C-C1C-NC	4.38	114.58	109.98
12	cA	813	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
12	cA	836	CLA	C3D-C2D-C1D	-4.38	99.86	105.83
12	bA	830	CLA	C3B-C4B-NB	4.38	114.44	110.53
12	cA	832	CLA	C2C-C1C-NC	4.38	114.58	109.98
12	aB	920	CLA	C3D-C4D-ND	4.38	117.10	109.99
12	cB	935	CLA	C3C-C4C-NC	4.37	116.03	110.43
12	cB	918	CLA	C2B-C1B-NB	4.37	114.86	110.33
12	bB	913	CLA	C3D-C4D-ND	4.37	117.10	109.99
12	aA	806	CLA	CHD-C4C-C3C	-4.37	118.40	124.77
12	aB	902	CLA	CHD-C4C-C3C	-4.37	118.40	124.77
12	bA	836	CLA	C3D-C2D-C1D	-4.37	99.86	105.83
12	cA	809	CLA	C2C-C1C-NC	4.37	114.58	109.98
12	bB	906	CLA	C3D-C4D-ND	4.37	117.09	109.99
12	cA	838	CLA	C3D-C4D-ND	4.37	117.09	109.99
12	aB	911	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
12	bL	204	CLA	C3D-C4D-ND	4.37	117.09	109.99
12	bB	931	CLA	C3B-C2B-C1B	-4.37	102.02	107.17
12	bA	838	CLA	C3D-C4D-ND	4.37	117.09	109.99
12	bB	925	CLA	C2C-C1C-NC	4.37	114.57	109.98
12	bB	935	CLA	C3C-C4C-NC	4.37	116.03	110.43
12	aA	811	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
12	aB	926	CLA	C3C-C4C-NC	4.37	116.02	110.43
12	cB	921	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
12	aB	932	CLA	CHD-C1D-ND	-4.36	118.66	124.80
12	cB	913	CLA	C3D-C4D-ND	4.36	117.08	109.99
12	bB	932	CLA	CHD-C1D-ND	-4.36	118.67	124.80
12	cB	906	CLA	C3D-C4D-ND	4.36	117.07	109.99
12	cB	932	CLA	CHD-C1D-ND	-4.36	118.67	124.80
12	aA	840	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
12	bA	840	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
12	cB	920	CLA	C3D-C4D-ND	4.36	117.07	109.99
12	bB	918	CLA	C3D-C2D-C1D	-4.36	99.89	105.83
12	aB	906	CLA	C3D-C4D-ND	4.36	117.07	109.99
12	cA	806	CLA	CHD-C4C-C3C	-4.36	118.42	124.77
12	aB	934	CLA	C3D-C2D-C1D	-4.36	99.89	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cB	936	CLA	CHD-C1D-ND	-4.36	118.67	124.80
12	bA	806	CLA	CHD-C4C-C3C	-4.35	118.42	124.77
12	bA	811	CLA	C3D-C2D-C1D	-4.35	99.89	105.83
12	cA	836	CLA	O2D-CGD-CBD	4.35	118.84	111.23
12	cB	902	CLA	CHD-C4C-C3C	-4.35	118.43	124.77
12	aB	931	CLA	C3B-C2B-C1B	-4.35	102.04	107.17
12	bA	809	CLA	C2C-C1C-NC	4.35	114.55	109.98
12	cB	934	CLA	C3D-C2D-C1D	-4.35	99.90	105.83
12	aA	838	CLA	C3D-C4D-ND	4.35	117.05	109.99
12	cB	911	CLA	C3D-C2D-C1D	-4.35	99.90	105.83
12	aB	936	CLA	C3D-C4D-ND	4.35	117.05	109.99
12	bB	921	CLA	C3D-C2D-C1D	-4.35	99.90	105.83
12	bA	817	CLA	C4A-NA-C1A	-4.35	104.70	106.68
12	bB	910	CLA	C3B-C2B-C1B	-4.35	102.05	107.17
12	bA	813	CLA	C3D-C2D-C1D	-4.35	99.90	105.83
12	cB	931	CLA	C3B-C2B-C1B	-4.35	102.05	107.17
12	bF	202	CLA	C4A-NA-C1A	-4.34	104.70	106.68
12	cB	931	CLA	C4A-NA-C1A	-4.34	104.70	106.68
12	cB	917	CLA	C2B-C1B-NB	4.34	114.83	110.33
12	bB	910	CLA	C2B-C1B-NB	4.34	114.83	110.33
12	bA	804	CLA	C3D-C4D-ND	4.34	117.05	109.99
12	aB	918	CLA	C3D-C2D-C1D	-4.34	99.91	105.83
12	bF	202	CLA	C3D-C4D-ND	4.34	117.04	109.99
12	aB	936	CLA	CHD-C1D-ND	-4.34	118.69	124.80
12	bB	923	CLA	C2B-C1B-NB	4.34	114.83	110.33
12	bB	919	CLA	C4A-NA-C1A	-4.34	104.70	106.68
12	aB	921	CLA	C3D-C2D-C1D	-4.34	99.91	105.83
12	aA	809	CLA	C2C-C1C-NC	4.34	114.54	109.98
12	aA	832	CLA	CAA-C2A-C3A	-4.34	101.27	113.00
12	bA	840	CLA	C3D-C4D-ND	4.34	117.04	109.99
12	cB	910	CLA	C3B-C2B-C1B	-4.34	102.06	107.17
12	aA	836	CLA	C3D-C2D-C1D	-4.34	99.91	105.83
12	cA	817	CLA	C4A-NA-C1A	-4.34	104.70	106.68
12	aA	840	CLA	C3D-C4D-ND	4.34	117.03	109.99
12	aA	824	CLA	C1C-C2C-C3C	-4.33	102.42	106.98
12	bA	824	CLA	C1C-C2C-C3C	-4.33	102.42	106.98
12	bA	806	CLA	CAC-C3C-C4C	4.33	130.43	124.79
12	cB	919	CLA	C4A-NA-C1A	-4.33	104.70	106.68
12	aA	843	CLA	C3D-C4D-ND	4.33	117.03	109.99
12	cB	905	CLA	C2C-C1C-NC	4.33	114.53	109.98
12	aA	823	CLA	C3D-C4D-ND	4.33	117.03	109.99
12	aF	202	CLA	C3D-C4D-ND	4.33	117.02	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	806	CLA	CAC-C3C-C4C	4.33	130.42	124.79
12	aA	827	CLA	C2C-C1C-NC	4.33	114.53	109.98
12	bB	936	CLA	C3D-C4D-ND	4.33	117.02	109.99
12	cB	936	CLA	C3D-C4D-ND	4.33	117.02	109.99
12	cA	802	CLA	C4A-NA-C1A	-4.33	104.70	106.68
12	aB	930	CLA	C3D-C4D-ND	4.33	117.02	109.99
12	bA	835	CLA	C3D-C4D-ND	4.33	117.02	109.99
12	aA	835	CLA	C3D-C4D-ND	4.33	117.02	109.99
12	cB	926	CLA	C3C-C4C-NC	4.33	115.97	110.43
12	bA	822	CLA	C3D-C4D-ND	4.33	117.02	109.99
12	bB	950	CLA	C3D-C2D-C1D	-4.32	99.93	105.83
12	cA	832	CLA	CAA-C2A-C3A	-4.32	101.32	113.00
12	cA	803	CLA	C3D-C4D-ND	4.32	117.01	109.99
12	aB	937	CLA	CHD-C1D-ND	-4.32	118.72	124.80
12	aB	931	CLA	C4A-NA-C1A	-4.32	104.71	106.68
12	aA	844	CLA	C3D-C2D-C1D	-4.32	99.93	105.83
12	aA	822	CLA	C3D-C4D-ND	4.32	117.01	109.99
12	cA	843	CLA	C3D-C4D-ND	4.32	117.01	109.99
12	cB	901	CLA	CMA-C3A-C2A	-4.32	97.27	113.98
12	cB	918	CLA	C3D-C2D-C1D	-4.32	99.93	105.83
12	bA	832	CLA	CAA-C2A-C3A	-4.32	101.32	113.00
12	aA	836	CLA	O2D-CGD-CBD	4.32	118.78	111.23
12	cA	820	CLA	C2B-C1B-NB	4.32	114.81	110.33
12	bB	934	CLA	C3D-C2D-C1D	-4.32	99.93	105.83
12	aB	939	CLA	C3B-C4B-NB	4.32	114.39	110.53
12	bA	802	CLA	C4A-NA-C1A	-4.32	104.71	106.68
12	cA	828	CLA	C3B-C4B-NB	4.32	114.38	110.53
12	bB	905	CLA	C2C-C1C-NC	4.32	114.52	109.98
12	aA	814	CLA	C3B-C4B-NB	4.32	114.38	110.53
12	bB	937	CLA	CHD-C1D-ND	-4.31	118.73	124.80
12	aB	901	CLA	CMA-C3A-C2A	-4.31	97.30	113.98
12	bA	843	CLA	C3D-C4D-ND	4.31	117.00	109.99
12	cB	923	CLA	C2B-C1B-NB	4.31	114.80	110.33
12	aB	950	CLA	C3D-C2D-C1D	-4.31	99.94	105.83
12	cB	937	CLA	CHD-C1D-ND	-4.31	118.73	124.80
12	bA	823	CLA	C3D-C4D-ND	4.31	117.00	109.99
12	bA	836	CLA	O2D-CGD-CBD	4.31	118.77	111.23
12	cA	835	CLA	C3D-C4D-ND	4.31	116.99	109.99
12	bB	901	CLA	CMA-C3A-C2A	-4.31	97.32	113.98
12	bA	814	CLA	C3B-C4B-NB	4.31	114.38	110.53
12	bB	930	CLA	C3D-C4D-ND	4.31	116.99	109.99
12	cB	915	CLA	C3D-C4D-ND	4.31	116.99	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cB	921	CLA	C3D-C4D-ND	4.30	116.98	109.99
12	bA	828	CLA	C3B-C4B-NB	4.30	114.37	110.53
12	bB	950	CLA	CMD-C2D-C1D	4.30	132.31	124.73
12	aB	923	CLA	C2B-C1B-NB	4.30	114.79	110.33
12	aB	901	CLA	C3C-C4C-NC	4.30	115.94	110.43
12	bB	911	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
12	cA	822	CLA	C3D-C4D-ND	4.30	116.98	109.99
12	bB	913	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
12	aB	929	CLA	CHD-C1D-ND	-4.30	118.75	124.80
12	bB	929	CLA	CHD-C1D-ND	-4.30	118.75	124.80
12	cB	913	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
12	cB	910	CLA	C2B-C1B-NB	4.30	114.79	110.33
12	aB	919	CLA	C4A-NA-C1A	-4.30	104.72	106.68
12	cB	913	CLA	C3B-C4B-NB	4.30	114.37	110.53
12	aA	808	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
12	bA	803	CLA	C3D-C4D-ND	4.30	116.97	109.99
12	cA	826	CLA	C3D-C4D-ND	4.30	116.97	109.99
12	aB	950	CLA	CMD-C2D-C1D	4.30	132.30	124.73
12	bB	933	CLA	C1C-C2C-C3C	-4.30	102.46	106.98
12	aA	828	CLA	C3B-C4B-NB	4.30	114.37	110.53
12	cA	823	CLA	C3D-C4D-ND	4.30	116.97	109.99
12	bA	824	CLA	O2D-CGD-CBD	4.30	118.74	111.23
12	bB	921	CLA	C3D-C4D-ND	4.30	116.97	109.99
12	cB	939	CLA	C3B-C4B-NB	4.30	114.36	110.53
12	bA	820	CLA	C2B-C1B-NB	4.30	114.78	110.33
12	bA	810	CLA	C3D-C4D-ND	4.30	116.97	109.99
12	cA	810	CLA	C3D-C4D-ND	4.30	116.97	109.99
12	bB	921	CLA	C4-C3-C5	4.29	122.68	115.23
12	cA	808	CLA	C3D-C2D-C1D	-4.29	99.97	105.83
12	bA	826	CLA	C3D-C4D-ND	4.29	116.97	109.99
12	cL	204	CLA	CHD-C1D-ND	-4.29	118.76	124.80
12	cF	202	CLA	C3D-C4D-ND	4.29	116.96	109.99
12	cB	911	CLA	C3D-C4D-ND	4.29	116.96	109.99
12	aB	910	CLA	C3B-C2B-C1B	-4.29	102.11	107.17
12	cA	814	CLA	C3B-C4B-NB	4.29	114.36	110.53
12	aB	905	CLA	C2C-C1C-NC	4.29	114.49	109.98
12	bB	911	CLA	C3D-C4D-ND	4.29	116.96	109.99
12	bB	901	CLA	C2B-C1B-NB	4.29	114.77	110.33
12	aB	915	CLA	CHD-C1D-ND	-4.29	118.77	124.80
12	aA	820	CLA	C2B-C1B-NB	4.29	114.77	110.33
12	aA	803	CLA	C3D-C4D-ND	4.29	116.96	109.99
12	cB	930	CLA	C3D-C4D-ND	4.29	116.95	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aB	915	CLA	C3D-C4D-ND	4.29	116.95	109.99
12	aB	913	CLA	C3D-C2D-C1D	-4.28	99.98	105.83
12	cA	824	CLA	C1C-C2C-C3C	-4.28	102.47	106.98
12	cB	921	CLA	C4-C3-C5	4.28	122.66	115.23
12	bB	950	CLA	CAC-C3C-C4C	4.28	130.36	124.79
12	aA	826	CLA	C3D-C4D-ND	4.28	116.95	109.99
12	aB	901	CLA	C2B-C1B-NB	4.28	114.77	110.33
12	aB	911	CLA	C3D-C4D-ND	4.28	116.94	109.99
12	cA	827	CLA	C2C-C1C-NC	4.28	114.48	109.98
12	bB	907	CLA	C3D-C2D-C1D	-4.28	99.99	105.83
12	bA	808	CLA	C3D-C2D-C1D	-4.28	99.99	105.83
12	aB	913	CLA	C3B-C4B-NB	4.28	114.35	110.53
12	aA	824	CLA	O2D-CGD-CBD	4.28	118.71	111.23
12	aB	921	CLA	C3D-C4D-ND	4.28	116.94	109.99
12	bA	822	CLA	C2C-C1C-NC	4.28	114.47	109.98
12	aA	844	CLA	C3B-C4B-NB	4.28	114.35	110.53
12	bB	915	CLA	CHD-C1D-ND	-4.27	118.79	124.80
12	bL	204	CLA	CHD-C1D-ND	-4.27	118.79	124.80
12	cB	929	CLA	C3D-C4D-ND	4.27	116.94	109.99
12	cA	824	CLA	O2D-CGD-CBD	4.27	118.70	111.23
12	cA	840	CLA	C3D-C4D-ND	4.27	116.94	109.99
12	cB	901	CLA	C3C-C4C-NC	4.27	115.90	110.43
12	bB	915	CLA	C1C-C2C-C3C	-4.27	102.49	106.98
12	cB	933	CLA	C1C-C2C-C3C	-4.27	102.49	106.98
12	aA	810	CLA	C3D-C4D-ND	4.27	116.93	109.99
12	cB	929	CLA	CHD-C1D-ND	-4.27	118.79	124.80
12	aB	950	CLA	CAC-C3C-C4C	4.27	130.35	124.79
12	aA	804	CLA	C2B-C1B-NB	4.27	114.75	110.33
12	aA	844	CLA	CMD-C2D-C1D	4.27	132.25	124.73
12	bA	804	CLA	C2B-C1B-NB	4.27	114.75	110.33
12	bB	939	CLA	C3B-C4B-NB	4.27	114.34	110.53
16	bB	948	LHG	O4-P-O5	4.27	132.29	112.44
12	cB	915	CLA	CHD-C1D-ND	-4.27	118.80	124.80
12	aB	907	CLA	C3D-C2D-C1D	-4.26	100.01	105.83
12	aA	844	CLA	CAC-C3C-C4C	4.26	130.34	124.79
12	aL	204	CLA	CHD-C1D-ND	-4.26	118.80	124.80
16	cB	948	LHG	O4-P-O5	4.26	132.27	112.44
12	cB	901	CLA	C2B-C1B-NB	4.26	114.75	110.33
12	aB	921	CLA	C4-C3-C5	4.26	122.63	115.23
12	bA	827	CLA	C2C-C1C-NC	4.26	114.46	109.98
16	aB	948	LHG	O4-P-O5	4.26	132.27	112.44
12	bB	913	CLA	C3B-C4B-NB	4.26	114.33	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	836	CLA	C3B-C2B-C1B	-4.26	102.15	107.17
12	aB	933	CLA	C1C-C2C-C3C	-4.26	102.50	106.98
12	cB	915	CLA	C1C-C2C-C3C	-4.26	102.50	106.98
12	aB	929	CLA	C3D-C4D-ND	4.26	116.91	109.99
12	cB	949	CLA	C1D-CHD-C4C	-4.26	116.97	126.02
12	bA	815	CLA	C3D-C4D-ND	4.26	116.91	109.99
12	aB	938	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
12	bB	949	CLA	C1D-CHD-C4C	-4.25	116.98	126.02
12	bB	908	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
12	cB	937	CLA	C3D-C4D-ND	4.25	116.90	109.99
12	bB	950	CLA	C3B-C4B-NB	4.25	114.33	110.53
12	aA	815	CLA	C3D-C4D-ND	4.25	116.90	109.99
12	bA	834	CLA	C1C-C2C-C3C	-4.25	102.51	106.98
12	aB	949	CLA	C1D-CHD-C4C	-4.25	116.99	126.02
12	cB	938	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
12	cB	924	CLA	CHD-C1D-ND	-4.25	118.82	124.80
12	bB	915	CLA	C3D-C4D-ND	4.25	116.89	109.99
12	aB	915	CLA	C1C-C2C-C3C	-4.25	102.51	106.98
12	cA	834	CLA	C1C-C2C-C3C	-4.25	102.51	106.98
12	bB	929	CLA	C3D-C4D-ND	4.25	116.89	109.99
12	aF	202	CLA	C4A-NA-C1A	-4.25	104.74	106.68
12	aB	910	CLA	C2B-C1B-NB	4.24	114.73	110.33
12	cA	815	CLA	C3D-C4D-ND	4.24	116.89	109.99
12	bB	949	CLA	C2C-C1C-NC	4.24	114.44	109.98
12	cA	841	CLA	C3D-C4D-ND	4.24	116.89	109.99
12	bA	841	CLA	C3D-C4D-ND	4.24	116.89	109.99
12	aA	826	CLA	CHD-C1D-ND	-4.24	118.83	124.80
12	bB	914	CLA	C3C-C4C-NC	4.24	115.86	110.43
12	bA	826	CLA	CHD-C1D-ND	-4.24	118.83	124.80
12	aA	836	CLA	C3B-C2B-C1B	-4.24	102.17	107.17
12	bB	924	CLA	C3D-C4D-ND	4.24	116.88	109.99
12	aB	918	CLA	C3D-C4D-ND	4.24	116.88	109.99
12	aB	938	CLA	C3D-C4D-ND	4.24	116.88	109.99
12	aB	914	CLA	C3C-C4C-NC	4.24	115.86	110.43
12	aA	822	CLA	C2C-C1C-NC	4.24	114.43	109.98
12	bB	901	CLA	C3C-C4C-NC	4.24	115.86	110.43
12	bB	938	CLA	C3D-C2D-C1D	-4.24	100.05	105.83
12	bB	917	CLA	C3B-C2B-C1B	-4.24	102.18	107.17
12	bA	836	CLA	C3B-C2B-C1B	-4.24	102.18	107.17
12	bA	803	CLA	C2C-C1C-NC	4.23	114.43	109.98
12	cA	822	CLA	C2C-C1C-NC	4.23	114.43	109.98
12	bA	806	CLA	C3B-C4B-NB	4.23	114.31	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	826	CLA	CHD-C1D-ND	-4.23	118.84	124.80
12	bB	937	CLA	C3D-C4D-ND	4.23	116.87	109.99
12	cA	803	CLA	C2C-C1C-NC	4.23	114.43	109.98
12	cB	907	CLA	C3D-C2D-C1D	-4.23	100.06	105.83
12	cB	912	CLA	C3C-C4C-NC	4.23	115.85	110.43
12	cA	835	CLA	C3D-C2D-C1D	-4.23	100.06	105.83
12	cB	924	CLA	C3D-C4D-ND	4.23	116.86	109.99
12	bB	915	CLA	C4A-NA-C1A	-4.23	104.75	106.68
12	cB	901	CLA	CAA-C2A-C3A	-4.23	101.57	113.00
12	bA	830	CLA	C4A-NA-C1A	-4.23	104.75	106.68
12	bB	901	CLA	CAA-C2A-C3A	-4.23	101.58	113.00
12	bB	938	CLA	C3D-C4D-ND	4.23	116.86	109.99
12	bA	804	CLA	CMD-C2D-C1D	4.23	132.17	124.73
12	aA	828	CLA	C3C-C4C-NC	4.23	115.84	110.43
12	bA	835	CLA	C3D-C2D-C1D	-4.22	100.07	105.83
12	aA	834	CLA	C1C-C2C-C3C	-4.22	102.54	106.98
12	aB	917	CLA	C3B-C2B-C1B	-4.22	102.19	107.17
12	aB	934	CLA	CHD-C1D-ND	-4.22	118.86	124.80
12	cA	804	CLA	C2B-C1B-NB	4.22	114.70	110.33
12	aB	937	CLA	C3D-C4D-ND	4.22	116.85	109.99
12	aB	916	CLA	CHD-C1D-ND	-4.22	118.86	124.80
12	aA	806	CLA	C3B-C4B-NB	4.22	114.30	110.53
12	cB	917	CLA	C3B-C2B-C1B	-4.22	102.20	107.17
12	aB	924	CLA	C3D-C4D-ND	4.22	116.84	109.99
12	cB	938	CLA	C3D-C4D-ND	4.22	116.84	109.99
12	bB	916	CLA	CHD-C1D-ND	-4.22	118.87	124.80
12	cB	918	CLA	C3D-C4D-ND	4.22	116.84	109.99
12	aA	835	CLA	C3D-C2D-C1D	-4.22	100.08	105.83
12	bA	812	CLA	C4A-NA-C1A	-4.22	104.76	106.68
12	aB	908	CLA	C3D-C2D-C1D	-4.21	100.08	105.83
12	aA	817	CLA	C4A-NA-C1A	-4.21	104.76	106.68
12	aB	901	CLA	CAA-C2A-C3A	-4.21	101.62	113.00
12	cB	914	CLA	C3C-C4C-NC	4.21	115.83	110.43
12	aA	841	CLA	C3D-C4D-ND	4.21	116.83	109.99
12	bB	904	CLA	CHD-C1D-ND	-4.21	118.88	124.80
12	bA	837	CLA	C4A-NA-C1A	-4.21	104.76	106.68
12	bB	909	CLA	C3C-C4C-NC	4.21	115.82	110.43
12	cA	838	CLA	C2B-C1B-NB	4.21	114.69	110.33
12	bB	924	CLA	CHD-C1D-ND	-4.21	118.88	124.80
12	aA	821	CLA	C3D-C4D-ND	4.21	116.83	109.99
12	aB	924	CLA	CHD-C1D-ND	-4.21	118.88	124.80
11	cA	801	CL0	CMA-C3A-C2A	-4.21	97.88	114.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cB	915	CLA	C4A-NA-C1A	-4.21	104.76	106.68
12	aA	838	CLA	C2B-C1B-NB	4.21	114.69	110.33
12	aB	912	CLA	C3C-C4C-NC	4.21	115.82	110.43
12	bB	910	CLA	C3D-C4D-ND	4.20	116.82	109.99
12	bB	912	CLA	C3C-C4C-NC	4.20	115.81	110.43
12	cB	909	CLA	C3C-C4C-NC	4.20	115.81	110.43
12	cB	908	CLA	C3D-C2D-C1D	-4.20	100.09	105.83
12	aB	950	CLA	C3B-C4B-NB	4.20	114.28	110.53
12	bB	925	CLA	C3C-C4C-NC	4.20	115.81	110.43
11	aA	801	CL0	CMA-C3A-C2A	-4.20	97.90	114.13
12	aA	812	CLA	C4A-NA-C1A	-4.20	104.76	106.68
12	cA	832	CLA	C3D-C4D-ND	4.20	116.82	109.99
12	aA	803	CLA	C2C-C1C-NC	4.20	114.39	109.98
11	bA	801	CL0	CMA-C3A-C2A	-4.20	97.90	114.13
12	bB	934	CLA	CHD-C1D-ND	-4.20	118.89	124.80
12	bB	918	CLA	C3D-C4D-ND	4.20	116.81	109.99
12	cB	916	CLA	CHD-C1D-ND	-4.20	118.89	124.80
12	aB	949	CLA	C2C-C1C-NC	4.20	114.39	109.98
12	aB	904	CLA	CHD-C1D-ND	-4.20	118.90	124.80
12	cA	806	CLA	C3B-C4B-NB	4.19	114.27	110.53
12	aA	830	CLA	C4A-NA-C1A	-4.19	104.77	106.68
12	bL	203	CLA	C2C-C1C-NC	4.19	114.39	109.98
12	bB	923	CLA	C3C-C4C-NC	4.19	115.80	110.43
12	cB	910	CLA	C3D-C4D-ND	4.19	116.80	109.99
12	aA	804	CLA	CMD-C2D-C1D	4.19	132.11	124.73
12	aB	909	CLA	C3C-C4C-NC	4.19	115.80	110.43
12	cA	828	CLA	C3C-C4C-NC	4.19	115.80	110.43
12	aB	910	CLA	C3D-C4D-ND	4.19	116.80	109.99
12	cA	811	CLA	CHD-C1D-ND	-4.19	118.91	124.80
12	cA	821	CLA	C2B-C1B-NB	4.19	114.67	110.33
12	aB	904	CLA	C3B-C4B-NB	4.19	114.27	110.53
12	cA	811	CLA	C3D-C4D-ND	4.19	116.79	109.99
15	aL	201	BCR	C2-C1-C6	4.19	116.52	110.44
12	bA	832	CLA	C3D-C4D-ND	4.19	116.79	109.99
12	cB	904	CLA	CHD-C1D-ND	-4.18	118.91	124.80
12	bA	811	CLA	C3D-C4D-ND	4.18	116.79	109.99
12	cB	925	CLA	C3C-C4C-NC	4.18	115.79	110.43
12	aA	826	CLA	C1C-C2C-C3C	-4.18	102.58	106.98
12	cA	842	CLA	C1C-C2C-C3C	-4.18	102.58	106.98
12	aL	203	CLA	C2C-C1C-NC	4.18	114.38	109.98
12	cB	949	CLA	C2C-C1C-NC	4.18	114.38	109.98
12	cA	811	CLA	C4A-NA-C1A	-4.18	104.77	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	838	CLA	C2B-C1B-NB	4.18	114.66	110.33
12	cA	802	CLA	C3D-C4D-ND	4.18	116.78	109.99
12	aB	932	CLA	C2C-C1C-NC	4.18	114.37	109.98
12	cA	804	CLA	CMD-C2D-C1D	4.18	132.09	124.73
12	aA	802	CLA	C3D-C4D-ND	4.18	116.78	109.99
12	aB	925	CLA	C3C-C4C-NC	4.18	115.78	110.43
12	aA	820	CLA	C3D-C4D-ND	4.18	116.78	109.99
12	cB	949	CLA	C3D-C4D-ND	4.18	116.78	109.99
12	bB	949	CLA	C3D-C4D-ND	4.18	116.78	109.99
12	aA	819	CLA	C3D-C4D-ND	4.17	116.77	109.99
12	aA	811	CLA	CHD-C1D-ND	-4.17	118.93	124.80
12	bA	811	CLA	CHD-C1D-ND	-4.17	118.93	124.80
12	bB	932	CLA	C2C-C1C-NC	4.17	114.36	109.98
12	aB	920	CLA	C1C-C2C-C3C	-4.17	102.59	106.98
12	cB	917	CLA	CHD-C1D-ND	-4.17	118.93	124.80
12	cA	837	CLA	C4A-NA-C1A	-4.17	104.78	106.68
12	aA	834	CLA	CHD-C1D-ND	-4.17	118.93	124.80
12	aA	832	CLA	C3D-C4D-ND	4.17	116.77	109.99
12	cB	922	CLA	C3D-C2D-C1D	-4.17	100.14	105.83
12	aA	842	CLA	C1C-C2C-C3C	-4.17	102.59	106.98
12	cA	834	CLA	CHD-C1D-ND	-4.17	118.94	124.80
12	aB	922	CLA	C3D-C2D-C1D	-4.17	100.14	105.83
12	cB	934	CLA	CHD-C1D-ND	-4.17	118.94	124.80
12	bA	821	CLA	C3D-C4D-ND	4.17	116.76	109.99
12	bA	834	CLA	CHD-C1D-ND	-4.17	118.94	124.80
12	cB	923	CLA	C3C-C4C-NC	4.17	115.77	110.43
12	cL	203	CLA	C2C-C1C-NC	4.17	114.36	109.98
12	aB	925	CLA	C1D-CHD-C4C	-4.17	117.17	126.02
12	cA	819	CLA	C3D-C4D-ND	4.17	116.76	109.99
12	bA	826	CLA	C1C-C2C-C3C	-4.17	102.60	106.98
12	cB	910	CLA	C1C-C2C-C3C	-4.17	102.60	106.98
15	cL	201	BCR	C2-C1-C6	4.16	116.49	110.44
12	bA	819	CLA	C3D-C4D-ND	4.16	116.76	109.99
12	cA	830	CLA	C4A-NA-C1A	-4.16	104.78	106.68
12	bB	910	CLA	CHD-C1D-ND	-4.16	118.94	124.80
12	cB	915	CLA	C1D-CHD-C4C	-4.16	117.17	126.02
12	bA	828	CLA	C3C-C4C-NC	4.16	115.76	110.43
12	bA	821	CLA	C2B-C1B-NB	4.16	114.64	110.33
12	bB	915	CLA	C1D-CHD-C4C	-4.16	117.17	126.02
12	cB	927	CLA	C3D-C4D-ND	4.16	116.75	109.99
12	aB	926	CLA	C2C-C1C-NC	4.16	114.35	109.98
12	cA	821	CLA	C3D-C4D-ND	4.16	116.75	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aB	917	CLA	CHD-C1D-ND	-4.16	118.95	124.80
12	bA	820	CLA	C3D-C4D-ND	4.16	116.75	109.99
12	cB	904	CLA	C3B-C4B-NB	4.16	114.24	110.53
12	cA	838	CLA	C3B-C2B-C1B	-4.16	102.27	107.17
12	bB	926	CLA	C2C-C1C-NC	4.16	114.35	109.98
12	bB	922	CLA	C3D-C2D-C1D	-4.16	100.16	105.83
12	aB	923	CLA	C3C-C4C-NC	4.16	115.76	110.43
12	bB	904	CLA	C3B-C4B-NB	4.16	114.24	110.53
12	aA	831	CLA	C3D-C2D-C1D	-4.16	100.16	105.83
12	aB	915	CLA	C1D-CHD-C4C	-4.16	117.19	126.02
12	bA	819	CLA	C4A-NA-C1A	-4.15	104.78	106.68
12	cB	935	CLA	C4A-NA-C1A	-4.15	104.78	106.68
12	bA	842	CLA	C1C-C2C-C3C	-4.15	102.61	106.98
12	bA	836	CLA	C3D-C4D-ND	4.15	116.74	109.99
12	cB	926	CLA	C2C-C1C-NC	4.15	114.34	109.98
12	cA	836	CLA	C3D-C4D-ND	4.15	116.73	109.99
12	cA	820	CLA	C3D-C4D-ND	4.15	116.73	109.99
12	cA	831	CLA	C3D-C2D-C1D	-4.15	100.17	105.83
12	bB	925	CLA	C1D-CHD-C4C	-4.15	117.20	126.02
12	cB	932	CLA	C2C-C1C-NC	4.15	114.34	109.98
12	aB	910	CLA	CHD-C1D-ND	-4.15	118.96	124.80
12	aB	949	CLA	C3D-C4D-ND	4.15	116.73	109.99
12	cA	804	CLA	C1-O2A-CGA	4.15	126.69	116.65
12	cB	927	CLA	C3B-C2B-C1B	-4.15	102.28	107.17
12	aA	835	CLA	O2D-CGD-CBD	4.15	118.48	111.23
12	bA	802	CLA	C3D-C4D-ND	4.15	116.73	109.99
12	cA	826	CLA	C1C-C2C-C3C	-4.14	102.62	106.98
12	cB	925	CLA	C1D-CHD-C4C	-4.14	117.21	126.02
12	bB	910	CLA	C1C-C2C-C3C	-4.14	102.62	106.98
12	cB	920	CLA	C1C-C2C-C3C	-4.14	102.62	106.98
12	aA	836	CLA	C3D-C4D-ND	4.14	116.72	109.99
12	aA	821	CLA	C2B-C1B-NB	4.14	114.62	110.33
12	bB	931	CLA	C2C-C1C-NC	4.14	114.33	109.98
12	aB	927	CLA	C3B-C2B-C1B	-4.14	102.29	107.17
12	bB	927	CLA	C3C-C4C-NC	4.14	115.73	110.43
15	bL	201	BCR	C2-C1-C6	4.14	116.45	110.44
12	bA	831	CLA	C3D-C2D-C1D	-4.14	100.18	105.83
12	aA	804	CLA	C1-O2A-CGA	4.14	126.67	116.65
12	bA	804	CLA	C1-O2A-CGA	4.14	126.67	116.65
12	aB	927	CLA	C3C-C4C-NC	4.14	115.73	110.43
12	cA	827	CLA	C3C-C4C-NC	4.14	115.73	110.43
12	cA	838	CLA	CHD-C1D-ND	-4.14	118.98	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	811	CLA	C3D-C4D-ND	4.14	116.71	109.99
12	aB	927	CLA	C3D-C4D-ND	4.14	116.71	109.99
12	bB	920	CLA	C1C-C2C-C3C	-4.14	102.63	106.98
12	aB	914	CLA	C3D-C4D-ND	4.13	116.71	109.99
12	aA	814	CLA	C3D-C4D-ND	4.13	116.71	109.99
12	cB	921	CLA	CHD-C1D-ND	-4.13	118.99	124.80
12	aB	928	CLA	C3C-C4C-NC	4.13	115.72	110.43
12	cB	929	CLA	C3C-C4C-NC	4.13	115.72	110.43
12	bB	917	CLA	CHD-C1D-ND	-4.13	118.99	124.80
12	bA	827	CLA	C3C-C4C-NC	4.13	115.72	110.43
12	bB	934	CLA	C3D-C4D-ND	4.13	116.70	109.99
12	cA	835	CLA	O2D-CGD-CBD	4.13	118.45	111.23
12	aA	838	CLA	C3B-C2B-C1B	-4.13	102.30	107.17
12	cB	917	CLA	C4A-NA-C1A	-4.13	104.80	106.68
12	aA	821	CLA	O2D-CGD-CBD	4.13	118.45	111.23
12	cB	910	CLA	CHD-C1D-ND	-4.13	118.99	124.80
12	cA	814	CLA	C3D-C4D-ND	4.13	116.69	109.99
12	aB	931	CLA	C2C-C1C-NC	4.13	114.32	109.98
12	aB	915	CLA	C4A-NA-C1A	-4.13	104.80	106.68
12	cA	819	CLA	O2A-CGA-CBA	4.12	124.41	111.83
12	aA	838	CLA	CHD-C1D-ND	-4.12	119.00	124.80
12	bA	815	CLA	C4A-NA-C1A	-4.12	104.80	106.68
12	aA	835	CLA	C3B-C2B-C1B	-4.12	102.31	107.17
12	bA	838	CLA	C3B-C2B-C1B	-4.12	102.31	107.17
12	aA	808	CLA	CHD-C1D-ND	-4.12	119.00	124.80
12	bA	838	CLA	CHD-C1D-ND	-4.12	119.00	124.80
12	bA	822	CLA	C1C-C2C-C3C	-4.12	102.65	106.98
12	aA	827	CLA	C3C-C4C-NC	4.12	115.71	110.43
12	cB	931	CLA	C2C-C1C-NC	4.12	114.31	109.98
12	cA	808	CLA	CHD-C1D-ND	-4.12	119.00	124.80
12	bA	811	CLA	C4A-NA-C1A	-4.12	104.80	106.68
12	cA	823	CLA	C4A-NA-C1A	-4.12	104.80	106.68
12	aB	904	CLA	C3D-C4D-ND	4.12	116.68	109.99
12	bA	821	CLA	O2D-CGD-CBD	4.12	118.43	111.23
12	cB	927	CLA	C3C-C4C-NC	4.12	115.70	110.43
12	bA	814	CLA	C3D-C4D-ND	4.12	116.68	109.99
12	bB	914	CLA	C3D-C4D-ND	4.12	116.68	109.99
12	bA	835	CLA	O2D-CGD-CBD	4.11	118.42	111.23
12	bB	927	CLA	C3D-C4D-ND	4.11	116.67	109.99
12	bB	927	CLA	C4B-C3B-C2B	-4.11	102.19	107.30
12	aA	819	CLA	O2A-CGA-CBA	4.11	124.36	111.83
12	cB	934	CLA	C3D-C4D-ND	4.11	116.67	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	812	CLA	C4A-NA-C1A	-4.11	104.81	106.68
12	cA	817	CLA	CHD-C1D-ND	-4.11	119.02	124.80
12	bA	819	CLA	O2A-CGA-CBA	4.11	124.36	111.83
12	cB	927	CLA	C4B-C3B-C2B	-4.11	102.20	107.30
12	cB	928	CLA	C3C-C4C-NC	4.11	115.69	110.43
12	aB	907	CLA	C1D-CHD-C4C	-4.11	117.29	126.02
12	cA	821	CLA	O2D-CGD-CBD	4.10	118.41	111.23
12	aB	910	CLA	C1C-C2C-C3C	-4.10	102.66	106.98
12	aB	950	CLA	C3D-C4D-ND	4.10	116.66	109.99
12	bB	928	CLA	C3C-C4C-NC	4.10	115.69	110.43
12	cA	825	CLA	C3C-C4C-NC	4.10	115.69	110.43
12	aA	805	CLA	C3D-C4D-ND	4.10	116.66	109.99
12	aA	825	CLA	C3C-C4C-NC	4.10	115.68	110.43
12	aA	842	CLA	C3C-C4C-NC	4.10	115.68	110.43
12	bB	921	CLA	CHD-C1D-ND	-4.10	119.03	124.80
12	aB	921	CLA	CHD-C1D-ND	-4.10	119.03	124.80
12	bB	924	CLA	C3B-C4B-NB	4.10	114.19	110.53
12	cB	907	CLA	C1D-CHD-C4C	-4.10	117.31	126.02
12	bB	933	CLA	C3D-C4D-ND	4.10	116.65	109.99
12	cA	805	CLA	C3D-C4D-ND	4.10	116.65	109.99
12	aA	807	CLA	C1D-CHD-C4C	-4.10	117.31	126.02
12	aB	909	CLA	C3B-C2B-C1B	-4.10	102.34	107.17
12	bB	907	CLA	C1D-CHD-C4C	-4.10	117.32	126.02
12	aB	923	CLA	C3D-C4D-ND	4.09	116.64	109.99
12	cB	914	CLA	C3D-C4D-ND	4.09	116.64	109.99
12	aB	917	CLA	C4A-NA-C1A	-4.09	104.81	106.68
12	bA	838	CLA	C4A-NA-C1A	-4.09	104.81	106.68
12	cA	842	CLA	C3C-C4C-NC	4.09	115.67	110.43
12	bA	808	CLA	CHD-C1D-ND	-4.09	119.05	124.80
12	bB	917	CLA	C4A-NA-C1A	-4.09	104.81	106.68
12	bB	904	CLA	C3D-C4D-ND	4.09	116.64	109.99
12	bB	927	CLA	C3B-C2B-C1B	-4.09	102.35	107.17
12	bA	817	CLA	CHD-C1D-ND	-4.09	119.05	124.80
12	cA	835	CLA	C3B-C2B-C1B	-4.09	102.35	107.17
12	aA	823	CLA	C4A-NA-C1A	-4.09	104.81	106.68
12	cA	838	CLA	C4A-NA-C1A	-4.09	104.81	106.68
12	cB	904	CLA	C3D-C4D-ND	4.09	116.63	109.99
12	bB	935	CLA	C4A-NA-C1A	-4.09	104.81	106.68
12	aA	833	CLA	CHD-C1D-ND	-4.09	119.05	124.80
12	aA	844	CLA	C3D-C4D-ND	4.08	116.62	109.99
12	aB	934	CLA	C3D-C4D-ND	4.08	116.62	109.99
12	bA	805	CLA	C3D-C4D-ND	4.08	116.62	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cB	923	CLA	C3D-C4D-ND	4.08	116.62	109.99
12	aA	822	CLA	C1C-C2C-C3C	-4.08	102.69	106.98
12	bB	902	CLA	C3D-C4D-ND	4.08	116.62	109.99
12	cA	839	CLA	C3D-C4D-ND	4.08	116.62	109.99
12	cB	933	CLA	C3D-C4D-ND	4.08	116.62	109.99
12	cA	807	CLA	C1D-CHD-C4C	-4.08	117.35	126.02
12	aA	813	CLA	C3C-C4C-NC	4.08	115.66	110.43
12	aB	924	CLA	C3B-C4B-NB	4.08	114.17	110.53
12	cB	901	CLA	O2D-CGD-CBD	4.08	118.36	111.23
12	bA	807	CLA	C1D-CHD-C4C	-4.08	117.35	126.02
12	bB	909	CLA	C2B-C1B-NB	4.08	114.55	110.33
12	aA	837	CLA	C4A-NA-C1A	-4.08	104.82	106.68
12	cB	902	CLA	C3D-C4D-ND	4.08	116.61	109.99
12	aB	909	CLA	C2B-C1B-NB	4.08	114.55	110.33
12	cA	833	CLA	CHD-C1D-ND	-4.08	119.07	124.80
12	aB	902	CLA	C3D-C4D-ND	4.07	116.61	109.99
12	aB	925	CLA	C4A-NA-C1A	-4.07	104.82	106.68
12	bA	839	CLA	C3D-C4D-ND	4.07	116.61	109.99
13	bA	844	1L3	C24-C25-C26	-4.07	118.30	127.62
12	aB	932	CLA	CMB-C2B-C1B	4.07	131.62	125.42
12	bB	950	CLA	C3D-C4D-ND	4.07	116.61	109.99
12	aB	912	CLA	C3D-C4D-ND	4.07	116.61	109.99
12	cA	828	CLA	C3D-C4D-ND	4.07	116.61	109.99
12	bA	835	CLA	C3B-C2B-C1B	-4.07	102.37	107.17
12	aB	901	CLA	CMB-C2B-C1B	4.07	131.62	125.42
12	cB	927	CLA	C3B-C4B-NB	4.07	114.16	110.53
12	aB	927	CLA	C4B-C3B-C2B	-4.07	102.24	107.30
12	cB	909	CLA	C2B-C1B-NB	4.07	114.55	110.33
12	bB	901	CLA	O2D-CGD-CBD	4.07	118.34	111.23
12	aA	816	CLA	C1D-CHD-C4C	-4.07	117.37	126.02
12	bA	816	CLA	C1D-CHD-C4C	-4.06	117.38	126.02
12	bB	909	CLA	C3B-C2B-C1B	-4.06	102.38	107.17
12	bA	813	CLA	C3C-C4C-NC	4.06	115.64	110.43
12	cB	925	CLA	C4A-NA-C1A	-4.06	104.83	106.68
12	aA	828	CLA	C3D-C4D-ND	4.06	116.59	109.99
12	bB	923	CLA	C3D-C4D-ND	4.06	116.59	109.99
12	bB	901	CLA	CMB-C2B-C1B	4.06	131.60	125.42
12	cB	912	CLA	C3D-C4D-ND	4.06	116.59	109.99
12	bA	828	CLA	C3D-C4D-ND	4.06	116.59	109.99
12	cB	932	CLA	CMB-C2B-C1B	4.06	131.60	125.42
12	aB	929	CLA	C3C-C4C-NC	4.06	115.63	110.43
12	aA	834	CLA	C3D-C4D-ND	4.06	116.58	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aB	922	CLA	C3D-C4D-ND	4.06	116.58	109.99
12	cA	818	CLA	C3D-C4D-ND	4.06	116.58	109.99
12	aA	839	CLA	C3D-C4D-ND	4.06	116.58	109.99
12	cL	202	CLA	C4A-NA-C1A	-4.06	104.83	106.68
12	aA	839	CLA	C3C-C4C-NC	4.05	115.62	110.43
12	cB	901	CLA	CMB-C2B-C1B	4.05	131.59	125.42
12	cA	816	CLA	C1D-CHD-C4C	-4.05	117.41	126.02
12	cA	810	CLA	CHD-C1D-ND	-4.05	119.10	124.80
12	aA	817	CLA	CHD-C1D-ND	-4.05	119.10	124.80
12	bB	912	CLA	C3D-C4D-ND	4.05	116.57	109.99
12	bA	825	CLA	C3C-C4C-NC	4.05	115.62	110.43
12	bA	809	CLA	C3D-C4D-ND	4.05	116.57	109.99
12	aB	929	CLA	C1C-C2C-C3C	-4.05	102.72	106.98
12	bB	915	CLA	C3C-C4C-NC	4.05	115.62	110.43
12	aB	933	CLA	C3D-C4D-ND	4.05	116.57	109.99
13	cA	844	1L3	C24-C25-C26	-4.05	118.36	127.62
12	bB	929	CLA	C3C-C4C-NC	4.05	115.61	110.43
12	bA	842	CLA	C3C-C4C-NC	4.05	115.61	110.43
12	bB	921	CLA	C1C-C2C-C3C	-4.05	102.72	106.98
12	cB	915	CLA	C3C-C4C-NC	4.04	115.61	110.43
12	aA	809	CLA	C3D-C4D-ND	4.04	116.56	109.99
12	aA	834	CLA	O2D-CGD-O1D	-4.04	115.98	123.85
12	aA	811	CLA	C4A-NA-C1A	-4.04	104.83	106.68
12	cB	935	CLA	C1C-C2C-C3C	-4.04	102.73	106.98
12	cA	809	CLA	C3D-C4D-ND	4.04	116.56	109.99
12	cB	909	CLA	C3B-C2B-C1B	-4.04	102.41	107.17
12	bA	804	CLA	C3B-C4B-NB	4.04	114.14	110.53
12	aA	810	CLA	CHD-C1D-ND	-4.04	119.12	124.80
12	cA	822	CLA	C1C-C2C-C3C	-4.04	102.73	106.98
12	aA	842	CLA	C3D-C4D-ND	4.04	116.55	109.99
12	cA	838	CLA	C1C-C2C-C3C	-4.04	102.73	106.98
13	aA	845	1L3	C24-C25-C26	-4.04	118.38	127.62
12	bA	839	CLA	C3C-C4C-NC	4.04	115.60	110.43
12	bB	932	CLA	CMB-C2B-C1B	4.04	131.56	125.42
12	cA	813	CLA	C3C-C4C-NC	4.04	115.60	110.43
12	bA	818	CLA	C3D-C4D-ND	4.03	116.55	109.99
12	cA	839	CLA	C1C-C2C-C3C	-4.03	102.74	106.98
12	cA	839	CLA	C3C-C4C-NC	4.03	115.60	110.43
12	cA	834	CLA	O2D-CGD-O1D	-4.03	116.00	123.85
12	aB	901	CLA	O2D-CGD-CBD	4.03	118.28	111.23
12	aA	816	CLA	C3C-C4C-NC	4.03	115.59	110.43
12	cB	929	CLA	C1C-C2C-C3C	-4.03	102.74	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	815	CLA	C4A-NA-C1A	-4.03	104.84	106.68
12	aA	839	CLA	C1C-C2C-C3C	-4.03	102.74	106.98
12	cB	924	CLA	C3B-C4B-NB	4.03	114.13	110.53
12	cA	834	CLA	C3D-C4D-ND	4.03	116.53	109.99
12	bA	834	CLA	O2D-CGD-O1D	-4.03	116.01	123.85
12	aB	935	CLA	C4A-NA-C1A	-4.03	104.84	106.68
12	bL	202	CLA	C4A-NA-C1A	-4.03	104.84	106.68
12	cA	842	CLA	C3D-C4D-ND	4.03	116.53	109.99
12	bB	927	CLA	C3B-C4B-NB	4.02	114.12	110.53
12	bA	823	CLA	C4A-NA-C1A	-4.02	104.84	106.68
12	bA	839	CLA	C1C-C2C-C3C	-4.02	102.75	106.98
12	bA	834	CLA	C3D-C4D-ND	4.02	116.53	109.99
12	bA	816	CLA	C3C-C4C-NC	4.02	115.58	110.43
12	bA	842	CLA	C3D-C4D-ND	4.02	116.52	109.99
12	aA	818	CLA	C3D-C4D-ND	4.02	116.52	109.99
12	bB	935	CLA	C1C-C2C-C3C	-4.02	102.75	106.98
12	aA	854	CLA	C3D-C4D-ND	4.02	116.52	109.99
12	aA	838	CLA	C1C-C2C-C3C	-4.02	102.75	106.98
12	aB	915	CLA	C3C-C4C-NC	4.02	115.58	110.43
12	aB	935	CLA	C1C-C2C-C3C	-4.02	102.76	106.98
12	aB	927	CLA	C3B-C4B-NB	4.02	114.11	110.53
12	aA	819	CLA	C4A-NA-C1A	-4.02	104.85	106.68
12	bA	833	CLA	CHD-C1D-ND	-4.01	119.15	124.80
12	bA	810	CLA	CHD-C1D-ND	-4.01	119.15	124.80
12	bA	825	CLA	CHD-C1D-ND	-4.01	119.16	124.80
12	bA	830	CLA	C3C-C4C-NC	4.01	115.57	110.43
12	bA	853	CLA	C3D-C4D-ND	4.01	116.50	109.99
12	cA	816	CLA	C3C-C4C-NC	4.01	115.56	110.43
12	cA	819	CLA	C1C-C2C-C3C	-4.01	102.77	106.98
12	cA	832	CLA	CHD-C1D-ND	-4.00	119.17	124.80
12	aA	832	CLA	CHD-C1D-ND	-4.00	119.17	124.80
12	aA	838	CLA	C4A-NA-C1A	-4.00	104.85	106.68
12	cB	904	CLA	C4A-NA-C1A	-4.00	104.85	106.68
12	bA	832	CLA	CHD-C1D-ND	-4.00	119.17	124.80
12	bB	927	CLA	C1C-C2C-C3C	-4.00	102.77	106.98
12	cA	805	CLA	CHD-C1D-ND	-4.00	119.17	124.80
12	aA	815	CLA	C4A-NA-C1A	-4.00	104.85	106.68
12	aA	854	CLA	C4A-NA-C1A	-4.00	104.85	106.68
12	aA	843	CLA	C1C-C2C-C3C	-4.00	102.77	106.98
12	aB	921	CLA	C1C-C2C-C3C	-4.00	102.77	106.98
12	bB	922	CLA	C3D-C4D-ND	4.00	116.49	109.99
12	cB	934	CLA	C4B-C3B-C2B	-4.00	102.33	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	805	CLA	CHD-C1D-ND	-4.00	119.18	124.80
12	aA	835	CLA	C3C-C4C-NC	4.00	115.55	110.43
12	bA	835	CLA	C3C-C4C-NC	3.99	115.55	110.43
12	bB	918	CLA	C4A-NA-C1A	-3.99	104.86	106.68
12	cB	921	CLA	C1C-C2C-C3C	-3.99	102.78	106.98
12	bA	838	CLA	C1C-C2C-C3C	-3.99	102.78	106.98
12	aA	805	CLA	CHD-C1D-ND	-3.99	119.19	124.80
12	cA	825	CLA	CHD-C1D-ND	-3.99	119.19	124.80
12	bB	934	CLA	C4B-C3B-C2B	-3.99	102.34	107.30
12	aB	918	CLA	C4A-NA-C1A	-3.99	104.86	106.68
12	cA	853	CLA	C3D-C4D-ND	3.99	116.47	109.99
12	cB	922	CLA	C3D-C4D-ND	3.99	116.47	109.99
12	aA	827	CLA	C1D-CHD-C4C	-3.99	117.54	126.02
12	aA	825	CLA	CHD-C1D-ND	-3.99	119.19	124.80
12	cA	812	CLA	CHD-C1D-ND	-3.99	119.19	124.80
12	bB	929	CLA	C1C-C2C-C3C	-3.98	102.79	106.98
12	bA	827	CLA	C1D-CHD-C4C	-3.98	117.55	126.02
12	cL	202	CLA	C1C-C2C-C3C	-3.98	102.79	106.98
12	bB	925	CLA	C4A-NA-C1A	-3.98	104.86	106.68
12	cA	827	CLA	C1D-CHD-C4C	-3.98	117.56	126.02
12	cA	833	CLA	C3D-C4D-ND	3.98	116.46	109.99
12	aA	802	CLA	C2B-C1B-NB	3.98	114.45	110.33
12	cA	804	CLA	C3B-C4B-NB	3.98	114.08	110.53
12	cB	939	CLA	CMB-C2B-C1B	3.97	131.47	125.42
12	aL	202	CLA	C1C-C2C-C3C	-3.97	102.80	106.98
12	bB	911	CLA	C1C-C2C-C3C	-3.97	102.80	106.98
12	bA	812	CLA	C3D-C4D-ND	3.97	116.44	109.99
12	cA	804	CLA	C3C-C4C-NC	3.97	115.52	110.43
12	bA	824	CLA	CAC-C3C-C4C	3.97	129.95	124.79
12	cA	802	CLA	C2B-C1B-NB	3.97	114.44	110.33
12	aA	804	CLA	C3B-C4B-NB	3.97	114.07	110.53
15	bA	850	BCR	C2-C1-C6	3.97	116.20	110.44
12	aA	833	CLA	C3D-C4D-ND	3.96	116.43	109.99
12	bB	939	CLA	CMB-C2B-C1B	3.96	131.46	125.42
12	aA	819	CLA	C1C-C2C-C3C	-3.96	102.81	106.98
12	cA	830	CLA	C3C-C4C-NC	3.96	115.51	110.43
12	cB	918	CLA	CHD-C1D-ND	-3.96	119.22	124.80
12	aA	813	CLA	C3D-C4D-ND	3.96	116.43	109.99
12	cA	823	CLA	C3C-C4C-NC	3.96	115.50	110.43
12	aA	823	CLA	C3C-C4C-NC	3.96	115.50	110.43
12	aA	830	CLA	C3C-C4C-NC	3.96	115.50	110.43
12	aA	812	CLA	C1C-C2C-C3C	-3.96	102.82	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	816	CLA	C3D-C4D-ND	3.96	116.42	109.99
12	bA	831	CLA	C3C-C4C-NC	3.96	115.50	110.43
15	cA	850	BCR	C2-C1-C6	3.96	116.19	110.44
12	cA	805	CLA	C2C-C1C-NC	3.96	114.14	109.98
12	aB	934	CLA	C4B-C3B-C2B	-3.96	102.38	107.30
12	bL	202	CLA	C1C-C2C-C3C	-3.96	102.82	106.98
12	aB	913	CLA	C1C-C2C-C3C	-3.96	102.82	106.98
12	cB	927	CLA	C1C-C2C-C3C	-3.96	102.82	106.98
12	cA	813	CLA	C3D-C4D-ND	3.96	116.42	109.99
12	aA	804	CLA	C3C-C4C-NC	3.96	115.50	110.43
12	cA	812	CLA	C1C-C2C-C3C	-3.96	102.82	106.98
12	aB	918	CLA	CHD-C1D-ND	-3.96	119.24	124.80
12	aA	812	CLA	CHD-C1D-ND	-3.95	119.24	124.80
12	bA	823	CLA	C3C-C4C-NC	3.95	115.50	110.43
12	aA	808	CLA	C1C-C2C-C3C	-3.95	102.82	106.98
12	bA	819	CLA	C1C-C2C-C3C	-3.95	102.82	106.98
12	aA	812	CLA	C3D-C4D-ND	3.95	116.41	109.99
12	aB	939	CLA	CMB-C2B-C1B	3.95	131.44	125.42
12	cA	812	CLA	C3D-C4D-ND	3.95	116.41	109.99
15	aA	851	BCR	C2-C1-C6	3.95	116.18	110.44
12	bA	813	CLA	C3D-C4D-ND	3.95	116.41	109.99
12	cA	816	CLA	C3D-C4D-ND	3.95	116.41	109.99
12	bA	843	CLA	C1C-C2C-C3C	-3.95	102.83	106.98
12	bA	833	CLA	C3D-C4D-ND	3.95	116.40	109.99
12	aA	837	CLA	C3C-C4C-NC	3.95	115.49	110.43
12	cA	835	CLA	C3C-C4C-NC	3.95	115.48	110.43
12	bA	812	CLA	C1C-C2C-C3C	-3.95	102.83	106.98
12	cB	913	CLA	C1C-C2C-C3C	-3.95	102.83	106.98
12	aA	842	CLA	CHD-C1D-ND	-3.95	119.25	124.80
12	bA	823	CLA	CHD-C1D-ND	-3.95	119.25	124.80
12	bB	901	CLA	C3D-C4D-ND	3.94	116.40	109.99
12	bA	815	CLA	CHD-C1D-ND	-3.94	119.25	124.80
12	bA	812	CLA	CHD-C1D-ND	-3.94	119.25	124.80
12	bA	840	CLA	CHD-C1D-ND	-3.94	119.25	124.80
12	aB	911	CLA	C1C-C2C-C3C	-3.94	102.83	106.98
12	aA	816	CLA	C3D-C4D-ND	3.94	116.40	109.99
12	bA	805	CLA	C2C-C1C-NC	3.94	114.12	109.98
12	bA	837	CLA	C3C-C4C-NC	3.94	115.48	110.43
12	aA	831	CLA	C3C-C4C-NC	3.94	115.48	110.43
12	cA	819	CLA	C4A-NA-C1A	-3.94	104.88	106.68
12	cB	936	CLA	C4A-NA-C1A	-3.94	104.88	106.68
12	aB	927	CLA	C1C-C2C-C3C	-3.94	102.83	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	808	CLA	C1C-C2C-C3C	-3.94	102.83	106.98
12	bA	833	CLA	C1C-C2C-C3C	-3.94	102.84	106.98
12	cA	843	CLA	C1C-C2C-C3C	-3.94	102.84	106.98
12	bB	909	CLA	C1C-C2C-C3C	-3.94	102.84	106.98
12	bB	914	CLA	CHD-C1D-ND	-3.94	119.26	124.80
12	bB	926	CLA	C3D-C4D-ND	3.94	116.39	109.99
12	bB	949	CLA	C4A-NA-C1A	-3.94	104.88	106.68
12	cB	907	CLA	C3D-C4D-ND	3.94	116.39	109.99
12	aA	829	CLA	C3B-C4B-NB	3.94	114.04	110.53
12	cB	901	CLA	C3D-C4D-ND	3.93	116.38	109.99
12	aA	854	CLA	CHD-C1D-ND	-3.93	119.27	124.80
12	bA	804	CLA	C3C-C4C-NC	3.93	115.47	110.43
12	aA	835	CLA	C4A-NA-C1A	-3.93	104.89	106.68
12	cB	926	CLA	C3D-C4D-ND	3.93	116.38	109.99
12	bA	802	CLA	C2B-C1B-NB	3.93	114.40	110.33
12	cA	842	CLA	CHD-C1D-ND	-3.93	119.27	124.80
12	aB	907	CLA	C2B-C1B-NB	3.93	114.40	110.33
12	aB	901	CLA	C3D-C4D-ND	3.93	116.37	109.99
12	bB	907	CLA	C2B-C1B-NB	3.93	114.40	110.33
12	aA	821	CLA	C3C-C4C-NC	3.93	115.46	110.43
12	bB	902	CLA	C4C-C3C-C2C	-3.93	101.18	106.89
12	cB	918	CLA	C4A-NA-C1A	-3.93	104.89	106.68
12	bA	842	CLA	CHD-C1D-ND	-3.92	119.28	124.80
12	bB	918	CLA	CHD-C1D-ND	-3.92	119.28	124.80
12	cA	815	CLA	CHD-C1D-ND	-3.92	119.28	124.80
12	bA	802	CLA	C4B-C3B-C2B	-3.92	102.42	107.30
12	aB	909	CLA	C3D-C4D-ND	3.92	116.36	109.99
12	aA	815	CLA	CHD-C1D-ND	-3.92	119.28	124.80
12	aB	914	CLA	CHD-C1D-ND	-3.92	119.28	124.80
12	bA	853	CLA	CHD-C1D-ND	-3.92	119.28	124.80
12	cA	824	CLA	CAC-C3C-C4C	3.92	129.89	124.79
12	cB	907	CLA	C2B-C1B-NB	3.92	114.39	110.33
12	aB	926	CLA	C3D-C4D-ND	3.92	116.36	109.99
12	bB	913	CLA	C1C-C2C-C3C	-3.92	102.86	106.98
12	cA	808	CLA	C1C-C2C-C3C	-3.92	102.86	106.98
12	cA	837	CLA	C3B-C4B-NB	3.92	114.03	110.53
12	bB	904	CLA	C4A-NA-C1A	-3.92	104.89	106.68
12	cB	909	CLA	C3D-C4D-ND	3.92	116.35	109.99
12	aA	840	CLA	CHD-C1D-ND	-3.92	119.29	124.80
12	bA	821	CLA	C3C-C4C-NC	3.92	115.45	110.43
12	cA	818	CLA	C3C-C4C-NC	3.92	115.45	110.43
12	aA	824	CLA	CAC-C3C-C4C	3.91	129.88	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aL	202	CLA	C4A-NA-C1A	-3.91	104.89	106.68
12	aA	833	CLA	C1C-C2C-C3C	-3.91	102.86	106.98
12	cA	835	CLA	C1C-C2C-C3C	-3.91	102.86	106.98
12	cB	930	CLA	C1C-C2C-C3C	-3.91	102.86	106.98
12	cA	821	CLA	C3C-C4C-NC	3.91	115.44	110.43
12	bA	837	CLA	C1D-CHD-C4C	-3.91	117.70	126.02
12	aA	818	CLA	C3C-C4C-NC	3.91	115.44	110.43
12	aA	844	CLA	C3C-C4C-NC	3.91	115.44	110.43
12	aA	837	CLA	C3B-C4B-NB	3.91	114.02	110.53
12	cA	840	CLA	CHD-C1D-ND	-3.91	119.30	124.80
12	cA	833	CLA	C1C-C2C-C3C	-3.91	102.86	106.98
12	aA	841	CLA	C3C-C4C-NC	3.91	115.44	110.43
12	bA	841	CLA	C3C-C4C-NC	3.91	115.44	110.43
12	bA	807	CLA	CHD-C1D-ND	-3.91	119.30	124.80
12	bA	803	CLA	CAA-C2A-C3A	-3.91	102.43	113.00
12	aA	823	CLA	C1C-C2C-C3C	-3.91	102.87	106.98
12	cA	837	CLA	C3C-C4C-NC	3.91	115.44	110.43
12	cA	818	CLA	O2D-CGD-CBD	3.91	118.06	111.23
12	cA	807	CLA	CHD-C1D-ND	-3.91	119.30	124.80
12	cA	831	CLA	C3D-C4D-ND	3.91	116.34	109.99
12	bA	824	CLA	C3D-C4D-ND	3.91	116.34	109.99
12	aA	803	CLA	CAA-C2A-C3A	-3.91	102.44	113.00
12	cB	914	CLA	CHD-C1D-ND	-3.91	119.31	124.80
12	cA	823	CLA	C1C-C2C-C3C	-3.91	102.87	106.98
12	bA	823	CLA	C1C-C2C-C3C	-3.90	102.87	106.98
12	aA	809	CLA	CHD-C1D-ND	-3.90	119.31	124.80
12	bB	933	CLA	C2B-C1B-NB	3.90	114.37	110.33
12	aB	935	CLA	C1D-CHD-C4C	-3.90	117.72	126.02
12	cB	909	CLA	C1C-C2C-C3C	-3.90	102.88	106.98
12	cA	807	CLA	O2A-CGA-CBA	3.90	123.73	111.83
12	aA	807	CLA	O2A-CGA-CBA	3.90	123.73	111.83
12	cA	831	CLA	C3C-C4C-NC	3.90	115.43	110.43
12	bB	909	CLA	C3D-C4D-ND	3.90	116.33	109.99
12	bB	933	CLA	C3C-C4C-NC	3.90	115.43	110.43
12	bB	904	CLA	C1C-C2C-C3C	-3.90	102.88	106.98
12	aA	819	CLA	C3B-C2B-C1B	-3.90	102.57	107.17
12	aA	818	CLA	O2D-CGD-CBD	3.90	118.05	111.23
12	bB	950	CLA	C3C-C4C-NC	3.90	115.43	110.43
12	cB	933	CLA	C3C-C4C-NC	3.90	115.43	110.43
12	aL	203	CLA	CHD-C1D-ND	-3.90	119.31	124.80
12	cA	803	CLA	CAA-C2A-C3A	-3.90	102.46	113.00
12	bA	819	CLA	CHD-C1D-ND	-3.90	119.32	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	819	CLA	C3B-C2B-C1B	-3.90	102.57	107.17
12	cB	935	CLA	C1D-CHD-C4C	-3.90	117.74	126.02
12	aB	936	CLA	C4A-NA-C1A	-3.90	104.90	106.68
12	bA	837	CLA	C3B-C4B-NB	3.90	114.01	110.53
12	cA	837	CLA	C1D-CHD-C4C	-3.90	117.74	126.02
12	cA	809	CLA	CHD-C1D-ND	-3.90	119.32	124.80
12	aB	907	CLA	C3D-C4D-ND	3.90	116.32	109.99
12	cA	823	CLA	CHD-C1D-ND	-3.90	119.32	124.80
12	aA	837	CLA	C1D-CHD-C4C	-3.89	117.74	126.02
12	cA	853	CLA	CHD-C1D-ND	-3.89	119.32	124.80
12	aA	805	CLA	C2C-C1C-NC	3.89	114.07	109.98
12	cA	819	CLA	CHD-C1D-ND	-3.89	119.32	124.80
12	cA	841	CLA	C3C-C4C-NC	3.89	115.42	110.43
12	cA	824	CLA	CHD-C1D-ND	-3.89	119.32	124.80
12	aB	902	CLA	C4C-C3C-C2C	-3.89	101.23	106.89
12	bB	907	CLA	C3D-C4D-ND	3.89	116.31	109.99
12	bA	810	CLA	C4A-NA-C1A	-3.89	104.90	106.68
12	bA	829	CLA	C3B-C4B-NB	3.89	114.00	110.53
12	bA	837	CLA	CAC-C3C-C4C	3.89	129.85	124.79
12	cB	939	CLA	O2D-CGD-CBD	3.89	118.03	111.23
12	bB	935	CLA	C1D-CHD-C4C	-3.89	117.75	126.02
12	bB	931	CLA	C3C-C4C-NC	3.89	115.41	110.43
12	bB	931	CLA	O2A-CGA-CBA	3.89	123.69	111.83
12	bA	835	CLA	C1C-C2C-C3C	-3.89	102.89	106.98
12	aA	823	CLA	CHD-C1D-ND	-3.89	119.33	124.80
12	cB	916	CLA	CAA-C2A-C3A	-3.89	102.49	113.00
12	cB	931	CLA	O2A-CGA-CBA	3.89	123.69	111.83
12	bB	916	CLA	CAA-C2A-C3A	-3.89	102.49	113.00
12	cA	802	CLA	C4B-C3B-C2B	-3.89	102.47	107.30
12	cA	824	CLA	C3D-C4D-ND	3.89	116.31	109.99
12	aB	916	CLA	CAA-C2A-C3A	-3.89	102.50	113.00
12	bA	819	CLA	C3B-C2B-C1B	-3.89	102.59	107.17
12	aA	831	CLA	C3D-C4D-ND	3.89	116.30	109.99
12	bA	807	CLA	O2A-CGA-CBA	3.89	123.68	111.83
12	bA	809	CLA	CHD-C1D-ND	-3.89	119.33	124.80
12	aB	931	CLA	O2A-CGA-CBA	3.89	123.68	111.83
12	aB	909	CLA	C1C-C2C-C3C	-3.88	102.89	106.98
12	bB	930	CLA	C1C-C2C-C3C	-3.88	102.89	106.98
12	aB	933	CLA	C3C-C4C-NC	3.88	115.41	110.43
12	bB	936	CLA	C4A-NA-C1A	-3.88	104.91	106.68
12	cA	810	CLA	C4A-NA-C1A	-3.88	104.91	106.68
12	bA	818	CLA	O2D-CGD-CBD	3.88	118.02	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	824	CLA	CHD-C1D-ND	-3.88	119.34	124.80
12	aB	903	CLA	C3C-C4C-NC	3.88	115.40	110.43
12	cB	911	CLA	C1C-C2C-C3C	-3.88	102.90	106.98
12	aB	950	CLA	C3C-C4C-NC	3.88	115.40	110.43
12	bB	903	CLA	C3C-C4C-NC	3.88	115.40	110.43
12	bB	939	CLA	O2D-CGD-CBD	3.88	118.01	111.23
12	aB	904	CLA	C1C-C2C-C3C	-3.88	102.90	106.98
12	cB	904	CLA	C1C-C2C-C3C	-3.88	102.90	106.98
12	aA	824	CLA	C3D-C4D-ND	3.88	116.29	109.99
12	aB	931	CLA	C3C-C4C-NC	3.88	115.40	110.43
12	cB	936	CLA	C1C-C2C-C3C	-3.88	102.90	106.98
12	bB	928	CLA	C3D-C4D-ND	3.88	116.29	109.99
12	bA	824	CLA	CHD-C1D-ND	-3.88	119.34	124.80
12	bB	933	CLA	C1D-CHD-C4C	-3.88	117.78	126.02
12	aB	933	CLA	C2B-C1B-NB	3.88	114.35	110.33
12	aA	837	CLA	CAC-C3C-C4C	3.88	129.83	124.79
12	cL	203	CLA	CHD-C1D-ND	-3.88	119.35	124.80
12	aA	802	CLA	C4B-C3B-C2B	-3.88	102.48	107.30
12	aB	928	CLA	C3D-C4D-ND	3.88	116.29	109.99
12	bA	818	CLA	C3C-C4C-NC	3.87	115.39	110.43
12	cA	841	CLA	CAA-C2A-C3A	-3.87	102.53	113.00
12	bA	829	CLA	C3D-C4D-ND	3.87	116.28	109.99
12	bB	938	CLA	CHD-C1D-ND	-3.87	119.35	124.80
12	bA	831	CLA	C3D-C4D-ND	3.87	116.28	109.99
12	cB	933	CLA	C2B-C1B-NB	3.87	114.34	110.33
12	aA	841	CLA	CAA-C2A-C3A	-3.87	102.54	113.00
12	aA	835	CLA	C1C-C2C-C3C	-3.87	102.91	106.98
12	cA	813	CLA	C1D-CHD-C4C	-3.87	117.79	126.02
12	cB	928	CLA	CAC-C3C-C4C	3.87	129.83	124.79
12	cB	907	CLA	C3C-C4C-NC	3.87	115.39	110.43
12	cA	853	CLA	C4A-NA-C1A	-3.87	104.91	106.68
12	aB	939	CLA	O2D-CGD-CBD	3.87	118.00	111.23
12	cA	829	CLA	C3D-C4D-ND	3.87	116.28	109.99
12	aA	819	CLA	CHD-C1D-ND	-3.87	119.36	124.80
12	aA	829	CLA	C3D-C4D-ND	3.87	116.28	109.99
12	aB	933	CLA	C1D-CHD-C4C	-3.87	117.80	126.02
12	cA	818	CLA	C1D-CHD-C4C	-3.87	117.80	126.02
12	aA	810	CLA	C4A-NA-C1A	-3.87	104.91	106.68
12	cB	902	CLA	C4C-C3C-C2C	-3.87	101.26	106.89
12	aA	807	CLA	CHD-C1D-ND	-3.87	119.36	124.80
12	cA	825	CLA	C3D-C4D-ND	3.87	116.27	109.99
12	cL	203	CLA	C3C-C4C-NC	3.87	115.38	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cB	928	CLA	C3D-C4D-ND	3.87	116.27	109.99
12	cB	933	CLA	C1D-CHD-C4C	-3.86	117.81	126.02
12	bA	818	CLA	C1D-CHD-C4C	-3.86	117.81	126.02
12	aB	935	CLA	C3D-C4D-ND	3.86	116.27	109.99
12	aB	918	CLA	C3B-C2B-C1B	-3.86	102.62	107.17
12	aA	813	CLA	C1D-CHD-C4C	-3.86	117.81	126.02
12	aA	825	CLA	C3D-C4D-ND	3.86	116.27	109.99
12	aB	909	CLA	C1D-CHD-C4C	-3.86	117.81	126.02
12	aB	930	CLA	C1C-C2C-C3C	-3.86	102.92	106.98
12	cB	935	CLA	C3D-C4D-ND	3.86	116.26	109.99
12	cB	903	CLA	C3C-C4C-NC	3.86	115.38	110.43
12	bB	907	CLA	C3C-C4C-NC	3.86	115.37	110.43
12	bL	203	CLA	CHD-C1D-ND	-3.86	119.37	124.80
12	cB	938	CLA	CHD-C1D-ND	-3.86	119.37	124.80
12	bA	825	CLA	C3D-C4D-ND	3.86	116.26	109.99
12	cB	906	CLA	C1C-C2C-C3C	-3.86	102.92	106.98
12	cB	906	CLA	C3C-C4C-NC	3.86	115.37	110.43
12	cA	837	CLA	CAC-C3C-C4C	3.86	129.81	124.79
12	bB	906	CLA	C1C-C2C-C3C	-3.86	102.92	106.98
12	cA	802	CLA	C3C-C4C-NC	3.86	115.37	110.43
12	aB	938	CLA	CHD-C1D-ND	-3.85	119.38	124.80
12	bA	841	CLA	CAA-C2A-C3A	-3.85	102.58	113.00
12	bB	922	CLA	C3C-C4C-NC	3.85	115.36	110.43
12	aA	818	CLA	C1D-CHD-C4C	-3.85	117.83	126.02
12	cA	835	CLA	C4A-NA-C1A	-3.85	104.92	106.68
12	bA	813	CLA	C1D-CHD-C4C	-3.85	117.84	126.02
12	bB	909	CLA	C1D-CHD-C4C	-3.85	117.84	126.02
12	cB	909	CLA	C1D-CHD-C4C	-3.85	117.84	126.02
12	cA	830	CLA	C2B-C1B-NB	3.85	114.31	110.33
12	cA	816	CLA	CAA-C2A-C3A	-3.85	102.61	113.00
12	aA	817	CLA	C3C-C4C-NC	3.85	115.36	110.43
12	bA	853	CLA	C4A-NA-C1A	-3.84	104.92	106.68
12	bL	203	CLA	C3C-C4C-NC	3.84	115.36	110.43
12	aB	928	CLA	CAC-C3C-C4C	3.84	129.79	124.79
12	aB	906	CLA	C1C-C2C-C3C	-3.84	102.94	106.98
12	aA	816	CLA	CAA-C2A-C3A	-3.84	102.61	113.00
12	cA	829	CLA	C3B-C4B-NB	3.84	113.96	110.53
12	bA	843	CLA	C3B-C2B-C1B	-3.84	102.64	107.17
12	cA	839	CLA	C1D-CHD-C4C	-3.84	117.86	126.02
12	bB	917	CLA	C3D-C4D-ND	3.84	116.23	109.99
12	bB	935	CLA	C3D-C4D-ND	3.84	116.23	109.99
12	cB	949	CLA	O2D-CGD-O1D	-3.84	116.38	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aB	938	CLA	C1D-CHD-C4C	-3.83	117.87	126.02
12	cA	808	CLA	C4A-NA-C1A	-3.83	104.93	106.68
12	cA	843	CLA	C3B-C2B-C1B	-3.83	102.65	107.17
12	bA	816	CLA	CAA-C2A-C3A	-3.83	102.64	113.00
12	cA	817	CLA	C3C-C4C-NC	3.83	115.34	110.43
12	bB	928	CLA	C1C-C2C-C3C	-3.83	102.95	106.98
12	cA	828	CLA	CHD-C1D-ND	-3.83	119.41	124.80
12	cA	830	CLA	C3D-C4D-ND	3.83	116.22	109.99
12	aB	936	CLA	C1C-C2C-C3C	-3.83	102.95	106.98
12	aB	906	CLA	C3C-C4C-NC	3.83	115.34	110.43
12	aL	203	CLA	C3C-C4C-NC	3.83	115.34	110.43
12	aA	815	CLA	C3B-C4B-NB	3.83	113.95	110.53
12	cB	912	CLA	CHD-C1D-ND	-3.83	119.41	124.80
12	bB	928	CLA	CAC-C3C-C4C	3.83	129.77	124.79
12	aB	922	CLA	C3C-C4C-NC	3.83	115.33	110.43
12	bB	906	CLA	C3C-C4C-NC	3.83	115.33	110.43
12	bB	930	CLA	CHD-C1D-ND	-3.83	119.42	124.80
12	aA	841	CLA	CHD-C1D-ND	-3.83	119.42	124.80
12	bA	830	CLA	C3D-C4D-ND	3.83	116.21	109.99
12	bA	841	CLA	CHD-C1D-ND	-3.82	119.42	124.80
12	bB	949	CLA	O2D-CGD-O1D	-3.82	116.41	123.85
12	cB	917	CLA	C3D-C4D-ND	3.82	116.20	109.99
12	bA	828	CLA	CHD-C1D-ND	-3.82	119.42	124.80
12	bB	902	CLA	O2D-CGD-CBD	3.82	117.91	111.23
12	cB	922	CLA	C3C-C4C-NC	3.82	115.33	110.43
12	cB	938	CLA	C1D-CHD-C4C	-3.82	117.89	126.02
12	aB	949	CLA	O2D-CGD-O1D	-3.82	116.41	123.85
12	aB	928	CLA	C1C-C2C-C3C	-3.82	102.96	106.98
12	aA	818	CLA	CHD-C1D-ND	-3.82	119.43	124.80
12	aA	830	CLA	C3D-C4D-ND	3.82	116.20	109.99
12	bB	938	CLA	C1D-CHD-C4C	-3.82	117.90	126.02
12	bA	802	CLA	C3C-C4C-NC	3.82	115.32	110.43
12	aB	930	CLA	CHD-C1D-ND	-3.82	119.43	124.80
12	aB	907	CLA	C3C-C4C-NC	3.82	115.32	110.43
12	aB	902	CLA	O2D-CGD-CBD	3.82	117.90	111.23
12	cB	931	CLA	C3C-C4C-NC	3.81	115.31	110.43
12	aB	904	CLA	C4A-NA-C1A	-3.81	104.94	106.68
12	bA	839	CLA	C1D-CHD-C4C	-3.81	117.92	126.02
12	cA	811	CLA	C1C-C2C-C3C	-3.81	102.97	106.98
12	bA	815	CLA	C3B-C4B-NB	3.81	113.93	110.53
12	aA	828	CLA	CHD-C1D-ND	-3.81	119.44	124.80
12	cB	902	CLA	O2D-CGD-CBD	3.81	117.89	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cB	939	CLA	C3B-C2B-C1B	-3.81	102.68	107.17
12	bA	817	CLA	C3C-C4C-NC	3.81	115.31	110.43
12	bB	903	CLA	C1D-CHD-C4C	-3.81	117.93	126.02
12	cB	903	CLA	C1D-CHD-C4C	-3.80	117.93	126.02
12	aA	839	CLA	C1D-CHD-C4C	-3.80	117.94	126.02
12	cB	905	CLA	C3C-C4C-NC	3.80	115.30	110.43
12	cB	928	CLA	C1C-C2C-C3C	-3.80	102.98	106.98
12	aA	843	CLA	C3B-C2B-C1B	-3.80	102.69	107.17
12	cA	818	CLA	CHD-C1D-ND	-3.80	119.45	124.80
12	cA	841	CLA	CHD-C1D-ND	-3.80	119.45	124.80
12	aB	949	CLA	C4A-NA-C1A	-3.80	104.94	106.68
12	bB	936	CLA	C1C-C2C-C3C	-3.80	102.98	106.98
12	cB	911	CLA	C3C-C4C-NC	3.80	115.30	110.43
12	cB	949	CLA	C4A-NA-C1A	-3.80	104.95	106.68
12	aA	811	CLA	C1C-C2C-C3C	-3.80	102.99	106.98
12	aB	917	CLA	C3D-C4D-ND	3.80	116.16	109.99
12	aB	903	CLA	C1D-CHD-C4C	-3.80	117.95	126.02
12	cB	930	CLA	CHD-C1D-ND	-3.80	119.46	124.80
12	aB	914	CLA	C1C-C2C-C3C	-3.80	102.99	106.98
12	aA	802	CLA	C3C-C4C-NC	3.80	115.29	110.43
12	aA	830	CLA	C2B-C1B-NB	3.79	114.26	110.33
12	bB	905	CLA	C3C-C4C-NC	3.79	115.29	110.43
12	aA	820	CLA	C1C-C2C-C3C	-3.79	102.99	106.98
12	aB	919	CLA	C1C-C2C-C3C	-3.79	102.99	106.98
12	bA	830	CLA	C2B-C1B-NB	3.79	114.26	110.33
12	cB	918	CLA	C3B-C2B-C1B	-3.79	102.70	107.17
12	cA	841	CLA	C1D-CHD-C4C	-3.79	117.96	126.02
12	bA	835	CLA	C4A-NA-C1A	-3.79	104.95	106.68
12	bB	912	CLA	CHD-C1D-ND	-3.79	119.47	124.80
12	cB	914	CLA	C1C-C2C-C3C	-3.79	102.99	106.98
12	aB	939	CLA	C3B-C2B-C1B	-3.79	102.70	107.17
12	aB	923	CLA	C1C-C2C-C3C	-3.79	102.99	106.98
12	cF	202	CLA	C1C-C2C-C3C	-3.79	102.99	106.98
12	bB	918	CLA	C3B-C2B-C1B	-3.79	102.70	107.17
12	cA	803	CLA	CHD-C1D-ND	-3.79	119.47	124.80
12	bA	811	CLA	C1C-C2C-C3C	-3.79	103.00	106.98
12	bA	841	CLA	C1D-CHD-C4C	-3.79	117.97	126.02
12	cB	914	CLA	C1D-CHD-C4C	-3.79	117.97	126.02
12	aA	833	CLA	CMB-C2B-C1B	3.79	131.19	125.42
12	bA	818	CLA	CHD-C1D-ND	-3.79	119.47	124.80
12	bA	833	CLA	CMB-C2B-C1B	3.79	131.19	125.42
12	bB	939	CLA	C3B-C2B-C1B	-3.79	102.71	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	833	CLA	CMB-C2B-C1B	3.79	131.18	125.42
12	bA	808	CLA	C4A-NA-C1A	-3.79	104.95	106.68
12	cF	202	CLA	CHD-C1D-ND	-3.78	119.48	124.80
12	aB	911	CLA	C3C-C4C-NC	3.78	115.28	110.43
12	bB	911	CLA	C3C-C4C-NC	3.78	115.28	110.43
12	cB	923	CLA	C1C-C2C-C3C	-3.78	103.00	106.98
12	bB	919	CLA	CHD-C1D-ND	-3.78	119.48	124.80
12	cA	815	CLA	C3B-C4B-NB	3.78	113.91	110.53
12	aF	202	CLA	CHD-C1D-ND	-3.78	119.48	124.80
12	bF	202	CLA	CHD-C1D-ND	-3.78	119.48	124.80
12	bB	939	CLA	CBC-CAC-C3C	-3.78	102.17	112.42
12	bB	914	CLA	C1C-C2C-C3C	-3.78	103.00	106.98
12	bB	937	CLA	C4A-NA-C1A	-3.78	104.95	106.68
12	bA	830	CLA	O2D-CGD-O1D	-3.78	116.49	123.85
12	cB	919	CLA	CHD-C1D-ND	-3.78	119.48	124.80
12	aA	841	CLA	C1D-CHD-C4C	-3.78	117.99	126.02
12	bB	914	CLA	C1D-CHD-C4C	-3.78	118.00	126.02
12	cB	937	CLA	C4A-NA-C1A	-3.77	104.96	106.68
12	bB	913	CLA	C3C-C4C-NC	3.77	115.27	110.43
12	cB	939	CLA	CBC-CAC-C3C	-3.77	102.19	112.42
12	cB	939	CLA	C1D-CHD-C4C	-3.77	118.00	126.02
12	aB	905	CLA	C3D-C4D-ND	3.77	116.12	109.99
12	aA	808	CLA	C4A-NA-C1A	-3.77	104.96	106.68
12	bA	803	CLA	CHD-C1D-ND	-3.77	119.49	124.80
12	aA	836	CLA	CHD-C1D-ND	-3.77	119.50	124.80
12	bB	939	CLA	C4B-C3B-C2B	-3.77	102.61	107.30
12	cB	928	CLA	C3B-C4B-NB	3.77	113.90	110.53
12	cB	919	CLA	C1C-C2C-C3C	-3.77	103.02	106.98
12	aB	932	CLA	CAA-C2A-C3A	-3.77	102.81	113.00
12	aB	939	CLA	CBC-CAC-C3C	-3.77	102.20	112.42
12	bB	949	CLA	CHD-C1D-ND	-3.77	119.50	124.80
12	aB	914	CLA	C1D-CHD-C4C	-3.77	118.01	126.02
12	bB	939	CLA	C1D-CHD-C4C	-3.77	118.01	126.02
12	aA	805	CLA	C3C-C4C-NC	3.77	115.26	110.43
12	aA	803	CLA	CHD-C1D-ND	-3.77	119.50	124.80
12	cB	939	CLA	C4B-C3B-C2B	-3.77	102.62	107.30
12	aB	928	CLA	C3B-C4B-NB	3.77	113.89	110.53
12	aB	949	CLA	CHD-C1D-ND	-3.77	119.50	124.80
12	bA	836	CLA	CHD-C1D-ND	-3.77	119.50	124.80
12	aB	939	CLA	C4B-C3B-C2B	-3.77	102.62	107.30
12	aB	912	CLA	CHD-C1D-ND	-3.77	119.50	124.80
12	aB	919	CLA	CHD-C1D-ND	-3.77	119.50	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	814	CLA	CHD-C1D-ND	-3.77	119.50	124.80
12	aA	830	CLA	O2D-CGD-O1D	-3.76	116.52	123.85
12	cA	842	CLA	C1D-CHD-C4C	-3.76	118.02	126.02
12	cA	837	CLA	C4-C3-C5	3.76	120.56	116.13
12	aB	938	CLA	C1C-C2C-C3C	-3.76	103.02	106.98
12	aB	939	CLA	CHD-C1D-ND	-3.76	119.51	124.80
12	cB	913	CLA	C3C-C4C-NC	3.76	115.25	110.43
12	aB	939	CLA	C1D-CHD-C4C	-3.76	118.03	126.02
12	cA	827	CLA	C3D-C4D-ND	3.76	116.10	109.99
12	aF	202	CLA	C1C-C2C-C3C	-3.76	103.03	106.98
12	bB	910	CLA	C3C-C4C-NC	3.76	115.25	110.43
12	aB	905	CLA	C3C-C4C-NC	3.76	115.24	110.43
12	bB	932	CLA	CAA-C2A-C3A	-3.76	102.84	113.00
12	bB	923	CLA	C1C-C2C-C3C	-3.76	103.03	106.98
12	aA	837	CLA	C4-C3-C5	3.76	120.55	116.13
12	cB	908	CLA	CHC-C1C-C2C	-3.76	116.28	126.95
12	bA	832	CLA	C1C-C2C-C3C	-3.75	103.03	106.98
12	aB	908	CLA	CHC-C1C-C2C	-3.75	116.28	126.95
12	cA	830	CLA	O2D-CGD-O1D	-3.75	116.54	123.85
12	cA	836	CLA	CHD-C1D-ND	-3.75	119.52	124.80
12	bB	938	CLA	C3C-C4C-NC	3.75	115.24	110.43
12	cB	910	CLA	C3C-C4C-NC	3.75	115.24	110.43
12	aB	907	CLA	C1C-C2C-C3C	-3.75	103.03	106.98
12	aB	930	CLA	C3B-C4B-NB	3.75	113.88	110.53
12	cB	932	CLA	CAA-C2A-C3A	-3.75	102.86	113.00
12	aA	814	CLA	C3C-C4C-NC	3.75	115.23	110.43
12	cB	949	CLA	CHD-C1D-ND	-3.75	119.52	124.80
12	aB	910	CLA	C3B-C4B-NB	3.75	113.88	110.53
12	aB	913	CLA	C1D-CHD-C4C	-3.75	118.05	126.02
12	aB	913	CLA	C3C-C4C-NC	3.75	115.23	110.43
12	bB	910	CLA	C3B-C4B-NB	3.75	113.88	110.53
12	bA	842	CLA	C1D-CHD-C4C	-3.75	118.05	126.02
12	aB	938	CLA	C3C-C4C-NC	3.75	115.23	110.43
12	aA	843	CLA	O2A-CGA-CBA	3.75	123.25	111.83
12	cB	921	CLA	C3B-C4B-NB	3.74	113.87	110.53
12	bB	919	CLA	C1C-C2C-C3C	-3.74	103.04	106.98
12	aA	827	CLA	C3D-C4D-ND	3.74	116.07	109.99
12	bB	908	CLA	CHC-C1C-C2C	-3.74	116.31	126.95
12	aB	903	CLA	C3D-C4D-ND	3.74	116.07	109.99
12	bF	202	CLA	C1C-C2C-C3C	-3.74	103.04	106.98
12	aB	910	CLA	C3C-C4C-NC	3.74	115.22	110.43
12	bA	843	CLA	O2A-CGA-CBA	3.74	123.25	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	829	CLA	C1C-C2C-C3C	-3.74	103.05	106.98
12	cB	938	CLA	C1C-C2C-C3C	-3.74	103.05	106.98
12	bB	905	CLA	C3D-C4D-ND	3.74	116.07	109.99
12	cA	843	CLA	O2A-CGA-CBA	3.74	123.24	111.83
12	cA	807	CLA	C2C-C1C-NC	3.74	113.91	109.98
12	aA	814	CLA	CHD-C1D-ND	-3.74	119.54	124.80
12	bA	814	CLA	C3C-C4C-NC	3.74	115.22	110.43
12	aB	935	CLA	CHD-C1D-ND	-3.74	119.54	124.80
12	cA	814	CLA	C3C-C4C-NC	3.74	115.22	110.43
12	cA	836	CLA	CAC-C3C-C4C	3.74	129.65	124.79
12	bB	935	CLA	CHD-C1D-ND	-3.73	119.55	124.80
12	aA	832	CLA	C1C-C2C-C3C	-3.73	103.05	106.98
12	cB	913	CLA	C1D-CHD-C4C	-3.73	118.08	126.02
12	bA	814	CLA	CHD-C1D-ND	-3.73	119.55	124.80
12	cB	917	CLA	O2A-CGA-CBA	3.73	123.22	111.83
12	bA	827	CLA	C3D-C4D-ND	3.73	116.06	109.99
12	cA	829	CLA	C3C-C4C-NC	3.73	115.21	110.43
12	bA	820	CLA	C1C-C2C-C3C	-3.73	103.05	106.98
12	bB	928	CLA	C3B-C4B-NB	3.73	113.86	110.53
12	cA	806	CLA	C1C-C2C-C3C	-3.73	103.06	106.98
12	cA	829	CLA	C1C-C2C-C3C	-3.73	103.06	106.98
12	aB	921	CLA	C3B-C4B-NB	3.73	113.86	110.53
12	bB	921	CLA	C3B-C4B-NB	3.73	113.86	110.53
12	aA	810	CLA	O2D-CGD-CBD	3.73	117.75	111.23
12	cB	918	CLA	C4B-C3B-C2B	-3.73	102.66	107.30
12	cB	930	CLA	C3C-C4C-NC	3.73	115.21	110.43
12	cA	820	CLA	C1C-C2C-C3C	-3.73	103.06	106.98
12	cA	810	CLA	CAC-C3C-C4C	3.73	129.64	124.79
12	cA	805	CLA	C3C-C4C-NC	3.73	115.21	110.43
12	aB	916	CLA	O2A-CGA-CBA	3.73	123.21	111.83
12	bA	807	CLA	C3D-C4D-ND	3.73	116.05	109.99
12	aA	842	CLA	C1D-CHD-C4C	-3.73	118.10	126.02
12	cA	832	CLA	C1C-C2C-C3C	-3.73	103.06	106.98
12	bA	829	CLA	C3C-C4C-NC	3.73	115.20	110.43
12	cB	935	CLA	CHD-C1D-ND	-3.73	119.56	124.80
12	aF	202	CLA	CAC-C3C-C4C	3.73	129.64	124.79
12	cF	202	CLA	CAC-C3C-C4C	3.73	129.64	124.79
12	bB	939	CLA	CHD-C1D-ND	-3.73	119.56	124.80
12	bB	913	CLA	C1D-CHD-C4C	-3.72	118.11	126.02
12	bB	934	CLA	C1D-CHD-C4C	-3.72	118.11	126.02
12	bB	938	CLA	C1C-C2C-C3C	-3.72	103.06	106.98
12	cB	932	CLA	C1D-CHD-C4C	-3.72	118.11	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bB	916	CLA	O2A-CGA-CBA	3.72	123.19	111.83
12	cB	904	CLA	C3C-C4C-NC	3.72	115.20	110.43
12	cB	905	CLA	C3D-C4D-ND	3.72	116.04	109.99
12	aA	822	CLA	C4A-NA-C1A	-3.72	104.98	106.68
12	cB	907	CLA	C1C-C2C-C3C	-3.72	103.07	106.98
12	aA	807	CLA	C3D-C4D-ND	3.72	116.04	109.99
12	bA	837	CLA	C4-C3-C5	3.72	120.51	116.13
12	bA	811	CLA	C3B-C4B-NB	3.72	113.85	110.53
12	bA	805	CLA	C4A-NA-C1A	-3.72	104.98	106.68
12	bA	805	CLA	C3C-C4C-NC	3.72	115.19	110.43
12	aA	804	CLA	C1D-CHD-C4C	-3.72	118.11	126.02
12	aB	932	CLA	C1D-CHD-C4C	-3.72	118.11	126.02
12	bB	903	CLA	C3D-C4D-ND	3.72	116.03	109.99
12	bB	930	CLA	C3C-C4C-NC	3.72	115.19	110.43
12	cB	934	CLA	C1D-CHD-C4C	-3.72	118.12	126.02
12	aA	830	CLA	C1C-C2C-C3C	-3.72	103.07	106.98
12	aA	837	CLA	C3D-C4D-ND	3.72	116.03	109.99
12	bA	810	CLA	CAC-C3C-C4C	3.72	129.63	124.79
12	cA	810	CLA	O2D-CGD-CBD	3.72	117.73	111.23
12	aA	821	CLA	C4B-C3B-C2B	-3.72	102.68	107.30
12	cA	802	CLA	C3B-C4B-NB	3.72	113.85	110.53
12	bB	917	CLA	O2A-CGA-CBA	3.72	123.17	111.83
12	aB	934	CLA	C1D-CHD-C4C	-3.72	118.12	126.02
12	aA	810	CLA	CAC-C3C-C4C	3.72	129.62	124.79
12	aA	829	CLA	C1C-C2C-C3C	-3.71	103.07	106.98
12	cB	938	CLA	C3C-C4C-NC	3.71	115.19	110.43
12	bB	918	CLA	C4B-C3B-C2B	-3.71	102.69	107.30
12	aB	906	CLA	CHD-C1D-ND	-3.71	119.58	124.80
12	aB	939	CLA	C3C-C4C-NC	3.71	115.19	110.43
12	cB	939	CLA	CHD-C1D-ND	-3.71	119.58	124.80
12	bB	939	CLA	C3C-C4C-NC	3.71	115.18	110.43
12	cB	939	CLA	C3C-C4C-NC	3.71	115.18	110.43
12	aB	918	CLA	C4B-C3B-C2B	-3.71	102.69	107.30
12	cB	916	CLA	O2A-CGA-CBA	3.71	123.14	111.83
12	aA	832	CLA	CAA-C2A-C1A	-3.71	99.82	111.97
12	cB	903	CLA	C3D-C4D-ND	3.71	116.01	109.99
12	bA	807	CLA	C2C-C1C-NC	3.71	113.88	109.98
12	aB	917	CLA	O2A-CGA-CBA	3.71	123.14	111.83
12	aB	914	CLA	CAA-C2A-C3A	-3.71	102.98	113.00
12	cB	910	CLA	C3B-C4B-NB	3.71	113.84	110.53
12	bA	832	CLA	CAA-C2A-C1A	-3.71	99.83	111.97
12	bF	202	CLA	CAC-C3C-C4C	3.71	129.61	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	825	CLA	C1D-CHD-C4C	-3.70	118.14	126.02
12	bB	932	CLA	C1D-CHD-C4C	-3.70	118.15	126.02
12	aA	825	CLA	C1D-CHD-C4C	-3.70	118.15	126.02
12	cA	810	CLA	C3C-C4C-NC	3.70	115.17	110.43
12	cA	821	CLA	C4B-C3B-C2B	-3.70	102.70	107.30
12	bA	804	CLA	C1D-CHD-C4C	-3.70	118.15	126.02
12	cA	832	CLA	CAA-C2A-C1A	-3.70	99.85	111.97
12	bB	925	CLA	C3D-C4D-ND	3.70	116.00	109.99
12	bB	907	CLA	C1C-C2C-C3C	-3.70	103.09	106.98
12	aB	905	CLA	CHD-C1D-ND	-3.70	119.60	124.80
12	cA	825	CLA	C1D-CHD-C4C	-3.70	118.16	126.02
12	aB	903	CLA	CHD-C1D-ND	-3.70	119.60	124.80
12	aA	807	CLA	C2C-C1C-NC	3.70	113.86	109.98
12	cB	903	CLA	C4-C3-C5	3.70	120.48	116.13
12	cA	804	CLA	C1D-CHD-C4C	-3.70	118.17	126.02
12	cA	853	CLA	C1D-CHD-C4C	-3.69	118.17	126.02
12	cA	830	CLA	C1C-C2C-C3C	-3.69	103.09	106.98
12	cB	930	CLA	C3B-C4B-NB	3.69	113.83	110.53
12	cB	914	CLA	CAA-C2A-C3A	-3.69	103.02	113.00
13	cA	844	1L3	C14-C15-C16	-3.69	120.47	126.83
12	aA	836	CLA	CAC-C3C-C4C	3.69	129.59	124.79
12	bB	903	CLA	C1C-C2C-C3C	-3.69	103.10	106.98
12	cA	807	CLA	C3D-C4D-ND	3.69	115.99	109.99
12	bB	914	CLA	CAA-C2A-C3A	-3.69	103.02	113.00
12	bA	810	CLA	O2D-CGD-CBD	3.69	117.68	111.23
12	cA	805	CLA	C4A-NA-C1A	-3.69	105.00	106.68
12	bA	802	CLA	C3B-C4B-NB	3.69	113.83	110.53
12	aA	829	CLA	C3C-C4C-NC	3.69	115.16	110.43
12	bA	836	CLA	CAC-C3C-C4C	3.69	129.59	124.79
12	bF	202	CLA	CAA-C2A-C3A	-3.69	103.03	113.00
12	cF	202	CLA	CAA-C2A-C3A	-3.69	103.03	113.00
12	bB	903	CLA	C4-C3-C5	3.69	120.47	116.13
12	bB	903	CLA	CHD-C1D-ND	-3.69	119.61	124.80
12	bA	830	CLA	C1C-C2C-C3C	-3.69	103.10	106.98
12	bL	204	CLA	C1C-C2C-C3C	-3.69	103.10	106.98
12	bB	904	CLA	C3C-C4C-NC	3.69	115.15	110.43
12	cA	836	CLA	C3B-C4B-NB	3.69	113.82	110.53
12	cB	919	CLA	C3D-C4D-ND	3.69	115.98	109.99
12	aB	903	CLA	C4-C3-C5	3.69	120.47	116.13
12	bA	830	CLA	CAC-C3C-C4C	3.69	129.59	124.79
15	bJ	101	BCR	C11-C10-C9	-3.68	122.11	127.28
12	aB	938	CLA	O2D-CGD-CBD	3.68	117.67	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	837	CLA	C3D-C4D-ND	3.68	115.97	109.99
12	aA	836	CLA	C3B-C4B-NB	3.68	113.82	110.53
12	cB	911	CLA	CHD-C1D-ND	-3.68	119.62	124.80
12	cB	916	CLA	C1D-CHD-C4C	-3.68	118.20	126.02
12	cB	903	CLA	CHD-C1D-ND	-3.68	119.62	124.80
12	bA	838	CLA	C3C-C4C-NC	3.68	115.14	110.43
12	aB	919	CLA	C3D-C4D-ND	3.68	115.96	109.99
12	bA	821	CLA	C4B-C3B-C2B	-3.68	102.73	107.30
12	aB	930	CLA	C3C-C4C-NC	3.68	115.14	110.43
12	bA	810	CLA	C3C-C4C-NC	3.68	115.14	110.43
12	bB	938	CLA	O2D-CGD-CBD	3.68	117.66	111.23
12	bA	830	CLA	CHD-C1D-ND	-3.68	119.63	124.80
12	aA	854	CLA	C1D-CHD-C4C	-3.68	118.21	126.02
12	bB	916	CLA	C1D-CHD-C4C	-3.68	118.21	126.02
12	aB	912	CLA	C4C-C3C-C2C	-3.67	101.54	106.89
12	cA	811	CLA	C1D-CHD-C4C	-3.67	118.21	126.02
12	bA	806	CLA	C1C-C2C-C3C	-3.67	103.11	106.98
12	aB	903	CLA	C1C-C2C-C3C	-3.67	103.12	106.98
12	bA	829	CLA	O2D-CGD-CBD	3.67	117.65	111.23
12	cF	202	CLA	C1D-CHD-C4C	-3.67	118.21	126.02
12	aF	202	CLA	CAA-C2A-C3A	-3.67	103.07	113.00
12	bA	811	CLA	C1D-CHD-C4C	-3.67	118.21	126.02
13	bA	844	1L3	C14-C03-C02	-3.67	118.59	124.89
12	bA	819	CLA	C4B-C3B-C2B	-3.67	102.74	107.30
12	aA	815	CLA	C1C-C2C-C3C	-3.67	103.12	106.98
12	bF	202	CLA	C1D-CHD-C4C	-3.67	118.22	126.02
12	cB	938	CLA	O2D-CGD-CBD	3.67	117.65	111.23
12	cB	937	CLA	C1C-C2C-C3C	-3.67	103.12	106.98
12	aB	904	CLA	C3C-C4C-NC	3.67	115.13	110.43
12	aA	816	CLA	C4A-NA-C1A	-3.67	105.00	106.68
12	bA	853	CLA	C1D-CHD-C4C	-3.67	118.22	126.02
12	aB	934	CLA	C1C-C2C-C3C	-3.67	103.12	106.98
12	cB	925	CLA	C3D-C4D-ND	3.67	115.95	109.99
12	cA	809	CLA	C3C-C4C-NC	3.67	115.13	110.43
12	cL	204	CLA	C1C-C2C-C3C	-3.67	103.12	106.98
12	aF	202	CLA	C1D-CHD-C4C	-3.67	118.22	126.02
12	cA	829	CLA	O2D-CGD-CBD	3.67	117.64	111.23
12	bB	906	CLA	CHD-C1D-ND	-3.67	119.64	124.80
12	aA	802	CLA	C3B-C2B-C1B	-3.67	102.85	107.17
12	cA	802	CLA	C3B-C2B-C1B	-3.67	102.85	107.17
12	aB	916	CLA	C1D-CHD-C4C	-3.66	118.23	126.02
12	aA	840	CLA	O2D-CGD-CBD	3.66	117.64	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	837	CLA	C3D-C4D-ND	3.66	115.94	109.99
12	aA	806	CLA	C1C-C2C-C3C	-3.66	103.13	106.98
12	cB	903	CLA	C1C-C2C-C3C	-3.66	103.13	106.98
12	cA	819	CLA	C4B-C3B-C2B	-3.66	102.75	107.30
15	aJ	101	BCR	C11-C10-C9	-3.66	122.14	127.28
12	aA	809	CLA	C3C-C4C-NC	3.66	115.12	110.43
12	aA	810	CLA	C3C-C4C-NC	3.66	115.12	110.43
12	aB	911	CLA	CHD-C1D-ND	-3.66	119.65	124.80
12	bB	919	CLA	C3D-C4D-ND	3.66	115.94	109.99
12	aA	814	CLA	CAC-C3C-C4C	3.66	129.55	124.79
13	aA	845	1L3	C14-C15-C16	-3.66	120.52	126.83
12	cA	802	CLA	C1C-C2C-C3C	-3.66	103.13	106.98
13	aA	845	1L3	C14-C03-C02	-3.66	118.62	124.89
12	bB	905	CLA	CHD-C1D-ND	-3.66	119.65	124.80
12	aA	811	CLA	C1D-CHD-C4C	-3.66	118.25	126.02
12	bB	912	CLA	C4C-C3C-C2C	-3.66	101.57	106.89
12	aB	913	CLA	CHD-C1D-ND	-3.66	119.66	124.80
12	bA	809	CLA	C3C-C4C-NC	3.66	115.11	110.43
12	aA	802	CLA	C3B-C4B-NB	3.66	113.79	110.53
12	bB	922	CLA	C1D-CHD-C4C	-3.66	118.25	126.02
12	aB	907	CLA	CAA-C2A-C3A	-3.66	103.12	113.00
12	cB	906	CLA	CHD-C1D-ND	-3.66	119.66	124.80
12	bA	840	CLA	O2D-CGD-CBD	3.66	117.62	111.23
12	bB	934	CLA	C1C-C2C-C3C	-3.65	103.14	106.98
12	cA	830	CLA	CAC-C3C-C4C	3.65	129.54	124.79
12	aB	925	CLA	C3D-C4D-ND	3.65	115.93	109.99
12	aA	812	CLA	C1D-CHD-C4C	-3.65	118.25	126.02
12	cB	912	CLA	C4C-C3C-C2C	-3.65	101.57	106.89
12	aA	829	CLA	O2D-CGD-CBD	3.65	117.62	111.23
12	bA	812	CLA	C1D-CHD-C4C	-3.65	118.26	126.02
12	bA	843	CLA	C1D-CHD-C4C	-3.65	118.26	126.02
15	cJ	101	BCR	C11-C10-C9	-3.65	122.16	127.28
12	aA	830	CLA	CAC-C3C-C4C	3.65	129.54	124.79
12	aA	819	CLA	C4B-C3B-C2B	-3.65	102.76	107.30
12	cB	922	CLA	O2D-CGD-CBD	3.65	117.61	111.23
12	aB	922	CLA	O2D-CGD-CBD	3.65	117.61	111.23
12	aA	802	CLA	C1C-C2C-C3C	-3.65	103.14	106.98
12	bB	922	CLA	O2D-CGD-CBD	3.65	117.61	111.23
12	bB	937	CLA	C1C-C2C-C3C	-3.65	103.14	106.98
12	cA	843	CLA	C1D-CHD-C4C	-3.65	118.27	126.02
12	cA	838	CLA	C3C-C4C-NC	3.65	115.10	110.43
12	aA	840	CLA	C1C-C2C-C3C	-3.65	103.14	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	817	CLA	C1C-C2C-C3C	-3.65	103.14	106.98
12	cB	934	CLA	C1C-C2C-C3C	-3.65	103.14	106.98
12	cB	905	CLA	CHD-C1D-ND	-3.65	119.67	124.80
12	bA	853	CLA	C4C-C3C-C2C	-3.65	101.58	106.89
12	aB	949	CLA	C3C-C4C-NC	3.65	115.10	110.43
12	cB	916	CLA	C3C-C4C-NC	3.65	115.10	110.43
12	cA	840	CLA	C1C-C2C-C3C	-3.65	103.15	106.98
12	cB	937	CLA	CAC-C3C-C4C	3.65	129.53	124.79
12	cA	812	CLA	C1D-CHD-C4C	-3.64	118.27	126.02
12	cA	843	CLA	C4B-C3B-C2B	-3.64	102.77	107.30
12	cB	939	CLA	C2B-C1B-NB	3.64	114.11	110.33
12	aB	937	CLA	CAC-C3C-C4C	3.64	129.53	124.79
12	bA	840	CLA	C1C-C2C-C3C	-3.64	103.15	106.98
12	aA	843	CLA	C4B-C3B-C2B	-3.64	102.77	107.30
12	bB	926	CLA	C4C-C3C-C2C	-3.64	101.59	106.89
12	cB	922	CLA	C1D-CHD-C4C	-3.64	118.28	126.02
12	bB	913	CLA	CHD-C1D-ND	-3.64	119.68	124.80
13	bA	844	1L3	C14-C15-C16	-3.64	120.56	126.83
12	bA	818	CLA	C1-O2A-CGA	3.64	125.46	116.65
12	cA	820	CLA	C1D-CHD-C4C	-3.64	118.29	126.02
12	cB	907	CLA	CAA-C2A-C3A	-3.64	103.17	113.00
12	bB	907	CLA	CAA-C2A-C3A	-3.64	103.17	113.00
12	aA	818	CLA	C1-O2A-CGA	3.64	125.45	116.65
12	aA	820	CLA	C1D-CHD-C4C	-3.64	118.29	126.02
12	bB	905	CLA	C1D-CHD-C4C	-3.64	118.29	126.02
12	bA	820	CLA	C1D-CHD-C4C	-3.63	118.29	126.02
12	aA	814	CLA	C1D-CHD-C4C	-3.63	118.30	126.02
12	cA	814	CLA	C1D-CHD-C4C	-3.63	118.30	126.02
12	cB	913	CLA	CHD-C1D-ND	-3.63	119.69	124.80
12	cA	811	CLA	C3B-C4B-NB	3.63	113.77	110.53
12	aA	843	CLA	C1D-CHD-C4C	-3.63	118.30	126.02
12	bA	814	CLA	CAC-C3C-C4C	3.63	129.52	124.79
12	bA	815	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
12	bB	911	CLA	CHD-C1D-ND	-3.63	119.69	124.80
12	cB	925	CLA	O2D-CGD-O1D	-3.63	116.78	123.85
12	cA	840	CLA	O2D-CGD-CBD	3.63	117.58	111.23
12	bB	930	CLA	C3B-C4B-NB	3.63	113.77	110.53
12	bB	925	CLA	O2D-CGD-O1D	-3.63	116.78	123.85
12	aA	817	CLA	C1D-CHD-C4C	-3.63	118.31	126.02
12	aB	922	CLA	C1D-CHD-C4C	-3.63	118.31	126.02
12	cA	818	CLA	C1-O2A-CGA	3.63	125.43	116.65
12	bA	808	CLA	C1D-CHD-C4C	-3.63	118.31	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	814	CLA	C1D-CHD-C4C	-3.63	118.31	126.02
12	cB	949	CLA	C3C-C4C-NC	3.63	115.08	110.43
13	cA	844	1L3	C14-C03-C02	-3.63	118.67	124.89
12	cA	816	CLA	C4A-NA-C1A	-3.63	105.02	106.68
12	aB	921	CLA	C3C-C4C-NC	3.63	115.08	110.43
12	aA	808	CLA	C1D-CHD-C4C	-3.63	118.31	126.02
12	bA	836	CLA	C3B-C4B-NB	3.63	113.77	110.53
12	cA	808	CLA	C1D-CHD-C4C	-3.63	118.31	126.02
12	cA	822	CLA	C4A-NA-C1A	-3.63	105.03	106.68
12	aB	937	CLA	C1C-C2C-C3C	-3.63	103.17	106.98
12	aB	925	CLA	O2D-CGD-O1D	-3.62	116.79	123.85
12	aL	204	CLA	C1C-C2C-C3C	-3.62	103.17	106.98
12	cA	814	CLA	CAC-C3C-C4C	3.62	129.50	124.79
12	cA	817	CLA	C1C-C2C-C3C	-3.62	103.17	106.98
12	bA	802	CLA	C3B-C2B-C1B	-3.62	102.90	107.17
12	cA	817	CLA	C1D-CHD-C4C	-3.62	118.32	126.02
12	bL	203	CLA	C1C-C2C-C3C	-3.62	103.17	106.98
12	bB	937	CLA	CAC-C3C-C4C	3.62	129.50	124.79
12	aA	811	CLA	C3B-C4B-NB	3.62	113.76	110.53
12	cB	905	CLA	C1D-CHD-C4C	-3.62	118.33	126.02
12	aA	805	CLA	C4A-NA-C1A	-3.62	105.03	106.68
12	aA	817	CLA	C1C-C2C-C3C	-3.62	103.18	106.98
12	bA	802	CLA	C1C-C2C-C3C	-3.62	103.18	106.98
12	aA	819	CLA	C3C-C4C-NC	3.62	115.06	110.43
12	aB	907	CLA	C3B-C4B-NB	3.61	113.76	110.53
12	bB	933	CLA	C3B-C2B-C1B	-3.61	102.91	107.17
12	aA	828	CLA	C1C-C2C-C3C	-3.61	103.18	106.98
12	aA	854	CLA	C4C-C3C-C2C	-3.61	101.63	106.89
12	bB	921	CLA	C3C-C4C-NC	3.61	115.06	110.43
12	aB	926	CLA	C4C-C3C-C2C	-3.61	101.64	106.89
12	bA	803	CLA	CMD-C2D-C1D	3.61	131.09	124.73
12	aA	838	CLA	C3C-C4C-NC	3.61	115.06	110.43
12	aB	939	CLA	C2B-C1B-NB	3.61	114.07	110.33
12	aB	908	CLA	C3D-C4D-ND	3.61	115.85	109.99
12	bA	828	CLA	C1C-C2C-C3C	-3.61	103.19	106.98
12	cB	905	CLA	C4A-NA-C1A	-3.61	105.03	106.68
12	aB	933	CLA	C4B-C3B-C2B	-3.61	102.82	107.30
12	cA	803	CLA	CMD-C2D-C1D	3.60	131.08	124.73
12	bA	822	CLA	C4A-NA-C1A	-3.60	105.03	106.68
12	aA	829	CLA	C1D-CHD-C4C	-3.60	118.36	126.02
12	cA	843	CLA	C2B-C1B-NB	3.60	114.06	110.33
12	aB	905	CLA	C1D-CHD-C4C	-3.60	118.36	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cB	933	CLA	C3B-C2B-C1B	-3.60	102.92	107.17
12	aA	831	CLA	C1C-C2C-C3C	-3.60	103.19	106.98
12	cB	926	CLA	C4C-C3C-C2C	-3.60	101.65	106.89
12	bB	937	CLA	O2D-CGD-O1D	-3.60	116.84	123.85
12	cA	830	CLA	CHD-C1D-ND	-3.60	119.73	124.80
12	bB	939	CLA	C2B-C1B-NB	3.60	114.06	110.33
12	aB	937	CLA	O2D-CGD-O1D	-3.60	116.84	123.85
12	bA	817	CLA	C1D-CHD-C4C	-3.60	118.37	126.02
12	aA	830	CLA	CHD-C1D-ND	-3.60	119.74	124.80
12	cA	816	CLA	C3B-C4B-NB	3.60	113.74	110.53
12	aA	803	CLA	CMD-C2D-C1D	3.60	131.06	124.73
12	bA	839	CLA	O2D-CGD-O1D	-3.60	116.85	123.85
12	cB	933	CLA	C4B-C3B-C2B	-3.60	102.83	107.30
12	bB	916	CLA	C3C-C4C-NC	3.60	115.04	110.43
12	aB	905	CLA	C4A-NA-C1A	-3.60	105.04	106.68
12	bA	809	CLA	C1C-C2C-C3C	-3.60	103.20	106.98
12	aA	815	CLA	C1D-CHD-C4C	-3.60	118.38	126.02
12	bB	949	CLA	C3C-C4C-NC	3.60	115.04	110.43
12	aA	838	CLA	C1D-CHD-C4C	-3.60	118.38	126.02
12	bB	933	CLA	C4B-C3B-C2B	-3.60	102.83	107.30
12	cA	809	CLA	C1C-C2C-C3C	-3.59	103.20	106.98
12	cB	918	CLA	C3C-C4C-NC	3.59	115.03	110.43
12	aA	823	CLA	C1D-CHD-C4C	-3.59	118.38	126.02
12	cB	908	CLA	C3D-C4D-ND	3.59	115.83	109.99
12	bA	829	CLA	C1D-CHD-C4C	-3.59	118.38	126.02
12	cA	820	CLA	C3C-C4C-NC	3.59	115.03	110.43
12	bA	838	CLA	C1D-CHD-C4C	-3.59	118.38	126.02
12	cA	824	CLA	C3B-C4B-NB	3.59	113.74	110.53
12	bB	918	CLA	C3C-C4C-NC	3.59	115.03	110.43
12	cA	821	CLA	CHD-C1D-ND	-3.59	119.75	124.80
12	cL	203	CLA	C1C-C2C-C3C	-3.59	103.20	106.98
12	cA	834	CLA	C1D-CHD-C4C	-3.59	118.39	126.02
12	bB	905	CLA	C1C-C2C-C3C	-3.59	103.20	106.98
12	bA	819	CLA	C3C-C4C-NC	3.59	115.03	110.43
12	cB	937	CLA	O2D-CGD-O1D	-3.59	116.86	123.85
12	cB	914	CLA	C4A-NA-C1A	-3.59	105.04	106.68
12	aL	203	CLA	C1C-C2C-C3C	-3.59	103.20	106.98
12	bA	843	CLA	C4B-C3B-C2B	-3.59	102.84	107.30
12	cA	853	CLA	C4C-C3C-C2C	-3.59	101.67	106.89
12	cA	809	CLA	CAA-C2A-C3A	-3.59	103.30	113.00
12	cA	828	CLA	C1C-C2C-C3C	-3.59	103.20	106.98
12	cA	827	CLA	C4C-C3C-C2C	-3.59	101.67	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	815	CLA	C1C-C2C-C3C	-3.59	103.21	106.98
12	bA	843	CLA	C2B-C1B-NB	3.59	114.05	110.33
12	cA	829	CLA	C1D-CHD-C4C	-3.59	118.39	126.02
12	aA	809	CLA	CAA-C2A-C3A	-3.59	103.31	113.00
12	cA	823	CLA	C1D-CHD-C4C	-3.59	118.40	126.02
12	bA	809	CLA	CAA-C2A-C3A	-3.59	103.31	113.00
12	cA	815	CLA	C1D-CHD-C4C	-3.58	118.40	126.02
12	cB	905	CLA	C1C-C2C-C3C	-3.58	103.21	106.98
12	bA	834	CLA	C1D-CHD-C4C	-3.58	118.40	126.02
12	cA	819	CLA	C3C-C4C-NC	3.58	115.02	110.43
12	cB	921	CLA	C3C-C4C-NC	3.58	115.02	110.43
12	aA	827	CLA	C4C-C3C-C2C	-3.58	101.68	106.89
12	aB	933	CLA	C3B-C2B-C1B	-3.58	102.95	107.17
12	bB	908	CLA	C3D-C4D-ND	3.58	115.81	109.99
12	aA	833	CLA	C3C-C4C-NC	3.58	115.02	110.43
12	bA	811	CLA	C3C-C4C-NC	3.58	115.02	110.43
12	aA	837	CLA	C4B-C3B-C2B	-3.58	102.85	107.30
12	aA	816	CLA	C3B-C4B-NB	3.58	113.72	110.53
12	aA	821	CLA	CHD-C1D-ND	-3.58	119.77	124.80
12	aB	922	CLA	CHD-C1D-ND	-3.58	119.77	124.80
12	aA	839	CLA	O2D-CGD-O1D	-3.58	116.89	123.85
12	aB	937	CLA	C4A-NA-C1A	-3.58	105.05	106.68
12	aA	837	CLA	C4C-C3C-C2C	-3.58	101.69	106.89
12	aB	917	CLA	CBA-CAA-C2A	3.58	124.44	113.79
12	bB	922	CLA	CHD-C1D-ND	-3.58	119.77	124.80
12	aB	926	CLA	C3B-C4B-NB	3.58	113.72	110.53
12	cB	907	CLA	C3B-C4B-NB	3.58	113.72	110.53
12	bB	917	CLA	CBA-CAA-C2A	3.58	124.43	113.79
12	aB	916	CLA	C3C-C4C-NC	3.58	115.01	110.43
12	bA	820	CLA	C3C-C4C-NC	3.58	115.01	110.43
12	bA	833	CLA	C3C-C4C-NC	3.58	115.01	110.43
12	bL	204	CLA	C3B-C4B-NB	3.57	113.72	110.53
12	aB	949	CLA	C4C-C3C-C2C	-3.57	101.69	106.89
12	aA	809	CLA	C1C-C2C-C3C	-3.57	103.22	106.98
12	bA	816	CLA	C3B-C4B-NB	3.57	113.72	110.53
12	bA	812	CLA	C3C-C4C-NC	3.57	115.01	110.43
12	aA	824	CLA	C3B-C4B-NB	3.57	113.72	110.53
12	bB	923	CLA	CHD-C1D-ND	-3.57	119.78	124.80
12	cB	917	CLA	CBA-CAA-C2A	3.57	124.42	113.79
12	aB	925	CLA	CHD-C1D-ND	-3.57	119.78	124.80
12	bA	815	CLA	C1D-CHD-C4C	-3.57	118.43	126.02
12	bA	831	CLA	C1C-C2C-C3C	-3.57	103.23	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bB	907	CLA	C3B-C4B-NB	3.57	113.72	110.53
12	cL	204	CLA	C3B-C4B-NB	3.57	113.72	110.53
12	cA	803	CLA	O2D-CGD-CBD	3.57	117.47	111.23
12	cA	838	CLA	C1D-CHD-C4C	-3.57	118.44	126.02
12	aA	820	CLA	C3C-C4C-NC	3.57	115.00	110.43
12	bA	821	CLA	CHD-C1D-ND	-3.57	119.78	124.80
12	cA	835	CLA	C4B-C3B-C2B	-3.57	102.87	107.30
12	bA	816	CLA	C4A-NA-C1A	-3.57	105.05	106.68
12	aA	825	CLA	C1C-C2C-C3C	-3.57	103.23	106.98
12	bA	823	CLA	C1D-CHD-C4C	-3.57	118.44	126.02
12	bB	925	CLA	CHD-C1D-ND	-3.56	119.79	124.80
12	aB	918	CLA	C3C-C4C-NC	3.56	115.00	110.43
12	bA	827	CLA	C4C-C3C-C2C	-3.56	101.70	106.89
12	cA	841	CLA	C1C-C2C-C3C	-3.56	103.23	106.98
12	cA	833	CLA	C3C-C4C-NC	3.56	115.00	110.43
12	cB	906	CLA	C1D-CHD-C4C	-3.56	118.45	126.02
12	aA	843	CLA	C2B-C1B-NB	3.56	114.02	110.33
12	aA	834	CLA	C1D-CHD-C4C	-3.56	118.45	126.02
12	aA	811	CLA	C3C-C4C-NC	3.56	114.99	110.43
12	bA	841	CLA	C1C-C2C-C3C	-3.56	103.23	106.98
12	cA	827	CLA	CHD-C1D-ND	-3.56	119.79	124.80
12	cB	923	CLA	CHD-C1D-ND	-3.56	119.79	124.80
12	bA	810	CLA	C1C-C2C-C3C	-3.56	103.23	106.98
12	aB	923	CLA	CHD-C1D-ND	-3.56	119.79	124.80
12	cB	905	CLA	C1-C2-C3	-3.56	120.36	126.20
12	bB	906	CLA	C1D-CHD-C4C	-3.56	118.45	126.02
12	cA	839	CLA	O2D-CGD-O1D	-3.56	116.92	123.85
12	aB	905	CLA	C1C-C2C-C3C	-3.56	103.24	106.98
12	bB	924	CLA	C3C-C4C-NC	3.56	114.99	110.43
12	bB	928	CLA	C3D-C2D-C1D	-3.56	100.97	105.83
12	bA	808	CLA	C4-C3-C5	3.56	120.31	116.13
12	aB	928	CLA	C3D-C2D-C1D	-3.56	100.98	105.83
12	cB	922	CLA	CHD-C1D-ND	-3.56	119.80	124.80
12	cB	923	CLA	C1D-CHD-C4C	-3.56	118.46	126.02
12	bB	905	CLA	C1-C2-C3	-3.56	120.37	126.20
12	aA	827	CLA	CHD-C1D-ND	-3.56	119.80	124.80
12	cB	928	CLA	C3D-C2D-C1D	-3.55	100.98	105.83
12	bA	826	CLA	C3C-C4C-NC	3.55	114.98	110.43
12	aA	831	CLA	C1D-CHD-C4C	-3.55	118.47	126.02
12	bA	837	CLA	C4C-C3C-C2C	-3.55	101.72	106.89
12	bA	803	CLA	C4B-C3B-C2B	-3.55	102.89	107.30
12	bA	835	CLA	C4B-C3B-C2B	-3.55	102.89	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	808	CLA	C4-C3-C5	3.55	120.31	116.13
12	bA	837	CLA	C4B-C3B-C2B	-3.55	102.89	107.30
12	aB	924	CLA	C3C-C4C-NC	3.55	114.98	110.43
12	cB	926	CLA	C1D-CHD-C4C	-3.55	118.48	126.02
12	aA	803	CLA	O2D-CGD-CBD	3.55	117.43	111.23
12	cB	925	CLA	CHD-C1D-ND	-3.55	119.81	124.80
12	cA	811	CLA	C3C-C4C-NC	3.55	114.97	110.43
12	bB	926	CLA	C3B-C4B-NB	3.55	113.70	110.53
12	cB	934	CLA	CAA-C2A-C3A	-3.55	103.41	113.00
12	cA	821	CLA	C1D-CHD-C4C	-3.55	118.48	126.02
12	cA	810	CLA	C1C-C2C-C3C	-3.55	103.25	106.98
12	cA	831	CLA	C1C-C2C-C3C	-3.55	103.25	106.98
12	cA	837	CLA	C4C-C3C-C2C	-3.55	101.73	106.89
12	aA	828	CLA	C1D-CHD-C4C	-3.55	118.48	126.02
12	cA	821	CLA	C1C-C2C-C3C	-3.55	103.25	106.98
12	aL	204	CLA	C3B-C4B-NB	3.54	113.69	110.53
12	aB	904	CLA	C1D-CHD-C4C	-3.54	118.49	126.02
12	aA	821	CLA	C1D-CHD-C4C	-3.54	118.49	126.02
12	bA	821	CLA	C1D-CHD-C4C	-3.54	118.49	126.02
12	bA	803	CLA	O2D-CGD-CBD	3.54	117.42	111.23
12	bA	821	CLA	C1C-C2C-C3C	-3.54	103.25	106.98
12	cA	831	CLA	C1D-CHD-C4C	-3.54	118.49	126.02
12	aB	934	CLA	CAA-C2A-C3A	-3.54	103.43	113.00
12	cA	803	CLA	C4B-C3B-C2B	-3.54	102.90	107.30
12	aA	812	CLA	C3C-C4C-NC	3.54	114.97	110.43
12	bA	831	CLA	C1D-CHD-C4C	-3.54	118.50	126.02
12	aA	808	CLA	C4-C3-C5	3.54	120.29	116.13
12	bB	939	CLA	CAA-C2A-C3A	-3.54	103.44	113.00
12	bA	808	CLA	C3B-C4B-NB	3.54	113.69	110.53
12	aA	821	CLA	C1C-C2C-C3C	-3.54	103.26	106.98
12	cB	920	CLA	C3B-C4B-NB	3.54	113.69	110.53
12	cB	936	CLA	C3C-C4C-NC	3.54	114.96	110.43
12	bB	918	CLA	CAC-C3C-C4C	3.54	129.39	124.79
12	bA	828	CLA	C1D-CHD-C4C	-3.54	118.50	126.02
12	aB	905	CLA	C1-C2-C3	-3.54	120.40	126.20
12	aA	810	CLA	C1C-C2C-C3C	-3.53	103.26	106.98
12	cB	928	CLA	C1D-CHD-C4C	-3.53	118.51	126.02
12	aB	939	CLA	CAA-C2A-C3A	-3.53	103.45	113.00
12	cA	826	CLA	C3C-C4C-NC	3.53	114.96	110.43
12	bB	949	CLA	C4C-C3C-C2C	-3.53	101.75	106.89
12	bB	934	CLA	CAA-C2A-C3A	-3.53	103.45	113.00
12	bB	926	CLA	C1D-CHD-C4C	-3.53	118.51	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aB	934	CLA	C3B-C2B-C1B	-3.53	103.01	107.17
12	bA	824	CLA	C3B-C4B-NB	3.53	113.68	110.53
12	aB	923	CLA	C1D-CHD-C4C	-3.53	118.52	126.02
12	bA	824	CLA	C4A-NA-C1A	-3.53	105.07	106.68
12	bA	827	CLA	CHD-C1D-ND	-3.53	119.84	124.80
12	bB	936	CLA	C3C-C4C-NC	3.53	114.95	110.43
12	cA	837	CLA	C4B-C3B-C2B	-3.53	102.92	107.30
12	cB	910	CLA	CAA-C2A-C3A	-3.53	103.47	113.00
12	cA	840	CLA	C1D-CHD-C4C	-3.53	118.53	126.02
12	bA	832	CLA	C3C-C4C-NC	3.53	114.95	110.43
12	aA	809	CLA	C1D-CHD-C4C	-3.53	118.53	126.02
12	bA	805	CLA	CAA-C2A-C3A	-3.52	103.47	113.00
12	cA	808	CLA	C3B-C4B-NB	3.52	113.68	110.53
12	cB	949	CLA	C4C-C3C-C2C	-3.52	101.76	106.89
12	cA	812	CLA	C3C-C4C-NC	3.52	114.94	110.43
12	cA	828	CLA	C1D-CHD-C4C	-3.52	118.53	126.02
12	bA	809	CLA	C1D-CHD-C4C	-3.52	118.53	126.02
12	aB	901	CLA	C4C-C3C-C2C	-3.52	101.76	106.89
12	bB	950	CLA	C4B-C3B-C2B	-3.52	102.92	107.30
12	aB	906	CLA	C1D-CHD-C4C	-3.52	118.53	126.02
12	cA	809	CLA	C1D-CHD-C4C	-3.52	118.53	126.02
12	cB	926	CLA	C3B-C4B-NB	3.52	113.67	110.53
12	cB	918	CLA	CAC-C3C-C4C	3.52	129.37	124.79
12	cB	939	CLA	CAA-C2A-C3A	-3.52	103.48	113.00
12	aA	840	CLA	C1D-CHD-C4C	-3.52	118.54	126.02
12	cA	828	CLA	CAA-C2A-C3A	-3.52	103.49	113.00
12	aA	803	CLA	C4B-C3B-C2B	-3.52	102.93	107.30
12	aA	835	CLA	C4B-C3B-C2B	-3.52	102.93	107.30
12	bB	928	CLA	C1D-CHD-C4C	-3.52	118.54	126.02
12	aA	828	CLA	CAA-C2A-C3A	-3.52	103.49	113.00
12	bB	905	CLA	C4A-NA-C1A	-3.52	105.07	106.68
12	aA	826	CLA	C3C-C4C-NC	3.52	114.94	110.43
12	aB	926	CLA	C1D-CHD-C4C	-3.52	118.55	126.02
12	aB	928	CLA	C1D-CHD-C4C	-3.52	118.55	126.02
12	cB	904	CLA	C1D-CHD-C4C	-3.52	118.55	126.02
12	cA	832	CLA	C3C-C4C-NC	3.52	114.94	110.43
12	aA	839	CLA	C3B-C4B-NB	3.52	113.67	110.53
12	bA	840	CLA	C1D-CHD-C4C	-3.52	118.55	126.02
12	bA	825	CLA	C1C-C2C-C3C	-3.52	103.28	106.98
12	cA	825	CLA	C1C-C2C-C3C	-3.52	103.28	106.98
12	aA	832	CLA	C3C-C4C-NC	3.52	114.93	110.43
12	bB	919	CLA	C3C-C4C-NC	3.52	114.93	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aB	919	CLA	C3C-C4C-NC	3.52	114.93	110.43
12	bB	910	CLA	CAA-C2A-C3A	-3.51	103.50	113.00
12	cB	918	CLA	CAA-C2A-C3A	-3.51	103.50	113.00
12	bB	923	CLA	C1D-CHD-C4C	-3.51	118.55	126.02
12	aB	918	CLA	CAA-C2A-C3A	-3.51	103.51	113.00
12	bB	920	CLA	C3C-C4C-NC	3.51	114.93	110.43
12	cB	924	CLA	C3C-C4C-NC	3.51	114.93	110.43
12	aA	844	CLA	C4B-C3B-C2B	-3.51	102.94	107.30
12	bB	904	CLA	C1D-CHD-C4C	-3.51	118.56	126.02
12	aB	922	CLA	C1C-C2C-C3C	-3.51	103.29	106.98
12	bB	925	CLA	C4-C3-C5	3.51	121.32	115.23
12	aB	950	CLA	C4B-C3B-C2B	-3.51	102.94	107.30
12	aB	936	CLA	C3C-C4C-NC	3.51	114.93	110.43
12	bA	828	CLA	CAA-C2A-C3A	-3.51	103.52	113.00
12	bA	836	CLA	C1D-CHD-C4C	-3.51	118.56	126.02
15	bA	849	BCR	C15-C14-C13	-3.51	122.36	127.28
12	aB	925	CLA	C4-C3-C5	3.51	121.32	115.23
12	aA	808	CLA	C3B-C4B-NB	3.51	113.66	110.53
12	bA	839	CLA	C3B-C4B-NB	3.51	113.66	110.53
12	bB	920	CLA	C3B-C4B-NB	3.51	113.66	110.53
12	aB	920	CLA	C3B-C4B-NB	3.51	113.66	110.53
12	bB	918	CLA	CAA-C2A-C3A	-3.51	103.52	113.00
12	cA	805	CLA	CAA-C2A-C3A	-3.51	103.52	113.00
12	cA	853	CLA	O2D-CGD-O1D	-3.51	117.03	123.85
12	aB	902	CLA	C2C-C1C-NC	3.50	113.66	109.98
15	aA	850	BCR	C15-C14-C13	-3.50	122.36	127.28
12	aA	805	CLA	CAA-C2A-C3A	-3.50	103.53	113.00
12	aB	910	CLA	CAA-C2A-C3A	-3.50	103.53	113.00
12	aA	841	CLA	C1C-C2C-C3C	-3.50	103.30	106.98
12	bB	924	CLA	C1C-C2C-C3C	-3.50	103.30	106.98
12	cB	934	CLA	C3B-C2B-C1B	-3.50	103.04	107.17
12	cB	902	CLA	C2C-C1C-NC	3.50	113.66	109.98
12	aA	814	CLA	C4C-C3C-C2C	-3.50	101.80	106.89
12	aA	834	CLA	CMB-C2B-C1B	3.50	130.75	125.42
12	aA	854	CLA	O2D-CGD-O1D	-3.50	117.04	123.85
15	cA	849	BCR	C15-C14-C13	-3.50	122.37	127.28
12	bB	921	CLA	C1D-CHD-C4C	-3.50	118.58	126.02
12	aB	920	CLA	C3C-C4C-NC	3.50	114.91	110.43
12	cB	908	CLA	C1D-CHD-C4C	-3.50	118.59	126.02
12	cB	901	CLA	C4C-C3C-C2C	-3.50	101.80	106.89
12	cB	920	CLA	C3C-C4C-NC	3.50	114.91	110.43
12	cB	936	CLA	O2D-CGD-O1D	-3.50	117.04	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aB	918	CLA	CAC-C3C-C4C	3.50	129.34	124.79
12	bA	853	CLA	O2D-CGD-O1D	-3.50	117.05	123.85
12	aB	936	CLA	O2D-CGD-O1D	-3.49	117.05	123.85
12	cA	834	CLA	CMB-C2B-C1B	3.49	130.74	125.42
12	cB	909	CLA	CHD-C1D-ND	-3.49	119.89	124.80
12	cB	919	CLA	C3C-C4C-NC	3.49	114.90	110.43
12	bA	831	CLA	CHD-C1D-ND	-3.49	119.89	124.80
12	bB	909	CLA	C4B-C3B-C2B	-3.49	102.96	107.30
12	cA	836	CLA	C1D-CHD-C4C	-3.49	118.60	126.02
12	cA	816	CLA	C1C-C2C-C3C	-3.49	103.31	106.98
12	cB	925	CLA	C4-C3-C5	3.49	121.29	115.23
12	aB	909	CLA	CHD-C1D-ND	-3.49	119.89	124.80
12	cA	824	CLA	C4A-NA-C1A	-3.49	105.09	106.68
12	cA	839	CLA	C3B-C4B-NB	3.49	113.64	110.53
12	aB	921	CLA	C1D-CHD-C4C	-3.49	118.61	126.02
12	bA	816	CLA	C1C-C2C-C3C	-3.49	103.31	106.98
12	bA	834	CLA	CMB-C2B-C1B	3.49	130.73	125.42
12	aA	811	CLA	CAA-C2A-C3A	-3.49	103.58	113.00
12	cB	909	CLA	C4B-C3B-C2B	-3.49	102.97	107.30
12	cA	814	CLA	C4C-C3C-C2C	-3.49	101.82	106.89
12	aB	924	CLA	C1C-C2C-C3C	-3.49	103.31	106.98
12	aA	824	CLA	C4A-NA-C1A	-3.49	105.09	106.68
12	aA	816	CLA	C1C-C2C-C3C	-3.48	103.31	106.98
12	cA	803	CLA	C1C-C2C-C3C	-3.48	103.31	106.98
12	cA	804	CLA	C1C-C2C-C3C	-3.48	103.31	106.98
12	cA	805	CLA	C1C-C2C-C3C	-3.48	103.31	106.98
12	aA	831	CLA	CHD-C1D-ND	-3.48	119.90	124.80
12	cA	819	CLA	C1D-CHD-C4C	-3.48	118.61	126.02
12	bB	908	CLA	C1D-CHD-C4C	-3.48	118.62	126.02
12	bB	911	CLA	C1D-CHD-C4C	-3.48	118.62	126.02
12	aA	819	CLA	C1D-CHD-C4C	-3.48	118.62	126.02
12	aB	908	CLA	C1D-CHD-C4C	-3.48	118.62	126.02
12	bA	819	CLA	C1D-CHD-C4C	-3.48	118.62	126.02
12	bA	802	CLA	O2D-CGD-O1D	-3.48	117.08	123.85
12	cA	811	CLA	CAA-C2A-C3A	-3.48	103.60	113.00
12	bA	811	CLA	CAA-C2A-C3A	-3.48	103.60	113.00
12	aB	911	CLA	C1D-CHD-C4C	-3.48	118.63	126.02
12	cA	831	CLA	CHD-C1D-ND	-3.48	119.91	124.80
12	bB	934	CLA	C3B-C2B-C1B	-3.48	103.07	107.17
12	bA	820	CLA	CHD-C1D-ND	-3.48	119.91	124.80
12	cB	922	CLA	C1C-C2C-C3C	-3.48	103.33	106.98
12	cB	923	CLA	O2D-CGD-O1D	-3.47	117.08	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	836	CLA	C1D-CHD-C4C	-3.47	118.64	126.02
12	aA	844	CLA	C4C-C3C-C2C	-3.47	101.84	106.89
12	cB	924	CLA	C1C-C2C-C3C	-3.47	103.33	106.98
12	aA	802	CLA	O2D-CGD-O1D	-3.47	117.09	123.85
12	bB	908	CLA	C3C-C4C-NC	3.47	114.88	110.43
12	bB	922	CLA	C1C-C2C-C3C	-3.47	103.33	106.98
12	bB	901	CLA	C4C-C3C-C2C	-3.47	101.84	106.89
12	cB	921	CLA	C1D-CHD-C4C	-3.47	118.64	126.02
12	cA	802	CLA	O2D-CGD-O1D	-3.47	117.10	123.85
12	aA	843	CLA	C1-C2-C3	-3.47	120.51	126.20
12	bB	909	CLA	CHD-C1D-ND	-3.47	119.92	124.80
12	aA	803	CLA	C1C-C2C-C3C	-3.47	103.33	106.98
12	aL	203	CLA	O2D-CGD-O1D	-3.47	117.10	123.85
12	aB	914	CLA	C4A-NA-C1A	-3.47	105.10	106.68
12	bA	814	CLA	C4C-C3C-C2C	-3.47	101.84	106.89
12	bA	804	CLA	C1C-C2C-C3C	-3.47	103.33	106.98
12	bB	918	CLA	C1D-CHD-C4C	-3.47	118.65	126.02
12	aA	843	CLA	C3B-C4B-NB	3.46	113.62	110.53
12	cB	908	CLA	C3C-C4C-NC	3.46	114.87	110.43
12	bL	204	CLA	C3C-C4C-NC	3.46	114.87	110.43
12	bA	813	CLA	C4C-C3C-C2C	-3.46	101.85	106.89
12	aA	820	CLA	CHD-C1D-ND	-3.46	119.93	124.80
12	cA	843	CLA	C1-C2-C3	-3.46	120.53	126.20
12	aA	828	CLA	C4C-C3C-C2C	-3.46	101.86	106.89
12	aB	918	CLA	O2D-CGD-CBD	3.46	117.28	111.23
12	bB	902	CLA	C2C-C1C-NC	3.46	113.61	109.98
12	aA	835	CLA	C1D-CHD-C4C	-3.46	118.67	126.02
12	bB	950	CLA	C4C-C3C-C2C	-3.46	101.86	106.89
12	aB	905	CLA	O2D-CGD-CBD	3.46	117.28	111.23
12	bB	918	CLA	O2D-CGD-CBD	3.46	117.28	111.23
12	bB	927	CLA	C1D-CHD-C4C	-3.46	118.67	126.02
12	bA	805	CLA	C1C-C2C-C3C	-3.46	103.34	106.98
12	bB	923	CLA	O2D-CGD-O1D	-3.46	117.12	123.85
12	cA	813	CLA	C4C-C3C-C2C	-3.46	101.86	106.89
12	bB	936	CLA	O2D-CGD-O1D	-3.45	117.12	123.85
12	aB	916	CLA	C2C-C1C-NC	3.45	113.61	109.98
12	bA	843	CLA	C1-C2-C3	-3.45	120.54	126.20
12	cA	829	CLA	CHD-C1D-ND	-3.45	119.94	124.80
12	aB	950	CLA	C1D-CHD-C4C	-3.45	118.68	126.02
12	aB	950	CLA	C4C-C3C-C2C	-3.45	101.86	106.89
12	cA	843	CLA	C3B-C4B-NB	3.45	113.61	110.53
12	bB	905	CLA	O2D-CGD-CBD	3.45	117.26	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cB	918	CLA	C1D-CHD-C4C	-3.45	118.69	126.02
12	cA	812	CLA	CAA-C2A-C3A	-3.45	103.67	113.00
12	aA	829	CLA	CHD-C1D-ND	-3.45	119.95	124.80
12	bA	835	CLA	C1D-CHD-C4C	-3.45	118.69	126.02
15	bA	849	BCR	C15-C16-C17	-3.45	116.47	123.52
12	cB	918	CLA	O2D-CGD-CBD	3.45	117.26	111.23
12	cA	820	CLA	CHD-C1D-ND	-3.45	119.95	124.80
12	aB	909	CLA	C4B-C3B-C2B	-3.45	103.02	107.30
12	cB	911	CLA	C1D-CHD-C4C	-3.45	118.70	126.02
12	aA	812	CLA	CAA-C2A-C3A	-3.44	103.69	113.00
12	aB	918	CLA	C1D-CHD-C4C	-3.44	118.70	126.02
12	bA	803	CLA	C1C-C2C-C3C	-3.44	103.36	106.98
12	aA	839	CLA	CHD-C1D-ND	-3.44	119.95	124.80
12	cL	203	CLA	O2D-CGD-O1D	-3.44	117.14	123.85
12	cA	835	CLA	C1D-CHD-C4C	-3.44	118.70	126.02
12	aB	927	CLA	C1D-CHD-C4C	-3.44	118.70	126.02
12	cB	927	CLA	C1D-CHD-C4C	-3.44	118.71	126.02
12	bA	812	CLA	CAA-C2A-C3A	-3.44	103.70	113.00
12	bB	950	CLA	C1D-CHD-C4C	-3.44	118.71	126.02
12	bA	810	CLA	C1D-CHD-C4C	-3.44	118.71	126.02
12	aB	937	CLA	C3C-C4C-NC	3.44	114.83	110.43
12	cA	843	CLA	CBA-CAA-C2A	3.44	124.02	113.79
12	bA	828	CLA	C4C-C3C-C2C	-3.44	101.89	106.89
12	cA	835	CLA	CHD-C1D-ND	-3.44	119.97	124.80
12	aA	844	CLA	C1D-CHD-C4C	-3.44	118.72	126.02
12	cA	828	CLA	C4C-C3C-C2C	-3.43	101.89	106.89
12	bA	843	CLA	CBA-CAA-C2A	3.43	124.01	113.79
15	aL	205	BCR	C27-C26-C25	3.43	127.34	122.70
12	cB	905	CLA	O2D-CGD-CBD	3.43	117.23	111.23
12	bB	916	CLA	C2C-C1C-NC	3.43	113.59	109.98
12	aB	923	CLA	O2D-CGD-O1D	-3.43	117.17	123.85
15	cA	849	BCR	C15-C16-C17	-3.43	116.50	123.52
12	bA	839	CLA	CHD-C1D-ND	-3.43	119.97	124.80
12	aA	804	CLA	C1C-C2C-C3C	-3.43	103.37	106.98
12	aA	813	CLA	C4C-C3C-C2C	-3.43	101.90	106.89
12	aA	843	CLA	CBA-CAA-C2A	3.43	124.00	113.79
12	aA	810	CLA	C1D-CHD-C4C	-3.43	118.73	126.02
12	cL	204	CLA	C3C-C4C-NC	3.43	114.82	110.43
12	aA	803	CLA	C3C-C4C-NC	3.43	114.82	110.43
12	bB	936	CLA	C3B-C4B-NB	3.43	113.59	110.53
12	aA	813	CLA	C1C-C2C-C3C	-3.43	103.38	106.98
12	bA	808	CLA	C3C-C4C-NC	3.43	114.82	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cB	911	CLA	C4A-NA-C1A	-3.43	105.12	106.68
12	bL	203	CLA	O2D-CGD-O1D	-3.42	117.18	123.85
12	bA	835	CLA	CHD-C1D-ND	-3.42	119.98	124.80
12	cB	936	CLA	C3B-C4B-NB	3.42	113.59	110.53
12	cA	839	CLA	CHD-C1D-ND	-3.42	119.98	124.80
12	aL	204	CLA	C3C-C4C-NC	3.42	114.82	110.43
12	bB	925	CLA	C4C-C3C-C2C	-3.42	101.91	106.89
12	aB	908	CLA	C3C-C4C-NC	3.42	114.81	110.43
12	cB	930	CLA	C1D-CHD-C4C	-3.42	118.75	126.02
12	bB	914	CLA	C4A-NA-C1A	-3.42	105.12	106.68
12	aA	825	CLA	CMB-C2B-C1B	3.42	130.62	125.42
12	bA	829	CLA	CHD-C1D-ND	-3.42	119.99	124.80
15	bL	205	BCR	C27-C26-C25	3.42	127.32	122.70
12	aF	202	CLA	C3C-C4C-NC	3.42	114.81	110.43
12	bA	843	CLA	C3B-C4B-NB	3.42	113.58	110.53
12	cA	818	CLA	C3B-C4B-NB	3.42	113.58	110.53
12	cA	822	CLA	C3B-C4B-NB	3.42	113.58	110.53
12	aB	912	CLA	C1D-CHD-C4C	-3.41	118.76	126.02
12	cA	823	CLA	C4-C3-C5	3.41	120.15	116.13
12	bA	825	CLA	CMB-C2B-C1B	3.41	130.62	125.42
12	cB	930	CLA	CAA-C2A-C3A	-3.41	103.78	113.00
12	aA	805	CLA	C1C-C2C-C3C	-3.41	103.39	106.98
12	bA	803	CLA	C3C-C4C-NC	3.41	114.80	110.43
12	bA	823	CLA	C4-C3-C5	3.41	120.14	116.13
12	cA	825	CLA	CMB-C2B-C1B	3.41	130.61	125.42
12	aA	818	CLA	C3B-C4B-NB	3.41	113.57	110.53
12	aA	808	CLA	C3C-C4C-NC	3.41	114.79	110.43
12	bA	830	CLA	C4C-C3C-C2C	-3.41	101.93	106.89
12	bB	919	CLA	O2D-CGD-O1D	-3.41	117.22	123.85
12	cA	802	CLA	C1D-CHD-C4C	-3.40	118.78	126.02
15	aA	850	BCR	C15-C16-C17	-3.40	116.55	123.52
12	bB	930	CLA	CAA-C2A-C3A	-3.40	103.80	113.00
12	cB	932	CLA	C3C-C4C-NC	3.40	114.79	110.43
12	cB	919	CLA	O2D-CGD-O1D	-3.40	117.22	123.85
12	cB	937	CLA	C3C-C4C-NC	3.40	114.79	110.43
12	cA	840	CLA	C4A-NA-C1A	-3.40	105.13	106.68
12	cA	836	CLA	C4B-C3B-C2B	-3.40	103.07	107.30
12	cA	830	CLA	C4C-C3C-C2C	-3.40	101.94	106.89
15	cL	205	BCR	C27-C26-C25	3.40	127.30	122.70
12	bB	912	CLA	C1D-CHD-C4C	-3.40	118.79	126.02
12	aB	930	CLA	C1D-CHD-C4C	-3.40	118.79	126.02
12	aA	836	CLA	C4B-C3B-C2B	-3.40	103.07	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	833	CLA	C1D-CHD-C4C	-3.40	118.80	126.02
12	bB	930	CLA	C1D-CHD-C4C	-3.40	118.80	126.02
12	cA	810	CLA	C1D-CHD-C4C	-3.40	118.80	126.02
12	bA	813	CLA	C1C-C2C-C3C	-3.40	103.41	106.98
12	cB	916	CLA	C2C-C1C-NC	3.40	113.55	109.98
12	aB	930	CLA	CAA-C2A-C3A	-3.40	103.82	113.00
12	aB	919	CLA	C1D-CHD-C4C	-3.39	118.81	126.02
12	cA	803	CLA	C3C-C4C-NC	3.39	114.78	110.43
12	aB	932	CLA	C4A-NA-C1A	-3.39	105.13	106.68
12	aA	835	CLA	CHD-C1D-ND	-3.39	120.03	124.80
12	cA	813	CLA	C1C-C2C-C3C	-3.39	103.41	106.98
12	aA	818	CLA	C4C-C3C-C2C	-3.39	101.96	106.89
12	aA	805	CLA	C1D-CHD-C4C	-3.39	118.81	126.02
12	aB	919	CLA	O2D-CGD-O1D	-3.39	117.25	123.85
12	bA	836	CLA	C4B-C3B-C2B	-3.39	103.09	107.30
12	cB	925	CLA	C4C-C3C-C2C	-3.39	101.96	106.89
12	aB	936	CLA	C3B-C4B-NB	3.39	113.55	110.53
12	cB	916	CLA	C4C-C3C-C2C	-3.39	101.96	106.89
12	bB	903	CLA	CMC-C2C-C1C	3.39	130.33	125.03
12	bF	202	CLA	C3C-C4C-NC	3.39	114.77	110.43
12	bA	805	CLA	C1D-CHD-C4C	-3.39	118.82	126.02
12	bB	937	CLA	C3C-C4C-NC	3.39	114.77	110.43
12	cB	912	CLA	C1D-CHD-C4C	-3.39	118.82	126.02
12	bB	922	CLA	C3B-C4B-NB	3.38	113.55	110.53
12	aB	932	CLA	C3C-C4C-NC	3.38	114.77	110.43
12	bB	932	CLA	C3C-C4C-NC	3.38	114.76	110.43
12	bA	802	CLA	C1D-CHD-C4C	-3.38	118.83	126.02
12	aB	903	CLA	CMC-C2C-C1C	3.38	130.32	125.03
12	aA	823	CLA	C4-C3-C5	3.38	120.11	116.13
12	bA	817	CLA	C3B-C4B-NB	3.38	113.55	110.53
12	aB	920	CLA	C1D-CHD-C4C	-3.38	118.84	126.02
12	cA	818	CLA	C4C-C3C-C2C	-3.38	101.97	106.89
12	cB	903	CLA	CMC-C2C-C1C	3.38	130.31	125.03
12	cA	818	CLA	CAA-C2A-C3A	-3.38	103.87	113.00
12	bB	920	CLA	C1D-CHD-C4C	-3.38	118.84	126.02
12	cA	805	CLA	C1D-CHD-C4C	-3.38	118.84	126.02
12	bA	822	CLA	C3C-C4C-NC	3.38	114.76	110.43
12	bB	919	CLA	C1D-CHD-C4C	-3.38	118.84	126.02
12	bB	908	CLA	CAA-C2A-C3A	-3.38	103.87	113.00
12	cB	919	CLA	C1D-CHD-C4C	-3.38	118.84	126.02
12	aB	911	CLA	CAC-C3C-C4C	3.38	129.18	124.79
12	cA	829	CLA	C4A-NA-C1A	-3.38	105.14	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aB	901	CLA	C1C-C2C-C3C	-3.37	103.43	106.98
12	bA	829	CLA	C4A-NA-C1A	-3.37	105.14	106.68
12	cB	908	CLA	CAA-C2A-C3A	-3.37	103.89	113.00
12	aA	820	CLA	C3B-C4B-NB	3.37	113.54	110.53
12	aB	925	CLA	C4C-C3C-C2C	-3.37	101.98	106.89
12	cF	202	CLA	C3C-C4C-NC	3.37	114.75	110.43
12	aA	818	CLA	CAA-C2A-C3A	-3.37	103.89	113.00
12	bB	902	CLA	C3C-C4C-NC	3.37	114.75	110.43
12	bB	901	CLA	C1C-C2C-C3C	-3.37	103.44	106.98
12	bA	807	CLA	CHD-C4C-NC	3.37	129.45	124.23
12	cA	820	CLA	C1-O2A-CGA	3.37	124.80	116.65
12	bB	916	CLA	C4C-C3C-C2C	-3.37	101.99	106.89
12	aA	807	CLA	CHD-C4C-NC	3.37	129.45	124.23
12	aA	822	CLA	C3B-C4B-NB	3.37	113.54	110.53
12	bA	808	CLA	C4B-C3B-C2B	-3.37	103.11	107.30
12	cB	922	CLA	C4A-NA-C1A	-3.37	105.14	106.68
12	bB	911	CLA	CAC-C3C-C4C	3.37	129.17	124.79
12	cA	840	CLA	O2A-CGA-CBA	3.37	122.10	111.83
12	aB	925	CLA	C1C-C2C-C3C	-3.36	103.44	106.98
12	bB	909	CLA	CAC-C3C-C4C	3.36	129.17	124.79
12	cA	808	CLA	C3C-C4C-NC	3.36	114.74	110.43
12	aA	802	CLA	C1D-CHD-C4C	-3.36	118.87	126.02
12	bA	840	CLA	O2A-CGA-CBA	3.36	122.09	111.83
12	cA	803	CLA	CMB-C2B-C3B	3.36	134.46	126.55
12	cB	909	CLA	CAC-C3C-C4C	3.36	129.17	124.79
12	bB	950	CLA	C1C-C2C-C3C	-3.36	103.44	106.98
12	aA	830	CLA	C4C-C3C-C2C	-3.36	102.00	106.89
12	cA	808	CLA	C4B-C3B-C2B	-3.36	103.12	107.30
12	bA	818	CLA	C3B-C4B-NB	3.36	113.53	110.53
12	bA	821	CLA	C3B-C2B-C1B	-3.36	103.21	107.17
12	cA	837	CLA	CHD-C1D-ND	-3.36	120.07	124.80
12	aA	841	CLA	C1-C2-C3	-3.36	120.69	126.20
12	cB	901	CLA	C1C-C2C-C3C	-3.36	103.44	106.98
12	cB	920	CLA	C1D-CHD-C4C	-3.36	118.88	126.02
12	aA	843	CLA	CMC-C2C-C1C	3.36	130.28	125.03
12	cA	833	CLA	C1D-CHD-C4C	-3.36	118.88	126.02
12	cB	911	CLA	CAC-C3C-C4C	3.36	129.16	124.79
12	aA	817	CLA	C3B-C4B-NB	3.36	113.53	110.53
12	aB	908	CLA	CAA-C2A-C3A	-3.36	103.92	113.00
12	bA	841	CLA	C1-C2-C3	-3.36	120.69	126.20
12	bA	820	CLA	C1-O2A-CGA	3.36	124.78	116.65
12	cB	928	CLA	CHD-C1D-ND	-3.36	120.08	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	833	CLA	C1D-CHD-C4C	-3.36	118.89	126.02
12	aA	808	CLA	C4B-C3B-C2B	-3.36	103.13	107.30
12	bA	843	CLA	CMC-C2C-C1C	3.36	130.28	125.03
12	aA	843	CLA	C3C-C4C-NC	3.36	114.73	110.43
12	aA	820	CLA	C1-O2A-CGA	3.36	124.77	116.65
12	bA	818	CLA	CAA-C2A-C3A	-3.36	103.93	113.00
12	cA	836	CLA	CHC-C1C-C2C	-3.36	117.41	126.95
12	aA	837	CLA	CHD-C1D-ND	-3.35	120.08	124.80
12	aA	844	CLA	C1C-C2C-C3C	-3.35	103.45	106.98
12	aA	803	CLA	CMB-C2B-C3B	3.35	134.44	126.55
12	aB	922	CLA	C3B-C4B-NB	3.35	113.52	110.53
12	cA	821	CLA	C3B-C2B-C1B	-3.35	103.22	107.17
12	aB	902	CLA	C3C-C4C-NC	3.35	114.73	110.43
12	cB	902	CLA	C3C-C4C-NC	3.35	114.73	110.43
12	bA	839	CLA	C4B-C3B-C2B	-3.35	103.13	107.30
12	aA	811	CLA	CMA-C3A-C2A	-3.35	101.02	113.98
12	bA	811	CLA	CMA-C3A-C2A	-3.35	101.02	113.98
12	cB	917	CLA	C3C-C4C-NC	3.35	114.72	110.43
12	cB	925	CLA	C1C-C2C-C3C	-3.35	103.45	106.98
12	aA	822	CLA	C3C-C4C-NC	3.35	114.72	110.43
12	cA	822	CLA	C3C-C4C-NC	3.35	114.72	110.43
12	cA	811	CLA	CMA-C3A-C2A	-3.35	101.02	113.98
12	bA	820	CLA	C3B-C4B-NB	3.35	113.52	110.53
12	aA	807	CLA	C3C-C4C-NC	3.35	114.72	110.43
12	aA	839	CLA	C4B-C3B-C2B	-3.35	103.14	107.30
12	cB	929	CLA	C1D-CHD-C4C	-3.35	118.90	126.02
12	bA	816	CLA	C4C-C3C-C2C	-3.35	102.02	106.89
12	aB	910	CLA	C4B-C3B-C2B	-3.35	103.14	107.30
12	bB	929	CLA	C1D-CHD-C4C	-3.35	118.91	126.02
12	aB	916	CLA	C4C-C3C-C2C	-3.35	102.02	106.89
12	aB	927	CLA	C3D-C2D-C1D	-3.35	101.26	105.83
12	bA	822	CLA	C3B-C4B-NB	3.35	113.52	110.53
12	aB	929	CLA	C1D-CHD-C4C	-3.35	118.91	126.02
12	aA	840	CLA	O2A-CGA-CBA	3.35	122.04	111.83
12	bB	931	CLA	C4C-C3C-C2C	-3.35	102.02	106.89
12	bA	818	CLA	C4C-C3C-C2C	-3.34	102.02	106.89
12	cA	824	CLA	C1D-CHD-C4C	-3.34	118.91	126.02
12	cA	807	CLA	C3C-C4C-NC	3.34	114.71	110.43
12	aB	928	CLA	CHD-C1D-ND	-3.34	120.10	124.80
12	cA	815	CLA	C3C-C4C-NC	3.34	114.71	110.43
12	cA	807	CLA	CHD-C4C-NC	3.34	129.41	124.23
12	cB	928	CLA	C4C-C3C-C2C	-3.34	102.03	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bB	928	CLA	CHD-C1D-ND	-3.34	120.10	124.80
12	aB	931	CLA	C4C-C3C-C2C	-3.34	102.03	106.89
12	bA	837	CLA	CHD-C1D-ND	-3.34	120.10	124.80
12	bA	843	CLA	C4A-NA-C1A	-3.34	105.16	106.68
12	bA	803	CLA	CMB-C2B-C3B	3.34	134.41	126.55
12	aB	950	CLA	C1C-C2C-C3C	-3.34	103.47	106.98
12	bB	910	CLA	C4B-C3B-C2B	-3.34	103.15	107.30
12	bB	909	CLA	CMB-C2B-C1B	3.34	130.50	125.42
12	aB	909	CLA	CAC-C3C-C4C	3.34	129.13	124.79
12	bL	204	CLA	CAC-C3C-C4C	3.34	129.13	124.79
12	bA	824	CLA	C1D-CHD-C4C	-3.34	118.92	126.02
12	aA	821	CLA	C3B-C2B-C1B	-3.34	103.23	107.17
12	cB	932	CLA	C4A-NA-C1A	-3.34	105.16	106.68
12	cB	910	CLA	C4B-C3B-C2B	-3.34	103.15	107.30
12	cB	935	CLA	C3B-C4B-NB	3.34	113.51	110.53
12	aA	840	CLA	C4A-NA-C1A	-3.33	105.16	106.68
12	cA	806	CLA	CHB-C4A-NA	3.33	129.21	124.40
12	cA	843	CLA	CMC-C2C-C1C	3.33	130.24	125.03
12	aA	841	CLA	CAC-C3C-C4C	3.33	129.13	124.79
12	bA	836	CLA	CHC-C1C-C2C	-3.33	117.47	126.95
12	bA	807	CLA	C3C-C4C-NC	3.33	114.70	110.43
12	aA	815	CLA	C3C-C4C-NC	3.33	114.70	110.43
12	aB	928	CLA	C4C-C3C-C2C	-3.33	102.04	106.89
12	cA	817	CLA	C3B-C4B-NB	3.33	113.50	110.53
12	bA	815	CLA	C3C-C4C-NC	3.33	114.70	110.43
12	aA	834	CLA	CAA-C2A-C3A	-3.33	104.00	113.00
12	aA	816	CLA	C4C-C3C-C2C	-3.33	102.05	106.89
12	aB	917	CLA	C3C-C4C-NC	3.33	114.69	110.43
12	aA	843	CLA	C4A-NA-C1A	-3.33	105.16	106.68
12	bA	840	CLA	C4A-NA-C1A	-3.33	105.16	106.68
12	bA	831	CLA	CMA-C3A-C4A	-3.33	102.83	111.77
12	cA	817	CLA	O2D-CGD-O1D	-3.33	117.37	123.85
12	bA	803	CLA	CMA-C3A-C2A	-3.32	101.13	113.98
12	cA	803	CLA	CMA-C3A-C2A	-3.32	101.13	113.98
12	aA	824	CLA	C1D-CHD-C4C	-3.32	118.95	126.02
12	bB	926	CLA	C4B-C3B-C2B	-3.32	103.17	107.30
12	cB	922	CLA	C3B-C4B-NB	3.32	113.50	110.53
12	cA	841	CLA	C1-C2-C3	-3.32	120.75	126.20
12	aB	926	CLA	C4B-C3B-C2B	-3.32	103.17	107.30
12	cA	816	CLA	C4C-C3C-C2C	-3.32	102.06	106.89
12	cA	841	CLA	CAC-C3C-C4C	3.32	129.11	124.79
12	cA	831	CLA	CMA-C3A-C4A	-3.32	102.85	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	843	CLA	CMB-C2B-C1B	3.32	130.47	125.42
12	aA	836	CLA	CHC-C1C-C2C	-3.32	117.52	126.95
12	bB	924	CLA	C4B-C3B-C2B	-3.32	103.17	107.30
12	cA	820	CLA	C4-C3-C5	3.32	120.99	115.23
12	bB	917	CLA	C3C-C4C-NC	3.32	114.68	110.43
12	aA	831	CLA	CMA-C3A-C4A	-3.32	102.86	111.77
12	cA	843	CLA	C3C-C4C-NC	3.32	114.68	110.43
12	aA	803	CLA	CMA-C3A-C2A	-3.32	101.16	113.98
12	bA	817	CLA	O2D-CGD-O1D	-3.32	117.39	123.85
12	bB	918	CLA	C1C-C2C-C3C	-3.32	103.49	106.98
12	cA	805	CLA	CMC-C2C-C1C	3.32	130.22	125.03
12	cB	931	CLA	C4C-C3C-C2C	-3.32	102.07	106.89
12	aA	821	CLA	CAC-C3C-C4C	3.31	129.10	124.79
12	aB	909	CLA	CMB-C2B-C1B	3.31	130.47	125.42
12	bB	931	CLA	CAA-C2A-C3A	-3.31	104.04	113.00
12	bA	832	CLA	C1D-CHD-C4C	-3.31	118.98	126.02
12	bA	843	CLA	C3C-C4C-NC	3.31	114.67	110.43
12	bA	818	CLA	C1C-C2C-C3C	-3.31	103.50	106.98
12	aA	820	CLA	C4-C3-C5	3.31	120.98	115.23
12	bA	834	CLA	CAA-C2A-C3A	-3.31	104.05	113.00
12	aB	931	CLA	C1C-C2C-C3C	-3.31	103.50	106.98
12	aB	931	CLA	CAA-C2A-C3A	-3.31	104.06	113.00
12	bB	927	CLA	C3D-C2D-C1D	-3.31	101.31	105.83
12	cA	840	CLA	CAC-C3C-C4C	3.31	129.09	124.79
12	aB	909	CLA	C4C-C3C-C2C	-3.31	102.08	106.89
12	cA	834	CLA	CAA-C2A-C3A	-3.31	104.06	113.00
12	cB	931	CLA	C1C-C2C-C3C	-3.31	103.50	106.98
12	aA	804	CLA	C4C-C3C-C2C	-3.31	102.08	106.89
12	cB	931	CLA	CAA-C2A-C3A	-3.31	104.06	113.00
12	bA	843	CLA	CMB-C2B-C1B	3.31	130.45	125.42
12	aA	832	CLA	C1D-CHD-C4C	-3.31	118.99	126.02
12	bA	830	CLA	C1-C2-C3	-3.31	120.78	126.20
12	cB	918	CLA	C1C-C2C-C3C	-3.30	103.50	106.98
12	cB	927	CLA	C3D-C2D-C1D	-3.30	101.32	105.83
12	aA	843	CLA	CHD-C1D-ND	-3.30	120.15	124.80
12	bA	806	CLA	CHB-C4A-NA	3.30	129.17	124.40
12	aA	843	CLA	CMB-C2B-C1B	3.30	130.45	125.42
12	cA	837	CLA	C1C-C2C-C3C	-3.30	103.50	106.98
12	aB	908	CLA	CHD-C1D-ND	-3.30	120.15	124.80
12	bA	804	CLA	C4C-C3C-C2C	-3.30	102.08	106.89
12	bB	928	CLA	C4C-C3C-C2C	-3.30	102.08	106.89
12	bB	911	CLA	C4A-NA-C1A	-3.30	105.17	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	839	CLA	C4B-C3B-C2B	-3.30	103.20	107.30
12	aA	817	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
12	bA	841	CLA	CAC-C3C-C4C	3.30	129.08	124.79
12	cA	832	CLA	C1D-CHD-C4C	-3.30	119.01	126.02
12	aB	934	CLA	C3C-C4C-NC	3.30	114.66	110.43
12	cA	843	CLA	C4A-NA-C1A	-3.30	105.17	106.68
12	bA	813	CLA	CHD-C1D-ND	-3.30	120.16	124.80
12	bA	821	CLA	CAC-C3C-C4C	3.30	129.08	124.79
12	bA	824	CLA	C3C-C4C-NC	3.30	114.66	110.43
12	bB	925	CLA	C1C-C2C-C3C	-3.30	103.51	106.98
12	cB	909	CLA	C4C-C3C-C2C	-3.30	102.09	106.89
12	bA	820	CLA	C4-C3-C5	3.30	120.95	115.23
12	cA	821	CLA	CAC-C3C-C4C	3.30	129.08	124.79
12	bB	931	CLA	C1C-C2C-C3C	-3.30	103.51	106.98
12	bB	914	CLA	C3B-C4B-NB	3.30	113.47	110.53
12	bB	917	CLA	C4B-C3B-C2B	-3.30	103.20	107.30
12	aA	806	CLA	CHB-C4A-NA	3.30	129.16	124.40
12	aL	204	CLA	CAC-C3C-C4C	3.29	129.08	124.79
12	aB	924	CLA	C4B-C3B-C2B	-3.29	103.20	107.30
12	aA	837	CLA	C1C-C2C-C3C	-3.29	103.52	106.98
12	aB	936	CLA	C1D-CHD-C4C	-3.29	119.02	126.02
12	bA	837	CLA	C1C-C2C-C3C	-3.29	103.52	106.98
12	aB	917	CLA	C4B-C3B-C2B	-3.29	103.21	107.30
12	cA	820	CLA	C3B-C4B-NB	3.29	113.47	110.53
12	cB	909	CLA	CMB-C2B-C1B	3.29	130.43	125.42
12	aB	935	CLA	C3B-C4B-NB	3.29	113.47	110.53
12	bB	934	CLA	C3C-C4C-NC	3.29	114.64	110.43
12	cA	813	CLA	CHD-C1D-ND	-3.29	120.17	124.80
12	cA	830	CLA	C1-C2-C3	-3.29	120.81	126.20
12	cL	204	CLA	CAC-C3C-C4C	3.29	129.07	124.79
12	cB	923	CLA	C4A-NA-C1A	-3.29	105.18	106.68
12	bA	842	CLA	C4B-C3B-C2B	-3.29	103.22	107.30
12	aA	828	CLA	C4B-C3B-C2B	-3.29	103.22	107.30
12	bB	909	CLA	C4C-C3C-C2C	-3.29	102.11	106.89
12	cB	905	CLA	CMC-C2C-C1C	3.29	130.17	125.03
12	cB	936	CLA	C1D-CHD-C4C	-3.29	119.04	126.02
12	cA	828	CLA	C4B-C3B-C2B	-3.29	103.22	107.30
12	cA	804	CLA	C4C-C3C-C2C	-3.28	102.11	106.89
12	aB	918	CLA	C1C-C2C-C3C	-3.28	103.53	106.98
12	bB	922	CLA	C4A-NA-C1A	-3.28	105.18	106.68
12	bA	840	CLA	CHC-C1C-C2C	-3.28	117.62	126.95
12	aA	813	CLA	CHD-C1D-ND	-3.28	120.18	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	811	CLA	C4B-C3B-C2B	-3.28	103.22	107.30
12	bA	825	CLA	C4C-C3C-C2C	-3.28	102.12	106.89
12	cB	907	CLA	CHC-C1C-C2C	-3.28	117.62	126.95
15	bB	945	BCR	C15-C14-C13	-3.28	122.68	127.28
12	bA	805	CLA	CMC-C2C-C1C	3.28	130.16	125.03
12	cB	924	CLA	C4B-C3B-C2B	-3.28	103.23	107.30
12	aB	902	CLA	CAA-C2A-C3A	-3.28	104.14	113.00
12	cA	809	CLA	C4A-NA-C1A	-3.28	105.18	106.68
12	cB	907	CLA	C4C-C3C-C2C	-3.28	102.12	106.89
12	bA	840	CLA	CAC-C3C-C4C	3.28	129.05	124.79
12	aA	840	CLA	CHC-C1C-C2C	-3.28	117.64	126.95
12	bA	806	CLA	CAA-C2A-C3A	-3.28	104.15	113.00
12	cA	843	CLA	CHD-C1D-ND	-3.27	120.20	124.80
12	cB	908	CLA	CHD-C1D-ND	-3.27	120.20	124.80
12	aB	911	CLA	C4A-NA-C1A	-3.27	105.19	106.68
12	aB	923	CLA	C4A-NA-C1A	-3.27	105.19	106.68
12	cB	930	CLA	C4A-NA-C1A	-3.27	105.19	106.68
12	bB	908	CLA	CHD-C1D-ND	-3.27	120.20	124.80
12	bA	814	CLA	C4B-C3B-C2B	-3.27	103.23	107.30
12	cA	853	CLA	C3B-C4B-NB	3.27	113.45	110.53
12	aA	830	CLA	C1-C2-C3	-3.27	120.84	126.20
12	cA	814	CLA	C4B-C3B-C2B	-3.27	103.23	107.30
12	cB	917	CLA	C4B-C3B-C2B	-3.27	103.23	107.30
12	cA	830	CLA	C3B-C2B-C1B	-3.27	103.31	107.17
12	cB	932	CLA	C4C-C3C-C2C	-3.27	102.13	106.89
12	bB	935	CLA	C3B-C4B-NB	3.27	113.45	110.53
12	cA	806	CLA	CAA-C2A-C3A	-3.27	104.16	113.00
12	aA	842	CLA	C4B-C3B-C2B	-3.27	103.24	107.30
12	cA	811	CLA	C4B-C3B-C2B	-3.27	103.24	107.30
12	bB	902	CLA	CAA-C2A-C3A	-3.27	104.16	113.00
12	bB	905	CLA	CMC-C2C-C1C	3.27	130.14	125.03
12	aL	202	CLA	C3C-C4C-NC	3.27	114.62	110.43
12	cA	842	CLA	C4B-C3B-C2B	-3.27	103.24	107.30
15	cB	945	BCR	C15-C14-C13	-3.27	122.69	127.28
12	aA	824	CLA	C3C-C4C-NC	3.27	114.62	110.43
12	bA	831	CLA	C4C-C3C-C2C	-3.27	102.13	106.89
12	aA	840	CLA	CAC-C3C-C4C	3.27	129.04	124.79
12	cA	825	CLA	C4C-C3C-C2C	-3.27	102.14	106.89
12	cA	824	CLA	C3C-C4C-NC	3.27	114.62	110.43
12	aA	805	CLA	CMC-C2C-C1C	3.27	130.14	125.03
12	aB	905	CLA	CMC-C2C-C1C	3.27	130.14	125.03
12	cA	818	CLA	C1C-C2C-C3C	-3.27	103.54	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	813	CLA	C3B-C4B-NB	3.27	113.45	110.53
12	bL	204	CLA	C1D-CHD-C4C	-3.27	119.08	126.02
12	aB	907	CLA	CHC-C1C-C2C	-3.27	117.67	126.95
12	bB	936	CLA	C1D-CHD-C4C	-3.27	119.08	126.02
12	cA	807	CLA	CMC-C2C-C1C	3.26	130.14	125.03
12	cA	840	CLA	CHC-C1C-C2C	-3.26	117.67	126.95
12	aB	926	CLA	CHD-C1D-ND	-3.26	120.21	124.80
12	aA	832	CLA	C4A-NA-C1A	-3.26	105.19	106.68
12	cA	829	CLA	O2A-CGA-CBA	3.26	121.79	111.83
12	cB	902	CLA	CAA-C2A-C3A	-3.26	104.18	113.00
12	bB	939	CLA	CHC-C1C-C2C	-3.26	117.68	126.95
12	bA	820	CLA	C4A-NA-C1A	-3.26	105.19	106.68
12	cB	912	CLA	CAC-C3C-C4C	3.26	129.03	124.79
12	cB	926	CLA	C4B-C3B-C2B	-3.26	103.25	107.30
12	bB	907	CLA	CHC-C1C-C2C	-3.26	117.68	126.95
12	aA	806	CLA	CAA-C2A-C3A	-3.26	104.19	113.00
12	aA	830	CLA	C3B-C2B-C1B	-3.26	103.33	107.17
12	aA	818	CLA	C1C-C2C-C3C	-3.26	103.55	106.98
12	aL	204	CLA	C1D-CHD-C4C	-3.26	119.09	126.02
12	bA	828	CLA	C4B-C3B-C2B	-3.26	103.25	107.30
12	bB	932	CLA	C4C-C3C-C2C	-3.26	102.15	106.89
12	bA	829	CLA	O2A-CGA-CBA	3.26	121.77	111.83
12	aB	932	CLA	C4C-C3C-C2C	-3.26	102.15	106.89
12	cB	918	CLA	C4C-C3C-C2C	-3.26	102.15	106.89
12	cB	901	CLA	CHD-C1D-ND	-3.26	120.22	124.80
12	aA	821	CLA	C4C-C3C-C2C	-3.26	102.15	106.89
12	cA	821	CLA	C4C-C3C-C2C	-3.26	102.15	106.89
12	cB	934	CLA	C3C-C4C-NC	3.26	114.60	110.43
12	aB	939	CLA	CHC-C1C-C2C	-3.25	117.70	126.95
12	aB	910	CLA	C1D-CHD-C4C	-3.25	119.10	126.02
12	aA	807	CLA	CMC-C2C-C1C	3.25	130.12	125.03
12	cB	926	CLA	CHD-C1D-ND	-3.25	120.22	124.80
12	aA	829	CLA	O2A-CGA-CBA	3.25	121.75	111.83
12	cB	939	CLA	CHC-C1C-C2C	-3.25	117.70	126.95
12	bB	907	CLA	C4C-C3C-C2C	-3.25	102.16	106.89
12	cB	910	CLA	C1D-CHD-C4C	-3.25	119.11	126.02
12	bB	937	CLA	O2A-CGA-CBA	3.25	121.75	111.83
12	aB	922	CLA	C4A-NA-C1A	-3.25	105.20	106.68
12	bB	927	CLA	CED-O2D-CGD	3.25	123.29	115.92
12	bA	813	CLA	C3B-C4B-NB	3.25	113.43	110.53
12	bA	843	CLA	CHD-C1D-ND	-3.25	120.23	124.80
12	cB	922	CLA	C4C-C3C-C2C	-3.25	102.16	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	832	CLA	C4A-NA-C1A	-3.25	105.20	106.68
12	bA	807	CLA	CMC-C2C-C1C	3.25	130.11	125.03
12	cL	202	CLA	C3C-C4C-NC	3.25	114.59	110.43
12	bB	913	CLA	C4B-C3B-C2B	-3.25	103.26	107.30
12	aA	841	CLA	C4C-C3C-C2C	-3.25	102.16	106.89
12	cB	927	CLA	CED-O2D-CGD	3.25	123.28	115.92
12	bB	901	CLA	CHD-C1D-ND	-3.25	120.23	124.80
12	cA	816	CLA	CHD-C1D-ND	-3.25	120.23	124.80
12	bB	917	CLA	C1D-CHD-C4C	-3.25	119.12	126.02
12	aA	811	CLA	C4B-C3B-C2B	-3.25	103.27	107.30
12	cA	841	CLA	C4C-C3C-C2C	-3.24	102.17	106.89
12	aB	912	CLA	CAC-C3C-C4C	3.24	129.01	124.79
12	bB	912	CLA	CAC-C3C-C4C	3.24	129.01	124.79
12	aB	927	CLA	CED-O2D-CGD	3.24	123.28	115.92
12	bB	949	CLA	C3B-C4B-NB	3.24	113.43	110.53
12	bB	926	CLA	CHD-C1D-ND	-3.24	120.24	124.80
12	cA	853	CLA	C1C-C2C-C3C	-3.24	103.57	106.98
12	bB	907	CLA	CMB-C2B-C1B	3.24	130.36	125.42
12	aB	914	CLA	C3B-C4B-NB	3.24	113.42	110.53
12	aA	830	CLA	C1D-CHD-C4C	-3.24	119.13	126.02
12	cB	901	CLA	C3B-C4B-NB	3.24	113.42	110.53
12	aA	814	CLA	C4B-C3B-C2B	-3.24	103.27	107.30
12	cA	831	CLA	C4C-C3C-C2C	-3.24	102.17	106.89
12	cL	204	CLA	C1D-CHD-C4C	-3.24	119.13	126.02
12	aA	854	CLA	C3B-C4B-NB	3.24	113.42	110.53
12	bA	819	CLA	C3B-C4B-NB	3.24	113.42	110.53
12	cB	914	CLA	C3B-C4B-NB	3.24	113.42	110.53
12	aB	917	CLA	C1D-CHD-C4C	-3.24	119.13	126.02
15	bI	101	BCR	C2-C1-C6	3.24	115.14	110.44
12	bB	910	CLA	C1D-CHD-C4C	-3.24	119.14	126.02
12	cB	949	CLA	C3B-C4B-NB	3.24	113.42	110.53
12	bB	918	CLA	C4C-C3C-C2C	-3.24	102.18	106.89
12	aB	937	CLA	O2A-CGA-CBA	3.24	121.71	111.83
15	aB	945	BCR	C15-C14-C13	-3.24	122.74	127.28
12	aA	829	CLA	C4A-NA-C1A	-3.24	105.20	106.68
12	aA	854	CLA	C1C-C2C-C3C	-3.24	103.58	106.98
12	aB	918	CLA	C4C-C3C-C2C	-3.24	102.18	106.89
12	bB	910	CLA	CMA-C3A-C2A	-3.24	101.47	113.98
12	bL	202	CLA	C3C-C4C-NC	3.24	114.58	110.43
12	bB	922	CLA	C4C-C3C-C2C	-3.24	102.18	106.89
12	bA	853	CLA	C1C-C2C-C3C	-3.24	103.58	106.98
12	cB	923	CLA	CMC-C2C-C1C	3.24	130.09	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	820	CLA	C4A-NA-C1A	-3.24	105.20	106.68
12	bA	853	CLA	C3B-C4B-NB	3.24	113.42	110.53
12	aB	949	CLA	CMB-C2B-C1B	3.24	130.34	125.42
12	aA	825	CLA	C4C-C3C-C2C	-3.23	102.18	106.89
12	bA	804	CLA	CAA-C2A-C3A	-3.23	104.26	113.00
12	bA	805	CLA	O2D-CGD-O1D	-3.23	117.55	123.85
12	cB	910	CLA	CMA-C3A-C2A	-3.23	101.48	113.98
12	bA	821	CLA	C4C-C3C-C2C	-3.23	102.19	106.89
12	aB	910	CLA	CMA-C3A-C2A	-3.23	101.48	113.98
12	aB	930	CLA	C4A-NA-C1A	-3.23	105.20	106.68
12	cB	913	CLA	C4B-C3B-C2B	-3.23	103.28	107.30
12	bA	816	CLA	CHD-C1D-ND	-3.23	120.25	124.80
12	aB	949	CLA	C3B-C4B-NB	3.23	113.42	110.53
12	aB	913	CLA	CMC-C2C-C1C	3.23	130.08	125.03
12	aA	804	CLA	CAA-C2A-C3A	-3.23	104.27	113.00
12	cB	917	CLA	C1D-CHD-C4C	-3.23	119.15	126.02
12	bB	949	CLA	CMB-C2B-C1B	3.23	130.34	125.42
12	cA	830	CLA	C1D-CHD-C4C	-3.23	119.16	126.02
12	bB	932	CLA	C3B-C4B-NB	3.23	113.41	110.53
12	cA	813	CLA	C3B-C4B-NB	3.23	113.41	110.53
12	aA	830	CLA	CMA-C3A-C2A	-3.23	101.50	113.98
15	cI	101	BCR	C2-C1-C6	3.23	115.13	110.44
12	cA	830	CLA	CMA-C3A-C2A	-3.23	101.50	113.98
12	bB	926	CLA	C4A-NA-C1A	-3.23	105.21	106.68
12	aB	922	CLA	C4C-C3C-C2C	-3.23	102.19	106.89
12	aB	932	CLA	C3B-C4B-NB	3.23	113.41	110.53
12	aB	923	CLA	CMC-C2C-C1C	3.23	130.07	125.03
12	bA	841	CLA	C4C-C3C-C2C	-3.23	102.20	106.89
12	cB	911	CLA	C4B-C3B-C2B	-3.23	103.29	107.30
12	bB	932	CLA	C4A-NA-C1A	-3.22	105.21	106.68
12	aA	819	CLA	C3B-C4B-NB	3.22	113.41	110.53
12	aA	822	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
12	aB	928	CLA	CMA-C3A-C2A	-3.22	101.52	113.98
12	cA	843	CLA	CMA-C3A-C2A	-3.22	101.52	113.98
12	bB	923	CLA	CMC-C2C-C1C	3.22	130.07	125.03
12	bA	830	CLA	CMA-C3A-C2A	-3.22	101.53	113.98
12	bA	843	CLA	CMA-C3A-C2A	-3.22	101.53	113.98
12	aB	907	CLA	CMB-C2B-C1B	3.22	130.32	125.42
12	bB	928	CLA	CMA-C3A-C2A	-3.22	101.53	113.98
12	cA	805	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
12	cA	804	CLA	CAA-C2A-C3A	-3.22	104.30	113.00
12	aA	843	CLA	CMA-C3A-C2A	-3.22	101.53	113.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cB	928	CLA	CMA-C3A-C2A	-3.22	101.54	113.98
12	cB	937	CLA	O2A-CGA-CBA	3.22	121.64	111.83
12	bB	911	CLA	C4B-C3B-C2B	-3.22	103.30	107.30
12	aA	831	CLA	C4C-C3C-C2C	-3.22	102.21	106.89
12	bA	830	CLA	C3B-C2B-C1B	-3.22	103.38	107.17
12	bB	905	CLA	C4-C3-C5	3.22	120.81	115.23
12	aA	806	CLA	O2D-CGD-O1D	-3.22	117.59	123.85
12	aA	805	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
12	aA	816	CLA	CHD-C1D-ND	-3.21	120.28	124.80
12	aB	933	CLA	CHD-C1D-ND	-3.21	120.28	124.80
12	cA	819	CLA	C3B-C4B-NB	3.21	113.40	110.53
15	aI	101	BCR	C2-C1-C6	3.21	115.11	110.44
12	bA	853	CLA	O2A-CGA-CBA	3.21	121.63	111.83
12	cA	839	CLA	C4C-C3C-C2C	-3.21	102.22	106.89
12	aA	812	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
12	bB	923	CLA	C4A-NA-C1A	-3.21	105.21	106.68
12	bA	806	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
12	aA	833	CLA	C3B-C4B-NB	3.21	113.40	110.53
12	aB	914	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
12	aB	907	CLA	C4C-C3C-C2C	-3.21	102.22	106.89
12	bA	835	CLA	C4C-C3C-C2C	-3.21	102.22	106.89
12	cA	826	CLA	C1D-CHD-C4C	-3.21	119.20	126.02
12	cB	916	CLA	C4A-NA-C1A	-3.21	105.22	106.68
12	cA	822	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
12	cB	914	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
12	aB	913	CLA	C4B-C3B-C2B	-3.21	103.31	107.30
12	cB	924	CLA	C4C-C3C-C2C	-3.21	102.22	106.89
12	bB	933	CLA	CHD-C1D-ND	-3.21	120.29	124.80
12	bB	914	CLA	O2D-CGD-O1D	-3.21	117.61	123.85
12	aA	839	CLA	C4C-C3C-C2C	-3.20	102.23	106.89
12	bA	839	CLA	C4C-C3C-C2C	-3.20	102.23	106.89
12	cA	806	CLA	O2D-CGD-O1D	-3.20	117.61	123.85
12	aA	820	CLA	C4B-C3B-C2B	-3.20	103.32	107.30
12	cA	840	CLA	C3C-C4C-NC	3.20	114.53	110.43
12	cB	933	CLA	CHD-C1D-ND	-3.20	120.30	124.80
12	cB	916	CLA	C1-C2-C3	-3.20	120.95	126.20
12	aB	936	CLA	CAA-C2A-C3A	-3.20	104.34	113.00
12	bA	822	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
12	cB	907	CLA	CMB-C2B-C1B	3.20	130.29	125.42
12	bA	830	CLA	C1D-CHD-C4C	-3.20	119.22	126.02
12	bA	820	CLA	C4B-C3B-C2B	-3.20	103.32	107.30
12	bA	831	CLA	C3B-C4B-NB	3.20	113.39	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bB	901	CLA	C3B-C4B-NB	3.20	113.39	110.53
12	bA	832	CLA	C4A-NA-C1A	-3.20	105.22	106.68
12	aB	924	CLA	C4C-C3C-C2C	-3.20	102.23	106.89
12	cB	928	CLA	C2B-C1B-NB	3.20	113.64	110.33
12	aA	831	CLA	C3B-C4B-NB	3.20	113.39	110.53
12	aB	901	CLA	CHD-C1D-ND	-3.20	120.30	124.80
12	bB	909	CLA	C3B-C4B-NB	3.20	113.39	110.53
12	bB	917	CLA	C3B-C4B-NB	3.20	113.39	110.53
12	aA	829	CLA	CAC-C3C-C4C	3.20	128.95	124.79
12	cA	853	CLA	O2A-CGA-CBA	3.20	121.58	111.83
12	aA	854	CLA	O2A-CGA-CBA	3.20	121.58	111.83
12	aA	818	CLA	C4-C3-C5	3.20	120.78	115.23
12	bA	829	CLA	CAC-C3C-C4C	3.20	128.95	124.79
12	cB	949	CLA	CMB-C2B-C1B	3.20	130.28	125.42
13	cB	940	1L3	C14-C15-C16	-3.19	121.33	126.83
12	aB	915	CLA	CHD-C4C-NC	3.19	129.18	124.23
12	cA	829	CLA	CAC-C3C-C4C	3.19	128.95	124.79
12	bB	902	CLA	C1D-CHD-C4C	-3.19	119.23	126.02
12	bB	931	CLA	C1D-CHD-C4C	-3.19	119.23	126.02
12	bB	913	CLA	CMC-C2C-C1C	3.19	130.03	125.03
12	cB	913	CLA	CMC-C2C-C1C	3.19	130.03	125.03
12	cB	909	CLA	C3B-C4B-NB	3.19	113.38	110.53
12	aA	809	CLA	C4A-NA-C1A	-3.19	105.22	106.68
12	cA	812	CLA	O2D-CGD-O1D	-3.19	117.63	123.85
12	cB	936	CLA	CAA-C2A-C3A	-3.19	104.37	113.00
12	aA	835	CLA	C4C-C3C-C2C	-3.19	102.24	106.89
12	aA	826	CLA	C1D-CHD-C4C	-3.19	119.23	126.02
12	aB	905	CLA	C4-C3-C5	3.19	120.77	115.23
12	bB	924	CLA	C4C-C3C-C2C	-3.19	102.25	106.89
12	cA	840	CLA	C3B-C4B-NB	3.19	113.38	110.53
12	cA	820	CLA	C4B-C3B-C2B	-3.19	103.34	107.30
12	aA	815	CLA	CHC-C1C-C2C	-3.19	117.89	126.95
12	aB	919	CLA	CMB-C2B-C1B	3.19	130.27	125.42
12	bB	915	CLA	CHD-C4C-NC	3.19	129.17	124.23
12	cB	901	CLA	CMA-C3A-C4A	-3.19	103.21	111.77
12	bA	826	CLA	C1D-CHD-C4C	-3.19	119.25	126.02
12	bB	908	CLA	CAC-C3C-C4C	3.19	128.94	124.79
12	bA	809	CLA	C4A-NA-C1A	-3.19	105.22	106.68
12	aB	911	CLA	C4B-C3B-C2B	-3.19	103.34	107.30
12	cL	203	CLA	C1D-CHD-C4C	-3.19	119.25	126.02
12	bB	901	CLA	CMA-C3A-C4A	-3.19	103.21	111.77
12	aB	904	CLA	C4B-C3B-C2B	-3.19	103.34	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bL	203	CLA	C1D-CHD-C4C	-3.19	119.25	126.02
12	cA	804	CLA	C4B-C3B-C2B	-3.19	103.34	107.30
12	cB	915	CLA	CHD-C4C-NC	3.19	129.17	124.23
12	aA	840	CLA	C3B-C4B-NB	3.18	113.37	110.53
15	cB	945	BCR	C2-C1-C6	3.18	115.06	110.44
12	bA	804	CLA	C4B-C3B-C2B	-3.18	103.34	107.30
12	cB	931	CLA	C1D-CHD-C4C	-3.18	119.25	126.02
12	cB	932	CLA	C3B-C4B-NB	3.18	113.37	110.53
12	bA	831	CLA	O2A-CGA-CBA	3.18	121.54	111.83
12	cB	919	CLA	CMB-C2B-C1B	3.18	130.27	125.42
12	bB	936	CLA	CAA-C2A-C3A	-3.18	104.40	113.00
12	bB	916	CLA	C1-C2-C3	-3.18	120.98	126.20
12	cA	831	CLA	O2A-CGA-CBA	3.18	121.53	111.83
12	cL	203	CLA	C4C-C3C-C2C	-3.18	102.26	106.89
12	bA	834	CLA	CHC-C1C-C2C	-3.18	117.91	126.95
12	aB	927	CLA	O2D-CGD-CBD	3.18	116.79	111.23
12	bB	927	CLA	O2D-CGD-CBD	3.18	116.79	111.23
12	cB	902	CLA	C1D-CHD-C4C	-3.18	119.26	126.02
12	bB	928	CLA	C2B-C1B-NB	3.18	113.62	110.33
12	aB	901	CLA	C3B-C4B-NB	3.18	113.37	110.53
12	aA	831	CLA	O2A-CGA-CBA	3.18	121.53	111.83
12	aB	901	CLA	CMA-C3A-C4A	-3.18	103.23	111.77
13	bB	940	1L3	C14-C15-C16	-3.18	121.36	126.83
12	aL	203	CLA	C1D-CHD-C4C	-3.18	119.27	126.02
13	aB	940	1L3	C14-C15-C16	-3.18	121.36	126.83
12	aA	834	CLA	CHC-C1C-C2C	-3.18	117.92	126.95
12	cB	904	CLA	C4-C3-C5	3.17	120.74	115.23
12	aB	931	CLA	C1D-CHD-C4C	-3.17	119.27	126.02
12	bB	916	CLA	CHD-C4C-NC	3.17	129.15	124.23
12	bA	812	CLA	CAC-C3C-C4C	3.17	128.92	124.79
12	bA	815	CLA	CHC-C1C-C2C	-3.17	117.94	126.95
12	aB	916	CLA	C1-C2-C3	-3.17	121.00	126.20
12	aB	917	CLA	C3B-C4B-NB	3.17	113.36	110.53
12	cA	812	CLA	CAC-C3C-C4C	3.17	128.92	124.79
12	aA	838	CLA	CAA-C2A-C3A	-3.17	104.43	113.00
12	cB	927	CLA	O2D-CGD-CBD	3.17	116.77	111.23
12	bA	812	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
12	cA	831	CLA	C3B-C4B-NB	3.17	113.36	110.53
12	cA	834	CLA	CHC-C1C-C2C	-3.17	117.94	126.95
12	aA	833	CLA	C4A-NA-C1A	-3.17	105.23	106.68
12	aB	916	CLA	C4A-NA-C1A	-3.17	105.23	106.68
12	bA	803	CLA	C4A-NA-C1A	-3.17	105.23	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	824	CLA	CHC-C1C-C2C	-3.17	117.94	126.95
12	aB	928	CLA	C2B-C1B-NB	3.17	113.61	110.33
12	aB	927	CLA	C4C-C3C-C2C	-3.17	102.28	106.89
12	bB	914	CLA	C4C-C3C-C2C	-3.17	102.28	106.89
12	bB	904	CLA	C4B-C3B-C2B	-3.17	103.36	107.30
12	aB	902	CLA	C1D-CHD-C4C	-3.17	119.29	126.02
12	cB	905	CLA	C4-C3-C5	3.17	120.73	115.23
12	cA	838	CLA	CAA-C2A-C3A	-3.17	104.44	113.00
12	bL	203	CLA	C4C-C3C-C2C	-3.17	102.28	106.89
12	aB	935	CLA	C4C-C3C-C2C	-3.16	102.29	106.89
12	cB	908	CLA	CAC-C3C-C4C	3.16	128.91	124.79
12	bB	927	CLA	C4A-NA-C1A	-3.16	105.24	106.68
12	aB	916	CLA	CHD-C4C-NC	3.16	129.13	124.23
12	cA	832	CLA	O2A-CGA-CBA	3.16	121.48	111.83
12	cA	835	CLA	C4C-C3C-C2C	-3.16	102.29	106.89
12	bB	916	CLA	C4A-NA-C1A	-3.16	105.24	106.68
15	bB	945	BCR	C2-C1-C6	3.16	115.03	110.44
12	cB	935	CLA	C4B-C3B-C2B	-3.16	103.37	107.30
12	cA	824	CLA	CHC-C1C-C2C	-3.16	117.97	126.95
12	bA	832	CLA	O2A-CGA-CBA	3.16	121.47	111.83
12	aL	202	CLA	O2A-CGA-CBA	3.16	121.47	111.83
12	aA	810	CLA	C4C-C3C-C2C	-3.16	102.29	106.89
12	aA	832	CLA	O2A-CGA-CBA	3.16	121.47	111.83
12	bA	840	CLA	C3C-C4C-NC	3.16	114.48	110.43
12	bA	818	CLA	C4-C3-C5	3.16	120.71	115.23
12	aB	938	CLA	C3B-C4B-NB	3.16	113.35	110.53
12	aA	812	CLA	CAC-C3C-C4C	3.16	128.90	124.79
12	cB	903	CLA	CBC-CAC-C3C	-3.16	103.86	112.42
12	aL	203	CLA	C4C-C3C-C2C	-3.16	102.30	106.89
12	cB	907	CLA	CHD-C1D-ND	-3.16	120.36	124.80
12	aB	904	CLA	C4-C3-C5	3.16	120.71	115.23
12	cA	818	CLA	C4-C3-C5	3.16	120.71	115.23
12	cB	917	CLA	C3B-C4B-NB	3.16	113.35	110.53
12	bA	838	CLA	CAA-C2A-C3A	-3.16	104.47	113.00
12	aA	841	CLA	O2A-CGA-CBA	3.16	121.45	111.83
12	cB	912	CLA	C1C-C2C-C3C	-3.15	103.66	106.98
12	cA	815	CLA	CHC-C1C-C2C	-3.15	117.99	126.95
12	bB	903	CLA	C3B-C4B-NB	3.15	113.34	110.53
12	aB	908	CLA	CAC-C3C-C4C	3.15	128.89	124.79
12	bA	841	CLA	O2A-CGA-CBA	3.15	121.44	111.83
12	aA	804	CLA	C4B-C3B-C2B	-3.15	103.38	107.30
12	aA	824	CLA	C4B-C3B-C2B	-3.15	103.38	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cB	907	CLA	C4B-C3B-C2B	-3.15	103.38	107.30
12	cB	904	CLA	C4B-C3B-C2B	-3.15	103.38	107.30
12	cA	841	CLA	O2A-CGA-CBA	3.15	121.44	111.83
12	cB	916	CLA	CHD-C4C-NC	3.15	129.12	124.23
12	bA	824	CLA	CHC-C1C-C2C	-3.15	118.00	126.95
12	cL	202	CLA	C1D-CHD-C4C	-3.15	119.33	126.02
12	bB	938	CLA	C3B-C4B-NB	3.15	113.34	110.53
12	bL	202	CLA	O2A-CGA-CBA	3.15	121.44	111.83
12	bA	810	CLA	C4C-C3C-C2C	-3.15	102.31	106.89
12	cB	917	CLA	CHC-C1C-C2C	-3.15	118.00	126.95
12	bB	904	CLA	C4-C3-C5	3.15	120.69	115.23
12	bA	840	CLA	C3B-C4B-NB	3.15	113.34	110.53
12	cB	936	CLA	C4B-C3B-C2B	-3.15	103.39	107.30
12	bA	803	CLA	C3B-C4B-NB	3.15	113.34	110.53
12	bB	926	CLA	CAA-C2A-C3A	-3.15	104.50	113.00
12	cA	810	CLA	C4C-C3C-C2C	-3.14	102.31	106.89
12	cL	202	CLA	O2A-CGA-CBA	3.14	121.42	111.83
12	cA	807	CLA	C1-C2-C3	-3.14	121.05	126.20
12	cA	833	CLA	C3B-C4B-NB	3.14	113.34	110.53
12	bL	202	CLA	C1D-CHD-C4C	-3.14	119.34	126.02
12	bB	936	CLA	C4B-C3B-C2B	-3.14	103.39	107.30
12	bB	927	CLA	C4C-C3C-C2C	-3.14	102.32	106.89
12	cB	927	CLA	C4C-C3C-C2C	-3.14	102.32	106.89
12	bB	919	CLA	CMB-C2B-C1B	3.14	130.21	125.42
12	aB	907	CLA	C4B-C3B-C2B	-3.14	103.39	107.30
12	cA	806	CLA	CHC-C1C-C2C	-3.14	118.02	126.95
12	bA	824	CLA	C4B-C3B-C2B	-3.14	103.39	107.30
12	aB	917	CLA	CHC-C1C-C2C	-3.14	118.02	126.95
12	aB	903	CLA	CBC-CAC-C3C	-3.14	103.90	112.42
12	aB	909	CLA	C3B-C4B-NB	3.14	113.33	110.53
12	cA	820	CLA	C4A-NA-C1A	-3.14	105.25	106.68
12	aL	202	CLA	C1D-CHD-C4C	-3.14	119.35	126.02
12	bB	935	CLA	C4C-C3C-C2C	-3.14	102.32	106.89
12	bB	903	CLA	CBC-CAC-C3C	-3.14	103.91	112.42
12	aB	914	CLA	C4C-C3C-C2C	-3.14	102.32	106.89
12	bB	912	CLA	C1C-C2C-C3C	-3.14	103.68	106.98
12	bA	833	CLA	C3B-C4B-NB	3.14	113.33	110.53
12	aA	840	CLA	C3C-C4C-NC	3.14	114.45	110.43
12	cB	914	CLA	C4C-C3C-C2C	-3.14	102.33	106.89
12	aB	935	CLA	C4B-C3B-C2B	-3.14	103.40	107.30
15	aB	941	BCR	C15-C14-C13	-3.14	122.88	127.28
12	aB	932	CLA	C1C-C2C-C3C	-3.14	103.68	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cB	937	CLA	C1D-CHD-C4C	-3.14	119.36	126.02
12	bB	911	CLA	CMC-C2C-C1C	3.13	129.93	125.03
12	aA	807	CLA	CAC-C3C-C4C	3.13	128.87	124.79
12	bB	907	CLA	C4B-C3B-C2B	-3.13	103.41	107.30
12	bB	937	CLA	C1D-CHD-C4C	-3.13	119.36	126.02
12	bB	907	CLA	CHD-C1D-ND	-3.13	120.39	124.80
13	cB	940	1L3	C27-C26-C28	3.13	120.66	115.23
12	aA	806	CLA	CHC-C1C-C2C	-3.13	118.05	126.95
12	bB	917	CLA	CHC-C1C-C2C	-3.13	118.05	126.95
12	cA	826	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
15	cB	941	BCR	C15-C14-C13	-3.13	122.89	127.28
12	bA	806	CLA	CHC-C1C-C2C	-3.13	118.06	126.95
12	bA	827	CLA	C1C-C2C-C3C	-3.13	103.69	106.98
12	cB	926	CLA	CAA-C2A-C3A	-3.13	104.55	113.00
12	aA	842	CLA	C4C-C3C-C2C	-3.12	102.34	106.89
12	cB	935	CLA	C4C-C3C-C2C	-3.12	102.34	106.89
12	aB	926	CLA	CAA-C2A-C3A	-3.12	104.56	113.00
12	bB	949	CLA	CHD-C4C-NC	3.12	129.08	124.23
12	aB	911	CLA	CMC-C2C-C1C	3.12	129.92	125.03
13	aB	940	1L3	C27-C26-C28	3.12	120.65	115.23
12	bA	833	CLA	C4A-NA-C1A	-3.12	105.25	106.68
12	bB	906	CLA	C4A-NA-C1A	-3.12	105.25	106.68
15	aB	945	BCR	C2-C1-C6	3.12	114.98	110.44
12	cA	803	CLA	C3B-C4B-NB	3.12	113.32	110.53
13	bB	940	1L3	C27-C26-C28	3.12	120.65	115.23
12	bB	930	CLA	C4A-NA-C1A	-3.12	105.25	106.68
12	bB	935	CLA	C4B-C3B-C2B	-3.12	103.42	107.30
12	aB	949	CLA	CHD-C4C-NC	3.12	129.07	124.23
12	cB	923	CLA	C4C-C3C-C2C	-3.12	102.35	106.89
12	cB	938	CLA	C3B-C4B-NB	3.12	113.31	110.53
12	cB	931	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
12	bB	922	CLA	CBC-CAC-C3C	-3.12	103.97	112.42
12	bA	826	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
12	cA	833	CLA	C4A-NA-C1A	-3.12	105.26	106.68
12	aB	937	CLA	C1D-CHD-C4C	-3.12	119.40	126.02
12	aB	922	CLA	CBC-CAC-C3C	-3.12	103.97	112.42
12	cB	903	CLA	C3B-C4B-NB	3.12	113.31	110.53
12	cB	922	CLA	CBC-CAC-C3C	-3.11	103.98	112.42
12	aB	912	CLA	C1C-C2C-C3C	-3.11	103.70	106.98
12	bB	923	CLA	C4C-C3C-C2C	-3.11	102.36	106.89
12	aB	936	CLA	C4B-C3B-C2B	-3.11	103.43	107.30
12	cA	824	CLA	C4B-C3B-C2B	-3.11	103.43	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	842	CLA	C4C-C3C-C2C	-3.11	102.36	106.89
15	aA	850	BCR	C24-C23-C22	-3.11	121.63	126.23
12	aA	826	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
15	cA	847	BCR	C15-C14-C13	-3.11	122.92	127.28
12	aA	835	CLA	CAC-C3C-C4C	3.11	128.83	124.79
12	bA	807	CLA	CAC-C3C-C4C	3.11	128.83	124.79
12	bB	907	CLA	O2A-CGA-CBA	3.11	121.31	111.83
12	bA	842	CLA	C4C-C3C-C2C	-3.11	102.37	106.89
15	bA	847	BCR	C15-C14-C13	-3.11	122.92	127.28
12	bA	807	CLA	C1-C2-C3	-3.11	121.11	126.20
12	cB	929	CLA	C4C-C3C-C2C	-3.10	102.37	106.89
12	aB	924	CLA	CAC-C3C-C4C	3.10	128.83	124.79
12	aB	935	CLA	C1-C2-C3	-3.10	121.74	126.76
12	cB	949	CLA	CHD-C4C-NC	3.10	129.04	124.23
15	cA	849	BCR	C24-C23-C22	-3.10	121.64	126.23
12	bB	935	CLA	CHD-C4C-NC	3.10	129.04	124.23
12	aA	807	CLA	C1-C2-C3	-3.10	121.11	126.20
12	bA	806	CLA	C1D-CHD-C4C	-3.10	119.43	126.02
12	aA	812	CLA	C4B-C3B-C2B	-3.10	103.44	107.30
12	cB	909	CLA	C4A-NA-C1A	-3.10	105.26	106.68
12	cA	806	CLA	C1D-CHD-C4C	-3.10	119.43	126.02
12	cB	924	CLA	CAC-C3C-C4C	3.10	128.82	124.79
12	cB	911	CLA	CMC-C2C-C1C	3.10	129.88	125.03
12	cL	202	CLA	C3B-C4B-NB	3.10	113.30	110.53
12	bB	928	CLA	CHC-C1C-C2C	-3.10	118.14	126.95
15	bA	849	BCR	C24-C23-C22	-3.10	121.65	126.23
12	aB	928	CLA	CHC-C1C-C2C	-3.10	118.14	126.95
12	cA	812	CLA	C4B-C3B-C2B	-3.10	103.45	107.30
12	cA	807	CLA	CAC-C3C-C4C	3.10	128.82	124.79
12	aB	903	CLA	C3B-C4B-NB	3.10	113.30	110.53
12	aA	844	CLA	CHC-C1C-C2C	-3.10	118.15	126.95
12	cA	804	CLA	CHD-C1D-ND	-3.10	120.45	124.80
12	bA	812	CLA	C4B-C3B-C2B	-3.10	103.45	107.30
12	bB	924	CLA	CAC-C3C-C4C	3.10	128.82	124.79
12	aA	842	CLA	C4A-NA-C1A	-3.09	105.27	106.68
12	aA	827	CLA	C1C-C2C-C3C	-3.09	103.72	106.98
12	cA	807	CLA	C1C-C2C-C3C	-3.09	103.72	106.98
12	bL	202	CLA	C3B-C4B-NB	3.09	113.29	110.53
12	aA	829	CLA	C4C-C3C-C2C	-3.09	102.39	106.89
12	bB	913	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
12	bB	931	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
12	cB	928	CLA	CHC-C1C-C2C	-3.09	118.16	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	835	CLA	CAC-C3C-C4C	3.09	128.81	124.79
12	bB	932	CLA	C1C-C2C-C3C	-3.09	103.73	106.98
12	aB	907	CLA	O2A-CGA-CBA	3.09	121.26	111.83
12	cB	907	CLA	O2A-CGA-CBA	3.09	121.26	111.83
12	aB	923	CLA	C4C-C3C-C2C	-3.09	102.39	106.89
12	aL	202	CLA	C3B-C4B-NB	3.09	113.29	110.53
12	aB	907	CLA	CHD-C1D-ND	-3.09	120.45	124.80
12	aA	829	CLA	C1-C2-C3	-3.09	121.14	126.20
12	bA	814	CLA	C1C-C2C-C3C	-3.09	103.73	106.98
12	cB	932	CLA	C1C-C2C-C3C	-3.09	103.73	106.98
12	aB	913	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
12	cB	935	CLA	C1-C2-C3	-3.09	121.77	126.76
12	bA	804	CLA	CHD-C1D-ND	-3.09	120.46	124.80
12	bA	829	CLA	C4C-C3C-C2C	-3.09	102.40	106.89
12	bB	950	CLA	CHC-C1C-C2C	-3.09	118.18	126.95
12	aA	838	CLA	CMB-C2B-C1B	3.09	130.12	125.42
12	cB	913	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
12	bA	843	CLA	CHC-C1C-C2C	-3.09	118.18	126.95
15	aA	848	BCR	C15-C14-C13	-3.08	122.95	127.28
12	aB	931	CLA	O2D-CGD-O1D	-3.08	117.84	123.85
12	cB	903	CLA	O2D-CGD-O1D	-3.08	117.84	123.85
12	aB	906	CLA	C4A-NA-C1A	-3.08	105.27	106.68
12	cB	935	CLA	CHD-C4C-NC	3.08	129.01	124.23
12	cA	809	CLA	C4C-C3C-C2C	-3.08	102.40	106.89
12	aA	806	CLA	C4B-C3B-C2B	-3.08	103.47	107.30
12	cB	903	CLA	C4C-C3C-C2C	-3.08	102.40	106.89
12	aL	204	CLA	C4B-C3B-C2B	-3.08	103.47	107.30
12	cA	827	CLA	C1C-C2C-C3C	-3.08	103.74	106.98
12	aB	935	CLA	CHD-C4C-NC	3.08	129.01	124.23
15	aF	203	BCR	C16-C15-C14	-3.08	117.21	123.52
12	cB	933	CLA	CHC-C1C-C2C	-3.08	118.19	126.95
12	aA	809	CLA	C4C-C3C-C2C	-3.08	102.41	106.89
12	bB	929	CLA	C4C-C3C-C2C	-3.08	102.41	106.89
12	cL	204	CLA	C4B-C3B-C2B	-3.08	103.47	107.30
12	aA	806	CLA	C1D-CHD-C4C	-3.08	119.47	126.02
12	aB	950	CLA	CHC-C1C-C2C	-3.08	118.20	126.95
12	bB	903	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
12	bB	933	CLA	CHC-C1C-C2C	-3.08	118.20	126.95
12	aA	804	CLA	CHD-C1D-ND	-3.08	120.47	124.80
12	cA	830	CLA	CHC-C1C-C2C	-3.08	118.21	126.95
12	bL	204	CLA	C4B-C3B-C2B	-3.08	103.48	107.30
12	aB	912	CLA	CMB-C2B-C1B	3.08	130.10	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bB	933	CLA	C4A-NA-C1A	-3.08	105.28	106.68
12	aA	823	CLA	C3B-C4B-NB	3.07	113.28	110.53
12	bB	935	CLA	C1-C2-C3	-3.07	121.79	126.76
15	bB	941	BCR	C15-C14-C13	-3.07	122.97	127.28
12	cB	918	CLA	CHC-C1C-C2C	-3.07	118.21	126.95
12	aA	843	CLA	CHC-C1C-C2C	-3.07	118.21	126.95
12	aB	903	CLA	C4C-C3C-C2C	-3.07	102.42	106.89
12	bA	806	CLA	C4B-C3B-C2B	-3.07	103.48	107.30
12	bA	842	CLA	C3B-C4B-NB	3.07	113.27	110.53
12	bB	931	CLA	C4B-C3B-C2B	-3.07	103.48	107.30
12	bA	829	CLA	C1-C2-C3	-3.07	121.16	126.20
12	bB	903	CLA	C4C-C3C-C2C	-3.07	102.42	106.89
12	cA	823	CLA	C4C-C3C-C2C	-3.07	102.42	106.89
12	cA	806	CLA	C4B-C3B-C2B	-3.07	103.48	107.30
12	cA	838	CLA	CMB-C2B-C1B	3.07	130.09	125.42
12	cB	927	CLA	C4A-NA-C1A	-3.07	105.28	106.68
12	bA	830	CLA	CHC-C1C-C2C	-3.07	118.22	126.95
12	cA	829	CLA	C4C-C3C-C2C	-3.07	102.42	106.89
15	bF	203	BCR	C16-C15-C14	-3.07	117.24	123.52
12	aA	818	CLA	CAC-C3C-C4C	3.07	128.78	124.79
12	bA	803	CLA	C4C-C3C-C2C	-3.07	102.43	106.89
12	cA	807	CLA	CED-O2D-CGD	3.07	122.87	115.92
12	aB	931	CLA	C4B-C3B-C2B	-3.06	103.49	107.30
12	aB	903	CLA	O2D-CGD-O1D	-3.06	117.88	123.85
12	aB	918	CLA	CHC-C1C-C2C	-3.06	118.24	126.95
12	cA	843	CLA	CHC-C1C-C2C	-3.06	118.24	126.95
12	aA	803	CLA	C3B-C4B-NB	3.06	113.27	110.53
12	aA	803	CLA	C4C-C3C-C2C	-3.06	102.43	106.89
12	bB	918	CLA	CHC-C1C-C2C	-3.06	118.24	126.95
12	bB	939	CLA	CHD-C4C-NC	3.06	128.98	124.23
12	aB	927	CLA	C4A-NA-C1A	-3.06	105.28	106.68
12	cB	933	CLA	C4A-NA-C1A	-3.06	105.28	106.68
12	cA	818	CLA	CAC-C3C-C4C	3.06	128.77	124.79
12	bA	834	CLA	CAC-C3C-C4C	3.06	128.77	124.79
12	cA	824	CLA	CAA-C2A-C3A	-3.06	104.73	113.00
15	aA	848	BCR	C40-C30-C25	3.06	115.04	110.24
12	aA	822	CLA	CHD-C4C-NC	3.06	128.98	124.23
15	aA	849	BCR	C27-C26-C25	3.06	126.84	122.70
12	cA	802	CLA	CAC-C3C-C4C	3.06	128.77	124.79
12	bA	809	CLA	C4C-C3C-C2C	-3.06	102.44	106.89
12	bB	920	CLA	CHD-C4C-NC	3.06	128.97	124.23
12	aA	823	CLA	C4C-C3C-C2C	-3.06	102.44	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cF	203	BCR	C16-C15-C14	-3.06	117.26	123.52
12	aB	933	CLA	CHC-C1C-C2C	-3.06	118.26	126.95
12	cA	822	CLA	CHD-C4C-NC	3.06	128.97	124.23
12	cB	931	CLA	C4B-C3B-C2B	-3.06	103.50	107.30
12	bB	904	CLA	CHB-C4A-NA	3.06	128.81	124.40
12	cB	902	CLA	CHC-C1C-C2C	-3.06	118.26	126.95
12	cA	802	CLA	C4C-C3C-C2C	-3.06	102.44	106.89
13	bB	940	1L3	C22-C21-C23	3.06	120.53	115.23
12	cB	949	CLA	C4B-C3B-C2B	-3.06	103.50	107.30
12	aB	920	CLA	CHD-C4C-NC	3.05	128.97	124.23
12	aA	824	CLA	CAA-C2A-C3A	-3.05	104.74	113.00
12	cA	829	CLA	C1-C2-C3	-3.05	121.19	126.20
12	bA	802	CLA	CAC-C3C-C4C	3.05	128.76	124.79
12	aA	830	CLA	CHC-C1C-C2C	-3.05	118.27	126.95
12	bA	853	CLA	CAC-C3C-C4C	3.05	128.76	124.79
15	cA	847	BCR	C40-C30-C25	3.05	115.03	110.24
12	aB	939	CLA	CHD-C4C-NC	3.05	128.96	124.23
12	bA	802	CLA	C4C-C3C-C2C	-3.05	102.45	106.89
12	cA	817	CLA	CAA-C2A-C3A	-3.05	104.75	113.00
12	aA	805	CLA	C4C-C3C-C2C	-3.05	102.45	106.89
15	cA	848	BCR	C27-C26-C25	3.05	126.83	122.70
12	bA	824	CLA	CAA-C2A-C3A	-3.05	104.75	113.00
12	cB	926	CLA	C1C-C2C-C3C	-3.05	103.77	106.98
12	aB	929	CLA	C4C-C3C-C2C	-3.05	102.45	106.89
12	bA	807	CLA	CED-O2D-CGD	3.05	122.83	115.92
12	cA	814	CLA	C1C-C2C-C3C	-3.05	103.77	106.98
12	cA	834	CLA	CAC-C3C-C4C	3.05	128.76	124.79
12	aA	817	CLA	CAA-C2A-C3A	-3.05	104.76	113.00
12	bB	912	CLA	CMB-C2B-C1B	3.05	130.06	125.42
12	cA	817	CLA	C4C-C3C-C2C	-3.05	102.45	106.89
12	cB	912	CLA	CMB-C2B-C1B	3.05	130.06	125.42
12	cB	939	CLA	CHD-C4C-NC	3.05	128.96	124.23
15	bA	847	BCR	C40-C30-C25	3.05	115.02	110.24
12	bB	903	CLA	CAC-C3C-C4C	3.05	128.75	124.79
12	aA	802	CLA	C4C-C3C-C2C	-3.05	102.46	106.89
12	aB	949	CLA	C4B-C3B-C2B	-3.05	103.51	107.30
12	cA	823	CLA	C3B-C4B-NB	3.05	113.25	110.53
12	aB	933	CLA	C4A-NA-C1A	-3.05	105.29	106.68
12	bA	838	CLA	CMB-C2B-C1B	3.05	130.06	125.42
12	aB	902	CLA	CHC-C1C-C2C	-3.05	118.29	126.95
12	bA	823	CLA	C4C-C3C-C2C	-3.05	102.46	106.89
12	bB	938	CLA	C4C-C3C-C2C	-3.05	102.46	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	807	CLA	C1C-C2C-C3C	-3.05	103.78	106.98
12	cA	822	CLA	C4B-C3B-C2B	-3.04	103.52	107.30
12	aA	802	CLA	CAC-C3C-C4C	3.04	128.75	124.79
12	bA	817	CLA	CAA-C2A-C3A	-3.04	104.78	113.00
12	aB	920	CLA	CMC-C2C-C1C	3.04	129.79	125.03
12	aA	814	CLA	C1C-C2C-C3C	-3.04	103.78	106.98
12	cA	842	CLA	C4A-NA-C1A	-3.04	105.29	106.68
12	cB	922	CLA	C4B-C3B-C2B	-3.04	103.52	107.30
12	bB	926	CLA	CAC-C3C-C4C	3.04	128.75	124.79
12	bB	905	CLA	CHD-C4C-NC	3.04	128.95	124.23
12	aA	807	CLA	CED-O2D-CGD	3.04	122.81	115.92
12	bB	902	CLA	CHC-C1C-C2C	-3.04	118.31	126.95
12	bB	949	CLA	C4B-C3B-C2B	-3.04	103.52	107.30
12	bB	916	CLA	CAA-C2A-C1A	-3.04	102.01	111.97
12	bA	819	CLA	C2A-C3A-C4A	-3.04	96.96	101.87
12	cA	803	CLA	CHB-C4A-NA	3.04	128.79	124.40
12	bB	938	CLA	C4B-C3B-C2B	-3.04	103.52	107.30
12	bA	818	CLA	CAC-C3C-C4C	3.04	128.74	124.79
15	cA	846	BCR	C29-C30-C25	3.04	114.85	110.44
12	cA	803	CLA	C4C-C3C-C2C	-3.04	102.47	106.89
12	cB	902	CLA	C3B-C4B-NB	3.04	113.24	110.53
12	cB	906	CLA	C4B-C3B-C2B	-3.04	103.53	107.30
12	aB	916	CLA	CAA-C2A-C1A	-3.04	102.02	111.97
12	bB	920	CLA	CMC-C2C-C1C	3.04	129.78	125.03
12	cB	920	CLA	CHD-C4C-NC	3.04	128.94	124.23
13	aB	940	1L3	C22-C21-C23	3.04	120.50	115.23
12	aA	817	CLA	C4C-C3C-C2C	-3.04	102.47	106.89
12	cA	835	CLA	CAC-C3C-C4C	3.04	128.74	124.79
15	bA	848	BCR	C27-C26-C25	3.03	126.80	122.70
12	bA	807	CLA	C1C-C2C-C3C	-3.03	103.79	106.98
12	cB	920	CLA	CMC-C2C-C1C	3.03	129.78	125.03
12	cB	916	CLA	CAA-C2A-C1A	-3.03	102.03	111.97
12	aA	803	CLA	CHB-C4A-NA	3.03	128.78	124.40
12	bB	928	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
12	aB	905	CLA	CHD-C4C-NC	3.03	128.93	124.23
12	bA	822	CLA	C4B-C3B-C2B	-3.03	103.53	107.30
15	aA	847	BCR	C29-C30-C25	3.03	114.84	110.44
12	bA	823	CLA	C3B-C4B-NB	3.03	113.24	110.53
12	bL	202	CLA	CBC-CAC-C3C	-3.03	104.20	112.42
12	aA	834	CLA	CAC-C3C-C4C	3.03	128.73	124.79
13	cB	940	1L3	C22-C21-C23	3.03	120.49	115.23
12	bA	833	CLA	CMA-C3A-C4A	-3.03	103.63	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bA	846	BCR	C29-C30-C25	3.03	114.84	110.44
12	aB	920	CLA	C4A-NA-C1A	-3.03	105.30	106.68
12	aB	904	CLA	CHB-C4A-NA	3.03	128.77	124.40
12	aA	808	CLA	CHC-C1C-C2C	-3.03	118.34	126.95
12	aB	904	CLA	CMC-C2C-C1C	3.03	129.77	125.03
12	aA	822	CLA	C4B-C3B-C2B	-3.03	103.54	107.30
15	bB	941	BCR	C15-C16-C17	-3.03	117.32	123.52
12	bB	909	CLA	C4A-NA-C1A	-3.03	105.30	106.68
12	bB	929	CLA	C4A-NA-C1A	-3.03	105.30	106.68
12	bB	925	CLA	C4B-C3B-C2B	-3.03	103.54	107.30
12	aA	842	CLA	C3B-C4B-NB	3.03	113.23	110.53
12	aB	925	CLA	CHD-C4C-NC	3.03	128.92	124.23
12	bB	922	CLA	C4B-C3B-C2B	-3.03	103.54	107.30
12	cA	833	CLA	CMA-C3A-C4A	-3.03	103.64	111.77
12	aB	928	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
12	cB	903	CLA	CAC-C3C-C4C	3.03	128.73	124.79
12	bA	822	CLA	CHD-C4C-NC	3.03	128.92	124.23
12	bB	902	CLA	C3B-C4B-NB	3.03	113.23	110.53
12	cB	906	CLA	C4C-C3C-C2C	-3.03	102.49	106.89
12	aB	903	CLA	CAC-C3C-C4C	3.03	128.73	124.79
12	cA	803	CLA	C4A-NA-C1A	-3.02	105.30	106.68
12	cA	842	CLA	C3B-C4B-NB	3.02	113.23	110.53
12	aB	920	CLA	C4B-C3B-C2B	-3.02	103.54	107.30
12	aB	922	CLA	C4B-C3B-C2B	-3.02	103.54	107.30
12	aA	833	CLA	CMA-C3A-C4A	-3.02	103.64	111.77
12	bA	833	CLA	CHC-C1C-C2C	-3.02	118.35	126.95
12	cB	904	CLA	CHB-C4A-NA	3.02	128.76	124.40
12	bA	838	CLA	C4B-C3B-C2B	-3.02	103.54	107.30
12	bB	931	CLA	C1-C2-C3	-3.02	121.24	126.20
12	aA	826	CLA	C4A-NA-C1A	-3.02	105.30	106.68
12	aB	929	CLA	C4A-NA-C1A	-3.02	105.30	106.68
12	bA	803	CLA	CHB-C4A-NA	3.02	128.76	124.40
12	cA	812	CLA	C3B-C4B-NB	3.02	113.23	110.53
12	aB	925	CLA	C4B-C3B-C2B	-3.02	103.54	107.30
12	cB	914	CLA	CHD-C4C-NC	3.02	128.92	124.23
15	aB	941	BCR	C15-C16-C17	-3.02	117.34	123.52
12	aB	926	CLA	C1C-C2C-C3C	-3.02	103.80	106.98
12	bB	930	CLA	C4C-C3C-C2C	-3.02	102.50	106.89
12	bA	808	CLA	CHC-C1C-C2C	-3.02	118.37	126.95
12	cA	823	CLA	CMB-C2B-C1B	3.02	130.02	125.42
12	cB	926	CLA	C1-C2-C3	-3.02	121.25	126.20
12	cA	833	CLA	CHC-C1C-C2C	-3.02	118.37	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	818	CLA	C4A-NA-C1A	-3.02	105.30	106.68
12	aB	934	CLA	CHC-C1C-C2C	-3.02	118.37	126.95
12	bA	814	CLA	CHC-C1C-C2C	-3.02	118.37	126.95
12	aA	812	CLA	C3B-C4B-NB	3.02	113.22	110.53
12	cB	905	CLA	CHD-C4C-NC	3.02	128.91	124.23
15	cB	941	BCR	C15-C16-C17	-3.02	117.34	123.52
12	aB	938	CLA	C4C-C3C-C2C	-3.02	102.50	106.89
12	bB	929	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
12	aB	902	CLA	C3B-C4B-NB	3.02	113.22	110.53
12	aA	812	CLA	CHC-C1C-C2C	-3.02	118.38	126.95
15	bB	945	BCR	C15-C16-C17	-3.02	117.35	123.52
12	bL	202	CLA	CAA-C2A-C3A	-3.02	104.85	113.00
12	cL	202	CLA	CAA-C2A-C3A	-3.02	104.85	113.00
12	bA	805	CLA	C4C-C3C-C2C	-3.02	102.50	106.89
12	aA	833	CLA	CHC-C1C-C2C	-3.02	118.38	126.95
12	bB	926	CLA	C1-C2-C3	-3.02	121.26	126.20
12	aB	929	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
12	cA	832	CLA	C3B-C4B-NB	3.01	113.22	110.53
12	bB	909	CLA	CHC-C1C-C2C	-3.01	118.38	126.95
12	bB	914	CLA	CHD-C4C-NC	3.01	128.90	124.23
12	aA	838	CLA	C4B-C3B-C2B	-3.01	103.56	107.30
12	cA	853	CLA	CAC-C3C-C4C	3.01	128.71	124.79
12	aB	930	CLA	C4C-C3C-C2C	-3.01	102.51	106.89
12	aA	819	CLA	C2A-C3A-C4A	-3.01	97.00	101.87
12	cB	920	CLA	C4A-NA-C1A	-3.01	105.31	106.68
12	cB	934	CLA	CHC-C1C-C2C	-3.01	118.39	126.95
12	bB	906	CLA	C4C-C3C-C2C	-3.01	102.51	106.89
12	aB	919	CLA	CAC-C3C-C4C	3.01	128.71	124.79
12	aA	842	CLA	C1-O2A-CGA	3.01	123.94	116.65
12	aL	202	CLA	CAA-C2A-C3A	-3.01	104.86	113.00
12	cA	814	CLA	CHC-C1C-C2C	-3.01	118.39	126.95
12	cA	819	CLA	C2A-C3A-C4A	-3.01	97.01	101.87
12	bA	817	CLA	C4C-C3C-C2C	-3.01	102.51	106.89
12	cB	928	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
12	cB	907	CLA	CAC-C3C-C4C	3.01	128.71	124.79
12	cB	938	CLA	C4C-C3C-C2C	-3.01	102.51	106.89
12	cL	202	CLA	CBC-CAC-C3C	-3.01	104.26	112.42
12	aA	813	CLA	C4B-C3B-C2B	-3.01	103.56	107.30
12	bB	920	CLA	C4B-C3B-C2B	-3.01	103.56	107.30
15	cB	945	BCR	C15-C16-C17	-3.01	117.36	123.52
12	bB	907	CLA	O2A-CGA-O1A	-3.01	116.10	123.63
12	cA	808	CLA	CHC-C1C-C2C	-3.01	118.40	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	814	CLA	CHC-C1C-C2C	-3.01	118.40	126.95
12	aB	931	CLA	C1-C2-C3	-3.01	121.27	126.20
12	bA	842	CLA	C1-O2A-CGA	3.01	123.93	116.65
12	aA	844	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
12	bB	901	CLA	CHD-C4C-NC	3.01	128.89	124.23
12	cA	834	CLA	C3C-C4C-NC	3.01	114.28	110.43
12	bA	823	CLA	CMB-C2B-C1B	3.01	130.00	125.42
12	aB	909	CLA	CHC-C1C-C2C	-3.00	118.41	126.95
12	cB	925	CLA	CHD-C4C-NC	3.00	128.89	124.23
12	bB	919	CLA	CAC-C3C-C4C	3.00	128.70	124.79
12	bA	812	CLA	CHC-C1C-C2C	-3.00	118.41	126.95
12	cB	909	CLA	CHC-C1C-C2C	-3.00	118.41	126.95
12	aB	938	CLA	C4B-C3B-C2B	-3.00	103.57	107.30
12	bA	813	CLA	C4B-C3B-C2B	-3.00	103.57	107.30
12	cB	907	CLA	O2A-CGA-O1A	-3.00	116.11	123.63
12	aL	202	CLA	CBC-CAC-C3C	-3.00	104.28	112.42
12	bB	920	CLA	C4A-NA-C1A	-3.00	105.31	106.68
12	bB	949	CLA	CHC-C1C-C2C	-3.00	118.42	126.95
12	aB	926	CLA	C1-C2-C3	-3.00	121.28	126.20
12	aB	914	CLA	CHD-C4C-NC	3.00	128.88	124.23
12	aA	804	CLA	CAC-C3C-C4C	3.00	128.69	124.79
12	cF	202	CLA	C4B-C3B-C2B	-3.00	103.57	107.30
12	cA	805	CLA	C4C-C3C-C2C	-3.00	102.52	106.89
13	cA	844	1L3	C17-C16-C18	3.00	120.44	115.23
12	cB	901	CLA	CHD-C4C-NC	3.00	128.88	124.23
12	aB	926	CLA	C4A-NA-C1A	-3.00	105.31	106.68
12	cA	813	CLA	C4B-C3B-C2B	-3.00	103.57	107.30
13	aA	845	1L3	C17-C16-C18	3.00	120.44	115.23
12	aA	837	CLA	CHC-C1C-C2C	-3.00	118.42	126.95
12	aA	854	CLA	CAC-C3C-C4C	3.00	128.69	124.79
12	aB	907	CLA	CAC-C3C-C4C	3.00	128.69	124.79
12	cA	815	CLA	CAC-C3C-C4C	3.00	128.69	124.79
15	aB	945	BCR	C15-C16-C17	-3.00	117.38	123.52
12	aA	833	CLA	C4C-C3C-C2C	-3.00	102.53	106.89
12	cB	920	CLA	C4B-C3B-C2B	-3.00	103.57	107.30
13	bA	844	1L3	C17-C16-C18	3.00	120.43	115.23
12	cB	913	CLA	C4A-NA-C1A	-3.00	105.31	106.68
12	bB	950	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
12	cB	929	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
12	cA	838	CLA	C4B-C3B-C2B	-3.00	103.57	107.30
12	aB	908	CLA	C2B-C1B-NB	3.00	113.44	110.33
12	aA	803	CLA	C1D-CHD-C4C	-3.00	119.65	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	cA	844	1L3	C01-C02-C03	-3.00	119.52	124.45
12	aB	924	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
12	aB	906	CLA	C4C-C3C-C2C	-3.00	102.53	106.89
12	bB	925	CLA	CHD-C4C-NC	3.00	128.88	124.23
12	bA	834	CLA	C3C-C4C-NC	3.00	114.27	110.43
12	bA	835	CLA	C3B-C4B-NB	3.00	113.20	110.53
12	aB	930	CLA	C4B-C3B-C2B	-3.00	103.58	107.30
12	bB	906	CLA	C4B-C3B-C2B	-3.00	103.58	107.30
12	bB	907	CLA	CAC-C3C-C4C	3.00	128.69	124.79
12	aB	907	CLA	O2A-CGA-O1A	-3.00	116.13	123.63
12	bB	926	CLA	C1C-C2C-C3C	-3.00	103.83	106.98
12	bB	934	CLA	CHC-C1C-C2C	-3.00	118.44	126.95
12	aA	820	CLA	CHC-C1C-C2C	-2.99	118.44	126.95
12	cB	910	CLA	CHC-C1C-C2C	-2.99	118.44	126.95
12	cB	924	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
12	cA	812	CLA	CHC-C1C-C2C	-2.99	118.44	126.95
12	bF	202	CLA	C4B-C3B-C2B	-2.99	103.58	107.30
12	cB	949	CLA	CHC-C1C-C2C	-2.99	118.44	126.95
12	bB	924	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
12	aB	906	CLA	C4B-C3B-C2B	-2.99	103.58	107.30
12	aA	807	CLA	C4C-C3C-C2C	-2.99	102.54	106.89
12	cA	804	CLA	CAC-C3C-C4C	2.99	128.68	124.79
12	bA	842	CLA	C4A-NA-C1A	-2.99	105.31	106.68
12	cA	835	CLA	C3B-C4B-NB	2.99	113.20	110.53
12	bB	936	CLA	C4C-C3C-C2C	-2.99	102.54	106.89
12	cB	930	CLA	C4C-C3C-C2C	-2.99	102.54	106.89
12	cA	842	CLA	C1-O2A-CGA	2.99	123.89	116.65
12	bA	833	CLA	C4C-C3C-C2C	-2.99	102.54	106.89
12	cA	820	CLA	CHC-C1C-C2C	-2.99	118.45	126.95
12	bA	838	CLA	C4C-C3C-C2C	-2.99	102.54	106.89
12	aF	202	CLA	C4B-C3B-C2B	-2.99	103.59	107.30
12	cB	935	CLA	O2A-CGA-CBA	2.99	120.95	111.83
12	bA	841	CLA	C4-C3-C5	2.99	119.64	116.13
12	cA	818	CLA	C4A-NA-C1A	-2.99	105.32	106.68
12	cA	837	CLA	CHC-C1C-C2C	-2.99	118.46	126.95
15	bA	850	BCR	C15-C16-C17	-2.99	117.41	123.52
12	bA	820	CLA	CHC-C1C-C2C	-2.99	118.46	126.95
12	bA	803	CLA	C1D-CHD-C4C	-2.99	119.67	126.02
12	cA	827	CLA	C3B-C4B-NB	2.99	113.20	110.53
12	aB	926	CLA	CAC-C3C-C4C	2.99	128.68	124.79
12	cB	926	CLA	CAC-C3C-C4C	2.99	128.68	124.79
12	bA	829	CLA	C4B-C3B-C2B	-2.99	103.59	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cB	904	CLA	CMC-C2C-C1C	2.99	129.70	125.03
12	aB	935	CLA	O2A-CGA-CBA	2.99	120.94	111.83
12	cB	926	CLA	C4A-NA-C1A	-2.99	105.32	106.68
12	bA	807	CLA	C4C-C3C-C2C	-2.99	102.55	106.89
12	cA	842	CLA	CMB-C2B-C1B	2.98	129.96	125.42
12	cB	918	CLA	C3B-C4B-NB	2.98	113.19	110.53
12	bB	910	CLA	CHC-C1C-C2C	-2.98	118.47	126.95
12	bB	904	CLA	CMC-C2C-C1C	2.98	129.70	125.03
12	aB	933	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
12	aB	949	CLA	CHC-C1C-C2C	-2.98	118.47	126.95
12	aA	815	CLA	CAC-C3C-C4C	2.98	128.67	124.79
12	cA	803	CLA	C1D-CHD-C4C	-2.98	119.68	126.02
12	bA	820	CLA	C6-C5-C3	2.98	120.73	113.47
12	aB	910	CLA	CHC-C1C-C2C	-2.98	118.48	126.95
12	aA	823	CLA	CMB-C2B-C1B	2.98	129.96	125.42
12	bB	933	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
15	cA	850	BCR	C15-C16-C17	-2.98	117.42	123.52
12	cA	817	CLA	CHD-C4C-NC	2.98	128.85	124.23
12	cA	820	CLA	C6-C5-C3	2.98	120.73	113.47
12	cB	906	CLA	C4A-NA-C1A	-2.98	105.32	106.68
12	bB	937	CLA	CAA-C2A-C3A	-2.98	104.95	113.00
12	cB	908	CLA	C2B-C1B-NB	2.98	113.41	110.33
12	cB	931	CLA	C1-C2-C3	-2.98	121.32	126.20
12	cA	826	CLA	CBC-CAC-C3C	-2.98	104.35	112.42
12	bA	820	CLA	C4C-C3C-C2C	-2.98	102.56	106.89
12	cB	929	CLA	C4A-NA-C1A	-2.98	105.32	106.68
12	bA	811	CLA	C4C-C3C-C2C	-2.98	102.56	106.89
12	bB	933	CLA	CAA-C2A-C3A	-2.98	104.96	113.00
12	bA	837	CLA	CHC-C1C-C2C	-2.98	118.49	126.95
12	aA	822	CLA	C1D-CHD-C4C	-2.97	119.70	126.02
12	aA	826	CLA	CBC-CAC-C3C	-2.97	104.36	112.42
12	bA	826	CLA	CBC-CAC-C3C	-2.97	104.36	112.42
12	bB	930	CLA	C4B-C3B-C2B	-2.97	103.60	107.30
12	bB	914	CLA	CMC-C2C-C1C	2.97	129.68	125.03
12	aL	204	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
12	bA	812	CLA	C3B-C4B-NB	2.97	113.18	110.53
12	aL	204	CLA	CAA-C2A-C3A	-2.97	104.97	113.00
12	aB	937	CLA	C4C-C3C-C2C	-2.97	102.56	106.89
12	aA	803	CLA	C4A-NA-C1A	-2.97	105.32	106.68
12	bL	204	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
13	bA	844	1L3	C01-C02-C03	-2.97	119.56	124.45
12	bB	937	CLA	C4C-C3C-C2C	-2.97	102.57	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cB	921	CLA	C4B-C3B-C2B	-2.97	103.61	107.30
12	cB	930	CLA	C4B-C3B-C2B	-2.97	103.61	107.30
12	aA	811	CLA	C4C-C3C-C2C	-2.97	102.57	106.89
12	cA	820	CLA	C4C-C3C-C2C	-2.97	102.57	106.89
12	cB	933	CLA	CAA-C2A-C3A	-2.97	104.97	113.00
12	bB	903	CLA	CAA-C2A-C3A	-2.97	104.97	113.00
12	cB	905	CLA	C4C-C3C-C2C	-2.97	102.57	106.89
12	bB	935	CLA	O2A-CGA-CBA	2.97	120.89	111.83
12	aB	936	CLA	C4C-C3C-C2C	-2.97	102.57	106.89
13	aA	845	1L3	C01-C02-C03	-2.97	119.57	124.45
12	cA	833	CLA	C4C-C3C-C2C	-2.97	102.57	106.89
12	cB	937	CLA	C4C-C3C-C2C	-2.97	102.57	106.89
12	aA	817	CLA	CHD-C4C-NC	2.97	128.83	124.23
12	bA	804	CLA	CAC-C3C-C4C	2.97	128.65	124.79
12	aB	937	CLA	CAA-C2A-C3A	-2.97	104.98	113.00
12	cB	937	CLA	CAA-C2A-C3A	-2.97	104.98	113.00
12	bB	907	CLA	CBA-CAA-C2A	2.97	122.62	113.79
12	aA	834	CLA	C3C-C4C-NC	2.97	114.23	110.43
12	aA	829	CLA	C4B-C3B-C2B	-2.97	103.61	107.30
12	aB	909	CLA	C4A-NA-C1A	-2.97	105.33	106.68
12	aB	903	CLA	CAA-C2A-C3A	-2.97	104.98	113.00
12	bB	919	CLA	CHC-C1C-C2C	-2.97	118.52	126.95
12	cB	924	CLA	C1D-CHD-C4C	-2.97	119.72	126.02
15	aA	851	BCR	C15-C16-C17	-2.96	117.45	123.52
12	aB	921	CLA	C4B-C3B-C2B	-2.96	103.62	107.30
12	cB	925	CLA	C4B-C3B-C2B	-2.96	103.62	107.30
12	cB	938	CLA	C4B-C3B-C2B	-2.96	103.62	107.30
12	aB	919	CLA	CHC-C1C-C2C	-2.96	118.52	126.95
12	bB	924	CLA	C1D-CHD-C4C	-2.96	119.72	126.02
12	aB	950	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
12	bB	913	CLA	C4A-NA-C1A	-2.96	105.33	106.68
12	cL	204	CLA	CAA-C2A-C3A	-2.96	104.99	113.00
12	aA	803	CLA	CBC-CAC-C3C	-2.96	104.39	112.42
12	cB	903	CLA	CAA-C2A-C3A	-2.96	104.99	113.00
12	cA	823	CLA	C4B-C3B-C2B	-2.96	103.62	107.30
12	cA	829	CLA	C4B-C3B-C2B	-2.96	103.62	107.30
12	aA	835	CLA	C3B-C4B-NB	2.96	113.17	110.53
12	bA	815	CLA	CAC-C3C-C4C	2.96	128.64	124.79
12	bB	908	CLA	C2B-C1B-NB	2.96	113.40	110.33
12	cB	907	CLA	CBA-CAA-C2A	2.96	122.60	113.79
12	bB	905	CLA	C4C-C3C-C2C	-2.96	102.58	106.89
12	aA	826	CLA	CMC-C2C-C1C	2.96	129.66	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	823	CLA	C4B-C3B-C2B	-2.96	103.62	107.30
12	aB	924	CLA	C1D-CHD-C4C	-2.96	119.73	126.02
12	cA	811	CLA	C4C-C3C-C2C	-2.96	102.58	106.89
12	aB	933	CLA	CAA-C2A-C3A	-2.96	105.00	113.00
12	aB	918	CLA	C3B-C4B-NB	2.96	113.17	110.53
12	cB	911	CLA	C4C-C3C-C2C	-2.96	102.58	106.89
12	bA	817	CLA	CHD-C4C-NC	2.96	128.82	124.23
12	bA	822	CLA	C1D-CHD-C4C	-2.96	119.73	126.02
12	cB	919	CLA	CHC-C1C-C2C	-2.96	118.54	126.95
12	cA	841	CLA	C4-C3-C5	2.96	119.61	116.13
15	bB	946	BCR	C27-C26-C25	2.96	126.70	122.70
12	bA	835	CLA	CMC-C2C-C1C	2.96	129.65	125.03
12	bL	204	CLA	C4C-C3C-C2C	-2.96	102.59	106.89
15	bL	205	BCR	C2-C1-C6	2.96	114.73	110.44
15	cA	847	BCR	C7-C8-C9	-2.96	121.86	126.23
12	cA	807	CLA	C4C-C3C-C2C	-2.96	102.59	106.89
12	cB	936	CLA	C4C-C3C-C2C	-2.96	102.59	106.89
12	bA	826	CLA	C4A-NA-C1A	-2.95	105.33	106.68
12	aA	803	CLA	C1-O2A-CGA	2.95	123.80	116.65
12	cB	919	CLA	CAC-C3C-C4C	2.95	128.63	124.79
12	aB	905	CLA	C4C-C3C-C2C	-2.95	102.59	106.89
12	aA	841	CLA	C4-C3-C5	2.95	119.61	116.13
12	bA	827	CLA	C3B-C4B-NB	2.95	113.17	110.53
12	bB	906	CLA	CMC-C2C-C1C	2.95	129.65	125.03
12	bL	204	CLA	CAA-C2A-C3A	-2.95	105.02	113.00
12	aB	901	CLA	CHD-C4C-NC	2.95	128.81	124.23
12	bA	803	CLA	C1-O2A-CGA	2.95	123.80	116.65
12	aB	925	CLA	OBD-CAD-C3D	-2.95	121.51	128.42
12	cA	841	CLA	O2D-CGD-CBD	2.95	116.39	111.23
12	bA	840	CLA	C4C-C3C-C2C	-2.95	102.59	106.89
12	cL	204	CLA	C4C-C3C-C2C	-2.95	102.59	106.89
12	aL	204	CLA	C4C-C3C-C2C	-2.95	102.59	106.89
12	cA	838	CLA	C4C-C3C-C2C	-2.95	102.59	106.89
12	cB	914	CLA	CMC-C2C-C1C	2.95	129.65	125.03
12	aB	913	CLA	CAA-C2A-C3A	-2.95	105.02	113.00
12	aA	832	CLA	CAC-C3C-C4C	2.95	128.63	124.79
12	bB	921	CLA	C4B-C3B-C2B	-2.95	103.63	107.30
12	cA	822	CLA	C1D-CHD-C4C	-2.95	119.75	126.02
12	bA	831	CLA	CHC-C1C-C2C	-2.95	118.56	126.95
12	aA	820	CLA	C6-C5-C3	2.95	120.65	113.47
12	aB	907	CLA	CBA-CAA-C2A	2.95	122.57	113.79
12	bA	832	CLA	C3B-C4B-NB	2.95	113.16	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	820	CLA	C4C-C3C-C2C	-2.95	102.60	106.89
12	cA	835	CLA	CMC-C2C-C1C	2.95	129.64	125.03
15	aL	205	BCR	C2-C1-C6	2.95	114.72	110.44
12	bA	807	CLA	C4B-C3B-C2B	-2.95	103.64	107.30
12	bA	841	CLA	O2D-CGD-CBD	2.95	116.38	111.23
12	aA	838	CLA	C4C-C3C-C2C	-2.95	102.60	106.89
12	cA	807	CLA	C4B-C3B-C2B	-2.95	103.64	107.30
12	bB	925	CLA	OBD-CAD-C3D	-2.95	121.53	128.42
12	cA	803	CLA	C1-O2A-CGA	2.95	123.78	116.65
12	aB	914	CLA	CMC-C2C-C1C	2.94	129.64	125.03
12	bB	926	CLA	O2A-CGA-CBA	2.94	120.81	111.83
12	cA	826	CLA	CMC-C2C-C1C	2.94	129.63	125.03
12	bB	915	CLA	C4C-C3C-C2C	-2.94	102.61	106.89
12	cA	815	CLA	C4C-C3C-C2C	-2.94	102.61	106.89
12	aA	832	CLA	C3B-C4B-NB	2.94	113.16	110.53
12	cA	831	CLA	CHC-C1C-C2C	-2.94	118.59	126.95
15	cJ	101	BCR	C7-C8-C9	-2.94	121.89	126.23
12	bA	842	CLA	CMB-C2B-C1B	2.94	129.90	125.42
12	aA	840	CLA	C4B-C3B-C2B	-2.94	103.65	107.30
12	aB	911	CLA	C4C-C3C-C2C	-2.94	102.61	106.89
12	aA	811	CLA	CHC-C1C-C2C	-2.94	118.59	126.95
12	aA	831	CLA	CHC-C1C-C2C	-2.94	118.59	126.95
12	cB	933	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
12	cL	204	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
12	cB	906	CLA	CMC-C2C-C1C	2.94	129.63	125.03
12	bA	831	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
12	aA	841	CLA	O2D-CGD-CBD	2.94	116.37	111.23
12	bB	913	CLA	CAA-C2A-C3A	-2.94	105.06	113.00
15	bA	847	BCR	C7-C8-C9	-2.94	121.89	126.23
12	aA	834	CLA	O2A-CGA-CBA	2.94	120.79	111.83
12	cB	925	CLA	OBD-CAD-C3D	-2.94	121.55	128.42
15	aA	848	BCR	C7-C8-C9	-2.94	121.89	126.23
12	aB	915	CLA	C4C-C3C-C2C	-2.94	102.62	106.89
12	bB	911	CLA	C4C-C3C-C2C	-2.94	102.62	106.89
12	bB	918	CLA	C3B-C4B-NB	2.94	113.15	110.53
12	bA	823	CLA	C4B-C3B-C2B	-2.94	103.65	107.30
12	bA	832	CLA	CAC-C3C-C4C	2.94	128.61	124.79
12	aA	827	CLA	C3B-C4B-NB	2.93	113.15	110.53
12	aB	904	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
12	cB	932	CLA	CAC-C3C-C4C	2.93	128.61	124.79
12	cB	915	CLA	O2A-CGA-CBA	2.93	120.78	111.83
12	bB	915	CLA	O2A-CGA-CBA	2.93	120.78	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cB	905	CLA	C11-C12-C13	-2.93	106.22	115.97
12	aA	834	CLA	C1-C2-C3	-2.93	121.39	126.20
12	bA	815	CLA	C4C-C3C-C2C	-2.93	102.62	106.89
12	aB	926	CLA	O2A-CGA-CBA	2.93	120.78	111.83
12	bA	834	CLA	O2A-CGA-CBA	2.93	120.78	111.83
12	cB	913	CLA	CAA-C2A-C3A	-2.93	105.08	113.00
12	cA	803	CLA	CBC-CAC-C3C	-2.93	104.47	112.42
12	aB	932	CLA	CAC-C3C-C4C	2.93	128.60	124.79
12	cA	834	CLA	O2A-CGA-CBA	2.93	120.77	111.83
12	bB	927	CLA	CHC-C1C-C2C	-2.93	118.62	126.95
12	cB	915	CLA	C4C-C3C-C2C	-2.93	102.63	106.89
12	bA	811	CLA	CHC-C1C-C2C	-2.93	118.62	126.95
12	cA	838	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
12	cF	202	CLA	CMC-C2C-C1C	2.93	129.61	125.03
12	aB	905	CLA	C3B-C4B-NB	2.93	113.14	110.53
12	aF	202	CLA	CMC-C2C-C1C	2.93	129.61	125.03
12	cA	811	CLA	CHC-C1C-C2C	-2.93	118.62	126.95
15	aB	946	BCR	C27-C26-C25	2.93	126.66	122.70
12	cB	905	CLA	C3B-C4B-NB	2.93	113.14	110.53
12	cA	840	CLA	C4C-C3C-C2C	-2.93	102.63	106.89
12	bB	905	CLA	C11-C12-C13	-2.93	106.23	115.97
12	bA	812	CLA	C4C-C3C-C2C	-2.93	102.63	106.89
12	aA	819	CLA	C4C-C3C-C2C	-2.93	102.63	106.89
15	bJ	101	BCR	C7-C8-C9	-2.93	121.91	126.23
12	cA	826	CLA	C4A-NA-C1A	-2.93	105.34	106.68
12	cB	926	CLA	O2A-CGA-CBA	2.93	120.76	111.83
12	aA	831	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
12	aA	838	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
12	aA	806	CLA	C3C-C4C-NC	2.93	114.18	110.43
12	aB	915	CLA	O2A-CGA-CBA	2.93	120.75	111.83
12	bA	826	CLA	CMC-C2C-C1C	2.93	129.60	125.03
12	aA	807	CLA	C4B-C3B-C2B	-2.92	103.67	107.30
12	cB	904	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
12	aB	906	CLA	CMC-C2C-C1C	2.92	129.60	125.03
12	aB	905	CLA	C11-C12-C13	-2.92	106.25	115.97
12	cA	831	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
12	bA	803	CLA	CBC-CAC-C3C	-2.92	104.50	112.42
12	aA	832	CLA	C1-O2A-CGA	2.92	123.72	116.65
12	bA	832	CLA	C1-O2A-CGA	2.92	123.72	116.65
12	aA	822	CLA	O2A-CGA-CBA	2.92	120.74	111.83
12	bA	819	CLA	C4C-C3C-C2C	-2.92	102.64	106.89
12	bA	822	CLA	O2A-CGA-CBA	2.92	120.74	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	819	CLA	C1-C2-C3	-2.92	121.42	126.20
12	bA	834	CLA	C1-C2-C3	-2.92	121.42	126.20
12	bB	904	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
12	bF	202	CLA	CMC-C2C-C1C	2.92	129.59	125.03
12	aA	803	CLA	C4-C3-C5	2.92	120.29	115.23
12	aA	815	CLA	C4C-C3C-C2C	-2.92	102.64	106.89
12	aA	842	CLA	CMB-C2B-C1B	2.92	129.86	125.42
12	cA	803	CLA	C4-C3-C5	2.92	120.29	115.23
16	bA	852	LHG	O8-C23-C24	2.92	120.00	111.15
15	cL	205	BCR	C2-C1-C6	2.92	114.67	110.44
12	cA	832	CLA	CAC-C3C-C4C	2.92	128.58	124.79
12	aA	840	CLA	C4C-C3C-C2C	-2.92	102.65	106.89
12	bA	806	CLA	C3C-C4C-NC	2.91	114.16	110.43
12	aA	812	CLA	C4C-C3C-C2C	-2.91	102.65	106.89
12	bB	932	CLA	CAC-C3C-C4C	2.91	128.58	124.79
12	bA	838	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
12	aB	927	CLA	CHC-C1C-C2C	-2.91	118.67	126.95
12	bA	803	CLA	C4-C3-C5	2.91	120.28	115.23
16	aA	853	LHG	O8-C23-C24	2.91	119.99	111.15
12	cA	821	CLA	CHC-C1C-C2C	-2.91	118.67	126.95
12	cA	832	CLA	C1-O2A-CGA	2.91	123.69	116.65
12	cB	927	CLA	CHC-C1C-C2C	-2.91	118.68	126.95
12	cA	819	CLA	C1-C2-C3	-2.91	121.43	126.20
12	cA	843	CLA	O2A-CGA-O1A	-2.91	116.35	123.63
12	cB	905	CLA	CAC-C3C-C4C	2.91	128.57	124.79
17	aB	947	LMG	O6-C1-O1	-2.91	103.17	110.04
17	cB	947	LMG	O6-C1-O1	-2.91	103.17	110.04
12	aB	933	CLA	C3B-C4B-NB	2.91	113.13	110.53
12	cB	933	CLA	C3B-C4B-NB	2.91	113.13	110.53
12	cA	840	CLA	C4B-C3B-C2B	-2.91	103.69	107.30
12	cA	834	CLA	C1-C2-C3	-2.90	121.44	126.20
15	aJ	101	BCR	C7-C8-C9	-2.90	121.94	126.23
16	cA	852	LHG	O8-C23-C24	2.90	119.96	111.15
12	bA	840	CLA	C4B-C3B-C2B	-2.90	103.69	107.30
12	aA	835	CLA	CMC-C2C-C1C	2.90	129.57	125.03
12	bA	816	CLA	C4B-C3B-C2B	-2.90	103.69	107.30
12	bB	930	CLA	CHC-C1C-C2C	-2.90	118.70	126.95
12	bA	843	CLA	O2A-CGA-O1A	-2.90	116.37	123.63
12	cA	819	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
17	bB	947	LMG	O6-C1-O1	-2.90	103.19	110.04
12	bA	804	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
12	bB	938	CLA	CAC-C3C-C4C	2.90	128.56	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	821	CLA	CHC-C1C-C2C	-2.90	118.71	126.95
12	aA	815	CLA	C4B-C3B-C2B	-2.90	103.70	107.30
12	cA	804	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
12	cB	906	CLA	C3B-C4B-NB	2.90	113.12	110.53
12	aB	913	CLA	C4A-NA-C1A	-2.90	105.36	106.68
12	aA	829	CLA	CHC-C1C-C2C	-2.90	118.72	126.95
12	aA	816	CLA	C4B-C3B-C2B	-2.90	103.70	107.30
12	bB	937	CLA	CHC-C1C-C2C	-2.90	118.72	126.95
12	aL	202	CLA	CHC-C1C-C2C	-2.90	118.72	126.95
12	cB	930	CLA	CHC-C1C-C2C	-2.90	118.72	126.95
12	aB	932	CLA	CHC-C1C-C2C	-2.90	118.72	126.95
13	aB	940	1L3	C19-C20-C21	-2.90	121.00	127.62
12	aA	843	CLA	O2A-CGA-O1A	-2.89	116.39	123.63
12	aB	911	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
12	cB	937	CLA	CHC-C1C-C2C	-2.89	118.72	126.95
15	cB	944	BCR	C27-C26-C25	2.89	126.61	122.70
13	cB	940	1L3	C19-C20-C21	-2.89	121.00	127.62
12	cA	815	CLA	C4B-C3B-C2B	-2.89	103.71	107.30
12	bA	829	CLA	CHC-C1C-C2C	-2.89	118.73	126.95
12	bB	934	CLA	C3B-C4B-NB	2.89	113.11	110.53
12	bB	905	CLA	C3B-C4B-NB	2.89	113.11	110.53
12	aA	819	CLA	C1-C2-C3	-2.89	121.46	126.20
12	cL	202	CLA	CHC-C1C-C2C	-2.89	118.74	126.95
12	cA	812	CLA	C4C-C3C-C2C	-2.89	102.69	106.89
12	bA	816	CLA	CAC-C3C-C4C	2.89	128.55	124.79
12	bB	905	CLA	CAC-C3C-C4C	2.89	128.55	124.79
12	cL	202	CLA	C4B-C3B-C2B	-2.89	103.71	107.30
13	bB	940	1L3	C19-C20-C21	-2.89	121.02	127.62
12	cA	842	CLA	C4-C3-C5	2.89	120.24	115.23
12	cB	938	CLA	CAC-C3C-C4C	2.89	128.54	124.79
15	aI	101	BCR	C15-C16-C17	-2.89	117.61	123.52
12	bA	816	CLA	CHC-C1C-C2C	-2.89	118.75	126.95
12	bB	915	CLA	C3B-C4B-NB	2.89	113.11	110.53
12	bA	815	CLA	C4B-C3B-C2B	-2.89	103.71	107.30
15	aB	944	BCR	C27-C26-C25	2.89	126.60	122.70
12	aB	902	CLA	CHB-C4A-NA	2.89	128.56	124.40
12	cA	822	CLA	O2A-CGA-CBA	2.89	120.63	111.83
12	cA	806	CLA	C3C-C4C-NC	2.89	114.13	110.43
15	cB	946	BCR	C27-C26-C25	2.88	126.60	122.70
12	aB	938	CLA	CAC-C3C-C4C	2.88	128.54	124.79
12	aA	816	CLA	CAC-C3C-C4C	2.88	128.54	124.79
12	aA	842	CLA	C4-C3-C5	2.88	120.23	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cI	101	BCR	C15-C16-C17	-2.88	117.62	123.52
12	aB	915	CLA	C3B-C4B-NB	2.88	113.10	110.53
12	bL	202	CLA	CHC-C1C-C2C	-2.88	118.76	126.95
12	aA	804	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
12	cB	932	CLA	CHC-C1C-C2C	-2.88	118.76	126.95
12	aA	813	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
12	bB	925	CLA	C1-C2-C3	-2.88	121.48	126.20
12	aB	937	CLA	CHC-C1C-C2C	-2.88	118.76	126.95
12	cA	829	CLA	CHC-C1C-C2C	-2.88	118.76	126.95
12	cA	816	CLA	CAC-C3C-C4C	2.88	128.54	124.79
12	aB	925	CLA	C1-C2-C3	-2.88	121.48	126.20
12	bA	842	CLA	C4-C3-C5	2.88	120.23	115.23
12	cA	813	CLA	CMB-C2B-C3B	2.88	133.32	126.55
15	aB	942	BCR	C29-C30-C25	2.88	114.62	110.44
12	bB	924	CLA	C4A-NA-C1A	-2.88	105.37	106.68
12	cA	836	CLA	CMC-C2C-C1C	2.88	129.53	125.03
12	cB	925	CLA	C1-C2-C3	-2.88	121.48	126.20
12	aB	930	CLA	CHC-C1C-C2C	-2.88	118.77	126.95
12	cB	933	CLA	C4C-C3C-C2C	-2.88	102.70	106.89
12	cB	934	CLA	C4C-C3C-C2C	-2.88	102.70	106.89
12	cA	813	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
12	cA	819	CLA	CHC-C1C-C2C	-2.88	118.78	126.95
12	aL	202	CLA	C4B-C3B-C2B	-2.88	103.73	107.30
12	cA	816	CLA	CHC-C1C-C2C	-2.88	118.78	126.95
12	aA	816	CLA	CHC-C1C-C2C	-2.87	118.78	126.95
12	bB	906	CLA	C3B-C4B-NB	2.87	113.10	110.53
12	bA	821	CLA	CHC-C1C-C2C	-2.87	118.78	126.95
12	cB	924	CLA	C4A-NA-C1A	-2.87	105.37	106.68
12	bB	918	CLA	CMA-C3A-C4A	-2.87	104.05	111.77
12	aA	842	CLA	CHC-C1C-C2C	-2.87	118.79	126.95
12	bB	911	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
12	aB	901	CLA	C1-C2-C3	-2.87	121.49	126.20
12	bB	929	CLA	CHD-C4C-NC	2.87	128.68	124.23
12	aB	903	CLA	C4B-C3B-C2B	-2.87	103.73	107.30
12	cB	903	CLA	C4B-C3B-C2B	-2.87	103.73	107.30
12	bB	901	CLA	C1-C2-C3	-2.87	121.50	126.20
12	aA	818	CLA	C4A-NA-C1A	-2.87	105.37	106.68
12	bB	932	CLA	CHC-C1C-C2C	-2.87	118.80	126.95
12	aB	918	CLA	CMA-C3A-C4A	-2.87	104.06	111.77
12	aA	813	CLA	CMB-C2B-C3B	2.87	133.30	126.55
12	bA	818	CLA	CHC-C1C-C2C	-2.87	118.80	126.95
12	aA	827	CLA	O2D-CGD-O1D	-2.87	118.27	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aB	913	CLA	C4C-C3C-C2C	-2.87	102.72	106.89
12	cA	816	CLA	C4B-C3B-C2B	-2.87	103.74	107.30
12	bB	933	CLA	C3B-C4B-NB	2.87	113.09	110.53
12	cB	934	CLA	C3B-C4B-NB	2.87	113.09	110.53
12	cA	831	CLA	C1-C2-C3	-2.87	122.13	126.76
12	bL	202	CLA	C4B-C3B-C2B	-2.87	103.74	107.30
12	cB	918	CLA	CMA-C3A-C4A	-2.86	104.07	111.77
12	cB	936	CLA	CHC-C1C-C2C	-2.86	118.81	126.95
12	cA	817	CLA	C1-O2A-CGA	2.86	123.58	116.65
12	aB	934	CLA	C4C-C3C-C2C	-2.86	102.72	106.89
12	bA	817	CLA	C4B-C3B-C2B	-2.86	103.74	107.30
12	bA	836	CLA	CMC-C2C-C1C	2.86	129.51	125.03
12	cB	907	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
12	cA	827	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
12	bB	913	CLA	C4C-C3C-C2C	-2.86	102.72	106.89
12	cA	842	CLA	CHC-C1C-C2C	-2.86	118.81	126.95
12	cB	910	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
12	aB	931	CLA	CAC-C3C-C4C	2.86	128.51	124.79
12	aA	831	CLA	C1-C2-C3	-2.86	122.13	126.76
12	bB	933	CLA	C4C-C3C-C2C	-2.86	102.73	106.89
12	cB	913	CLA	C4C-C3C-C2C	-2.86	102.73	106.89
12	cB	916	CLA	CAC-C3C-C4C	2.86	128.51	124.79
15	bB	944	BCR	C27-C26-C25	2.86	126.57	122.70
12	aA	818	CLA	CHC-C1C-C2C	-2.86	118.82	126.95
12	aB	924	CLA	CHC-C1C-C2C	-2.86	118.82	126.95
12	aA	828	CLA	C4-C3-C5	2.86	120.19	115.23
12	cA	828	CLA	C4-C3-C5	2.86	120.19	115.23
12	cB	905	CLA	CED-O2D-CGD	2.86	122.40	115.92
12	bB	949	CLA	C1C-C2C-C3C	-2.86	103.97	106.98
12	cB	949	CLA	C1C-C2C-C3C	-2.86	103.97	106.98
12	cA	818	CLA	CHC-C1C-C2C	-2.86	118.82	126.95
12	aB	933	CLA	C4C-C3C-C2C	-2.86	102.73	106.89
12	aA	819	CLA	CHC-C1C-C2C	-2.86	118.82	126.95
12	cB	924	CLA	CHC-C1C-C2C	-2.86	118.82	126.95
12	bB	917	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
12	bA	819	CLA	CHC-C1C-C2C	-2.86	118.83	126.95
12	bA	813	CLA	CMB-C2B-C3B	2.86	133.27	126.55
12	cB	915	CLA	C3B-C4B-NB	2.86	113.08	110.53
12	cB	910	CLA	CAC-C3C-C4C	2.86	128.51	124.79
12	cB	911	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
12	bB	902	CLA	CHB-C4A-NA	2.86	128.52	124.40
12	bA	828	CLA	C4-C3-C5	2.86	120.18	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aB	936	CLA	CHC-C1C-C2C	-2.85	118.83	126.95
12	bB	950	CLA	CHD-C1D-ND	-2.85	120.78	124.80
15	bI	101	BCR	C15-C16-C17	-2.85	117.68	123.52
12	bB	901	CLA	CBC-CAC-C3C	-2.85	104.68	112.42
12	bA	817	CLA	C1-O2A-CGA	2.85	123.56	116.65
12	aB	905	CLA	CAC-C3C-C4C	2.85	128.50	124.79
15	bF	204	BCR	C2-C1-C6	2.85	114.58	110.44
12	bA	827	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
12	aB	905	CLA	CED-O2D-CGD	2.85	122.39	115.92
12	aB	929	CLA	CHD-C4C-NC	2.85	128.65	124.23
12	bB	934	CLA	C4C-C3C-C2C	-2.85	102.74	106.89
12	bB	924	CLA	CHC-C1C-C2C	-2.85	118.84	126.95
12	bB	936	CLA	CHC-C1C-C2C	-2.85	118.85	126.95
12	bB	905	CLA	CED-O2D-CGD	2.85	122.38	115.92
15	cF	204	BCR	C2-C1-C6	2.85	114.58	110.44
12	aA	836	CLA	CMC-C2C-C1C	2.85	129.49	125.03
12	aB	924	CLA	C4A-NA-C1A	-2.85	105.38	106.68
12	aA	809	CLA	CHB-C4A-NA	2.85	128.51	124.40
12	aB	910	CLA	CAC-C3C-C4C	2.85	128.50	124.79
12	cL	202	CLA	C4-C3-C5	2.85	120.17	115.23
12	cB	901	CLA	C1-C2-C3	-2.85	121.53	126.20
12	cB	901	CLA	CBC-CAC-C3C	-2.85	104.70	112.42
12	aB	907	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
12	bB	911	CLA	CHC-C1C-C2C	-2.85	118.86	126.95
12	cA	853	CLA	C4B-C3B-C2B	-2.85	103.76	107.30
15	aB	946	BCR	C16-C15-C14	-2.85	117.69	123.52
12	bB	903	CLA	C4B-C3B-C2B	-2.85	103.76	107.30
12	bA	842	CLA	CHC-C1C-C2C	-2.85	118.86	126.95
12	cA	836	CLA	CMB-C2B-C1B	2.85	129.75	125.42
12	bA	831	CLA	C1-C2-C3	-2.85	122.16	126.76
12	aA	817	CLA	C1-O2A-CGA	2.85	123.54	116.65
12	bB	910	CLA	CAC-C3C-C4C	2.85	128.49	124.79
12	cA	841	CLA	C4B-C3B-C2B	-2.85	103.76	107.30
12	bA	813	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
12	bB	907	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
15	cB	946	BCR	C16-C15-C14	-2.84	117.70	123.52
12	bA	809	CLA	CHB-C4A-NA	2.84	128.50	124.40
12	aA	827	CLA	CHD-C4C-NC	2.84	128.64	124.23
12	bA	827	CLA	CHD-C4C-NC	2.84	128.64	124.23
12	aB	901	CLA	CBC-CAC-C3C	-2.84	104.71	112.42
12	aB	906	CLA	C3B-C4B-NB	2.84	113.07	110.53
12	aL	202	CLA	C4-C3-C5	2.84	120.16	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aB	925	CLA	O2A-CGA-CBA	2.84	120.50	111.83
12	aA	802	CLA	CHC-C1C-C2C	-2.84	118.87	126.95
12	bB	937	CLA	C3B-C4B-NB	2.84	113.07	110.53
12	cA	802	CLA	CHC-C1C-C2C	-2.84	118.88	126.95
15	bB	942	BCR	C29-C30-C25	2.84	114.56	110.44
12	aB	915	CLA	C4-C3-C5	2.84	120.16	115.23
12	cA	827	CLA	CHD-C4C-NC	2.84	128.63	124.23
12	aA	832	CLA	C4C-C3C-C2C	-2.84	102.76	106.89
12	aA	841	CLA	C4B-C3B-C2B	-2.84	103.77	107.30
12	aB	930	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
12	cB	917	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
12	aB	937	CLA	C3B-C4B-NB	2.84	113.06	110.53
12	bA	810	CLA	C3B-C4B-NB	2.84	113.06	110.53
12	bB	905	CLA	CMB-C2B-C1B	2.84	129.74	125.42
12	aA	814	CLA	C4A-NA-C1A	-2.84	105.39	106.68
12	cB	902	CLA	CHB-C4A-NA	2.84	128.49	124.40
12	bA	841	CLA	C4B-C3B-C2B	-2.84	103.78	107.30
12	aA	812	CLA	C7-C6-C5	-2.84	105.70	113.26
15	aA	847	BCR	C15-C14-C13	-2.84	123.30	127.28
12	bB	910	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
12	bL	202	CLA	C4-C3-C5	2.83	120.15	115.23
12	bB	925	CLA	O2A-CGA-CBA	2.83	120.47	111.83
12	aB	921	CLA	C4C-C3C-C2C	-2.83	102.77	106.89
12	cA	805	CLA	CHD-C4C-NC	2.83	128.62	124.23
15	aF	204	BCR	C2-C1-C6	2.83	114.55	110.44
12	bA	812	CLA	C7-C6-C5	-2.83	105.72	113.26
12	cA	812	CLA	C7-C6-C5	-2.83	105.72	113.26
12	aB	905	CLA	CMB-C2B-C1B	2.83	129.73	125.42
12	aB	917	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
15	cB	942	BCR	C29-C30-C25	2.83	114.55	110.44
12	bA	808	CLA	C4C-C3C-C2C	-2.83	102.77	106.89
12	bA	805	CLA	CHD-C4C-NC	2.83	128.62	124.23
12	cB	925	CLA	O2A-CGA-CBA	2.83	120.46	111.83
12	aB	932	CLA	CHD-C4C-NC	2.83	128.62	124.23
12	cB	923	CLA	CHD-C4C-NC	2.83	128.62	124.23
12	cB	904	CLA	C4C-C3C-C2C	-2.83	102.77	106.89
12	cB	904	CLA	CMA-C3A-C2A	-2.83	103.05	113.98
12	aA	831	CLA	CHB-C4A-NA	2.83	128.48	124.40
12	aF	202	CLA	C3B-C4B-NB	2.83	113.05	110.53
12	cB	911	CLA	C3B-C4B-NB	2.83	113.05	110.53
12	bB	916	CLA	CAC-C3C-C4C	2.83	128.47	124.79
12	bB	931	CLA	CAC-C3C-C4C	2.83	128.47	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	832	CLA	C4C-C3C-C2C	-2.83	102.78	106.89
12	cA	802	CLA	CHA-C1A-NA	-2.83	119.99	126.39
12	aL	203	CLA	C4A-NA-C1A	-2.83	105.39	106.68
12	aA	836	CLA	CMB-C2B-C1B	2.83	129.72	125.42
12	cB	905	CLA	CMB-C2B-C1B	2.83	129.72	125.42
12	cB	929	CLA	CHD-C4C-NC	2.83	128.61	124.23
12	aF	202	CLA	C4C-C3C-C2C	-2.83	102.78	106.89
12	aA	817	CLA	C4B-C3B-C2B	-2.83	103.79	107.30
12	aA	805	CLA	CAC-C3C-C4C	2.82	128.47	124.79
12	bF	202	CLA	C4C-C3C-C2C	-2.82	102.78	106.89
12	aA	839	CLA	CHC-C1C-C2C	-2.82	118.92	126.95
12	bB	910	CLA	C4C-C3C-C2C	-2.82	102.78	106.89
12	bL	203	CLA	C4A-NA-C1A	-2.82	105.39	106.68
12	cB	931	CLA	CAC-C3C-C4C	2.82	128.46	124.79
12	aB	911	CLA	CHC-C1C-C2C	-2.82	118.92	126.95
12	bB	909	CLA	O2D-CGD-CBD	2.82	116.17	111.23
12	bA	839	CLA	CHC-C1C-C2C	-2.82	118.93	126.95
12	bA	802	CLA	CHC-C1C-C2C	-2.82	118.93	126.95
15	bB	946	BCR	C16-C15-C14	-2.82	117.75	123.52
12	cA	839	CLA	CHD-C4C-NC	2.82	128.60	124.23
12	aB	904	CLA	C4C-C3C-C2C	-2.82	102.79	106.89
12	aB	904	CLA	CMA-C3A-C2A	-2.82	103.08	113.98
12	bB	916	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
12	bB	930	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
12	cA	828	CLA	O2A-CGA-CBA	2.82	120.43	111.83
12	cB	910	CLA	C4C-C3C-C2C	-2.82	102.79	106.89
12	aB	910	CLA	C4C-C3C-C2C	-2.82	102.79	106.89
12	bB	929	CLA	CHC-C1C-C2C	-2.82	118.94	126.95
12	cA	839	CLA	CHC-C1C-C2C	-2.82	118.95	126.95
12	cB	905	CLA	CAA-C2A-C3A	-2.82	105.39	113.00
12	cB	932	CLA	CHD-C4C-NC	2.81	128.60	124.23
12	cB	911	CLA	CHC-C1C-C2C	-2.81	118.95	126.95
12	bB	904	CLA	CMA-C3A-C2A	-2.81	103.10	113.98
12	aB	949	CLA	C1C-C2C-C3C	-2.81	104.02	106.98
12	aA	805	CLA	CHD-C4C-NC	2.81	128.59	124.23
12	bB	905	CLA	CAA-C2A-C3A	-2.81	105.40	113.00
12	bA	802	CLA	CHA-C1A-NA	-2.81	120.02	126.39
12	cB	929	CLA	CHC-C1C-C2C	-2.81	118.96	126.95
12	cA	831	CLA	CHB-C4A-NA	2.81	128.46	124.40
12	aA	823	CLA	CHD-C4C-NC	2.81	128.59	124.23
12	aB	910	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
12	bB	921	CLA	CHC-C1C-C2C	-2.81	118.96	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bB	932	CLA	CHD-C4C-NC	2.81	128.59	124.23
12	cA	836	CLA	CED-O2D-CGD	2.81	122.29	115.92
12	aB	909	CLA	O2D-CGD-CBD	2.81	116.14	111.23
12	cB	909	CLA	O2D-CGD-CBD	2.81	116.14	111.23
12	aA	802	CLA	CHA-C1A-NA	-2.81	120.03	126.39
12	aB	934	CLA	C3B-C4B-NB	2.81	113.04	110.53
12	aA	828	CLA	O2A-CGA-CBA	2.81	120.40	111.83
12	bB	915	CLA	C4-C3-C5	2.81	120.11	115.23
12	aB	929	CLA	CHC-C1C-C2C	-2.81	118.96	126.95
12	bB	919	CLA	C4C-C3C-C2C	-2.81	102.80	106.89
12	aB	921	CLA	CHC-C1C-C2C	-2.81	118.97	126.95
12	bB	902	CLA	C4B-C3B-C2B	-2.81	103.81	107.30
12	cF	202	CLA	CHC-C1C-C2C	-2.81	118.97	126.95
12	aF	202	CLA	CHC-C1C-C2C	-2.81	118.97	126.95
12	aA	854	CLA	C4B-C3B-C2B	-2.81	103.81	107.30
13	cB	940	1L3	C24-C25-C26	-2.81	121.20	127.62
12	aB	916	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
12	bA	823	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
15	aF	203	BCR	C27-C26-C25	2.81	126.50	122.70
12	bA	832	CLA	C4C-C3C-C2C	-2.81	102.81	106.89
12	cA	818	CLA	CHD-C4C-NC	2.81	128.58	124.23
12	aB	902	CLA	O2A-CGA-CBA	2.81	120.39	111.83
12	bF	202	CLA	CHC-C1C-C2C	-2.81	118.98	126.95
12	aL	202	CLA	C4C-C3C-C2C	-2.80	102.81	106.89
12	cF	202	CLA	C4C-C3C-C2C	-2.80	102.81	106.89
12	aA	844	CLA	CHD-C1D-ND	-2.80	120.86	124.80
12	bA	853	CLA	C4B-C3B-C2B	-2.80	103.81	107.30
12	bA	813	CLA	CHC-C1C-C2C	-2.80	118.98	126.95
12	bB	921	CLA	C4C-C3C-C2C	-2.80	102.81	106.89
12	cA	817	CLA	CMC-C2C-C1C	2.80	129.41	125.03
12	cB	915	CLA	C4-C3-C5	2.80	120.09	115.23
12	aA	808	CLA	C4C-C3C-C2C	-2.80	102.81	106.89
12	cA	817	CLA	C4B-C3B-C2B	-2.80	103.82	107.30
12	aA	823	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
12	aB	916	CLA	CAC-C3C-C4C	2.80	128.44	124.79
12	cA	823	CLA	CHD-C4C-NC	2.80	128.57	124.23
12	cA	808	CLA	C4C-C3C-C2C	-2.80	102.81	106.89
13	aB	940	1L3	C24-C25-C26	-2.80	121.21	127.62
15	bF	203	BCR	C27-C26-C25	2.80	126.49	122.70
12	cB	930	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
12	cB	913	CLA	CAC-C3C-C4C	2.80	128.43	124.79
12	bB	904	CLA	C4C-C3C-C2C	-2.80	102.81	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aB	905	CLA	CAA-C2A-C3A	-2.80	105.43	113.00
12	aB	922	CLA	CHC-C1C-C2C	-2.80	118.99	126.95
12	aA	818	CLA	CHD-C4C-NC	2.80	128.57	124.23
12	cB	916	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
12	aB	950	CLA	CHD-C1D-ND	-2.80	120.86	124.80
12	bB	902	CLA	O2A-CGA-CBA	2.80	120.37	111.83
13	bB	940	1L3	C24-C25-C26	-2.80	121.22	127.62
12	bB	911	CLA	C3B-C4B-NB	2.80	113.03	110.53
12	cB	921	CLA	CHC-C1C-C2C	-2.80	119.00	126.95
12	aA	802	CLA	C4-C3-C5	2.80	120.08	115.23
12	cA	813	CLA	CHC-C1C-C2C	-2.80	119.00	126.95
12	aB	913	CLA	CAC-C3C-C4C	2.80	128.43	124.79
12	cA	809	CLA	CHB-C4A-NA	2.80	128.44	124.40
12	cB	921	CLA	C4C-C3C-C2C	-2.80	102.82	106.89
12	bA	818	CLA	CHD-C4C-NC	2.80	128.57	124.23
12	bA	836	CLA	CED-O2D-CGD	2.80	122.26	115.92
12	aB	911	CLA	C3B-C4B-NB	2.80	113.03	110.53
12	bA	828	CLA	O2A-CGA-CBA	2.80	120.36	111.83
12	bA	831	CLA	CHB-C4A-NA	2.80	128.43	124.40
12	bA	817	CLA	CMC-C2C-C1C	2.80	129.40	125.03
12	cB	922	CLA	CHC-C1C-C2C	-2.79	119.00	126.95
12	aA	836	CLA	CED-O2D-CGD	2.79	122.25	115.92
12	aB	901	CLA	CHC-C1C-C2C	-2.79	119.01	126.95
12	aA	832	CLA	C4-C3-C5	2.79	120.08	115.23
12	cA	843	CLA	C4-C3-C5	2.79	120.08	115.23
12	cB	916	CLA	CHB-C4A-NA	2.79	128.43	124.40
12	bA	836	CLA	CMB-C2B-C1B	2.79	129.67	125.42
12	aA	831	CLA	CHD-C4C-NC	2.79	128.56	124.23
12	cB	902	CLA	O2A-CGA-CBA	2.79	120.35	111.83
12	aA	838	CLA	CHD-C4C-NC	2.79	128.56	124.23
12	bB	933	CLA	CHD-C4C-NC	2.79	128.56	124.23
12	cB	903	CLA	CHD-C4C-NC	2.79	128.56	124.23
12	aB	914	CLA	C4B-C3B-C2B	-2.79	103.83	107.30
12	aB	923	CLA	CHD-C4C-NC	2.79	128.56	124.23
12	cA	831	CLA	CHD-C4C-NC	2.79	128.56	124.23
12	aA	813	CLA	CHC-C1C-C2C	-2.79	119.01	126.95
12	bA	823	CLA	CHD-C4C-NC	2.79	128.56	124.23
12	cB	937	CLA	C3B-C4B-NB	2.79	113.02	110.53
12	cA	814	CLA	C4A-NA-C1A	-2.79	105.41	106.68
12	cA	805	CLA	CAC-C3C-C4C	2.79	128.42	124.79
12	bB	922	CLA	CHC-C1C-C2C	-2.79	119.02	126.95
12	bB	915	CLA	CHC-C1C-C2C	-2.79	119.02	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	820	CLA	CAC-C3C-C4C	2.79	128.42	124.79
12	bB	927	CLA	CAC-C3C-C4C	2.79	128.42	124.79
12	cB	922	CLA	CHD-C4C-NC	2.79	128.56	124.23
12	aB	927	CLA	CHD-C1D-ND	-2.79	120.88	124.80
12	cA	823	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
12	cB	927	CLA	CHD-C1D-ND	-2.79	120.88	124.80
12	bA	826	CLA	CMB-C2B-C1B	2.79	129.66	125.42
12	bL	202	CLA	C4C-C3C-C2C	-2.79	102.83	106.89
12	bB	903	CLA	CHD-C4C-NC	2.79	128.55	124.23
15	cF	203	BCR	C27-C26-C25	2.79	126.47	122.70
12	bA	839	CLA	CHD-C4C-NC	2.79	128.55	124.23
12	aA	854	CLA	CHA-C1A-NA	-2.79	120.08	126.39
12	aB	927	CLA	CAC-C3C-C4C	2.79	128.41	124.79
12	cB	926	CLA	CHD-C4C-NC	2.79	128.55	124.23
12	cL	202	CLA	C4C-C3C-C2C	-2.78	102.84	106.89
12	bA	833	CLA	C4-C3-C5	2.78	119.41	116.13
12	cB	927	CLA	CAC-C3C-C4C	2.78	128.41	124.79
15	aB	945	BCR	C11-C10-C9	-2.78	123.37	127.28
12	bA	831	CLA	CHD-C4C-NC	2.78	128.55	124.23
12	cA	832	CLA	C4-C3-C5	2.78	120.06	115.23
15	bA	846	BCR	C15-C14-C13	-2.78	123.38	127.28
12	bA	805	CLA	CAC-C3C-C4C	2.78	128.41	124.79
12	cA	804	CLA	C4A-NA-C1A	-2.78	105.41	106.68
12	aB	933	CLA	CHD-C4C-NC	2.78	128.54	124.23
12	cB	901	CLA	CHC-C1C-C2C	-2.78	119.05	126.95
15	cB	945	BCR	C11-C10-C9	-2.78	123.38	127.28
12	bB	922	CLA	CHD-C4C-NC	2.78	128.54	124.23
12	aA	820	CLA	CAC-C3C-C4C	2.78	128.41	124.79
15	bB	945	BCR	C11-C10-C9	-2.78	123.38	127.28
12	aA	826	CLA	CMB-C2B-C1B	2.78	129.65	125.42
12	aB	919	CLA	C4C-C3C-C2C	-2.78	102.85	106.89
12	bB	949	CLA	CMA-C3A-C2A	-2.78	109.86	116.23
12	aB	907	CLA	CBC-CAC-C3C	-2.78	104.89	112.42
12	bA	832	CLA	C4-C3-C5	2.78	120.05	115.23
12	aA	806	CLA	C4C-C3C-C2C	-2.78	102.85	106.89
12	aB	915	CLA	CHC-C1C-C2C	-2.78	119.06	126.95
12	aB	949	CLA	CMA-C3A-C2A	-2.78	109.86	116.23
12	bB	901	CLA	CHC-C1C-C2C	-2.78	119.06	126.95
12	bL	204	CLA	CHC-C1C-C2C	-2.78	119.06	126.95
12	aA	839	CLA	CHD-C4C-NC	2.77	128.53	124.23
12	cA	810	CLA	C3B-C4B-NB	2.77	113.01	110.53
12	cF	202	CLA	C3B-C4B-NB	2.77	113.01	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	804	CLA	O1D-CGD-CBD	-2.77	119.05	124.52
12	aB	913	CLA	CHC-C1C-C2C	-2.77	119.06	126.95
12	cB	933	CLA	CHD-C4C-NC	2.77	128.53	124.23
12	bL	202	CLA	O2A-CGA-O1A	-2.77	116.69	123.63
12	aB	922	CLA	CHD-C4C-NC	2.77	128.53	124.23
12	aB	902	CLA	C4B-C3B-C2B	-2.77	103.85	107.30
12	cA	836	CLA	C3C-C4C-NC	2.77	113.98	110.43
12	aB	916	CLA	CHB-C4A-NA	2.77	128.40	124.40
12	bB	913	CLA	CAC-C3C-C4C	2.77	128.40	124.79
12	cA	820	CLA	CAC-C3C-C4C	2.77	128.40	124.79
12	cA	820	CLA	CMB-C2B-C1B	2.77	129.64	125.42
12	aA	833	CLA	C4-C3-C5	2.77	119.39	116.13
12	cL	202	CLA	O2A-CGA-O1A	-2.77	116.70	123.63
15	cA	846	BCR	C15-C14-C13	-2.77	123.39	127.28
12	aA	818	CLA	C1-C2-C3	-2.77	121.66	126.20
12	bA	808	CLA	CAC-C3C-C4C	2.77	128.39	124.79
12	aL	202	CLA	O2A-CGA-O1A	-2.77	116.70	123.63
12	bA	843	CLA	C4-C3-C5	2.77	120.03	115.23
12	aB	935	CLA	CMB-C2B-C3B	2.77	133.06	126.55
12	cA	823	CLA	CHC-C1C-C2C	-2.77	119.08	126.95
12	cB	915	CLA	CHC-C1C-C2C	-2.77	119.08	126.95
12	cB	917	CLA	CMC-C2C-C1C	2.77	129.36	125.03
12	bA	823	CLA	CHC-C1C-C2C	-2.77	119.08	126.95
12	aB	903	CLA	CHD-C4C-NC	2.77	128.52	124.23
12	cA	853	CLA	CHA-C1A-NA	-2.77	120.13	126.39
12	bB	935	CLA	CMB-C2B-C3B	2.77	133.06	126.55
12	aA	823	CLA	CHC-C1C-C2C	-2.77	119.09	126.95
12	cB	919	CLA	C4C-C3C-C2C	-2.77	102.86	106.89
12	aB	917	CLA	CMC-C2C-C1C	2.77	129.36	125.03
12	cL	204	CLA	CHC-C1C-C2C	-2.77	119.09	126.95
12	cB	913	CLA	O2A-CGA-CBA	2.77	120.27	111.83
16	aA	852	LHG	O8-C23-C24	2.76	120.26	111.83
12	cB	935	CLA	CMB-C2B-C3B	2.76	133.05	126.55
12	aA	843	CLA	C4-C3-C5	2.76	120.03	115.23
12	cA	838	CLA	CHD-C4C-NC	2.76	128.51	124.23
12	aA	804	CLA	O1D-CGD-CBD	-2.76	119.07	124.52
12	cA	826	CLA	C4C-C3C-C2C	-2.76	102.87	106.89
12	bA	804	CLA	CHC-C1C-C2C	-2.76	119.10	126.95
12	bA	822	CLA	CHC-C1C-C2C	-2.76	119.10	126.95
12	cB	913	CLA	CHC-C1C-C2C	-2.76	119.10	126.95
12	cA	802	CLA	C4-C3-C5	2.76	120.02	115.23
12	bA	818	CLA	C1-C2-C3	-2.76	121.67	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	bA	851	LHG	O8-C23-C24	2.76	120.25	111.83
12	aA	817	CLA	CMC-C2C-C1C	2.76	129.35	125.03
12	bA	853	CLA	CHA-C1A-NA	-2.76	120.14	126.39
12	cB	949	CLA	CMA-C3A-C2A	-2.76	109.90	116.23
12	cB	907	CLA	CBC-CAC-C3C	-2.76	104.94	112.42
12	aB	921	CLA	CAA-C2A-C3A	-2.76	105.54	113.00
12	cA	818	CLA	C1-C2-C3	-2.76	121.68	126.20
12	bB	921	CLA	CAA-C2A-C3A	-2.76	105.55	113.00
12	bB	907	CLA	CBC-CAC-C3C	-2.76	104.94	112.42
12	bA	836	CLA	C3C-C4C-NC	2.76	113.96	110.43
12	bF	202	CLA	C3B-C4B-NB	2.76	112.99	110.53
13	aB	940	1L3	C17-C16-C18	2.76	120.01	115.23
15	cM	101	BCR	C27-C26-C25	2.76	126.43	122.70
12	bB	913	CLA	CHC-C1C-C2C	-2.76	119.12	126.95
12	aB	913	CLA	O2A-CGA-CBA	2.75	120.23	111.83
16	cA	851	LHG	O8-C23-C24	2.75	120.23	111.83
12	bB	912	CLA	C4-C3-C5	2.75	120.01	115.23
12	cA	826	CLA	CMB-C2B-C1B	2.75	129.61	125.42
12	bB	917	CLA	CMC-C2C-C1C	2.75	129.34	125.03
12	bB	917	CLA	CHD-C4C-NC	2.75	128.50	124.23
12	aB	917	CLA	CHD-C4C-NC	2.75	128.50	124.23
12	aB	919	CLA	CHD-C4C-NC	2.75	128.50	124.23
12	bB	927	CLA	CHD-C1D-ND	-2.75	120.93	124.80
12	cB	902	CLA	C4B-C3B-C2B	-2.75	103.88	107.30
12	bB	916	CLA	CHB-C4A-NA	2.75	128.37	124.40
12	aL	204	CLA	CHC-C1C-C2C	-2.75	119.14	126.95
12	cA	804	CLA	CHC-C1C-C2C	-2.75	119.14	126.95
12	aB	916	CLA	O2A-CGA-O1A	-2.75	116.75	123.63
12	bA	802	CLA	C4-C3-C5	2.75	120.00	115.23
12	cB	912	CLA	C4-C3-C5	2.75	120.00	115.23
12	cB	921	CLA	CAA-C2A-C3A	-2.75	105.58	113.00
12	bB	923	CLA	CHD-C4C-NC	2.75	128.49	124.23
12	bB	914	CLA	C4B-C3B-C2B	-2.75	103.89	107.30
12	cA	833	CLA	C4-C3-C5	2.75	119.36	116.13
15	cA	847	BCR	C2-C1-C6	2.75	114.43	110.44
12	bA	843	CLA	C4C-C3C-C2C	-2.75	102.89	106.89
12	cB	912	CLA	CHC-C1C-C2C	-2.75	119.15	126.95
12	bA	820	CLA	CMB-C2B-C1B	2.75	129.60	125.42
12	bB	919	CLA	CHD-C4C-NC	2.74	128.49	124.23
12	aB	938	CLA	CHC-C1C-C2C	-2.74	119.15	126.95
12	bB	912	CLA	CHC-C1C-C2C	-2.74	119.15	126.95
12	bB	913	CLA	O2A-CGA-CBA	2.74	120.20	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	810	CLA	C3B-C4B-NB	2.74	112.98	110.53
12	bB	938	CLA	CHC-C1C-C2C	-2.74	119.15	126.95
12	cB	917	CLA	CHD-C4C-NC	2.74	128.48	124.23
12	aA	822	CLA	CHC-C1C-C2C	-2.74	119.16	126.95
12	aA	805	CLA	CHB-C4A-NA	2.74	128.36	124.40
12	aA	808	CLA	CAC-C3C-C4C	2.74	128.36	124.79
12	cB	938	CLA	CHC-C1C-C2C	-2.74	119.16	126.95
12	bB	934	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
12	aB	912	CLA	C4-C3-C5	2.74	119.99	115.23
12	cB	912	CLA	O2A-CGA-CBA	2.74	120.19	111.83
12	aA	820	CLA	CMB-C2B-C1B	2.74	129.59	125.42
12	bA	806	CLA	C4A-NA-C1A	-2.74	105.43	106.68
12	cA	804	CLA	O1D-CGD-CBD	-2.74	119.11	124.52
12	aA	826	CLA	CHC-C1C-C2C	-2.74	119.16	126.95
12	bA	841	CLA	CMB-C2B-C1B	2.74	129.59	125.42
12	cA	822	CLA	CHC-C1C-C2C	-2.74	119.16	126.95
12	bB	912	CLA	C1-C2-C3	-2.74	121.71	126.20
12	cB	904	CLA	CHC-C1C-C2C	-2.74	119.17	126.95
12	bA	814	CLA	CHB-C4A-NA	2.74	128.35	124.40
12	bA	835	CLA	CHC-C1C-C2C	-2.74	119.17	126.95
15	aA	848	BCR	C27-C26-C25	2.74	126.40	122.70
12	aA	826	CLA	C4C-C3C-C2C	-2.74	102.91	106.89
12	bA	806	CLA	C4C-C3C-C2C	-2.74	102.91	106.89
12	bA	838	CLA	CHD-C4C-NC	2.74	128.47	124.23
12	aA	810	CLA	CHC-C1C-C2C	-2.74	119.17	126.95
12	aB	912	CLA	O2A-CGA-CBA	2.74	120.18	111.83
12	cB	928	CLA	C3B-C2B-C1B	-2.74	103.94	107.17
12	cB	914	CLA	C4B-C3B-C2B	-2.74	103.90	107.30
12	aA	806	CLA	C4A-NA-C1A	-2.74	105.43	106.68
12	bA	826	CLA	C4C-C3C-C2C	-2.74	102.91	106.89
12	bB	903	CLA	CHC-C1C-C2C	-2.74	119.17	126.95
12	bB	916	CLA	O2A-CGA-O1A	-2.73	116.79	123.63
12	aA	836	CLA	C3C-C4C-NC	2.73	113.93	110.43
12	aA	804	CLA	CHC-C1C-C2C	-2.73	119.18	126.95
12	aB	904	CLA	CHC-C1C-C2C	-2.73	119.18	126.95
12	cA	808	CLA	CAC-C3C-C4C	2.73	128.35	124.79
12	cB	919	CLA	CHD-C4C-NC	2.73	128.47	124.23
12	aB	932	CLA	CAA-C2A-C1A	-2.73	103.02	111.97
12	aB	934	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
12	bA	810	CLA	CHC-C1C-C2C	-2.73	119.18	126.95
12	aA	832	CLA	CMC-C2C-C1C	2.73	129.30	125.03
12	cA	841	CLA	CMC-C2C-C1C	2.73	129.30	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	843	CLA	C4C-C3C-C2C	-2.73	102.92	106.89
12	cA	842	CLA	CHD-C4C-NC	2.73	128.47	124.23
12	bA	820	CLA	CHD-C4C-NC	2.73	128.46	124.23
12	bA	825	CLA	CHD-C4C-NC	2.73	128.46	124.23
12	cA	824	CLA	CMC-C2C-C1C	2.73	129.30	125.03
12	bB	928	CLA	C3B-C2B-C1B	-2.73	103.95	107.17
12	bB	932	CLA	CAA-C2A-C1A	-2.73	103.03	111.97
12	aB	903	CLA	CHC-C1C-C2C	-2.73	119.19	126.95
12	cB	932	CLA	CAA-C2A-C1A	-2.73	103.03	111.97
12	aB	912	CLA	CHC-C1C-C2C	-2.73	119.19	126.95
12	cA	805	CLA	O2A-CGA-CBA	2.73	120.15	111.83
12	cA	810	CLA	CHC-C1C-C2C	-2.73	119.20	126.95
12	aA	841	CLA	CMB-C2B-C1B	2.73	129.57	125.42
12	aB	912	CLA	C1-C2-C3	-2.73	121.73	126.20
12	cL	203	CLA	C4A-NA-C1A	-2.73	105.44	106.68
12	cA	805	CLA	C3B-C4B-NB	2.73	112.96	110.53
13	cB	940	1L3	C17-C16-C18	2.73	119.96	115.23
12	bB	904	CLA	CHC-C1C-C2C	-2.73	119.20	126.95
12	cB	909	CLA	C1-C2-C3	-2.73	121.73	126.20
12	cB	912	CLA	C1-C2-C3	-2.73	121.73	126.20
12	bA	842	CLA	CHD-C4C-NC	2.73	128.46	124.23
12	cA	835	CLA	CHC-C1C-C2C	-2.73	119.20	126.95
12	cA	806	CLA	C4C-C3C-C2C	-2.72	102.92	106.89
15	cA	847	BCR	C27-C26-C25	2.72	126.39	122.70
12	aB	932	CLA	CAA-CBA-CGA	-2.72	105.23	112.49
12	cA	803	CLA	CHC-C1C-C2C	-2.72	119.21	126.95
12	aA	813	CLA	CAC-C3C-C4C	2.72	128.33	124.79
12	bB	912	CLA	O2A-CGA-CBA	2.72	120.14	111.83
15	bA	850	BCR	C24-C23-C22	-2.72	122.21	126.23
12	aA	820	CLA	CHD-C4C-NC	2.72	128.45	124.23
12	bA	805	CLA	O2A-CGA-CBA	2.72	120.13	111.83
15	bF	203	BCR	C35-C13-C14	-2.72	118.41	122.82
12	cA	809	CLA	CHD-C4C-NC	2.72	128.45	124.23
12	bA	813	CLA	CAC-C3C-C4C	2.72	128.33	124.79
12	aL	203	CLA	CBC-CAC-C3C	-2.72	105.05	112.42
12	cA	814	CLA	CHB-C4A-NA	2.72	128.32	124.40
12	cB	903	CLA	CHC-C1C-C2C	-2.72	119.22	126.95
12	aA	805	CLA	O2A-CGA-CBA	2.72	120.12	111.83
12	cA	813	CLA	CAC-C3C-C4C	2.72	128.33	124.79
12	bB	928	CLA	O2A-CGA-CBA	2.72	120.12	111.83
12	cB	932	CLA	CAA-CBA-CGA	-2.72	105.24	112.49
15	aF	203	BCR	C35-C13-C14	-2.72	118.41	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aB	912	CLA	C4B-C3B-C2B	-2.72	103.92	107.30
12	cB	928	CLA	O2A-CGA-CBA	2.72	120.12	111.83
12	cB	934	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
12	cA	811	CLA	CHD-C4C-NC	2.72	128.44	124.23
12	cA	826	CLA	CHC-C1C-C2C	-2.72	119.23	126.95
12	aB	928	CLA	C3B-C2B-C1B	-2.72	103.97	107.17
12	aA	828	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
12	bA	805	CLA	CHB-C4A-NA	2.71	128.32	124.40
12	bB	928	CLA	CMB-C2B-C3B	2.71	132.94	126.55
12	aA	843	CLA	C4C-C3C-C2C	-2.71	102.94	106.89
13	bB	940	1L3	C17-C16-C18	2.71	119.94	115.23
12	aA	824	CLA	CMC-C2C-C1C	2.71	129.28	125.03
12	bB	909	CLA	C1-C2-C3	-2.71	121.75	126.20
12	cA	805	CLA	CHB-C4A-NA	2.71	128.32	124.40
12	aB	928	CLA	O2A-CGA-CBA	2.71	120.11	111.83
12	cA	832	CLA	CHC-C1C-C2C	-2.71	119.24	126.95
15	cF	203	BCR	C40-C30-C25	2.71	114.50	110.24
12	cB	912	CLA	C4B-C3B-C2B	-2.71	103.93	107.30
15	aA	848	BCR	C2-C1-C6	2.71	114.38	110.44
12	bA	826	CLA	CHC-C1C-C2C	-2.71	119.24	126.95
12	aA	835	CLA	CHC-C1C-C2C	-2.71	119.24	126.95
12	bA	832	CLA	CMC-C2C-C1C	2.71	129.27	125.03
11	bA	801	CL0	C4C-C3C-C2C	-2.71	102.67	113.37
12	aL	204	CLA	C4A-NA-C1A	-2.71	105.44	106.68
12	cB	935	CLA	CHC-C1C-C2C	-2.71	119.25	126.95
12	bB	912	CLA	C4B-C3B-C2B	-2.71	103.93	107.30
12	aB	901	CLA	CMC-C2C-C1C	2.71	129.27	125.03
15	bM	101	BCR	C27-C26-C25	2.71	126.36	122.70
12	cA	828	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
11	cA	801	CL0	C4C-C3C-C2C	-2.71	102.68	113.37
12	cL	204	CLA	C4A-NA-C1A	-2.71	105.44	106.68
12	bA	803	CLA	CHC-C1C-C2C	-2.71	119.25	126.95
12	aA	812	CLA	C1-O2A-CGA	2.71	123.20	116.65
12	cA	820	CLA	CHD-C4C-NC	2.71	128.43	124.23
12	aA	832	CLA	CHC-C1C-C2C	-2.71	119.26	126.95
12	bA	828	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
12	cB	928	CLA	CMB-C2B-C3B	2.71	132.91	126.55
12	bL	203	CLA	CBC-CAC-C3C	-2.71	105.09	112.42
12	cB	916	CLA	O2A-CGA-O1A	-2.70	116.86	123.63
12	bA	819	CLA	CHD-C4C-NC	2.70	128.43	124.23
12	aA	803	CLA	CHC-C1C-C2C	-2.70	119.26	126.95
15	bA	847	BCR	C2-C1-C6	2.70	114.37	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	831	CLA	C4B-C3B-C2B	-2.70	103.94	107.30
12	aB	926	CLA	CHD-C4C-NC	2.70	128.42	124.23
12	cA	819	CLA	CHD-C4C-NC	2.70	128.42	124.23
11	aA	801	CL0	C4C-C3C-C2C	-2.70	102.70	113.37
12	bB	935	CLA	CHC-C1C-C2C	-2.70	119.27	126.95
12	aA	804	CLA	C4A-NA-C1A	-2.70	105.45	106.68
12	cL	203	CLA	CBC-CAC-C3C	-2.70	105.09	112.42
12	bB	926	CLA	CHD-C4C-NC	2.70	128.42	124.23
12	bL	202	CLA	O1D-CGD-CBD	-2.70	119.19	124.52
12	bL	204	CLA	CMC-C2C-C1C	2.70	129.26	125.03
12	aB	901	CLA	O2A-CGA-CBA	2.70	120.07	111.83
12	bA	812	CLA	O2A-CGA-CBA	2.70	120.07	111.83
12	aA	805	CLA	C3B-C4B-NB	2.70	112.94	110.53
12	aA	842	CLA	CHD-C4C-NC	2.70	128.42	124.23
12	bA	811	CLA	CHD-C4C-NC	2.70	128.42	124.23
15	aF	203	BCR	C40-C30-C25	2.70	114.48	110.24
12	aA	811	CLA	CHD-C4C-NC	2.70	128.42	124.23
12	cL	202	CLA	O1D-CGD-CBD	-2.70	119.19	124.52
12	cB	926	CLA	C4-C3-C5	2.70	119.91	115.23
12	cL	204	CLA	CMC-C2C-C1C	2.70	129.25	125.03
12	aA	821	CLA	CAA-C2A-C3A	-2.70	105.71	113.00
12	bA	828	CLA	CHD-C4C-NC	2.70	128.41	124.23
15	aM	101	BCR	C27-C26-C25	2.70	126.35	122.70
12	cA	841	CLA	CMB-C2B-C1B	2.70	129.53	125.42
12	aA	831	CLA	C4B-C3B-C2B	-2.70	103.95	107.30
12	aB	909	CLA	C1-C2-C3	-2.70	121.78	126.20
12	aB	926	CLA	CHC-C1C-C2C	-2.70	119.28	126.95
12	aL	202	CLA	O1D-CGD-CBD	-2.70	119.20	124.52
12	aB	915	CLA	C4B-C3B-C2B	-2.70	103.95	107.30
12	aB	935	CLA	CHC-C1C-C2C	-2.70	119.28	126.95
12	bA	832	CLA	CHC-C1C-C2C	-2.70	119.28	126.95
12	aA	809	CLA	CHD-C4C-NC	2.70	128.41	124.23
12	bB	930	CLA	O2A-CGA-CBA	2.70	120.06	111.83
12	cB	930	CLA	O2A-CGA-CBA	2.70	120.06	111.83
12	cB	926	CLA	CHC-C1C-C2C	-2.70	119.29	126.95
12	aB	909	CLA	O2A-CGA-CBA	2.70	120.05	111.83
12	bA	824	CLA	CMC-C2C-C1C	2.70	129.25	125.03
12	bA	809	CLA	CHD-C4C-NC	2.69	128.41	124.23
12	bA	821	CLA	CAA-C2A-C3A	-2.69	105.72	113.00
12	bB	932	CLA	CAA-CBA-CGA	-2.69	105.30	112.49
12	bA	831	CLA	C4A-NA-C1A	-2.69	105.45	106.68
12	cA	832	CLA	CMC-C2C-C1C	2.69	129.24	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cB	901	CLA	O2A-CGA-CBA	2.69	120.05	111.83
12	bA	805	CLA	C3B-C4B-NB	2.69	112.93	110.53
12	cB	906	CLA	CAC-C3C-C4C	2.69	128.29	124.79
15	bA	847	BCR	C27-C26-C25	2.69	126.34	122.70
12	aA	827	CLA	CHC-C1C-C2C	-2.69	119.30	126.95
12	aB	930	CLA	O2A-CGA-CBA	2.69	120.04	111.83
12	aA	812	CLA	O2A-CGA-CBA	2.69	120.04	111.83
12	cA	831	CLA	C4B-C3B-C2B	-2.69	103.96	107.30
12	bB	909	CLA	O2A-CGA-CBA	2.69	120.04	111.83
12	bB	923	CLA	C1-C2-C3	-2.69	121.79	126.20
12	bA	827	CLA	CHC-C1C-C2C	-2.69	119.30	126.95
12	aB	928	CLA	CMB-C2B-C3B	2.69	132.88	126.55
12	cA	812	CLA	O2A-CGA-CBA	2.69	120.03	111.83
15	cF	203	BCR	C35-C13-C14	-2.69	118.46	122.82
12	aB	920	CLA	CHC-C1C-C2C	-2.69	119.31	126.95
12	aA	815	CLA	CHD-C4C-NC	2.69	128.40	124.23
12	cB	929	CLA	CMB-C2B-C1B	2.69	129.51	125.42
12	bA	814	CLA	C4A-NA-C1A	-2.69	105.45	106.68
12	bB	912	CLA	C4A-NA-C1A	-2.69	105.45	106.68
15	cF	204	BCR	C27-C26-C25	2.69	126.33	122.70
12	bB	915	CLA	C4B-C3B-C2B	-2.69	103.96	107.30
12	aB	913	CLA	CHD-C4C-NC	2.69	128.40	124.23
12	cA	802	CLA	O2A-CGA-CBA	2.69	120.03	111.83
12	aB	929	CLA	CMB-C2B-C1B	2.69	129.51	125.42
12	aA	802	CLA	O2A-CGA-CBA	2.69	120.02	111.83
12	bA	812	CLA	C1-O2A-CGA	2.68	123.15	116.65
12	cB	923	CLA	C1-C2-C3	-2.68	121.80	126.20
12	cA	816	CLA	O2D-CGD-O1D	-2.68	118.62	123.85
12	cA	827	CLA	CHC-C1C-C2C	-2.68	119.32	126.95
12	cA	828	CLA	CHD-C4C-NC	2.68	128.39	124.23
12	bB	926	CLA	CHC-C1C-C2C	-2.68	119.32	126.95
12	cA	821	CLA	CAA-C2A-C3A	-2.68	105.75	113.00
15	bF	203	BCR	C40-C30-C25	2.68	114.45	110.24
12	bB	901	CLA	O2A-CGA-CBA	2.68	120.01	111.83
12	aB	923	CLA	C1-C2-C3	-2.68	121.80	126.20
12	aA	804	CLA	O2A-CGA-CBA	2.68	120.01	111.83
15	aA	851	BCR	C7-C8-C9	-2.68	122.27	126.23
12	cA	812	CLA	C1-O2A-CGA	2.68	123.14	116.65
12	aA	819	CLA	CHD-C4C-NC	2.68	128.39	124.23
12	bA	808	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
15	aI	101	BCR	C3-C4-C5	-2.68	109.28	114.06
12	cB	926	CLA	CMC-C2C-C1C	2.68	129.22	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bB	920	CLA	O1D-CGD-CBD	-2.68	119.24	124.52
12	bB	920	CLA	CHC-C1C-C2C	-2.68	119.34	126.95
12	aA	828	CLA	CHD-C4C-NC	2.68	128.38	124.23
12	bA	802	CLA	O2A-CGA-CBA	2.68	120.00	111.83
12	aA	810	CLA	CHD-C4C-NC	2.68	128.38	124.23
12	cB	913	CLA	CHD-C4C-NC	2.68	128.38	124.23
12	aA	854	CLA	CMC-C2C-C1C	2.68	129.22	125.03
12	bA	853	CLA	CMC-C2C-C1C	2.68	129.22	125.03
12	aA	814	CLA	CHB-C4A-NA	2.68	128.26	124.40
12	cB	920	CLA	CHC-C1C-C2C	-2.68	119.34	126.95
12	bA	841	CLA	CMC-C2C-C1C	2.68	129.22	125.03
12	cB	908	CLA	CMC-C2C-C1C	2.68	129.22	125.03
12	bA	832	CLA	C4B-C3B-C2B	-2.68	103.97	107.30
15	aA	851	BCR	C24-C23-C22	-2.67	122.28	126.23
15	bI	101	BCR	C3-C4-C5	-2.67	109.29	114.06
12	cA	804	CLA	O2A-CGA-CBA	2.67	119.99	111.83
15	aF	204	BCR	C27-C26-C25	2.67	126.32	122.70
12	aB	926	CLA	C4-C3-C5	2.67	119.87	115.23
12	cA	832	CLA	C4B-C3B-C2B	-2.67	103.98	107.30
12	cB	915	CLA	C4B-C3B-C2B	-2.67	103.98	107.30
12	cA	817	CLA	CHC-C1C-C2C	-2.67	119.36	126.95
15	cA	850	BCR	C24-C23-C22	-2.67	122.28	126.23
12	cB	909	CLA	O2A-CGA-CBA	2.67	119.98	111.83
12	bA	817	CLA	CHC-C1C-C2C	-2.67	119.36	126.95
12	cA	815	CLA	CHD-C4C-NC	2.67	128.37	124.23
12	bA	804	CLA	O2A-CGA-CBA	2.67	119.97	111.83
12	cB	917	CLA	CAC-C3C-C4C	2.67	128.26	124.79
12	bB	926	CLA	C4-C3-C5	2.67	119.86	115.23
12	bA	833	CLA	CHD-C4C-NC	2.67	128.37	124.23
15	bA	850	BCR	C7-C8-C9	-2.67	122.29	126.23
12	aA	825	CLA	CHD-C4C-NC	2.67	128.37	124.23
12	bA	816	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
12	cB	920	CLA	O1D-CGD-CBD	-2.67	119.26	124.52
12	aA	816	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
12	cA	831	CLA	C4A-NA-C1A	-2.67	105.46	106.68
15	cA	850	BCR	C7-C8-C9	-2.67	122.29	126.23
12	aA	817	CLA	CHC-C1C-C2C	-2.66	119.38	126.95
12	aB	935	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
12	aB	920	CLA	O1D-CGD-CBD	-2.66	119.26	124.52
12	bA	815	CLA	CHD-C4C-NC	2.66	128.36	124.23
12	bB	935	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
12	aA	805	CLA	CBC-CAC-C3C	-2.66	105.20	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	809	CLA	CHC-C1C-C2C	-2.66	119.38	126.95
12	bA	805	CLA	CBC-CAC-C3C	-2.66	105.20	112.42
12	bB	939	CLA	C4C-C3C-C2C	-2.66	103.02	106.89
12	cA	841	CLA	CHC-C1C-C2C	-2.66	119.38	126.95
12	bB	919	CLA	CBC-CAC-C3C	-2.66	105.21	112.42
15	bI	101	BCR	C15-C14-C13	-2.66	123.55	127.28
12	aA	832	CLA	C4B-C3B-C2B	-2.66	103.99	107.30
12	aB	908	CLA	CMC-C2C-C1C	2.66	129.19	125.03
12	bA	809	CLA	CMC-C2C-C1C	2.66	129.19	125.03
12	cA	853	CLA	CMC-C2C-C1C	2.66	129.19	125.03
15	cI	101	BCR	C3-C4-C5	-2.66	109.31	114.06
12	bB	901	CLA	CMC-C2C-C1C	2.66	129.19	125.03
12	bB	927	CLA	CMC-C2C-C1C	2.66	129.19	125.03
12	aA	833	CLA	CHD-C4C-NC	2.66	128.35	124.23
12	bA	804	CLA	C4A-NA-C1A	-2.66	105.47	106.68
12	bB	917	CLA	CAC-C3C-C4C	2.66	128.25	124.79
15	bA	849	BCR	C11-C10-C9	-2.66	123.55	127.28
12	cA	824	CLA	C4C-C3C-C2C	-2.66	103.02	106.89
12	aA	841	CLA	CMC-C2C-C1C	2.66	129.19	125.03
12	aB	936	CLA	CHD-C4C-NC	2.66	128.35	124.23
12	cA	825	CLA	CHD-C4C-NC	2.66	128.35	124.23
12	bA	831	CLA	CMB-C2B-C1B	2.66	129.47	125.42
12	bB	901	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
12	aA	809	CLA	CMC-C2C-C1C	2.66	129.19	125.03
12	bA	809	CLA	CHC-C1C-C2C	-2.66	119.40	126.95
12	bB	908	CLA	CMC-C2C-C1C	2.66	129.18	125.03
12	aB	938	CLA	CMC-C2C-C1C	2.66	129.18	125.03
12	cA	805	CLA	CBC-CAC-C3C	-2.65	105.22	112.42
12	bB	906	CLA	CAC-C3C-C4C	2.65	128.24	124.79
15	cL	201	BCR	C1-C6-C5	-2.65	119.01	122.64
12	aB	926	CLA	CMC-C2C-C1C	2.65	129.18	125.03
12	bB	929	CLA	CMB-C2B-C1B	2.65	129.46	125.42
12	bB	932	CLA	C4B-C3B-C2B	-2.65	104.00	107.30
12	bL	203	CLA	C4B-C3B-C2B	-2.65	104.00	107.30
12	aA	809	CLA	CHC-C1C-C2C	-2.65	119.41	126.95
12	aL	204	CLA	CMC-C2C-C1C	2.65	129.18	125.03
12	cB	901	CLA	CMC-C2C-C1C	2.65	129.18	125.03
12	aB	917	CLA	CAC-C3C-C4C	2.65	128.24	124.79
12	bB	926	CLA	CMC-C2C-C1C	2.65	129.18	125.03
12	aA	831	CLA	C4A-NA-C1A	-2.65	105.47	106.68
15	aL	201	BCR	C1-C6-C5	-2.65	119.01	122.64
15	cA	849	BCR	C27-C26-C25	2.65	126.29	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	841	CLA	CHC-C1C-C2C	-2.65	119.42	126.95
12	aB	936	CLA	CBA-CAA-C2A	2.65	121.68	113.79
12	cB	912	CLA	C3B-C4B-NB	2.65	112.90	110.53
12	cB	919	CLA	C3B-C4B-NB	2.65	112.90	110.53
12	aB	939	CLA	C4C-C3C-C2C	-2.65	103.03	106.89
12	bL	204	CLA	C4A-NA-C1A	-2.65	105.47	106.68
12	cB	901	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
12	aB	921	CLA	O2A-CGA-CBA	2.65	119.91	111.83
12	bA	836	CLA	CBC-CAC-C3C	-2.65	105.24	112.42
12	cB	917	CLA	C4-C3-C5	2.65	119.83	115.23
15	aI	101	BCR	C15-C14-C13	-2.65	123.56	127.28
12	aB	927	CLA	CMC-C2C-C1C	2.65	129.17	125.03
12	cA	833	CLA	CHD-C4C-NC	2.65	128.34	124.23
12	cL	202	CLA	CHD-C4C-NC	2.65	128.34	124.23
12	bA	828	CLA	CHC-C1C-C2C	-2.65	119.42	126.95
12	cA	836	CLA	CBC-CAC-C3C	-2.65	105.24	112.42
12	bA	810	CLA	CHD-C4C-NC	2.65	128.34	124.23
12	aA	828	CLA	CHC-C1C-C2C	-2.65	119.42	126.95
12	cA	808	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
12	cA	825	CLA	CMC-C2C-C1C	2.65	129.17	125.03
12	aB	921	CLA	CAC-C3C-C4C	2.65	128.23	124.79
12	aB	917	CLA	C4-C3-C5	2.65	119.82	115.23
12	cB	939	CLA	C4C-C3C-C2C	-2.65	103.04	106.89
12	bB	913	CLA	CHD-C4C-NC	2.64	128.33	124.23
12	cB	927	CLA	CMC-C2C-C1C	2.64	129.16	125.03
12	aA	841	CLA	CHC-C1C-C2C	-2.64	119.44	126.95
12	bA	825	CLA	CMC-C2C-C1C	2.64	129.16	125.03
12	cB	936	CLA	CBA-CAA-C2A	2.64	121.66	113.79
12	bB	921	CLA	CAC-C3C-C4C	2.64	128.23	124.79
12	aB	901	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
12	bB	936	CLA	CHD-C4C-NC	2.64	128.33	124.23
15	bF	204	BCR	C27-C26-C25	2.64	126.27	122.70
12	bA	836	CLA	CHD-C4C-NC	2.64	128.33	124.23
12	cB	921	CLA	O2A-CGA-CBA	2.64	119.89	111.83
12	aB	920	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
12	aB	913	CLA	C1-C2-C3	-2.64	121.87	126.20
12	bB	920	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
12	bB	938	CLA	CMC-C2C-C1C	2.64	129.16	125.03
12	cA	842	CLA	CMC-C2C-C1C	2.64	129.16	125.03
12	cA	809	CLA	CMC-C2C-C1C	2.64	129.16	125.03
12	cA	831	CLA	CMB-C2B-C1B	2.64	129.43	125.42
12	aA	831	CLA	CBC-CAC-C3C	-2.64	105.27	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	836	CLA	CBC-CAC-C3C	-2.64	105.27	112.42
12	cB	935	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
12	aL	203	CLA	C4B-C3B-C2B	-2.64	104.03	107.30
12	cB	919	CLA	CBC-CAC-C3C	-2.63	105.28	112.42
12	aB	936	CLA	C1-C2-C3	-2.63	121.88	126.20
15	cA	846	BCR	C27-C26-C25	2.63	126.26	122.70
12	aB	902	CLA	C4-C3-C5	2.63	119.80	115.23
12	cA	839	CLA	CAA-CBA-CGA	-2.63	105.47	112.49
12	bB	913	CLA	C1-C2-C3	-2.63	121.88	126.20
12	aB	908	CLA	C3B-C2B-C1B	-2.63	104.06	107.17
12	aB	906	CLA	CAC-C3C-C4C	2.63	128.22	124.79
11	bA	801	CL0	C1-C2-C3	-2.63	121.88	126.20
12	aB	901	CLA	C4B-C3B-C2B	-2.63	104.03	107.30
12	bA	842	CLA	CMC-C2C-C1C	2.63	129.15	125.03
12	aB	919	CLA	CBC-CAC-C3C	-2.63	105.28	112.42
12	cB	920	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
12	aA	842	CLA	CMC-C2C-C1C	2.63	129.15	125.03
12	aA	833	CLA	C4B-C3B-C2B	-2.63	104.03	107.30
12	cB	901	CLA	C4B-C3B-C2B	-2.63	104.03	107.30
12	cA	842	CLA	C1-C2-C3	-2.63	121.89	126.20
12	bB	921	CLA	O2A-CGA-CBA	2.63	119.86	111.83
12	bA	831	CLA	CBC-CAC-C3C	-2.63	105.29	112.42
15	aA	848	BCR	C15-C16-C17	-2.63	118.14	123.52
12	bB	936	CLA	C1-C2-C3	-2.63	121.89	126.20
12	bB	936	CLA	CBA-CAA-C2A	2.63	121.62	113.79
12	bL	202	CLA	CHD-C4C-NC	2.63	128.31	124.23
12	cA	822	CLA	C4C-C3C-C2C	-2.63	103.06	106.89
12	aL	202	CLA	CHD-C4C-NC	2.63	128.31	124.23
12	bA	824	CLA	C4C-C3C-C2C	-2.63	103.06	106.89
12	bA	810	CLA	CMC-C2C-C1C	2.63	129.14	125.03
12	aA	808	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
12	aA	831	CLA	CMB-C2B-C1B	2.63	129.42	125.42
12	cA	828	CLA	CHC-C1C-C2C	-2.63	119.48	126.95
12	bB	917	CLA	C4-C3-C5	2.63	119.79	115.23
12	aA	836	CLA	C4A-NA-C1A	-2.63	105.48	106.68
12	aB	932	CLA	C4B-C3B-C2B	-2.63	104.03	107.30
12	cA	831	CLA	CBC-CAC-C3C	-2.63	105.30	112.42
15	bA	849	BCR	C27-C26-C25	2.63	126.25	122.70
12	aA	839	CLA	CAA-CBA-CGA	-2.63	105.48	112.49
12	cA	832	CLA	CED-O2D-CGD	2.63	121.88	115.92
15	cJ	101	BCR	C15-C14-C13	-2.63	123.59	127.28
12	bA	839	CLA	CAA-CBA-CGA	-2.63	105.48	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bA	847	BCR	C15-C16-C17	-2.63	118.14	123.52
15	aA	850	BCR	C27-C26-C25	2.63	126.25	122.70
12	aA	842	CLA	C1-C2-C3	-2.63	121.89	126.20
12	cA	820	CLA	O2A-CGA-CBA	2.63	119.84	111.83
12	aA	832	CLA	CED-O2D-CGD	2.63	121.87	115.92
12	aB	916	CLA	CMC-C2C-C1C	2.62	129.13	125.03
12	cA	805	CLA	C4B-C3B-C2B	-2.62	104.04	107.30
12	bA	842	CLA	CAA-C2A-C3A	-2.62	105.91	113.00
12	cA	834	CLA	C3B-C4B-NB	2.62	112.87	110.53
11	aA	801	CL0	C1-C2-C3	-2.62	121.90	126.20
12	bA	823	CLA	O2A-CGA-CBA	2.62	119.83	111.83
12	aA	824	CLA	C4C-C3C-C2C	-2.62	103.08	106.89
12	bB	901	CLA	C4B-C3B-C2B	-2.62	104.04	107.30
12	cB	936	CLA	CHD-C4C-NC	2.62	128.30	124.23
12	aA	823	CLA	O2A-CGA-CBA	2.62	119.83	111.83
12	cB	913	CLA	C1-C2-C3	-2.62	121.90	126.20
12	cL	203	CLA	C4B-C3B-C2B	-2.62	104.04	107.30
12	cB	902	CLA	C4-C3-C5	2.62	119.78	115.23
12	cB	932	CLA	C4B-C3B-C2B	-2.62	104.05	107.30
12	cA	842	CLA	CAA-C2A-C3A	-2.62	105.92	113.00
15	bJ	101	BCR	C15-C14-C13	-2.62	123.61	127.28
12	bB	921	CLA	CHD-C4C-NC	2.62	128.29	124.23
12	cA	840	CLA	CAA-C2A-C3A	-2.62	105.92	113.00
12	bA	820	CLA	O2A-CGA-CBA	2.62	119.82	111.83
15	cI	101	BCR	C15-C14-C13	-2.62	123.61	127.28
12	bA	805	CLA	C4B-C3B-C2B	-2.62	104.05	107.30
12	bA	832	CLA	CED-O2D-CGD	2.62	121.85	115.92
12	bL	203	CLA	CMC-C2C-C1C	2.62	129.12	125.03
12	cB	938	CLA	CMC-C2C-C1C	2.62	129.12	125.03
12	bB	912	CLA	C3B-C4B-NB	2.62	112.86	110.53
12	aA	820	CLA	O2A-CGA-CBA	2.62	119.81	111.83
12	aA	820	CLA	O2D-CGD-O1D	-2.62	118.76	123.85
12	bA	820	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
12	aA	842	CLA	CAA-C2A-C3A	-2.61	105.93	113.00
11	cA	801	CL0	C1-C2-C3	-2.61	121.91	126.20
12	aA	834	CLA	C3B-C4B-NB	2.61	112.86	110.53
12	cA	810	CLA	CHD-C4C-NC	2.61	128.28	124.23
12	aA	825	CLA	CMC-C2C-C1C	2.61	129.12	125.03
12	aL	204	CLA	CHD-C4C-NC	2.61	128.28	124.23
12	bB	908	CLA	C3B-C2B-C1B	-2.61	104.09	107.17
12	cB	934	CLA	CHD-C4C-NC	2.61	128.28	124.23
15	aB	941	BCR	C33-C5-C6	-2.61	121.64	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	825	CLA	CHA-C1A-NA	-2.61	120.48	126.39
12	bA	842	CLA	C1-C2-C3	-2.61	121.92	126.20
12	cA	820	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
12	bA	840	CLA	CAA-C2A-C3A	-2.61	105.95	113.00
12	cA	826	CLA	CHD-C4C-NC	2.61	128.28	124.23
12	bL	204	CLA	CHD-C4C-NC	2.61	128.28	124.23
12	aB	912	CLA	C4A-NA-C1A	-2.61	105.49	106.68
12	aL	203	CLA	CMC-C2C-C1C	2.61	129.11	125.03
15	aA	850	BCR	C11-C10-C9	-2.61	123.62	127.28
12	bA	834	CLA	C4C-C3C-C2C	-2.61	103.10	106.89
12	cB	936	CLA	C1-C2-C3	-2.61	121.92	126.20
12	aA	854	CLA	CHC-C1C-C2C	-2.61	119.54	126.95
12	cB	921	CLA	CAC-C3C-C4C	2.61	128.18	124.79
12	cA	818	CLA	C4B-C3B-C2B	-2.61	104.06	107.30
12	aB	921	CLA	CHD-C4C-NC	2.61	128.27	124.23
12	cA	823	CLA	O2A-CGA-CBA	2.61	119.78	111.83
12	bB	902	CLA	C4-C3-C5	2.61	119.75	115.23
12	cA	833	CLA	C4B-C3B-C2B	-2.60	104.06	107.30
12	cB	906	CLA	CHC-C1C-C2C	-2.60	119.55	126.95
12	bA	808	CLA	C1-C2-C3	-2.60	121.93	126.20
12	cA	834	CLA	C4C-C3C-C2C	-2.60	103.10	106.89
12	aB	933	CLA	CAC-C3C-C4C	2.60	128.18	124.79
12	aA	815	CLA	CBC-CAC-C3C	-2.60	105.36	112.42
12	aB	916	CLA	C1C-C2C-C3C	-2.60	104.24	106.98
12	cB	921	CLA	CHD-C4C-NC	2.60	128.27	124.23
12	bB	933	CLA	CAC-C3C-C4C	2.60	128.18	124.79
11	aA	801	CL0	C4-C3-C5	2.60	119.74	115.23
12	cB	907	CLA	CHD-C4C-NC	2.60	128.26	124.23
12	aA	822	CLA	C4C-C3C-C2C	-2.60	103.11	106.89
12	bB	916	CLA	C1C-C2C-C3C	-2.60	104.24	106.98
12	bA	822	CLA	C4C-C3C-C2C	-2.60	103.11	106.89
15	bL	201	BCR	C1-C6-C5	-2.60	119.08	122.64
12	aA	819	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
12	aA	810	CLA	CMC-C2C-C1C	2.60	129.10	125.03
15	cB	941	BCR	C33-C5-C6	-2.60	121.65	124.48
12	cA	806	CLA	C4A-NA-C1A	-2.60	105.49	106.68
12	aA	818	CLA	C4B-C3B-C2B	-2.60	104.07	107.30
12	cA	819	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
12	aA	805	CLA	C4B-C3B-C2B	-2.60	104.07	107.30
12	cA	836	CLA	CHD-C4C-NC	2.60	128.26	124.23
11	cA	801	CL0	C4-C3-C5	2.60	119.74	115.23
12	cA	808	CLA	CHD-C4C-NC	2.60	128.26	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cA	847	BCR	C15-C16-C17	-2.60	118.21	123.52
12	bB	906	CLA	CHC-C1C-C2C	-2.60	119.57	126.95
12	bA	819	CLA	O2D-CGD-O1D	-2.60	118.80	123.85
12	aA	836	CLA	CHD-C4C-NC	2.60	128.26	124.23
12	aB	907	CLA	CHD-C4C-NC	2.60	128.26	124.23
12	bB	906	CLA	CHD-C4C-NC	2.60	128.26	124.23
12	aA	840	CLA	CAA-C2A-C3A	-2.60	105.99	113.00
12	aA	826	CLA	CHD-C4C-NC	2.59	128.25	124.23
12	bA	853	CLA	CHC-C1C-C2C	-2.59	119.57	126.95
12	aA	829	CLA	CHD-C4C-NC	2.59	128.25	124.23
12	cA	814	CLA	CHD-C4C-NC	2.59	128.25	124.23
12	cL	204	CLA	CHD-C4C-NC	2.59	128.25	124.23
12	bA	832	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
12	aB	912	CLA	C3B-C4B-NB	2.59	112.84	110.53
11	bA	801	CL0	C4-C3-C5	2.59	119.73	115.23
12	cA	853	CLA	CHC-C1C-C2C	-2.59	119.58	126.95
12	aA	832	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
12	bA	815	CLA	CBC-CAC-C3C	-2.59	105.39	112.42
12	aA	834	CLA	C4C-C3C-C2C	-2.59	103.12	106.89
13	cA	844	1L3	C22-C21-C20	-2.59	116.97	123.63
15	bB	941	BCR	C33-C5-C6	-2.59	121.66	124.48
15	aJ	101	BCR	C15-C14-C13	-2.59	123.64	127.28
12	bA	838	CLA	CMC-C2C-C1C	2.59	129.08	125.03
12	cB	916	CLA	CMC-C2C-C1C	2.59	129.08	125.03
12	cA	815	CLA	CBC-CAC-C3C	-2.59	105.40	112.42
15	aA	847	BCR	C27-C26-C25	2.59	126.20	122.70
12	cL	203	CLA	CMC-C2C-C1C	2.59	129.08	125.03
15	cF	204	BCR	C7-C8-C9	-2.59	122.41	126.23
13	cA	844	1L3	C22-C21-C23	2.59	119.72	115.23
12	bB	916	CLA	CMC-C2C-C1C	2.59	129.08	125.03
12	cA	810	CLA	CMC-C2C-C1C	2.59	129.08	125.03
15	bA	846	BCR	C27-C26-C25	2.59	126.20	122.70
13	bA	844	1L3	C22-C21-C23	2.59	119.72	115.23
12	aB	904	CLA	CHD-C4C-NC	2.59	128.24	124.23
12	cB	933	CLA	CAC-C3C-C4C	2.58	128.15	124.79
12	cB	906	CLA	CHD-C4C-NC	2.58	128.24	124.23
12	bA	818	CLA	C4B-C3B-C2B	-2.58	104.09	107.30
12	bA	833	CLA	C4B-C3B-C2B	-2.58	104.09	107.30
12	bA	836	CLA	C4A-NA-C1A	-2.58	105.50	106.68
12	cA	808	CLA	C1-C2-C3	-2.58	121.97	126.20
12	bF	202	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
12	bA	808	CLA	CHD-C4C-NC	2.58	128.23	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bB	934	CLA	CHD-C4C-NC	2.58	128.23	124.23
12	cB	916	CLA	C1C-C2C-C3C	-2.58	104.27	106.98
12	cB	905	CLA	C4B-C3B-C2B	-2.58	104.09	107.30
15	bL	201	BCR	C27-C26-C25	2.58	126.19	122.70
12	aB	905	CLA	C4B-C3B-C2B	-2.58	104.09	107.30
12	aA	825	CLA	CHA-C1A-NA	-2.58	120.55	126.39
12	aA	814	CLA	CHD-C4C-NC	2.58	128.23	124.23
13	aA	845	1L3	C22-C21-C23	2.58	119.70	115.23
12	aA	838	CLA	CHC-C1C-C2C	-2.58	119.62	126.95
12	bA	838	CLA	CHC-C1C-C2C	-2.58	119.62	126.95
13	bA	844	1L3	C22-C21-C20	-2.58	117.01	123.63
12	aB	906	CLA	CHC-C1C-C2C	-2.58	119.62	126.95
13	aA	845	1L3	C22-C21-C20	-2.58	117.01	123.63
12	cA	825	CLA	CHA-C1A-NA	-2.58	120.56	126.39
12	bB	907	CLA	CHD-C4C-NC	2.58	128.23	124.23
12	cA	838	CLA	CHC-C1C-C2C	-2.58	119.62	126.95
12	aA	808	CLA	CHD-C4C-NC	2.58	128.23	124.23
12	aA	821	CLA	O2A-CGA-CBA	2.58	119.69	111.83
12	aB	927	CLA	CMB-C2B-C3B	2.58	132.61	126.55
12	cA	832	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
12	aA	808	CLA	C1-C2-C3	-2.58	121.98	126.20
12	cA	842	CLA	CAC-C3C-C4C	2.58	128.14	124.79
12	cB	912	CLA	C4A-NA-C1A	-2.58	105.50	106.68
12	cB	938	CLA	CHD-C4C-NC	2.58	128.22	124.23
12	aA	838	CLA	CMC-C2C-C1C	2.57	129.06	125.03
12	bA	825	CLA	CAC-C3C-C4C	2.57	128.14	124.79
15	aF	204	BCR	C7-C8-C9	-2.57	122.43	126.23
15	cA	849	BCR	C11-C10-C9	-2.57	123.67	127.28
12	cA	821	CLA	O2A-CGA-CBA	2.57	119.67	111.83
12	bA	814	CLA	CHD-C4C-NC	2.57	128.22	124.23
12	cF	202	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
15	bB	946	BCR	C29-C30-C25	2.57	114.17	110.44
12	aA	825	CLA	CAC-C3C-C4C	2.57	128.13	124.79
12	aA	842	CLA	CAC-C3C-C4C	2.57	128.13	124.79
12	aB	934	CLA	CHD-C4C-NC	2.57	128.22	124.23
12	aB	938	CLA	CHD-C4C-NC	2.57	128.21	124.23
12	bB	906	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
12	aB	928	CLA	C1-C2-C3	-2.57	122.61	126.76
12	bB	928	CLA	CMA-C3A-C4A	-2.57	104.88	111.77
12	cA	825	CLA	CAC-C3C-C4C	2.57	128.13	124.79
12	bA	803	CLA	O2A-CGA-CBA	2.56	119.65	111.83
12	bB	920	CLA	C4C-C3C-C2C	-2.56	103.16	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aF	202	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
12	bL	202	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
15	bM	101	BCR	C7-C8-C9	-2.56	122.44	126.23
15	aB	943	BCR	C27-C26-C25	2.56	126.17	122.70
12	bB	919	CLA	C3B-C4B-NB	2.56	112.82	110.53
12	cA	836	CLA	C4A-NA-C1A	-2.56	105.51	106.68
12	bB	938	CLA	CHD-C4C-NC	2.56	128.20	124.23
15	bF	204	BCR	C7-C8-C9	-2.56	122.44	126.23
12	bA	826	CLA	CHD-C4C-NC	2.56	128.20	124.23
12	aB	919	CLA	O1D-CGD-CBD	-2.56	119.47	124.52
12	cB	908	CLA	C3B-C2B-C1B	-2.56	104.15	107.17
12	cA	838	CLA	CMC-C2C-C1C	2.56	129.03	125.03
12	aB	906	CLA	CHD-C4C-NC	2.56	128.20	124.23
12	bA	834	CLA	C3B-C4B-NB	2.56	112.81	110.53
12	cA	839	CLA	C4A-NA-C1A	-2.56	105.51	106.68
12	aA	803	CLA	CAC-C3C-C4C	2.56	128.12	124.79
12	aB	930	CLA	CHD-C4C-NC	2.56	128.19	124.23
12	bB	905	CLA	C4B-C3B-C2B	-2.56	104.12	107.30
11	cA	801	CL0	C1C-CHC-C4B	2.56	125.21	116.07
12	bF	202	CLA	CMB-C2B-C1B	2.56	129.31	125.42
12	aB	909	CLA	CAA-C2A-C3A	-2.55	106.10	113.00
12	cL	202	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
12	aA	803	CLA	O2A-CGA-CBA	2.55	119.62	111.83
15	cB	943	BCR	C27-C26-C25	2.55	126.16	122.70
12	cB	909	CLA	CAA-C2A-C3A	-2.55	106.10	113.00
12	aA	839	CLA	C4A-NA-C1A	-2.55	105.51	106.68
12	aA	804	CLA	CHD-C4C-NC	2.55	128.19	124.23
12	cB	906	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
12	bB	909	CLA	CAA-C2A-C3A	-2.55	106.10	113.00
12	cA	809	CLA	C3B-C4B-NB	2.55	112.81	110.53
12	aB	928	CLA	CMA-C3A-C4A	-2.55	104.92	111.77
12	bA	808	CLA	CED-O2D-CGD	2.55	121.70	115.92
12	bB	924	CLA	O1D-CGD-CBD	-2.55	119.49	124.52
12	bA	821	CLA	O2A-CGA-CBA	2.55	119.61	111.83
12	bB	928	CLA	C1-C2-C3	-2.55	122.64	126.76
12	cB	929	CLA	O1D-CGD-CBD	-2.55	119.49	124.52
12	cA	819	CLA	CBC-CAC-C3C	-2.55	105.51	112.42
12	bA	843	CLA	CHD-C4C-NC	2.55	128.19	124.23
12	cA	803	CLA	O2A-CGA-CBA	2.55	119.61	111.83
12	cB	926	CLA	CHB-C4A-NA	2.55	128.08	124.40
12	bB	925	CLA	CHC-C1C-C2C	-2.55	119.70	126.95
12	cB	927	CLA	CMB-C2B-C3B	2.55	132.55	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cB	932	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
12	cA	830	CLA	CMB-C2B-C3B	2.55	132.54	126.55
12	cA	836	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
15	cL	201	BCR	C27-C26-C25	2.55	126.15	122.70
12	bA	829	CLA	CHD-C4C-NC	2.55	128.18	124.23
15	cB	946	BCR	C29-C30-C25	2.55	114.14	110.44
12	cB	920	CLA	C4C-C3C-C2C	-2.55	103.18	106.89
12	aB	923	CLA	O2A-CGA-O1A	-2.55	117.26	123.63
12	bB	923	CLA	O2A-CGA-O1A	-2.55	117.26	123.63
12	bA	843	CLA	C11-C12-C13	-2.55	107.50	115.97
12	aB	919	CLA	C3B-C4B-NB	2.55	112.80	110.53
12	bB	927	CLA	CMB-C2B-C3B	2.55	132.54	126.55
12	bA	825	CLA	CHC-C1C-C2C	-2.55	119.71	126.95
12	cA	806	CLA	O2A-CGA-CBA	2.55	119.60	111.83
12	cA	829	CLA	CHD-C4C-NC	2.55	128.18	124.23
15	aB	946	BCR	C29-C30-C25	2.55	114.14	110.44
12	cA	825	CLA	CHC-C1C-C2C	-2.55	119.71	126.95
11	aA	801	CL0	C1C-CHC-C4B	2.55	125.18	116.07
12	aB	925	CLA	CHC-C1C-C2C	-2.55	119.72	126.95
12	cA	843	CLA	C11-C12-C13	-2.54	107.51	115.97
12	bA	832	CLA	CHD-C4C-NC	2.54	128.18	124.23
12	aA	832	CLA	CHD-C4C-NC	2.54	128.18	124.23
12	cB	929	CLA	CBB-CAB-C3B	-2.54	114.82	127.53
12	cB	928	CLA	CMA-C3A-C4A	-2.54	104.94	111.77
12	aA	843	CLA	C11-C12-C13	-2.54	107.51	115.97
12	bA	821	CLA	CED-O2D-CGD	2.54	121.68	115.92
12	aA	809	CLA	C3B-C4B-NB	2.54	112.80	110.53
12	bA	819	CLA	CBC-CAC-C3C	-2.54	105.53	112.42
12	aA	811	CLA	CAC-C3C-C4C	2.54	128.10	124.79
12	aB	929	CLA	CBB-CAB-C3B	-2.54	114.82	127.53
12	bA	822	CLA	CMC-C2C-C1C	2.54	129.01	125.03
12	cA	838	CLA	C4-C3-C5	2.54	119.64	115.23
12	cB	925	CLA	CHC-C1C-C2C	-2.54	119.72	126.95
11	bA	801	CL0	C1C-CHC-C4B	2.54	125.17	116.07
12	cA	808	CLA	CED-O2D-CGD	2.54	121.68	115.92
15	bB	943	BCR	C27-C26-C25	2.54	126.14	122.70
12	aB	924	CLA	O1D-CGD-CBD	-2.54	119.50	124.52
12	cB	924	CLA	O1D-CGD-CBD	-2.54	119.50	124.52
12	aL	202	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
12	bB	929	CLA	O1D-CGD-CBD	-2.54	119.51	124.52
12	cL	202	CLA	CAC-C3C-C4C	2.54	128.10	124.79
12	aB	920	CLA	C4C-C3C-C2C	-2.54	103.19	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bB	904	CLA	CHD-C4C-NC	2.54	128.17	124.23
12	cA	843	CLA	CHD-C4C-NC	2.54	128.17	124.23
12	aA	825	CLA	CHC-C1C-C2C	-2.54	119.73	126.95
12	aB	929	CLA	O1D-CGD-CBD	-2.54	119.51	124.52
12	aA	838	CLA	C4-C3-C5	2.54	119.64	115.23
12	cB	930	CLA	CHD-C4C-NC	2.54	128.17	124.23
15	aL	201	BCR	C27-C26-C25	2.54	126.14	122.70
12	aL	202	CLA	CAC-C3C-C4C	2.54	128.09	124.79
12	bB	918	CLA	CED-O2D-CGD	2.54	121.67	115.92
12	aF	202	CLA	CMB-C2B-C1B	2.54	129.28	125.42
12	bA	838	CLA	CBC-CAC-C3C	-2.54	105.54	112.42
12	aA	844	CLA	C4A-NA-C1A	-2.54	105.52	106.68
12	bB	938	CLA	C4A-NA-C1A	-2.54	105.52	106.68
12	aB	918	CLA	CED-O2D-CGD	2.54	121.67	115.92
12	cB	918	CLA	CED-O2D-CGD	2.54	121.67	115.92
12	cB	928	CLA	C1-C2-C3	-2.54	122.66	126.76
12	bA	806	CLA	O2A-CGA-CBA	2.54	119.57	111.83
12	aA	819	CLA	CBC-CAC-C3C	-2.54	105.54	112.42
12	aA	806	CLA	O2A-CGA-CBA	2.54	119.57	111.83
12	cA	832	CLA	CHD-C4C-NC	2.54	128.16	124.23
12	aA	809	CLA	C4B-C3B-C2B	-2.54	104.15	107.30
15	cF	201	BCR	C27-C26-C25	2.54	126.13	122.70
12	bB	929	CLA	CBB-CAB-C3B	-2.54	114.86	127.53
12	aB	907	CLA	O1D-CGD-CBD	-2.54	119.52	124.52
12	aB	930	CLA	CHB-C4A-NA	2.53	128.06	124.40
12	cB	919	CLA	O1D-CGD-CBD	-2.53	119.52	124.52
12	bA	804	CLA	CHD-C4C-NC	2.53	128.16	124.23
12	bA	811	CLA	CAC-C3C-C4C	2.53	128.09	124.79
12	bB	930	CLA	CHD-C4C-NC	2.53	128.16	124.23
12	cB	904	CLA	CHD-C4C-NC	2.53	128.16	124.23
12	bB	932	CLA	CBC-CAC-C3C	-2.53	105.56	112.42
12	bA	809	CLA	O1D-CGD-CBD	-2.53	119.53	124.52
12	aA	821	CLA	CED-O2D-CGD	2.53	121.66	115.92
12	bB	933	CLA	CMB-C2B-C1B	2.53	129.27	125.42
12	cA	811	CLA	CAC-C3C-C4C	2.53	128.08	124.79
12	aB	934	CLA	CHB-C1B-C2B	-2.53	120.08	127.43
12	aA	830	CLA	CMB-C2B-C3B	2.53	132.50	126.55
15	cA	847	BCR	C11-C10-C9	-2.53	123.73	127.28
12	bB	904	CLA	CBC-CAC-C3C	-2.53	105.56	112.42
12	bB	930	CLA	CHB-C4A-NA	2.53	128.05	124.40
11	bA	801	CL0	C1-O2A-CGA	2.53	122.77	116.65
12	aB	932	CLA	CBC-CAC-C3C	-2.53	105.56	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	809	CLA	O1D-CGD-CBD	-2.53	119.53	124.52
11	aA	801	CL0	C1-O2A-CGA	2.53	122.77	116.65
12	cA	826	CLA	CAC-C3C-C4C	2.53	128.08	124.79
12	aA	830	CLA	O2A-CGA-CBA	2.53	119.54	111.83
15	cM	101	BCR	C7-C8-C9	-2.53	122.50	126.23
12	cA	838	CLA	CBC-CAC-C3C	-2.53	105.57	112.42
12	cA	805	CLA	CHC-C1C-C2C	-2.53	119.77	126.95
12	cA	809	CLA	C4B-C3B-C2B	-2.53	104.16	107.30
12	bB	919	CLA	O1D-CGD-CBD	-2.53	119.54	124.52
12	bA	842	CLA	CAC-C3C-C4C	2.53	128.08	124.79
12	cA	819	CLA	CHB-C1B-C2B	-2.53	120.09	127.43
12	bA	830	CLA	CMB-C2B-C3B	2.53	132.49	126.55
12	cB	923	CLA	O2A-CGA-O1A	-2.53	117.31	123.63
15	aA	848	BCR	C11-C10-C9	-2.52	123.74	127.28
12	aA	819	CLA	CHB-C1B-C2B	-2.52	120.10	127.43
12	cA	809	CLA	O1D-CGD-CBD	-2.52	119.54	124.52
12	aA	830	CLA	CAA-C2A-C3A	-2.52	106.18	113.00
15	aM	101	BCR	C7-C8-C9	-2.52	122.50	126.23
12	aA	838	CLA	CBC-CAC-C3C	-2.52	105.58	112.42
12	aB	904	CLA	CBC-CAC-C3C	-2.52	105.58	112.42
15	aF	201	BCR	C27-C26-C25	2.52	126.11	122.70
12	bA	809	CLA	C4B-C3B-C2B	-2.52	104.17	107.30
12	cB	907	CLA	O1D-CGD-CBD	-2.52	119.54	124.52
12	bA	839	CLA	CMB-C2B-C1B	2.52	129.26	125.42
12	cB	934	CLA	CHB-C1B-C2B	-2.52	120.11	127.43
12	cB	904	CLA	CBC-CAC-C3C	-2.52	105.59	112.42
11	cA	801	CL0	C1-O2A-CGA	2.52	122.75	116.65
12	bA	819	CLA	CHB-C1B-C2B	-2.52	120.11	127.43
12	aA	815	CLA	CMB-C2B-C1B	2.52	129.26	125.42
12	bA	826	CLA	CAC-C3C-C4C	2.52	128.07	124.79
12	aB	906	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
12	aB	926	CLA	CHB-C4A-NA	2.52	128.03	124.40
12	bA	805	CLA	CHC-C1C-C2C	-2.52	119.79	126.95
12	aB	927	CLA	CMA-C3A-C2A	-2.52	104.25	113.98
12	bA	830	CLA	CAA-C2A-C3A	-2.52	106.20	113.00
12	cA	830	CLA	CAA-C2A-C3A	-2.52	106.20	113.00
12	aA	808	CLA	CED-O2D-CGD	2.52	121.63	115.92
12	cB	932	CLA	CBC-CAC-C3C	-2.52	105.60	112.42
12	aB	932	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
12	bA	839	CLA	C4A-NA-C1A	-2.52	105.53	106.68
12	bA	827	CLA	C4B-C3B-C2B	-2.52	104.17	107.30
12	bB	907	CLA	O1D-CGD-CBD	-2.52	119.56	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	840	CLA	CED-O2D-CGD	2.51	121.62	115.92
12	aL	203	CLA	CHC-C1C-C2C	-2.51	119.80	126.95
12	cF	202	CLA	CMB-C2B-C1B	2.51	129.25	125.42
12	cB	901	CLA	CAC-C3C-C4C	2.51	128.06	124.79
12	aB	908	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
15	bF	201	BCR	C27-C26-C25	2.51	126.10	122.70
12	cA	821	CLA	CED-O2D-CGD	2.51	121.62	115.92
12	aA	843	CLA	CHD-C4C-NC	2.51	128.13	124.23
12	aA	834	CLA	CMA-C3A-C2A	-2.51	104.27	113.98
12	cA	804	CLA	CHD-C4C-NC	2.51	128.13	124.23
12	bA	840	CLA	CED-O2D-CGD	2.51	121.61	115.92
12	bA	836	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
12	cL	203	CLA	CHC-C1C-C2C	-2.51	119.81	126.95
12	cF	202	CLA	CHD-C4C-NC	2.51	128.12	124.23
12	bA	809	CLA	CMB-C2B-C1B	2.51	129.24	125.42
12	aA	805	CLA	CHC-C1C-C2C	-2.51	119.81	126.95
12	aB	908	CLA	O2A-CGA-CBA	2.51	119.49	111.83
12	cA	830	CLA	O2A-CGA-CBA	2.51	119.49	111.83
12	bL	203	CLA	CHC-C1C-C2C	-2.51	119.81	126.95
15	aA	848	BCR	C16-C15-C14	-2.51	118.38	123.52
12	bA	833	CLA	CAA-C2A-C3A	-2.51	106.22	113.00
12	cA	809	CLA	CMB-C2B-C1B	2.51	129.24	125.42
12	bB	914	CLA	CHC-C1C-C2C	-2.51	119.81	126.95
12	cB	904	CLA	CMB-C2B-C3B	2.51	132.45	126.55
12	aA	836	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
15	bA	847	BCR	C16-C15-C14	-2.51	118.38	123.52
12	aB	914	CLA	CHC-C1C-C2C	-2.51	119.82	126.95
12	bL	202	CLA	CAC-C3C-C4C	2.51	128.05	124.79
12	aB	904	CLA	CMB-C2B-C3B	2.51	132.45	126.55
12	aA	854	CLA	O2A-CGA-O1A	-2.51	117.35	123.63
12	cB	908	CLA	O2A-CGA-CBA	2.51	119.48	111.83
15	bA	847	BCR	C11-C10-C9	-2.51	123.76	127.28
12	aA	826	CLA	CAC-C3C-C4C	2.51	128.05	124.79
12	aB	923	CLA	CHC-C1C-C2C	-2.51	119.82	126.95
12	cA	840	CLA	CED-O2D-CGD	2.51	121.60	115.92
12	cA	808	CLA	CBC-CAC-C3C	-2.51	105.63	112.42
12	cB	914	CLA	CHC-C1C-C2C	-2.50	119.83	126.95
12	bB	908	CLA	O2A-CGA-CBA	2.50	119.47	111.83
12	aA	809	CLA	O2D-CGD-O1D	-2.50	118.97	123.85
15	cA	847	BCR	C16-C15-C14	-2.50	118.40	123.52
12	aF	202	CLA	O1D-CGD-CBD	-2.50	119.58	124.52
11	aA	801	CL0	CMC-C2C-C1C	2.50	129.24	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bB	932	CLA	O2D-CGD-O1D	-2.50	118.97	123.85
12	bA	809	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
12	aB	933	CLA	CMB-C2B-C1B	2.50	129.23	125.42
12	cA	843	CLA	CBC-CAC-C3C	-2.50	105.64	112.42
12	bB	934	CLA	CHB-C1B-C2B	-2.50	120.16	127.43
12	cA	834	CLA	CMA-C3A-C2A	-2.50	104.31	113.98
12	cA	822	CLA	CMC-C2C-C1C	2.50	128.94	125.03
12	bA	838	CLA	C4-C3-C5	2.50	119.57	115.23
11	bA	801	CL0	CMC-C2C-C1C	2.50	129.24	124.73
12	cB	925	CLA	CMC-C2C-C1C	2.50	128.94	125.03
12	cB	908	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
12	bA	809	CLA	C3B-C4B-NB	2.50	112.76	110.53
12	bA	803	CLA	CAC-C3C-C4C	2.50	128.04	124.79
12	aB	938	CLA	C4A-NA-C1A	-2.50	105.54	106.68
12	bA	815	CLA	CMB-C2B-C1B	2.50	129.23	125.42
12	cA	853	CLA	O2A-CGA-O1A	-2.50	117.37	123.63
12	cA	827	CLA	C4B-C3B-C2B	-2.50	104.19	107.30
12	bB	927	CLA	CMA-C3A-C2A	-2.50	104.32	113.98
12	cB	927	CLA	CMA-C3A-C2A	-2.50	104.32	113.98
12	bA	816	CLA	CHD-C4C-NC	2.50	128.11	124.23
12	aA	824	CLA	O2A-CGA-CBA	2.50	119.45	111.83
12	aB	907	CLA	C4-C3-C5	2.50	119.56	115.23
12	bA	830	CLA	O2A-CGA-CBA	2.50	119.45	111.83
12	cA	834	CLA	CHD-C4C-NC	2.50	128.10	124.23
12	bA	834	CLA	CMA-C3A-C2A	-2.50	104.33	113.98
12	aA	843	CLA	CBC-CAC-C3C	-2.50	105.65	112.42
12	aB	913	CLA	CBC-CAC-C3C	-2.50	105.65	112.42
12	bA	808	CLA	CBC-CAC-C3C	-2.50	105.65	112.42
12	bA	843	CLA	CBC-CAC-C3C	-2.50	105.65	112.42
12	bB	913	CLA	CBC-CAC-C3C	-2.50	105.65	112.42
12	cB	912	CLA	O2A-CGA-O1A	-2.50	117.39	123.63
12	cA	809	CLA	CAC-C3C-C4C	2.50	128.04	124.79
12	aA	822	CLA	CMC-C2C-C1C	2.50	128.93	125.03
12	cA	839	CLA	CMB-C2B-C1B	2.50	129.22	125.42
12	cF	202	CLA	O1D-CGD-CBD	-2.50	119.60	124.52
12	bB	908	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
12	bB	923	CLA	CHC-C1C-C2C	-2.50	119.86	126.95
12	bA	834	CLA	CHD-C4C-NC	2.50	128.10	124.23
12	bA	853	CLA	O2A-CGA-O1A	-2.50	117.39	123.63
12	cB	923	CLA	CHC-C1C-C2C	-2.49	119.86	126.95
12	bB	935	CLA	C5-C3-C4	2.49	120.33	114.59
12	cB	938	CLA	CHB-C4A-NA	2.49	128.00	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	833	CLA	O2A-CGA-CBA	2.49	119.44	111.83
12	bB	904	CLA	CMB-C2B-C3B	2.49	132.42	126.55
12	aA	827	CLA	C4B-C3B-C2B	-2.49	104.20	107.30
12	cB	933	CLA	CMC-C2C-C1C	2.49	128.93	125.03
12	cA	816	CLA	CHD-C4C-NC	2.49	128.10	124.23
12	aA	823	CLA	CMA-C3A-C2A	-2.49	104.35	113.98
12	bA	833	CLA	O2A-CGA-CBA	2.49	119.43	111.83
12	bF	202	CLA	O1D-CGD-CBD	-2.49	119.60	124.52
12	cB	928	CLA	CMD-C2D-C3D	-2.49	121.97	127.69
12	bA	824	CLA	O2A-CGA-CBA	2.49	119.43	111.83
12	aB	928	CLA	CMD-C2D-C3D	-2.49	121.98	127.69
12	bB	931	CLA	CMC-C2C-C1C	2.49	128.93	125.03
12	bA	817	CLA	C4-C3-C5	2.49	119.55	115.23
12	aB	901	CLA	CAC-C3C-C4C	2.49	128.03	124.79
12	bB	928	CLA	CMD-C2D-C3D	-2.49	121.98	127.69
12	aB	950	CLA	C4A-NA-C1A	-2.49	105.54	106.68
12	aA	816	CLA	CHD-C4C-NC	2.49	128.09	124.23
12	aA	823	CLA	CAA-C2A-C3A	-2.49	106.27	113.00
12	aB	938	CLA	CHB-C4A-NA	2.49	127.99	124.40
12	aA	833	CLA	CAA-C2A-C3A	-2.49	106.27	113.00
12	aB	933	CLA	CMC-C2C-C1C	2.49	128.92	125.03
12	bF	202	CLA	CHD-C4C-NC	2.49	128.09	124.23
12	aB	931	CLA	CHC-C1C-C2C	-2.49	119.87	126.95
12	bB	930	CLA	CAC-C3C-C4C	2.49	128.03	124.79
12	cB	930	CLA	CAC-C3C-C4C	2.49	128.03	124.79
15	aB	946	BCR	C2-C1-C6	2.49	114.05	110.44
11	cA	801	CL0	CMC-C2C-C1C	2.49	129.21	124.73
12	aB	926	CLA	O1D-CGD-CBD	-2.49	119.61	124.52
12	cA	824	CLA	O2A-CGA-CBA	2.49	119.42	111.83
12	aA	823	CLA	CBC-CAC-C3C	-2.49	105.68	112.42
12	cA	838	CLA	CAC-C3C-C4C	2.49	128.03	124.79
12	bB	925	CLA	CMC-C2C-C1C	2.49	128.92	125.03
12	aB	937	CLA	C4B-C3B-C2B	-2.49	104.21	107.30
12	aB	921	CLA	CMC-C2C-C1C	2.49	128.92	125.03
12	bB	907	CLA	C4-C3-C5	2.49	119.54	115.23
12	cA	803	CLA	CAC-C3C-C4C	2.49	128.02	124.79
12	aA	817	CLA	C4-C3-C2	-2.49	117.24	123.63
12	aB	935	CLA	C5-C3-C4	2.49	120.31	114.59
12	cA	817	CLA	C4-C3-C2	-2.48	117.25	123.63
12	bB	937	CLA	C4B-C3B-C2B	-2.48	104.21	107.30
12	aB	931	CLA	CMC-C2C-C1C	2.48	128.92	125.03
12	bB	901	CLA	C4-C3-C5	2.48	119.54	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	823	CLA	CAA-C2A-C3A	-2.48	106.29	113.00
12	aB	923	CLA	C4B-C3B-C2B	-2.48	104.21	107.30
12	bB	921	CLA	CMC-C2C-C1C	2.48	128.91	125.03
12	cA	833	CLA	CAA-C2A-C3A	-2.48	106.29	113.00
12	bB	901	CLA	CAC-C3C-C4C	2.48	128.02	124.79
12	cA	823	CLA	CAA-C2A-C3A	-2.48	106.29	113.00
12	aA	809	CLA	CMB-C2B-C1B	2.48	129.20	125.42
12	bB	933	CLA	CMC-C2C-C1C	2.48	128.91	125.03
12	aA	808	CLA	CBC-CAC-C3C	-2.48	105.69	112.42
12	aB	925	CLA	CMC-C2C-C1C	2.48	128.91	125.03
12	bA	840	CLA	CHD-C4C-NC	2.48	128.08	124.23
12	cA	809	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
12	aA	839	CLA	CMB-C2B-C1B	2.48	129.19	125.42
15	aI	101	BCR	C38-C26-C27	-2.48	108.31	113.60
12	cB	913	CLA	CBC-CAC-C3C	-2.48	105.70	112.42
12	bA	823	CLA	C1-C2-C3	-2.48	122.14	126.20
12	bA	817	CLA	C4-C3-C2	-2.48	117.26	123.63
12	aA	834	CLA	CHD-C4C-NC	2.48	128.07	124.23
12	cB	933	CLA	CMB-C2B-C1B	2.48	129.19	125.42
15	cF	203	BCR	C30-C25-C26	-2.48	119.25	122.64
12	bB	931	CLA	CHC-C1C-C2C	-2.48	119.91	126.95
12	aA	837	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
12	aA	817	CLA	C4-C3-C5	2.48	119.53	115.23
12	cA	833	CLA	O2A-CGA-CBA	2.48	119.39	111.83
12	cB	935	CLA	C5-C3-C4	2.48	120.29	114.59
15	cI	101	BCR	C38-C26-C27	-2.48	108.32	113.60
15	bB	946	BCR	C2-C1-C6	2.48	114.04	110.44
15	cL	206	BCR	C27-C26-C25	2.48	126.05	122.70
12	cB	907	CLA	C4-C3-C5	2.48	119.53	115.23
12	bA	804	CLA	CHB-C4A-NA	2.48	127.97	124.40
12	bB	902	CLA	CHC-C1C-NC	2.48	128.04	124.31
12	aA	831	CLA	CAC-C3C-C4C	2.48	128.01	124.79
12	cB	910	CLA	CED-O2D-CGD	2.48	121.53	115.92
12	cA	823	CLA	CMA-C3A-C2A	-2.48	104.41	113.98
12	cB	902	CLA	CHC-C1C-NC	2.48	128.04	124.31
12	cA	815	CLA	CMB-C2B-C1B	2.47	129.19	125.42
12	aA	809	CLA	CAC-C3C-C4C	2.47	128.01	124.79
12	bA	831	CLA	CAC-C3C-C4C	2.47	128.01	124.79
15	aL	206	BCR	C2-C1-C6	2.47	114.03	110.44
15	cB	944	BCR	C30-C25-C26	-2.47	119.26	122.64
12	aA	840	CLA	CHD-C4C-NC	2.47	128.07	124.23
12	aB	912	CLA	O2A-CGA-O1A	-2.47	117.44	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	837	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
15	aF	203	BCR	C30-C25-C26	-2.47	119.26	122.64
12	cA	833	CLA	CHB-C4A-NA	2.47	127.97	124.40
15	cB	946	BCR	C2-C1-C6	2.47	114.03	110.44
12	cB	931	CLA	CHC-C1C-C2C	-2.47	119.92	126.95
12	bA	838	CLA	CAC-C3C-C4C	2.47	128.00	124.79
12	cB	930	CLA	CHB-C4A-NA	2.47	127.97	124.40
12	cB	901	CLA	C4-C3-C5	2.47	119.52	115.23
12	bB	926	CLA	O1D-CGD-CBD	-2.47	119.64	124.52
12	bB	912	CLA	O2A-CGA-O1A	-2.47	117.45	123.63
12	cB	931	CLA	CMC-C2C-C1C	2.47	128.89	125.03
12	cB	935	CLA	O2A-CGA-O1A	-2.47	117.45	123.63
12	cB	923	CLA	C4B-C3B-C2B	-2.47	104.23	107.30
12	cA	817	CLA	C4-C3-C5	2.47	119.51	115.23
12	cA	823	CLA	CBC-CAC-C3C	-2.47	105.73	112.42
15	cA	847	BCR	C31-C1-C6	2.47	114.11	110.24
12	cA	834	CLA	O1D-CGD-CBD	-2.47	119.65	124.52
12	bB	916	CLA	CHC-C1C-C2C	-2.47	119.94	126.95
12	cA	837	CLA	CMB-C2B-C3B	2.47	132.35	126.55
12	aF	202	CLA	CHD-C4C-NC	2.47	128.06	124.23
12	bB	938	CLA	C1-C2-C3	-2.47	122.16	126.20
12	bA	834	CLA	O1D-CGD-CBD	-2.47	119.66	124.52
12	bB	926	CLA	CHB-C4A-NA	2.47	127.96	124.40
12	aB	935	CLA	O2A-CGA-O1A	-2.47	117.46	123.63
12	aA	833	CLA	CHB-C4A-NA	2.46	127.96	124.40
12	bA	809	CLA	CAC-C3C-C4C	2.46	128.00	124.79
15	bI	101	BCR	C38-C26-C27	-2.46	108.34	113.60
12	bA	839	CLA	CAA-C2A-C3A	-2.46	106.34	113.00
12	bB	911	CLA	CHD-C4C-NC	2.46	128.05	124.23
12	aA	832	CLA	CBC-CAC-C3C	-2.46	105.74	112.42
12	bA	823	CLA	CBC-CAC-C3C	-2.46	105.74	112.42
15	cA	848	BCR	C24-C23-C22	-2.46	122.59	126.23
12	bA	837	CLA	O2D-CGD-O1D	-2.46	119.05	123.85
15	cF	204	BCR	C15-C14-C13	-2.46	123.83	127.28
12	aB	911	CLA	CHD-C4C-NC	2.46	128.05	124.23
12	bA	823	CLA	CMA-C3A-C2A	-2.46	104.46	113.98
12	cA	832	CLA	CBC-CAC-C3C	-2.46	105.75	112.42
12	cB	919	CLA	C4B-C3B-C2B	-2.46	104.24	107.30
12	bB	915	CLA	CMB-C2B-C1B	2.46	129.17	125.42
12	bB	938	CLA	CHB-C4A-NA	2.46	127.95	124.40
12	bB	910	CLA	CED-O2D-CGD	2.46	121.50	115.92
12	cB	938	CLA	C1-C2-C3	-2.46	122.17	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bB	935	CLA	O2A-CGA-O1A	-2.46	117.48	123.63
12	cB	916	CLA	CHC-C1C-C2C	-2.46	119.96	126.95
15	aL	206	BCR	C27-C26-C25	2.46	126.03	122.70
12	bA	837	CLA	CMB-C2B-C3B	2.46	132.33	126.55
12	aA	823	CLA	C1-C2-C3	-2.46	122.17	126.20
12	aB	938	CLA	C1-C2-C3	-2.46	122.17	126.20
12	cA	839	CLA	CAA-C2A-C3A	-2.46	106.35	113.00
12	bA	825	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
15	bL	206	BCR	C27-C26-C25	2.46	126.03	122.70
12	aA	802	CLA	CMC-C2C-C1C	2.46	128.88	125.03
12	bB	908	CLA	C4C-C3C-C2C	-2.46	103.31	106.89
12	cA	807	CLA	O2A-CGA-O1A	-2.46	117.48	123.63
12	aB	930	CLA	CAC-C3C-C4C	2.46	127.99	124.79
15	aB	944	BCR	C30-C25-C26	-2.46	119.28	122.64
12	aB	916	CLA	CHC-C1C-C2C	-2.46	119.97	126.95
12	cB	926	CLA	O1D-CGD-CBD	-2.46	119.67	124.52
12	bA	819	CLA	C4-C3-C5	2.46	119.49	115.23
12	aB	902	CLA	CHC-C1C-NC	2.46	128.01	124.31
12	bA	833	CLA	CHB-C4A-NA	2.46	127.94	124.40
12	cA	825	CLA	O2D-CGD-O1D	-2.46	119.07	123.85
15	bF	203	BCR	C30-C25-C26	-2.46	119.28	122.64
12	cA	842	CLA	O2D-CGD-O1D	-2.46	119.07	123.85
12	bB	923	CLA	C4B-C3B-C2B	-2.46	104.25	107.30
12	aB	912	CLA	CHB-C4A-NA	2.45	127.94	124.40
12	bB	919	CLA	C4B-C3B-C2B	-2.45	104.25	107.30
12	aB	925	CLA	C3B-C4B-NB	2.45	112.72	110.53
12	aB	908	CLA	C4C-C3C-C2C	-2.45	103.32	106.89
12	bA	808	CLA	CMB-C2B-C1B	2.45	129.16	125.42
12	bA	807	CLA	O2A-CGA-O1A	-2.45	117.49	123.63
12	bA	811	CLA	O2D-CGD-O1D	-2.45	119.07	123.85
12	bA	842	CLA	O2D-CGD-O1D	-2.45	119.07	123.85
12	cA	811	CLA	O2D-CGD-O1D	-2.45	119.07	123.85
12	bA	832	CLA	CBC-CAC-C3C	-2.45	105.77	112.42
12	aB	928	CLA	CMC-C2C-C1C	2.45	128.87	125.03
12	aA	825	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
12	aA	839	CLA	CAA-C2A-C3A	-2.45	106.37	113.00
12	cB	912	CLA	CHB-C4A-NA	2.45	127.94	124.40
12	bB	928	CLA	CMC-C2C-C1C	2.45	128.86	125.03
15	bM	101	BCR	C33-C5-C6	-2.45	121.81	124.48
12	aA	811	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
12	cA	840	CLA	CHD-C4C-NC	2.45	128.03	124.23
12	cA	819	CLA	C4-C3-C5	2.45	119.48	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bA	847	BCR	C31-C1-C6	2.45	114.08	110.24
12	aA	834	CLA	O1D-CGD-CBD	-2.45	119.69	124.52
12	aB	915	CLA	CMB-C2B-C1B	2.45	129.15	125.42
12	cB	937	CLA	C4B-C3B-C2B	-2.45	104.26	107.30
12	aB	931	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
12	cB	915	CLA	CMB-C2B-C1B	2.45	129.15	125.42
12	cA	802	CLA	CMC-C2C-C1C	2.45	128.86	125.03
12	cA	817	CLA	CAC-C3C-C4C	2.45	127.98	124.79
15	aA	849	BCR	C24-C23-C22	-2.45	122.61	126.23
12	aB	934	CLA	CAC-C3C-C4C	2.45	127.97	124.79
12	cB	905	CLA	CHC-C1C-C2C	-2.45	119.99	126.95
12	cB	921	CLA	CMC-C2C-C1C	2.45	128.86	125.03
12	aA	804	CLA	CHB-C4A-NA	2.45	127.93	124.40
12	cB	934	CLA	CAC-C3C-C4C	2.45	127.97	124.79
12	aB	901	CLA	C4-C3-C5	2.45	119.48	115.23
12	bA	825	CLA	C1-C2-C3	-2.45	122.19	126.20
12	aA	817	CLA	CAC-C3C-C4C	2.45	127.97	124.79
11	bA	801	CL0	O2D-CGD-O1D	-2.45	119.09	123.85
15	cB	946	BCR	C10-C11-C12	-2.45	116.11	123.20
12	cA	831	CLA	CAC-C3C-C4C	2.45	127.97	124.79
12	bB	909	CLA	CED-O2D-CGD	2.44	121.46	115.92
12	cB	908	CLA	C4C-C3C-C2C	-2.44	103.33	106.89
12	cA	823	CLA	C1-C2-C3	-2.44	122.19	126.20
11	aA	801	CL0	O2D-CGD-O1D	-2.44	119.09	123.85
12	aA	808	CLA	CMB-C2B-C1B	2.44	129.14	125.42
12	bB	906	CLA	CMB-C2B-C1B	2.44	129.14	125.42
12	aA	837	CLA	CMB-C2B-C3B	2.44	132.29	126.55
15	bF	204	BCR	C24-C23-C22	-2.44	122.62	126.23
12	cA	835	CLA	CHD-C4C-NC	2.44	128.02	124.23
15	bA	848	BCR	C24-C23-C22	-2.44	122.62	126.23
12	aA	819	CLA	C4-C3-C5	2.44	119.47	115.23
12	cB	917	CLA	C4C-C3C-C2C	-2.44	103.34	106.89
15	aA	848	BCR	C31-C1-C6	2.44	114.07	110.24
12	cB	928	CLA	CMC-C2C-C1C	2.44	128.85	125.03
15	cB	945	BCR	C29-C30-C25	2.44	113.98	110.44
12	aA	838	CLA	CAC-C3C-C4C	2.44	127.97	124.79
12	cA	821	CLA	CHD-C4C-NC	2.44	128.01	124.23
12	aB	906	CLA	C1-O2A-CGA	2.44	122.56	116.65
12	aA	807	CLA	O2A-CGA-O1A	-2.44	117.53	123.63
12	aA	835	CLA	CED-O2D-CGD	2.44	121.45	115.92
12	aB	910	CLA	CED-O2D-CGD	2.44	121.45	115.92
12	aA	842	CLA	O2D-CGD-O1D	-2.44	119.10	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bB	946	BCR	C10-C11-C12	-2.44	116.14	123.20
12	aA	821	CLA	C3B-C4B-NB	2.44	112.71	110.53
12	aB	919	CLA	C4B-C3B-C2B	-2.44	104.27	107.30
12	cB	906	CLA	C1-O2A-CGA	2.44	122.55	116.65
12	bB	905	CLA	CHC-C1C-C2C	-2.44	120.02	126.95
12	bB	906	CLA	C1-O2A-CGA	2.44	122.55	116.65
12	aB	933	CLA	CBC-CAC-C3C	-2.44	105.82	112.42
12	cA	808	CLA	CMB-C2B-C1B	2.44	129.13	125.42
12	cB	906	CLA	CMB-C2B-C1B	2.44	129.13	125.42
12	aL	203	CLA	CHD-C4C-NC	2.44	128.01	124.23
12	bL	203	CLA	CHD-C4C-NC	2.44	128.01	124.23
12	bA	803	CLA	CHB-C1B-C2B	-2.43	120.36	127.43
12	aB	909	CLA	CED-O2D-CGD	2.43	121.44	115.92
12	aB	905	CLA	CHC-C1C-C2C	-2.43	120.03	126.95
12	aB	911	CLA	O2A-CGA-CBA	2.43	121.69	114.00
15	cL	206	BCR	C2-C1-C6	2.43	113.97	110.44
11	cA	801	CL0	O2D-CGD-O1D	-2.43	119.11	123.85
12	cB	909	CLA	CED-O2D-CGD	2.43	121.44	115.92
12	cA	804	CLA	CHB-C4A-NA	2.43	127.91	124.40
12	aA	825	CLA	C1-C2-C3	-2.43	122.21	126.20
12	bB	912	CLA	CHB-C4A-NA	2.43	127.91	124.40
12	cA	835	CLA	CED-O2D-CGD	2.43	121.43	115.92
12	bB	934	CLA	CAC-C3C-C4C	2.43	127.95	124.79
12	bA	835	CLA	CHD-C4C-NC	2.43	128.00	124.23
12	cL	203	CLA	CHD-C4C-NC	2.43	128.00	124.23
15	aB	946	BCR	C10-C11-C12	-2.43	116.15	123.20
12	aB	917	CLA	C4C-C3C-C2C	-2.43	103.35	106.89
15	bL	206	BCR	C2-C1-C6	2.43	113.97	110.44
12	bA	842	CLA	CMA-C3A-C2A	-2.43	104.58	113.98
12	aA	835	CLA	CHD-C4C-NC	2.43	128.00	124.23
15	bF	204	BCR	C15-C14-C13	-2.43	123.87	127.28
12	aA	842	CLA	CMA-C3A-C2A	-2.43	104.59	113.98
12	aA	814	CLA	CMC-C2C-C1C	2.43	128.83	125.03
12	bA	814	CLA	CMC-C2C-C1C	2.43	128.83	125.03
12	aA	807	CLA	CMB-C2B-C1B	2.43	129.11	125.42
12	bB	917	CLA	C4C-C3C-C2C	-2.43	103.36	106.89
12	bA	808	CLA	CAA-C2A-C3A	-2.43	106.44	113.00
12	aA	821	CLA	CHD-C4C-NC	2.43	127.99	124.23
12	cL	203	CLA	CHB-C4A-NA	2.43	127.90	124.40
12	aA	803	CLA	CHB-C1B-C2B	-2.42	120.39	127.43
15	cF	204	BCR	C24-C23-C22	-2.42	122.65	126.23
12	bB	931	CLA	O2A-CGA-O1A	-2.42	117.56	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	827	CLA	OBD-CAD-C3D	-2.42	122.75	128.42
12	bA	828	CLA	CMA-C3A-C2A	-2.42	104.61	113.98
12	cA	821	CLA	C3B-C4B-NB	2.42	112.69	110.53
12	bA	802	CLA	CMC-C2C-C1C	2.42	128.82	125.03
12	cB	916	CLA	C4-C3-C5	2.42	119.44	115.23
12	cB	935	CLA	CMC-C2C-C1C	2.42	128.82	125.03
12	cB	907	CLA	CHB-C4A-NA	2.42	127.90	124.40
12	aA	808	CLA	CAA-C2A-C3A	-2.42	106.45	113.00
12	bB	907	CLA	C1-C2-C3	-2.42	122.23	126.20
12	cB	911	CLA	O2A-CGA-CBA	2.42	121.65	114.00
12	bA	820	CLA	O1D-CGD-CBD	-2.42	119.74	124.52
12	cA	828	CLA	CMA-C3A-C2A	-2.42	104.62	113.98
15	aF	204	BCR	C15-C14-C13	-2.42	123.88	127.28
12	bB	911	CLA	O2A-CGA-CBA	2.42	121.65	114.00
12	cB	931	CLA	O2A-CGA-O1A	-2.42	117.57	123.63
12	bA	842	CLA	CHB-C4A-NA	2.42	127.89	124.40
12	bA	835	CLA	CED-O2D-CGD	2.42	121.41	115.92
12	cA	842	CLA	CMA-C3A-C2A	-2.42	104.62	113.98
12	cA	825	CLA	C1-C2-C3	-2.42	122.23	126.20
12	cB	926	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
12	bA	821	CLA	C3B-C4B-NB	2.42	112.69	110.53
12	aA	820	CLA	O1D-CGD-CBD	-2.42	119.74	124.52
15	cF	201	BCR	C15-C16-C17	-2.42	118.57	123.52
12	cA	803	CLA	CHB-C1B-C2B	-2.42	120.40	127.43
15	aA	848	BCR	C16-C17-C18	-2.42	123.89	127.28
12	bL	203	CLA	CHB-C4A-NA	2.42	127.89	124.40
12	bB	909	CLA	CMC-C2C-C1C	2.42	128.81	125.03
12	bB	949	CLA	C2A-C1A-NA	2.42	116.14	110.21
12	bA	821	CLA	CHD-C4C-NC	2.42	127.98	124.23
17	cB	947	LMG	C1-C2-C3	-2.42	104.92	110.01
12	aA	828	CLA	CMA-C3A-C2A	-2.42	104.63	113.98
12	bA	836	CLA	CAA-C2A-C3A	-2.42	106.47	113.00
12	bB	916	CLA	C4-C3-C5	2.42	119.42	115.23
12	aA	812	CLA	CMB-C2B-C1B	2.42	129.10	125.42
12	cB	933	CLA	CBC-CAC-C3C	-2.42	105.87	112.42
12	cA	808	CLA	CAA-C2A-C3A	-2.42	106.47	113.00
12	aA	804	CLA	C4-C3-C5	2.42	119.42	115.23
15	aL	206	BCR	C40-C30-C25	2.42	114.03	110.24
12	bB	950	CLA	C4A-NA-C1A	-2.42	105.58	106.68
12	aB	938	CLA	CAA-C2A-C3A	-2.42	106.47	113.00
12	aL	203	CLA	CHB-C4A-NA	2.41	127.89	124.40
17	aB	947	LMG	C1-C2-C3	-2.41	104.93	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bB	944	BCR	C30-C25-C26	-2.41	119.34	122.64
12	aB	935	CLA	CMC-C2C-C1C	2.41	128.81	125.03
12	cA	803	CLA	CMC-C2C-C1C	2.41	128.81	125.03
15	bA	847	BCR	C16-C17-C18	-2.41	123.89	127.28
12	aB	916	CLA	C4B-C3B-C2B	-2.41	104.30	107.30
12	cA	804	CLA	C4-C3-C5	2.41	119.42	115.23
12	aA	836	CLA	CAA-C2A-C3A	-2.41	106.48	113.00
12	aA	840	CLA	CHB-C4A-NA	2.41	127.88	124.40
12	cB	907	CLA	C1-C2-C3	-2.41	122.24	126.20
12	cB	911	CLA	CHD-C4C-NC	2.41	127.97	124.23
12	cA	805	CLA	O1D-CGD-CBD	-2.41	119.76	124.52
12	bB	933	CLA	CBC-CAC-C3C	-2.41	105.88	112.42
17	bB	947	LMG	C1-C2-C3	-2.41	104.94	110.01
12	bA	803	CLA	CMC-C2C-C1C	2.41	128.80	125.03
12	cA	836	CLA	CAA-C2A-C3A	-2.41	106.48	113.00
12	cA	813	CLA	CHD-C4C-NC	2.41	127.97	124.23
12	bA	817	CLA	CAC-C3C-C4C	2.41	127.92	124.79
12	cA	827	CLA	OBD-CAD-C3D	-2.41	122.79	128.42
12	cA	815	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
15	aF	201	BCR	C15-C16-C17	-2.41	118.59	123.52
12	cA	812	CLA	CMB-C2B-C1B	2.41	129.08	125.42
12	aB	909	CLA	CMC-C2C-C1C	2.41	128.79	125.03
12	bB	926	CLA	O2D-CGD-O1D	-2.41	119.17	123.85
12	aA	842	CLA	CHB-C4A-NA	2.41	127.87	124.40
12	bA	825	CLA	CHB-C1B-C2B	-2.40	120.44	127.43
12	bB	914	CLA	O1D-CGD-CBD	-2.40	119.78	124.52
15	bF	201	BCR	C15-C16-C17	-2.40	118.60	123.52
15	bL	206	BCR	C40-C30-C25	2.40	114.01	110.24
12	aA	827	CLA	OBD-CAD-C3D	-2.40	122.80	128.42
12	cA	840	CLA	CHB-C4A-NA	2.40	127.87	124.40
12	bB	919	CLA	CMC-C2C-C1C	2.40	128.79	125.03
12	cA	842	CLA	CHB-C4A-NA	2.40	127.87	124.40
15	aF	204	BCR	C24-C23-C22	-2.40	122.68	126.23
12	cB	949	CLA	C2A-C1A-NA	2.40	116.10	110.21
12	bB	935	CLA	CMC-C2C-C1C	2.40	128.79	125.03
12	aB	929	CLA	CBC-CAC-C3C	-2.40	105.91	112.42
12	cB	916	CLA	C4B-C3B-C2B	-2.40	104.31	107.30
12	cA	820	CLA	O1D-CGD-CBD	-2.40	119.78	124.52
12	bB	936	CLA	O2A-CGA-CBA	2.40	119.16	111.83
12	cB	906	CLA	C4-C3-C5	2.40	119.39	115.23
12	bB	910	CLA	CBC-CAC-C3C	-2.40	105.91	112.42
15	cM	101	BCR	C33-C5-C6	-2.40	121.86	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	804	CLA	C4-C3-C5	2.40	119.39	115.23
12	cA	807	CLA	CMB-C2B-C1B	2.40	129.07	125.42
12	cB	931	CLA	CHD-C4C-NC	2.40	127.95	124.23
15	aF	201	BCR	C16-C15-C14	-2.40	118.61	123.52
12	aB	910	CLA	CBC-CAC-C3C	-2.40	105.92	112.42
15	aB	945	BCR	C29-C30-C25	2.40	113.92	110.44
12	aB	906	CLA	CMB-C2B-C1B	2.40	129.07	125.42
12	aB	929	CLA	C3B-C4B-NB	2.40	112.67	110.53
12	cA	814	CLA	CMC-C2C-C1C	2.40	128.78	125.03
15	bB	945	BCR	C29-C30-C25	2.40	113.92	110.44
15	cF	201	BCR	C16-C15-C14	-2.40	118.61	123.52
12	aA	805	CLA	O1D-CGD-CBD	-2.40	119.79	124.52
12	bB	907	CLA	CHB-C4A-NA	2.40	127.86	124.40
12	aB	919	CLA	O2A-CGA-CBA	2.40	119.14	111.83
12	aA	825	CLA	CHB-C1B-C2B	-2.40	120.47	127.43
12	aB	915	CLA	CAC-C3C-C2C	2.40	131.96	127.56
12	cB	935	CLA	O1D-CGD-CBD	-2.40	119.79	124.52
12	aB	907	CLA	CHB-C4A-NA	2.40	127.86	124.40
12	cB	936	CLA	O2A-CGA-CBA	2.40	119.14	111.83
15	cL	206	BCR	C40-C30-C25	2.40	114.00	110.24
12	cA	820	CLA	CHB-C4A-NA	2.40	127.86	124.40
12	bB	925	CLA	C3B-C4B-NB	2.40	112.67	110.53
12	cA	828	CLA	C4A-NA-C1A	-2.40	105.59	106.68
13	cA	844	1L3	C01-C02-C12	2.40	121.09	116.68
12	aA	828	CLA	CHB-C4A-NA	2.39	127.86	124.40
12	cB	938	CLA	CAA-C2A-C3A	-2.39	106.53	113.00
12	cB	915	CLA	CAC-C3C-C2C	2.39	131.96	127.56
12	bB	915	CLA	CAC-C3C-C2C	2.39	131.96	127.56
12	aB	936	CLA	O2A-CGA-CBA	2.39	119.13	111.83
12	aA	810	CLA	CED-O2D-CGD	2.39	121.34	115.92
12	cB	914	CLA	O1D-CGD-CBD	-2.39	119.80	124.52
12	bB	919	CLA	O2A-CGA-CBA	2.39	119.13	111.83
12	bB	939	CLA	CED-O2D-CGD	2.39	121.34	115.92
15	cL	206	BCR	C16-C15-C14	-2.39	118.62	123.52
12	bB	929	CLA	CBC-CAC-C3C	-2.39	105.93	112.42
12	bA	840	CLA	CHB-C4A-NA	2.39	127.85	124.40
12	bB	913	CLA	CMB-C2B-C1B	2.39	129.06	125.42
12	cB	929	CLA	CBC-CAC-C3C	-2.39	105.94	112.42
12	bB	906	CLA	C4-C3-C5	2.39	119.38	115.23
12	aB	949	CLA	C2A-C1A-NA	2.39	116.07	110.21
12	cA	810	CLA	CED-O2D-CGD	2.39	121.34	115.92
12	cA	807	CLA	C3B-C4B-NB	2.39	112.66	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aB	914	CLA	O1D-CGD-CBD	-2.39	119.81	124.52
12	bA	815	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
12	bB	906	CLA	CAA-C2A-C3A	-2.39	106.54	113.00
13	bA	844	1L3	C01-C02-C12	2.39	121.08	116.68
12	aA	815	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
15	bL	206	BCR	C16-C15-C14	-2.39	118.63	123.52
12	cB	909	CLA	CMC-C2C-C1C	2.39	128.77	125.03
12	aB	916	CLA	C4-C3-C5	2.39	119.37	115.23
12	bB	938	CLA	CAA-C2A-C3A	-2.39	106.55	113.00
12	cB	919	CLA	CMC-C2C-C1C	2.39	128.77	125.03
12	cB	913	CLA	CMB-C2B-C1B	2.39	129.05	125.42
15	aA	847	BCR	C15-C16-C17	-2.39	118.64	123.52
12	bA	828	CLA	CHB-C4A-NA	2.39	127.84	124.40
12	aB	912	CLA	O1D-CGD-CBD	-2.38	119.81	124.52
12	cB	919	CLA	O2A-CGA-CBA	2.38	119.10	111.83
12	cB	910	CLA	CBC-CAC-C3C	-2.38	105.96	112.42
12	cB	937	CLA	CHD-C4C-NC	2.38	127.93	124.23
12	bB	937	CLA	CHD-C4C-NC	2.38	127.93	124.23
12	cA	828	CLA	C1-O2A-CGA	2.38	122.42	116.65
15	cA	847	BCR	C16-C17-C18	-2.38	123.94	127.28
12	cA	825	CLA	CHB-C1B-C2B	-2.38	120.52	127.43
12	cB	929	CLA	C3B-C4B-NB	2.38	112.66	110.53
12	cA	826	CLA	C1-C2-C3	-2.38	122.30	126.20
11	bA	801	CL0	O2A-CGA-CBA	2.38	119.09	111.83
12	cA	823	CLA	CMC-C2C-C1C	2.38	128.75	125.03
12	aB	907	CLA	C1-C2-C3	-2.38	122.30	126.20
15	cA	846	BCR	C15-C16-C17	-2.38	118.65	123.52
12	bA	810	CLA	CED-O2D-CGD	2.38	121.31	115.92
12	aA	803	CLA	CMC-C2C-C1C	2.38	128.75	125.03
12	cB	938	CLA	C4A-NA-C1A	-2.38	105.59	106.68
12	bB	929	CLA	C3B-C4B-NB	2.38	112.65	110.53
12	cB	906	CLA	CAA-C2A-C3A	-2.38	106.57	113.00
12	bA	809	CLA	O2A-CGA-CBA	2.38	121.51	114.00
12	bB	931	CLA	CGD-CBD-CAD	-2.38	103.15	110.85
12	bA	807	CLA	CMB-C2B-C1B	2.38	129.04	125.42
12	aB	924	CLA	CMC-C2C-C1C	2.38	128.75	125.03
12	cB	925	CLA	C3B-C4B-NB	2.38	112.65	110.53
12	cB	939	CLA	CED-O2D-CGD	2.38	121.31	115.92
12	aA	831	CLA	O1D-CGD-CBD	-2.38	119.83	124.52
12	bA	826	CLA	C1-C2-C3	-2.38	122.30	126.20
12	cA	833	CLA	CBC-CAC-C3C	-2.38	105.98	112.42
12	cB	931	CLA	CGD-CBD-CAD	-2.38	103.15	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cB	922	CLA	CED-O2D-CGD	2.38	121.31	115.92
12	bA	805	CLA	O1D-CGD-CBD	-2.38	119.83	124.52
12	aA	809	CLA	O2A-CGA-CBA	2.38	121.51	114.00
12	cB	912	CLA	O1D-CGD-CBD	-2.37	119.83	124.52
12	bA	812	CLA	CMB-C2B-C1B	2.37	129.03	125.42
15	aL	206	BCR	C16-C15-C14	-2.37	118.66	123.52
12	aA	828	CLA	C1-O2A-CGA	2.37	122.40	116.65
12	aB	909	CLA	C4-C3-C5	2.37	119.35	115.23
12	aB	906	CLA	CAA-C2A-C3A	-2.37	106.58	113.00
12	aA	826	CLA	C1-C2-C3	-2.37	122.31	126.20
12	cA	828	CLA	CHB-C4A-NA	2.37	127.83	124.40
12	aB	931	CLA	CGD-CBD-CAD	-2.37	103.16	110.85
12	aB	919	CLA	CMC-C2C-C1C	2.37	128.74	125.03
12	aB	939	CLA	CED-O2D-CGD	2.37	121.30	115.92
13	aA	845	1L3	C01-C02-C12	2.37	121.05	116.68
12	aB	908	CLA	CBC-CAC-C3C	-2.37	105.99	112.42
12	bA	839	CLA	CAC-C3C-C4C	2.37	127.88	124.79
12	aA	807	CLA	CHC-C1C-C2C	-2.37	120.20	126.95
12	cA	807	CLA	CHC-C1C-C2C	-2.37	120.20	126.95
12	aA	813	CLA	CHD-C4C-NC	2.37	127.91	124.23
12	bA	813	CLA	CHD-C4C-NC	2.37	127.91	124.23
13	bB	940	1L3	C14-C03-C02	-2.37	120.83	124.89
12	aA	839	CLA	CAC-C3C-C4C	2.37	127.88	124.79
12	aB	913	CLA	CMB-C2B-C1B	2.37	129.03	125.42
12	bA	833	CLA	CBC-CAC-C3C	-2.37	105.99	112.42
12	cB	909	CLA	C4-C3-C5	2.37	119.34	115.23
12	bA	826	CLA	C3B-C4B-NB	2.37	112.65	110.53
12	bB	909	CLA	C4-C3-C5	2.37	119.34	115.23
12	aB	910	CLA	CHD-C4C-NC	2.37	127.91	124.23
13	aB	940	1L3	C14-C03-C02	-2.37	120.83	124.89
12	aB	906	CLA	C4-C3-C5	2.37	119.34	115.23
11	cA	801	CL0	O2A-CGA-CBA	2.37	119.06	111.83
12	aA	816	CLA	CHB-C4A-NA	2.37	127.82	124.40
12	cB	901	CLA	CHB-C4A-NA	2.37	127.82	124.40
15	bA	846	BCR	C15-C16-C17	-2.37	118.67	123.52
12	bA	816	CLA	CHB-C4A-NA	2.37	127.82	124.40
12	cA	831	CLA	O1D-CGD-CBD	-2.37	119.85	124.52
12	cB	908	CLA	CBC-CAC-C3C	-2.37	106.00	112.42
12	cA	809	CLA	O2A-CGA-CBA	2.37	121.48	114.00
12	bB	924	CLA	CMC-C2C-C1C	2.37	128.73	125.03
12	aB	901	CLA	CHB-C4A-NA	2.37	127.81	124.40
12	cA	816	CLA	CHB-C4A-NA	2.37	127.81	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bB	935	CLA	O1D-CGD-CBD	-2.37	119.85	124.52
12	aB	931	CLA	CHD-C4C-NC	2.37	127.90	124.23
12	cB	924	CLA	CMC-C2C-C1C	2.37	128.73	125.03
11	aA	801	CL0	O2A-CGA-CBA	2.36	119.05	111.83
12	aB	926	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
12	aA	814	CLA	CAA-C2A-C3A	-2.36	106.61	113.00
12	bA	807	CLA	C3B-C4B-NB	2.36	112.64	110.53
12	bA	807	CLA	CHC-C1C-C2C	-2.36	120.23	126.95
12	bB	922	CLA	CED-O2D-CGD	2.36	121.27	115.92
12	aA	826	CLA	C3B-C4B-NB	2.36	112.64	110.53
12	cA	841	CLA	C3B-C4B-NB	2.36	112.64	110.53
12	bA	814	CLA	CAA-C2A-C3A	-2.36	106.62	113.00
15	aM	101	BCR	C33-C5-C6	-2.36	121.91	124.48
15	cA	846	BCR	C33-C5-C6	-2.36	121.91	124.48
12	cA	819	CLA	CMC-C2C-C1C	2.36	128.72	125.03
12	aB	935	CLA	O1D-CGD-CBD	-2.36	119.86	124.52
12	bB	912	CLA	O1D-CGD-CBD	-2.36	119.86	124.52
12	aB	922	CLA	CED-O2D-CGD	2.36	121.27	115.92
12	aB	938	CLA	O2A-CGA-CBA	2.36	119.03	111.83
12	bA	823	CLA	CMC-C2C-C1C	2.36	128.72	125.03
12	bB	916	CLA	C4B-C3B-C2B	-2.36	104.37	107.30
12	bB	910	CLA	CHD-C4C-NC	2.36	127.89	124.23
12	cA	841	CLA	CHD-C4C-NC	2.36	127.89	124.23
12	aA	823	CLA	CMC-C2C-C1C	2.36	128.72	125.03
12	bA	831	CLA	O1D-CGD-CBD	-2.36	119.87	124.52
12	bB	938	CLA	O2A-CGA-CBA	2.36	119.02	111.83
12	aA	818	CLA	CHB-C4A-NA	2.36	127.80	124.40
12	bB	938	CLA	CMB-C2B-C1B	2.36	129.01	125.42
12	bA	820	CLA	CHB-C4A-NA	2.36	127.80	124.40
12	aA	828	CLA	CBA-CAA-C2A	2.36	120.80	113.79
12	cB	938	CLA	O2A-CGA-CBA	2.36	119.02	111.83
12	bB	924	CLA	CHB-C4A-NA	2.36	127.80	124.40
12	aA	833	CLA	CAC-C3C-C4C	2.36	127.85	124.79
12	aB	911	CLA	CBC-CAC-C3C	-2.35	106.04	112.42
12	bA	828	CLA	C1-O2A-CGA	2.35	122.35	116.65
12	cA	815	CLA	CAA-C2A-C3A	-2.35	106.64	113.00
12	aA	833	CLA	CBC-CAC-C3C	-2.35	106.04	112.42
12	cB	925	CLA	O1D-CGD-CBD	-2.35	119.88	124.52
12	bB	908	CLA	CBC-CAC-C3C	-2.35	106.04	112.42
12	aA	820	CLA	CHB-C4A-NA	2.35	127.80	124.40
15	aA	847	BCR	C33-C5-C6	-2.35	121.92	124.48
12	bA	828	CLA	CBA-CAA-C2A	2.35	120.79	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bB	932	CLA	CHB-C4A-NA	2.35	127.79	124.40
12	cB	911	CLA	CBC-CAC-C3C	-2.35	106.05	112.42
12	cB	910	CLA	CHD-C4C-NC	2.35	127.88	124.23
12	bB	901	CLA	CHB-C4A-NA	2.35	127.79	124.40
12	cA	827	CLA	CAA-C2A-C3A	-2.35	106.65	113.00
12	bB	911	CLA	CBC-CAC-C3C	-2.35	106.05	112.42
12	bA	828	CLA	C4A-NA-C1A	-2.35	105.61	106.68
12	cA	814	CLA	CAA-C2A-C3A	-2.35	106.65	113.00
12	bB	925	CLA	O1D-CGD-CBD	-2.35	119.88	124.52
12	aA	815	CLA	CHB-C4A-NA	2.35	127.79	124.40
15	bF	201	BCR	C16-C15-C14	-2.35	118.71	123.52
12	aA	840	CLA	CBC-CAC-C3C	-2.35	106.05	112.42
12	bA	802	CLA	CHD-C4C-NC	2.35	127.87	124.23
12	cA	828	CLA	CBA-CAA-C2A	2.35	120.78	113.79
12	aB	912	CLA	CHD-C4C-NC	2.35	127.87	124.23
13	cB	940	1L3	C14-C03-C02	-2.35	120.87	124.89
12	bA	837	CLA	O1D-CGD-CBD	-2.35	119.89	124.52
12	bA	833	CLA	CAC-C3C-C4C	2.35	127.84	124.79
12	aA	802	CLA	CHD-C4C-NC	2.35	127.87	124.23
12	cA	815	CLA	CHB-C4A-NA	2.35	127.79	124.40
12	bA	820	CLA	CMC-C2C-C1C	2.35	128.70	125.03
15	bJ	101	BCR	C15-C16-C17	-2.35	118.72	123.52
15	cJ	101	BCR	C15-C16-C17	-2.35	118.72	123.52
12	cA	837	CLA	O1D-CGD-CBD	-2.34	119.89	124.52
12	aA	837	CLA	O1D-CGD-CBD	-2.34	119.90	124.52
12	aB	932	CLA	CHB-C4A-NA	2.34	127.78	124.40
12	cA	839	CLA	CAC-C3C-C4C	2.34	127.84	124.79
12	aB	938	CLA	CMB-C2B-C1B	2.34	128.99	125.42
12	cB	924	CLA	CHD-C4C-NC	2.34	127.86	124.23
12	bB	908	CLA	C4A-NA-C1A	-2.34	105.61	106.68
12	cA	821	CLA	CMC-C2C-C1C	2.34	128.69	125.03
12	aA	827	CLA	CAA-C2A-C3A	-2.34	106.67	113.00
15	bB	942	BCR	C28-C27-C26	-2.34	109.88	114.06
12	aB	924	CLA	CHB-C4A-NA	2.34	127.78	124.40
12	aA	809	CLA	CAA-C2A-C1A	-2.34	104.31	111.97
12	bA	840	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
12	bA	827	CLA	CAA-C2A-C3A	-2.34	106.68	113.00
12	bB	931	CLA	CHD-C4C-NC	2.34	127.86	124.23
12	cB	912	CLA	CHD-C4C-NC	2.34	127.86	124.23
12	aA	827	CLA	O1D-CGD-CBD	-2.34	119.91	124.52
15	bA	848	BCR	C15-C14-C13	-2.34	124.00	127.28
12	bA	853	CLA	CGD-CBD-CAD	-2.34	103.28	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bB	912	CLA	CHD-C4C-NC	2.34	127.85	124.23
12	aB	925	CLA	O1D-CGD-CBD	-2.34	119.91	124.52
12	bA	829	CLA	CMC-C2C-C1C	2.34	128.68	125.03
12	cA	840	CLA	CBC-CAC-C3C	-2.34	106.09	112.42
12	bA	819	CLA	CMC-C2C-C1C	2.34	128.68	125.03
12	aA	841	CLA	CHD-C4C-NC	2.34	127.85	124.23
12	bA	815	CLA	CAA-C2A-C3A	-2.33	106.69	113.00
12	aA	820	CLA	CMC-C2C-C1C	2.33	128.68	125.03
12	cA	820	CLA	CMC-C2C-C1C	2.33	128.68	125.03
12	cA	803	CLA	C1-C2-C3	-2.33	122.38	126.20
12	cA	829	CLA	C4-C3-C5	2.33	119.28	115.23
12	bA	841	CLA	CHD-C4C-NC	2.33	127.85	124.23
12	cA	802	CLA	CHD-C4C-NC	2.33	127.85	124.23
12	aB	937	CLA	CHD-C4C-NC	2.33	127.85	124.23
15	cB	942	BCR	C28-C27-C26	-2.33	109.90	114.06
12	aB	929	CLA	CMC-C2C-C1C	2.33	128.68	125.03
12	cA	809	CLA	CAA-C2A-C1A	-2.33	104.34	111.97
12	cA	827	CLA	O1D-CGD-CBD	-2.33	119.92	124.52
12	cB	914	CLA	CMB-C2B-C1B	2.33	128.97	125.42
15	aB	942	BCR	C28-C27-C26	-2.33	109.90	114.06
12	bA	829	CLA	C4-C3-C5	2.33	119.27	115.23
12	bA	818	CLA	CHB-C4A-NA	2.33	127.76	124.40
15	aJ	101	BCR	C33-C5-C6	-2.33	121.94	124.48
12	cA	810	CLA	CAA-C2A-C1A	-2.33	104.34	111.97
12	cB	924	CLA	CHB-C4A-NA	2.33	127.76	124.40
15	cJ	101	BCR	C33-C5-C6	-2.33	121.94	124.48
12	bA	831	CLA	O2A-CGA-O1A	-2.33	117.81	123.63
12	cA	822	CLA	CHB-C4A-NA	2.33	127.76	124.40
12	aA	831	CLA	O2A-CGA-O1A	-2.33	117.81	123.63
12	cB	932	CLA	CHB-C4A-NA	2.33	127.76	124.40
12	aA	854	CLA	CGD-CBD-CAD	-2.33	103.31	110.85
12	aA	841	CLA	C3B-C4B-NB	2.33	112.61	110.53
12	aA	829	CLA	C4-C3-C5	2.33	119.27	115.23
12	cB	938	CLA	CMB-C2B-C1B	2.33	128.96	125.42
12	bA	840	CLA	CBC-CAC-C3C	-2.33	106.12	112.42
12	cA	820	CLA	C4-C3-C2	-2.32	117.66	123.63
15	bA	850	BCR	C27-C26-C25	2.32	125.84	122.70
12	aA	819	CLA	CMC-C2C-C1C	2.32	128.67	125.03
15	bA	847	BCR	C3-C4-C5	-2.32	109.91	114.06
12	aB	936	CLA	C4-C3-C5	2.32	119.26	115.23
12	aA	838	CLA	C1-O2A-CGA	2.32	122.27	116.65
15	bF	201	BCR	C2-C1-C6	2.32	113.81	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	853	CLA	CGD-CBD-CAD	-2.32	103.33	110.85
12	aA	807	CLA	C3B-C4B-NB	2.32	112.60	110.53
12	cB	929	CLA	CMC-C2C-C1C	2.32	128.66	125.03
12	cB	937	CLA	CMB-C2B-C1B	2.32	128.95	125.42
12	cA	831	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
15	cF	201	BCR	C2-C1-C6	2.32	113.81	110.44
12	aA	807	CLA	CHA-C1A-NA	-2.32	121.14	126.39
12	bB	938	CLA	CED-O2D-CGD	2.32	121.18	115.92
12	bA	809	CLA	CAA-C2A-C1A	-2.32	104.37	111.97
12	aA	822	CLA	CHB-C4A-NA	2.32	127.75	124.40
12	cB	904	CLA	CAC-C3C-C4C	2.32	127.81	124.79
12	aA	820	CLA	C4-C3-C2	-2.32	117.67	123.63
12	bA	815	CLA	CHB-C4A-NA	2.32	127.75	124.40
12	cA	853	CLA	CHB-C1B-C2B	-2.32	120.69	127.43
12	aA	810	CLA	CMB-C2B-C1B	2.32	128.95	125.42
12	aA	810	CLA	CAA-C2A-C1A	-2.32	104.38	111.97
12	cB	904	CLA	C1-O2A-CGA	2.32	122.26	116.65
12	bA	807	CLA	CHA-C1A-NA	-2.32	121.14	126.39
12	aB	914	CLA	CMB-C2B-C1B	2.32	128.95	125.42
15	cA	848	BCR	C15-C14-C13	-2.32	124.03	127.28
12	aA	825	CLA	O2A-CGA-CBA	2.32	118.90	111.83
12	cA	825	CLA	O2A-CGA-CBA	2.32	118.90	111.83
12	bA	853	CLA	CHB-C1B-C2B	-2.32	120.70	127.43
12	aA	829	CLA	CMC-C2C-C1C	2.32	128.65	125.03
12	aA	840	CLA	O2A-CGA-O1A	-2.32	117.84	123.63
12	bA	827	CLA	O1D-CGD-CBD	-2.32	119.95	124.52
12	bA	810	CLA	CAA-C2A-C1A	-2.31	104.39	111.97
12	aA	815	CLA	CAA-C2A-C3A	-2.31	106.74	113.00
12	bB	914	CLA	CMB-C2B-C1B	2.31	128.94	125.42
12	cA	840	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
12	aB	938	CLA	CED-O2D-CGD	2.31	121.17	115.92
12	bA	803	CLA	C1-C2-C3	-2.31	122.41	126.20
12	bA	822	CLA	CHB-C4A-NA	2.31	127.74	124.40
15	aI	101	BCR	C27-C26-C25	2.31	125.83	122.70
12	aA	821	CLA	CMC-C2C-C1C	2.31	128.65	125.03
12	cA	826	CLA	C3B-C4B-NB	2.31	112.59	110.53
12	aB	904	CLA	C1-O2A-CGA	2.31	122.25	116.65
12	cA	818	CLA	CHB-C4A-NA	2.31	127.74	124.40
15	aF	201	BCR	C2-C1-C6	2.31	113.80	110.44
12	cA	833	CLA	CAC-C3C-C4C	2.31	127.80	124.79
12	cA	839	CLA	CMC-C2C-C1C	2.31	128.65	125.03
12	bA	835	CLA	CMA-C3A-C4A	-2.31	105.56	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	803	CLA	C1-C2-C3	-2.31	122.41	126.20
12	aA	854	CLA	CHB-C1B-C2B	-2.31	120.72	127.43
12	bL	202	CLA	CMC-C2C-C1C	2.31	128.65	125.03
12	cB	908	CLA	C4A-NA-C1A	-2.31	105.62	106.68
12	aB	938	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
12	cA	807	CLA	CHA-C1A-NA	-2.31	121.16	126.39
12	cA	838	CLA	C1-O2A-CGA	2.31	122.24	116.65
12	cB	938	CLA	CED-O2D-CGD	2.31	121.16	115.92
15	aJ	101	BCR	C15-C16-C17	-2.31	118.80	123.52
12	cB	915	CLA	O2D-CGD-O1D	-2.31	119.36	123.85
12	aB	922	CLA	O2A-CGA-CBA	2.31	121.29	114.00
17	bB	947	LMG	O7-C10-O9	-2.31	118.31	123.70
12	aB	937	CLA	CMB-C2B-C1B	2.31	128.93	125.42
12	bA	825	CLA	O2A-CGA-CBA	2.31	118.87	111.83
15	bA	846	BCR	C33-C5-C6	-2.31	121.97	124.48
12	bB	929	CLA	CMC-C2C-C1C	2.31	128.64	125.03
12	cB	936	CLA	C4-C3-C5	2.31	119.23	115.23
12	aA	835	CLA	CMA-C3A-C4A	-2.31	105.58	111.77
12	bA	820	CLA	C4-C3-C2	-2.31	117.71	123.63
12	bB	938	CLA	CMD-C2D-C3D	-2.31	122.40	127.69
12	bB	922	CLA	O2A-CGA-CBA	2.30	121.28	114.00
12	bA	810	CLA	CMB-C2B-C1B	2.30	128.93	125.42
12	aL	204	CLA	O2A-CGA-CBA	2.30	121.28	114.00
17	cB	947	LMG	O7-C10-O9	-2.30	118.32	123.70
12	bA	839	CLA	CMC-C2C-C1C	2.30	128.63	125.03
12	cA	829	CLA	CMC-C2C-C1C	2.30	128.63	125.03
15	bI	101	BCR	C27-C26-C25	2.30	125.82	122.70
12	bA	825	CLA	CAA-CBA-CGA	-2.30	106.67	113.21
12	bB	904	CLA	C1-O2A-CGA	2.30	122.22	116.65
12	bA	841	CLA	C3B-C4B-NB	2.30	112.58	110.53
12	aA	834	CLA	CBB-CAB-C3B	-2.30	116.03	127.53
12	bA	834	CLA	CBB-CAB-C3B	-2.30	116.03	127.53
12	bB	936	CLA	C4-C3-C5	2.30	119.22	115.23
15	cI	101	BCR	C27-C26-C25	2.30	125.81	122.70
12	aA	834	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
12	bA	821	CLA	CMC-C2C-C1C	2.30	128.63	125.03
12	cB	938	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
12	bA	833	CLA	CMA-C3A-C2A	-2.30	105.09	113.98
15	cA	850	BCR	C20-C21-C22	-2.30	124.05	127.28
15	bJ	101	BCR	C33-C5-C6	-2.30	121.98	124.48
12	cB	922	CLA	O2A-CGA-CBA	2.30	121.26	114.00
12	cA	825	CLA	CAA-CBA-CGA	-2.30	106.69	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aA	848	BCR	C3-C4-C5	-2.30	109.96	114.06
12	aA	833	CLA	CHA-C1A-NA	-2.30	121.19	126.39
12	cL	202	CLA	CMC-C2C-C1C	2.30	128.62	125.03
12	bB	910	CLA	CMB-C2B-C1B	2.30	128.91	125.42
12	aB	924	CLA	CHD-C4C-NC	2.30	127.79	124.23
12	aA	828	CLA	C4A-NA-C1A	-2.29	105.63	106.68
12	cA	834	CLA	CBB-CAB-C3B	-2.29	116.06	127.53
12	cA	833	CLA	CMA-C3A-C2A	-2.29	105.11	113.98
12	bB	939	CLA	CAA-CBA-CGA	-2.29	106.37	112.49
12	bB	904	CLA	CAC-C3C-C4C	2.29	127.78	124.79
12	cA	810	CLA	CMB-C2B-C1B	2.29	128.91	125.42
12	aA	825	CLA	CAA-CBA-CGA	-2.29	106.70	113.21
12	bB	937	CLA	CMB-C2B-C1B	2.29	128.91	125.42
12	bB	924	CLA	CHD-C4C-NC	2.29	127.79	124.23
12	bB	911	CLA	CHB-C4A-NA	2.29	127.71	124.40
12	aA	803	CLA	CHD-C4C-NC	2.29	127.79	124.23
12	bB	915	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
17	aB	947	LMG	O7-C10-O9	-2.29	118.35	123.70
12	cB	923	CLA	CAC-C3C-C4C	2.29	127.77	124.79
15	cA	850	BCR	C27-C26-C25	2.29	125.80	122.70
12	bL	204	CLA	O2A-CGA-CBA	2.29	121.24	114.00
12	cA	835	CLA	CMA-C3A-C4A	-2.29	105.62	111.77
15	aA	851	BCR	C27-C26-C25	2.29	125.80	122.70
12	cL	204	CLA	O2A-CGA-CBA	2.29	121.23	114.00
12	bA	838	CLA	C1-O2A-CGA	2.29	122.19	116.65
12	cB	910	CLA	CMB-C2B-C1B	2.29	128.91	125.42
12	aB	918	CLA	CHB-C1B-C2B	-2.29	120.78	127.43
12	cB	903	CLA	CHB-C4A-NA	2.29	127.70	124.40
15	aB	942	BCR	C30-C25-C26	-2.29	119.51	122.64
12	bA	826	CLA	C4B-C3B-C2B	-2.29	104.46	107.30
12	cA	836	CLA	CHB-C4A-NA	2.29	127.70	124.40
12	aA	810	CLA	CAA-CBA-CGA	-2.29	106.39	112.49
12	aA	839	CLA	CMC-C2C-C1C	2.29	128.61	125.03
12	aA	837	CLA	CBA-CAA-C2A	-2.29	106.99	113.79
12	cA	834	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
12	cB	939	CLA	CAA-CBA-CGA	-2.29	106.39	112.49
12	bA	834	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
12	aA	833	CLA	CMA-C3A-C2A	-2.28	105.15	113.98
12	aA	822	CLA	CAA-C2A-C3A	-2.28	106.83	113.00
12	bA	835	CLA	CAA-C2A-C3A	-2.28	106.83	113.00
15	aA	849	BCR	C15-C14-C13	-2.28	124.08	127.28
12	aB	939	CLA	CAA-CBA-CGA	-2.28	106.40	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	810	CLA	CAA-CBA-CGA	-2.28	106.40	112.49
12	bA	827	CLA	CAC-C3C-C4C	2.28	127.76	124.79
12	aA	819	CLA	C11-C10-C8	-2.28	108.38	115.97
12	aB	911	CLA	CHB-C4A-NA	2.28	127.69	124.40
12	bB	936	CLA	CAC-C3C-C4C	2.28	127.76	124.79
12	cA	837	CLA	CHA-C1A-NA	-2.28	121.22	126.39
15	cM	101	BCR	C10-C11-C12	-2.28	116.59	123.20
12	cB	936	CLA	CAC-C3C-C4C	2.28	127.76	124.79
12	bA	822	CLA	CAA-C2A-C3A	-2.28	106.83	113.00
12	aA	817	CLA	CHB-C4A-NA	2.28	127.69	124.40
12	bA	829	CLA	CED-O2D-CGD	2.28	121.09	115.92
12	cB	915	CLA	CED-O2D-CGD	2.28	121.09	115.92
12	cA	819	CLA	C11-C10-C8	-2.28	108.39	115.97
12	aB	915	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
15	bA	850	BCR	C20-C21-C22	-2.28	124.08	127.28
12	aL	202	CLA	CMC-C2C-C1C	2.28	128.59	125.03
12	bA	833	CLA	CHA-C1A-NA	-2.28	121.23	126.39
15	cB	943	BCR	C30-C25-C26	-2.28	119.52	122.64
12	cA	833	CLA	CHA-C1A-NA	-2.28	121.23	126.39
12	aB	908	CLA	C4A-NA-C1A	-2.28	105.64	106.68
12	aA	826	CLA	CAA-C2A-C1A	-2.28	104.51	111.97
12	aA	826	CLA	C4B-C3B-C2B	-2.28	104.47	107.30
12	aA	837	CLA	CHA-C1A-NA	-2.27	121.24	126.39
12	cB	936	CLA	CHB-C4A-NA	2.27	127.68	124.40
15	cA	847	BCR	C3-C4-C5	-2.27	110.00	114.06
15	bB	943	BCR	C30-C25-C26	-2.27	119.53	122.64
12	bA	837	CLA	CHA-C1A-NA	-2.27	121.24	126.39
15	cB	944	BCR	C33-C5-C6	-2.27	122.00	124.48
12	aB	904	CLA	CAC-C3C-C4C	2.27	127.75	124.79
12	bA	819	CLA	C11-C10-C8	-2.27	108.41	115.97
12	bA	803	CLA	CHD-C4C-NC	2.27	127.76	124.23
12	cB	933	CLA	CHB-C4A-NA	2.27	127.68	124.40
12	aA	819	CLA	CED-O2D-CGD	2.27	121.07	115.92
12	cA	810	CLA	CAA-CBA-CGA	-2.27	106.43	112.49
12	aB	923	CLA	CAC-C3C-C4C	2.27	127.75	124.79
12	cA	803	CLA	CHD-C4C-NC	2.27	127.75	124.23
12	aB	903	CLA	O1D-CGD-CBD	-2.27	120.04	124.52
12	cB	949	CLA	CGD-CBD-CAD	-2.27	103.50	110.85
12	aA	835	CLA	CAA-C2A-C3A	-2.27	106.86	113.00
16	bA	851	LHG	O8-C23-O10	-2.27	117.95	123.63
12	aA	825	CLA	O1D-CGD-CBD	-2.27	120.04	124.52
12	aA	836	CLA	CHB-C4A-NA	2.27	127.67	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	837	CLA	CBA-CAA-C2A	-2.27	107.04	113.79
12	bB	918	CLA	CHB-C1B-C2B	-2.27	120.84	127.43
12	cA	826	CLA	CAA-C2A-C1A	-2.27	104.54	111.97
12	cA	825	CLA	O1D-CGD-CBD	-2.27	120.05	124.52
12	aB	902	CLA	C1-O2A-CGA	2.27	122.14	116.65
12	cB	936	CLA	CMC-C2C-C1C	2.27	128.58	125.03
15	aB	944	BCR	C33-C5-C6	-2.27	122.01	124.48
12	aB	909	CLA	CHD-C4C-NC	2.27	127.74	124.23
12	bA	831	CLA	CMC-C2C-C1C	2.27	128.57	125.03
12	bA	817	CLA	CHB-C4A-NA	2.27	127.67	124.40
12	cB	918	CLA	CHB-C1B-C2B	-2.26	120.85	127.43
15	bM	101	BCR	C10-C11-C12	-2.26	116.64	123.20
15	bB	942	BCR	C30-C25-C26	-2.26	119.54	122.64
12	cB	911	CLA	CHB-C4A-NA	2.26	127.67	124.40
12	aB	933	CLA	CHB-C4A-NA	2.26	127.67	124.40
12	aA	808	CLA	O2A-CGA-CBA	2.26	118.74	111.83
12	cA	808	CLA	O2A-CGA-CBA	2.26	118.74	111.83
12	cA	827	CLA	O2A-CGA-CBA	2.26	120.69	112.14
12	bA	836	CLA	CHB-C4A-NA	2.26	127.67	124.40
17	bB	947	LMG	C38-C37-C36	-2.26	102.93	114.37
12	cB	903	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
12	bB	903	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
12	aB	936	CLA	CAC-C3C-C4C	2.26	127.73	124.79
12	cA	829	CLA	CED-O2D-CGD	2.26	121.05	115.92
15	aB	943	BCR	C30-C25-C26	-2.26	119.55	122.64
12	cB	902	CLA	C1-O2A-CGA	2.26	122.12	116.65
17	cB	947	LMG	C38-C37-C36	-2.26	102.94	114.37
12	bL	203	CLA	CAC-C3C-C4C	2.26	127.73	124.79
12	bA	811	CLA	CBC-CAC-C3C	-2.26	106.29	112.42
12	bB	902	CLA	C1-O2A-CGA	2.26	122.12	116.65
12	cA	826	CLA	C4B-C3B-C2B	-2.26	104.49	107.30
12	cA	819	CLA	CED-O2D-CGD	2.26	121.04	115.92
12	aB	949	CLA	CGD-CBD-CAD	-2.26	103.53	110.85
12	bA	826	CLA	CAA-C2A-C1A	-2.26	104.57	111.97
17	aB	947	LMG	C38-C37-C36	-2.26	102.95	114.37
12	cB	917	CLA	C1-C2-C3	-2.26	122.50	126.20
12	cA	822	CLA	CAA-C2A-C3A	-2.26	106.89	113.00
12	cA	827	CLA	CAC-C3C-C4C	2.26	127.73	124.79
12	bB	933	CLA	CHB-C4A-NA	2.26	127.66	124.40
12	bB	906	CLA	CED-O2D-CGD	2.26	121.04	115.92
12	aB	908	CLA	CHD-C4C-NC	2.26	127.73	124.23
15	aM	101	BCR	C10-C11-C12	-2.26	116.66	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	829	CLA	CED-O2D-CGD	2.26	121.04	115.92
12	cA	838	CLA	C3B-C4B-NB	2.26	112.55	110.53
12	cA	817	CLA	CHB-C4A-NA	2.26	127.66	124.40
12	aB	937	CLA	CHB-C4A-NA	2.26	127.66	124.40
12	bB	915	CLA	CED-O2D-CGD	2.26	121.03	115.92
12	aA	811	CLA	CBC-CAC-C3C	-2.26	106.31	112.42
12	bA	815	CLA	O2A-CGA-CBA	2.26	121.13	114.00
12	bB	918	CLA	CHB-C4A-NA	2.26	127.66	124.40
12	bA	837	CLA	CBA-CAA-C2A	-2.26	107.08	113.79
12	bB	949	CLA	CGD-CBD-CAD	-2.25	103.55	110.85
12	aB	918	CLA	CHB-C4A-NA	2.25	127.65	124.40
12	cL	204	CLA	CHB-C4A-NA	2.25	127.65	124.40
12	cA	811	CLA	CBC-CAC-C3C	-2.25	106.31	112.42
12	cL	203	CLA	CAC-C3C-C4C	2.25	127.72	124.79
15	cB	942	BCR	C30-C25-C26	-2.25	119.56	122.64
12	bB	924	CLA	CBC-CAC-C3C	-2.25	106.31	112.42
12	bB	903	CLA	CHB-C4A-NA	2.25	127.65	124.40
12	cA	835	CLA	CAA-C2A-C3A	-2.25	106.91	113.00
12	bB	937	CLA	CHB-C4A-NA	2.25	127.65	124.40
12	cB	906	CLA	CED-O2D-CGD	2.25	121.03	115.92
12	bA	825	CLA	O1D-CGD-CBD	-2.25	120.07	124.52
12	bA	819	CLA	CED-O2D-CGD	2.25	121.03	115.92
12	aB	915	CLA	CHB-C4A-NA	2.25	127.65	124.40
15	bB	944	BCR	C33-C5-C6	-2.25	122.03	124.48
12	aB	915	CLA	CED-O2D-CGD	2.25	121.03	115.92
12	aB	917	CLA	C1-C2-C3	-2.25	122.51	126.20
12	bB	904	CLA	CBA-CAA-C2A	2.25	120.49	113.79
12	bA	827	CLA	O2A-CGA-CBA	2.25	120.65	112.14
15	cB	943	BCR	C40-C30-C25	2.25	113.77	110.24
12	bA	808	CLA	O2A-CGA-CBA	2.25	118.70	111.83
12	bA	836	CLA	C4C-C3C-C2C	-2.25	103.62	106.89
16	aA	852	LHG	O8-C23-O10	-2.25	118.00	123.63
12	cA	824	CLA	CED-O2D-CGD	2.25	121.02	115.92
12	aB	910	CLA	CMB-C2B-C1B	2.25	128.84	125.42
12	aA	829	CLA	CHB-C4A-NA	2.25	127.65	124.40
12	aA	827	CLA	O2A-CGA-CBA	2.25	120.64	112.14
12	aA	831	CLA	CAA-C2A-C3A	-2.25	106.92	113.00
12	aF	202	CLA	CHB-C4A-NA	2.25	127.64	124.40
12	aB	918	CLA	CHD-C4C-NC	2.25	127.72	124.23
12	aB	936	CLA	CHB-C4A-NA	2.25	127.64	124.40
12	cB	918	CLA	CHB-C4A-NA	2.25	127.64	124.40
12	aA	815	CLA	O2A-CGA-CBA	2.25	121.10	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	830	CLA	CMC-C2C-C1C	2.25	128.54	125.03
12	bL	204	CLA	CHB-C4A-NA	2.25	127.64	124.40
15	aA	851	BCR	C20-C21-C22	-2.25	124.13	127.28
16	cA	851	LHG	O8-C23-O10	-2.25	118.01	123.63
12	bA	834	CLA	CHB-C1B-C2B	-2.25	120.91	127.43
12	bB	917	CLA	C1-C2-C3	-2.25	122.52	126.20
12	bB	906	CLA	O2A-CGA-CBA	2.25	118.68	111.83
12	aB	936	CLA	CMC-C2C-C1C	2.24	128.54	125.03
12	cA	831	CLA	CAA-C2A-C3A	-2.24	106.93	113.00
12	aB	906	CLA	O2A-CGA-CBA	2.24	118.68	111.83
12	bB	936	CLA	CHB-C4A-NA	2.24	127.64	124.40
12	aB	904	CLA	CBA-CAA-C2A	2.24	120.47	113.79
12	aA	827	CLA	CAC-C3C-C4C	2.24	127.71	124.79
12	bB	923	CLA	CAC-C3C-C4C	2.24	127.71	124.79
12	cA	815	CLA	O2A-CGA-CBA	2.24	121.09	114.00
12	aB	902	CLA	CMA-C3A-C2A	-2.24	105.31	113.98
12	aB	930	CLA	CMC-C2C-C1C	2.24	128.54	125.03
12	aB	903	CLA	C4A-NA-C1A	-2.24	105.66	106.68
12	aA	824	CLA	CED-O2D-CGD	2.24	121.00	115.92
12	bB	918	CLA	CHD-C4C-NC	2.24	127.71	124.23
12	bA	824	CLA	CED-O2D-CGD	2.24	121.00	115.92
12	bB	930	CLA	CMC-C2C-C1C	2.24	128.53	125.03
12	cB	936	CLA	CMB-C2B-C1B	2.24	128.83	125.42
12	cB	904	CLA	CBA-CAA-C2A	2.24	120.46	113.79
12	aA	816	CLA	O1D-CGD-CBD	-2.24	120.10	124.52
12	aB	924	CLA	CBC-CAC-C3C	-2.24	106.35	112.42
12	aA	812	CLA	CMC-C2C-C1C	2.24	128.53	125.03
12	cA	837	CLA	C1-C2-C3	-2.24	122.53	126.20
12	bB	931	CLA	CHB-C1B-C2B	-2.24	120.93	127.43
12	cB	902	CLA	CMA-C3A-C2A	-2.24	105.33	113.98
12	aA	807	CLA	C16-C15-C13	-2.24	108.52	115.97
12	cA	834	CLA	CHB-C1B-C2B	-2.24	120.93	127.43
12	aA	834	CLA	CHB-C1B-C2B	-2.24	120.93	127.43
12	aB	926	CLA	CBA-CAA-C2A	2.24	120.45	113.79
12	bA	812	CLA	CMC-C2C-C1C	2.24	128.53	125.03
15	aB	943	BCR	C40-C30-C25	2.24	113.75	110.24
12	cB	926	CLA	CBA-CAA-C2A	2.24	120.45	113.79
12	aL	203	CLA	CAC-C3C-C4C	2.24	127.70	124.79
12	aF	202	CLA	CBC-CAC-C3C	-2.24	106.36	112.42
12	aB	914	CLA	CHB-C4A-NA	2.24	127.63	124.40
12	bF	202	CLA	CHB-C4A-NA	2.24	127.63	124.40
12	bA	829	CLA	CBC-CAC-C3C	-2.24	106.36	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cB	924	CLA	CBC-CAC-C3C	-2.24	106.36	112.42
12	bB	914	CLA	CHB-C4A-NA	2.24	127.63	124.40
12	bB	902	CLA	CMA-C3A-C2A	-2.24	105.34	113.98
12	cB	921	CLA	CBC-CAC-C3C	-2.24	106.36	112.42
16	bA	851	LHG	C20-C19-C18	-2.23	103.07	114.37
12	aB	906	CLA	CED-O2D-CGD	2.23	120.98	115.92
12	bA	830	CLA	CMC-C2C-C1C	2.23	128.53	125.03
12	bA	807	CLA	C16-C15-C13	-2.23	108.54	115.97
11	aA	801	CL0	CGD-CBD-CAD	-2.23	103.62	110.85
12	cA	811	CLA	CMB-C2B-C1B	2.23	128.82	125.42
12	bB	936	CLA	CMC-C2C-C1C	2.23	128.52	125.03
15	bF	201	BCR	C24-C23-C22	-2.23	122.93	126.23
12	cB	918	CLA	CHD-C4C-NC	2.23	127.69	124.23
12	cA	807	CLA	C16-C15-C13	-2.23	108.55	115.97
12	bB	950	CLA	CHB-C4A-NA	2.23	127.62	124.40
12	aB	931	CLA	CHB-C1B-C2B	-2.23	120.95	127.43
12	aA	829	CLA	CBC-CAC-C3C	-2.23	106.37	112.42
12	aB	921	CLA	CBC-CAC-C3C	-2.23	106.37	112.42
12	bB	938	CLA	CBC-CAC-C3C	-2.23	106.37	112.42
12	aL	204	CLA	CHB-C4A-NA	2.23	127.62	124.40
16	aA	852	LHG	C20-C19-C18	-2.23	103.09	114.37
12	bA	831	CLA	CAA-C2A-C3A	-2.23	106.97	113.00
12	aA	831	CLA	CMC-C2C-C1C	2.23	128.52	125.03
12	aB	936	CLA	CMB-C2B-C1B	2.23	128.81	125.42
15	cA	850	BCR	C20-C19-C18	-2.23	120.25	126.36
12	bA	811	CLA	CMB-C2B-C1B	2.23	128.81	125.42
12	cA	827	CLA	CMB-C2B-C3B	2.23	131.79	126.55
12	bB	936	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
16	cA	851	LHG	C20-C19-C18	-2.23	103.10	114.37
12	aA	827	CLA	CMB-C2B-C3B	2.23	131.79	126.55
12	aA	835	CLA	CHB-C1B-C2B	-2.23	120.96	127.43
11	cA	801	CL0	CGD-CBD-CAD	-2.23	103.63	110.85
12	cA	836	CLA	C4C-C3C-C2C	-2.23	103.65	106.89
12	aB	923	CLA	O1D-CGD-CBD	-2.23	120.13	124.52
12	bB	909	CLA	CHD-C4C-NC	2.23	127.68	124.23
15	cM	101	BCR	C24-C23-C22	-2.23	122.94	126.23
12	cB	906	CLA	O2A-CGA-CBA	2.23	118.62	111.83
12	aA	836	CLA	C4C-C3C-C2C	-2.23	103.65	106.89
12	cB	909	CLA	CHD-C4C-NC	2.23	127.68	124.23
12	cA	837	CLA	O2A-CGA-CBA	2.23	118.62	111.83
12	cA	826	CLA	CHB-C4A-NA	2.23	127.61	124.40
12	bA	816	CLA	O1D-CGD-CBD	-2.22	120.13	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	bM	101	BCR	C24-C23-C22	-2.22	122.94	126.23
12	aB	903	CLA	CHB-C4A-NA	2.22	127.61	124.40
12	bB	936	CLA	CMB-C2B-C1B	2.22	128.81	125.42
12	bF	202	CLA	CBC-CAC-C3C	-2.22	106.39	112.42
12	bA	807	CLA	C4-C3-C5	2.22	119.09	115.23
15	bB	943	BCR	C40-C30-C25	2.22	113.73	110.24
12	cA	816	CLA	O1D-CGD-CBD	-2.22	120.13	124.52
12	cB	903	CLA	C1-C2-C3	-2.22	122.55	126.20
12	cB	931	CLA	CHB-C1B-C2B	-2.22	120.97	127.43
12	cB	910	CLA	CMC-C2C-C1C	2.22	128.51	125.03
12	bA	826	CLA	CHB-C4A-NA	2.22	127.61	124.40
12	cA	829	CLA	CHB-C4A-NA	2.22	127.61	124.40
12	bB	926	CLA	CBA-CAA-C2A	2.22	120.41	113.79
12	aB	938	CLA	CBC-CAC-C3C	-2.22	106.39	112.42
12	cB	915	CLA	CHB-C4A-NA	2.22	127.61	124.40
12	cF	202	CLA	CBC-CAC-C3C	-2.22	106.40	112.42
12	bB	921	CLA	CBC-CAC-C3C	-2.22	106.40	112.42
12	bA	837	CLA	C1-C2-C3	-2.22	122.56	126.20
12	bB	916	CLA	CHB-C1B-C2B	-2.22	120.98	127.43
12	bB	903	CLA	C1-C2-C3	-2.22	122.56	126.20
12	cF	202	CLA	CHB-C4A-NA	2.22	127.61	124.40
12	cB	908	CLA	CHD-C4C-NC	2.22	127.67	124.23
12	cB	916	CLA	CHB-C1B-C2B	-2.22	120.98	127.43
12	cB	925	CLA	CAC-C3C-C4C	2.22	127.68	124.79
12	cA	835	CLA	CHB-C1B-C2B	-2.22	120.98	127.43
12	aB	916	CLA	CHB-C1B-C2B	-2.22	120.98	127.43
12	aA	829	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
12	cB	914	CLA	CHB-C4A-NA	2.22	127.60	124.40
12	cA	829	CLA	CBC-CAC-C3C	-2.22	106.40	112.42
12	cA	824	CLA	CHB-C4A-NA	2.22	127.60	124.40
12	aA	830	CLA	CMC-C2C-C1C	2.22	128.50	125.03
15	aF	201	BCR	C24-C23-C22	-2.22	122.95	126.23
12	cB	903	CLA	C4A-NA-C1A	-2.22	105.67	106.68
12	cA	807	CLA	C7-C6-C5	-2.22	107.35	113.26
12	aA	811	CLA	CMB-C2B-C1B	2.22	128.80	125.42
11	bA	801	CL0	CGD-CBD-CAD	-2.22	103.67	110.85
15	aM	101	BCR	C24-C23-C22	-2.22	122.95	126.23
12	aA	833	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
12	cA	831	CLA	CMC-C2C-C1C	2.22	128.50	125.03
15	bA	848	BCR	C15-C16-C17	-2.22	118.98	123.52
12	aA	829	CLA	CMB-C2B-C3B	2.22	131.76	126.55
15	bA	850	BCR	C20-C19-C18	-2.22	120.29	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cB	926	CLA	CMB-C2B-C1B	2.22	128.79	125.42
12	aA	807	CLA	C7-C6-C5	-2.22	107.36	113.26
12	cB	931	CLA	C3B-C4B-NB	2.21	112.51	110.53
12	cB	939	CLA	CHB-C4A-NA	2.21	127.59	124.40
15	bF	201	BCR	C10-C11-C12	-2.21	116.78	123.20
15	cF	201	BCR	C10-C11-C12	-2.21	116.78	123.20
12	bA	827	CLA	CMB-C2B-C3B	2.21	131.76	126.55
12	aB	903	CLA	C1-C2-C3	-2.21	122.57	126.20
12	bA	835	CLA	CHB-C1B-C2B	-2.21	121.00	127.43
12	cB	930	CLA	CMC-C2C-C1C	2.21	128.49	125.03
15	aF	203	BCR	C38-C26-C27	-2.21	108.88	113.60
12	cA	807	CLA	C4-C3-C5	2.21	119.07	115.23
12	aB	931	CLA	C3B-C4B-NB	2.21	112.50	110.53
12	cB	938	CLA	CBC-CAC-C3C	-2.21	106.43	112.42
12	cB	937	CLA	CHB-C4A-NA	2.21	127.59	124.40
15	cF	201	BCR	C24-C23-C22	-2.21	122.97	126.23
12	aB	936	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
12	cA	829	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
12	cA	833	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
11	aA	801	CL0	C3D-C4D-ND	2.21	116.48	112.94
12	bA	838	CLA	C3B-C4B-NB	2.21	112.50	110.53
15	aB	945	BCR	C7-C8-C9	-2.21	122.97	126.23
12	aA	807	CLA	C4-C3-C5	2.21	119.06	115.23
12	bB	925	CLA	CAC-C3C-C4C	2.21	127.66	124.79
12	bB	923	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
15	aA	851	BCR	C20-C19-C18	-2.21	120.31	126.36
12	bB	926	CLA	CMB-C2B-C1B	2.21	128.78	125.42
12	bA	833	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
12	bA	829	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
12	aA	838	CLA	C3B-C4B-NB	2.21	112.50	110.53
11	bA	801	CL0	C3D-C4D-ND	2.21	116.48	112.94
12	bA	829	CLA	CHB-C4A-NA	2.21	127.58	124.40
12	aA	826	CLA	CHB-C4A-NA	2.21	127.58	124.40
12	bA	807	CLA	C7-C6-C5	-2.21	107.38	113.26
12	cA	829	CLA	CMB-C2B-C3B	2.21	131.74	126.55
12	cA	821	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
12	bA	837	CLA	O2A-CGA-CBA	2.20	118.56	111.83
12	bA	843	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
15	bF	203	BCR	C38-C26-C27	-2.20	108.90	113.60
12	aB	926	CLA	CMB-C2B-C1B	2.20	128.77	125.42
12	aB	903	CLA	C1-O2A-CGA	2.20	121.98	116.65
12	bB	950	CLA	CBC-CAC-C3C	-2.20	106.45	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	824	CLA	CHB-C4A-NA	2.20	127.58	124.40
12	aA	837	CLA	O2A-CGA-CBA	2.20	118.55	111.83
12	bB	908	CLA	CHD-C4C-NC	2.20	127.64	124.23
12	bB	909	CLA	C1-O2A-CGA	2.20	121.98	116.65
12	cA	812	CLA	CHD-C4C-NC	2.20	127.64	124.23
12	cB	936	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
12	aA	828	CLA	C1-C2-C3	-2.20	122.59	126.20
15	cB	945	BCR	C7-C8-C9	-2.20	122.98	126.23
12	aA	808	CLA	CMC-C2C-C1C	2.20	128.47	125.03
12	cA	812	CLA	CMC-C2C-C1C	2.20	128.47	125.03
12	aB	936	CLA	CMA-C3A-C2A	-2.20	105.48	113.98
12	aB	925	CLA	CAC-C3C-C4C	2.20	127.65	124.79
15	cA	848	BCR	C15-C16-C17	-2.20	119.02	123.52
12	bA	811	CLA	CHB-C4A-NA	2.20	127.57	124.40
12	aB	923	CLA	C3B-C4B-NB	2.20	112.49	110.53
12	aA	844	CLA	CBC-CAC-C3C	-2.20	106.46	112.42
15	cF	203	BCR	C38-C26-C27	-2.20	108.91	113.60
12	bB	935	CLA	CHA-C1A-NA	-2.20	121.42	126.39
17	cB	947	LMG	O2-C2-C1	-2.20	104.84	110.08
12	bB	936	CLA	CMA-C3A-C2A	-2.20	105.49	113.98
12	bB	910	CLA	CMC-C2C-C1C	2.20	128.47	125.03
12	bB	903	CLA	C1-O2A-CGA	2.20	121.97	116.65
12	aA	821	CLA	O2A-CGA-O1A	-2.20	118.14	123.63
15	aA	848	BCR	C38-C26-C27	-2.19	108.92	113.60
13	aA	845	1L3	C14-C03-C04	2.19	120.89	118.58
12	bB	933	CLA	CED-O2D-CGD	2.19	120.89	115.92
15	bB	945	BCR	C27-C26-C25	2.19	125.67	122.70
12	bA	838	CLA	CBA-CAA-C2A	2.19	120.32	113.79
15	aA	849	BCR	C15-C16-C17	-2.19	119.03	123.52
12	cB	935	CLA	CHA-C1A-NA	-2.19	121.42	126.39
12	aL	203	CLA	C3B-C4B-NB	2.19	112.49	110.53
12	bA	824	CLA	CHB-C4A-NA	2.19	127.56	124.40
12	cA	802	CLA	CHB-C1B-C2B	-2.19	121.06	127.43
15	bA	847	BCR	C38-C26-C27	-2.19	108.92	113.60
12	cB	936	CLA	CMA-C3A-C2A	-2.19	105.51	113.98
12	cA	843	CLA	O2D-CGD-O1D	-2.19	119.58	123.85
12	bA	829	CLA	CMB-C2B-C3B	2.19	131.71	126.55
12	aB	933	CLA	CED-O2D-CGD	2.19	120.89	115.92
12	aA	812	CLA	CMA-C3A-C2A	-2.19	105.51	113.98
12	bB	915	CLA	CHB-C4A-NA	2.19	127.56	124.40
12	aA	802	CLA	CHB-C1B-C2B	-2.19	121.07	127.43
12	aB	950	CLA	CBC-CAC-C3C	-2.19	106.48	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cB	945	BCR	C27-C26-C25	2.19	125.66	122.70
12	bB	939	CLA	CHB-C4A-NA	2.19	127.56	124.40
12	aA	829	CLA	CMA-C3A-C2A	-2.19	105.51	113.98
12	aB	950	CLA	CHB-C4A-NA	2.19	127.56	124.40
12	aA	811	CLA	CHB-C4A-NA	2.19	127.56	124.40
12	cA	828	CLA	C1-C2-C3	-2.19	122.61	126.20
12	aB	939	CLA	CHB-C4A-NA	2.19	127.56	124.40
12	bA	802	CLA	CHB-C1B-C2B	-2.19	121.08	127.43
11	cA	801	CL0	C3D-C4D-ND	2.19	116.44	112.94
12	aA	837	CLA	C1-C2-C3	-2.19	122.62	126.20
12	cB	949	CLA	CHB-C4A-NA	2.19	127.55	124.40
15	cM	101	BCR	C16-C15-C14	-2.19	119.05	123.52
12	bA	812	CLA	CMA-C3A-C2A	-2.19	105.53	113.98
12	aB	909	CLA	C1-O2A-CGA	2.19	121.94	116.65
12	cA	838	CLA	CBA-CAA-C2A	2.18	120.29	113.79
12	cB	909	CLA	C1-O2A-CGA	2.18	121.94	116.65
15	aM	101	BCR	C16-C15-C14	-2.18	119.05	123.52
12	bA	808	CLA	CMC-C2C-C1C	2.18	128.45	125.03
15	bB	945	BCR	C7-C8-C9	-2.18	123.00	126.23
12	cA	812	CLA	CMA-C3A-C2A	-2.18	105.54	113.98
12	cA	829	CLA	CMA-C3A-C2A	-2.18	105.54	113.98
12	bA	825	CLA	CED-O2D-CGD	2.18	120.87	115.92
12	cB	923	CLA	O1D-CGD-CBD	-2.18	120.21	124.52
15	bL	205	BCR	C11-C10-C9	-2.18	124.22	127.28
12	aA	812	CLA	CHD-C4C-NC	2.18	127.61	124.23
15	aF	201	BCR	C10-C11-C12	-2.18	116.88	123.20
12	aA	838	CLA	CBA-CAA-C2A	2.18	120.28	113.79
12	bB	915	CLA	C4-C3-C2	-2.18	118.03	123.63
12	bA	829	CLA	CMA-C3A-C2A	-2.18	105.55	113.98
12	cA	808	CLA	CMC-C2C-C1C	2.18	128.44	125.03
12	cB	903	CLA	C1-O2A-CGA	2.18	121.93	116.65
12	bL	203	CLA	C3B-C4B-NB	2.18	112.48	110.53
12	cB	933	CLA	CED-O2D-CGD	2.18	120.86	115.92
12	cB	925	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
12	aB	915	CLA	C4-C3-C2	-2.18	118.03	123.63
12	bA	843	CLA	CED-O2D-CGD	2.18	120.86	115.92
12	bA	804	CLA	CMC-C2C-C1C	2.18	128.44	125.03
15	aL	205	BCR	C11-C10-C9	-2.18	124.22	127.28
12	aB	927	CLA	C1-C2-C3	-2.18	122.63	126.20
12	bB	949	CLA	C2A-C3A-C4A	-2.18	99.04	101.59
17	aB	947	LMG	O2-C2-C1	-2.18	104.89	110.08
12	bB	931	CLA	C3B-C4B-NB	2.18	112.47	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	cA	847	BCR	C38-C26-C27	-2.18	108.96	113.60
12	bA	816	CLA	CMC-C2C-C1C	2.18	128.43	125.03
12	aA	825	CLA	CED-O2D-CGD	2.17	120.85	115.92
15	bM	101	BCR	C16-C15-C14	-2.17	119.07	123.52
12	cA	824	CLA	CHD-C4C-NC	2.17	127.60	124.23
12	aB	935	CLA	CHA-C1A-NA	-2.17	121.47	126.39
13	bA	844	1L3	C14-C03-C04	2.17	120.87	118.58
12	bA	828	CLA	C1-C2-C3	-2.17	122.64	126.20
15	bB	944	BCR	C40-C30-C25	2.17	113.65	110.24
12	cB	915	CLA	C4-C3-C2	-2.17	118.05	123.63
12	aB	909	CLA	CGD-CBD-CAD	-2.17	103.82	110.85
12	aA	816	CLA	CMC-C2C-C1C	2.17	128.43	125.03
12	cA	853	CLA	CHD-C4C-NC	2.17	127.60	124.23
15	cA	847	BCR	C30-C25-C26	-2.17	119.67	122.64
12	cB	923	CLA	C3B-C4B-NB	2.17	112.47	110.53
12	aA	835	CLA	CBC-CAC-C3C	-2.17	106.53	112.42
12	aA	843	CLA	O2D-CGD-O1D	-2.17	119.62	123.85
12	aA	854	CLA	CHD-C4C-NC	2.17	127.60	124.23
12	bA	808	CLA	CHB-C4A-NA	2.17	127.53	124.40
12	aA	840	CLA	C4-C3-C5	2.17	119.00	115.23
12	aA	844	CLA	CHB-C4A-NA	2.17	127.53	124.40
12	bA	824	CLA	O2D-CGD-O1D	-2.17	119.62	123.85
12	bA	821	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
12	aA	824	CLA	O2D-CGD-O1D	-2.17	119.63	123.85
12	bA	835	CLA	CHB-C4A-NA	2.17	127.53	124.40
12	cA	811	CLA	CHB-C4A-NA	2.17	127.53	124.40
12	bB	923	CLA	C3B-C4B-NB	2.17	112.47	110.53
12	cA	824	CLA	CBC-CAC-C3C	-2.17	106.54	112.42
15	cA	846	BCR	C38-C26-C27	-2.17	108.97	113.60
12	bA	853	CLA	CHD-C4C-NC	2.17	127.59	124.23
12	aA	825	CLA	C7-C6-C5	-2.17	107.48	113.26
12	bA	835	CLA	CBC-CAC-C3C	-2.17	106.54	112.42
12	bB	925	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
12	aA	820	CLA	C1-C2-C3	-2.17	122.65	126.20
17	bB	947	LMG	O2-C2-C1	-2.17	104.91	110.08
12	cA	825	CLA	CED-O2D-CGD	2.17	120.83	115.92
12	aA	828	CLA	CMC-C2C-C1C	2.17	128.42	125.03
12	aB	921	CLA	O2D-CGD-O1D	-2.16	119.64	123.85
15	aA	848	BCR	C30-C25-C26	-2.16	119.68	122.64
12	cA	820	CLA	C1-C2-C3	-2.16	122.65	126.20
12	aA	824	CLA	CBC-CAC-C3C	-2.16	106.55	112.42
12	cB	920	CLA	CAC-C3C-C4C	2.16	127.61	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bA	818	CLA	CHA-C1A-NA	-2.16	121.49	126.39
12	cA	831	CLA	C5-C3-C4	2.16	119.56	114.59
12	aB	910	CLA	CMC-C2C-C1C	2.16	128.41	125.03
12	cA	835	CLA	CBC-CAC-C3C	-2.16	106.56	112.42
15	bA	846	BCR	C38-C26-C27	-2.16	108.99	113.60
15	aA	847	BCR	C38-C26-C27	-2.16	108.99	113.60
12	bB	920	CLA	CAC-C3C-C4C	2.16	127.60	124.79
12	aA	808	CLA	C1-O2A-CGA	2.16	121.88	116.65
12	cA	833	CLA	C1-C2-C3	-2.16	122.66	126.20
12	aB	925	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
12	cB	929	CLA	CHB-C4A-NA	2.16	127.52	124.40
12	aA	804	CLA	CMC-C2C-C1C	2.16	128.41	125.03
12	cB	904	CLA	CAA-C2A-C3A	-2.16	107.17	113.00
12	bA	820	CLA	C1-C2-C3	-2.16	122.66	126.20
12	aB	904	CLA	CAA-C2A-C3A	-2.16	107.17	113.00
12	bB	904	CLA	CAA-C2A-C3A	-2.16	107.17	113.00
12	cB	913	CLA	O1D-CGD-CBD	-2.16	120.26	124.52
15	aB	944	BCR	C40-C30-C25	2.16	113.62	110.24
12	bB	949	CLA	CHB-C4A-NA	2.16	127.51	124.40
15	aB	945	BCR	C27-C26-C25	2.16	125.62	122.70
12	bA	812	CLA	CHD-C4C-NC	2.16	127.58	124.23
12	aA	819	CLA	CAC-C3C-C4C	2.16	127.59	124.79
12	cA	843	CLA	CED-O2D-CGD	2.16	120.81	115.92
12	cB	919	CLA	CHA-C1A-NA	-2.16	121.51	126.39
12	cA	808	CLA	C1-O2A-CGA	2.16	121.87	116.65
15	aI	101	BCR	C31-C1-C6	2.16	113.62	110.24
12	bA	840	CLA	C4-C3-C5	2.16	118.97	115.23
12	cA	805	CLA	C1-C2-C3	-2.16	122.67	126.20
12	cA	816	CLA	CMC-C2C-C1C	2.15	128.40	125.03
12	cA	807	CLA	CHB-C4A-NA	2.15	127.51	124.40
12	bB	923	CLA	CMB-C2B-C1B	2.15	128.70	125.42
12	bB	913	CLA	O1D-CGD-CBD	-2.15	120.27	124.52
12	aB	939	CLA	O2A-CGA-CBA	2.15	120.80	114.00
15	cI	101	BCR	C31-C1-C6	2.15	113.62	110.24
12	aB	930	CLA	CMB-C2B-C3B	2.15	131.61	126.55
12	cB	911	CLA	CAA-C2A-C3A	-2.15	107.18	113.00
12	bA	824	CLA	CBC-CAC-C3C	-2.15	106.58	112.42
12	bB	911	CLA	CAA-C2A-C3A	-2.15	107.18	113.00
12	bA	824	CLA	CHD-C4C-NC	2.15	127.57	124.23
12	cA	840	CLA	C4-C3-C5	2.15	118.96	115.23
12	bB	909	CLA	CGD-CBD-CAD	-2.15	103.88	110.85
12	aA	823	CLA	O2A-CGA-O1A	-2.15	118.25	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cB	909	CLA	CGD-CBD-CAD	-2.15	103.88	110.85
12	cA	808	CLA	CHB-C4A-NA	2.15	127.50	124.40
12	aA	824	CLA	CMB-C2B-C1B	2.15	128.69	125.42
12	bA	828	CLA	CMC-C2C-C1C	2.15	128.39	125.03
12	cB	927	CLA	C1-C2-C3	-2.15	122.68	126.20
15	bB	946	BCR	C38-C26-C27	-2.15	109.02	113.60
12	cB	930	CLA	CMB-C2B-C3B	2.15	131.60	126.55
12	cA	835	CLA	CHB-C4A-NA	2.15	127.50	124.40
15	bJ	101	BCR	C28-C27-C26	-2.15	110.22	114.06
12	aA	805	CLA	CHB-C1B-C2B	-2.15	121.19	127.43
12	aA	824	CLA	CHD-C4C-NC	2.15	127.56	124.23
12	bB	927	CLA	CHD-C4C-NC	2.15	127.56	124.23
12	cB	927	CLA	CHD-C4C-NC	2.15	127.56	124.23
12	aA	833	CLA	C1-C2-C3	-2.15	122.68	126.20
12	cA	804	CLA	CMC-C2C-C1C	2.15	128.39	125.03
12	bB	922	CLA	CAC-C3C-C4C	2.15	127.58	124.79
12	aB	949	CLA	C2A-C3A-C4A	-2.15	99.08	101.59
12	aB	911	CLA	CAA-C2A-C3A	-2.15	107.20	113.00
12	aA	818	CLA	CHA-C1A-NA	-2.15	121.53	126.39
12	aB	920	CLA	O2A-CGA-CBA	2.15	120.78	114.00
12	cB	927	CLA	CHB-C4A-NA	2.15	127.50	124.40
12	aB	927	CLA	CHD-C4C-NC	2.15	127.56	124.23
15	cB	944	BCR	C40-C30-C25	2.15	113.61	110.24
12	aA	831	CLA	C5-C3-C4	2.14	119.53	114.59
12	bB	930	CLA	CMB-C2B-C3B	2.14	131.59	126.55
12	bB	928	CLA	O1D-CGD-CBD	-2.14	120.29	124.52
15	bI	101	BCR	C31-C1-C6	2.14	113.61	110.24
12	bB	921	CLA	O2D-CGD-O1D	-2.14	119.67	123.85
12	aB	923	CLA	CMB-C2B-C1B	2.14	128.68	125.42
12	bB	921	CLA	CHA-C1A-NA	-2.14	121.54	126.39
12	cA	824	CLA	O2D-CGD-O1D	-2.14	119.68	123.85
12	cB	935	CLA	CHB-C1B-C2B	-2.14	121.20	127.43
12	aB	922	CLA	CAC-C3C-C4C	2.14	127.58	124.79
12	bA	808	CLA	C1-O2A-CGA	2.14	121.84	116.65
12	aB	919	CLA	CHA-C1A-NA	-2.14	121.54	126.39
12	aB	913	CLA	O1D-CGD-CBD	-2.14	120.29	124.52
12	aB	949	CLA	CHB-C4A-NA	2.14	127.49	124.40
15	aJ	101	BCR	C28-C27-C26	-2.14	110.24	114.06
12	cA	825	CLA	C7-C6-C5	-2.14	107.56	113.26
12	aA	808	CLA	CHB-C4A-NA	2.14	127.49	124.40
12	bA	805	CLA	C1-C2-C3	-2.14	122.69	126.20
12	cB	949	CLA	C2A-C3A-C4A	-2.14	99.08	101.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bB	903	CLA	O2A-CGA-CBA	2.14	118.36	111.83
15	bA	847	BCR	C30-C25-C26	-2.14	119.71	122.64
12	cA	818	CLA	CHA-C1A-NA	-2.14	121.55	126.39
12	bA	832	CLA	C2A-C1A-CHA	-2.14	120.16	123.87
12	cB	921	CLA	O2D-CGD-O1D	-2.14	119.69	123.85
12	bB	919	CLA	CHA-C1A-NA	-2.14	121.55	126.39
15	bB	944	BCR	C15-C16-C17	-2.14	119.14	123.52
12	cA	807	CLA	CHB-C1B-C2B	-2.14	121.22	127.43
12	bA	823	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
12	aB	921	CLA	CHA-C1A-NA	-2.14	121.55	126.39
12	aA	832	CLA	C2A-C1A-CHA	-2.14	120.16	123.87
12	aB	934	CLA	CHB-C4A-NA	2.14	127.48	124.40
12	cA	832	CLA	C2A-C1A-CHA	-2.14	120.16	123.87
12	bA	814	CLA	O1D-CGD-CBD	-2.14	120.30	124.52
12	aB	903	CLA	O2A-CGA-CBA	2.14	118.35	111.83
12	aB	935	CLA	CHB-C1B-C2B	-2.14	121.23	127.43
12	cA	853	CLA	CHB-C4A-NA	2.14	127.48	124.40
12	aB	920	CLA	CAC-C3C-C4C	2.14	127.57	124.79
15	bB	941	BCR	C28-C27-C26	-2.14	110.25	114.06
12	cB	923	CLA	CMB-C2B-C1B	2.14	128.67	125.42
13	cA	844	1L3	C14-C03-C04	2.14	120.83	118.58
12	bB	927	CLA	C1-C2-C3	-2.14	122.70	126.20
15	aB	946	BCR	C38-C26-C27	-2.13	109.04	113.60
12	bB	926	CLA	CMA-C3A-C2A	-2.13	105.73	113.98
12	bB	935	CLA	CHB-C1B-C2B	-2.13	121.23	127.43
12	cB	928	CLA	O1D-CGD-CBD	-2.13	120.31	124.52
12	aB	927	CLA	CHB-C4A-NA	2.13	127.48	124.40
15	cB	944	BCR	C15-C16-C17	-2.13	119.15	123.52
12	aB	922	CLA	O2A-CGA-O1A	-2.13	117.84	123.33
12	bA	825	CLA	C7-C6-C5	-2.13	107.57	113.26
12	bB	908	CLA	CED-O2D-CGD	2.13	120.76	115.92
12	cA	805	CLA	CHB-C1B-C2B	-2.13	121.23	127.43
12	bA	853	CLA	CHB-C4A-NA	2.13	127.48	124.40
12	bB	913	CLA	CMA-C3A-C2A	-2.13	105.73	113.98
12	aB	908	CLA	CED-O2D-CGD	2.13	120.75	115.92
12	aA	807	CLA	CHB-C1B-C2B	-2.13	121.23	127.43
12	aA	821	CLA	CHB-C1B-C2B	-2.13	121.23	127.43
12	cB	922	CLA	O2A-CGA-O1A	-2.13	117.85	123.33
12	bB	920	CLA	O2A-CGA-CBA	2.13	120.74	114.00
12	cB	922	CLA	CMA-C3A-C2A	-2.13	105.74	113.98
12	cB	917	CLA	O1A-CGA-CBA	-2.13	115.44	123.78
12	bB	937	CLA	O2A-CGA-O1A	-2.13	118.30	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aB	913	CLA	CMA-C3A-C2A	-2.13	105.74	113.98
15	cB	946	BCR	C38-C26-C27	-2.13	109.05	113.60
12	bA	831	CLA	C5-C3-C4	2.13	119.49	114.59
15	cL	205	BCR	C11-C10-C9	-2.13	124.29	127.28
12	aB	931	CLA	CHB-C4A-NA	2.13	127.47	124.40
12	cB	935	CLA	CBA-CAA-C2A	-2.13	107.45	113.79
12	cB	926	CLA	CMA-C3A-C2A	-2.13	105.75	113.98
12	cA	806	CLA	CMC-C2C-C1C	2.13	128.36	125.03
12	cA	828	CLA	CMC-C2C-C1C	2.13	128.36	125.03
12	bB	906	CLA	CBC-CAC-C3C	-2.13	106.65	112.42
12	cB	906	CLA	CBC-CAC-C3C	-2.13	106.65	112.42
12	aA	843	CLA	CED-O2D-CGD	2.13	120.75	115.92
12	bA	821	CLA	CHB-C1B-C2B	-2.13	121.25	127.43
12	cA	821	CLA	CHB-C1B-C2B	-2.13	121.25	127.43
12	aB	937	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
12	bB	903	CLA	C4A-NA-C1A	-2.13	105.71	106.68
12	aA	812	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
12	bA	824	CLA	CMB-C2B-C1B	2.13	128.66	125.42
12	bB	927	CLA	CHB-C4A-NA	2.13	127.47	124.40
12	cA	807	CLA	O2D-CGD-CBD	2.13	114.95	111.23
15	aB	941	BCR	C28-C27-C26	-2.13	110.26	114.06
12	cB	913	CLA	CMA-C3A-C2A	-2.13	105.76	113.98
12	bA	805	CLA	CHB-C1B-C2B	-2.13	121.25	127.43
12	cA	824	CLA	CMB-C2B-C1B	2.13	128.66	125.42
12	cB	920	CLA	O2A-CGA-CBA	2.13	120.72	114.00
12	bB	931	CLA	CMB-C2B-C1B	2.13	128.66	125.42
12	aA	854	CLA	C1-C2-C3	-2.13	122.71	126.20
12	cB	908	CLA	CED-O2D-CGD	2.13	120.74	115.92
12	bB	939	CLA	O2A-CGA-CBA	2.13	120.72	114.00
15	bF	204	BCR	C1-C6-C5	-2.13	119.73	122.64
15	aB	944	BCR	C15-C16-C17	-2.13	119.17	123.52
12	bA	819	CLA	CAC-C3C-C4C	2.13	127.56	124.79
12	aA	805	CLA	C1-C2-C3	-2.13	122.72	126.20
16	cA	851	LHG	C18-C17-C16	-2.12	103.63	114.37
12	bA	807	CLA	CHB-C1B-C2B	-2.12	121.26	127.43
12	bB	935	CLA	CBA-CAA-C2A	-2.12	107.47	113.79
12	aB	929	CLA	CHB-C4A-NA	2.12	127.47	124.40
12	bA	810	CLA	C4B-C3B-C2B	-2.12	104.66	107.30
12	aA	806	CLA	CMA-C3A-C2A	-2.12	105.77	113.98
12	cA	813	CLA	CHA-C1A-NA	-2.12	121.58	126.39
16	aA	852	LHG	C18-C17-C16	-2.12	103.63	114.37
12	cB	922	CLA	CAC-C3C-C4C	2.12	127.55	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aB	926	CLA	CMA-C3A-C2A	-2.12	105.78	113.98
12	bA	813	CLA	CHB-C4A-NA	2.12	127.46	124.40
12	cB	913	CLA	CHB-C4A-NA	2.12	127.46	124.40
12	bB	922	CLA	O2A-CGA-O1A	-2.12	117.88	123.33
12	bA	806	CLA	CMA-C3A-C2A	-2.12	105.78	113.98
12	aA	825	CLA	C1-O2A-CGA	2.12	121.78	116.65
12	bA	807	CLA	CHB-C4A-NA	2.12	127.46	124.40
16	bA	851	LHG	C18-C17-C16	-2.12	103.65	114.37
12	bB	929	CLA	CHB-C4A-NA	2.12	127.46	124.40
12	cB	903	CLA	O2A-CGA-CBA	2.12	118.30	111.83
15	cL	205	BCR	C16-C15-C14	-2.12	119.18	123.52
12	cB	939	CLA	O2A-CGA-CBA	2.12	120.70	114.00
12	cL	203	CLA	C3B-C4B-NB	2.12	112.42	110.53
12	aB	928	CLA	O1D-CGD-CBD	-2.12	120.34	124.52
12	cB	928	CLA	CBC-CAC-C3C	-2.12	106.67	112.42
12	cF	202	CLA	O2A-CGA-CBA	2.12	120.69	114.00
12	bB	928	CLA	CBC-CAC-C3C	-2.12	106.68	112.42
12	cB	921	CLA	CHA-C1A-NA	-2.12	121.59	126.39
12	aA	813	CLA	CHA-C1A-NA	-2.12	121.59	126.39
12	cA	813	CLA	CAA-C2A-C3A	-2.12	107.28	113.00
12	bA	825	CLA	C1-O2A-CGA	2.12	121.78	116.65
12	bB	922	CLA	CMA-C3A-C2A	-2.12	105.80	113.98
12	aA	814	CLA	O1D-CGD-CBD	-2.12	120.34	124.52
12	bA	813	CLA	CAA-C2A-C3A	-2.12	107.28	113.00
12	bB	913	CLA	CHB-C4A-NA	2.12	127.45	124.40
12	aA	806	CLA	CMC-C2C-C1C	2.12	128.34	125.03
12	bA	812	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
12	bB	918	CLA	O2A-CGA-CBA	2.12	120.14	112.14
12	aB	917	CLA	O1A-CGA-CBA	-2.12	115.50	123.78
12	cA	813	CLA	CHB-C4A-NA	2.12	127.45	124.40
12	cB	937	CLA	O2A-CGA-O1A	-2.12	118.34	123.63
15	cF	203	BCR	C11-C10-C9	-2.12	124.31	127.28
15	cJ	101	BCR	C28-C27-C26	-2.12	110.28	114.06
12	cA	811	CLA	CMC-C2C-C1C	2.11	128.34	125.03
12	cB	906	CLA	CHB-C4A-NA	2.11	127.45	124.40
12	bA	813	CLA	CHA-C1A-NA	-2.11	121.60	126.39
12	cA	819	CLA	CAC-C3C-C4C	2.11	127.54	124.79
12	aA	806	CLA	CMB-C2B-C3B	2.11	131.52	126.55
12	aB	935	CLA	CBA-CAA-C2A	-2.11	107.51	113.79
12	aB	922	CLA	CMA-C3A-C2A	-2.11	105.81	113.98
12	aA	830	CLA	CMA-C3A-C4A	-2.11	106.10	111.77
12	aA	814	CLA	O2D-CGD-O1D	-2.11	119.74	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aB	911	CLA	CMB-C2B-C1B	2.11	128.63	125.42
12	bA	833	CLA	C1-C2-C3	-2.11	122.74	126.20
12	bB	917	CLA	O1A-CGA-CBA	-2.11	115.53	123.78
12	aB	906	CLA	CBC-CAC-C3C	-2.11	106.70	112.42
12	cB	917	CLA	CHA-C1A-NA	-2.11	121.61	126.39
12	aA	813	CLA	CAA-C2A-C3A	-2.11	107.30	113.00
15	cB	941	BCR	C28-C27-C26	-2.11	110.29	114.06
12	bB	912	CLA	CHA-C1A-NA	-2.11	121.61	126.39
12	bB	917	CLA	CHA-C1A-NA	-2.11	121.61	126.39
15	aB	945	BCR	C40-C30-C25	2.11	113.55	110.24
12	cA	823	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
12	aA	807	CLA	CHB-C4A-NA	2.11	127.44	124.40
12	cA	810	CLA	C4B-C3B-C2B	-2.11	104.68	107.30
12	bA	830	CLA	CMA-C3A-C4A	-2.11	106.10	111.77
12	bA	819	CLA	C3A-C2A-C1A	2.11	104.50	101.34
12	cA	806	CLA	CMB-C2B-C3B	2.11	131.51	126.55
12	cA	834	CLA	C4B-C3B-C2B	-2.11	104.68	107.30
15	aF	204	BCR	C20-C21-C22	-2.11	124.32	127.28
15	cF	204	BCR	C11-C10-C9	-2.11	124.32	127.28
12	aB	928	CLA	CBC-CAC-C3C	-2.11	106.70	112.42
12	cA	814	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
15	cF	204	BCR	C1-C6-C5	-2.11	119.75	122.64
12	cA	825	CLA	C1-O2A-CGA	2.11	121.75	116.65
12	cA	836	CLA	O2A-CGA-CBA	2.11	120.66	114.00
12	cB	918	CLA	O2A-CGA-CBA	2.11	120.10	112.14
12	bB	905	CLA	CHB-C4A-NA	2.11	127.44	124.40
12	aA	822	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
12	bB	934	CLA	CHB-C4A-NA	2.11	127.44	124.40
12	cB	934	CLA	CHB-C4A-NA	2.11	127.44	124.40
12	bB	912	CLA	CMC-C2C-C1C	2.11	128.33	125.03
12	cB	911	CLA	CMB-C2B-C1B	2.11	128.62	125.42
12	aB	922	CLA	CMC-C2C-C1C	2.11	128.32	125.03
12	cA	806	CLA	CMA-C3A-C2A	-2.10	105.84	113.98
15	bF	204	BCR	C11-C10-C9	-2.10	124.33	127.28
12	bA	853	CLA	C1-C2-C3	-2.10	122.75	126.20
12	bB	911	CLA	CMB-C2B-C1B	2.10	128.62	125.42
12	aB	917	CLA	CHA-C1A-NA	-2.10	121.63	126.39
12	cA	853	CLA	C1-C2-C3	-2.10	122.75	126.20
12	aB	913	CLA	CHB-C4A-NA	2.10	127.43	124.40
15	cB	945	BCR	C40-C30-C25	2.10	113.54	110.24
12	cA	822	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
12	aA	835	CLA	CHB-C4A-NA	2.10	127.43	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	819	CLA	C3A-C2A-C1A	2.10	104.48	101.34
12	aB	918	CLA	O2A-CGA-CBA	2.10	120.07	112.14
15	cL	206	BCR	C30-C25-C26	-2.10	119.77	122.64
12	bA	806	CLA	CMB-C2B-C3B	2.10	131.49	126.55
12	cA	830	CLA	CMA-C3A-C4A	-2.10	106.13	111.77
15	aL	205	BCR	C16-C15-C14	-2.10	119.22	123.52
15	cJ	101	BCR	C40-C30-C25	2.10	113.53	110.24
12	cA	812	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
12	cB	909	CLA	CBC-CAC-C3C	-2.10	106.73	112.42
11	cA	801	CL0	O1D-CGD-CBD	-2.10	121.54	124.72
12	bF	202	CLA	O2A-CGA-CBA	2.10	120.62	114.00
12	bA	806	CLA	CMC-C2C-C1C	2.10	128.31	125.03
12	aA	836	CLA	O2A-CGA-CBA	2.10	120.62	114.00
12	cA	837	CLA	CHD-C4C-NC	2.10	127.48	124.23
12	aA	810	CLA	CHB-C4A-NA	2.09	127.42	124.40
12	aB	922	CLA	CHB-C4A-NA	2.09	127.42	124.40
12	aF	202	CLA	O2A-CGA-CBA	2.09	120.62	114.00
15	bI	101	BCR	C30-C25-C26	-2.09	119.77	122.64
12	aB	930	CLA	O2A-C1-C2	2.09	113.97	108.99
12	aB	935	CLA	CAA-C2A-C3A	-2.09	107.34	113.00
12	cA	814	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
12	bB	929	CLA	O2A-CGA-CBA	2.09	120.61	114.00
15	bL	205	BCR	C16-C15-C14	-2.09	119.24	123.52
12	cA	837	CLA	OBD-CAD-C3D	-2.09	123.53	128.42
15	aI	101	BCR	C30-C25-C26	-2.09	119.78	122.64
12	aA	813	CLA	CHB-C4A-NA	2.09	127.42	124.40
12	cA	803	CLA	C6-C7-C8	-2.09	109.02	115.97
12	cB	935	CLA	CAA-C2A-C3A	-2.09	107.35	113.00
12	cB	929	CLA	O2A-CGA-CBA	2.09	120.61	114.00
15	cF	204	BCR	C15-C16-C17	-2.09	119.24	123.52
12	bA	811	CLA	CMC-C2C-C1C	2.09	128.30	125.03
12	cB	912	CLA	CMC-C2C-C1C	2.09	128.30	125.03
15	cF	203	BCR	C33-C5-C6	-2.09	122.20	124.48
12	bA	834	CLA	C4B-C3B-C2B	-2.09	104.70	107.30
12	cB	931	CLA	CHB-C4A-NA	2.09	127.42	124.40
11	aA	801	CL0	O1D-CGD-CBD	-2.09	121.55	124.72
12	aA	806	CLA	C4-C3-C5	2.09	118.86	115.23
12	aA	810	CLA	C4B-C3B-C2B	-2.09	104.70	107.30
12	aA	822	CLA	CMB-C2B-C3B	2.09	131.46	126.55
12	cB	930	CLA	O2A-C1-C2	2.09	113.96	108.99
12	aB	931	CLA	CMB-C2B-C1B	2.09	128.60	125.42
12	aA	803	CLA	C6-C7-C8	-2.09	109.03	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aA	807	CLA	O2D-CGD-CBD	2.09	114.88	111.23
12	cA	819	CLA	C3A-C2A-C1A	2.09	104.46	101.34
12	aA	834	CLA	C4B-C3B-C2B	-2.09	104.71	107.30
12	cB	925	CLA	CHA-C1A-NA	-2.09	121.67	126.39
12	bA	803	CLA	C6-C7-C8	-2.09	109.03	115.97
12	bA	842	CLA	CED-O2D-CGD	2.09	120.65	115.92
12	aB	929	CLA	O2A-CGA-CBA	2.09	120.59	114.00
12	aA	812	CLA	C4-C3-C5	2.08	118.85	115.23
12	cA	812	CLA	C4-C3-C5	2.08	118.85	115.23
12	bB	925	CLA	CHA-C1A-NA	-2.08	121.67	126.39
12	cA	823	CLA	CAC-C3C-C4C	2.08	127.50	124.79
12	bB	931	CLA	CHB-C4A-NA	2.08	127.41	124.40
12	cB	912	CLA	CHA-C1A-NA	-2.08	121.67	126.39
12	cA	809	CLA	CBC-CAC-C3C	-2.08	106.77	112.42
12	bA	822	CLA	CMB-C2B-C3B	2.08	131.45	126.55
12	cB	931	CLA	CMB-C2B-C1B	2.08	128.59	125.42
15	aF	204	BCR	C1-C6-C5	-2.08	119.79	122.64
12	bA	828	CLA	CHB-C1B-C2B	-2.08	121.38	127.43
15	aF	204	BCR	C11-C10-C9	-2.08	124.36	127.28
12	aB	905	CLA	CHB-C4A-NA	2.08	127.41	124.40
12	cB	922	CLA	CMC-C2C-C1C	2.08	128.29	125.03
12	bA	836	CLA	O2A-CGA-CBA	2.08	120.58	114.00
12	bB	911	CLA	O2A-CGA-O1A	-2.08	117.98	123.33
15	aF	204	BCR	C15-C16-C17	-2.08	119.26	123.52
12	aB	909	CLA	CBC-CAC-C3C	-2.08	106.78	112.42
12	bA	807	CLA	O2D-CGD-CBD	2.08	114.87	111.23
15	cI	101	BCR	C30-C25-C26	-2.08	119.79	122.64
12	aB	925	CLA	CHA-C1A-NA	-2.08	121.68	126.39
12	aB	912	CLA	CMC-C2C-C1C	2.08	128.28	125.03
12	bA	822	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
12	aL	202	CLA	CHB-C4A-NA	2.08	127.40	124.40
12	cB	905	CLA	CHB-C4A-NA	2.08	127.40	124.40
12	aB	912	CLA	CHA-C1A-NA	-2.08	121.68	126.39
12	cA	822	CLA	CMB-C2B-C3B	2.08	131.44	126.55
15	bF	203	BCR	C11-C10-C9	-2.08	124.36	127.28
12	bB	926	CLA	CHA-C1A-NA	-2.08	121.68	126.39
12	bA	837	CLA	CHD-C4C-NC	2.08	127.45	124.23
12	aA	854	CLA	CHB-C4A-NA	2.08	127.40	124.40
12	aA	828	CLA	CHB-C1B-C2B	-2.08	121.39	127.43
12	aA	809	CLA	CBC-CAC-C3C	-2.08	106.78	112.42
12	bA	802	CLA	CBC-CAC-C3C	-2.08	106.78	112.42
12	aA	811	CLA	CMC-C2C-C1C	2.08	128.28	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aF	203	BCR	C11-C10-C9	-2.08	124.36	127.28
12	bB	930	CLA	CHB-C1B-C2B	-2.08	121.40	127.43
12	cB	908	CLA	CHA-C1A-NA	-2.08	121.69	126.39
12	aA	837	CLA	OBD-CAD-C3D	-2.08	123.56	128.42
15	bF	204	BCR	C15-C16-C17	-2.08	119.27	123.52
12	aA	812	CLA	CHB-C4A-NA	2.08	127.40	124.40
12	bB	922	CLA	CHB-C4A-NA	2.08	127.40	124.40
12	aA	832	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
12	bB	922	CLA	CMC-C2C-C1C	2.08	128.28	125.03
12	cA	806	CLA	CHD-C4C-NC	2.08	127.45	124.23
15	bF	204	BCR	C20-C21-C22	-2.08	124.37	127.28
12	bB	935	CLA	CAA-C2A-C3A	-2.08	107.39	113.00
12	bB	909	CLA	CBC-CAC-C3C	-2.07	106.80	112.42
12	bA	814	CLA	O2D-CGD-O1D	-2.07	119.81	123.85
12	bA	809	CLA	CBC-CAC-C3C	-2.07	106.80	112.42
12	bB	925	CLA	CAA-C2A-C3A	-2.07	107.39	113.00
17	aB	947	LMG	C3-C4-C5	-2.07	106.47	110.23
15	bJ	101	BCR	C40-C30-C25	2.07	113.50	110.24
12	bA	806	CLA	C4-C3-C5	2.07	118.83	115.23
12	aB	906	CLA	CHB-C4A-NA	2.07	127.39	124.40
12	bB	906	CLA	CHB-C4A-NA	2.07	127.39	124.40
12	bB	908	CLA	CHA-C1A-NA	-2.07	121.70	126.39
15	bJ	101	BCR	C29-C30-C25	2.07	113.45	110.44
15	aJ	101	BCR	C40-C30-C25	2.07	113.49	110.24
15	bB	945	BCR	C40-C30-C25	2.07	113.49	110.24
12	aA	802	CLA	CBC-CAC-C3C	-2.07	106.80	112.42
12	aA	842	CLA	CED-O2D-CGD	2.07	120.62	115.92
15	cF	204	BCR	C20-C21-C22	-2.07	124.37	127.28
15	bA	846	BCR	C35-C13-C14	-2.07	119.46	122.82
12	aB	908	CLA	CHA-C1A-NA	-2.07	121.70	126.39
15	aJ	101	BCR	C29-C30-C25	2.07	113.45	110.44
12	bA	835	CLA	CMB-C2B-C3B	2.07	131.42	126.55
12	bB	930	CLA	O2A-C1-C2	2.07	113.92	108.99
12	aA	837	CLA	CHD-C4C-NC	2.07	127.44	124.23
12	cA	842	CLA	CED-O2D-CGD	2.07	120.61	115.92
12	aB	913	CLA	CHB-C1B-NB	-2.07	120.94	124.05
15	cJ	101	BCR	C29-C30-C25	2.07	113.44	110.44
12	bA	823	CLA	CAC-C3C-C4C	2.07	127.48	124.79
15	bJ	101	BCR	C4-C5-C6	2.07	125.50	122.70
12	cA	802	CLA	CBC-CAC-C3C	-2.07	106.81	112.42
12	cB	917	CLA	C2A-C3A-C4A	-2.07	98.53	101.87
12	cA	812	CLA	CHB-C4A-NA	2.07	127.39	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aB	911	CLA	O2A-CGA-O1A	-2.07	118.01	123.33
12	cB	922	CLA	O2D-CGD-O1D	-2.07	119.82	123.85
15	cA	847	BCR	C21-C20-C19	-2.07	117.21	123.20
12	cB	926	CLA	CHA-C1A-NA	-2.07	121.71	126.39
12	aB	925	CLA	CAA-C2A-C3A	-2.07	107.41	113.00
12	aA	810	CLA	O2A-CGA-CBA	2.07	120.53	114.00
15	cA	846	BCR	C1-C6-C5	-2.07	119.81	122.64
16	cA	852	LHG	C11-C10-C9	-2.07	103.92	114.37
12	bB	922	CLA	O2D-CGD-O1D	-2.07	119.83	123.85
12	bA	837	CLA	OBD-CAD-C3D	-2.07	123.59	128.42
15	aL	206	BCR	C30-C25-C26	-2.07	119.81	122.64
12	cB	913	CLA	CHB-C1B-NB	-2.07	120.95	124.05
12	cA	821	CLA	CMA-C3A-C4A	-2.06	106.22	111.77
17	bB	947	LMG	C3-C4-C5	-2.06	106.49	110.23
12	cA	818	CLA	CMB-C2B-C3B	2.06	131.41	126.55
15	aL	201	BCR	C3-C4-C5	-2.06	110.38	114.06
12	bA	821	CLA	CBC-CAC-C3C	-2.06	106.83	112.42
12	bA	821	CLA	CMA-C3A-C4A	-2.06	106.23	111.77
12	bB	917	CLA	C2A-C3A-C4A	-2.06	98.54	101.87
12	bA	814	CLA	CMB-C2B-C1B	2.06	128.56	125.42
12	aA	821	CLA	CBC-CAC-C3C	-2.06	106.83	112.42
16	bA	852	LHG	C11-C10-C9	-2.06	103.94	114.37
12	bA	833	CLA	O2D-CGD-O1D	-2.06	119.83	123.85
12	bA	812	CLA	C4-C3-C5	2.06	118.81	115.23
12	aA	821	CLA	CMA-C3A-C4A	-2.06	106.23	111.77
12	cB	925	CLA	CHB-C4A-NA	2.06	127.37	124.40
16	aA	853	LHG	C11-C10-C9	-2.06	103.95	114.37
12	aA	818	CLA	CMB-C2B-C3B	2.06	131.40	126.55
12	bA	810	CLA	O2A-CGA-CBA	2.06	120.51	114.00
12	cB	929	CLA	C4B-C3B-C2B	-2.06	104.74	107.30
15	aJ	101	BCR	C4-C5-C6	2.06	125.49	122.70
12	bB	931	CLA	C4-C3-C5	2.06	118.80	115.23
12	cA	806	CLA	C4-C3-C5	2.06	118.80	115.23
12	cB	929	CLA	CAC-C3C-C4C	2.06	127.47	124.79
15	aA	851	BCR	C10-C11-C12	-2.06	117.23	123.20
15	aI	101	BCR	C11-C10-C9	-2.06	124.39	127.28
15	cA	850	BCR	C10-C11-C12	-2.06	117.23	123.20
12	cA	821	CLA	CBC-CAC-C3C	-2.06	106.84	112.42
12	bB	918	CLA	CMC-C2C-C1C	2.06	128.25	125.03
12	aA	806	CLA	CHD-C4C-NC	2.06	127.42	124.23
12	cA	830	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
12	cA	833	CLA	O2D-CGD-O1D	-2.06	119.84	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aB	930	CLA	CHB-C1B-C2B	-2.06	121.45	127.43
15	bL	201	BCR	C3-C4-C5	-2.06	110.39	114.06
12	aA	827	CLA	CHA-C1A-NA	-2.06	121.73	126.39
12	cA	832	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
12	aB	926	CLA	CHA-C1A-NA	-2.06	121.73	126.39
15	aA	848	BCR	C21-C20-C19	-2.06	117.24	123.20
12	cB	918	CLA	CMC-C2C-C1C	2.06	128.25	125.03
15	cA	846	BCR	C35-C13-C14	-2.06	119.48	122.82
12	aA	833	CLA	O2D-CGD-O1D	-2.06	119.85	123.85
12	bB	925	CLA	CHB-C4A-NA	2.05	127.36	124.40
12	aA	823	CLA	CAC-C3C-C4C	2.05	127.46	124.79
12	bA	832	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
12	bA	839	CLA	CHB-C4A-NA	2.05	127.36	124.40
12	cA	810	CLA	O2A-CGA-CBA	2.05	120.49	114.00
12	cB	925	CLA	CAA-C2A-C3A	-2.05	107.45	113.00
15	cL	205	BCR	C15-C16-C17	-2.05	119.32	123.52
12	cB	913	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
12	cA	827	CLA	CHA-C1A-NA	-2.05	121.74	126.39
12	cB	930	CLA	CHB-C1B-C2B	-2.05	121.47	127.43
15	bA	847	BCR	C21-C20-C19	-2.05	117.25	123.20
12	cB	904	CLA	CMA-C3A-C4A	-2.05	106.26	111.77
12	bA	810	CLA	CHB-C4A-NA	2.05	127.36	124.40
12	cB	911	CLA	O2A-CGA-O1A	-2.05	118.06	123.33
15	cJ	101	BCR	C4-C5-C6	2.05	125.47	122.70
12	cB	939	CLA	O2D-CGD-O1D	-2.05	119.86	123.85
12	cA	828	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
11	bA	801	CL0	O1D-CGD-CBD	-2.05	121.61	124.72
12	bA	806	CLA	CHD-C4C-NC	2.05	127.41	124.23
12	bA	812	CLA	CHB-C4A-NA	2.05	127.36	124.40
12	cB	923	CLA	CAA-C2A-C3A	-2.05	107.46	113.00
15	bA	850	BCR	C10-C11-C12	-2.05	117.26	123.20
12	aB	917	CLA	C2A-C3A-C4A	-2.05	98.56	101.87
12	cB	922	CLA	CHB-C4A-NA	2.05	127.36	124.40
12	aA	814	CLA	CMB-C2B-C1B	2.05	128.54	125.42
12	cA	814	CLA	CMB-C2B-C1B	2.05	128.54	125.42
12	bA	827	CLA	CHA-C1A-NA	-2.05	121.75	126.39
12	bA	831	CLA	CHA-C1A-NA	-2.05	121.75	126.39
12	cA	828	CLA	CHB-C1B-C2B	-2.05	121.48	127.43
15	aF	201	BCR	C7-C8-C9	-2.05	123.21	126.23
12	aA	835	CLA	CMB-C2B-C3B	2.05	131.36	126.55
12	bA	818	CLA	CMB-C2B-C3B	2.05	131.36	126.55
12	bB	913	CLA	CHB-C1B-NB	-2.05	120.98	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bB	904	CLA	CMA-C3A-C4A	-2.04	106.28	111.77
17	cB	947	LMG	C3-C4-C5	-2.04	106.53	110.23
12	cB	909	CLA	CHA-C1A-NA	-2.04	121.76	126.39
12	aA	821	CLA	O1D-CGD-CBD	-2.04	120.49	124.52
12	cB	931	CLA	C4-C3-C5	2.04	118.78	115.23
12	cB	928	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
12	aB	925	CLA	CHB-C4A-NA	2.04	127.35	124.40
12	cA	810	CLA	CHB-C4A-NA	2.04	127.35	124.40
12	cA	839	CLA	CHB-C4A-NA	2.04	127.35	124.40
15	aF	203	BCR	C33-C5-C6	-2.04	122.25	124.48
12	bA	813	CLA	CHB-C1B-C2B	-2.04	121.50	127.43
12	cA	818	CLA	CBC-CAC-C3C	-2.04	106.88	112.42
12	aA	831	CLA	CHA-C1A-NA	-2.04	121.77	126.39
12	cA	835	CLA	CMB-C2B-C3B	2.04	131.35	126.55
15	cL	201	BCR	C3-C4-C5	-2.04	110.42	114.06
12	aB	904	CLA	CMA-C3A-C4A	-2.04	106.29	111.77
12	bB	928	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
12	aA	834	CLA	CBC-CAC-C3C	-2.04	106.89	112.42
12	aB	923	CLA	CAA-C2A-C3A	-2.04	107.48	113.00
15	cI	101	BCR	C11-C10-C9	-2.04	124.42	127.28
12	bA	834	CLA	CBC-CAC-C3C	-2.04	106.89	112.42
12	cB	935	CLA	CAC-C3C-C2C	2.04	131.31	127.56
15	cB	943	BCR	C7-C8-C9	-2.04	123.22	126.23
15	bF	201	BCR	C7-C8-C9	-2.04	123.22	126.23
12	aA	818	CLA	CBC-CAC-C3C	-2.04	106.89	112.42
12	bL	204	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
12	cB	919	CLA	CHB-C4A-NA	2.04	127.34	124.40
12	cL	202	CLA	CHB-C4A-NA	2.04	127.34	124.40
12	bA	828	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
12	aB	917	CLA	CAA-C2A-C3A	-2.04	107.50	113.00
12	aB	930	CLA	CED-O2D-CGD	2.04	120.53	115.92
12	bB	917	CLA	CAA-C2A-C3A	-2.03	107.50	113.00
12	cA	831	CLA	CHA-C1A-NA	-2.03	121.78	126.39
12	bB	935	CLA	CAC-C3C-C2C	2.03	131.30	127.56
12	cA	829	CLA	CHA-C1A-NA	-2.03	121.78	126.39
15	cL	206	BCR	C29-C30-C25	2.03	113.39	110.44
16	aA	852	LHG	C11-C10-C9	-2.03	104.09	114.37
15	aL	205	BCR	C15-C16-C17	-2.03	119.36	123.52
12	bB	930	CLA	CED-O2D-CGD	2.03	120.53	115.92
12	cB	930	CLA	CED-O2D-CGD	2.03	120.53	115.92
15	bL	206	BCR	C30-C25-C26	-2.03	119.86	122.64
12	bA	818	CLA	CBC-CAC-C3C	-2.03	106.91	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bB	917	CLA	CHB-C1B-C2B	-2.03	121.53	127.43
12	aA	830	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
15	bL	205	BCR	C15-C16-C17	-2.03	119.36	123.52
12	cB	910	CLA	CMA-C3A-C4A	-2.03	106.31	111.77
12	bA	830	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
16	bA	851	LHG	C11-C10-C9	-2.03	104.09	114.37
12	bB	902	CLA	CED-O2D-CGD	2.03	120.53	115.92
12	aB	907	CLA	C4A-NA-C1A	-2.03	105.75	106.68
12	aB	922	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
12	aB	928	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
12	cB	902	CLA	CED-O2D-CGD	2.03	120.52	115.92
12	cB	932	CLA	CED-O2D-CGD	2.03	120.52	115.92
15	cF	201	BCR	C7-C8-C9	-2.03	123.23	126.23
15	aA	847	BCR	C1-C6-C5	-2.03	119.86	122.64
12	cB	916	CLA	C3B-C4B-NB	2.03	112.34	110.53
12	aB	932	CLA	CED-O2D-CGD	2.03	120.52	115.92
16	cA	851	LHG	C11-C10-C9	-2.03	104.11	114.37
12	cB	904	CLA	O2A-CGA-CBA	2.03	118.02	111.83
12	bB	919	CLA	CHB-C4A-NA	2.03	127.33	124.40
15	bA	846	BCR	C1-C6-C5	-2.03	119.86	122.64
15	bL	206	BCR	C20-C21-C22	-2.03	124.43	127.28
12	aA	840	CLA	O2D-CGD-O1D	-2.03	119.90	123.85
12	bB	910	CLA	CMA-C3A-C4A	-2.03	106.32	111.77
15	bJ	101	BCR	C27-C26-C25	2.03	125.44	122.70
12	aB	902	CLA	CED-O2D-CGD	2.03	120.51	115.92
15	aB	943	BCR	C7-C8-C9	-2.03	123.24	126.23
12	aB	910	CLA	CMA-C3A-C4A	-2.03	106.33	111.77
12	cA	834	CLA	CBC-CAC-C3C	-2.03	106.92	112.42
12	aL	204	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
12	bL	202	CLA	CHB-C4A-NA	2.03	127.33	124.40
12	bA	815	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
12	cL	204	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
12	cB	917	CLA	CAA-C2A-C3A	-2.03	107.53	113.00
12	bB	909	CLA	CHA-C1A-NA	-2.03	121.80	126.39
12	aA	828	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
12	aB	935	CLA	CAC-C3C-C2C	2.03	131.28	127.56
12	aA	824	CLA	CHA-C1A-NA	-2.03	121.81	126.39
12	bA	810	CLA	CBC-CAC-C3C	-2.02	106.93	112.42
12	aB	925	CLA	CHB-C1B-C2B	-2.02	121.55	127.43
12	cA	821	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
15	bI	101	BCR	C11-C10-C9	-2.02	124.44	127.28
12	bA	840	CLA	O2D-CGD-O1D	-2.02	119.91	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aB	941	BCR	C27-C26-C25	2.02	125.44	122.70
12	aB	931	CLA	C4-C3-C5	2.02	118.74	115.23
12	bB	950	CLA	CAA-C2A-C3A	-2.02	107.53	113.00
12	aB	939	CLA	O2D-CGD-O1D	-2.02	119.91	123.85
12	bB	923	CLA	CAA-C2A-C3A	-2.02	107.53	113.00
12	aA	810	CLA	CBC-CAC-C3C	-2.02	106.94	112.42
12	aL	203	CLA	CHB-C1B-C2B	-2.02	121.55	127.43
12	bB	939	CLA	O2D-CGD-O1D	-2.02	119.91	123.85
12	aB	909	CLA	CHA-C1A-NA	-2.02	121.81	126.39
12	aB	929	CLA	C4B-C3B-C2B	-2.02	104.79	107.30
12	aB	904	CLA	O2A-CGA-CBA	2.02	118.00	111.83
12	aA	840	CLA	CMB-C2B-C1B	2.02	128.50	125.42
12	cL	203	CLA	CHB-C1B-C2B	-2.02	121.56	127.43
12	aB	917	CLA	CHB-C1B-C2B	-2.02	121.56	127.43
12	aB	919	CLA	CHB-C4A-NA	2.02	127.31	124.40
12	cA	824	CLA	CHA-C1A-NA	-2.02	121.82	126.39
15	cB	941	BCR	C24-C23-C22	-2.02	123.25	126.23
12	cA	813	CLA	CHB-C1B-C2B	-2.02	121.56	127.43
12	bB	904	CLA	O2A-CGA-CBA	2.02	117.99	111.83
12	aA	815	CLA	O1D-CGD-CBD	-2.02	120.54	124.52
12	cA	819	CLA	CHB-C4A-NA	2.02	127.31	124.40
12	cB	917	CLA	CHB-C1B-C2B	-2.02	121.57	127.43
12	cB	925	CLA	CHB-C1B-C2B	-2.02	121.57	127.43
15	aA	847	BCR	C35-C13-C14	-2.02	119.55	122.82
12	bA	821	CLA	O1D-CGD-CBD	-2.02	120.54	124.52
12	cA	803	CLA	C11-C10-C8	-2.02	109.26	115.97
15	cB	941	BCR	C27-C26-C25	2.02	125.43	122.70
12	aA	803	CLA	C11-C10-C8	-2.02	109.26	115.97
12	aA	813	CLA	CHB-C1B-C2B	-2.02	121.57	127.43
15	cA	849	BCR	C8-C7-C6	-2.02	121.61	127.00
12	aA	819	CLA	CHB-C4A-NA	2.02	127.31	124.40
15	bB	941	BCR	C24-C23-C22	-2.02	123.25	126.23
12	aA	833	CLA	CMC-C2C-C1C	2.02	128.19	125.03
12	cA	810	CLA	CBC-CAC-C3C	-2.02	106.95	112.42
12	bA	803	CLA	C11-C10-C8	-2.02	109.26	115.97
12	bA	826	CLA	O1D-CGD-CBD	-2.02	120.54	124.52
12	bB	932	CLA	CED-O2D-CGD	2.02	120.49	115.92
15	aJ	101	BCR	C1-C6-C5	-2.02	119.88	122.64
12	aA	844	CLA	CAA-C2A-C3A	-2.02	107.55	113.00
12	cA	815	CLA	O1D-CGD-CBD	-2.01	120.54	124.52
12	bA	824	CLA	CHA-C1A-NA	-2.01	121.83	126.39
12	cA	853	CLA	C4D-C3D-CAD	-2.01	105.92	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	aB	918	CLA	CMC-C2C-C1C	2.01	128.18	125.03
12	aB	913	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
12	aA	826	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
12	cA	826	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
12	bA	840	CLA	CMB-C2B-C1B	2.01	128.49	125.42
12	bB	925	CLA	CHB-C1B-C2B	-2.01	121.58	127.43
15	bA	849	BCR	C8-C7-C6	-2.01	121.62	127.00
15	aB	946	BCR	C39-C30-C25	2.01	113.40	110.24
12	cB	927	CLA	O2A-CGA-CBA	2.01	117.97	111.83
15	aB	941	BCR	C24-C23-C22	-2.01	123.26	126.23
12	bB	913	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
15	bB	943	BCR	C7-C8-C9	-2.01	123.26	126.23
15	cB	946	BCR	C39-C30-C25	2.01	113.39	110.24
15	bB	941	BCR	C27-C26-C25	2.01	125.42	122.70
12	aB	950	CLA	CAA-C2A-C3A	-2.01	107.57	113.00
15	aA	850	BCR	C8-C7-C6	-2.01	121.63	127.00
12	bA	833	CLA	CMC-C2C-C1C	2.01	128.17	125.03
15	cB	943	BCR	C38-C26-C27	-2.01	109.31	113.60
12	bB	916	CLA	C3B-C4B-NB	2.01	112.32	110.53
12	cA	825	CLA	C4B-C3B-C2B	-2.01	104.81	107.30
12	cA	839	CLA	CHA-C1A-NA	-2.01	121.84	126.39
15	cL	206	BCR	C20-C21-C22	-2.01	124.46	127.28
12	cA	840	CLA	O2D-CGD-O1D	-2.01	119.94	123.85
12	cB	937	CLA	CMC-C2C-C1C	2.01	128.17	125.03
15	bB	943	BCR	C38-C26-C27	-2.01	109.32	113.60
12	bB	929	CLA	C4B-C3B-C2B	-2.01	104.81	107.30
12	aA	820	CLA	CHA-C1A-NA	-2.01	121.85	126.39
12	aA	839	CLA	CHB-C4A-NA	2.01	127.30	124.40
15	bJ	101	BCR	C1-C6-C5	-2.01	119.89	122.64
12	bB	937	CLA	CMC-C2C-C1C	2.01	128.17	125.03
15	bF	203	BCR	C33-C5-C6	-2.01	122.30	124.48
12	bB	923	CLA	C4-C3-C5	2.01	118.71	115.23
12	cA	840	CLA	CMB-C2B-C1B	2.01	128.47	125.42
15	aJ	101	BCR	C27-C26-C25	2.01	125.41	122.70
12	bA	826	CLA	O2A-CGA-CBA	2.01	117.95	111.83
12	aB	916	CLA	CMB-C2B-C1B	2.01	128.47	125.42
12	cA	833	CLA	CMC-C2C-C1C	2.00	128.17	125.03
15	bB	942	BCR	C15-C16-C17	-2.00	119.42	123.52
15	aB	943	BCR	C38-C26-C27	-2.00	109.32	113.60
12	aB	927	CLA	O2A-CGA-CBA	2.00	117.94	111.83
12	bA	839	CLA	CHA-C1A-NA	-2.00	121.86	126.39
12	bA	803	CLA	CBA-CAA-C2A	2.00	119.75	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	cA	811	CLA	O1D-CGD-CBD	-2.00	120.57	124.52
12	aB	904	CLA	CHB-C1B-NB	-2.00	121.05	124.05
12	cB	916	CLA	CMB-C2B-C1B	2.00	128.47	125.42
12	aB	916	CLA	C3B-C4B-NB	2.00	112.32	110.53
12	aA	803	CLA	CBA-CAA-C2A	2.00	119.75	113.79
12	bB	916	CLA	CMB-C2B-C1B	2.00	128.47	125.42
12	aA	841	CLA	CMA-C3A-C2A	-2.00	106.24	113.98
12	bA	841	CLA	CMA-C3A-C2A	-2.00	106.24	113.98
15	cF	204	BCR	C30-C25-C26	-2.00	119.90	122.64
15	cJ	101	BCR	C27-C26-C25	2.00	125.41	122.70
12	bL	203	CLA	CHB-C1B-C2B	-2.00	121.62	127.43
12	bA	820	CLA	CHA-C1A-NA	-2.00	121.86	126.39
15	bF	204	BCR	C30-C25-C26	-2.00	119.90	122.64
12	cB	923	CLA	C4-C3-C5	2.00	118.70	115.23

All (225) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	aA	801	CL0	ND
11	aA	801	CL0	NC
11	aA	801	CL0	NA
11	bA	801	CL0	ND
11	bA	801	CL0	NC
11	bA	801	CL0	NA
11	cA	801	CL0	ND
11	cA	801	CL0	NC
11	cA	801	CL0	NA
12	aA	802	CLA	ND
12	aA	803	CLA	ND
12	aA	804	CLA	ND
12	aA	805	CLA	ND
12	aA	806	CLA	ND
12	aA	807	CLA	ND
12	aA	808	CLA	ND
12	aA	809	CLA	ND
12	aA	810	CLA	ND
12	aA	811	CLA	ND
12	aA	812	CLA	ND
12	aA	813	CLA	ND
12	aA	814	CLA	ND
12	aA	816	CLA	ND
12	aA	818	CLA	ND

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Mol	Chain	Res	Type	Atom
12	aA	819	CLA	ND
12	aA	820	CLA	ND
12	aA	821	CLA	ND
12	aA	823	CLA	ND
12	aA	825	CLA	ND
12	aA	826	CLA	ND
12	aA	827	CLA	ND
12	aA	828	CLA	ND
12	aA	829	CLA	ND
12	aA	830	CLA	ND
12	aA	832	CLA	ND
12	aA	833	CLA	ND
12	aA	834	CLA	ND
12	aA	835	CLA	ND
12	aA	836	CLA	ND
12	aA	837	CLA	ND
12	aA	838	CLA	ND
12	aA	839	CLA	ND
12	aA	840	CLA	ND
12	aA	841	CLA	ND
12	aA	842	CLA	ND
12	aA	843	CLA	ND
12	aA	854	CLA	ND
12	aB	901	CLA	ND
12	aB	902	CLA	ND
12	aB	903	CLA	ND
12	aB	904	CLA	ND
12	aB	905	CLA	ND
12	aB	906	CLA	ND
12	aB	907	CLA	ND
12	aB	908	CLA	ND
12	aB	909	CLA	ND
12	aB	910	CLA	ND
12	aB	912	CLA	ND
12	aB	913	CLA	ND
12	aB	914	CLA	ND
12	aB	917	CLA	ND
12	aB	918	CLA	ND
12	aB	919	CLA	ND
12	aB	922	CLA	ND
12	aB	923	CLA	ND
12	aB	924	CLA	ND

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Mol	Chain	Res	Type	Atom
12	aB	925	CLA	ND
12	aB	926	CLA	ND
12	aB	927	CLA	ND
12	aB	928	CLA	ND
12	aB	930	CLA	ND
12	aB	931	CLA	ND
12	aB	933	CLA	ND
12	aB	934	CLA	ND
12	aB	935	CLA	ND
12	aB	936	CLA	ND
12	aB	937	CLA	ND
12	aB	938	CLA	ND
12	aB	939	CLA	ND
12	aB	949	CLA	ND
12	aF	202	CLA	ND
12	bA	802	CLA	ND
12	bA	803	CLA	ND
12	bA	804	CLA	ND
12	bA	805	CLA	ND
12	bA	806	CLA	ND
12	bA	807	CLA	ND
12	bA	808	CLA	ND
12	bA	809	CLA	ND
12	bA	810	CLA	ND
12	bA	811	CLA	ND
12	bA	812	CLA	ND
12	bA	813	CLA	ND
12	bA	814	CLA	ND
12	bA	816	CLA	ND
12	bA	818	CLA	ND
12	bA	819	CLA	ND
12	bA	820	CLA	ND
12	bA	821	CLA	ND
12	bA	823	CLA	ND
12	bA	825	CLA	ND
12	bA	826	CLA	ND
12	bA	827	CLA	ND
12	bA	828	CLA	ND
12	bA	829	CLA	ND
12	bA	830	CLA	ND
12	bA	832	CLA	ND
12	bA	833	CLA	ND

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Mol	Chain	Res	Type	Atom
12	bA	834	CLA	ND
12	bA	835	CLA	ND
12	bA	836	CLA	ND
12	bA	837	CLA	ND
12	bA	838	CLA	ND
12	bA	839	CLA	ND
12	bA	840	CLA	ND
12	bA	841	CLA	ND
12	bA	842	CLA	ND
12	bA	843	CLA	ND
12	bA	853	CLA	ND
12	bB	901	CLA	ND
12	bB	902	CLA	ND
12	bB	903	CLA	ND
12	bB	904	CLA	ND
12	bB	905	CLA	ND
12	bB	906	CLA	ND
12	bB	907	CLA	ND
12	bB	908	CLA	ND
12	bB	909	CLA	ND
12	bB	910	CLA	ND
12	bB	912	CLA	ND
12	bB	913	CLA	ND
12	bB	914	CLA	ND
12	bB	917	CLA	ND
12	bB	918	CLA	ND
12	bB	919	CLA	ND
12	bB	922	CLA	ND
12	bB	923	CLA	ND
12	bB	924	CLA	ND
12	bB	925	CLA	ND
12	bB	926	CLA	ND
12	bB	927	CLA	ND
12	bB	928	CLA	ND
12	bB	930	CLA	ND
12	bB	931	CLA	ND
12	bB	933	CLA	ND
12	bB	934	CLA	ND
12	bB	935	CLA	ND
12	bB	936	CLA	ND
12	bB	937	CLA	ND
12	bB	938	CLA	ND

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Mol	Chain	Res	Type	Atom
12	bB	939	CLA	ND
12	bB	949	CLA	ND
12	bF	202	CLA	ND
12	cA	802	CLA	ND
12	cA	803	CLA	ND
12	cA	804	CLA	ND
12	cA	805	CLA	ND
12	cA	806	CLA	ND
12	cA	807	CLA	ND
12	cA	808	CLA	ND
12	cA	809	CLA	ND
12	cA	810	CLA	ND
12	cA	811	CLA	ND
12	cA	812	CLA	ND
12	cA	813	CLA	ND
12	cA	814	CLA	ND
12	cA	816	CLA	ND
12	cA	818	CLA	ND
12	cA	819	CLA	ND
12	cA	820	CLA	ND
12	cA	821	CLA	ND
12	cA	823	CLA	ND
12	cA	825	CLA	ND
12	cA	826	CLA	ND
12	cA	827	CLA	ND
12	cA	828	CLA	ND
12	cA	829	CLA	ND
12	cA	830	CLA	ND
12	cA	832	CLA	ND
12	cA	833	CLA	ND
12	cA	834	CLA	ND
12	cA	835	CLA	ND
12	cA	836	CLA	ND
12	cA	837	CLA	ND
12	cA	838	CLA	ND
12	cA	839	CLA	ND
12	cA	840	CLA	ND
12	cA	841	CLA	ND
12	cA	842	CLA	ND
12	cA	843	CLA	ND
12	cA	853	CLA	ND
12	cB	901	CLA	ND

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Mol	Chain	Res	Type	Atom
12	cB	902	CLA	ND
12	cB	903	CLA	ND
12	cB	904	CLA	ND
12	cB	905	CLA	ND
12	cB	906	CLA	ND
12	cB	907	CLA	ND
12	cB	908	CLA	ND
12	cB	909	CLA	ND
12	cB	910	CLA	ND
12	cB	912	CLA	ND
12	cB	913	CLA	ND
12	cB	914	CLA	ND
12	cB	917	CLA	ND
12	cB	918	CLA	ND
12	cB	919	CLA	ND
12	cB	922	CLA	ND
12	cB	923	CLA	ND
12	cB	924	CLA	ND
12	cB	925	CLA	ND
12	cB	926	CLA	ND
12	cB	927	CLA	ND
12	cB	928	CLA	ND
12	cB	930	CLA	ND
12	cB	931	CLA	ND
12	cB	933	CLA	ND
12	cB	934	CLA	ND
12	cB	935	CLA	ND
12	cB	936	CLA	ND
12	cB	937	CLA	ND
12	cB	938	CLA	ND
12	cB	939	CLA	ND
12	cB	949	CLA	ND
12	cF	202	CLA	ND

All (2522) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	aA	804	CLA	C1A-C2A-CAA-CBA
12	aA	804	CLA	C3A-C2A-CAA-CBA
12	aA	807	CLA	C1A-C2A-CAA-CBA
12	aA	808	CLA	C2-C3-C5-C6
12	aA	809	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
12	aA	809	CLA	CHA-CBD-CGD-O2D
12	aA	820	CLA	C1A-C2A-CAA-CBA
12	aA	820	CLA	C3A-C2A-CAA-CBA
12	aA	823	CLA	C2-C3-C5-C6
12	aA	823	CLA	C4-C3-C5-C6
12	aA	830	CLA	CHA-CBD-CGD-O1D
12	aA	830	CLA	CHA-CBD-CGD-O2D
12	aA	833	CLA	C2B-C3B-CAB-CBB
12	aA	833	CLA	C4B-C3B-CAB-CBB
12	aA	833	CLA	C2-C3-C5-C6
12	aA	833	CLA	C4-C3-C5-C6
12	aA	834	CLA	C4B-C3B-CAB-CBB
12	aA	834	CLA	CHA-CBD-CGD-O1D
12	aA	834	CLA	CHA-CBD-CGD-O2D
12	aA	837	CLA	CBD-CGD-O2D-CED
12	aA	837	CLA	C2-C3-C5-C6
12	aA	837	CLA	C4-C3-C5-C6
12	aA	841	CLA	C2-C3-C5-C6
12	aA	841	CLA	C4-C3-C5-C6
12	aA	842	CLA	C2-C1-O2A-CGA
12	aB	903	CLA	CHA-CBD-CGD-O1D
12	aB	903	CLA	CHA-CBD-CGD-O2D
12	aB	903	CLA	C2-C3-C5-C6
12	aB	903	CLA	C4-C3-C5-C6
12	aB	904	CLA	C1A-C2A-CAA-CBA
12	aB	904	CLA	C3A-C2A-CAA-CBA
12	aB	905	CLA	C2B-C3B-CAB-CBB
12	aB	905	CLA	C4B-C3B-CAB-CBB
12	aB	907	CLA	CHA-CBD-CGD-O1D
12	aB	907	CLA	CHA-CBD-CGD-O2D
12	aB	914	CLA	CHA-CBD-CGD-O1D
12	aB	914	CLA	CHA-CBD-CGD-O2D
12	aB	917	CLA	C1A-C2A-CAA-CBA
12	aB	917	CLA	C3A-C2A-CAA-CBA
12	aB	919	CLA	C1A-C2A-CAA-CBA
12	aB	919	CLA	C3A-C2A-CAA-CBA
12	aB	919	CLA	C2B-C3B-CAB-CBB
12	aB	919	CLA	C4B-C3B-CAB-CBB
12	aB	924	CLA	CHA-CBD-CGD-O1D
12	aB	924	CLA	CHA-CBD-CGD-O2D
12	aB	926	CLA	C1A-C2A-CAA-CBA
12	aB	927	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	aB	927	CLA	C3A-C2A-CAA-CBA
12	aB	929	CLA	C1A-C2A-CAA-CBA
12	aB	929	CLA	C3A-C2A-CAA-CBA
12	aB	929	CLA	C2B-C3B-CAB-CBB
12	aB	929	CLA	C4B-C3B-CAB-CBB
12	aB	932	CLA	C2B-C3B-CAB-CBB
12	aB	932	CLA	C4B-C3B-CAB-CBB
12	aB	932	CLA	CHA-CBD-CGD-O1D
12	aB	932	CLA	CHA-CBD-CGD-O2D
12	aF	202	CLA	C1A-C2A-CAA-CBA
12	aF	202	CLA	C3A-C2A-CAA-CBA
12	aF	202	CLA	CHA-CBD-CGD-O1D
12	aF	202	CLA	CHA-CBD-CGD-O2D
12	bA	804	CLA	C1A-C2A-CAA-CBA
12	bA	804	CLA	C3A-C2A-CAA-CBA
12	bA	807	CLA	C1A-C2A-CAA-CBA
12	bA	808	CLA	C2-C3-C5-C6
12	bA	809	CLA	CHA-CBD-CGD-O1D
12	bA	809	CLA	CHA-CBD-CGD-O2D
12	bA	820	CLA	C1A-C2A-CAA-CBA
12	bA	820	CLA	C3A-C2A-CAA-CBA
12	bA	823	CLA	C2-C3-C5-C6
12	bA	823	CLA	C4-C3-C5-C6
12	bA	830	CLA	CHA-CBD-CGD-O1D
12	bA	830	CLA	CHA-CBD-CGD-O2D
12	bA	833	CLA	C2B-C3B-CAB-CBB
12	bA	833	CLA	C4B-C3B-CAB-CBB
12	bA	833	CLA	C2-C3-C5-C6
12	bA	833	CLA	C4-C3-C5-C6
12	bA	834	CLA	C4B-C3B-CAB-CBB
12	bA	834	CLA	CHA-CBD-CGD-O1D
12	bA	834	CLA	CHA-CBD-CGD-O2D
12	bA	837	CLA	CBD-CGD-O2D-CED
12	bA	837	CLA	C2-C3-C5-C6
12	bA	837	CLA	C4-C3-C5-C6
12	bA	841	CLA	C2-C3-C5-C6
12	bA	841	CLA	C4-C3-C5-C6
12	bA	842	CLA	C2-C1-O2A-CGA
12	bB	903	CLA	CHA-CBD-CGD-O1D
12	bB	903	CLA	CHA-CBD-CGD-O2D
12	bB	903	CLA	C2-C3-C5-C6
12	bB	903	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
12	bB	904	CLA	C1A-C2A-CAA-CBA
12	bB	904	CLA	C3A-C2A-CAA-CBA
12	bB	905	CLA	C2B-C3B-CAB-CBB
12	bB	905	CLA	C4B-C3B-CAB-CBB
12	bB	907	CLA	CHA-CBD-CGD-O1D
12	bB	907	CLA	CHA-CBD-CGD-O2D
12	bB	914	CLA	CHA-CBD-CGD-O1D
12	bB	914	CLA	CHA-CBD-CGD-O2D
12	bB	917	CLA	C1A-C2A-CAA-CBA
12	bB	917	CLA	C3A-C2A-CAA-CBA
12	bB	919	CLA	C1A-C2A-CAA-CBA
12	bB	919	CLA	C3A-C2A-CAA-CBA
12	bB	919	CLA	C2B-C3B-CAB-CBB
12	bB	919	CLA	C4B-C3B-CAB-CBB
12	bB	924	CLA	CHA-CBD-CGD-O1D
12	bB	924	CLA	CHA-CBD-CGD-O2D
12	bB	926	CLA	C1A-C2A-CAA-CBA
12	bB	927	CLA	C1A-C2A-CAA-CBA
12	bB	927	CLA	C3A-C2A-CAA-CBA
12	bB	929	CLA	C1A-C2A-CAA-CBA
12	bB	929	CLA	C3A-C2A-CAA-CBA
12	bB	929	CLA	C2B-C3B-CAB-CBB
12	bB	929	CLA	C4B-C3B-CAB-CBB
12	bB	932	CLA	C2B-C3B-CAB-CBB
12	bB	932	CLA	C4B-C3B-CAB-CBB
12	bB	932	CLA	CHA-CBD-CGD-O1D
12	bB	932	CLA	CHA-CBD-CGD-O2D
12	bF	202	CLA	C1A-C2A-CAA-CBA
12	bF	202	CLA	C3A-C2A-CAA-CBA
12	bF	202	CLA	CHA-CBD-CGD-O1D
12	bF	202	CLA	CHA-CBD-CGD-O2D
12	cA	804	CLA	C1A-C2A-CAA-CBA
12	cA	804	CLA	C3A-C2A-CAA-CBA
12	cA	807	CLA	C1A-C2A-CAA-CBA
12	cA	808	CLA	C2-C3-C5-C6
12	cA	809	CLA	CHA-CBD-CGD-O1D
12	cA	809	CLA	CHA-CBD-CGD-O2D
12	cA	820	CLA	C1A-C2A-CAA-CBA
12	cA	820	CLA	C3A-C2A-CAA-CBA
12	cA	823	CLA	C2-C3-C5-C6
12	cA	823	CLA	C4-C3-C5-C6
12	cA	830	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
12	cA	830	CLA	CHA-CBD-CGD-O2D
12	cA	833	CLA	C2B-C3B-CAB-CBB
12	cA	833	CLA	C4B-C3B-CAB-CBB
12	cA	833	CLA	C2-C3-C5-C6
12	cA	833	CLA	C4-C3-C5-C6
12	cA	834	CLA	C4B-C3B-CAB-CBB
12	cA	834	CLA	CHA-CBD-CGD-O1D
12	cA	834	CLA	CHA-CBD-CGD-O2D
12	cA	837	CLA	CBD-CGD-O2D-CED
12	cA	837	CLA	C2-C3-C5-C6
12	cA	837	CLA	C4-C3-C5-C6
12	cA	841	CLA	C2-C3-C5-C6
12	cA	841	CLA	C4-C3-C5-C6
12	cA	842	CLA	C2-C1-O2A-CGA
12	cB	903	CLA	CHA-CBD-CGD-O1D
12	cB	903	CLA	CHA-CBD-CGD-O2D
12	cB	903	CLA	C2-C3-C5-C6
12	cB	903	CLA	C4-C3-C5-C6
12	cB	904	CLA	C1A-C2A-CAA-CBA
12	cB	904	CLA	C3A-C2A-CAA-CBA
12	cB	905	CLA	C2B-C3B-CAB-CBB
12	cB	905	CLA	C4B-C3B-CAB-CBB
12	cB	907	CLA	CHA-CBD-CGD-O1D
12	cB	907	CLA	CHA-CBD-CGD-O2D
12	cB	914	CLA	CHA-CBD-CGD-O1D
12	cB	914	CLA	CHA-CBD-CGD-O2D
12	cB	917	CLA	C1A-C2A-CAA-CBA
12	cB	917	CLA	C3A-C2A-CAA-CBA
12	cB	919	CLA	C1A-C2A-CAA-CBA
12	cB	919	CLA	C3A-C2A-CAA-CBA
12	cB	919	CLA	C2B-C3B-CAB-CBB
12	cB	919	CLA	C4B-C3B-CAB-CBB
12	cB	924	CLA	CHA-CBD-CGD-O1D
12	cB	924	CLA	CHA-CBD-CGD-O2D
12	cB	926	CLA	C1A-C2A-CAA-CBA
12	cB	927	CLA	C1A-C2A-CAA-CBA
12	cB	927	CLA	C3A-C2A-CAA-CBA
12	cB	929	CLA	C1A-C2A-CAA-CBA
12	cB	929	CLA	C3A-C2A-CAA-CBA
12	cB	929	CLA	C2B-C3B-CAB-CBB
12	cB	929	CLA	C4B-C3B-CAB-CBB
12	cB	932	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
12	cB	932	CLA	C4B-C3B-CAB-CBB
12	cB	932	CLA	CHA-CBD-CGD-O1D
12	cB	932	CLA	CHA-CBD-CGD-O2D
12	cF	202	CLA	C1A-C2A-CAA-CBA
12	cF	202	CLA	C3A-C2A-CAA-CBA
12	cF	202	CLA	CHA-CBD-CGD-O1D
12	cF	202	CLA	CHA-CBD-CGD-O2D
13	aA	845	1L3	C22-C21-C23-C24
13	bA	844	1L3	C20-C21-C23-C24
13	bA	844	1L3	C22-C21-C23-C24
13	cA	844	1L3	C22-C21-C23-C24
15	aA	847	BCR	C7-C8-C9-C10
15	aA	847	BCR	C17-C18-C19-C20
15	aA	847	BCR	C37-C22-C23-C24
15	aA	847	BCR	C22-C23-C24-C25
15	aA	848	BCR	C7-C8-C9-C10
15	aA	849	BCR	C22-C23-C24-C25
15	aA	850	BCR	C17-C18-C19-C20
15	aA	850	BCR	C18-C19-C20-C21
15	aA	850	BCR	C21-C22-C23-C24
15	aA	851	BCR	C7-C8-C9-C10
15	aA	851	BCR	C20-C21-C22-C23
15	aA	851	BCR	C21-C22-C23-C24
15	aB	941	BCR	C37-C22-C23-C24
15	aB	942	BCR	C21-C22-C23-C24
15	aB	942	BCR	C37-C22-C23-C24
15	aB	943	BCR	C11-C10-C9-C8
15	aB	943	BCR	C11-C10-C9-C34
15	aB	944	BCR	C6-C7-C8-C9
15	aB	944	BCR	C7-C8-C9-C34
15	aB	944	BCR	C11-C10-C9-C8
15	aB	944	BCR	C18-C19-C20-C21
15	aB	944	BCR	C20-C21-C22-C23
15	aB	944	BCR	C20-C21-C22-C37
15	aB	944	BCR	C21-C22-C23-C24
15	aB	944	BCR	C37-C22-C23-C24
15	aF	201	BCR	C14-C15-C16-C17
15	aF	201	BCR	C21-C22-C23-C24
15	aF	203	BCR	C7-C8-C9-C34
15	aF	204	BCR	C7-C8-C9-C10
15	aF	204	BCR	C7-C8-C9-C34
15	aI	101	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
15	aI	101	BCR	C17-C18-C19-C20
15	aI	101	BCR	C20-C21-C22-C23
15	aI	101	BCR	C21-C22-C23-C24
15	aJ	101	BCR	C5-C6-C7-C8
15	aJ	101	BCR	C7-C8-C9-C10
15	aJ	101	BCR	C7-C8-C9-C34
15	aJ	101	BCR	C20-C21-C22-C37
15	aJ	101	BCR	C22-C23-C24-C25
15	aL	201	BCR	C7-C8-C9-C34
15	aL	205	BCR	C7-C8-C9-C10
15	aL	205	BCR	C7-C8-C9-C34
15	aL	205	BCR	C21-C22-C23-C24
15	aL	205	BCR	C23-C24-C25-C26
15	aL	205	BCR	C23-C24-C25-C30
15	aM	101	BCR	C7-C8-C9-C34
15	aM	101	BCR	C17-C18-C19-C20
15	aM	101	BCR	C20-C21-C22-C23
15	aM	101	BCR	C20-C21-C22-C37
15	aM	101	BCR	C21-C22-C23-C24
15	bA	846	BCR	C7-C8-C9-C10
15	bA	846	BCR	C17-C18-C19-C20
15	bA	846	BCR	C37-C22-C23-C24
15	bA	846	BCR	C22-C23-C24-C25
15	bA	847	BCR	C7-C8-C9-C10
15	bA	848	BCR	C22-C23-C24-C25
15	bA	849	BCR	C17-C18-C19-C20
15	bA	849	BCR	C18-C19-C20-C21
15	bA	849	BCR	C21-C22-C23-C24
15	bA	850	BCR	C7-C8-C9-C10
15	bA	850	BCR	C20-C21-C22-C23
15	bA	850	BCR	C21-C22-C23-C24
15	bB	941	BCR	C37-C22-C23-C24
15	bB	942	BCR	C21-C22-C23-C24
15	bB	942	BCR	C37-C22-C23-C24
15	bB	943	BCR	C11-C10-C9-C8
15	bB	943	BCR	C11-C10-C9-C34
15	bB	944	BCR	C6-C7-C8-C9
15	bB	944	BCR	C7-C8-C9-C34
15	bB	944	BCR	C11-C10-C9-C8
15	bB	944	BCR	C18-C19-C20-C21
15	bB	944	BCR	C20-C21-C22-C23
15	bB	944	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
15	bB	944	BCR	C21-C22-C23-C24
15	bB	944	BCR	C37-C22-C23-C24
15	bF	201	BCR	C14-C15-C16-C17
15	bF	201	BCR	C21-C22-C23-C24
15	bF	203	BCR	C7-C8-C9-C34
15	bF	204	BCR	C7-C8-C9-C10
15	bF	204	BCR	C7-C8-C9-C34
15	bI	101	BCR	C7-C8-C9-C34
15	bI	101	BCR	C17-C18-C19-C20
15	bI	101	BCR	C20-C21-C22-C23
15	bI	101	BCR	C21-C22-C23-C24
15	bJ	101	BCR	C5-C6-C7-C8
15	bJ	101	BCR	C7-C8-C9-C10
15	bJ	101	BCR	C7-C8-C9-C34
15	bJ	101	BCR	C20-C21-C22-C37
15	bJ	101	BCR	C22-C23-C24-C25
15	bL	201	BCR	C7-C8-C9-C34
15	bL	205	BCR	C7-C8-C9-C10
15	bL	205	BCR	C21-C22-C23-C24
15	bL	205	BCR	C23-C24-C25-C26
15	bL	205	BCR	C23-C24-C25-C30
15	bM	101	BCR	C7-C8-C9-C34
15	bM	101	BCR	C17-C18-C19-C20
15	bM	101	BCR	C20-C21-C22-C23
15	bM	101	BCR	C20-C21-C22-C37
15	bM	101	BCR	C21-C22-C23-C24
15	cA	846	BCR	C7-C8-C9-C10
15	cA	846	BCR	C17-C18-C19-C20
15	cA	846	BCR	C37-C22-C23-C24
15	cA	846	BCR	C22-C23-C24-C25
15	cA	847	BCR	C7-C8-C9-C10
15	cA	848	BCR	C22-C23-C24-C25
15	cA	849	BCR	C17-C18-C19-C20
15	cA	849	BCR	C18-C19-C20-C21
15	cA	849	BCR	C21-C22-C23-C24
15	cA	850	BCR	C7-C8-C9-C10
15	cA	850	BCR	C20-C21-C22-C23
15	cA	850	BCR	C21-C22-C23-C24
15	cB	941	BCR	C37-C22-C23-C24
15	cB	942	BCR	C21-C22-C23-C24
15	cB	942	BCR	C37-C22-C23-C24
15	cB	943	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
15	cB	943	BCR	C11-C10-C9-C34
15	cB	944	BCR	C6-C7-C8-C9
15	cB	944	BCR	C7-C8-C9-C34
15	cB	944	BCR	C11-C10-C9-C8
15	cB	944	BCR	C18-C19-C20-C21
15	cB	944	BCR	C20-C21-C22-C23
15	cB	944	BCR	C20-C21-C22-C37
15	cB	944	BCR	C21-C22-C23-C24
15	cB	944	BCR	C37-C22-C23-C24
15	cF	201	BCR	C14-C15-C16-C17
15	cF	201	BCR	C21-C22-C23-C24
15	cF	203	BCR	C7-C8-C9-C34
15	cF	204	BCR	C7-C8-C9-C10
15	cF	204	BCR	C7-C8-C9-C34
15	cI	101	BCR	C7-C8-C9-C34
15	cI	101	BCR	C17-C18-C19-C20
15	cI	101	BCR	C20-C21-C22-C23
15	cI	101	BCR	C21-C22-C23-C24
15	cJ	101	BCR	C5-C6-C7-C8
15	cJ	101	BCR	C7-C8-C9-C10
15	cJ	101	BCR	C7-C8-C9-C34
15	cJ	101	BCR	C20-C21-C22-C37
15	cJ	101	BCR	C22-C23-C24-C25
15	cL	201	BCR	C7-C8-C9-C34
15	cL	205	BCR	C7-C8-C9-C10
15	cL	205	BCR	C21-C22-C23-C24
15	cL	205	BCR	C23-C24-C25-C26
15	cL	205	BCR	C23-C24-C25-C30
15	cM	101	BCR	C7-C8-C9-C34
15	cM	101	BCR	C17-C18-C19-C20
15	cM	101	BCR	C20-C21-C22-C23
15	cM	101	BCR	C20-C21-C22-C37
15	cM	101	BCR	C21-C22-C23-C24
16	aA	852	LHG	C3-O3-P-O5
16	aA	852	LHG	O7-C5-C6-O8
16	aA	853	LHG	C3-O3-P-O5
16	aA	853	LHG	C3-O3-P-O6
16	aA	853	LHG	C4-O6-P-O3
16	aA	853	LHG	C4-O6-P-O5
16	aB	948	LHG	C3-O3-P-O6
16	aB	948	LHG	C4-O6-P-O5
16	bA	851	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
16	bA	851	LHG	O7-C5-C6-O8
16	bA	852	LHG	C3-O3-P-O6
16	bA	852	LHG	C4-O6-P-O3
16	bA	852	LHG	C4-O6-P-O5
16	bB	948	LHG	C3-O3-P-O6
16	bB	948	LHG	C4-O6-P-O5
16	cA	851	LHG	C3-O3-P-O5
16	cA	851	LHG	O7-C5-C6-O8
16	cA	852	LHG	C3-O3-P-O6
16	cA	852	LHG	C4-O6-P-O3
16	cA	852	LHG	C4-O6-P-O5
16	cB	948	LHG	C3-O3-P-O6
16	cB	948	LHG	C4-O6-P-O5
12	aA	844	CLA	CBD-CGD-O2D-CED
12	aB	950	CLA	CBD-CGD-O2D-CED
12	bB	950	CLA	CBD-CGD-O2D-CED
12	aA	837	CLA	O1A-CGA-O2A-C1
12	cA	837	CLA	O1A-CGA-O2A-C1
12	aA	822	CLA	O1A-CGA-O2A-C1
12	aB	930	CLA	O1A-CGA-O2A-C1
12	bA	822	CLA	O1A-CGA-O2A-C1
12	bA	837	CLA	O1A-CGA-O2A-C1
12	bB	930	CLA	O1A-CGA-O2A-C1
12	cA	822	CLA	O1A-CGA-O2A-C1
12	cB	930	CLA	O1A-CGA-O2A-C1
12	aB	915	CLA	O1A-CGA-O2A-C1
12	bB	915	CLA	O1A-CGA-O2A-C1
12	cB	915	CLA	O1A-CGA-O2A-C1
12	aA	807	CLA	C3-C5-C6-C7
12	aA	820	CLA	C3-C5-C6-C7
12	aA	832	CLA	C3-C5-C6-C7
12	aB	912	CLA	C3-C5-C6-C7
12	aL	202	CLA	C3-C5-C6-C7
12	bA	807	CLA	C3-C5-C6-C7
12	bA	820	CLA	C3-C5-C6-C7
12	bA	832	CLA	C3-C5-C6-C7
12	bB	912	CLA	C3-C5-C6-C7
12	bL	202	CLA	C3-C5-C6-C7
12	cA	807	CLA	C3-C5-C6-C7
12	cA	820	CLA	C3-C5-C6-C7
12	cA	832	CLA	C3-C5-C6-C7
12	cB	912	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
12	cL	202	CLA	C3-C5-C6-C7
12	aA	823	CLA	CBA-CGA-O2A-C1
12	aB	930	CLA	CBA-CGA-O2A-C1
12	bA	823	CLA	CBA-CGA-O2A-C1
12	bB	930	CLA	CBA-CGA-O2A-C1
12	cA	823	CLA	CBA-CGA-O2A-C1
12	cB	930	CLA	CBA-CGA-O2A-C1
12	aA	805	CLA	CBD-CGD-O2D-CED
12	aA	815	CLA	CBD-CGD-O2D-CED
12	aA	834	CLA	CBD-CGD-O2D-CED
12	aB	935	CLA	CBD-CGD-O2D-CED
12	bA	805	CLA	CBD-CGD-O2D-CED
12	bA	815	CLA	CBD-CGD-O2D-CED
12	bA	834	CLA	CBD-CGD-O2D-CED
12	bB	935	CLA	CBD-CGD-O2D-CED
12	cA	805	CLA	CBD-CGD-O2D-CED
12	cA	815	CLA	CBD-CGD-O2D-CED
12	cA	834	CLA	CBD-CGD-O2D-CED
12	cB	935	CLA	CBD-CGD-O2D-CED
12	aA	837	CLA	O1D-CGD-O2D-CED
12	bA	837	CLA	O1D-CGD-O2D-CED
12	cA	837	CLA	O1D-CGD-O2D-CED
12	aA	817	CLA	C4-C3-C5-C6
12	aA	818	CLA	C4-C3-C5-C6
12	aA	819	CLA	C4-C3-C5-C6
12	aA	832	CLA	C4-C3-C5-C6
12	aB	905	CLA	C4-C3-C5-C6
12	aB	915	CLA	C4-C3-C5-C6
12	aB	917	CLA	C4-C3-C5-C6
12	aB	921	CLA	C4-C3-C5-C6
12	aB	925	CLA	C4-C3-C5-C6
12	bA	817	CLA	C4-C3-C5-C6
12	bA	818	CLA	C4-C3-C5-C6
12	bA	819	CLA	C4-C3-C5-C6
12	bA	832	CLA	C4-C3-C5-C6
12	bB	905	CLA	C4-C3-C5-C6
12	bB	915	CLA	C4-C3-C5-C6
12	bB	917	CLA	C4-C3-C5-C6
12	bB	921	CLA	C4-C3-C5-C6
12	bB	925	CLA	C4-C3-C5-C6
12	cA	817	CLA	C4-C3-C5-C6
12	cA	818	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
12	cA	819	CLA	C4-C3-C5-C6
12	cA	832	CLA	C4-C3-C5-C6
12	cB	905	CLA	C4-C3-C5-C6
12	cB	915	CLA	C4-C3-C5-C6
12	cB	917	CLA	C4-C3-C5-C6
12	cB	921	CLA	C4-C3-C5-C6
12	cB	925	CLA	C4-C3-C5-C6
12	aA	817	CLA	C2-C3-C5-C6
12	aA	819	CLA	C2-C3-C5-C6
12	aA	832	CLA	C2-C3-C5-C6
12	aB	905	CLA	C2-C3-C5-C6
12	aB	917	CLA	C2-C3-C5-C6
12	aB	925	CLA	C2-C3-C5-C6
12	bA	817	CLA	C2-C3-C5-C6
12	bA	819	CLA	C2-C3-C5-C6
12	bA	832	CLA	C2-C3-C5-C6
12	bB	905	CLA	C2-C3-C5-C6
12	bB	917	CLA	C2-C3-C5-C6
12	bB	925	CLA	C2-C3-C5-C6
12	cA	817	CLA	C2-C3-C5-C6
12	cA	819	CLA	C2-C3-C5-C6
12	cA	832	CLA	C2-C3-C5-C6
12	cB	905	CLA	C2-C3-C5-C6
12	cB	917	CLA	C2-C3-C5-C6
12	cB	925	CLA	C2-C3-C5-C6
13	aA	845	1L3	C20-C21-C23-C24
13	cA	844	1L3	C20-C21-C23-C24
12	aA	808	CLA	C2A-CAA-CBA-CGA
12	aB	915	CLA	C3-C5-C6-C7
12	aB	923	CLA	C2A-CAA-CBA-CGA
12	bA	808	CLA	C2A-CAA-CBA-CGA
12	bB	915	CLA	C3-C5-C6-C7
12	bB	923	CLA	C2A-CAA-CBA-CGA
12	cA	808	CLA	C2A-CAA-CBA-CGA
12	cB	915	CLA	C3-C5-C6-C7
12	cB	923	CLA	C2A-CAA-CBA-CGA
12	aA	806	CLA	C3-C5-C6-C7
12	aA	818	CLA	C3-C5-C6-C7
12	bA	806	CLA	C3-C5-C6-C7
12	bA	818	CLA	C3-C5-C6-C7
12	cA	806	CLA	C3-C5-C6-C7
12	cA	818	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
12	aA	822	CLA	CBA-CGA-O2A-C1
12	aA	837	CLA	CBA-CGA-O2A-C1
12	aB	915	CLA	CBA-CGA-O2A-C1
12	bA	822	CLA	CBA-CGA-O2A-C1
12	bA	837	CLA	CBA-CGA-O2A-C1
12	bB	915	CLA	CBA-CGA-O2A-C1
12	cA	822	CLA	CBA-CGA-O2A-C1
12	cA	837	CLA	CBA-CGA-O2A-C1
12	cB	915	CLA	CBA-CGA-O2A-C1
12	aA	823	CLA	O1A-CGA-O2A-C1
12	bA	823	CLA	O1A-CGA-O2A-C1
12	cA	823	CLA	O1A-CGA-O2A-C1
16	aA	852	LHG	C28-C29-C30-C31
16	bA	851	LHG	C28-C29-C30-C31
16	cA	851	LHG	C28-C29-C30-C31
12	aA	832	CLA	CBA-CGA-O2A-C1
12	aB	917	CLA	CBA-CGA-O2A-C1
12	bA	832	CLA	CBA-CGA-O2A-C1
12	bB	917	CLA	CBA-CGA-O2A-C1
12	cA	832	CLA	CBA-CGA-O2A-C1
12	cB	917	CLA	CBA-CGA-O2A-C1
12	aB	902	CLA	CBD-CGD-O2D-CED
12	bB	902	CLA	CBD-CGD-O2D-CED
12	cB	902	CLA	CBD-CGD-O2D-CED
12	aB	921	CLA	CBD-CGD-O2D-CED
12	bB	921	CLA	CBD-CGD-O2D-CED
12	cB	921	CLA	CBD-CGD-O2D-CED
12	aA	818	CLA	C2-C3-C5-C6
12	aB	921	CLA	C2-C3-C5-C6
12	bA	818	CLA	C2-C3-C5-C6
12	bB	921	CLA	C2-C3-C5-C6
12	cA	818	CLA	C2-C3-C5-C6
12	cB	921	CLA	C2-C3-C5-C6
12	aA	832	CLA	O1A-CGA-O2A-C1
12	bA	832	CLA	O1A-CGA-O2A-C1
12	cA	832	CLA	O1A-CGA-O2A-C1
13	aA	845	1L3	C26-C28-C29-C30
13	bA	844	1L3	C26-C28-C29-C30
13	cA	844	1L3	C26-C28-C29-C30
12	aA	818	CLA	CBD-CGD-O2D-CED
12	aB	922	CLA	CBD-CGD-O2D-CED
12	bA	818	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	bB	922	CLA	CBD-CGD-O2D-CED
12	cA	818	CLA	CBD-CGD-O2D-CED
12	cB	922	CLA	CBD-CGD-O2D-CED
12	aA	804	CLA	CBA-CGA-O2A-C1
12	bA	804	CLA	CBA-CGA-O2A-C1
12	cB	921	CLA	CBA-CGA-O2A-C1
12	aA	829	CLA	CBD-CGD-O2D-CED
12	aB	905	CLA	CBD-CGD-O2D-CED
12	aB	908	CLA	CBD-CGD-O2D-CED
12	bA	829	CLA	CBD-CGD-O2D-CED
12	bB	905	CLA	CBD-CGD-O2D-CED
12	bB	908	CLA	CBD-CGD-O2D-CED
12	cA	829	CLA	CBD-CGD-O2D-CED
12	cB	905	CLA	CBD-CGD-O2D-CED
12	cB	908	CLA	CBD-CGD-O2D-CED
12	aA	808	CLA	CBD-CGD-O2D-CED
12	bA	808	CLA	CBD-CGD-O2D-CED
12	cA	808	CLA	CBD-CGD-O2D-CED
12	aA	807	CLA	CBA-CGA-O2A-C1
12	aA	812	CLA	CBA-CGA-O2A-C1
12	aA	818	CLA	CBA-CGA-O2A-C1
12	aA	820	CLA	CBA-CGA-O2A-C1
12	aB	921	CLA	CBA-CGA-O2A-C1
12	bA	807	CLA	CBA-CGA-O2A-C1
12	bA	812	CLA	CBA-CGA-O2A-C1
12	bA	818	CLA	CBA-CGA-O2A-C1
12	bA	820	CLA	CBA-CGA-O2A-C1
12	bB	921	CLA	CBA-CGA-O2A-C1
12	cA	804	CLA	CBA-CGA-O2A-C1
12	cA	807	CLA	CBA-CGA-O2A-C1
12	cA	812	CLA	CBA-CGA-O2A-C1
12	cA	818	CLA	CBA-CGA-O2A-C1
12	cA	820	CLA	CBA-CGA-O2A-C1
12	aB	915	CLA	C2-C3-C5-C6
12	bB	915	CLA	C2-C3-C5-C6
12	cB	915	CLA	C2-C3-C5-C6
12	aB	949	CLA	CBD-CGD-O2D-CED
12	bB	949	CLA	CBD-CGD-O2D-CED
12	aA	838	CLA	C11-C12-C13-C14
12	aA	842	CLA	C11-C10-C8-C9
12	aB	912	CLA	C6-C7-C8-C9
12	bA	838	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
12	bA	842	CLA	C11-C10-C8-C9
12	bB	912	CLA	C6-C7-C8-C9
12	cA	838	CLA	C11-C12-C13-C14
12	cA	842	CLA	C11-C10-C8-C9
12	cB	912	CLA	C6-C7-C8-C9
12	aA	844	CLA	O1D-CGD-O2D-CED
12	aB	950	CLA	O1D-CGD-O2D-CED
12	bB	950	CLA	O1D-CGD-O2D-CED
12	aA	804	CLA	O1A-CGA-O2A-C1
12	aB	917	CLA	O1A-CGA-O2A-C1
12	bA	804	CLA	O1A-CGA-O2A-C1
12	cA	804	CLA	O1A-CGA-O2A-C1
12	cB	949	CLA	CBD-CGD-O2D-CED
12	aA	834	CLA	O1D-CGD-O2D-CED
12	bA	834	CLA	O1D-CGD-O2D-CED
12	cA	834	CLA	O1D-CGD-O2D-CED
15	aA	847	BCR	C7-C8-C9-C34
15	aA	848	BCR	C7-C8-C9-C34
15	aA	848	BCR	C37-C22-C23-C24
15	aA	850	BCR	C7-C8-C9-C34
15	aA	851	BCR	C37-C22-C23-C24
15	aB	943	BCR	C7-C8-C9-C34
15	aF	201	BCR	C7-C8-C9-C34
15	aF	201	BCR	C37-C22-C23-C24
15	aI	101	BCR	C11-C12-C13-C35
15	aI	101	BCR	C37-C22-C23-C24
15	aJ	101	BCR	C37-C22-C23-C24
15	aL	206	BCR	C37-C22-C23-C24
15	aM	101	BCR	C36-C18-C19-C20
15	bA	846	BCR	C7-C8-C9-C34
15	bA	847	BCR	C7-C8-C9-C34
15	bA	847	BCR	C37-C22-C23-C24
15	bA	849	BCR	C7-C8-C9-C34
15	bA	850	BCR	C37-C22-C23-C24
15	bB	943	BCR	C7-C8-C9-C34
15	bF	201	BCR	C7-C8-C9-C34
15	bF	201	BCR	C37-C22-C23-C24
15	bI	101	BCR	C11-C12-C13-C35
15	bI	101	BCR	C37-C22-C23-C24
15	bJ	101	BCR	C37-C22-C23-C24
15	bL	205	BCR	C7-C8-C9-C34
15	bL	206	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
15	bM	101	BCR	C36-C18-C19-C20
15	cA	846	BCR	C7-C8-C9-C34
15	cA	847	BCR	C7-C8-C9-C34
15	cA	847	BCR	C37-C22-C23-C24
15	cA	849	BCR	C7-C8-C9-C34
15	cA	850	BCR	C37-C22-C23-C24
15	cB	943	BCR	C7-C8-C9-C34
15	cF	201	BCR	C7-C8-C9-C34
15	cF	201	BCR	C37-C22-C23-C24
15	cI	101	BCR	C11-C12-C13-C35
15	cI	101	BCR	C37-C22-C23-C24
15	cJ	101	BCR	C37-C22-C23-C24
15	cL	205	BCR	C7-C8-C9-C34
15	cL	206	BCR	C37-C22-C23-C24
15	cM	101	BCR	C36-C18-C19-C20
15	aB	941	BCR	C7-C8-C9-C10
15	aB	943	BCR	C7-C8-C9-C10
15	aF	201	BCR	C7-C8-C9-C10
15	bB	941	BCR	C7-C8-C9-C10
15	bB	943	BCR	C7-C8-C9-C10
15	bF	201	BCR	C7-C8-C9-C10
15	cB	941	BCR	C7-C8-C9-C10
15	cB	943	BCR	C7-C8-C9-C10
15	cF	201	BCR	C7-C8-C9-C10
12	aA	831	CLA	C2A-CAA-CBA-CGA
12	aA	841	CLA	C2A-CAA-CBA-CGA
12	bA	831	CLA	C2A-CAA-CBA-CGA
12	bA	841	CLA	C2A-CAA-CBA-CGA
12	cA	831	CLA	C2A-CAA-CBA-CGA
12	cA	841	CLA	C2A-CAA-CBA-CGA
12	aA	807	CLA	O1A-CGA-O2A-C1
12	aA	812	CLA	O1A-CGA-O2A-C1
12	aA	818	CLA	O1A-CGA-O2A-C1
12	aA	820	CLA	O1A-CGA-O2A-C1
12	bA	807	CLA	O1A-CGA-O2A-C1
12	bA	812	CLA	O1A-CGA-O2A-C1
12	bA	818	CLA	O1A-CGA-O2A-C1
12	bA	820	CLA	O1A-CGA-O2A-C1
12	bB	917	CLA	O1A-CGA-O2A-C1
12	cA	807	CLA	O1A-CGA-O2A-C1
12	cA	812	CLA	O1A-CGA-O2A-C1
12	cA	818	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	cA	820	CLA	O1A-CGA-O2A-C1
12	cB	917	CLA	O1A-CGA-O2A-C1
12	aA	831	CLA	CBA-CGA-O2A-C1
12	bA	831	CLA	CBA-CGA-O2A-C1
12	cA	831	CLA	CBA-CGA-O2A-C1
12	aA	804	CLA	C2-C1-O2A-CGA
12	bA	804	CLA	C2-C1-O2A-CGA
12	cA	804	CLA	C2-C1-O2A-CGA
12	aA	805	CLA	O1D-CGD-O2D-CED
12	bA	805	CLA	O1D-CGD-O2D-CED
12	cA	805	CLA	O1D-CGD-O2D-CED
12	aB	926	CLA	CBD-CGD-O2D-CED
12	bB	926	CLA	CBD-CGD-O2D-CED
12	cB	926	CLA	CBD-CGD-O2D-CED
12	aB	927	CLA	C5-C6-C7-C8
12	bB	927	CLA	C5-C6-C7-C8
12	cB	927	CLA	C5-C6-C7-C8
17	aB	947	LMG	C28-C29-C30-C31
17	bB	947	LMG	C28-C29-C30-C31
17	cB	947	LMG	C28-C29-C30-C31
12	aB	935	CLA	O1D-CGD-O2D-CED
12	bB	935	CLA	O1D-CGD-O2D-CED
12	cB	935	CLA	O1D-CGD-O2D-CED
12	aA	843	CLA	C13-C15-C16-C17
12	bA	843	CLA	C13-C15-C16-C17
12	aA	820	CLA	C5-C6-C7-C8
12	aB	931	CLA	C15-C16-C17-C18
12	bA	820	CLA	C5-C6-C7-C8
12	bB	931	CLA	C15-C16-C17-C18
12	cA	820	CLA	C5-C6-C7-C8
12	cA	843	CLA	C13-C15-C16-C17
12	cB	931	CLA	C15-C16-C17-C18
12	aA	809	CLA	C2A-CAA-CBA-CGA
12	aA	820	CLA	C2A-CAA-CBA-CGA
12	aA	829	CLA	C2A-CAA-CBA-CGA
12	aB	907	CLA	C3-C5-C6-C7
12	aF	202	CLA	C2A-CAA-CBA-CGA
12	bA	809	CLA	C2A-CAA-CBA-CGA
12	bA	820	CLA	C2A-CAA-CBA-CGA
12	bA	829	CLA	C2A-CAA-CBA-CGA
12	bB	907	CLA	C3-C5-C6-C7
12	bF	202	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
12	cA	809	CLA	C2A-CAA-CBA-CGA
12	cA	820	CLA	C2A-CAA-CBA-CGA
12	cA	829	CLA	C2A-CAA-CBA-CGA
12	cB	907	CLA	C3-C5-C6-C7
12	cF	202	CLA	C2A-CAA-CBA-CGA
16	aB	948	LHG	O10-C23-O8-C6
16	bB	948	LHG	O10-C23-O8-C6
16	cB	948	LHG	O10-C23-O8-C6
15	aJ	101	BCR	C18-C19-C20-C21
15	aM	101	BCR	C18-C19-C20-C21
15	bJ	101	BCR	C18-C19-C20-C21
15	bM	101	BCR	C18-C19-C20-C21
15	cJ	101	BCR	C18-C19-C20-C21
15	cM	101	BCR	C18-C19-C20-C21
12	aB	902	CLA	C5-C6-C7-C8
12	aB	904	CLA	C15-C16-C17-C18
12	aB	931	CLA	C10-C11-C12-C13
12	bB	902	CLA	C5-C6-C7-C8
12	bB	904	CLA	C15-C16-C17-C18
12	bB	931	CLA	C10-C11-C12-C13
12	cB	902	CLA	C5-C6-C7-C8
12	cB	904	CLA	C15-C16-C17-C18
12	cB	931	CLA	C10-C11-C12-C13
12	aA	843	CLA	C15-C16-C17-C18
12	bA	843	CLA	C15-C16-C17-C18
12	cA	843	CLA	C15-C16-C17-C18
12	aB	916	CLA	C10-C11-C12-C13
12	bB	916	CLA	C10-C11-C12-C13
12	cB	916	CLA	C10-C11-C12-C13
12	aA	806	CLA	CBD-CGD-O2D-CED
12	bA	806	CLA	CBD-CGD-O2D-CED
12	cA	806	CLA	CBD-CGD-O2D-CED
12	aB	921	CLA	O1A-CGA-O2A-C1
12	bB	921	CLA	O1A-CGA-O2A-C1
12	cB	921	CLA	O1A-CGA-O2A-C1
12	aA	825	CLA	C8-C10-C11-C12
12	aA	825	CLA	C10-C11-C12-C13
12	aB	925	CLA	C5-C6-C7-C8
12	bA	825	CLA	C8-C10-C11-C12
12	bA	825	CLA	C10-C11-C12-C13
12	bB	925	CLA	C5-C6-C7-C8
12	cA	825	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
12	cA	825	CLA	C10-C11-C12-C13
12	aA	831	CLA	O1A-CGA-O2A-C1
12	bA	831	CLA	O1A-CGA-O2A-C1
12	cA	831	CLA	O1A-CGA-O2A-C1
12	cB	925	CLA	C5-C6-C7-C8
12	aA	830	CLA	C3-C5-C6-C7
12	aB	909	CLA	C3-C5-C6-C7
12	bA	830	CLA	C3-C5-C6-C7
12	bB	909	CLA	C3-C5-C6-C7
12	bB	923	CLA	C3-C5-C6-C7
12	cB	909	CLA	C3-C5-C6-C7
12	bB	901	CLA	CBD-CGD-O2D-CED
12	aA	840	CLA	C8-C10-C11-C12
12	bA	840	CLA	C8-C10-C11-C12
12	cA	840	CLA	C8-C10-C11-C12
12	aA	844	CLA	C2A-CAA-CBA-CGA
12	aB	938	CLA	C2A-CAA-CBA-CGA
12	aB	950	CLA	C2A-CAA-CBA-CGA
12	bB	938	CLA	C2A-CAA-CBA-CGA
12	bB	950	CLA	C2A-CAA-CBA-CGA
12	cB	938	CLA	C2A-CAA-CBA-CGA
12	aA	803	CLA	C13-C15-C16-C17
12	aA	825	CLA	C15-C16-C17-C18
12	bA	803	CLA	C13-C15-C16-C17
12	cA	803	CLA	C13-C15-C16-C17
12	aB	901	CLA	CBD-CGD-O2D-CED
12	cB	901	CLA	CBD-CGD-O2D-CED
12	aA	815	CLA	O1D-CGD-O2D-CED
12	bA	815	CLA	O1D-CGD-O2D-CED
12	cA	815	CLA	O1D-CGD-O2D-CED
12	aA	838	CLA	C10-C11-C12-C13
12	bA	825	CLA	C15-C16-C17-C18
12	bA	838	CLA	C10-C11-C12-C13
12	aA	842	CLA	C8-C10-C11-C12
12	bA	842	CLA	C8-C10-C11-C12
12	cA	825	CLA	C15-C16-C17-C18
12	cA	838	CLA	C10-C11-C12-C13
12	cA	842	CLA	C8-C10-C11-C12
12	aB	923	CLA	C3-C5-C6-C7
12	cA	830	CLA	C3-C5-C6-C7
12	cB	923	CLA	C3-C5-C6-C7
15	aA	849	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
15	aB	942	BCR	C11-C10-C9-C34
15	aB	944	BCR	C11-C10-C9-C34
15	aF	203	BCR	C20-C21-C22-C37
15	aM	101	BCR	C16-C17-C18-C36
15	bA	848	BCR	C20-C21-C22-C37
15	bB	942	BCR	C11-C10-C9-C34
15	bB	944	BCR	C11-C10-C9-C34
15	bF	203	BCR	C20-C21-C22-C37
15	bM	101	BCR	C16-C17-C18-C36
15	cA	848	BCR	C20-C21-C22-C37
15	cB	942	BCR	C11-C10-C9-C34
15	cB	944	BCR	C11-C10-C9-C34
15	cF	203	BCR	C20-C21-C22-C37
15	cM	101	BCR	C16-C17-C18-C36
12	aA	832	CLA	C5-C6-C7-C8
12	bA	832	CLA	C5-C6-C7-C8
12	cA	832	CLA	C5-C6-C7-C8
15	aB	941	BCR	C7-C8-C9-C34
15	aL	205	BCR	C37-C22-C23-C24
15	aM	101	BCR	C37-C22-C23-C24
15	bA	848	BCR	C37-C22-C23-C24
15	bB	941	BCR	C7-C8-C9-C34
15	bL	205	BCR	C37-C22-C23-C24
15	bM	101	BCR	C37-C22-C23-C24
15	cA	848	BCR	C37-C22-C23-C24
15	cB	941	BCR	C7-C8-C9-C34
15	cL	205	BCR	C37-C22-C23-C24
15	cM	101	BCR	C37-C22-C23-C24
15	aA	847	BCR	C21-C22-C23-C24
15	aB	941	BCR	C21-C22-C23-C24
15	aJ	101	BCR	C21-C22-C23-C24
15	aL	206	BCR	C21-C22-C23-C24
15	bA	846	BCR	C21-C22-C23-C24
15	bB	941	BCR	C21-C22-C23-C24
15	bJ	101	BCR	C21-C22-C23-C24
15	bL	206	BCR	C21-C22-C23-C24
15	cA	846	BCR	C21-C22-C23-C24
15	cB	941	BCR	C21-C22-C23-C24
15	cJ	101	BCR	C21-C22-C23-C24
15	cL	206	BCR	C21-C22-C23-C24
12	aA	854	CLA	C2A-CAA-CBA-CGA
12	aB	915	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
12	bA	853	CLA	C2A-CAA-CBA-CGA
12	bB	915	CLA	C2A-CAA-CBA-CGA
12	cA	853	CLA	C2A-CAA-CBA-CGA
12	cB	915	CLA	C2A-CAA-CBA-CGA
12	aA	829	CLA	C5-C6-C7-C8
12	bA	829	CLA	C5-C6-C7-C8
12	cA	829	CLA	C5-C6-C7-C8
16	aA	852	LHG	O1-C1-C2-C3
16	bA	851	LHG	O1-C1-C2-C3
16	cA	851	LHG	O1-C1-C2-C3
12	aB	904	CLA	C16-C17-C18-C19
12	bB	904	CLA	C16-C17-C18-C19
12	cB	904	CLA	C16-C17-C18-C19
12	aA	854	CLA	C3-C5-C6-C7
12	bA	853	CLA	C3-C5-C6-C7
12	cA	853	CLA	C3-C5-C6-C7
15	aA	847	BCR	C11-C10-C9-C8
15	aA	849	BCR	C20-C21-C22-C23
15	aB	942	BCR	C11-C10-C9-C8
15	aF	203	BCR	C11-C10-C9-C8
15	aF	203	BCR	C20-C21-C22-C23
15	aM	101	BCR	C11-C10-C9-C8
15	aM	101	BCR	C16-C17-C18-C19
15	bA	846	BCR	C11-C10-C9-C8
15	bA	848	BCR	C20-C21-C22-C23
15	bB	942	BCR	C11-C10-C9-C8
15	bF	203	BCR	C11-C10-C9-C8
15	bF	203	BCR	C20-C21-C22-C23
15	bM	101	BCR	C11-C10-C9-C8
15	bM	101	BCR	C16-C17-C18-C19
15	cA	846	BCR	C11-C10-C9-C8
15	cA	848	BCR	C20-C21-C22-C23
15	cB	942	BCR	C11-C10-C9-C8
15	cF	203	BCR	C11-C10-C9-C8
15	cF	203	BCR	C20-C21-C22-C23
15	cM	101	BCR	C11-C10-C9-C8
15	cM	101	BCR	C16-C17-C18-C19
12	aB	905	CLA	O1D-CGD-O2D-CED
12	aB	935	CLA	CBA-CGA-O2A-C1
12	bB	935	CLA	CBA-CGA-O2A-C1
12	cB	935	CLA	CBA-CGA-O2A-C1
12	aA	824	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	aB	916	CLA	CBD-CGD-O2D-CED
12	bA	824	CLA	CBD-CGD-O2D-CED
12	bB	916	CLA	CBD-CGD-O2D-CED
12	cA	824	CLA	CBD-CGD-O2D-CED
12	cB	916	CLA	CBD-CGD-O2D-CED
12	cB	905	CLA	O1D-CGD-O2D-CED
12	cA	817	CLA	C2-C1-O2A-CGA
12	aB	908	CLA	O2A-C1-C2-C3
12	bB	908	CLA	O2A-C1-C2-C3
12	cB	908	CLA	O2A-C1-C2-C3
12	aA	854	CLA	CBD-CGD-O2D-CED
12	cA	853	CLA	CBD-CGD-O2D-CED
15	aA	847	BCR	C14-C15-C16-C17
15	bA	846	BCR	C14-C15-C16-C17
15	cA	846	BCR	C14-C15-C16-C17
12	bB	905	CLA	O1D-CGD-O2D-CED
16	aA	852	LHG	C13-C14-C15-C16
16	bA	851	LHG	C13-C14-C15-C16
16	cA	851	LHG	C13-C14-C15-C16
12	aA	818	CLA	O1D-CGD-O2D-CED
12	aB	921	CLA	O1D-CGD-O2D-CED
12	bA	818	CLA	O1D-CGD-O2D-CED
12	bB	921	CLA	O1D-CGD-O2D-CED
12	cA	818	CLA	O1D-CGD-O2D-CED
12	cB	921	CLA	O1D-CGD-O2D-CED
12	aA	810	CLA	C4B-C3B-CAB-CBB
12	aA	826	CLA	C4B-C3B-CAB-CBB
12	aB	901	CLA	C4B-C3B-CAB-CBB
12	aB	910	CLA	C4B-C3B-CAB-CBB
12	aB	912	CLA	C4B-C3B-CAB-CBB
12	aB	915	CLA	C4B-C3B-CAB-CBB
12	aB	916	CLA	C4B-C3B-CAB-CBB
12	aB	918	CLA	C4B-C3B-CAB-CBB
12	aB	923	CLA	C4B-C3B-CAB-CBB
12	bA	810	CLA	C4B-C3B-CAB-CBB
12	bA	826	CLA	C4B-C3B-CAB-CBB
12	bB	901	CLA	C4B-C3B-CAB-CBB
12	bB	910	CLA	C4B-C3B-CAB-CBB
12	bB	912	CLA	C4B-C3B-CAB-CBB
12	bB	915	CLA	C4B-C3B-CAB-CBB
12	bB	916	CLA	C4B-C3B-CAB-CBB
12	bB	918	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
12	bB	923	CLA	C4B-C3B-CAB-CBB
12	cA	810	CLA	C4B-C3B-CAB-CBB
12	cA	826	CLA	C4B-C3B-CAB-CBB
12	cB	901	CLA	C4B-C3B-CAB-CBB
12	cB	910	CLA	C4B-C3B-CAB-CBB
12	cB	912	CLA	C4B-C3B-CAB-CBB
12	cB	915	CLA	C4B-C3B-CAB-CBB
12	cB	916	CLA	C4B-C3B-CAB-CBB
12	cB	918	CLA	C4B-C3B-CAB-CBB
12	cB	923	CLA	C4B-C3B-CAB-CBB
12	aB	935	CLA	O1A-CGA-O2A-C1
12	bB	935	CLA	O1A-CGA-O2A-C1
12	cB	935	CLA	O1A-CGA-O2A-C1
12	aA	842	CLA	C11-C12-C13-C15
12	aB	926	CLA	C11-C12-C13-C15
12	bA	842	CLA	C11-C12-C13-C15
12	bB	926	CLA	C11-C12-C13-C15
12	cA	842	CLA	C11-C12-C13-C15
12	cB	926	CLA	C11-C12-C13-C15
16	bB	948	LHG	C24-C23-O8-C6
16	cB	948	LHG	C24-C23-O8-C6
16	aA	852	LHG	C26-C27-C28-C29
16	bA	851	LHG	C26-C27-C28-C29
16	cA	851	LHG	C26-C27-C28-C29
12	aB	921	CLA	C3-C5-C6-C7
12	bB	921	CLA	C3-C5-C6-C7
12	cB	921	CLA	C3-C5-C6-C7
12	aA	802	CLA	C3A-C2A-CAA-CBA
12	aA	807	CLA	C3A-C2A-CAA-CBA
12	aA	810	CLA	C3A-C2A-CAA-CBA
12	aA	816	CLA	C3A-C2A-CAA-CBA
12	aA	832	CLA	C3A-C2A-CAA-CBA
12	aB	914	CLA	C3A-C2A-CAA-CBA
12	aB	939	CLA	C3A-C2A-CAA-CBA
12	bA	802	CLA	C3A-C2A-CAA-CBA
12	bA	807	CLA	C3A-C2A-CAA-CBA
12	bA	810	CLA	C3A-C2A-CAA-CBA
12	bA	816	CLA	C3A-C2A-CAA-CBA
12	bA	832	CLA	C3A-C2A-CAA-CBA
12	bB	914	CLA	C3A-C2A-CAA-CBA
12	bB	939	CLA	C3A-C2A-CAA-CBA
12	cA	802	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	cA	807	CLA	C3A-C2A-CAA-CBA
12	cA	810	CLA	C3A-C2A-CAA-CBA
12	cA	816	CLA	C3A-C2A-CAA-CBA
12	cA	832	CLA	C3A-C2A-CAA-CBA
12	cB	914	CLA	C3A-C2A-CAA-CBA
12	cB	939	CLA	C3A-C2A-CAA-CBA
12	bA	853	CLA	CBD-CGD-O2D-CED
12	aB	902	CLA	O1D-CGD-O2D-CED
12	bB	902	CLA	O1D-CGD-O2D-CED
12	cB	902	CLA	O1D-CGD-O2D-CED
16	aB	948	LHG	C24-C23-O8-C6
15	aF	203	BCR	C19-C20-C21-C22
15	bF	203	BCR	C19-C20-C21-C22
15	cF	203	BCR	C19-C20-C21-C22
12	bB	934	CLA	CBD-CGD-O2D-CED
12	cB	934	CLA	CBD-CGD-O2D-CED
12	aA	834	CLA	C2B-C3B-CAB-CBB
12	aB	912	CLA	C2B-C3B-CAB-CBB
12	aB	915	CLA	C2B-C3B-CAB-CBB
12	aB	916	CLA	C2B-C3B-CAB-CBB
12	aB	918	CLA	C2B-C3B-CAB-CBB
12	bA	834	CLA	C2B-C3B-CAB-CBB
12	bB	912	CLA	C2B-C3B-CAB-CBB
12	bB	915	CLA	C2B-C3B-CAB-CBB
12	bB	916	CLA	C2B-C3B-CAB-CBB
12	bB	918	CLA	C2B-C3B-CAB-CBB
12	cA	834	CLA	C2B-C3B-CAB-CBB
12	cB	912	CLA	C2B-C3B-CAB-CBB
12	cB	915	CLA	C2B-C3B-CAB-CBB
12	cB	916	CLA	C2B-C3B-CAB-CBB
12	cB	918	CLA	C2B-C3B-CAB-CBB
15	aA	849	BCR	C23-C24-C25-C26
15	aA	849	BCR	C23-C24-C25-C30
15	aB	941	BCR	C1-C6-C7-C8
15	aB	941	BCR	C5-C6-C7-C8
15	aB	944	BCR	C1-C6-C7-C8
15	aJ	101	BCR	C1-C6-C7-C8
15	aJ	101	BCR	C23-C24-C25-C26
15	aJ	101	BCR	C23-C24-C25-C30
15	aM	101	BCR	C1-C6-C7-C8
15	aM	101	BCR	C5-C6-C7-C8
15	bA	848	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
15	bA	848	BCR	C23-C24-C25-C30
15	bB	941	BCR	C1-C6-C7-C8
15	bB	941	BCR	C5-C6-C7-C8
15	bB	944	BCR	C1-C6-C7-C8
15	bJ	101	BCR	C1-C6-C7-C8
15	bJ	101	BCR	C23-C24-C25-C26
15	bJ	101	BCR	C23-C24-C25-C30
15	bM	101	BCR	C1-C6-C7-C8
15	bM	101	BCR	C5-C6-C7-C8
15	cA	848	BCR	C23-C24-C25-C26
15	cA	848	BCR	C23-C24-C25-C30
15	cB	941	BCR	C1-C6-C7-C8
15	cB	941	BCR	C5-C6-C7-C8
15	cB	944	BCR	C1-C6-C7-C8
15	cJ	101	BCR	C1-C6-C7-C8
15	cJ	101	BCR	C23-C24-C25-C26
15	cJ	101	BCR	C23-C24-C25-C30
15	cM	101	BCR	C1-C6-C7-C8
15	cM	101	BCR	C5-C6-C7-C8
12	aB	934	CLA	CBD-CGD-O2D-CED
16	aA	852	LHG	C8-C7-O7-C5
16	bA	851	LHG	C8-C7-O7-C5
16	cA	851	LHG	C8-C7-O7-C5
17	aB	947	LMG	C35-C36-C37-C38
17	cB	947	LMG	C35-C36-C37-C38
12	aB	926	CLA	C2A-CAA-CBA-CGA
12	bB	926	CLA	C2A-CAA-CBA-CGA
12	cB	926	CLA	C2A-CAA-CBA-CGA
17	bB	947	LMG	C35-C36-C37-C38
15	aA	847	BCR	C18-C19-C20-C21
15	aB	942	BCR	C10-C11-C12-C13
15	bA	846	BCR	C18-C19-C20-C21
15	bB	942	BCR	C10-C11-C12-C13
15	cA	846	BCR	C18-C19-C20-C21
15	cB	942	BCR	C10-C11-C12-C13
12	aA	806	CLA	C8-C10-C11-C12
12	bA	806	CLA	C8-C10-C11-C12
12	cA	806	CLA	C8-C10-C11-C12
15	aM	101	BCR	C22-C23-C24-C25
15	bM	101	BCR	C22-C23-C24-C25
15	cM	101	BCR	C22-C23-C24-C25
15	aJ	101	BCR	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
15	bJ	101	BCR	C14-C15-C16-C17
15	cJ	101	BCR	C14-C15-C16-C17
12	aB	908	CLA	O1D-CGD-O2D-CED
12	cB	908	CLA	O1D-CGD-O2D-CED
17	aB	947	LMG	C36-C37-C38-C39
17	cB	947	LMG	C36-C37-C38-C39
12	aA	830	CLA	CBA-CGA-O2A-C1
12	bA	830	CLA	CBA-CGA-O2A-C1
12	cA	830	CLA	CBA-CGA-O2A-C1
12	aA	825	CLA	C16-C17-C18-C19
12	aB	904	CLA	C16-C17-C18-C20
12	bB	904	CLA	C16-C17-C18-C20
12	cB	904	CLA	C16-C17-C18-C20
17	bB	947	LMG	C36-C37-C38-C39
12	bB	908	CLA	O1D-CGD-O2D-CED
16	aA	852	LHG	C27-C28-C29-C30
16	bA	851	LHG	C27-C28-C29-C30
16	cA	851	LHG	C27-C28-C29-C30
15	aA	849	BCR	C37-C22-C23-C24
15	aA	850	BCR	C11-C12-C13-C35
15	bA	849	BCR	C11-C12-C13-C35
15	cA	849	BCR	C11-C12-C13-C35
12	aA	824	CLA	C2A-CAA-CBA-CGA
12	bA	824	CLA	C2A-CAA-CBA-CGA
12	cA	824	CLA	C2A-CAA-CBA-CGA
12	bA	825	CLA	C16-C17-C18-C19
12	cA	825	CLA	C16-C17-C18-C19
12	aA	830	CLA	CBD-CGD-O2D-CED
12	bA	830	CLA	CBD-CGD-O2D-CED
12	cA	830	CLA	CBD-CGD-O2D-CED
12	aA	808	CLA	O1D-CGD-O2D-CED
12	aB	922	CLA	O1D-CGD-O2D-CED
12	bA	808	CLA	O1D-CGD-O2D-CED
12	cA	808	CLA	O1D-CGD-O2D-CED
12	cB	922	CLA	O1D-CGD-O2D-CED
16	bB	948	LHG	O7-C5-C6-O8
16	cB	948	LHG	O7-C5-C6-O8
16	cA	851	LHG	C10-C11-C12-C13
12	bB	922	CLA	O1D-CGD-O2D-CED
16	aA	852	LHG	C10-C11-C12-C13
16	bA	851	LHG	C10-C11-C12-C13
12	aA	829	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	cA	829	CLA	O1D-CGD-O2D-CED
12	aA	817	CLA	C2-C1-O2A-CGA
12	bA	817	CLA	C2-C1-O2A-CGA
12	bA	829	CLA	O1D-CGD-O2D-CED
12	aA	802	CLA	C2A-CAA-CBA-CGA
12	bA	802	CLA	C2A-CAA-CBA-CGA
12	cA	802	CLA	C2A-CAA-CBA-CGA
12	aF	202	CLA	CBD-CGD-O2D-CED
12	bF	202	CLA	CBD-CGD-O2D-CED
12	cF	202	CLA	CBD-CGD-O2D-CED
12	aB	902	CLA	C3-C5-C6-C7
12	bB	902	CLA	C3-C5-C6-C7
12	cB	902	CLA	C3-C5-C6-C7
12	aA	810	CLA	C1A-C2A-CAA-CBA
12	aA	811	CLA	C1A-C2A-CAA-CBA
12	aA	812	CLA	C1A-C2A-CAA-CBA
12	aA	816	CLA	C1A-C2A-CAA-CBA
12	aA	818	CLA	C1A-C2A-CAA-CBA
12	aA	821	CLA	C1A-C2A-CAA-CBA
12	aA	824	CLA	C1A-C2A-CAA-CBA
12	aA	834	CLA	C1A-C2A-CAA-CBA
12	aB	910	CLA	C1A-C2A-CAA-CBA
12	aB	913	CLA	C1A-C2A-CAA-CBA
12	aB	914	CLA	C1A-C2A-CAA-CBA
12	aB	918	CLA	C1A-C2A-CAA-CBA
12	aB	922	CLA	C1A-C2A-CAA-CBA
12	aB	930	CLA	C1A-C2A-CAA-CBA
12	aB	931	CLA	C1A-C2A-CAA-CBA
12	aB	933	CLA	C1A-C2A-CAA-CBA
12	aB	934	CLA	C1A-C2A-CAA-CBA
12	aB	939	CLA	C1A-C2A-CAA-CBA
12	aL	202	CLA	C1A-C2A-CAA-CBA
12	bA	810	CLA	C1A-C2A-CAA-CBA
12	bA	811	CLA	C1A-C2A-CAA-CBA
12	bA	812	CLA	C1A-C2A-CAA-CBA
12	bA	816	CLA	C1A-C2A-CAA-CBA
12	bA	818	CLA	C1A-C2A-CAA-CBA
12	bA	821	CLA	C1A-C2A-CAA-CBA
12	bA	824	CLA	C1A-C2A-CAA-CBA
12	bA	834	CLA	C1A-C2A-CAA-CBA
12	bB	910	CLA	C1A-C2A-CAA-CBA
12	bB	913	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	bB	914	CLA	C1A-C2A-CAA-CBA
12	bB	918	CLA	C1A-C2A-CAA-CBA
12	bB	922	CLA	C1A-C2A-CAA-CBA
12	bB	930	CLA	C1A-C2A-CAA-CBA
12	bB	931	CLA	C1A-C2A-CAA-CBA
12	bB	933	CLA	C1A-C2A-CAA-CBA
12	bB	934	CLA	C1A-C2A-CAA-CBA
12	bB	939	CLA	C1A-C2A-CAA-CBA
12	bL	202	CLA	C1A-C2A-CAA-CBA
12	cA	810	CLA	C1A-C2A-CAA-CBA
12	cA	811	CLA	C1A-C2A-CAA-CBA
12	cA	812	CLA	C1A-C2A-CAA-CBA
12	cA	816	CLA	C1A-C2A-CAA-CBA
12	cA	818	CLA	C1A-C2A-CAA-CBA
12	cA	821	CLA	C1A-C2A-CAA-CBA
12	cA	824	CLA	C1A-C2A-CAA-CBA
12	cA	834	CLA	C1A-C2A-CAA-CBA
12	cB	910	CLA	C1A-C2A-CAA-CBA
12	cB	913	CLA	C1A-C2A-CAA-CBA
12	cB	914	CLA	C1A-C2A-CAA-CBA
12	cB	918	CLA	C1A-C2A-CAA-CBA
12	cB	922	CLA	C1A-C2A-CAA-CBA
12	cB	930	CLA	C1A-C2A-CAA-CBA
12	cB	931	CLA	C1A-C2A-CAA-CBA
12	cB	933	CLA	C1A-C2A-CAA-CBA
12	cB	934	CLA	C1A-C2A-CAA-CBA
12	cB	939	CLA	C1A-C2A-CAA-CBA
12	cL	202	CLA	C1A-C2A-CAA-CBA
12	bA	811	CLA	CBD-CGD-O2D-CED
16	aA	852	LHG	O9-C7-O7-C5
16	bA	851	LHG	O9-C7-O7-C5
16	cA	851	LHG	O9-C7-O7-C5
12	aB	925	CLA	C3-C5-C6-C7
12	bB	925	CLA	C3-C5-C6-C7
12	cB	925	CLA	C3-C5-C6-C7
12	aA	825	CLA	C12-C13-C15-C16
12	aA	838	CLA	C11-C10-C8-C7
12	aA	843	CLA	C11-C12-C13-C15
12	aB	902	CLA	C6-C7-C8-C10
12	aB	904	CLA	C12-C13-C15-C16
12	bA	825	CLA	C12-C13-C15-C16
12	bA	838	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
12	bA	843	CLA	C11-C12-C13-C15
12	bB	902	CLA	C6-C7-C8-C10
12	bB	904	CLA	C12-C13-C15-C16
12	cA	825	CLA	C12-C13-C15-C16
12	cA	838	CLA	C11-C10-C8-C7
12	cA	843	CLA	C11-C12-C13-C15
12	cB	902	CLA	C6-C7-C8-C10
12	cB	904	CLA	C12-C13-C15-C16
17	aB	947	LMG	C29-C30-C31-C32
17	bB	947	LMG	C29-C30-C31-C32
17	cB	947	LMG	C29-C30-C31-C32
12	aA	811	CLA	CBD-CGD-O2D-CED
12	cA	811	CLA	CBD-CGD-O2D-CED
12	aB	913	CLA	C4-C3-C5-C6
12	bB	913	CLA	C4-C3-C5-C6
12	cB	913	CLA	C4-C3-C5-C6
12	aB	902	CLA	C6-C7-C8-C9
12	aB	904	CLA	C14-C13-C15-C16
12	aB	905	CLA	C6-C7-C8-C9
12	aB	926	CLA	C11-C10-C8-C9
12	aB	926	CLA	C14-C13-C15-C16
12	aB	936	CLA	C6-C7-C8-C9
12	bB	902	CLA	C6-C7-C8-C9
12	bB	904	CLA	C14-C13-C15-C16
12	bB	905	CLA	C6-C7-C8-C9
12	bB	926	CLA	C11-C10-C8-C9
12	bB	926	CLA	C14-C13-C15-C16
12	bB	936	CLA	C6-C7-C8-C9
12	cB	902	CLA	C6-C7-C8-C9
12	cB	904	CLA	C14-C13-C15-C16
12	cB	905	CLA	C6-C7-C8-C9
12	cB	926	CLA	C11-C10-C8-C9
12	cB	926	CLA	C14-C13-C15-C16
12	cB	936	CLA	C6-C7-C8-C9
15	aM	101	BCR	C19-C20-C21-C22
15	bM	101	BCR	C19-C20-C21-C22
15	cM	101	BCR	C19-C20-C21-C22
12	aB	927	CLA	CBA-CGA-O2A-C1
12	bB	927	CLA	CBA-CGA-O2A-C1
12	cB	927	CLA	CBA-CGA-O2A-C1
16	aA	852	LHG	C4-C5-C6-O8
16	aB	948	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
16	bA	851	LHG	C4-C5-C6-O8
16	bB	948	LHG	C4-C5-C6-O8
16	cA	851	LHG	C4-C5-C6-O8
16	cB	948	LHG	C4-C5-C6-O8
12	aA	842	CLA	CBA-CGA-O2A-C1
12	bA	842	CLA	CBA-CGA-O2A-C1
12	cA	842	CLA	CBA-CGA-O2A-C1
16	bA	851	LHG	C14-C15-C16-C17
15	aB	942	BCR	C35-C13-C14-C15
15	bB	942	BCR	C35-C13-C14-C15
15	cB	942	BCR	C35-C13-C14-C15
16	aA	852	LHG	C14-C15-C16-C17
16	cA	851	LHG	C14-C15-C16-C17
12	aA	830	CLA	O1A-CGA-O2A-C1
12	bA	830	CLA	O1A-CGA-O2A-C1
12	cA	830	CLA	O1A-CGA-O2A-C1
12	bB	920	CLA	CBD-CGD-O2D-CED
12	cB	920	CLA	CBD-CGD-O2D-CED
12	aA	806	CLA	C2-C3-C5-C6
12	aB	913	CLA	C2-C3-C5-C6
12	bA	806	CLA	C2-C3-C5-C6
12	bB	913	CLA	C2-C3-C5-C6
12	cA	806	CLA	C2-C3-C5-C6
12	cB	913	CLA	C2-C3-C5-C6
15	aF	203	BCR	C21-C22-C23-C24
15	bF	203	BCR	C21-C22-C23-C24
15	cF	203	BCR	C21-C22-C23-C24
12	aA	834	CLA	C5-C6-C7-C8
12	bA	834	CLA	C5-C6-C7-C8
12	cA	834	CLA	C5-C6-C7-C8
12	aA	808	CLA	CBA-CGA-O2A-C1
12	aB	909	CLA	CBA-CGA-O2A-C1
12	bA	808	CLA	CBA-CGA-O2A-C1
12	bB	909	CLA	CBA-CGA-O2A-C1
12	cA	808	CLA	CBA-CGA-O2A-C1
12	cB	909	CLA	CBA-CGA-O2A-C1
12	aB	920	CLA	CBD-CGD-O2D-CED
15	aL	201	BCR	C11-C10-C9-C8
15	bL	201	BCR	C11-C10-C9-C8
15	cL	201	BCR	C11-C10-C9-C8
15	aB	941	BCR	C22-C23-C24-C25
15	aB	945	BCR	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
15	bB	941	BCR	C22-C23-C24-C25
15	bB	945	BCR	C6-C7-C8-C9
15	cB	941	BCR	C22-C23-C24-C25
15	cB	945	BCR	C6-C7-C8-C9
12	aA	817	CLA	CBA-CGA-O2A-C1
12	aB	912	CLA	CBA-CGA-O2A-C1
12	bA	817	CLA	CBA-CGA-O2A-C1
12	cA	817	CLA	CBA-CGA-O2A-C1
12	cB	916	CLA	O1D-CGD-O2D-CED
12	aB	931	CLA	C2-C3-C5-C6
12	bB	931	CLA	C2-C3-C5-C6
12	cB	931	CLA	C2-C3-C5-C6
12	aB	916	CLA	C11-C12-C13-C14
16	aB	948	LHG	O7-C5-C6-O8
12	bB	916	CLA	C11-C12-C13-C14
12	cB	916	CLA	C11-C12-C13-C14
12	bB	912	CLA	CBA-CGA-O2A-C1
12	cB	912	CLA	CBA-CGA-O2A-C1
12	aA	842	CLA	O1A-CGA-O2A-C1
12	aB	916	CLA	O1D-CGD-O2D-CED
12	bB	916	CLA	O1D-CGD-O2D-CED
12	aA	826	CLA	C3-C5-C6-C7
12	bA	826	CLA	C3-C5-C6-C7
12	cA	826	CLA	C3-C5-C6-C7
12	aA	840	CLA	C5-C6-C7-C8
12	bA	840	CLA	C5-C6-C7-C8
12	cA	840	CLA	C5-C6-C7-C8
12	bA	842	CLA	O1A-CGA-O2A-C1
12	cA	842	CLA	O1A-CGA-O2A-C1
12	aA	806	CLA	C4-C3-C5-C6
12	aA	807	CLA	C4-C3-C5-C6
12	aB	904	CLA	C4-C3-C5-C6
12	aB	923	CLA	C4-C3-C5-C6
12	bA	806	CLA	C4-C3-C5-C6
12	bA	807	CLA	C4-C3-C5-C6
12	bB	904	CLA	C4-C3-C5-C6
12	bB	923	CLA	C4-C3-C5-C6
12	cA	806	CLA	C4-C3-C5-C6
12	cA	807	CLA	C4-C3-C5-C6
12	cB	904	CLA	C4-C3-C5-C6
12	cB	923	CLA	C4-C3-C5-C6
16	aA	852	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
16	bA	851	LHG	O1-C1-C2-O2
16	cA	851	LHG	O1-C1-C2-O2
12	aA	825	CLA	C14-C13-C15-C16
12	aA	838	CLA	C11-C10-C8-C9
12	aA	840	CLA	C11-C10-C8-C9
12	aA	843	CLA	C11-C12-C13-C14
12	bA	825	CLA	C14-C13-C15-C16
12	bA	838	CLA	C11-C10-C8-C9
12	bA	840	CLA	C11-C10-C8-C9
12	bA	843	CLA	C11-C12-C13-C14
12	cA	825	CLA	C14-C13-C15-C16
12	cA	838	CLA	C11-C10-C8-C9
12	cA	840	CLA	C11-C10-C8-C9
12	cA	843	CLA	C11-C12-C13-C14
12	aB	927	CLA	O1A-CGA-O2A-C1
12	aA	831	CLA	C4B-C3B-CAB-CBB
12	aA	840	CLA	C4B-C3B-CAB-CBB
12	bA	831	CLA	C4B-C3B-CAB-CBB
12	bA	840	CLA	C4B-C3B-CAB-CBB
12	cA	831	CLA	C4B-C3B-CAB-CBB
12	cA	840	CLA	C4B-C3B-CAB-CBB
12	aA	806	CLA	C16-C17-C18-C20
12	bA	806	CLA	C16-C17-C18-C20
12	cA	806	CLA	C16-C17-C18-C20
12	bB	927	CLA	O1A-CGA-O2A-C1
12	cB	927	CLA	O1A-CGA-O2A-C1
17	aB	947	LMG	C31-C32-C33-C34
17	bB	947	LMG	C31-C32-C33-C34
17	cB	947	LMG	C31-C32-C33-C34
12	aA	805	CLA	C3-C5-C6-C7
12	aA	817	CLA	C3-C5-C6-C7
12	bA	805	CLA	C3-C5-C6-C7
12	bA	817	CLA	C3-C5-C6-C7
12	cA	805	CLA	C3-C5-C6-C7
12	cA	817	CLA	C3-C5-C6-C7
12	aB	923	CLA	C6-C7-C8-C9
12	aB	936	CLA	C11-C12-C13-C14
12	bB	923	CLA	C6-C7-C8-C9
12	bB	936	CLA	C11-C12-C13-C14
12	cB	923	CLA	C6-C7-C8-C9
12	cB	936	CLA	C11-C12-C13-C14
12	aA	834	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
12	aA	840	CLA	C11-C10-C8-C7
12	aB	905	CLA	C6-C7-C8-C10
12	aB	926	CLA	C11-C10-C8-C7
12	aB	926	CLA	C12-C13-C15-C16
12	aB	936	CLA	C6-C7-C8-C10
12	bA	834	CLA	C12-C13-C15-C16
12	bA	840	CLA	C11-C10-C8-C7
12	bB	905	CLA	C6-C7-C8-C10
12	bB	926	CLA	C11-C10-C8-C7
12	bB	926	CLA	C12-C13-C15-C16
12	bB	936	CLA	C6-C7-C8-C10
12	cA	834	CLA	C12-C13-C15-C16
12	cA	840	CLA	C11-C10-C8-C7
12	cB	905	CLA	C6-C7-C8-C10
12	cB	926	CLA	C11-C10-C8-C7
12	cB	926	CLA	C12-C13-C15-C16
12	cB	936	CLA	C6-C7-C8-C10
12	aA	854	CLA	C5-C6-C7-C8
12	bA	853	CLA	C5-C6-C7-C8
12	cA	853	CLA	C5-C6-C7-C8
12	aA	808	CLA	O1A-CGA-O2A-C1
12	aB	909	CLA	O1A-CGA-O2A-C1
12	bA	808	CLA	O1A-CGA-O2A-C1
12	bB	909	CLA	O1A-CGA-O2A-C1
12	cA	808	CLA	O1A-CGA-O2A-C1
12	cB	909	CLA	O1A-CGA-O2A-C1
12	aA	842	CLA	C4-C3-C5-C6
12	aB	926	CLA	C3A-C2A-CAA-CBA
12	aB	927	CLA	C4-C3-C5-C6
12	aL	203	CLA	C3A-C2A-CAA-CBA
12	bA	842	CLA	C4-C3-C5-C6
12	bB	926	CLA	C3A-C2A-CAA-CBA
12	bB	927	CLA	C4-C3-C5-C6
12	bL	203	CLA	C3A-C2A-CAA-CBA
12	cA	842	CLA	C4-C3-C5-C6
12	cB	926	CLA	C3A-C2A-CAA-CBA
12	cB	927	CLA	C4-C3-C5-C6
12	cL	203	CLA	C3A-C2A-CAA-CBA
16	aA	852	LHG	C29-C30-C31-C32
16	bA	851	LHG	C29-C30-C31-C32
12	aA	808	CLA	C4-C3-C5-C6
12	bA	808	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
12	cA	808	CLA	C4-C3-C5-C6
16	cA	851	LHG	C29-C30-C31-C32
12	bB	907	CLA	CBD-CGD-O2D-CED
15	aM	101	BCR	C7-C8-C9-C10
15	bM	101	BCR	C7-C8-C9-C10
15	cM	101	BCR	C7-C8-C9-C10
12	aB	907	CLA	CBD-CGD-O2D-CED
12	cB	907	CLA	CBD-CGD-O2D-CED
12	aB	931	CLA	C4-C3-C5-C6
12	bB	931	CLA	C4-C3-C5-C6
12	cB	931	CLA	C4-C3-C5-C6
12	aA	807	CLA	C2-C3-C5-C6
12	aA	825	CLA	C2-C3-C5-C6
12	aB	923	CLA	C2-C3-C5-C6
12	aB	927	CLA	C2-C3-C5-C6
12	bA	807	CLA	C2-C3-C5-C6
12	bA	825	CLA	C2-C3-C5-C6
12	bB	923	CLA	C2-C3-C5-C6
12	bB	927	CLA	C2-C3-C5-C6
12	cA	807	CLA	C2-C3-C5-C6
12	cA	825	CLA	C2-C3-C5-C6
12	cB	923	CLA	C2-C3-C5-C6
12	cB	927	CLA	C2-C3-C5-C6
12	bA	839	CLA	CBD-CGD-O2D-CED
12	aL	203	CLA	C2B-C3B-CAB-CBB
12	bL	203	CLA	C2B-C3B-CAB-CBB
12	cL	203	CLA	C2B-C3B-CAB-CBB
15	aA	847	BCR	C1-C6-C7-C8
15	aA	850	BCR	C1-C6-C7-C8
15	aB	942	BCR	C1-C6-C7-C8
15	aB	945	BCR	C23-C24-C25-C30
15	aB	946	BCR	C1-C6-C7-C8
15	aF	203	BCR	C1-C6-C7-C8
15	aF	204	BCR	C23-C24-C25-C30
15	aL	201	BCR	C23-C24-C25-C30
15	aL	206	BCR	C1-C6-C7-C8
15	aM	101	BCR	C23-C24-C25-C30
15	bA	846	BCR	C1-C6-C7-C8
15	bA	849	BCR	C1-C6-C7-C8
15	bB	942	BCR	C1-C6-C7-C8
15	bB	945	BCR	C23-C24-C25-C30
15	bB	946	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
15	bF	203	BCR	C1-C6-C7-C8
15	bF	204	BCR	C23-C24-C25-C30
15	bL	201	BCR	C23-C24-C25-C30
15	bL	206	BCR	C1-C6-C7-C8
15	bM	101	BCR	C23-C24-C25-C30
15	cA	846	BCR	C1-C6-C7-C8
15	cA	849	BCR	C1-C6-C7-C8
15	cB	942	BCR	C1-C6-C7-C8
15	cB	945	BCR	C23-C24-C25-C30
15	cB	946	BCR	C1-C6-C7-C8
15	cF	203	BCR	C1-C6-C7-C8
15	cF	204	BCR	C23-C24-C25-C30
15	cL	201	BCR	C23-C24-C25-C30
15	cL	206	BCR	C1-C6-C7-C8
15	cM	101	BCR	C23-C24-C25-C30
12	aA	839	CLA	CBD-CGD-O2D-CED
12	cA	839	CLA	CBD-CGD-O2D-CED
17	aB	947	LMG	C34-C35-C36-C37
17	bB	947	LMG	C34-C35-C36-C37
12	aA	825	CLA	C16-C17-C18-C20
12	bA	825	CLA	C16-C17-C18-C20
12	cA	825	CLA	C16-C17-C18-C20
17	cB	947	LMG	C34-C35-C36-C37
17	aB	947	LMG	C38-C39-C40-C41
17	bB	947	LMG	C38-C39-C40-C41
17	cB	947	LMG	C38-C39-C40-C41
12	aA	817	CLA	O1A-CGA-O2A-C1
12	bA	817	CLA	O1A-CGA-O2A-C1
12	aA	825	CLA	C4-C3-C5-C6
12	bA	825	CLA	C4-C3-C5-C6
12	cA	825	CLA	C4-C3-C5-C6
12	aA	842	CLA	C2-C3-C5-C6
12	bA	842	CLA	C2-C3-C5-C6
12	cA	842	CLA	C2-C3-C5-C6
16	bA	852	LHG	C9-C10-C11-C12
16	cA	852	LHG	C9-C10-C11-C12
16	aA	853	LHG	C9-C10-C11-C12
12	cA	817	CLA	O1A-CGA-O2A-C1
12	aA	834	CLA	C14-C13-C15-C16
12	bA	834	CLA	C14-C13-C15-C16
12	cA	834	CLA	C14-C13-C15-C16
12	bA	806	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	bB	949	CLA	O1D-CGD-O2D-CED
12	cA	806	CLA	O1D-CGD-O2D-CED
12	bA	812	CLA	C10-C11-C12-C13
15	aB	946	BCR	C6-C7-C8-C9
15	bB	946	BCR	C6-C7-C8-C9
15	cB	946	BCR	C6-C7-C8-C9
12	aA	806	CLA	O1D-CGD-O2D-CED
12	aB	949	CLA	O1D-CGD-O2D-CED
12	bA	807	CLA	C15-C16-C17-C18
15	aB	942	BCR	C14-C15-C16-C17
15	bB	942	BCR	C14-C15-C16-C17
15	cB	942	BCR	C14-C15-C16-C17
11	aA	801	CL0	C16-C17-C18-C20
12	cB	949	CLA	O1D-CGD-O2D-CED
12	aA	807	CLA	C15-C16-C17-C18
12	cA	807	CLA	C15-C16-C17-C18
12	cA	812	CLA	C10-C11-C12-C13
12	aB	915	CLA	C2C-C3C-CAC-CBC
12	aA	836	CLA	C2A-CAA-CBA-CGA
12	bA	836	CLA	C2A-CAA-CBA-CGA
12	cA	836	CLA	C2A-CAA-CBA-CGA
12	aA	812	CLA	C10-C11-C12-C13
12	aA	826	CLA	CBA-CGA-O2A-C1
12	aB	904	CLA	C2-C3-C5-C6
12	bB	904	CLA	C2-C3-C5-C6
12	cB	904	CLA	C2-C3-C5-C6
11	bA	801	CL0	C16-C17-C18-C20
11	cA	801	CL0	C16-C17-C18-C20
12	bB	915	CLA	C2C-C3C-CAC-CBC
12	cB	915	CLA	C2C-C3C-CAC-CBC
15	aA	851	BCR	C20-C21-C22-C37
15	aB	941	BCR	C20-C21-C22-C37
15	aB	943	BCR	C20-C21-C22-C37
15	aB	945	BCR	C35-C13-C14-C15
15	aF	204	BCR	C11-C10-C9-C34
15	bA	850	BCR	C20-C21-C22-C37
15	bB	941	BCR	C20-C21-C22-C37
15	bB	943	BCR	C20-C21-C22-C37
15	bB	945	BCR	C35-C13-C14-C15
15	bF	204	BCR	C11-C10-C9-C34
15	cA	850	BCR	C20-C21-C22-C37
15	cB	941	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
15	cB	943	BCR	C20-C21-C22-C37
15	cB	945	BCR	C35-C13-C14-C15
15	cF	204	BCR	C11-C10-C9-C34
12	aA	841	CLA	CBA-CGA-O2A-C1
12	bA	826	CLA	CBA-CGA-O2A-C1
12	bA	841	CLA	CBA-CGA-O2A-C1
12	cA	826	CLA	CBA-CGA-O2A-C1
12	cA	841	CLA	CBA-CGA-O2A-C1
12	aA	806	CLA	C16-C17-C18-C19
12	bA	806	CLA	C16-C17-C18-C19
12	cA	806	CLA	C16-C17-C18-C19
12	aA	838	CLA	C11-C12-C13-C15
12	aA	842	CLA	C12-C13-C15-C16
12	bA	838	CLA	C11-C12-C13-C15
12	bA	842	CLA	C12-C13-C15-C16
12	cA	838	CLA	C11-C12-C13-C15
12	cA	842	CLA	C12-C13-C15-C16
11	aA	801	CL0	C15-C16-C17-C18
11	bA	801	CL0	C15-C16-C17-C18
11	cA	801	CL0	C15-C16-C17-C18
12	bA	842	CLA	C10-C11-C12-C13
15	aA	849	BCR	C21-C22-C23-C24
15	aB	944	BCR	C7-C8-C9-C10
15	aI	101	BCR	C7-C8-C9-C10
15	aL	201	BCR	C7-C8-C9-C10
15	bA	848	BCR	C21-C22-C23-C24
15	bB	944	BCR	C7-C8-C9-C10
15	bI	101	BCR	C7-C8-C9-C10
15	bL	201	BCR	C7-C8-C9-C10
15	cA	848	BCR	C21-C22-C23-C24
15	cB	944	BCR	C7-C8-C9-C10
15	cI	101	BCR	C7-C8-C9-C10
15	cL	201	BCR	C7-C8-C9-C10
12	aA	824	CLA	O1D-CGD-O2D-CED
16	aA	853	LHG	C7-C8-C9-C10
16	bA	852	LHG	C7-C8-C9-C10
16	cA	852	LHG	C7-C8-C9-C10
12	bA	824	CLA	O1D-CGD-O2D-CED
12	aA	842	CLA	C10-C11-C12-C13
12	cA	842	CLA	C10-C11-C12-C13
12	cB	927	CLA	C2A-CAA-CBA-CGA
12	aA	812	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
12	bA	812	CLA	C4-C3-C5-C6
12	cA	812	CLA	C4-C3-C5-C6
12	aA	843	CLA	O1A-CGA-O2A-C1
12	aB	912	CLA	O1A-CGA-O2A-C1
12	bA	843	CLA	O1A-CGA-O2A-C1
12	bB	912	CLA	O1A-CGA-O2A-C1
12	cB	904	CLA	C13-C15-C16-C17
12	bB	905	CLA	C3-C5-C6-C7
12	aA	821	CLA	CBD-CGD-O2D-CED
12	cA	821	CLA	CBD-CGD-O2D-CED
12	cA	824	CLA	O1D-CGD-O2D-CED
12	bB	904	CLA	C13-C15-C16-C17
12	cA	843	CLA	O1A-CGA-O2A-C1
12	cB	912	CLA	O1A-CGA-O2A-C1
12	bA	821	CLA	CBD-CGD-O2D-CED
12	cA	818	CLA	C6-C7-C8-C9
16	aA	852	LHG	C30-C31-C32-C33
16	bA	851	LHG	C30-C31-C32-C33
16	cA	851	LHG	C30-C31-C32-C33
12	aA	818	CLA	C6-C7-C8-C9
12	aB	905	CLA	C3-C5-C6-C7
12	cB	905	CLA	C3-C5-C6-C7
12	aB	904	CLA	C13-C15-C16-C17
16	aA	853	LHG	C24-C23-O8-C6
16	bA	852	LHG	C24-C23-O8-C6
16	cA	852	LHG	C24-C23-O8-C6
15	aF	204	BCR	C11-C10-C9-C8
15	aJ	101	BCR	C20-C21-C22-C23
15	aL	205	BCR	C20-C21-C22-C23
15	bF	204	BCR	C11-C10-C9-C8
15	bJ	101	BCR	C20-C21-C22-C23
15	bL	205	BCR	C20-C21-C22-C23
15	cF	204	BCR	C11-C10-C9-C8
15	cJ	101	BCR	C20-C21-C22-C23
15	cL	205	BCR	C20-C21-C22-C23
12	bA	818	CLA	C6-C7-C8-C9
12	aA	841	CLA	O1A-CGA-O2A-C1
12	bA	841	CLA	O1A-CGA-O2A-C1
12	aB	916	CLA	C2A-CAA-CBA-CGA
12	aB	927	CLA	C2A-CAA-CBA-CGA
12	bB	916	CLA	C2A-CAA-CBA-CGA
12	bB	927	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
12	cB	916	CLA	C2A-CAA-CBA-CGA
17	aB	947	LMG	O7-C8-C9-O8
17	bB	947	LMG	O7-C8-C9-O8
17	cB	947	LMG	O7-C8-C9-O8
12	aA	819	CLA	C5-C6-C7-C8
12	bA	819	CLA	C5-C6-C7-C8
12	cA	819	CLA	C5-C6-C7-C8
12	cA	826	CLA	O1A-CGA-O2A-C1
12	cA	841	CLA	O1A-CGA-O2A-C1
12	cB	934	CLA	O1D-CGD-O2D-CED
12	aA	804	CLA	C5-C6-C7-C8
12	bA	804	CLA	C5-C6-C7-C8
12	cA	804	CLA	C5-C6-C7-C8
12	aA	826	CLA	O1A-CGA-O2A-C1
12	bA	826	CLA	O1A-CGA-O2A-C1
12	aA	827	CLA	CBA-CGA-O2A-C1
12	bA	827	CLA	CBA-CGA-O2A-C1
12	cA	827	CLA	CBA-CGA-O2A-C1
12	aB	934	CLA	O1D-CGD-O2D-CED
12	aA	830	CLA	O1D-CGD-O2D-CED
12	bA	830	CLA	O1D-CGD-O2D-CED
12	bB	934	CLA	O1D-CGD-O2D-CED
12	cA	830	CLA	O1D-CGD-O2D-CED
12	aF	202	CLA	O1D-CGD-O2D-CED
12	cF	202	CLA	O1D-CGD-O2D-CED
12	bB	926	CLA	O1D-CGD-O2D-CED
12	aB	926	CLA	O1D-CGD-O2D-CED
12	cB	926	CLA	O1D-CGD-O2D-CED
12	bA	821	CLA	O1A-CGA-O2A-C1
12	aA	809	CLA	C1A-C2A-CAA-CBA
12	aA	809	CLA	C4B-C3B-CAB-CBB
12	aA	817	CLA	C1A-C2A-CAA-CBA
12	aA	819	CLA	C4B-C3B-CAB-CBB
12	aA	820	CLA	C4B-C3B-CAB-CBB
12	aA	835	CLA	C4B-C3B-CAB-CBB
12	aA	836	CLA	C4B-C3B-CAB-CBB
12	aA	839	CLA	C1A-C2A-CAA-CBA
12	aB	907	CLA	C4B-C3B-CAB-CBB
12	aB	939	CLA	C4B-C3B-CAB-CBB
12	aL	203	CLA	C4B-C3B-CAB-CBB
12	bA	809	CLA	C1A-C2A-CAA-CBA
12	bA	809	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
12	bA	817	CLA	C1A-C2A-CAA-CBA
12	bA	819	CLA	C4B-C3B-CAB-CBB
12	bA	820	CLA	C4B-C3B-CAB-CBB
12	bA	835	CLA	C4B-C3B-CAB-CBB
12	bA	836	CLA	C4B-C3B-CAB-CBB
12	bA	839	CLA	C1A-C2A-CAA-CBA
12	bB	907	CLA	C4B-C3B-CAB-CBB
12	bB	939	CLA	C4B-C3B-CAB-CBB
12	bL	203	CLA	C4B-C3B-CAB-CBB
12	cA	809	CLA	C1A-C2A-CAA-CBA
12	cA	809	CLA	C4B-C3B-CAB-CBB
12	cA	817	CLA	C1A-C2A-CAA-CBA
12	cA	819	CLA	C4B-C3B-CAB-CBB
12	cA	820	CLA	C4B-C3B-CAB-CBB
12	cA	835	CLA	C4B-C3B-CAB-CBB
12	cA	836	CLA	C4B-C3B-CAB-CBB
12	cA	839	CLA	C1A-C2A-CAA-CBA
12	cB	907	CLA	C4B-C3B-CAB-CBB
12	cB	939	CLA	C4B-C3B-CAB-CBB
12	cL	203	CLA	C4B-C3B-CAB-CBB
12	bF	202	CLA	O1D-CGD-O2D-CED
12	aA	840	CLA	C4-C3-C5-C6
12	bA	840	CLA	C4-C3-C5-C6
12	cA	840	CLA	C4-C3-C5-C6
12	aA	821	CLA	O1A-CGA-O2A-C1
12	cA	821	CLA	O1A-CGA-O2A-C1
16	bA	851	LHG	C32-C33-C34-C35
16	cA	851	LHG	C32-C33-C34-C35
16	aA	852	LHG	C32-C33-C34-C35
12	aA	803	CLA	C11-C10-C8-C7
12	aA	803	CLA	C12-C13-C15-C16
12	aB	905	CLA	C12-C13-C15-C16
12	bA	803	CLA	C11-C10-C8-C7
12	bA	803	CLA	C12-C13-C15-C16
12	bB	905	CLA	C12-C13-C15-C16
12	cA	803	CLA	C11-C10-C8-C7
12	cA	803	CLA	C12-C13-C15-C16
12	cB	905	CLA	C12-C13-C15-C16
12	aA	821	CLA	CBA-CGA-O2A-C1
12	cA	828	CLA	CBD-CGD-O2D-CED
12	cB	915	CLA	C4C-C3C-CAC-CBC
17	aB	947	LMG	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
17	cB	947	LMG	C37-C38-C39-C40
12	aA	814	CLA	C3A-C2A-CAA-CBA
12	bA	814	CLA	C3A-C2A-CAA-CBA
12	cA	814	CLA	C3A-C2A-CAA-CBA
12	cA	821	CLA	CBA-CGA-O2A-C1
16	bA	851	LHG	O6-C4-C5-O7
16	cA	851	LHG	O6-C4-C5-O7
17	bB	947	LMG	C37-C38-C39-C40
12	aB	915	CLA	C4C-C3C-CAC-CBC
12	bB	915	CLA	C4C-C3C-CAC-CBC
12	aA	842	CLA	C14-C13-C15-C16
12	bA	842	CLA	C14-C13-C15-C16
12	cA	842	CLA	C14-C13-C15-C16
12	aA	822	CLA	C1-C2-C3-C4
12	aB	930	CLA	C1-C2-C3-C4
12	bA	822	CLA	C1-C2-C3-C4
12	bB	930	CLA	C1-C2-C3-C4
12	cA	822	CLA	C1-C2-C3-C4
12	cB	930	CLA	C1-C2-C3-C4
12	aB	901	CLA	O1D-CGD-O2D-CED
12	bB	901	CLA	O1D-CGD-O2D-CED
12	cB	901	CLA	O1D-CGD-O2D-CED
12	aA	828	CLA	CBD-CGD-O2D-CED
12	bA	828	CLA	CBD-CGD-O2D-CED
12	aB	935	CLA	CAD-CBD-CGD-O2D
12	bB	935	CLA	CAD-CBD-CGD-O2D
12	cB	904	CLA	CAD-CBD-CGD-O2D
12	cB	935	CLA	CAD-CBD-CGD-O2D
12	aB	907	CLA	O1D-CGD-O2D-CED
12	bA	821	CLA	CBA-CGA-O2A-C1
12	bB	917	CLA	C5-C6-C7-C8
12	cB	907	CLA	O1D-CGD-O2D-CED
12	aB	917	CLA	C5-C6-C7-C8
12	cB	917	CLA	C5-C6-C7-C8
12	bB	926	CLA	CAA-CBA-CGA-O2A
11	aA	801	CL0	CHA-CBD-CGD-O1D
11	aA	801	CL0	CHA-CBD-CGD-O2D
11	bA	801	CL0	CHA-CBD-CGD-O1D
11	bA	801	CL0	CHA-CBD-CGD-O2D
11	cA	801	CL0	CHA-CBD-CGD-O1D
11	cA	801	CL0	CHA-CBD-CGD-O2D
12	aA	812	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
12	aA	827	CLA	CAD-CBD-CGD-O1D
12	aB	904	CLA	CAD-CBD-CGD-O1D
12	aB	923	CLA	CHA-CBD-CGD-O1D
12	aB	923	CLA	CHA-CBD-CGD-O2D
12	aB	935	CLA	CAD-CBD-CGD-O1D
12	bA	812	CLA	CHA-CBD-CGD-O1D
12	bA	827	CLA	CAD-CBD-CGD-O1D
12	bB	904	CLA	CAD-CBD-CGD-O1D
12	bB	923	CLA	CHA-CBD-CGD-O1D
12	bB	923	CLA	CHA-CBD-CGD-O2D
12	bB	935	CLA	CAD-CBD-CGD-O1D
12	cA	812	CLA	CHA-CBD-CGD-O1D
12	cA	827	CLA	CAD-CBD-CGD-O1D
12	cB	904	CLA	CAD-CBD-CGD-O1D
12	cB	923	CLA	CHA-CBD-CGD-O1D
12	cB	923	CLA	CHA-CBD-CGD-O2D
12	cB	935	CLA	CAD-CBD-CGD-O1D
16	aA	853	LHG	C4-O6-P-O4
16	aB	948	LHG	C3-O3-P-O5
16	bA	852	LHG	C3-O3-P-O5
16	bA	852	LHG	C4-O6-P-O4
16	bB	948	LHG	C3-O3-P-O5
16	cA	852	LHG	C3-O3-P-O5
16	cA	852	LHG	C4-O6-P-O4
16	cB	948	LHG	C3-O3-P-O5
12	aA	810	CLA	C2B-C3B-CAB-CBB
12	aA	823	CLA	C2B-C3B-CAB-CBB
12	aA	826	CLA	C2B-C3B-CAB-CBB
12	aA	831	CLA	C2B-C3B-CAB-CBB
12	aA	836	CLA	C2B-C3B-CAB-CBB
12	aB	901	CLA	C2B-C3B-CAB-CBB
12	aB	907	CLA	C2B-C3B-CAB-CBB
12	aB	910	CLA	C2B-C3B-CAB-CBB
12	aB	923	CLA	C2B-C3B-CAB-CBB
12	bA	810	CLA	C2B-C3B-CAB-CBB
12	bA	823	CLA	C2B-C3B-CAB-CBB
12	bA	826	CLA	C2B-C3B-CAB-CBB
12	bA	831	CLA	C2B-C3B-CAB-CBB
12	bA	836	CLA	C2B-C3B-CAB-CBB
12	bB	901	CLA	C2B-C3B-CAB-CBB
12	bB	907	CLA	C2B-C3B-CAB-CBB
12	bB	910	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
12	bB	923	CLA	C2B-C3B-CAB-CBB
12	cA	810	CLA	C2B-C3B-CAB-CBB
12	cA	823	CLA	C2B-C3B-CAB-CBB
12	cA	826	CLA	C2B-C3B-CAB-CBB
12	cA	831	CLA	C2B-C3B-CAB-CBB
12	cA	836	CLA	C2B-C3B-CAB-CBB
12	cB	901	CLA	C2B-C3B-CAB-CBB
12	cB	907	CLA	C2B-C3B-CAB-CBB
12	cB	910	CLA	C2B-C3B-CAB-CBB
12	cB	923	CLA	C2B-C3B-CAB-CBB
12	aB	926	CLA	CAA-CBA-CGA-O2A
12	cB	926	CLA	CAA-CBA-CGA-O2A
12	aA	812	CLA	C2-C3-C5-C6
12	bA	812	CLA	C2-C3-C5-C6
12	cA	812	CLA	C2-C3-C5-C6
15	aF	203	BCR	C37-C22-C23-C24
15	bF	203	BCR	C37-C22-C23-C24
15	cF	203	BCR	C37-C22-C23-C24
12	bB	907	CLA	O1D-CGD-O2D-CED
12	aA	812	CLA	C16-C17-C18-C20
12	bA	812	CLA	C16-C17-C18-C20
12	cA	812	CLA	C16-C17-C18-C20
16	aA	852	LHG	C11-C10-C9-C8
16	bA	851	LHG	C11-C10-C9-C8
16	cA	851	LHG	C11-C10-C9-C8
12	aA	830	CLA	C10-C11-C12-C13
12	bA	830	CLA	C10-C11-C12-C13
12	cA	830	CLA	C10-C11-C12-C13
12	aA	842	CLA	C11-C12-C13-C14
12	aA	843	CLA	C14-C13-C15-C16
12	bA	842	CLA	C11-C12-C13-C14
12	bA	843	CLA	C14-C13-C15-C16
12	cA	842	CLA	C11-C12-C13-C14
12	cA	843	CLA	C14-C13-C15-C16
12	aB	912	CLA	C6-C7-C8-C10
12	bB	912	CLA	C6-C7-C8-C10
12	cB	912	CLA	C6-C7-C8-C10
12	aA	840	CLA	C15-C16-C17-C18
12	bA	840	CLA	C15-C16-C17-C18
12	cA	840	CLA	C15-C16-C17-C18
15	aB	943	BCR	C20-C21-C22-C23
15	bB	943	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
15	cB	943	BCR	C20-C21-C22-C23
16	aA	852	LHG	O6-C4-C5-O7
12	aA	818	CLA	C2A-CAA-CBA-CGA
12	bA	818	CLA	C2A-CAA-CBA-CGA
12	aB	916	CLA	CAA-CBA-CGA-O2A
12	bB	916	CLA	CAA-CBA-CGA-O2A
12	cB	916	CLA	CAA-CBA-CGA-O2A
12	aA	854	CLA	O1D-CGD-O2D-CED
12	cA	853	CLA	O1D-CGD-O2D-CED
12	aA	812	CLA	C16-C17-C18-C19
12	bA	812	CLA	C16-C17-C18-C19
12	cA	812	CLA	C16-C17-C18-C19
12	aB	912	CLA	C10-C11-C12-C13
12	cB	912	CLA	C10-C11-C12-C13
12	bA	853	CLA	O1D-CGD-O2D-CED
12	aA	843	CLA	CBA-CGA-O2A-C1
12	bA	843	CLA	CBA-CGA-O2A-C1
12	cA	843	CLA	CBA-CGA-O2A-C1
15	aA	849	BCR	C19-C20-C21-C22
15	aB	944	BCR	C9-C10-C11-C12
15	bA	848	BCR	C19-C20-C21-C22
15	bB	944	BCR	C9-C10-C11-C12
15	cA	848	BCR	C19-C20-C21-C22
15	cB	944	BCR	C9-C10-C11-C12
12	bB	912	CLA	C10-C11-C12-C13
12	aA	832	CLA	CAA-CBA-CGA-O2A
12	bA	832	CLA	CAA-CBA-CGA-O2A
12	cA	832	CLA	CAA-CBA-CGA-O2A
12	cA	818	CLA	C2A-CAA-CBA-CGA
12	aB	931	CLA	CBD-CGD-O2D-CED
12	cB	931	CLA	CBD-CGD-O2D-CED
12	aA	820	CLA	C2-C1-O2A-CGA
12	bA	820	CLA	C2-C1-O2A-CGA
12	cA	820	CLA	C2-C1-O2A-CGA
12	cB	920	CLA	O1D-CGD-O2D-CED
12	aB	920	CLA	O1D-CGD-O2D-CED
12	aB	921	CLA	CAA-CBA-CGA-O2A
12	aB	926	CLA	C16-C17-C18-C20
12	bB	926	CLA	C16-C17-C18-C20
12	cB	926	CLA	C16-C17-C18-C20
12	bB	921	CLA	CAA-CBA-CGA-O2A
12	cB	921	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
12	bB	931	CLA	CBD-CGD-O2D-CED
12	bB	920	CLA	O1D-CGD-O2D-CED
16	cA	851	LHG	C17-C18-C19-C20
12	cB	931	CLA	C3-C5-C6-C7
16	aA	852	LHG	C17-C18-C19-C20
16	bA	851	LHG	C17-C18-C19-C20
12	bA	840	CLA	C2-C3-C5-C6
12	cA	840	CLA	C2-C3-C5-C6
12	aA	814	CLA	C4B-C3B-CAB-CBB
12	aA	823	CLA	C4B-C3B-CAB-CBB
12	aB	936	CLA	C4B-C3B-CAB-CBB
12	bA	814	CLA	C4B-C3B-CAB-CBB
12	bA	823	CLA	C4B-C3B-CAB-CBB
12	bB	936	CLA	C4B-C3B-CAB-CBB
12	cA	814	CLA	C4B-C3B-CAB-CBB
12	cA	823	CLA	C4B-C3B-CAB-CBB
12	cB	936	CLA	C4B-C3B-CAB-CBB
12	aA	840	CLA	C2-C3-C5-C6
12	aB	931	CLA	C3-C5-C6-C7
12	bB	931	CLA	C3-C5-C6-C7
12	aB	926	CLA	C16-C17-C18-C19
12	bB	926	CLA	C16-C17-C18-C19
12	cB	926	CLA	C16-C17-C18-C19
12	aB	931	CLA	C6-C7-C8-C10
12	bB	931	CLA	C6-C7-C8-C10
12	cB	931	CLA	C6-C7-C8-C10
12	bA	811	CLA	O1D-CGD-O2D-CED
12	aA	811	CLA	O1D-CGD-O2D-CED
12	aA	802	CLA	C4-C3-C5-C6
12	aB	950	CLA	C3A-C2A-CAA-CBA
12	bA	802	CLA	C4-C3-C5-C6
12	cA	802	CLA	C4-C3-C5-C6
11	aA	801	CL0	CAA-CBA-CGA-O2A
11	bA	801	CL0	CAA-CBA-CGA-O2A
11	cA	801	CL0	CAA-CBA-CGA-O2A
15	aA	848	BCR	C6-C7-C8-C9
15	aA	850	BCR	C20-C21-C22-C37
15	aA	851	BCR	C16-C17-C18-C36
15	aB	943	BCR	C6-C7-C8-C9
15	aB	944	BCR	C35-C13-C14-C15
15	aF	203	BCR	C35-C13-C14-C15
15	aL	201	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
15	bA	847	BCR	C6-C7-C8-C9
15	bA	849	BCR	C20-C21-C22-C37
15	bA	850	BCR	C16-C17-C18-C36
15	bB	943	BCR	C6-C7-C8-C9
15	bB	944	BCR	C35-C13-C14-C15
15	bF	203	BCR	C35-C13-C14-C15
15	bL	201	BCR	C20-C21-C22-C37
15	cA	847	BCR	C6-C7-C8-C9
15	cA	849	BCR	C20-C21-C22-C37
15	cA	850	BCR	C16-C17-C18-C36
15	cB	944	BCR	C35-C13-C14-C15
15	cF	203	BCR	C35-C13-C14-C15
15	cL	201	BCR	C20-C21-C22-C37
12	cA	811	CLA	O1D-CGD-O2D-CED
16	bA	851	LHG	C7-C8-C9-C10
15	aF	203	BCR	C11-C12-C13-C35
15	bF	203	BCR	C11-C12-C13-C35
16	aA	852	LHG	C7-C8-C9-C10
16	cA	851	LHG	C7-C8-C9-C10
12	cA	814	CLA	CAA-CBA-CGA-O1A
12	aB	926	CLA	C4-C3-C5-C6
12	bB	926	CLA	C4-C3-C5-C6
12	cB	926	CLA	C4-C3-C5-C6
12	aA	814	CLA	CAA-CBA-CGA-O1A
12	bA	814	CLA	CAA-CBA-CGA-O1A
13	aB	940	1L3	C16-C18-C19-C20
13	bB	940	1L3	C16-C18-C19-C20
13	cB	940	1L3	C16-C18-C19-C20
12	aB	901	CLA	C14-C13-C15-C16
12	aB	931	CLA	C6-C7-C8-C9
12	bB	901	CLA	C14-C13-C15-C16
12	bB	931	CLA	C6-C7-C8-C9
12	cB	901	CLA	C14-C13-C15-C16
12	cB	931	CLA	C6-C7-C8-C9
11	aA	801	CL0	C16-C17-C18-C19
11	bA	801	CL0	C16-C17-C18-C19
11	cA	801	CL0	C16-C17-C18-C19
12	aA	838	CLA	C15-C16-C17-C18
12	cA	838	CLA	C15-C16-C17-C18
12	aA	816	CLA	CAA-CBA-CGA-O1A
12	bA	816	CLA	CAA-CBA-CGA-O1A
12	cA	816	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
12	bA	838	CLA	C15-C16-C17-C18
12	aA	806	CLA	C1A-C2A-CAA-CBA
12	aA	814	CLA	C1A-C2A-CAA-CBA
12	aA	822	CLA	C1A-C2A-CAA-CBA
12	aB	912	CLA	C1A-C2A-CAA-CBA
12	aB	923	CLA	C1A-C2A-CAA-CBA
12	bA	806	CLA	C1A-C2A-CAA-CBA
12	bA	814	CLA	C1A-C2A-CAA-CBA
12	bA	822	CLA	C1A-C2A-CAA-CBA
12	bB	912	CLA	C1A-C2A-CAA-CBA
12	bB	923	CLA	C1A-C2A-CAA-CBA
12	cA	806	CLA	C1A-C2A-CAA-CBA
12	cA	814	CLA	C1A-C2A-CAA-CBA
12	cA	822	CLA	C1A-C2A-CAA-CBA
12	cB	912	CLA	C1A-C2A-CAA-CBA
12	cB	923	CLA	C1A-C2A-CAA-CBA
15	aF	203	BCR	C12-C13-C14-C15
15	bF	203	BCR	C12-C13-C14-C15
15	cF	203	BCR	C12-C13-C14-C15
12	cB	912	CLA	C2C-C3C-CAC-CBC
12	aA	813	CLA	CAA-CBA-CGA-O1A
12	aA	814	CLA	CAA-CBA-CGA-O2A
12	bA	813	CLA	CAA-CBA-CGA-O1A
12	bA	814	CLA	CAA-CBA-CGA-O2A
12	cA	813	CLA	CAA-CBA-CGA-O1A
12	aB	912	CLA	C2C-C3C-CAC-CBC
12	aA	809	CLA	C2B-C3B-CAB-CBB
12	aA	814	CLA	C2B-C3B-CAB-CBB
12	aA	819	CLA	C2B-C3B-CAB-CBB
12	aA	820	CLA	C2B-C3B-CAB-CBB
12	aA	835	CLA	C2B-C3B-CAB-CBB
12	aB	902	CLA	C2B-C3B-CAB-CBB
12	aB	917	CLA	C2B-C3B-CAB-CBB
12	aB	926	CLA	C2B-C3B-CAB-CBB
12	aB	936	CLA	C2B-C3B-CAB-CBB
12	aB	939	CLA	C2B-C3B-CAB-CBB
12	bA	809	CLA	C2B-C3B-CAB-CBB
12	bA	814	CLA	C2B-C3B-CAB-CBB
12	bA	819	CLA	C2B-C3B-CAB-CBB
12	bA	820	CLA	C2B-C3B-CAB-CBB
12	bA	835	CLA	C2B-C3B-CAB-CBB
12	bB	902	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
12	bB	917	CLA	C2B-C3B-CAB-CBB
12	bB	926	CLA	C2B-C3B-CAB-CBB
12	bB	936	CLA	C2B-C3B-CAB-CBB
12	bB	939	CLA	C2B-C3B-CAB-CBB
12	cA	809	CLA	C2B-C3B-CAB-CBB
12	cA	814	CLA	C2B-C3B-CAB-CBB
12	cA	819	CLA	C2B-C3B-CAB-CBB
12	cA	820	CLA	C2B-C3B-CAB-CBB
12	cA	835	CLA	C2B-C3B-CAB-CBB
12	cB	902	CLA	C2B-C3B-CAB-CBB
12	cB	917	CLA	C2B-C3B-CAB-CBB
12	cB	926	CLA	C2B-C3B-CAB-CBB
12	cB	936	CLA	C2B-C3B-CAB-CBB
12	cB	939	CLA	C2B-C3B-CAB-CBB
15	aA	847	BCR	C5-C6-C7-C8
15	aA	848	BCR	C1-C6-C7-C8
15	aA	848	BCR	C5-C6-C7-C8
15	aA	850	BCR	C5-C6-C7-C8
15	aA	850	BCR	C23-C24-C25-C30
15	aB	942	BCR	C5-C6-C7-C8
15	aB	943	BCR	C1-C6-C7-C8
15	aB	943	BCR	C5-C6-C7-C8
15	aB	944	BCR	C5-C6-C7-C8
15	aB	945	BCR	C23-C24-C25-C26
15	aB	946	BCR	C5-C6-C7-C8
15	aF	203	BCR	C5-C6-C7-C8
15	aF	204	BCR	C23-C24-C25-C26
15	aI	101	BCR	C1-C6-C7-C8
15	aI	101	BCR	C5-C6-C7-C8
15	aL	201	BCR	C23-C24-C25-C26
15	aL	205	BCR	C1-C6-C7-C8
15	aL	205	BCR	C5-C6-C7-C8
15	aL	206	BCR	C5-C6-C7-C8
15	aL	206	BCR	C23-C24-C25-C30
15	aM	101	BCR	C23-C24-C25-C26
15	bA	846	BCR	C5-C6-C7-C8
15	bA	847	BCR	C1-C6-C7-C8
15	bA	847	BCR	C5-C6-C7-C8
15	bA	849	BCR	C5-C6-C7-C8
15	bA	849	BCR	C23-C24-C25-C30
15	bB	942	BCR	C5-C6-C7-C8
15	bB	943	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
15	bB	943	BCR	C5-C6-C7-C8
15	bB	944	BCR	C5-C6-C7-C8
15	bB	945	BCR	C23-C24-C25-C26
15	bB	946	BCR	C5-C6-C7-C8
15	bF	203	BCR	C5-C6-C7-C8
15	bF	204	BCR	C23-C24-C25-C26
15	bI	101	BCR	C1-C6-C7-C8
15	bI	101	BCR	C5-C6-C7-C8
15	bL	201	BCR	C23-C24-C25-C26
15	bL	205	BCR	C1-C6-C7-C8
15	bL	205	BCR	C5-C6-C7-C8
15	bL	206	BCR	C5-C6-C7-C8
15	bL	206	BCR	C23-C24-C25-C30
15	bM	101	BCR	C23-C24-C25-C26
15	cA	846	BCR	C5-C6-C7-C8
15	cA	847	BCR	C1-C6-C7-C8
15	cA	847	BCR	C5-C6-C7-C8
15	cA	849	BCR	C5-C6-C7-C8
15	cA	849	BCR	C23-C24-C25-C30
15	cB	942	BCR	C5-C6-C7-C8
15	cB	943	BCR	C1-C6-C7-C8
15	cB	943	BCR	C5-C6-C7-C8
15	cB	944	BCR	C5-C6-C7-C8
15	cB	945	BCR	C23-C24-C25-C26
15	cB	946	BCR	C5-C6-C7-C8
15	cF	203	BCR	C5-C6-C7-C8
15	cF	204	BCR	C23-C24-C25-C26
15	cI	101	BCR	C1-C6-C7-C8
15	cI	101	BCR	C5-C6-C7-C8
15	cL	201	BCR	C23-C24-C25-C26
15	cL	205	BCR	C1-C6-C7-C8
15	cL	205	BCR	C5-C6-C7-C8
15	cL	206	BCR	C5-C6-C7-C8
15	cL	206	BCR	C23-C24-C25-C30
15	cM	101	BCR	C23-C24-C25-C26
12	aF	202	CLA	CAA-CBA-CGA-O2A
12	bF	202	CLA	CAA-CBA-CGA-O2A
12	cA	814	CLA	CAA-CBA-CGA-O2A
12	cF	202	CLA	CAA-CBA-CGA-O2A
12	aB	936	CLA	C4-C3-C5-C6
12	bB	936	CLA	C4-C3-C5-C6
12	cB	936	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
12	bB	912	CLA	C2C-C3C-CAC-CBC
12	aB	931	CLA	C11-C10-C8-C7
12	bB	931	CLA	C11-C10-C8-C7
12	cB	931	CLA	C11-C10-C8-C7
12	aA	813	CLA	C2A-CAA-CBA-CGA
12	aB	912	CLA	C2A-CAA-CBA-CGA
12	bA	813	CLA	C2A-CAA-CBA-CGA
12	bB	912	CLA	C2A-CAA-CBA-CGA
12	cA	813	CLA	C2A-CAA-CBA-CGA
12	cB	912	CLA	C2A-CAA-CBA-CGA
16	aA	853	LHG	O7-C5-C6-O8
16	bA	852	LHG	O7-C5-C6-O8
16	cA	852	LHG	O7-C5-C6-O8
12	aA	816	CLA	CAA-CBA-CGA-O2A
12	bA	816	CLA	CAA-CBA-CGA-O2A
12	aA	813	CLA	CAA-CBA-CGA-O2A
12	aB	922	CLA	CAA-CBA-CGA-O2A
12	bA	813	CLA	CAA-CBA-CGA-O2A
12	bB	922	CLA	CAA-CBA-CGA-O2A
12	cA	813	CLA	CAA-CBA-CGA-O2A
12	cA	816	CLA	CAA-CBA-CGA-O2A
12	cB	922	CLA	CAA-CBA-CGA-O2A
15	aB	945	BCR	C36-C18-C19-C20
15	bB	945	BCR	C36-C18-C19-C20
15	cB	945	BCR	C36-C18-C19-C20
15	cF	203	BCR	C11-C12-C13-C35
12	aA	810	CLA	CAA-CBA-CGA-O2A
12	bA	810	CLA	CAA-CBA-CGA-O2A
12	cA	810	CLA	CAA-CBA-CGA-O2A
12	aA	838	CLA	C4-C3-C5-C6
12	aB	912	CLA	C4-C3-C5-C6
12	bA	838	CLA	C4-C3-C5-C6
12	bB	912	CLA	C4-C3-C5-C6
12	cA	838	CLA	C4-C3-C5-C6
12	cB	912	CLA	C4-C3-C5-C6
12	aA	802	CLA	C2-C3-C5-C6
12	aB	926	CLA	C2-C3-C5-C6
12	bA	802	CLA	C2-C3-C5-C6
12	bB	926	CLA	C2-C3-C5-C6
12	cA	802	CLA	C2-C3-C5-C6
12	cB	926	CLA	C2-C3-C5-C6
12	aA	843	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
12	bA	843	CLA	C16-C17-C18-C19
12	bA	839	CLA	O1D-CGD-O2D-CED
12	bA	842	CLA	CBD-CGD-O2D-CED
12	aF	202	CLA	CAA-CBA-CGA-O1A
12	bF	202	CLA	CAA-CBA-CGA-O1A
12	cF	202	CLA	CAA-CBA-CGA-O1A
12	aB	916	CLA	C5-C6-C7-C8
12	bB	916	CLA	C5-C6-C7-C8
12	cB	916	CLA	C5-C6-C7-C8
12	cA	827	CLA	O1A-CGA-O2A-C1
12	cA	843	CLA	C16-C17-C18-C19
15	cB	943	BCR	C6-C7-C8-C9
12	cB	922	CLA	CAA-CBA-CGA-O1A
12	aA	827	CLA	O1A-CGA-O2A-C1
12	bA	827	CLA	O1A-CGA-O2A-C1
12	cA	842	CLA	CBD-CGD-O2D-CED
12	aB	922	CLA	CAA-CBA-CGA-O1A
12	bB	922	CLA	CAA-CBA-CGA-O1A
12	aA	842	CLA	CBD-CGD-O2D-CED
12	cA	839	CLA	O1D-CGD-O2D-CED
12	bB	931	CLA	CAA-CBA-CGA-O2A
12	aA	839	CLA	CAA-CBA-CGA-O2A
12	bA	839	CLA	CAA-CBA-CGA-O2A
12	cA	839	CLA	CAA-CBA-CGA-O2A
12	cB	931	CLA	CAA-CBA-CGA-O2A
12	aA	815	CLA	C4B-C3B-CAB-CBB
12	aA	817	CLA	C4B-C3B-CAB-CBB
12	aB	902	CLA	C4B-C3B-CAB-CBB
12	aB	917	CLA	C4B-C3B-CAB-CBB
12	aB	926	CLA	C4B-C3B-CAB-CBB
12	aB	937	CLA	C4B-C3B-CAB-CBB
12	bA	815	CLA	C4B-C3B-CAB-CBB
12	bA	817	CLA	C4B-C3B-CAB-CBB
12	bB	902	CLA	C4B-C3B-CAB-CBB
12	bB	917	CLA	C4B-C3B-CAB-CBB
12	bB	926	CLA	C4B-C3B-CAB-CBB
12	bB	937	CLA	C4B-C3B-CAB-CBB
12	cA	815	CLA	C4B-C3B-CAB-CBB
12	cA	817	CLA	C4B-C3B-CAB-CBB
12	cB	902	CLA	C4B-C3B-CAB-CBB
12	cB	917	CLA	C4B-C3B-CAB-CBB
12	cB	926	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
12	cB	937	CLA	C4B-C3B-CAB-CBB
12	aB	913	CLA	O1A-CGA-O2A-C1
12	bB	913	CLA	O1A-CGA-O2A-C1
12	cB	913	CLA	O1A-CGA-O2A-C1
16	cA	852	LHG	C11-C10-C9-C8
12	aA	839	CLA	O1D-CGD-O2D-CED
16	aA	853	LHG	C11-C10-C9-C8
12	aB	931	CLA	CAA-CBA-CGA-O2A
16	bA	852	LHG	C11-C10-C9-C8
12	aA	810	CLA	CAA-CBA-CGA-O1A
12	aA	836	CLA	CAA-CBA-CGA-O2A
12	aB	929	CLA	CAA-CBA-CGA-O2A
12	bA	810	CLA	CAA-CBA-CGA-O1A
12	bA	836	CLA	CAA-CBA-CGA-O2A
12	bB	929	CLA	CAA-CBA-CGA-O2A
12	cA	810	CLA	CAA-CBA-CGA-O1A
12	cA	836	CLA	CAA-CBA-CGA-O2A
12	cB	929	CLA	CAA-CBA-CGA-O2A
15	aA	851	BCR	C11-C10-C9-C34
15	bA	850	BCR	C11-C10-C9-C34
15	cA	850	BCR	C11-C10-C9-C34
12	aB	912	CLA	C4C-C3C-CAC-CBC
12	bB	912	CLA	C4C-C3C-CAC-CBC
12	cB	912	CLA	C4C-C3C-CAC-CBC
12	aB	909	CLA	C5-C6-C7-C8
12	bB	909	CLA	C5-C6-C7-C8
12	aB	929	CLA	CAA-CBA-CGA-O1A
12	bB	929	CLA	CAA-CBA-CGA-O1A
12	aB	912	CLA	C2-C3-C5-C6
12	bB	912	CLA	C2-C3-C5-C6
12	cB	912	CLA	C2-C3-C5-C6
12	aA	830	CLA	C15-C16-C17-C18
12	bA	830	CLA	C15-C16-C17-C18
12	cA	830	CLA	C15-C16-C17-C18
12	cB	909	CLA	C5-C6-C7-C8
12	cB	929	CLA	CAA-CBA-CGA-O1A
12	bB	905	CLA	C8-C10-C11-C12
12	aB	905	CLA	C8-C10-C11-C12
12	aA	803	CLA	C14-C13-C15-C16
12	aB	905	CLA	C14-C13-C15-C16
12	bA	803	CLA	C14-C13-C15-C16
12	bB	905	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
12	cA	803	CLA	C14-C13-C15-C16
12	cB	905	CLA	C14-C13-C15-C16
12	cA	829	CLA	CAA-CBA-CGA-O2A
12	aA	814	CLA	C2A-CAA-CBA-CGA
12	aA	819	CLA	C2A-CAA-CBA-CGA
12	bA	814	CLA	C2A-CAA-CBA-CGA
12	bA	819	CLA	C2A-CAA-CBA-CGA
12	cA	814	CLA	C2A-CAA-CBA-CGA
12	cA	819	CLA	C2A-CAA-CBA-CGA
12	aA	829	CLA	C2-C1-O2A-CGA
12	aB	909	CLA	C2-C1-O2A-CGA
12	aB	925	CLA	C2-C1-O2A-CGA
12	aB	928	CLA	C2-C1-O2A-CGA
12	bA	829	CLA	C2-C1-O2A-CGA
12	bB	909	CLA	C2-C1-O2A-CGA
12	bB	925	CLA	C2-C1-O2A-CGA
12	bB	928	CLA	C2-C1-O2A-CGA
12	cA	829	CLA	C2-C1-O2A-CGA
12	cB	909	CLA	C2-C1-O2A-CGA
12	cB	925	CLA	C2-C1-O2A-CGA
12	cB	928	CLA	C2-C1-O2A-CGA
11	cA	801	CL0	C3-C5-C6-C7
12	cB	905	CLA	C8-C10-C11-C12
12	aB	926	CLA	CBA-CGA-O2A-C1
12	bB	926	CLA	CBA-CGA-O2A-C1
12	cB	926	CLA	CBA-CGA-O2A-C1
12	aA	809	CLA	C3A-C2A-CAA-CBA
12	aA	822	CLA	C3A-C2A-CAA-CBA
12	aA	844	CLA	C3A-C2A-CAA-CBA
12	aB	912	CLA	C3A-C2A-CAA-CBA
12	bA	809	CLA	C3A-C2A-CAA-CBA
12	bA	822	CLA	C3A-C2A-CAA-CBA
12	bB	912	CLA	C3A-C2A-CAA-CBA
12	bB	950	CLA	C3A-C2A-CAA-CBA
12	cA	809	CLA	C3A-C2A-CAA-CBA
12	cA	822	CLA	C3A-C2A-CAA-CBA
12	cB	912	CLA	C3A-C2A-CAA-CBA
12	aB	933	CLA	CAA-CBA-CGA-O2A
12	bB	933	CLA	CAA-CBA-CGA-O2A
12	cB	933	CLA	CAA-CBA-CGA-O2A
11	aA	801	CL0	C3-C5-C6-C7
11	bA	801	CL0	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
12	aB	913	CLA	CBA-CGA-O2A-C1
12	bB	913	CLA	CBA-CGA-O2A-C1
12	cB	913	CLA	CBA-CGA-O2A-C1
12	aA	829	CLA	CAA-CBA-CGA-O2A
12	bA	829	CLA	CAA-CBA-CGA-O2A
12	cA	843	CLA	CAA-CBA-CGA-O2A
15	aB	945	BCR	C18-C19-C20-C21
15	bB	945	BCR	C18-C19-C20-C21
15	bL	205	BCR	C18-C19-C20-C21
15	cB	945	BCR	C18-C19-C20-C21
15	cL	205	BCR	C18-C19-C20-C21
12	aA	843	CLA	CAA-CBA-CGA-O2A
12	bA	843	CLA	CAA-CBA-CGA-O2A
15	bB	945	BCR	C14-C15-C16-C17
12	aA	836	CLA	CAA-CBA-CGA-O1A
12	aB	933	CLA	CAA-CBA-CGA-O1A
12	bA	836	CLA	CAA-CBA-CGA-O1A
12	bA	839	CLA	CAA-CBA-CGA-O1A
12	bB	933	CLA	CAA-CBA-CGA-O1A
12	cA	836	CLA	CAA-CBA-CGA-O1A
12	cB	933	CLA	CAA-CBA-CGA-O1A
12	aB	902	CLA	C8-C10-C11-C12
12	bB	936	CLA	C2-C3-C5-C6
12	bB	902	CLA	C8-C10-C11-C12
12	cB	902	CLA	C8-C10-C11-C12
15	aA	851	BCR	C11-C10-C9-C8
15	aA	851	BCR	C16-C17-C18-C19
15	aL	201	BCR	C20-C21-C22-C23
15	bA	850	BCR	C11-C10-C9-C8
15	bA	850	BCR	C16-C17-C18-C19
15	bB	945	BCR	C12-C13-C14-C15
15	bL	201	BCR	C20-C21-C22-C23
15	cA	850	BCR	C11-C10-C9-C8
15	cA	850	BCR	C16-C17-C18-C19
15	cL	201	BCR	C20-C21-C22-C23
12	aA	839	CLA	CAA-CBA-CGA-O1A
12	cA	839	CLA	CAA-CBA-CGA-O1A
12	aB	909	CLA	C4-C3-C5-C6
12	bB	909	CLA	C4-C3-C5-C6
12	cB	909	CLA	C4-C3-C5-C6
12	aA	844	CLA	CAA-CBA-CGA-O1A
12	aB	950	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
12	bB	950	CLA	CAA-CBA-CGA-O1A
12	aB	936	CLA	C2-C3-C5-C6
12	cB	936	CLA	C2-C3-C5-C6
15	aB	945	BCR	C14-C15-C16-C17
15	cB	945	BCR	C14-C15-C16-C17
12	aA	803	CLA	C11-C10-C8-C9
12	aA	807	CLA	C6-C7-C8-C9
12	aB	926	CLA	C11-C12-C13-C14
12	bA	803	CLA	C11-C10-C8-C9
12	bA	807	CLA	C6-C7-C8-C9
12	bB	926	CLA	C11-C12-C13-C14
12	cA	803	CLA	C11-C10-C8-C9
12	cA	807	CLA	C6-C7-C8-C9
12	cB	926	CLA	C11-C12-C13-C14
12	aB	919	CLA	CAA-CBA-CGA-O2A
12	bB	919	CLA	CAA-CBA-CGA-O2A
12	cB	919	CLA	CAA-CBA-CGA-O2A
12	bA	826	CLA	C5-C6-C7-C8
12	aA	820	CLA	CAA-CBA-CGA-O2A
12	bB	928	CLA	CBA-CGA-O2A-C1
12	aA	807	CLA	C11-C10-C8-C7
12	aA	807	CLA	C12-C13-C15-C16
12	aA	842	CLA	C11-C10-C8-C7
12	aB	901	CLA	C12-C13-C15-C16
12	bA	807	CLA	C11-C10-C8-C7
12	bA	807	CLA	C12-C13-C15-C16
12	bA	842	CLA	C11-C10-C8-C7
12	bB	901	CLA	C12-C13-C15-C16
12	cA	807	CLA	C11-C10-C8-C7
12	cA	807	CLA	C12-C13-C15-C16
12	cA	842	CLA	C11-C10-C8-C7
12	cB	901	CLA	C12-C13-C15-C16
12	aA	815	CLA	C2B-C3B-CAB-CBB
12	aA	840	CLA	C2B-C3B-CAB-CBB
12	aB	908	CLA	C2B-C3B-CAB-CBB
12	bA	815	CLA	C2B-C3B-CAB-CBB
12	bA	840	CLA	C2B-C3B-CAB-CBB
12	bB	908	CLA	C2B-C3B-CAB-CBB
12	cA	815	CLA	C2B-C3B-CAB-CBB
12	cA	840	CLA	C2B-C3B-CAB-CBB
12	cB	908	CLA	C2B-C3B-CAB-CBB
15	aA	849	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
15	aA	849	BCR	C5-C6-C7-C8
15	aA	850	BCR	C23-C24-C25-C26
15	aB	941	BCR	C23-C24-C25-C26
15	aB	941	BCR	C23-C24-C25-C30
15	aB	944	BCR	C23-C24-C25-C26
15	aB	945	BCR	C1-C6-C7-C8
15	aB	945	BCR	C5-C6-C7-C8
15	aF	201	BCR	C1-C6-C7-C8
15	aF	201	BCR	C5-C6-C7-C8
15	aL	206	BCR	C23-C24-C25-C26
15	bA	848	BCR	C1-C6-C7-C8
15	bA	848	BCR	C5-C6-C7-C8
15	bA	849	BCR	C23-C24-C25-C26
15	bB	941	BCR	C23-C24-C25-C26
15	bB	941	BCR	C23-C24-C25-C30
15	bB	944	BCR	C23-C24-C25-C26
15	bB	945	BCR	C1-C6-C7-C8
15	bB	945	BCR	C5-C6-C7-C8
15	bF	201	BCR	C1-C6-C7-C8
15	bF	201	BCR	C5-C6-C7-C8
15	bL	206	BCR	C23-C24-C25-C26
15	cA	848	BCR	C1-C6-C7-C8
15	cA	848	BCR	C5-C6-C7-C8
15	cA	849	BCR	C23-C24-C25-C26
15	cB	941	BCR	C23-C24-C25-C26
15	cB	941	BCR	C23-C24-C25-C30
15	cB	944	BCR	C23-C24-C25-C26
15	cB	945	BCR	C1-C6-C7-C8
15	cB	945	BCR	C5-C6-C7-C8
15	cF	201	BCR	C1-C6-C7-C8
15	cF	201	BCR	C5-C6-C7-C8
15	cL	206	BCR	C23-C24-C25-C26
12	aA	822	CLA	CAA-CBA-CGA-O2A
12	bA	820	CLA	CAA-CBA-CGA-O2A
12	bA	822	CLA	CAA-CBA-CGA-O2A
12	cA	820	CLA	CAA-CBA-CGA-O2A
12	cA	822	CLA	CAA-CBA-CGA-O2A
12	aA	812	CLA	C2-C1-O2A-CGA
12	aA	826	CLA	C2-C1-O2A-CGA
12	aB	903	CLA	C2-C1-O2A-CGA
12	bA	812	CLA	C2-C1-O2A-CGA
12	bA	826	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
12	bB	903	CLA	C2-C1-O2A-CGA
12	cA	812	CLA	C2-C1-O2A-CGA
12	cA	826	CLA	C2-C1-O2A-CGA
12	cB	903	CLA	C2-C1-O2A-CGA
12	bA	818	CLA	C5-C6-C7-C8
12	aB	928	CLA	CBA-CGA-O2A-C1
12	aA	826	CLA	C5-C6-C7-C8
12	cA	826	CLA	C5-C6-C7-C8
12	aA	818	CLA	C5-C6-C7-C8
12	cA	818	CLA	C5-C6-C7-C8
12	aL	203	CLA	CAA-CBA-CGA-O2A
12	bL	203	CLA	CAA-CBA-CGA-O2A
12	cL	203	CLA	CAA-CBA-CGA-O2A
12	cB	928	CLA	CBA-CGA-O2A-C1
12	cA	834	CLA	C13-C15-C16-C17
12	aA	823	CLA	CAA-CBA-CGA-O2A
12	bA	823	CLA	CAA-CBA-CGA-O2A
12	cA	823	CLA	CAA-CBA-CGA-O2A
12	aA	834	CLA	C13-C15-C16-C17
12	bA	834	CLA	C13-C15-C16-C17
12	bB	926	CLA	O1A-CGA-O2A-C1
17	aB	947	LMG	O7-C10-C11-C12
17	bB	947	LMG	O7-C10-C11-C12
17	cB	947	LMG	O7-C10-C11-C12
12	cB	926	CLA	O1A-CGA-O2A-C1
15	aL	205	BCR	C18-C19-C20-C21
12	aA	828	CLA	O1D-CGD-O2D-CED
12	cA	828	CLA	O1D-CGD-O2D-CED
12	bB	926	CLA	C8-C10-C11-C12
12	aB	926	CLA	O1A-CGA-O2A-C1
12	bB	909	CLA	CAA-CBA-CGA-O2A
12	aB	926	CLA	C8-C10-C11-C12
12	aA	807	CLA	C11-C10-C8-C9
12	aB	931	CLA	C11-C10-C8-C9
12	bA	807	CLA	C11-C10-C8-C9
12	bB	931	CLA	C11-C10-C8-C9
12	cA	807	CLA	C11-C10-C8-C9
12	cB	931	CLA	C11-C10-C8-C9
12	cB	926	CLA	C8-C10-C11-C12
15	aA	851	BCR	C7-C8-C9-C34
15	bA	849	BCR	C37-C22-C23-C24
15	cA	850	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
12	aB	909	CLA	CAA-CBA-CGA-O2A
12	cB	909	CLA	CAA-CBA-CGA-O2A
16	aA	853	LHG	O7-C7-C8-C9
16	cA	852	LHG	O7-C7-C8-C9
12	aA	802	CLA	C1A-C2A-CAA-CBA
12	aA	815	CLA	C1A-C2A-CAA-CBA
12	aA	824	CLA	C4B-C3B-CAB-CBB
12	aA	832	CLA	C1A-C2A-CAA-CBA
12	aA	843	CLA	C4B-C3B-CAB-CBB
12	aB	906	CLA	C4B-C3B-CAB-CBB
12	aB	908	CLA	C4B-C3B-CAB-CBB
12	aB	937	CLA	C1A-C2A-CAA-CBA
12	bA	802	CLA	C1A-C2A-CAA-CBA
12	bA	815	CLA	C1A-C2A-CAA-CBA
12	bA	824	CLA	C4B-C3B-CAB-CBB
12	bA	832	CLA	C1A-C2A-CAA-CBA
12	bA	843	CLA	C4B-C3B-CAB-CBB
12	bB	906	CLA	C4B-C3B-CAB-CBB
12	bB	908	CLA	C4B-C3B-CAB-CBB
12	bB	937	CLA	C1A-C2A-CAA-CBA
12	cA	802	CLA	C1A-C2A-CAA-CBA
12	cA	815	CLA	C1A-C2A-CAA-CBA
12	cA	824	CLA	C4B-C3B-CAB-CBB
12	cA	832	CLA	C1A-C2A-CAA-CBA
12	cA	843	CLA	C4B-C3B-CAB-CBB
12	cB	906	CLA	C4B-C3B-CAB-CBB
12	cB	908	CLA	C4B-C3B-CAB-CBB
12	aL	203	CLA	CAA-CBA-CGA-O1A
12	bL	203	CLA	CAA-CBA-CGA-O1A
12	cL	203	CLA	CAA-CBA-CGA-O1A
12	aA	854	CLA	C4-C3-C5-C6
12	bA	853	CLA	C4-C3-C5-C6
12	cA	853	CLA	C4-C3-C5-C6
12	aA	805	CLA	CAA-CBA-CGA-O2A
12	aB	936	CLA	CAA-CBA-CGA-O2A
12	bA	805	CLA	CAA-CBA-CGA-O2A
12	bB	936	CLA	CAA-CBA-CGA-O2A
12	cA	805	CLA	CAA-CBA-CGA-O2A
12	cB	908	CLA	CAA-CBA-CGA-O2A
12	cB	936	CLA	CAA-CBA-CGA-O2A
16	bA	852	LHG	O7-C7-C8-C9
17	aB	947	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
12	aA	827	CLA	CAA-CBA-CGA-O2A
12	aB	905	CLA	CAA-CBA-CGA-O2A
12	aB	908	CLA	CAA-CBA-CGA-O2A
12	bB	905	CLA	CAA-CBA-CGA-O2A
12	bB	908	CLA	CAA-CBA-CGA-O2A
12	cB	905	CLA	CAA-CBA-CGA-O2A
17	bB	947	LMG	C14-C15-C16-C17
17	cB	947	LMG	C14-C15-C16-C17
12	aA	844	CLA	CAA-CBA-CGA-O2A
12	aB	914	CLA	CAA-CBA-CGA-O2A
12	bB	914	CLA	CAA-CBA-CGA-O2A
12	bB	950	CLA	CAA-CBA-CGA-O2A
12	cB	914	CLA	CAA-CBA-CGA-O2A
12	aB	928	CLA	O1A-CGA-O2A-C1
12	cB	928	CLA	O1A-CGA-O2A-C1
12	bA	827	CLA	CAA-CBA-CGA-O2A
12	cA	827	CLA	CAA-CBA-CGA-O2A
12	aB	950	CLA	CAA-CBA-CGA-O2A
12	bA	828	CLA	O1D-CGD-O2D-CED
12	aA	830	CLA	C2-C1-O2A-CGA
12	bA	830	CLA	C2-C1-O2A-CGA
12	cA	830	CLA	C2-C1-O2A-CGA
12	bB	928	CLA	O1A-CGA-O2A-C1
15	aB	942	BCR	C19-C20-C21-C22
12	aB	923	CLA	C3A-C2A-CAA-CBA
12	bB	923	CLA	C3A-C2A-CAA-CBA
12	cB	923	CLA	C3A-C2A-CAA-CBA
12	aA	828	CLA	C10-C11-C12-C13
12	bA	828	CLA	C10-C11-C12-C13
12	cA	828	CLA	C10-C11-C12-C13
15	aB	945	BCR	C12-C13-C14-C15
15	aF	201	BCR	C20-C21-C22-C23
15	bF	201	BCR	C20-C21-C22-C23
15	cB	945	BCR	C12-C13-C14-C15
15	cF	201	BCR	C20-C21-C22-C23
12	aA	822	CLA	CAA-CBA-CGA-O1A
12	cA	822	CLA	CAA-CBA-CGA-O1A
15	bB	942	BCR	C19-C20-C21-C22
15	cB	942	BCR	C19-C20-C21-C22
12	aA	834	CLA	C4-C3-C5-C6
12	bA	834	CLA	C4-C3-C5-C6
12	cA	834	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
12	aA	805	CLA	CAA-CBA-CGA-O1A
12	bA	805	CLA	CAA-CBA-CGA-O1A
12	aA	834	CLA	C2-C3-C5-C6
12	bA	834	CLA	C2-C3-C5-C6
12	cA	834	CLA	C2-C3-C5-C6
12	aA	823	CLA	CAA-CBA-CGA-O1A
12	aB	919	CLA	CAA-CBA-CGA-O1A
12	bA	822	CLA	CAA-CBA-CGA-O1A
12	bB	919	CLA	CAA-CBA-CGA-O1A
12	cA	805	CLA	CAA-CBA-CGA-O1A
12	cB	919	CLA	CAA-CBA-CGA-O1A
12	bB	914	CLA	CAA-CBA-CGA-O1A
12	bA	823	CLA	CAA-CBA-CGA-O1A
12	cA	823	CLA	CAA-CBA-CGA-O1A
12	aB	914	CLA	CAA-CBA-CGA-O1A
12	cB	914	CLA	CAA-CBA-CGA-O1A
12	aB	905	CLA	CAA-CBA-CGA-O1A
12	bB	905	CLA	CAA-CBA-CGA-O1A
12	cB	905	CLA	CAA-CBA-CGA-O1A
12	bA	807	CLA	CAA-CBA-CGA-O2A
12	cA	807	CLA	CAA-CBA-CGA-O2A
12	aB	909	CLA	CAA-CBA-CGA-O1A
12	bB	909	CLA	CAA-CBA-CGA-O1A
12	cB	909	CLA	CAA-CBA-CGA-O1A
12	aB	905	CLA	C15-C16-C17-C18
12	bB	905	CLA	C15-C16-C17-C18
12	cB	905	CLA	C15-C16-C17-C18
12	aA	807	CLA	CAA-CBA-CGA-O2A
16	aB	948	LHG	O7-C7-C8-C9
16	bB	948	LHG	O7-C7-C8-C9
16	aA	852	LHG	O10-C23-C24-C25
16	bA	851	LHG	O10-C23-C24-C25
16	cA	851	LHG	O10-C23-C24-C25
12	aA	804	CLA	CAD-CBD-CGD-O2D
12	aA	810	CLA	CAD-CBD-CGD-O2D
12	aA	815	CLA	CAD-CBD-CGD-O2D
12	aA	833	CLA	CAD-CBD-CGD-O2D
12	aB	904	CLA	CAD-CBD-CGD-O2D
12	aB	919	CLA	CAD-CBD-CGD-O2D
12	bA	804	CLA	CAD-CBD-CGD-O2D
12	bA	810	CLA	CAD-CBD-CGD-O2D
12	bA	815	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
12	bA	833	CLA	CAD-CBD-CGD-O2D
12	bB	904	CLA	CAD-CBD-CGD-O2D
12	bB	919	CLA	CAD-CBD-CGD-O2D
12	cA	804	CLA	CAD-CBD-CGD-O2D
12	cA	810	CLA	CAD-CBD-CGD-O2D
12	cA	815	CLA	CAD-CBD-CGD-O2D
12	cA	833	CLA	CAD-CBD-CGD-O2D
12	cB	919	CLA	CAD-CBD-CGD-O2D
16	cB	948	LHG	O7-C7-C8-C9
12	aA	818	CLA	C2-C1-O2A-CGA
12	aB	927	CLA	C2-C1-O2A-CGA
12	bA	818	CLA	C2-C1-O2A-CGA
12	cA	818	CLA	C2-C1-O2A-CGA
12	aB	908	CLA	CAA-CBA-CGA-O1A
12	bB	908	CLA	CAA-CBA-CGA-O1A
12	cB	908	CLA	CAA-CBA-CGA-O1A
12	aB	915	CLA	CAA-CBA-CGA-O2A
12	bB	915	CLA	CAA-CBA-CGA-O2A
12	cB	915	CLA	CAA-CBA-CGA-O2A
12	cB	920	CLA	CAA-CBA-CGA-O2A
16	aA	852	LHG	C11-C12-C13-C14
16	cA	851	LHG	C11-C12-C13-C14
12	aA	838	CLA	CAA-CBA-CGA-O2A
16	bA	851	LHG	C11-C12-C13-C14
12	aB	920	CLA	CAA-CBA-CGA-O2A
12	bB	920	CLA	CAA-CBA-CGA-O2A
12	aB	936	CLA	CAA-CBA-CGA-O1A
12	cB	936	CLA	CAA-CBA-CGA-O1A
12	aB	906	CLA	CAA-CBA-CGA-O2A
12	bA	838	CLA	CAA-CBA-CGA-O2A
12	bB	906	CLA	CAA-CBA-CGA-O2A
12	cA	838	CLA	CAA-CBA-CGA-O2A
12	cB	906	CLA	CAA-CBA-CGA-O2A
12	aA	827	CLA	CAA-CBA-CGA-O1A
12	bA	827	CLA	CAA-CBA-CGA-O1A
12	bB	936	CLA	CAA-CBA-CGA-O1A
12	cA	827	CLA	CAA-CBA-CGA-O1A
17	bB	947	LMG	O9-C10-C11-C12
17	cB	947	LMG	O9-C10-C11-C12

There are no ring outliers.

235 monomers are involved in 370 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	bB	906	CLA	1	0
12	bA	840	CLA	4	0
15	bB	945	BCR	2	0
12	bB	949	CLA	1	0
15	cB	946	BCR	1	0
12	bB	923	CLA	2	0
12	bB	921	CLA	1	0
16	bA	852	LHG	1	0
12	cA	809	CLA	3	0
15	cA	846	BCR	1	0
12	bA	817	CLA	1	0
15	cF	204	BCR	3	0
12	bB	929	CLA	2	0
12	cA	812	CLA	1	0
12	cB	926	CLA	3	0
12	cB	913	CLA	1	0
15	bB	943	BCR	3	0
12	aA	829	CLA	1	0
12	aB	936	CLA	2	0
15	aB	944	BCR	3	0
12	bB	911	CLA	1	0
12	aA	833	CLA	1	0
15	bB	944	BCR	3	0
12	aB	918	CLA	1	0
12	cA	840	CLA	4	0
12	aA	837	CLA	2	0
16	bA	851	LHG	1	0
15	cB	944	BCR	2	0
12	cA	819	CLA	3	0
12	aA	827	CLA	2	0
12	bB	936	CLA	2	0
15	bJ	101	BCR	1	0
12	bB	901	CLA	1	0
12	bB	915	CLA	2	0
12	cB	936	CLA	2	0
12	cA	838	CLA	2	0
12	cB	930	CLA	1	0
12	cB	935	CLA	1	0
12	cA	837	CLA	1	0
15	bI	101	BCR	2	0
12	bB	926	CLA	3	0
12	cA	821	CLA	2	0
12	aB	916	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	cA	822	CLA	1	0
12	aA	828	CLA	1	0
12	cB	915	CLA	2	0
12	aB	906	CLA	1	0
16	cA	851	LHG	1	0
12	cA	834	CLA	3	0
12	bA	812	CLA	1	0
12	cB	927	CLA	3	0
12	cB	905	CLA	2	0
12	aA	830	CLA	2	0
15	bB	946	BCR	2	0
12	aA	836	CLA	1	0
12	bA	838	CLA	1	0
12	cA	826	CLA	1	0
12	bA	809	CLA	3	0
12	bA	825	CLA	6	0
15	aF	203	BCR	2	0
15	aF	201	BCR	2	0
12	bA	834	CLA	2	0
12	cB	918	CLA	1	0
12	bB	935	CLA	1	0
15	aL	205	BCR	2	0
12	bA	821	CLA	2	0
15	cL	205	BCR	2	0
12	cA	806	CLA	5	0
12	bA	822	CLA	1	0
12	aA	818	CLA	2	0
12	aB	930	CLA	1	0
12	bA	826	CLA	1	0
12	aA	820	CLA	1	0
15	aA	848	BCR	2	0
12	cA	827	CLA	2	0
12	cB	933	CLA	1	0
12	bB	905	CLA	1	0
15	aB	943	BCR	3	0
12	bA	843	CLA	3	0
12	aB	911	CLA	1	0
12	aA	817	CLA	1	0
15	aA	850	BCR	3	0
12	aA	821	CLA	2	0
12	aA	841	CLA	2	0
12	aB	909	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	cB	911	CLA	1	0
15	cB	941	BCR	1	0
12	aA	814	CLA	1	0
12	aB	949	CLA	1	0
12	aA	803	CLA	1	0
12	aL	204	CLA	1	0
12	cB	912	CLA	5	0
12	cA	818	CLA	3	0
15	aB	945	BCR	1	0
12	aB	922	CLA	2	0
12	cA	842	CLA	4	0
15	cB	943	BCR	2	0
12	bB	917	CLA	1	0
15	aL	206	BCR	1	0
12	aB	935	CLA	1	0
15	aA	851	BCR	2	0
12	bB	912	CLA	4	0
12	bA	818	CLA	3	0
15	aI	101	BCR	2	0
15	cA	847	BCR	3	0
12	aB	904	CLA	1	0
15	aB	941	BCR	2	0
12	bB	931	CLA	5	0
12	aB	933	CLA	1	0
12	bL	204	CLA	1	0
12	bA	807	CLA	1	0
15	bL	201	BCR	2	0
12	cA	810	CLA	2	0
12	cA	830	CLA	2	0
12	bA	837	CLA	1	0
12	cB	929	CLA	2	0
12	cA	807	CLA	2	0
12	cA	814	CLA	1	0
15	aA	849	BCR	1	0
12	cB	917	CLA	1	0
12	cB	909	CLA	1	0
12	bA	806	CLA	4	0
12	cB	906	CLA	1	0
12	cA	832	CLA	2	0
12	bA	810	CLA	2	0
12	aB	931	CLA	6	0
12	bA	827	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	bA	842	CLA	4	0
12	bA	830	CLA	2	0
12	bB	914	CLA	1	0
12	bB	925	CLA	2	0
12	aA	854	CLA	2	0
12	bB	922	CLA	1	0
12	bA	814	CLA	1	0
12	cA	805	CLA	1	0
15	aL	201	BCR	1	0
15	cA	848	BCR	2	0
12	aA	834	CLA	2	0
12	cA	803	CLA	1	0
12	aB	912	CLA	5	0
12	aA	843	CLA	4	0
12	cB	923	CLA	3	0
12	bB	927	CLA	2	0
12	bA	841	CLA	2	0
12	cB	922	CLA	2	0
12	aL	202	CLA	2	0
12	cA	829	CLA	1	0
12	bA	820	CLA	1	0
15	cA	849	BCR	4	0
12	bL	202	CLA	2	0
12	bB	909	CLA	2	0
12	bA	803	CLA	1	0
12	bB	919	CLA	1	0
12	cB	916	CLA	2	0
12	bA	853	CLA	2	0
12	cB	919	CLA	1	0
15	bF	201	BCR	1	0
12	cA	808	CLA	1	0
12	aA	806	CLA	3	0
12	cA	843	CLA	4	0
15	bA	847	BCR	3	0
16	aA	853	LHG	1	0
12	cL	204	CLA	1	0
12	aB	927	CLA	3	0
12	aB	902	CLA	1	0
15	bA	848	BCR	2	0
12	cA	853	CLA	3	0
12	aA	842	CLA	3	0
12	cL	202	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	cL	201	BCR	3	0
12	cA	841	CLA	2	0
12	aB	905	CLA	2	0
15	bL	205	BCR	2	0
15	cI	101	BCR	1	0
12	bA	836	CLA	1	0
15	aF	204	BCR	3	0
12	aA	825	CLA	5	0
12	aB	923	CLA	3	0
12	bB	933	CLA	1	0
12	bA	828	CLA	1	0
12	bA	802	CLA	2	0
13	bB	940	1L3	1	0
12	cB	924	CLA	1	0
12	bA	832	CLA	2	0
12	aB	925	CLA	2	0
12	cA	828	CLA	1	0
12	aB	929	CLA	2	0
15	bB	941	BCR	1	0
12	cA	820	CLA	1	0
12	aA	810	CLA	2	0
12	aA	812	CLA	1	0
12	aB	926	CLA	2	0
12	cB	931	CLA	4	0
15	bA	850	BCR	3	0
12	cA	836	CLA	1	0
12	aA	804	CLA	2	0
15	bF	203	BCR	1	0
12	aB	915	CLA	2	0
12	cB	914	CLA	1	0
12	aA	819	CLA	3	0
12	aB	917	CLA	1	0
12	cA	802	CLA	1	0
12	cA	804	CLA	2	0
15	bF	204	BCR	3	0
16	cA	852	LHG	1	0
15	cL	206	BCR	1	0
12	cB	925	CLA	3	0
15	aB	946	BCR	2	0
12	bB	930	CLA	1	0
12	bA	829	CLA	1	0
15	aJ	101	BCR	1	0

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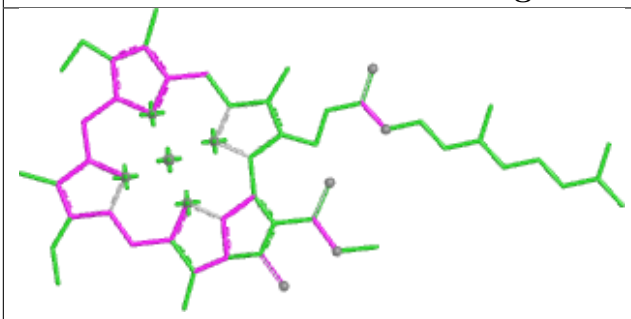
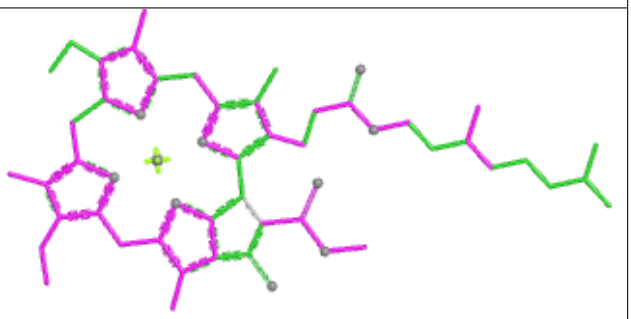
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	cB	945	BCR	3	0
12	aA	802	CLA	2	0
15	bA	849	BCR	2	0
12	bB	904	CLA	2	0
12	aA	840	CLA	4	0
12	aB	919	CLA	1	0
15	cF	203	BCR	2	0
15	cA	850	BCR	2	0
15	bB	942	BCR	1	0
12	aA	838	CLA	1	0
12	bA	808	CLA	1	0
12	aA	809	CLA	4	0
12	aB	914	CLA	1	0
12	aA	807	CLA	1	0
12	cA	817	CLA	1	0
12	aA	826	CLA	1	0
12	bA	804	CLA	2	0
12	bB	902	CLA	1	0
12	aA	832	CLA	2	0
12	bB	916	CLA	2	0
12	cA	825	CLA	6	0
15	cF	201	BCR	2	0
12	aA	808	CLA	1	0
12	bA	819	CLA	3	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.

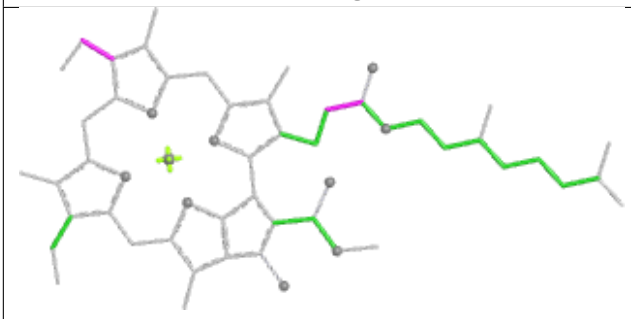
Ligand CLA bB 906



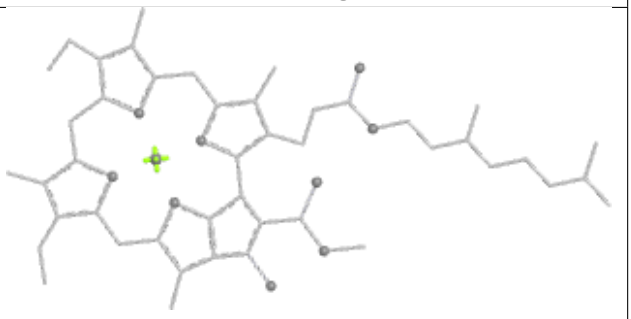
Bond lengths



Bond angles

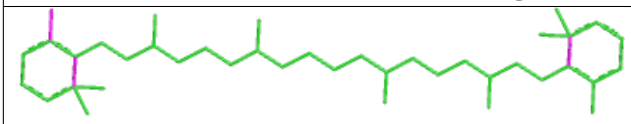


Torsions

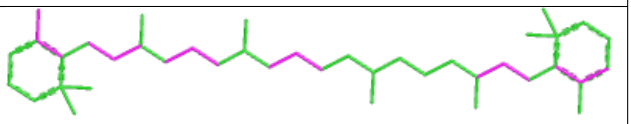


Rings

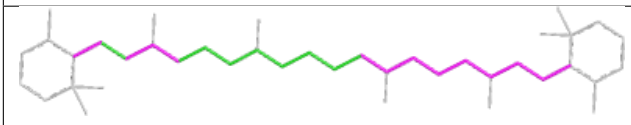
Ligand BCR cM 101



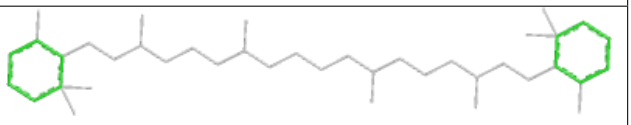
Bond lengths



Bond angles

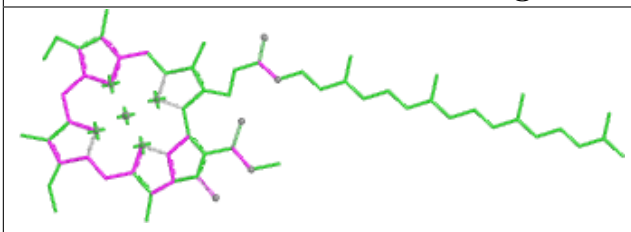


Torsions

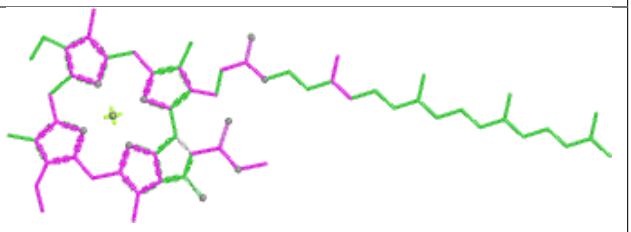


Rings

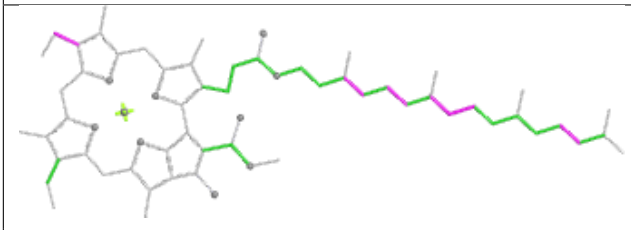
Ligand CLA bA 840



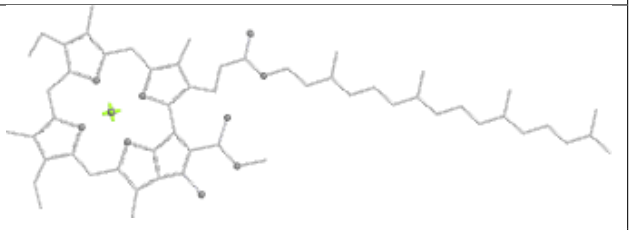
Bond lengths



Bond angles

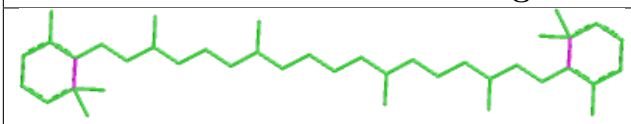


Torsions

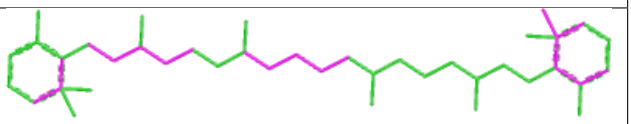


Rings

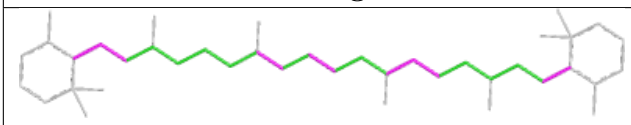
Ligand BCR bB 945



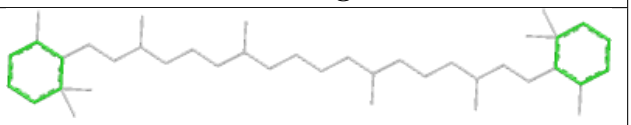
Bond lengths



Bond angles

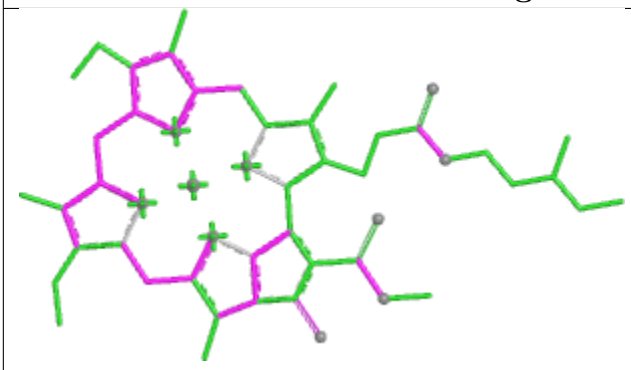


Torsions

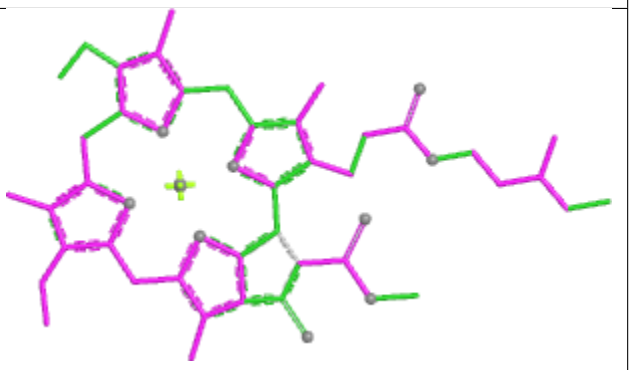


Rings

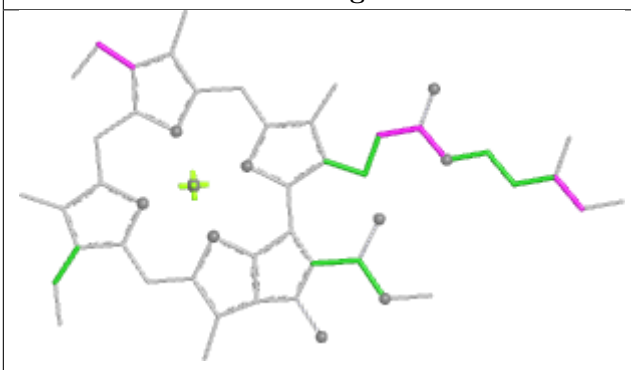
Ligand CLA aA 823



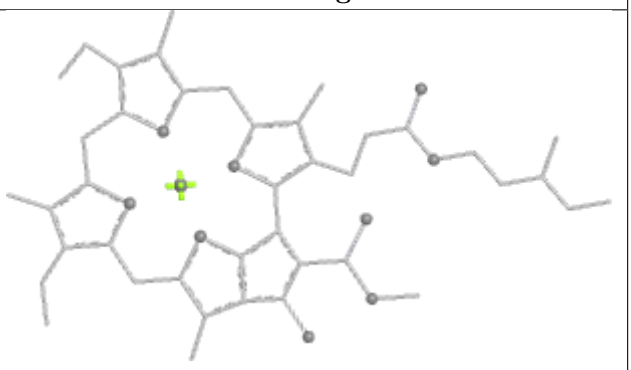
Bond lengths



Bond angles

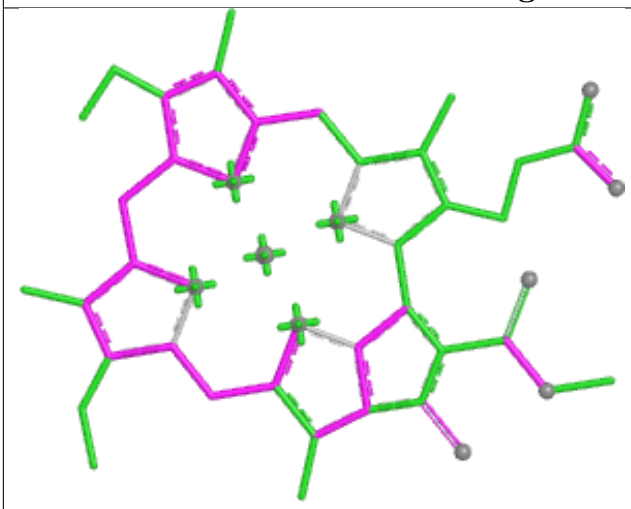


Torsions

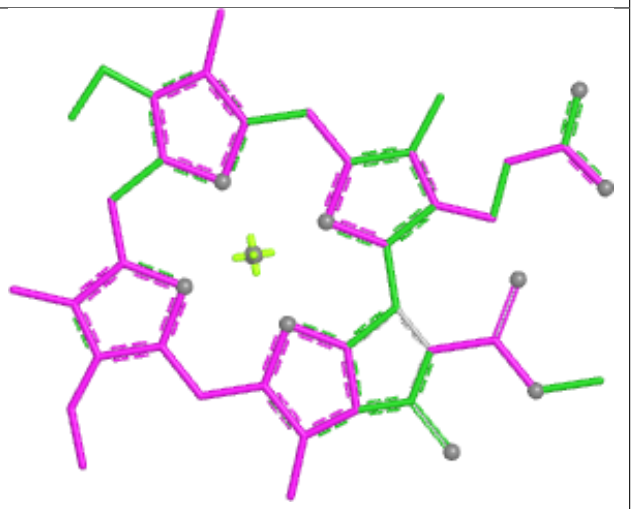


Rings

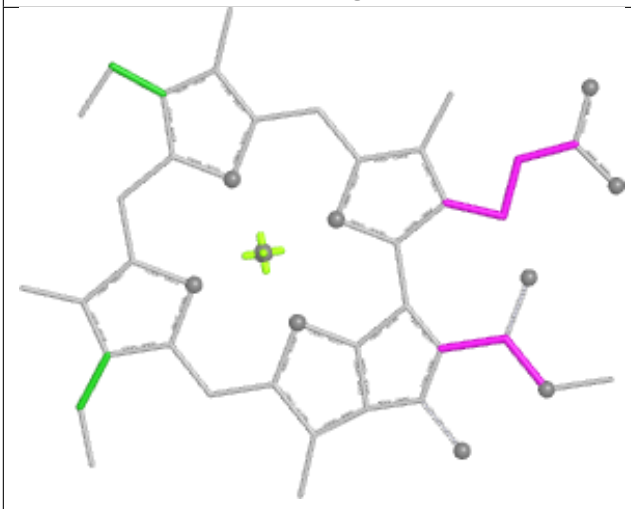
Ligand CLA cF 202



Bond lengths



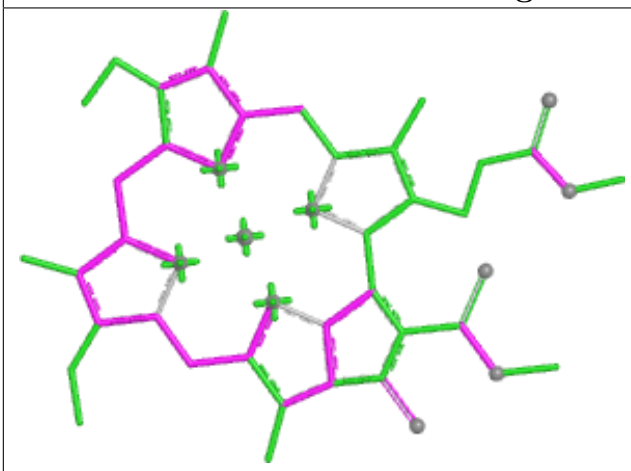
Bond angles



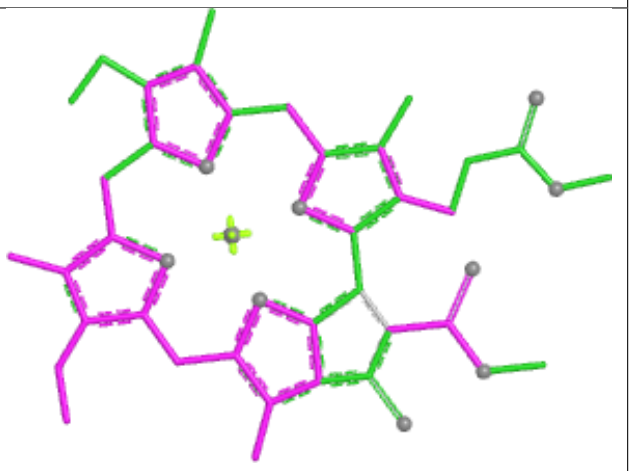
Torsions

Rings

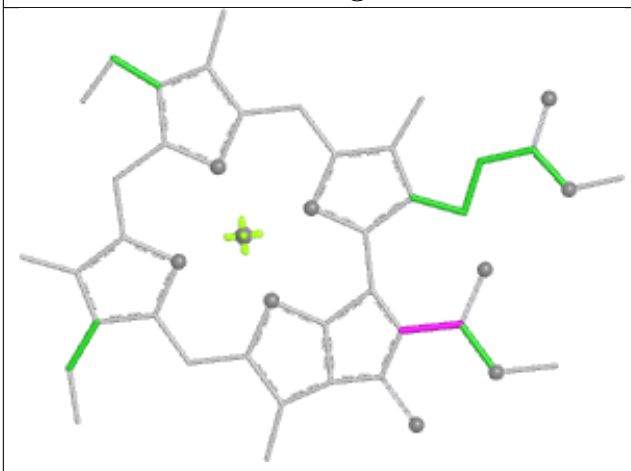
Ligand CLA aB 924



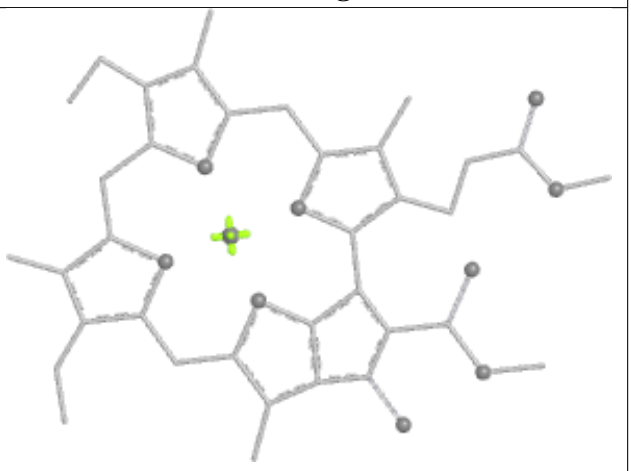
Bond lengths



Bond angles

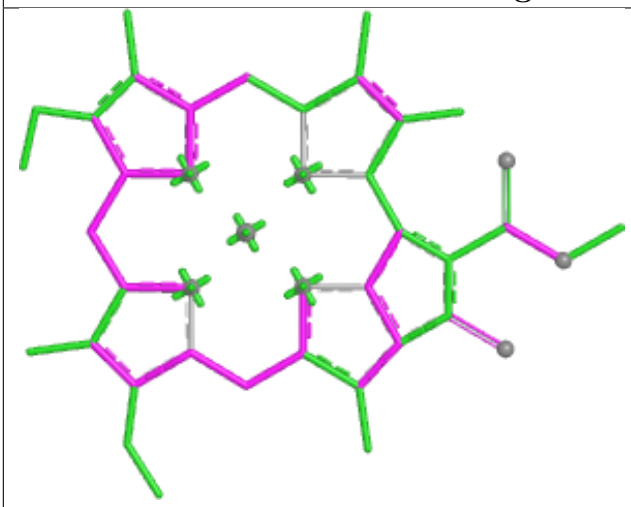


Torsions

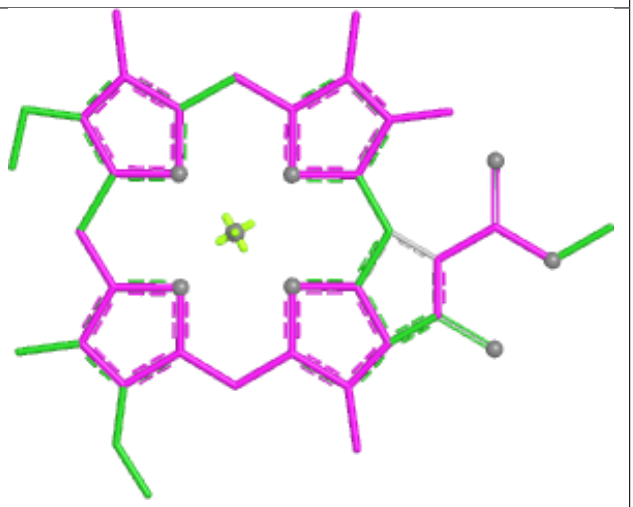


Rings

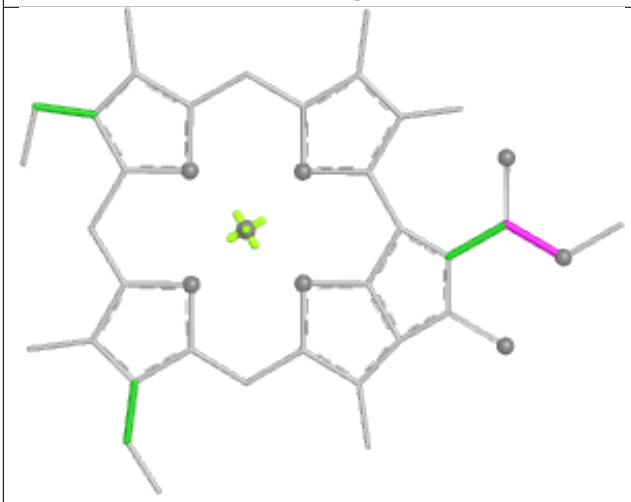
Ligand CLA bB 949



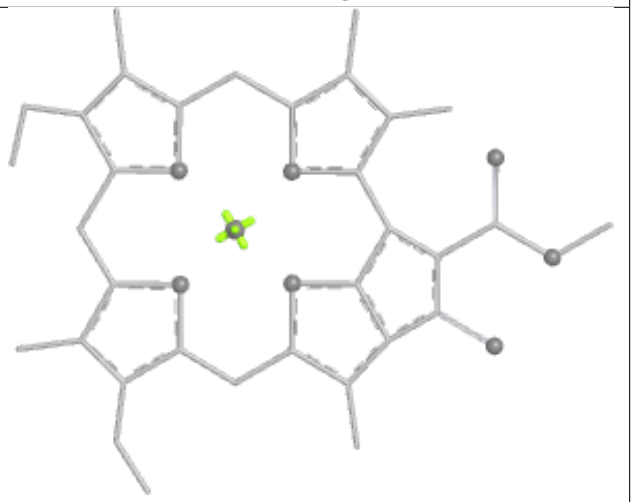
Bond lengths



Bond angles

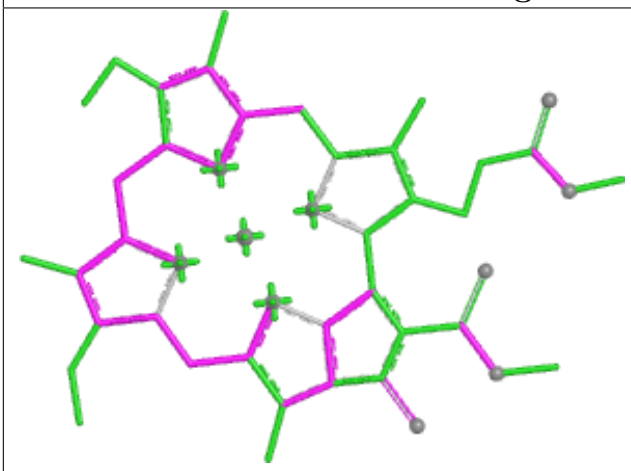


Torsions



Rings

Ligand CLA bB 924



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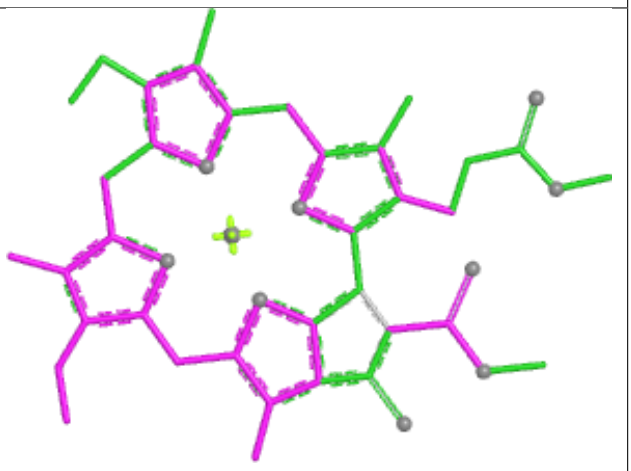
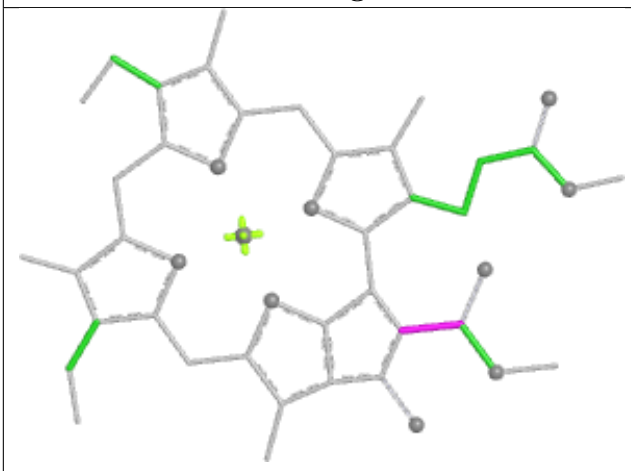
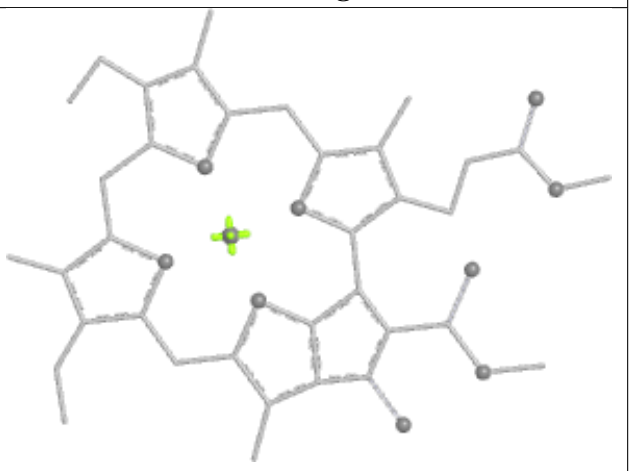


Bond angles



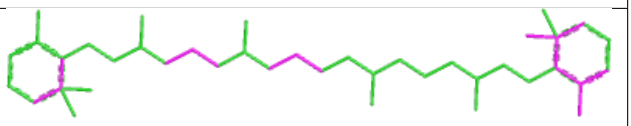
Torsions



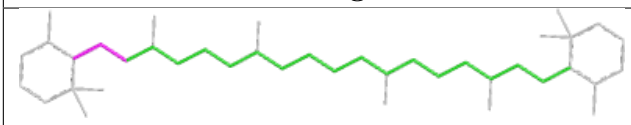
Rings

Ligand BCR cB 946

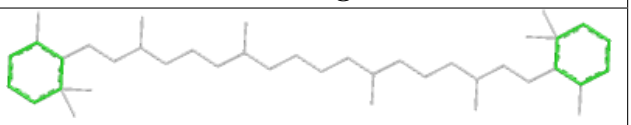
Bond lengths



Bond angles

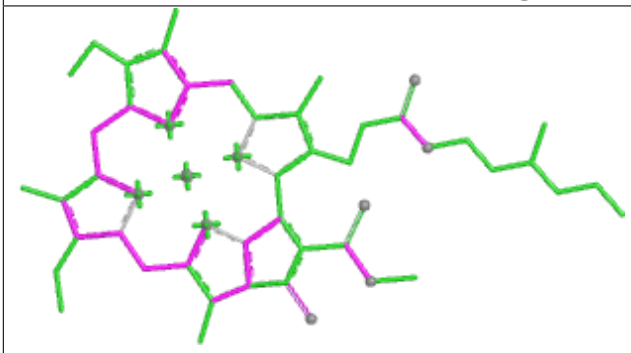


Torsions

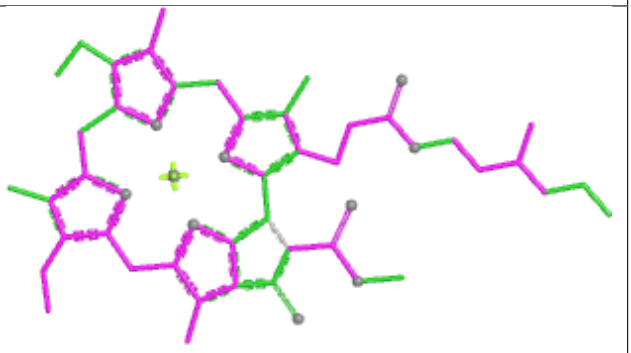


Rings

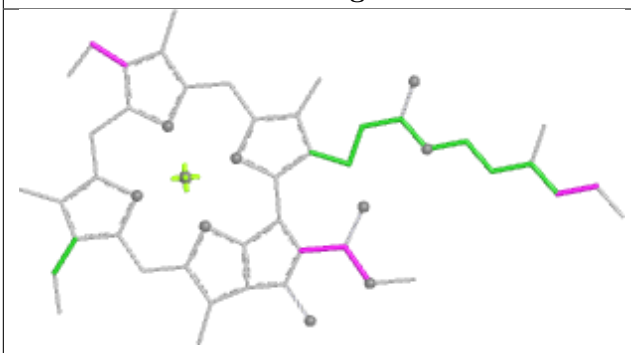
Ligand CLA aB 907



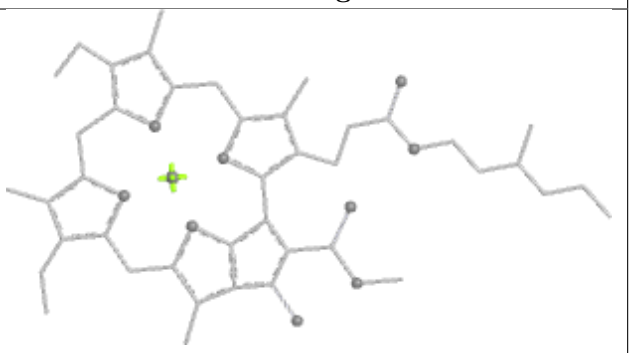
Bond lengths



Bond angles

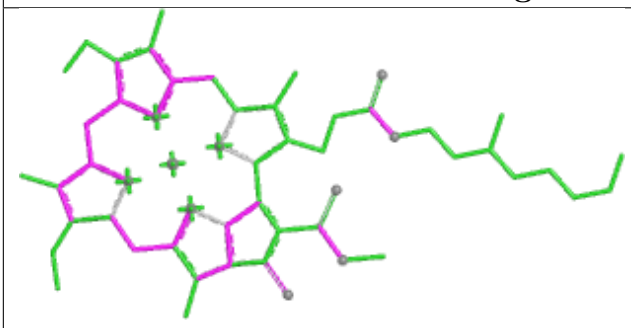


Torsions

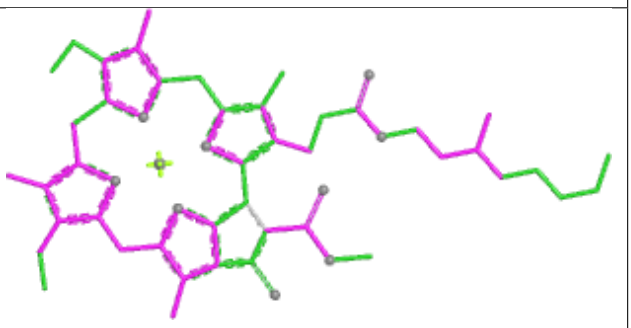


Rings

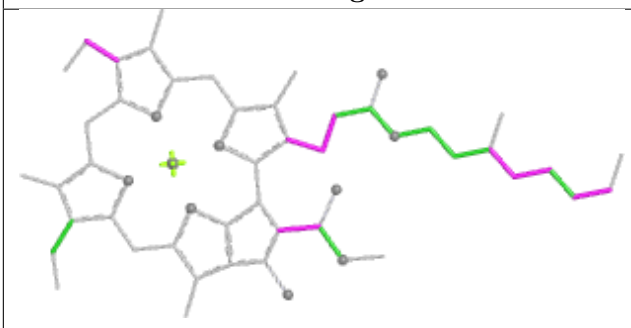
Ligand CLA bB 923



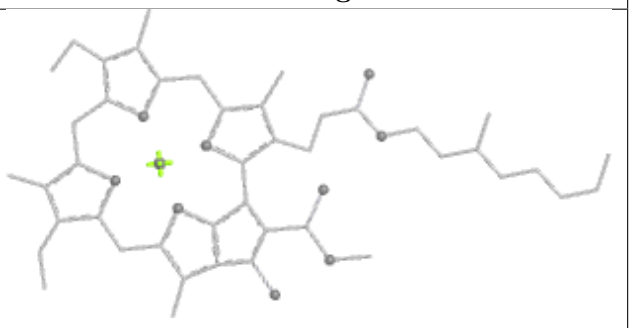
Bond lengths



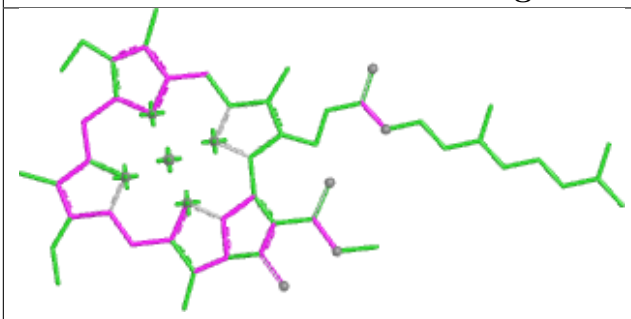
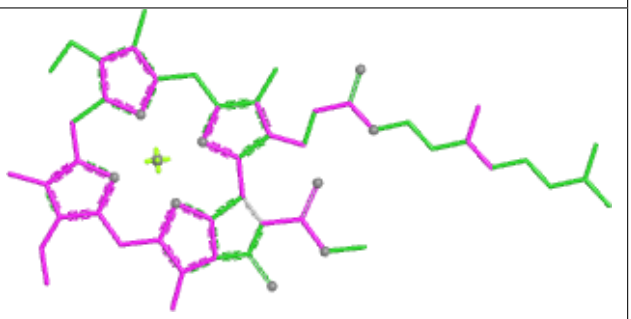
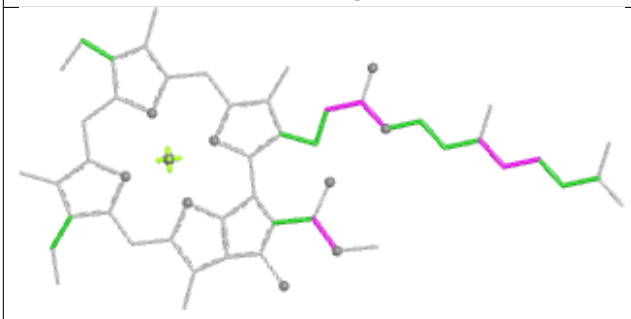
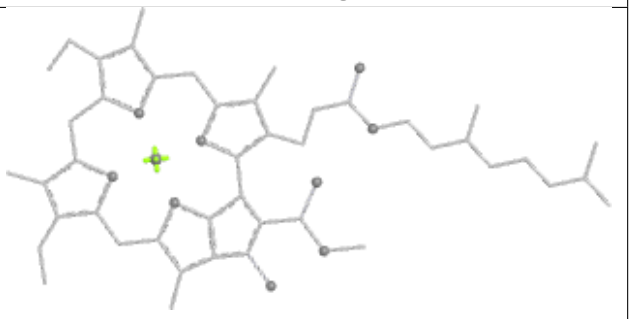
Bond angles

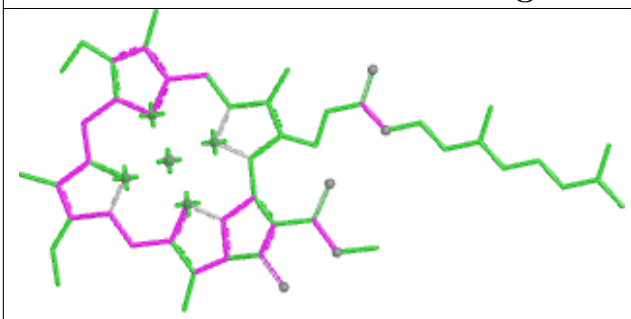
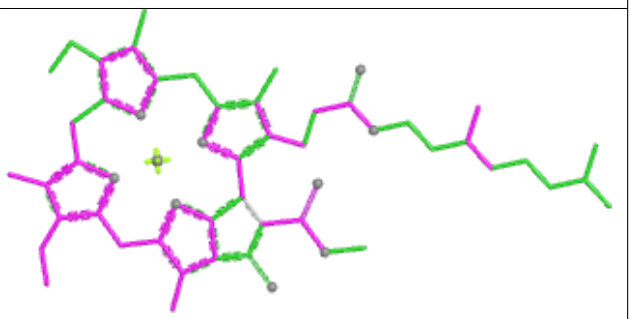
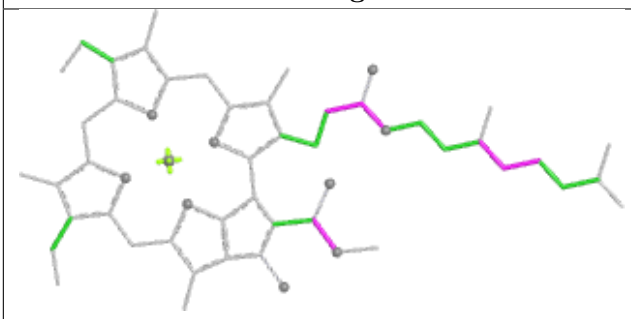
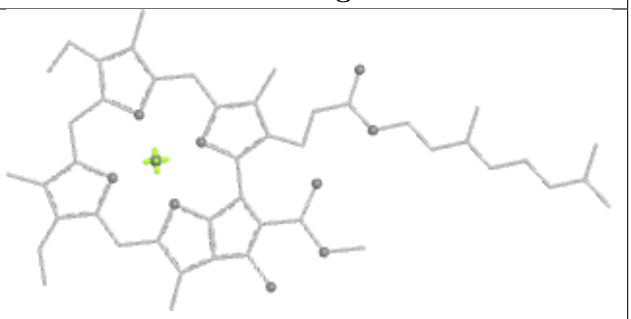


Torsions

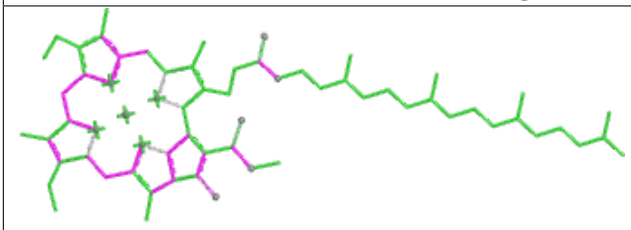


Rings

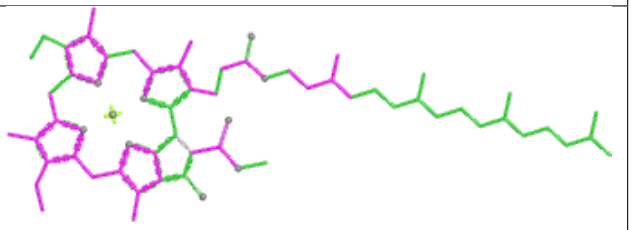
Ligand CLA bB 921	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA cB 921	
	
Bond lengths	Bond angles
	
Torsions	Rings

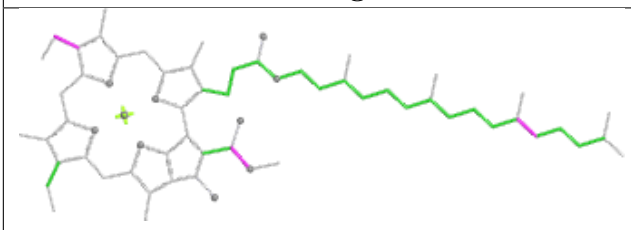
Ligand CLA aB 901



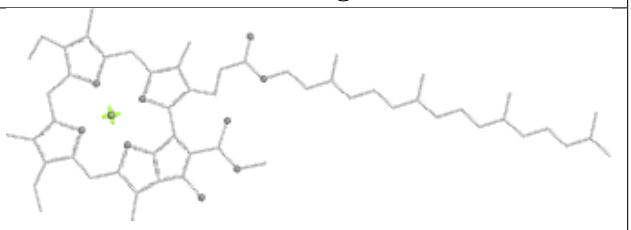
Bond lengths



Bond angles

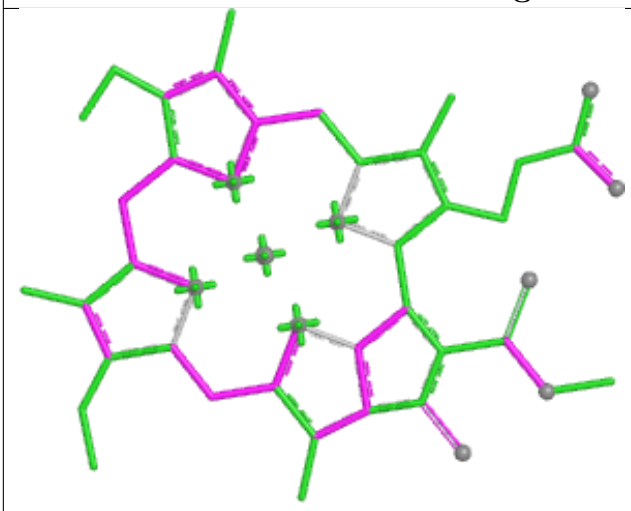


Torsions



Rings

Ligand CLA bA 811



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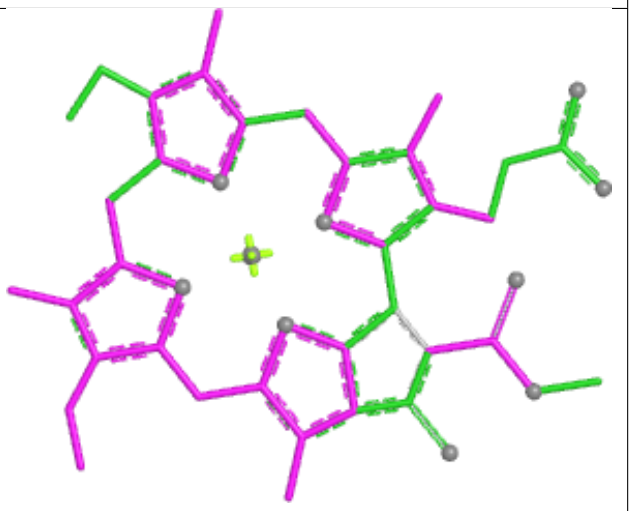
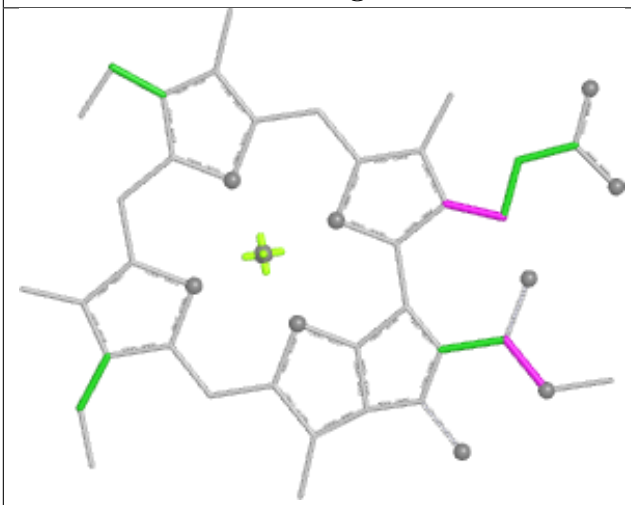
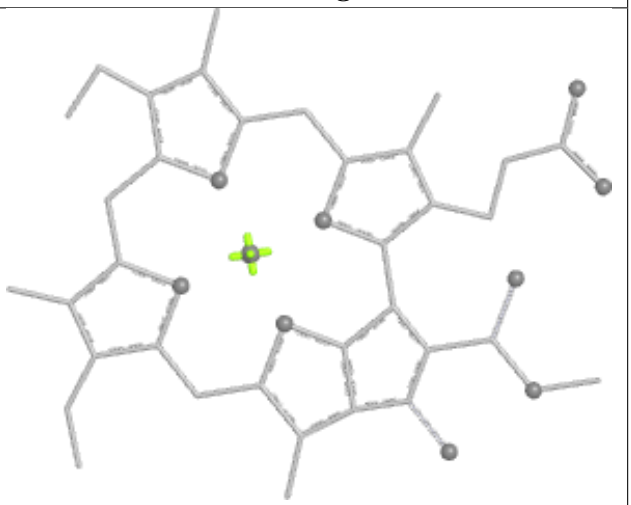


Bond angles

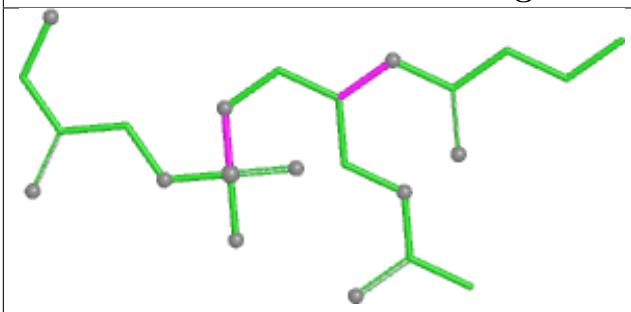


Torsions



Rings

Ligand LHG cB 948



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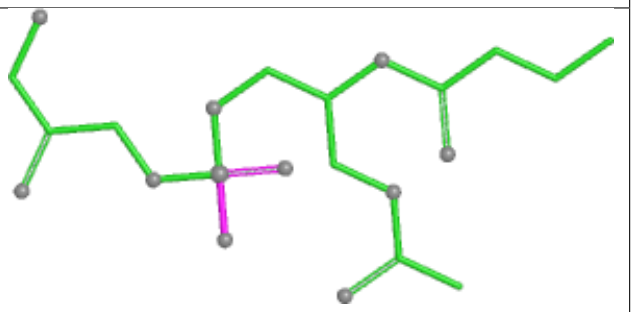
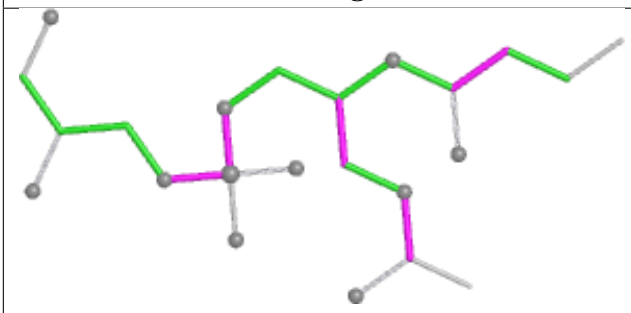
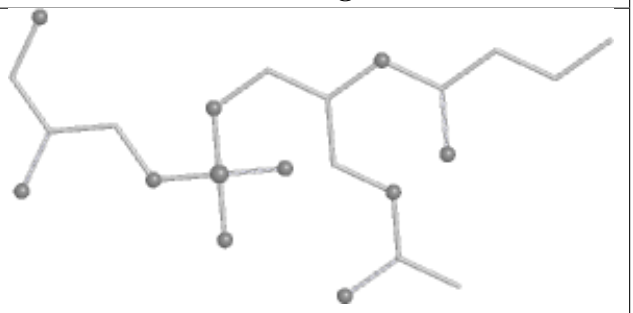


Bond angles

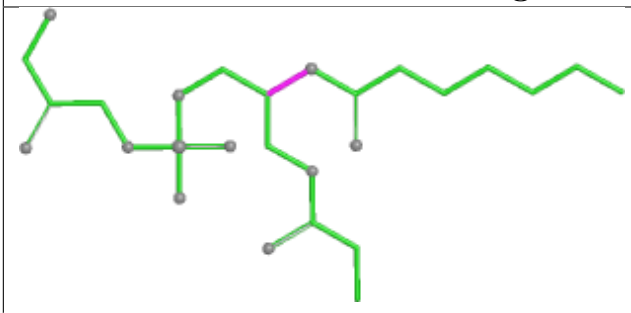


Torsions

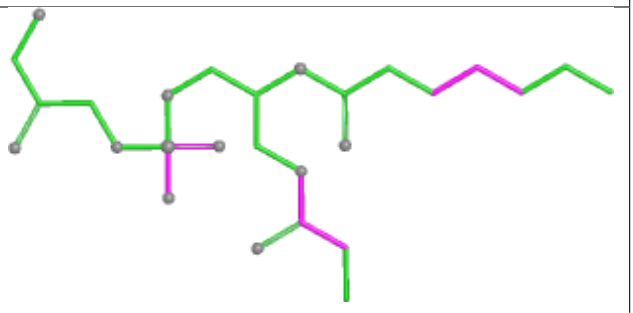


Rings

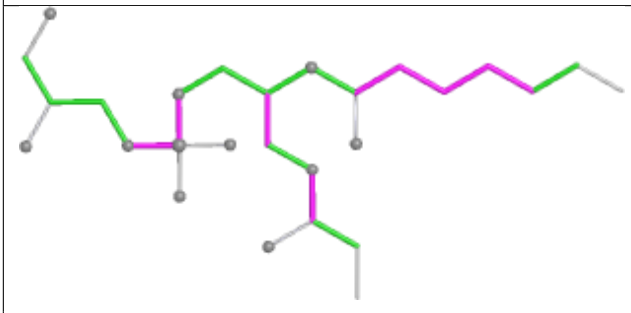
Ligand LHG bA 852



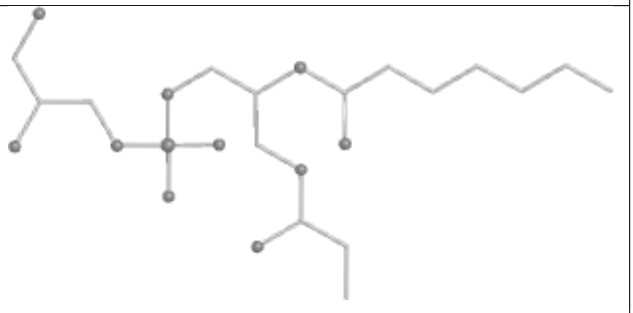
Bond lengths



Bond angles

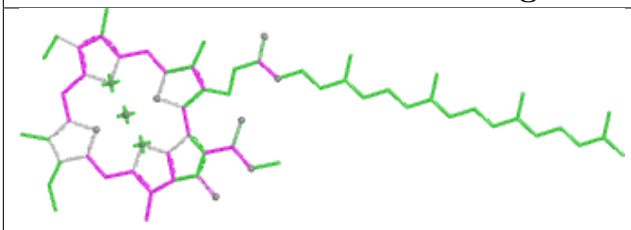


Torsions

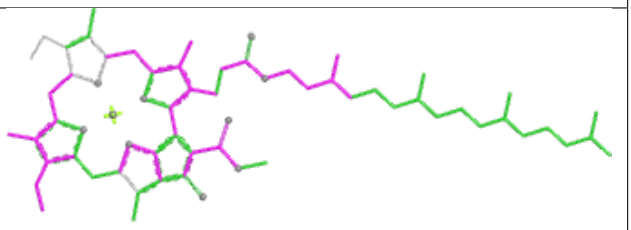


Rings

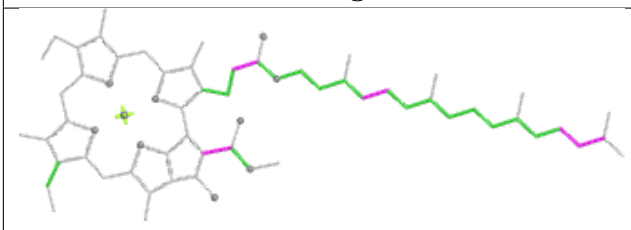
Ligand CL0 aA 801



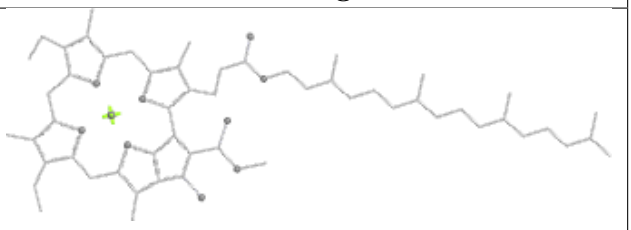
Bond lengths



Bond angles

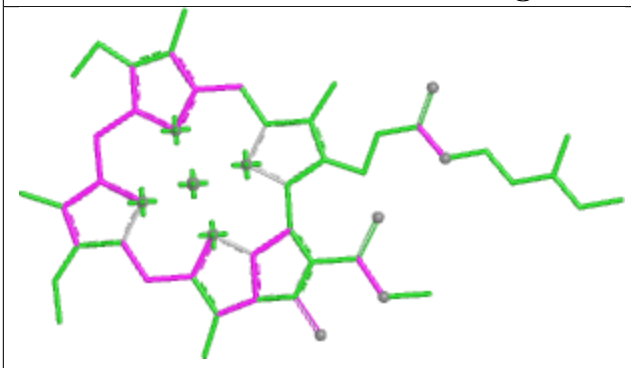


Torsions

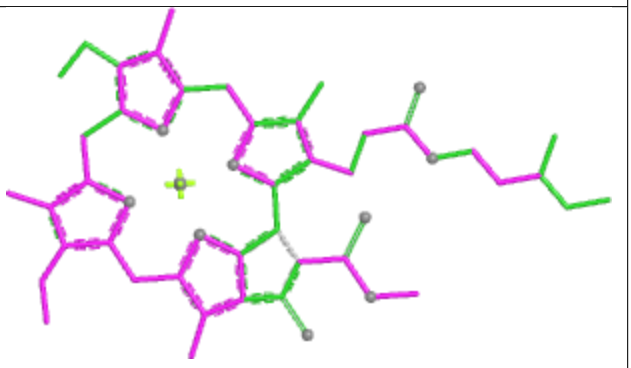


Rings

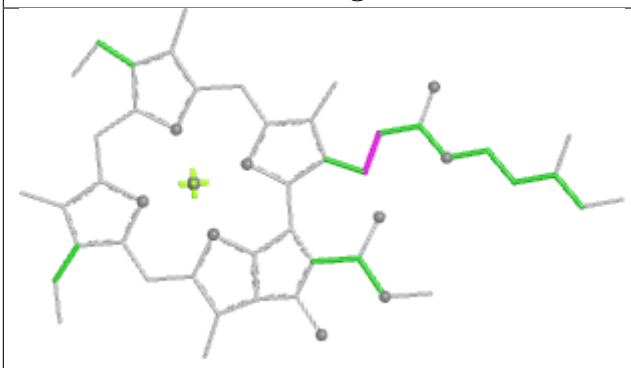
Ligand CLA bB 938



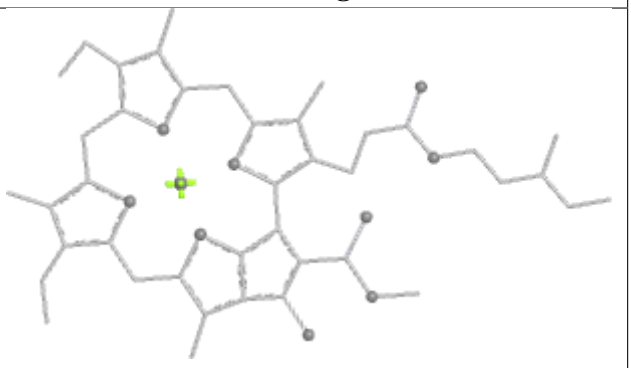
Bond lengths



Bond angles

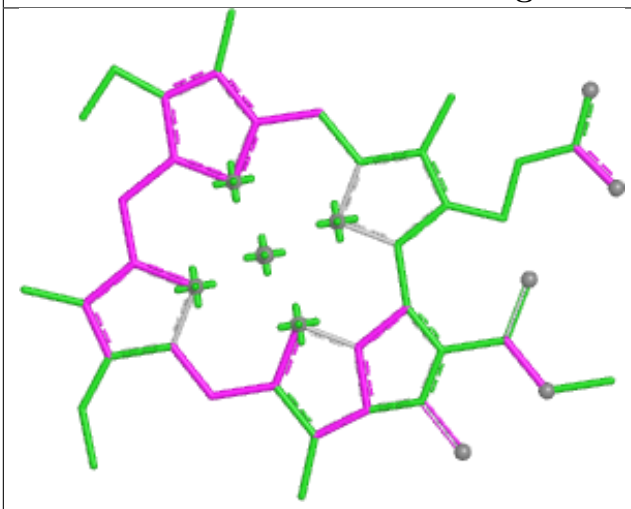


Torsions

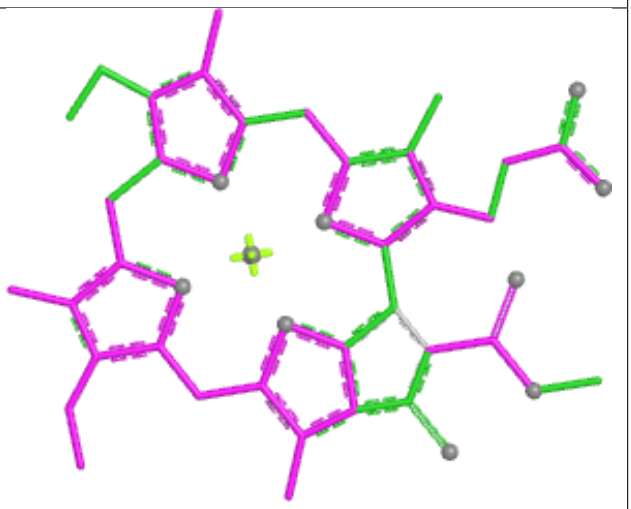


Rings

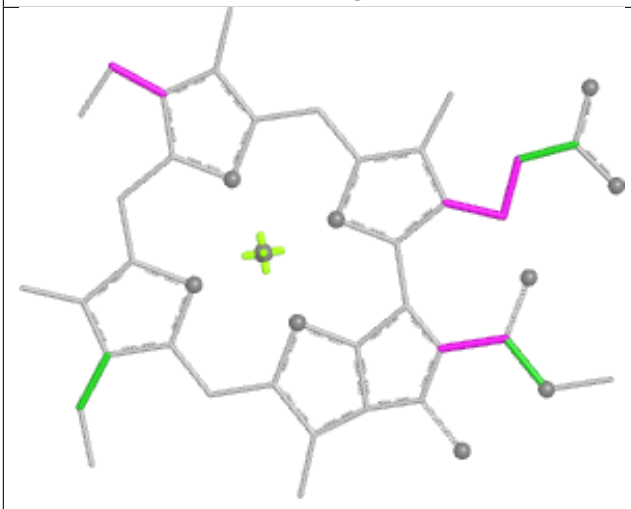
Ligand CLA cA 809



Bond lengths



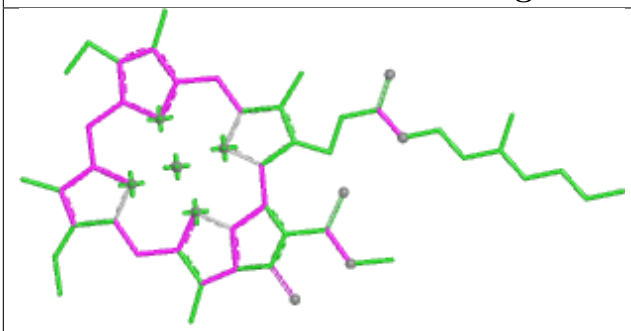
Bond angles



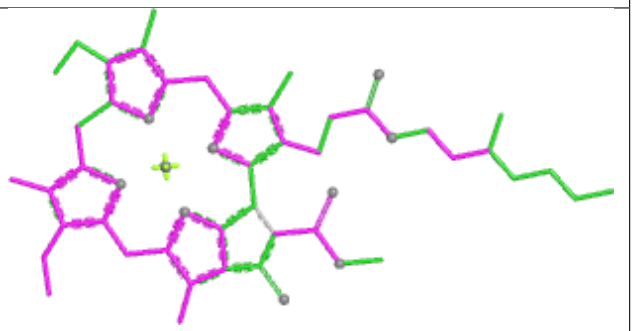
Torsions

Rings

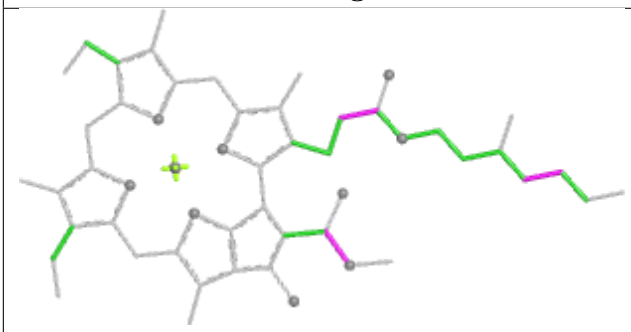
Ligand CLA aA 805



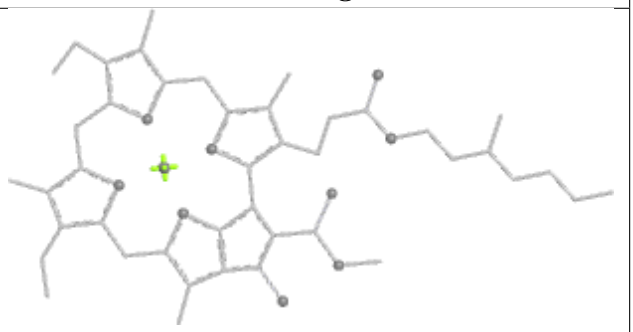
Bond lengths



Bond angles



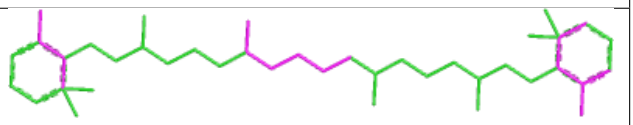
Torsions



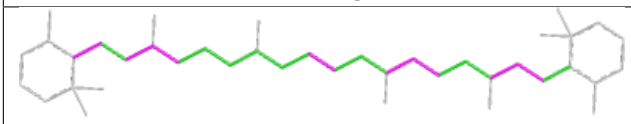
Rings

Ligand BCR cA 846

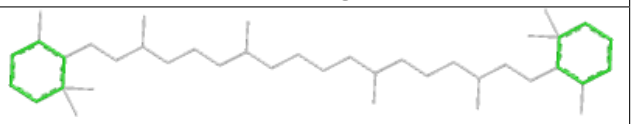
Bond lengths



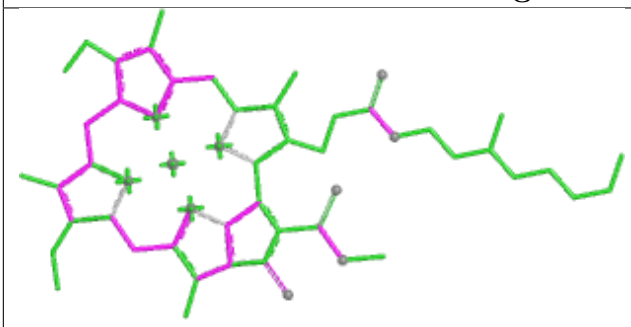
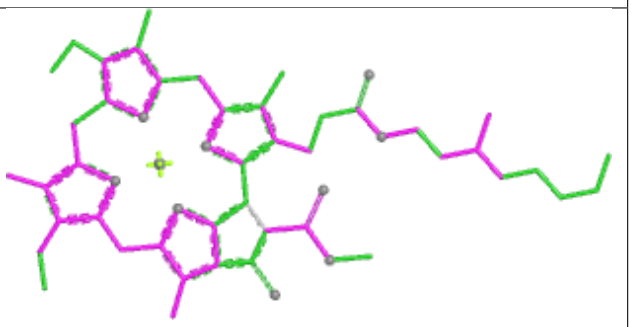
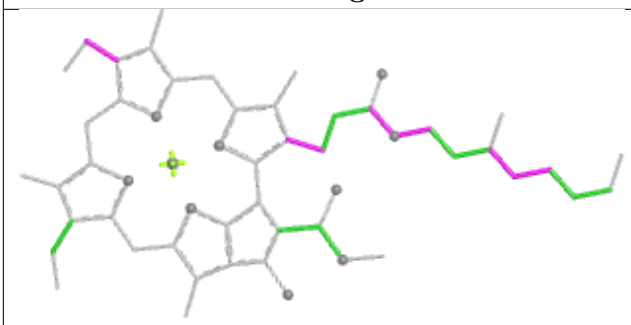
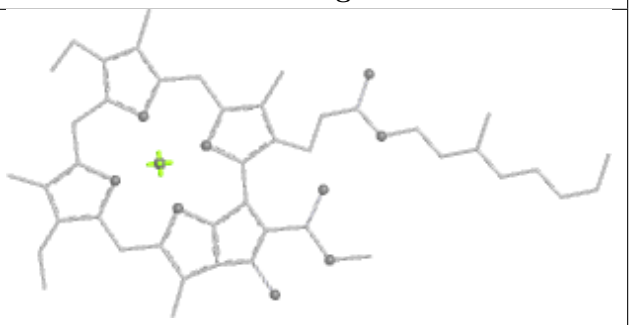
Bond angles

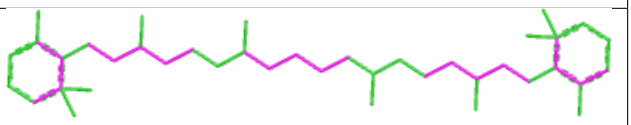
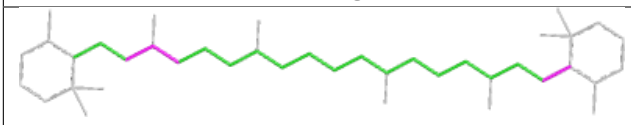
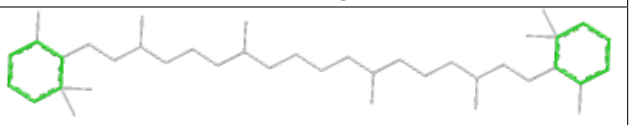


Torsions

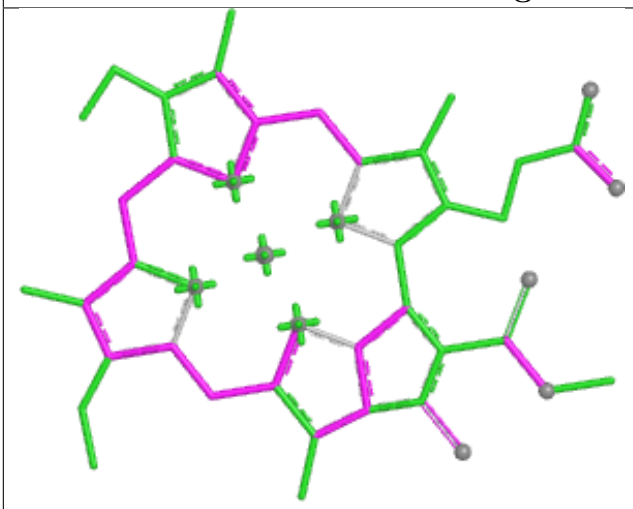


Rings

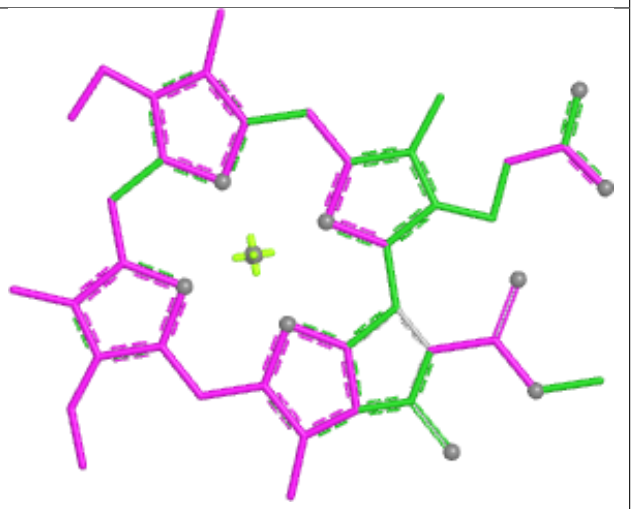
Ligand CLA bA 817	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR cF 204	
	
Bond lengths	Bond angles
	
Torsions	Rings

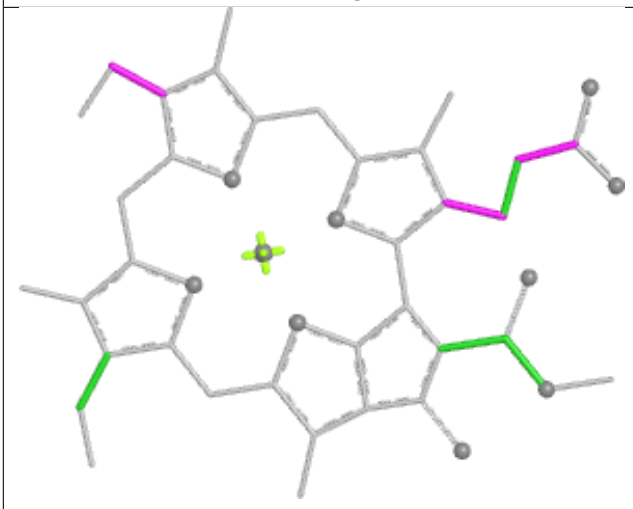
Ligand CLA bB 929



Bond lengths



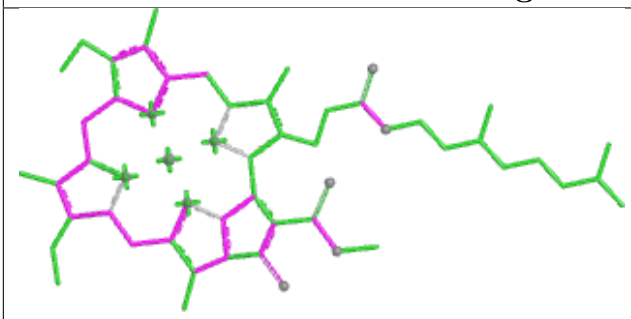
Bond angles



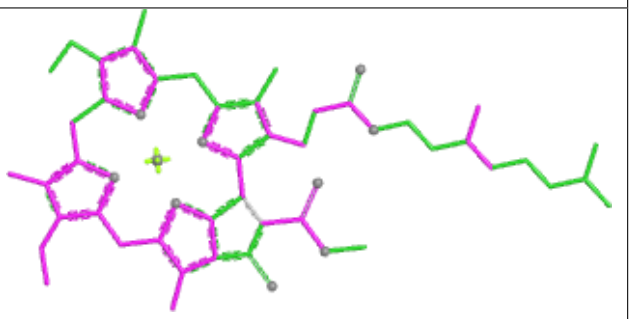
Torsions

Rings

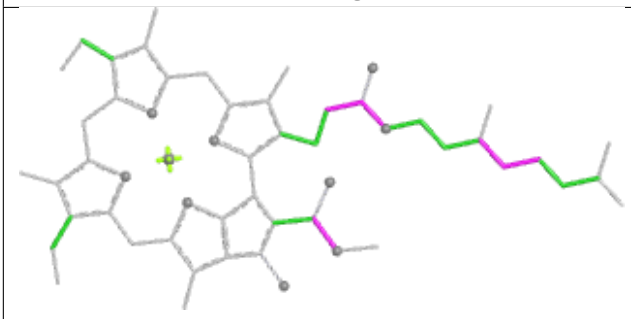
Ligand CLA aB 921



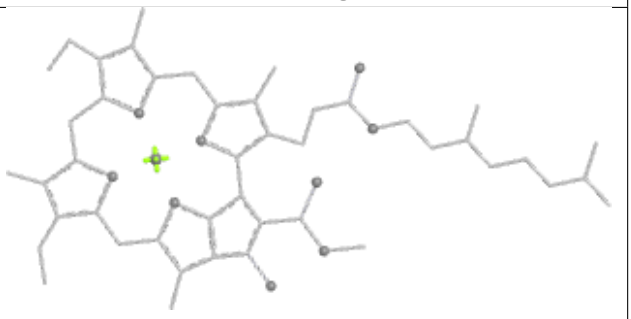
Bond lengths



Bond angles

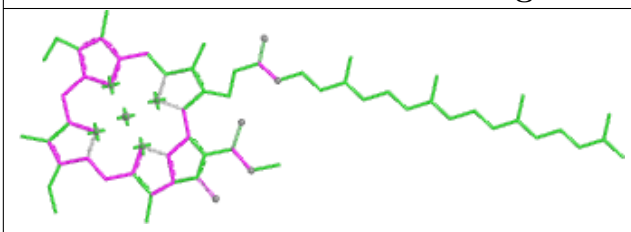


Torsions

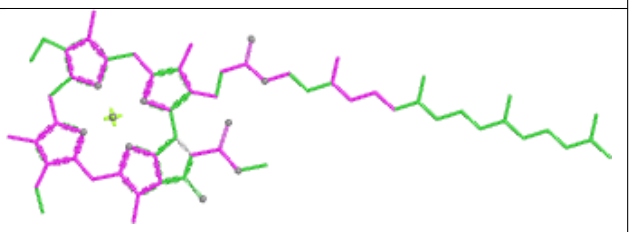


Rings

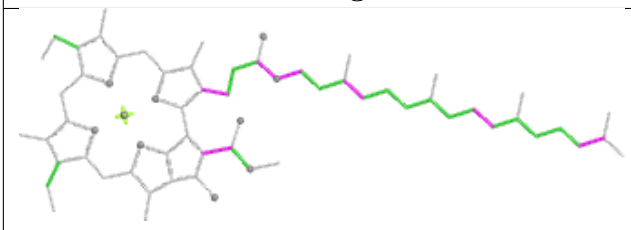
Ligand CLA cA 812



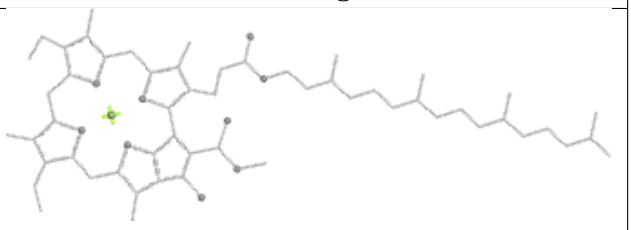
Bond lengths



Bond angles

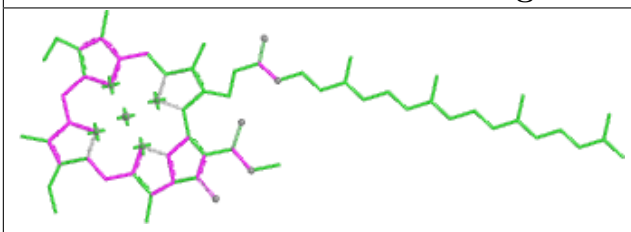


Torsions

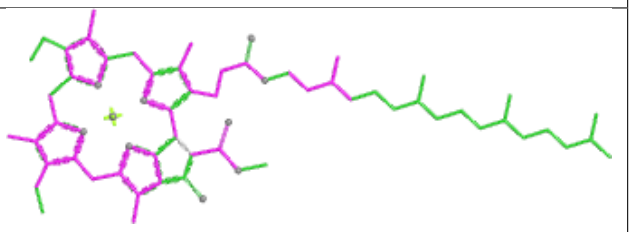


Rings

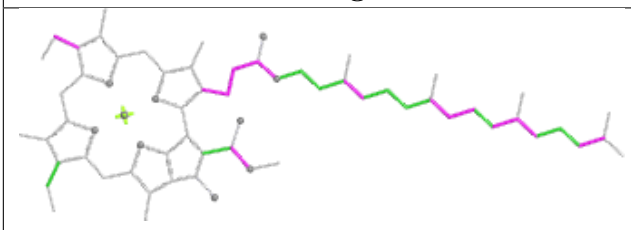
Ligand CLA cB 926



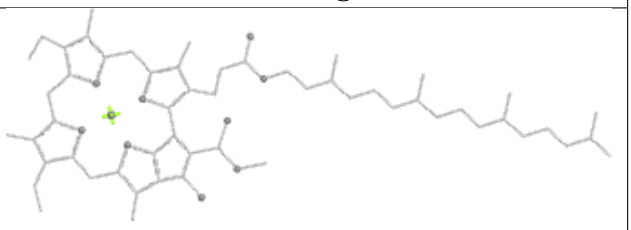
Bond lengths



Bond angles

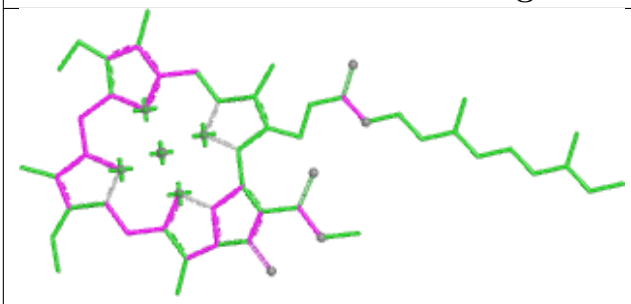


Torsions



Rings

Ligand CLA cB 913



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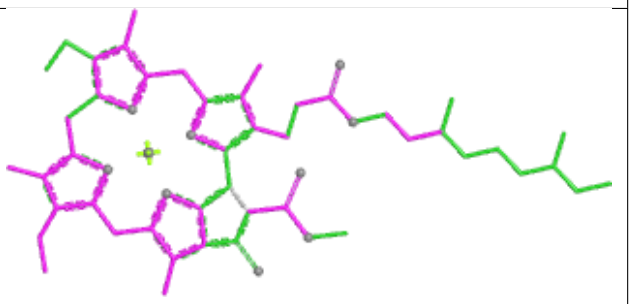
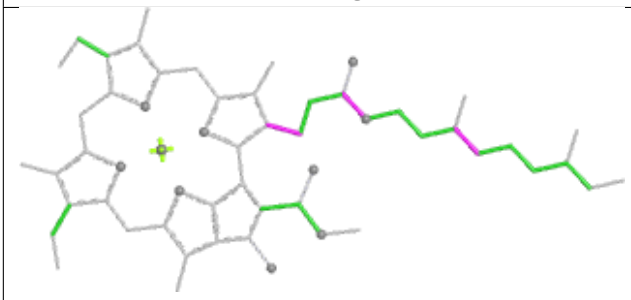
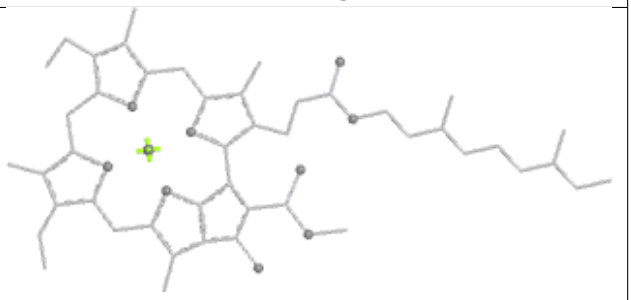


Bond angles



Torsions

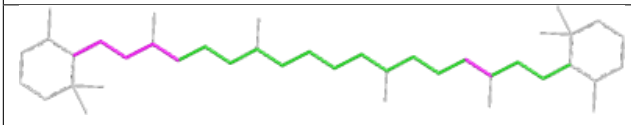


Rings

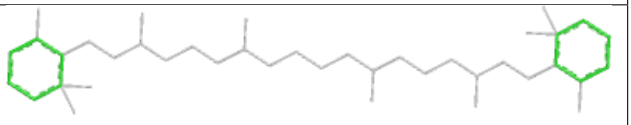
Ligand BCR bB 943

Bond lengths

Bond angles

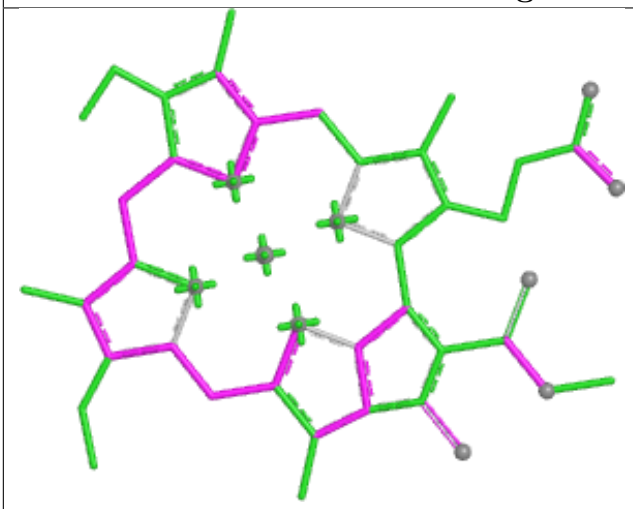


Torsions



Rings

Ligand CLA cB 910



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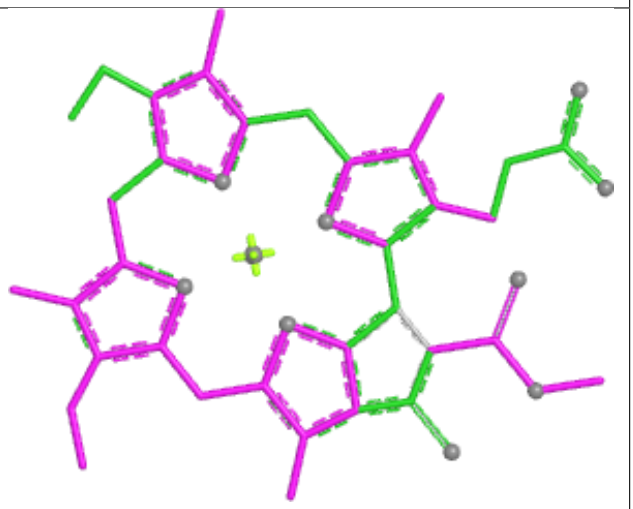
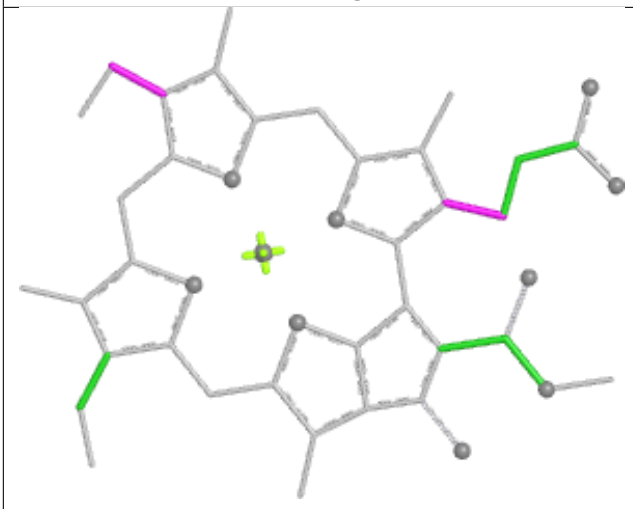


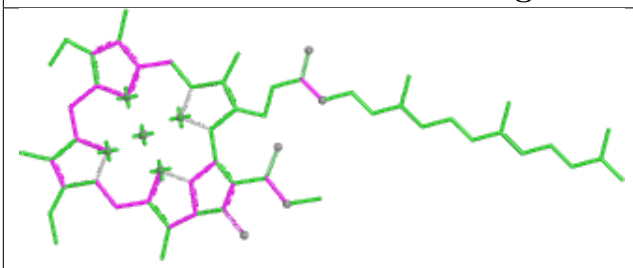
Bond angles



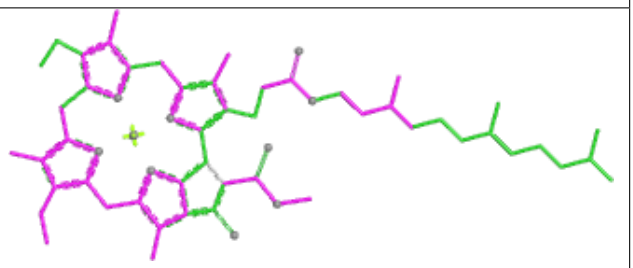
Torsions

Rings

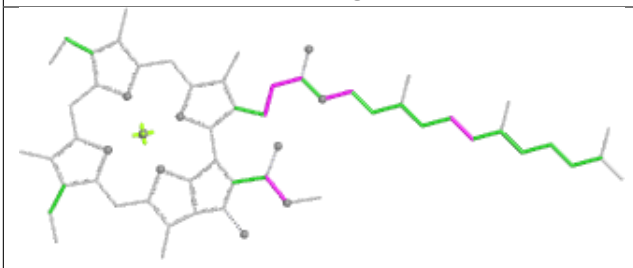
Ligand CLA aA 829



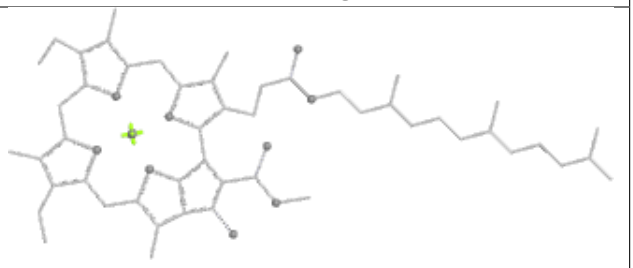
Bond lengths



Bond angles

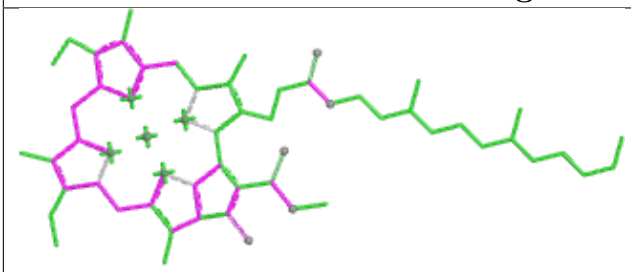


Torsions

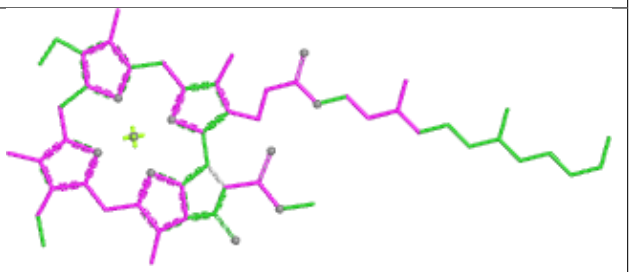


Rings

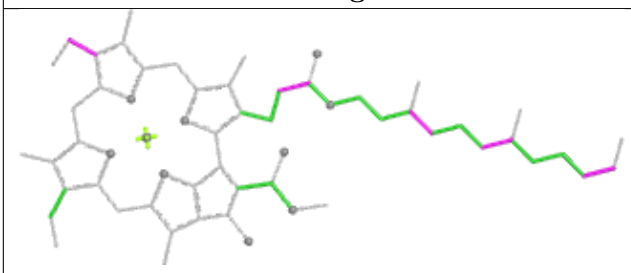
Ligand CLA aB 936



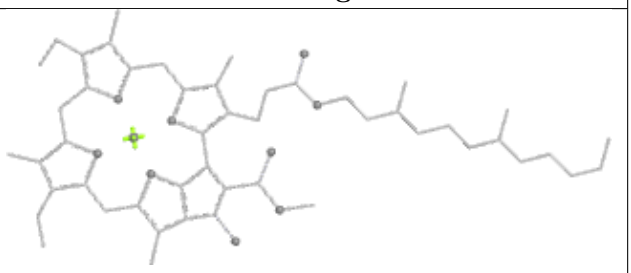
Bond lengths



Bond angles

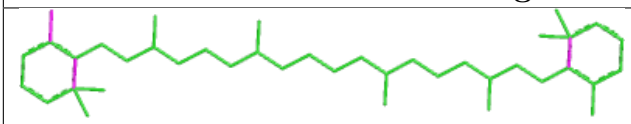


Torsions

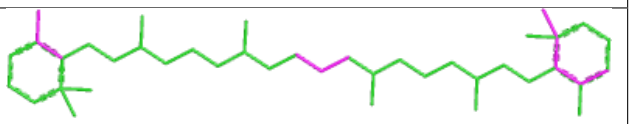


Rings

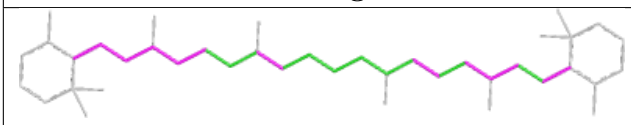
Ligand BCR aB 944



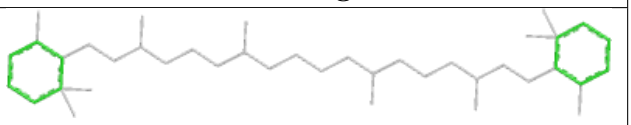
Bond lengths



Bond angles

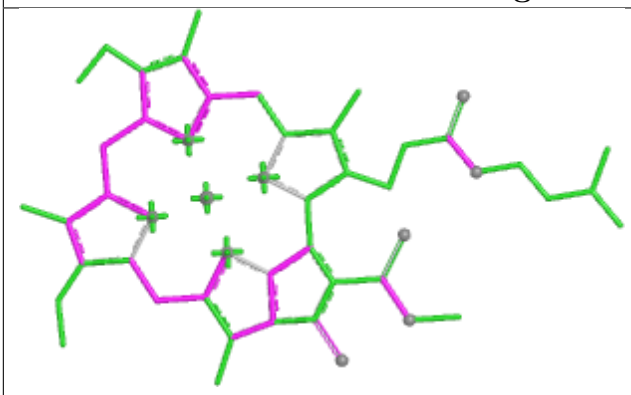


Torsions

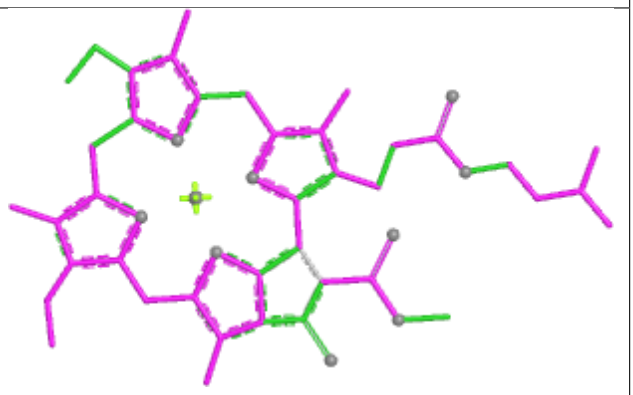


Rings

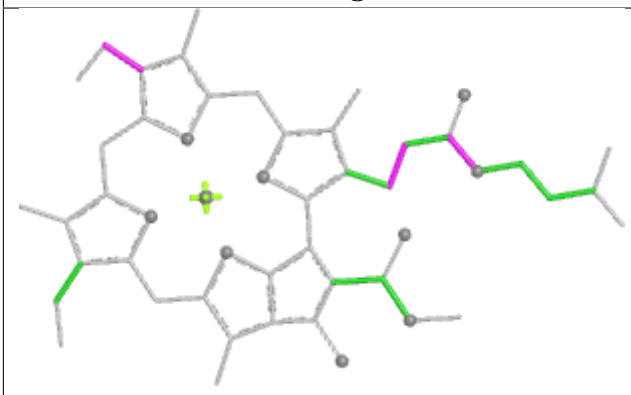
Ligand CLA bA 831



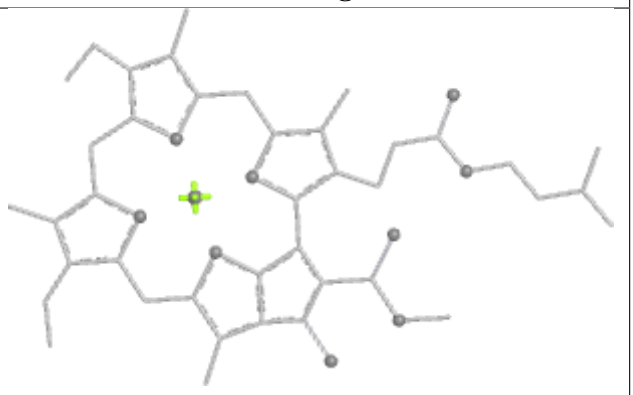
Bond lengths



Bond angles

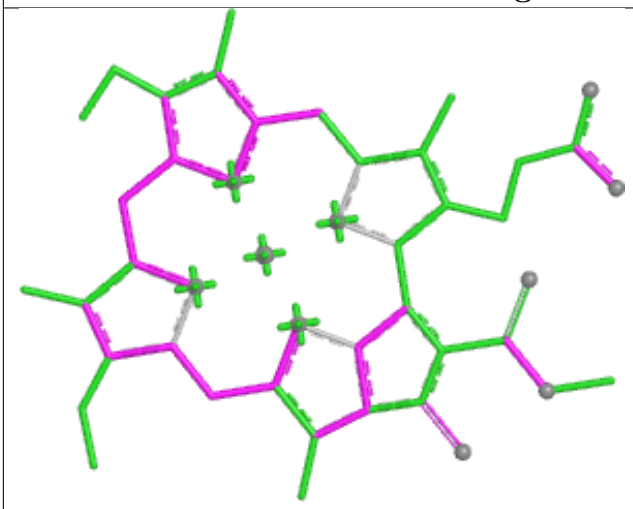


Torsions

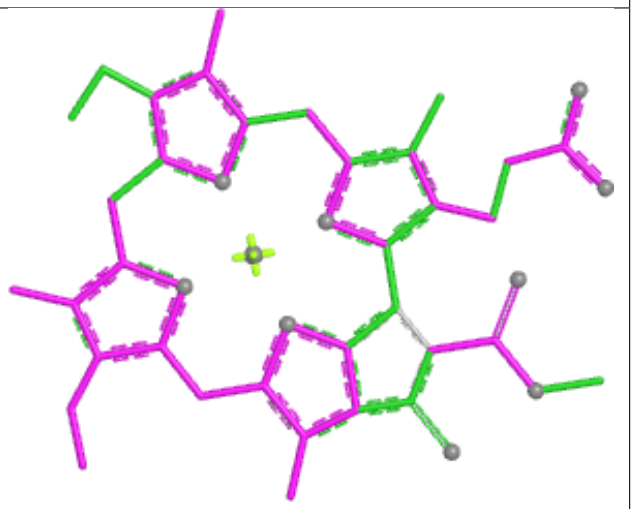


Rings

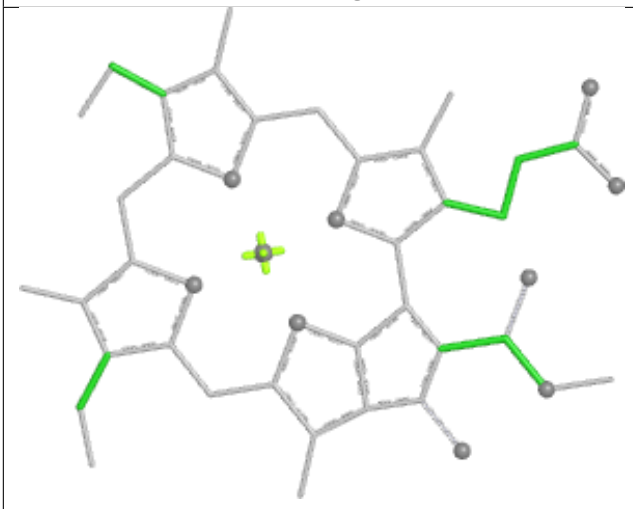
Ligand CLA bB 911



Bond lengths



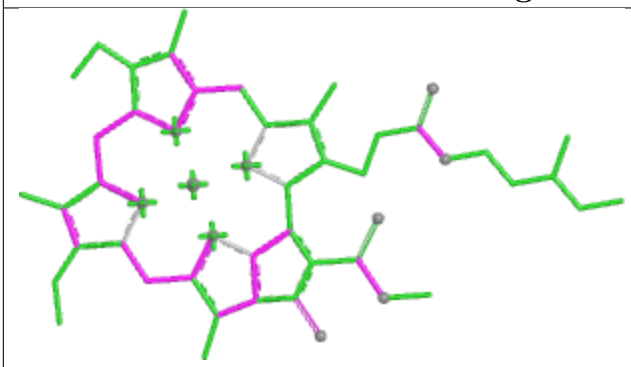
Bond angles



Torsions

Rings

Ligand CLA aA 833



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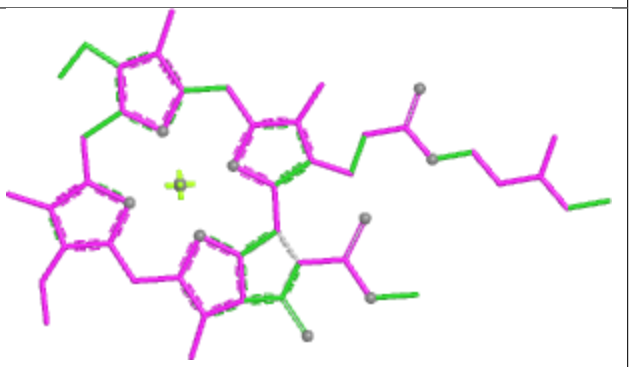
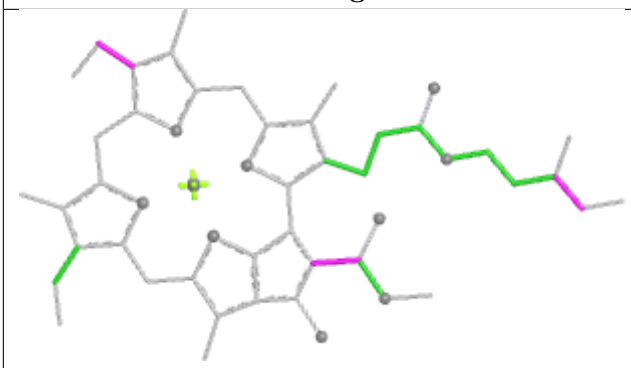
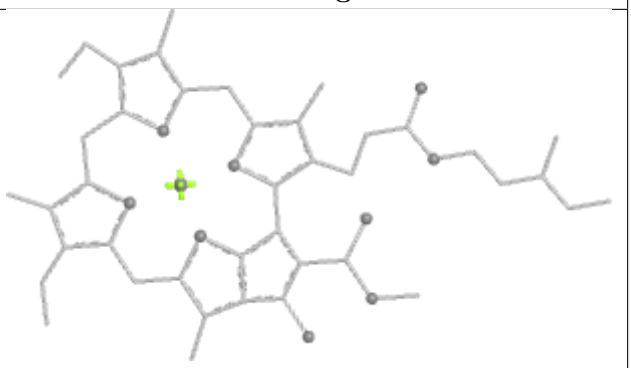


Bond angles

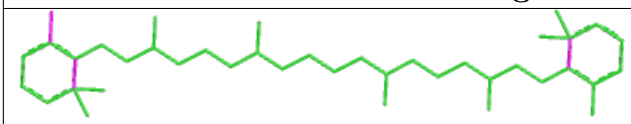


Torsions

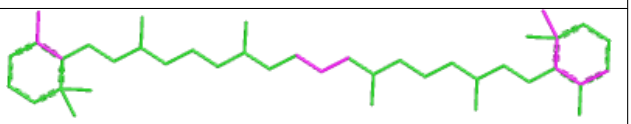


Rings

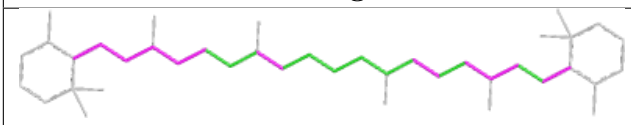
Ligand BCR bB 944



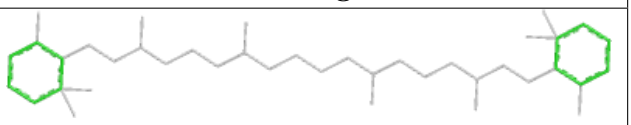
Bond lengths



Bond angles

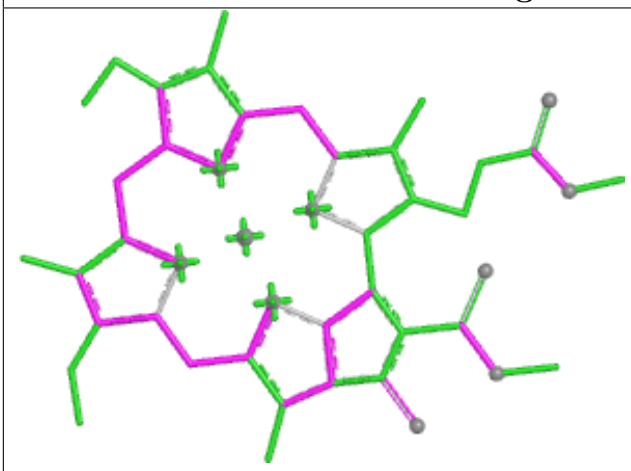


Torsions

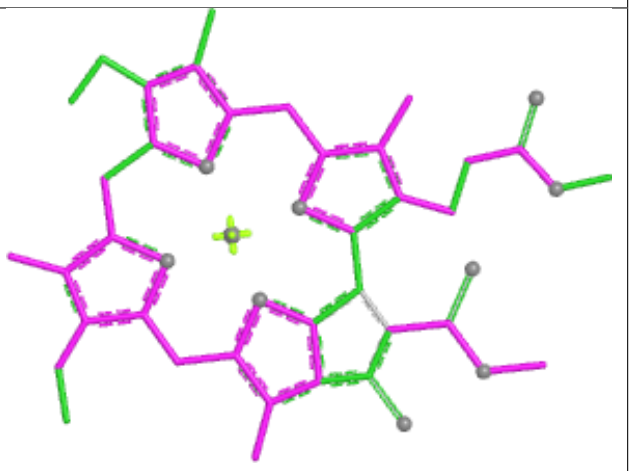


Rings

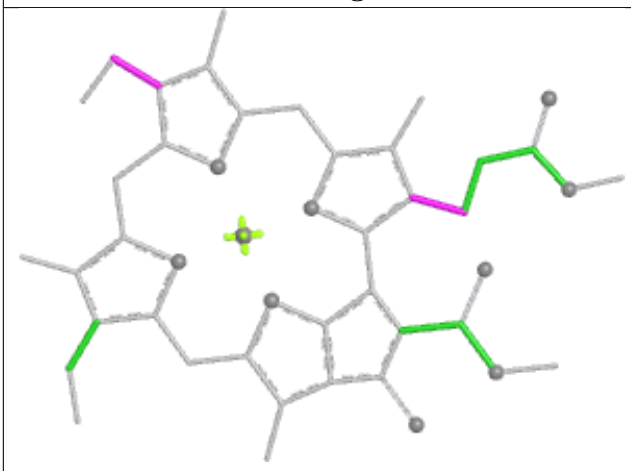
Ligand CLA aB 918



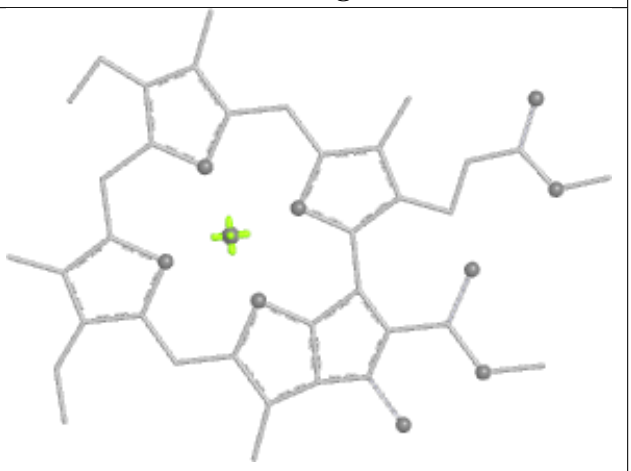
Bond lengths



Bond angles

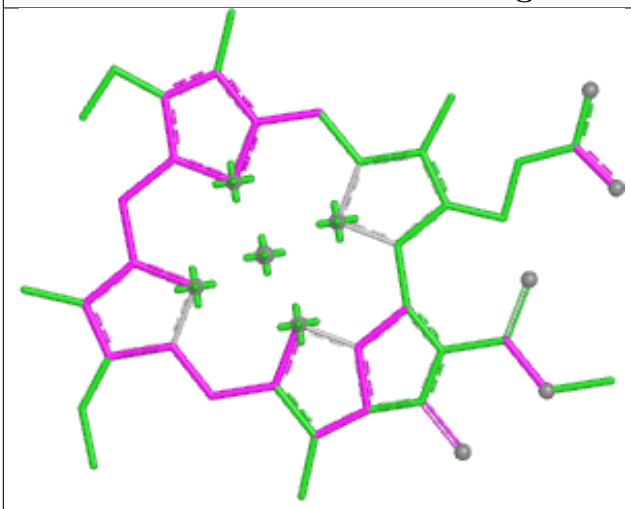


Torsions



Rings

Ligand CLA cA 813



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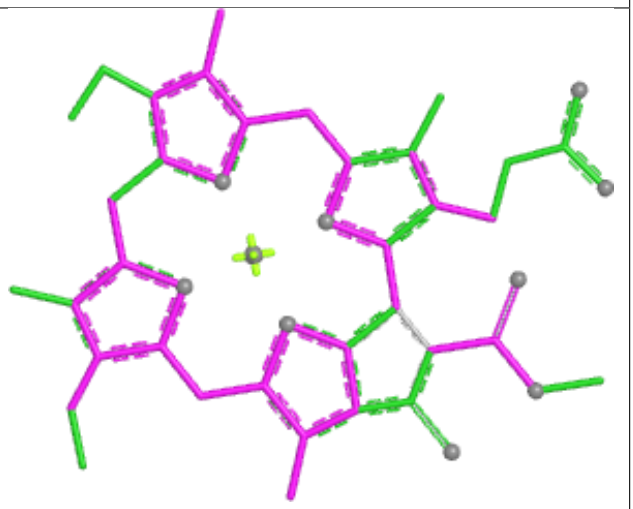
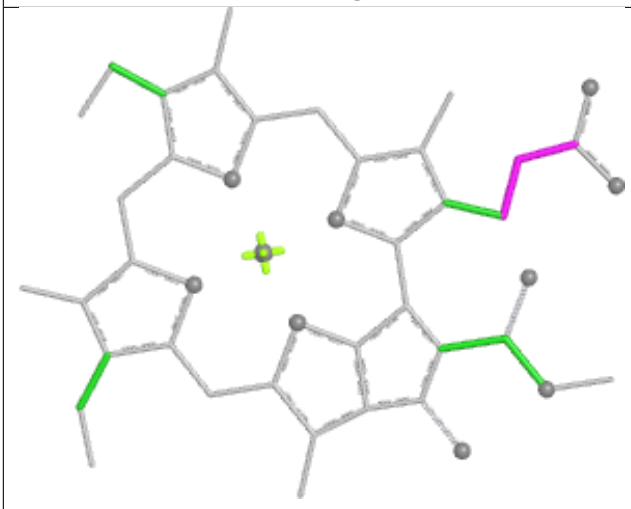


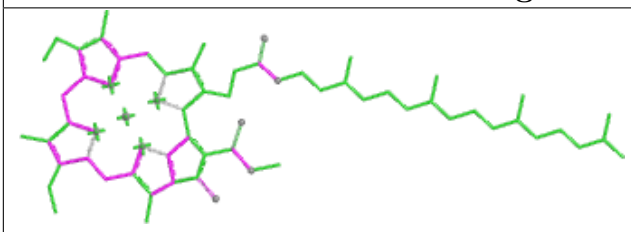
Bond angles



Torsions

Rings

Ligand CLA cA 840



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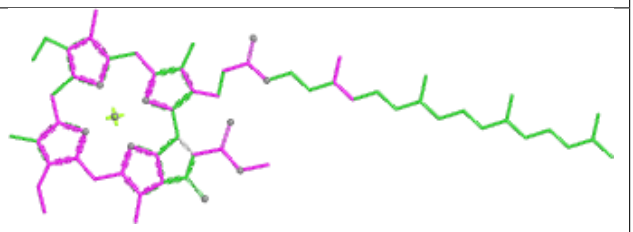
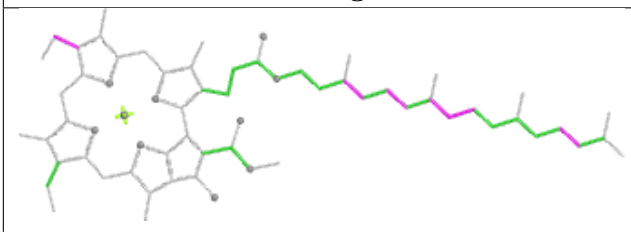
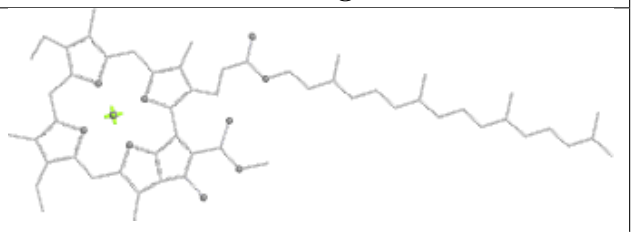


Bond angles

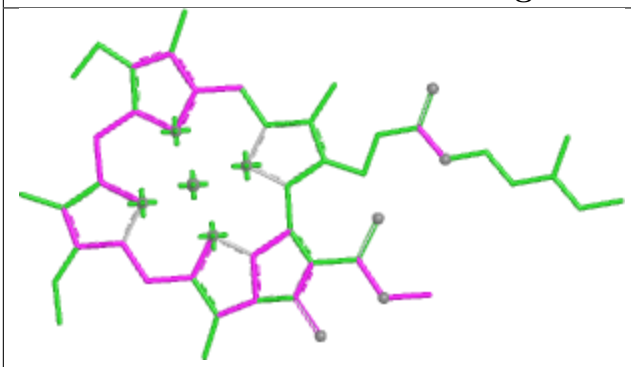


Torsions



Rings

Ligand CLA aA 837



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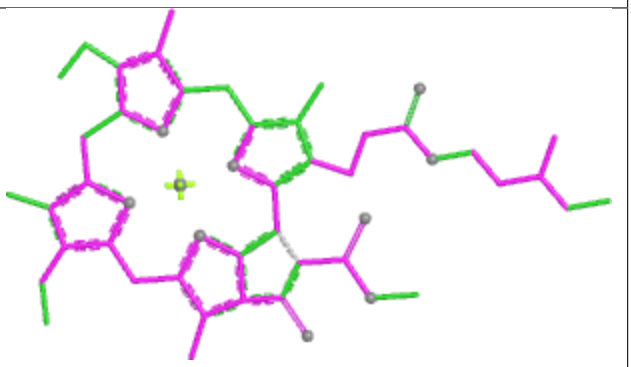
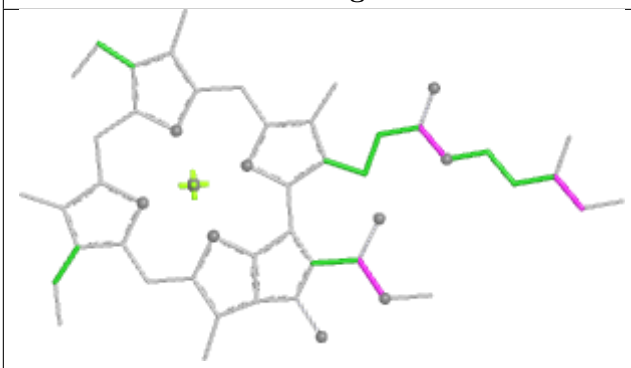
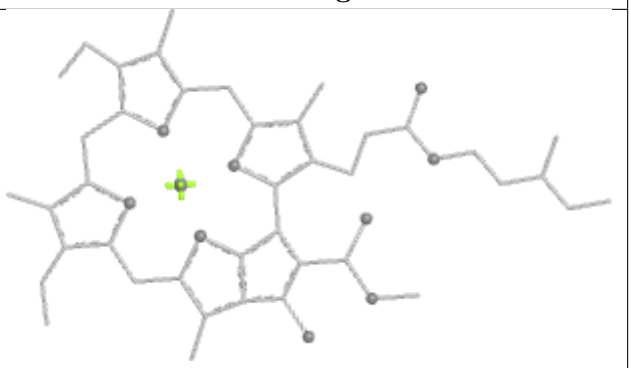


Bond angles

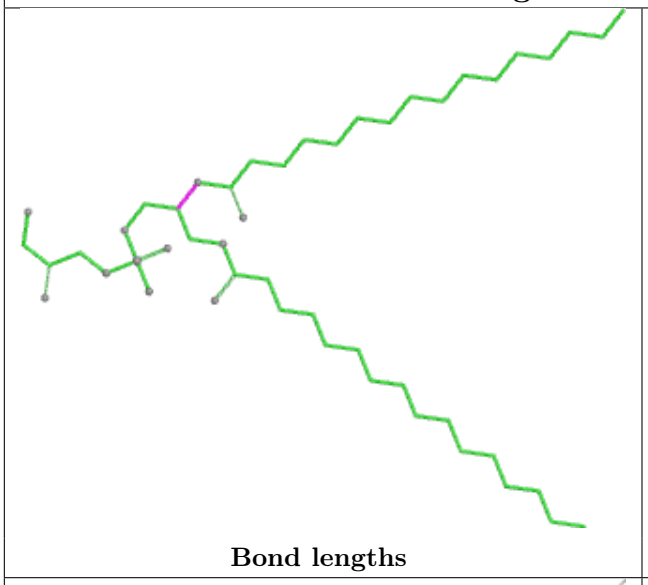


Torsions

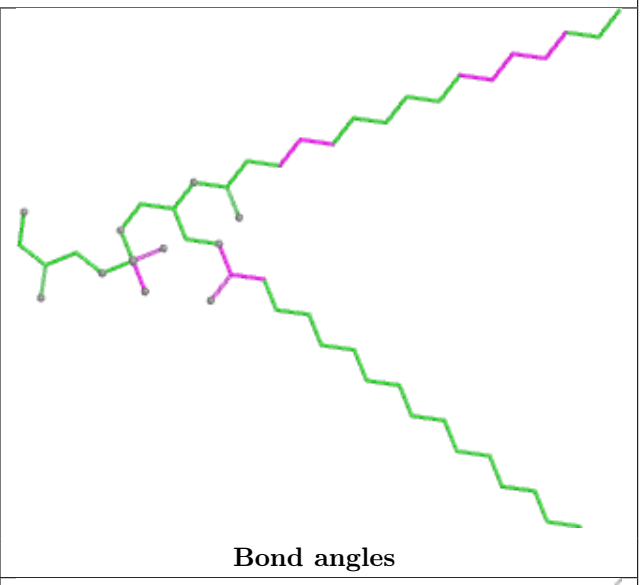


Rings

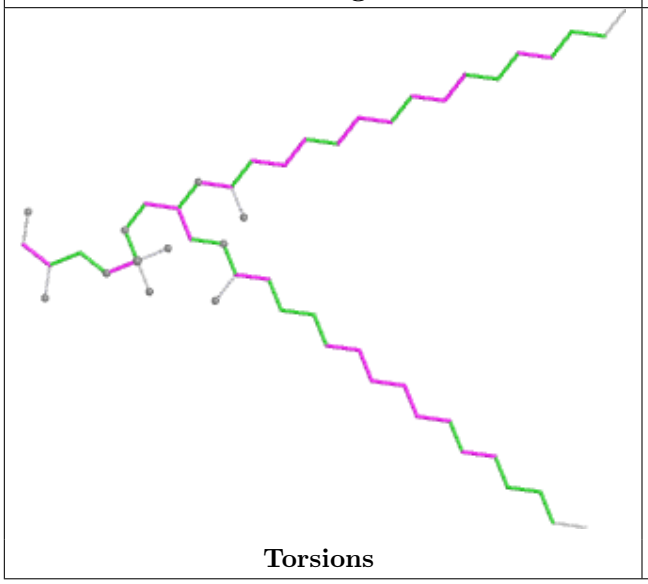
Ligand LHG bA 851



Bond lengths



Bond angles



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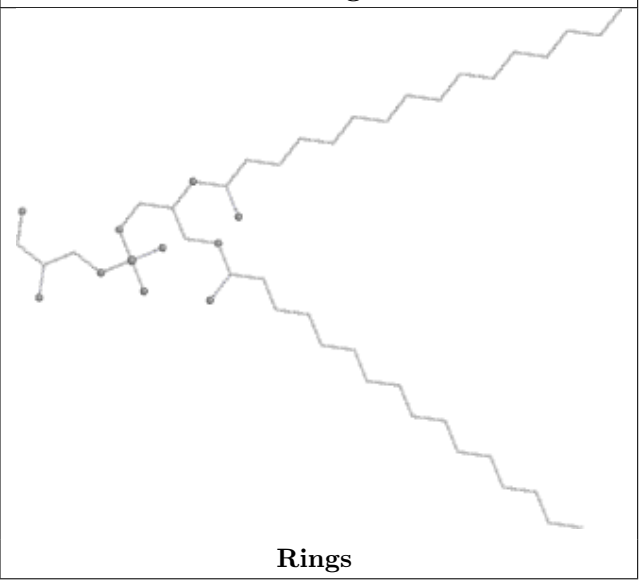
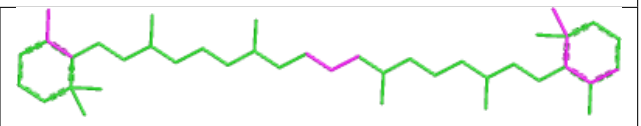


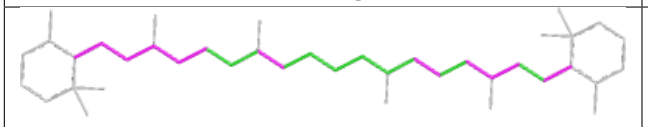
Rings

Ligand BCR cB 944

Bond lengths



Bond angles



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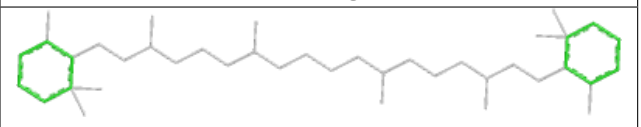
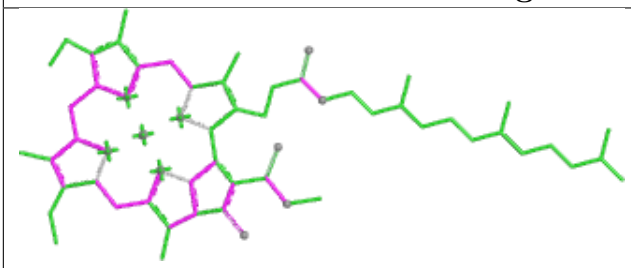


Rings

Ligand CLA cA 819



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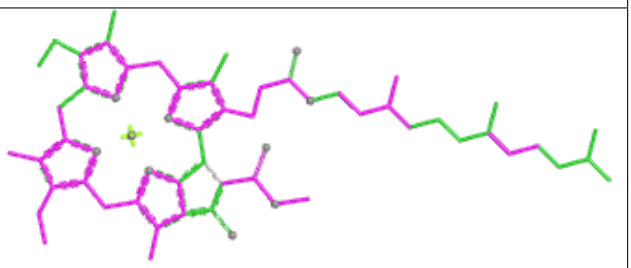
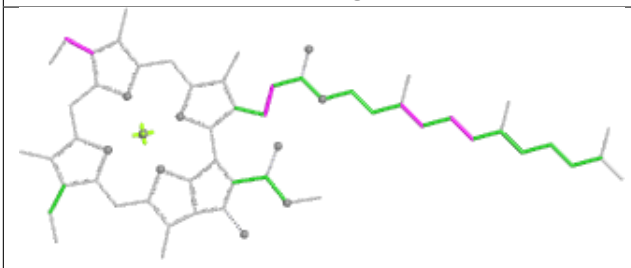
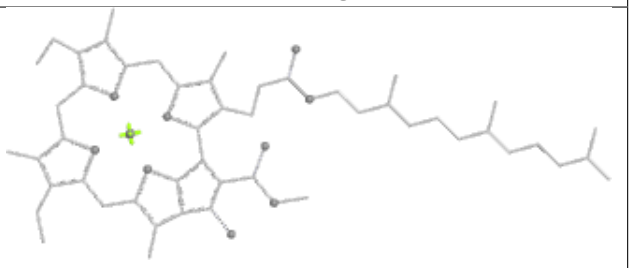


Bond angles

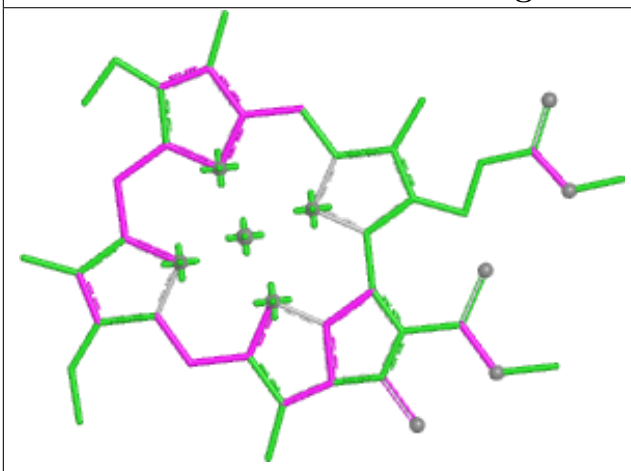


Torsions



Rings

Ligand CLA aA 827



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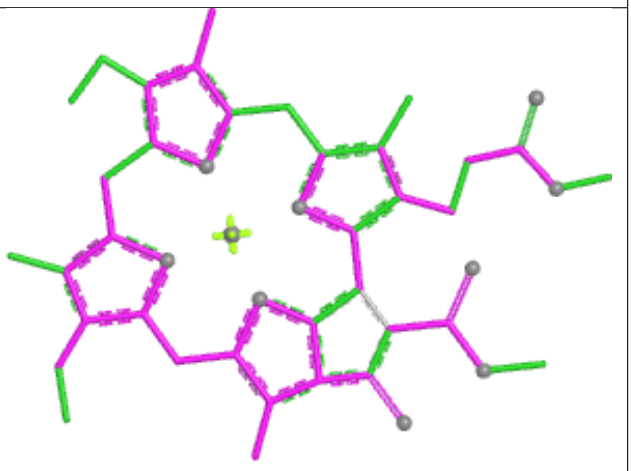
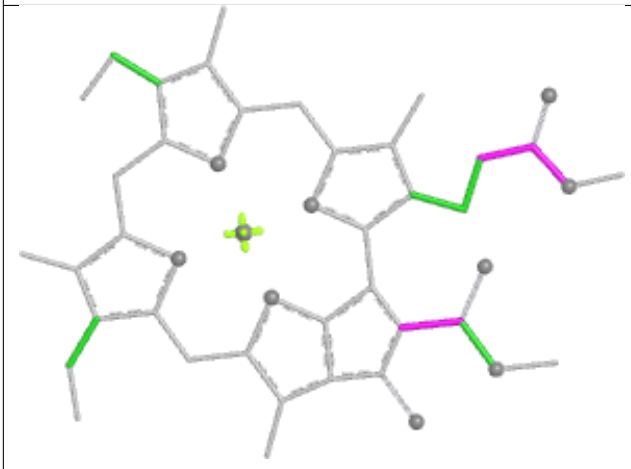
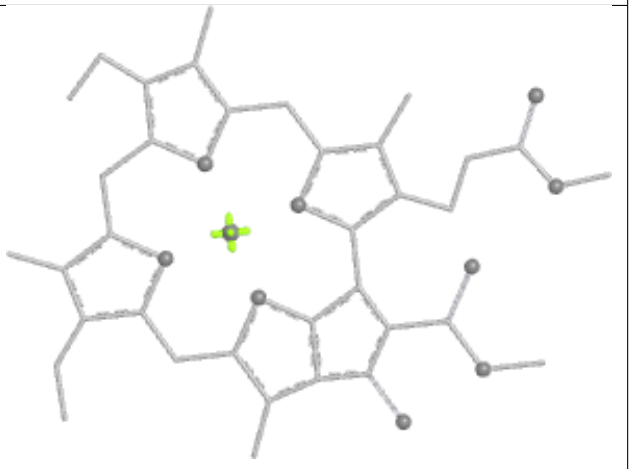


Bond angles

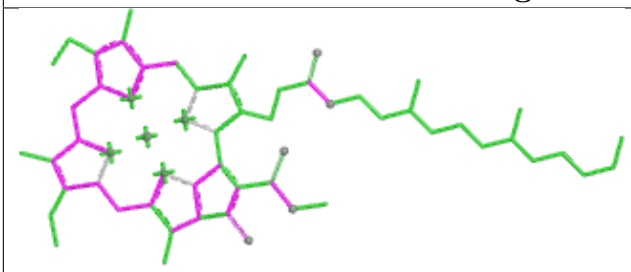


Torsions

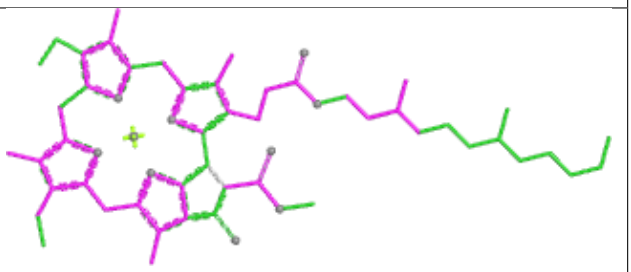


Rings

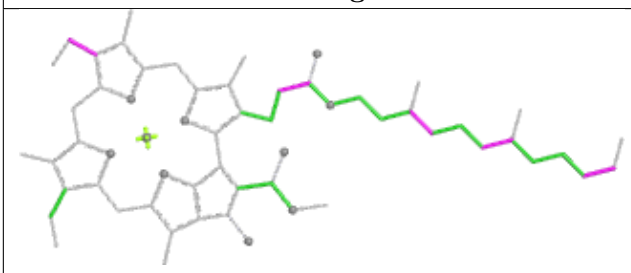
Ligand CLA bB 936



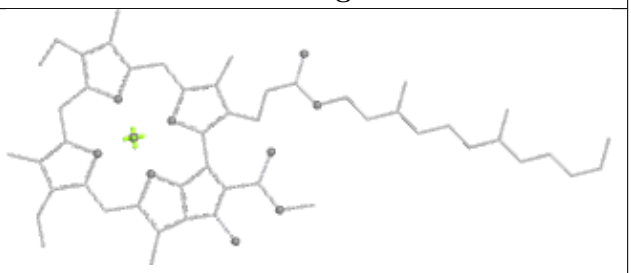
Bond lengths



Bond angles

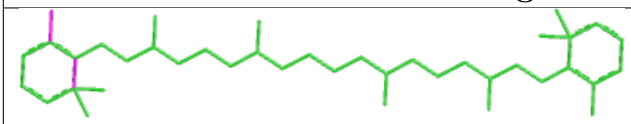


Torsions

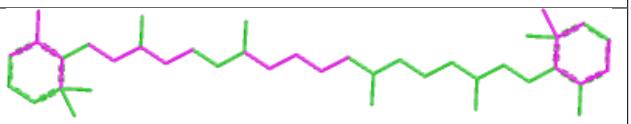


Rings

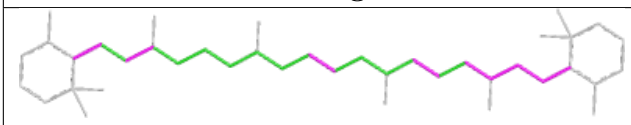
Ligand BCR bJ 101



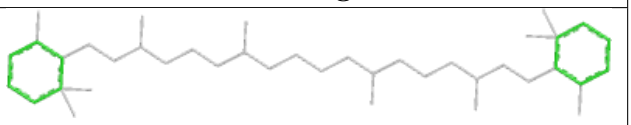
Bond lengths



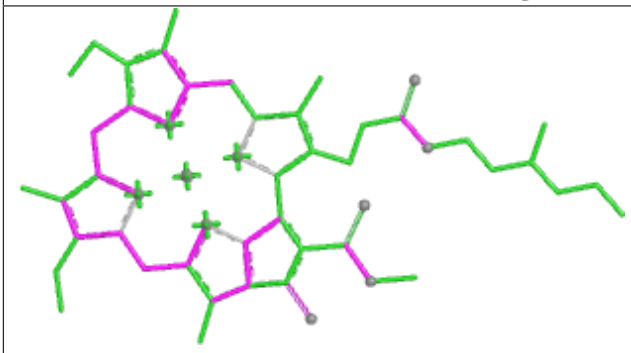
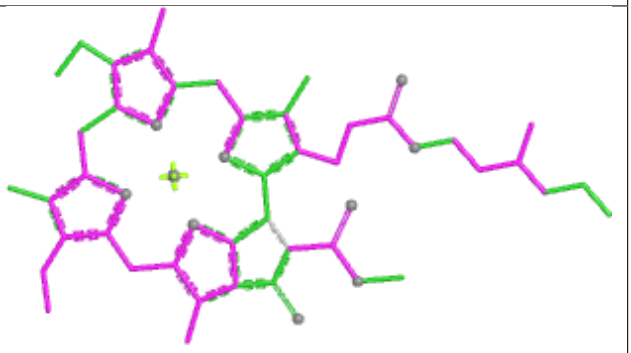
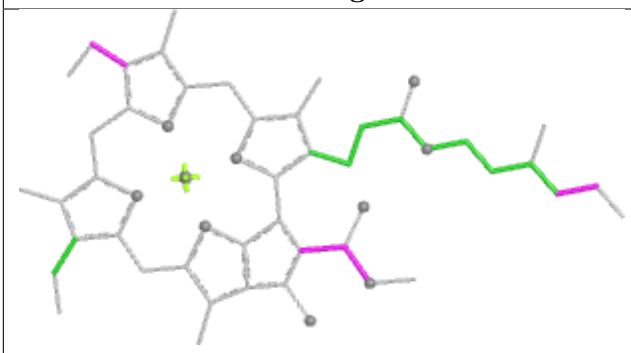
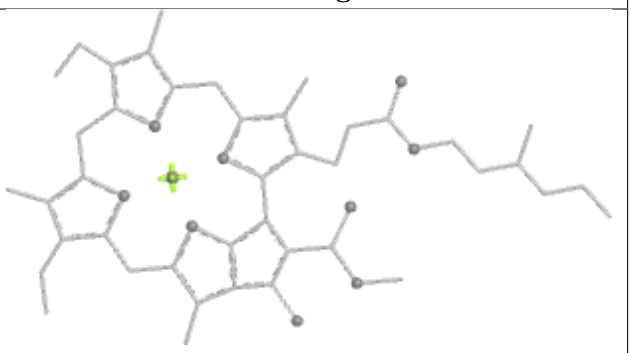
Bond angles

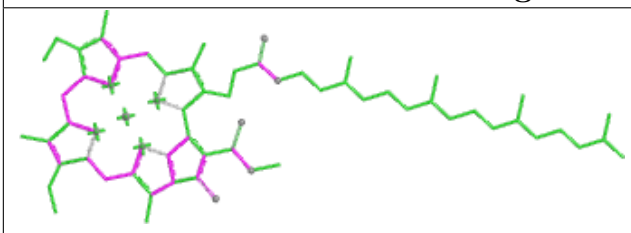
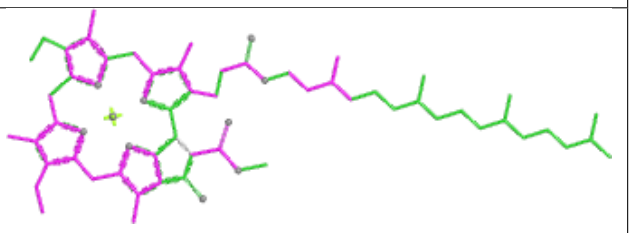
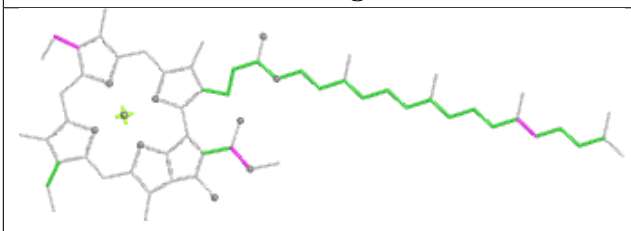
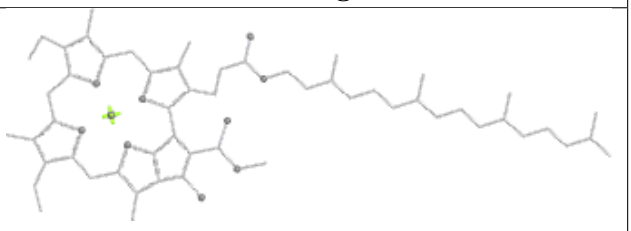


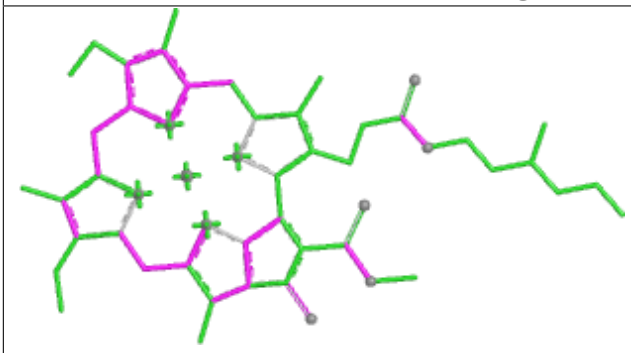
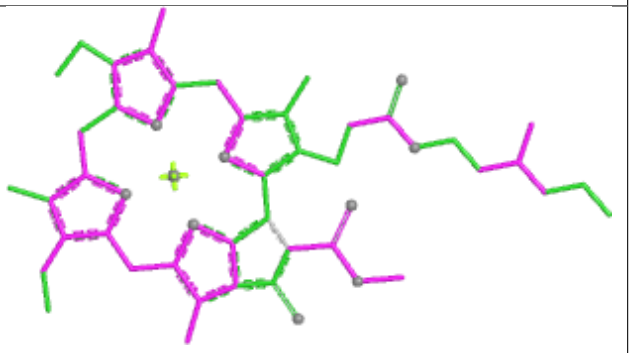
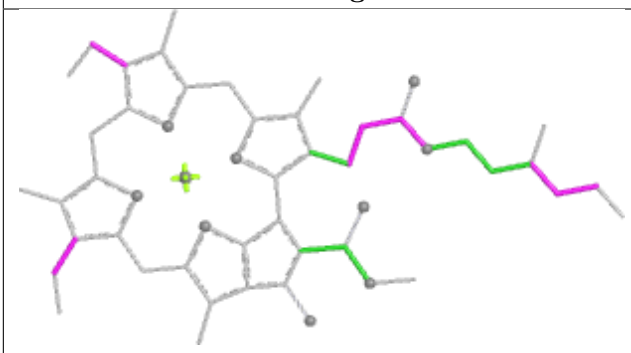
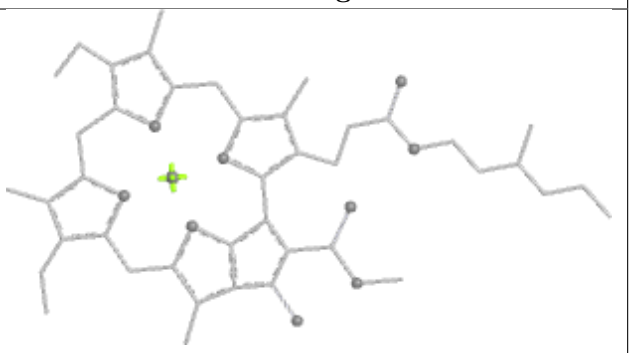
Torsions

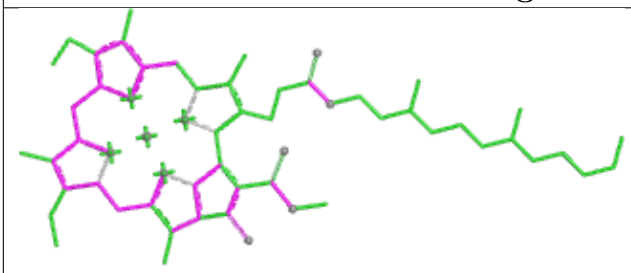
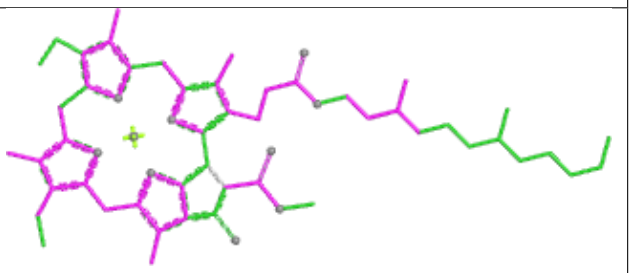
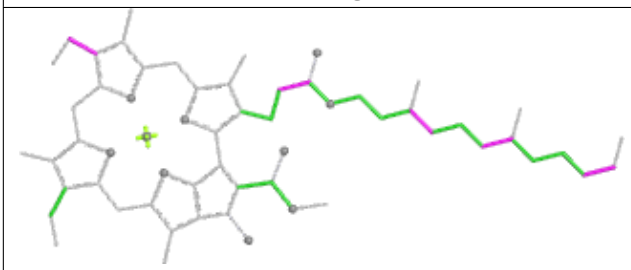
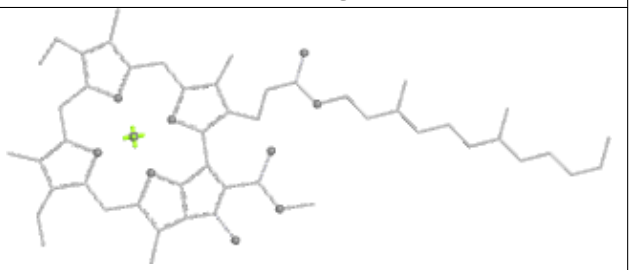


Rings

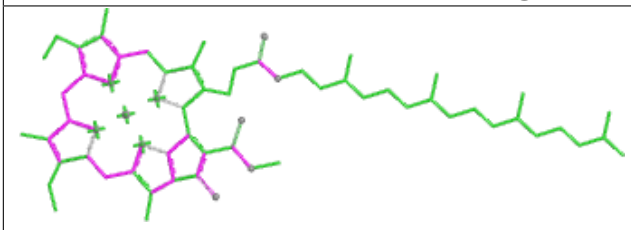
Ligand CLA cB 907	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA bB 901	
	
Bond lengths	Bond angles
	
Torsions	Rings

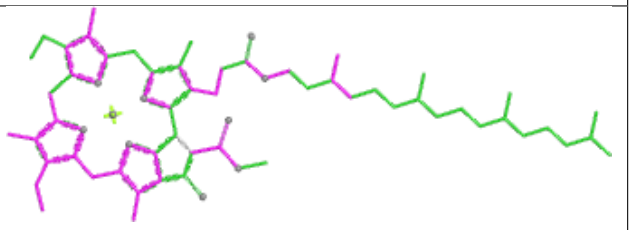
Ligand CLA bB 915	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA cB 936	
	
Bond lengths	Bond angles
	
Torsions	Rings

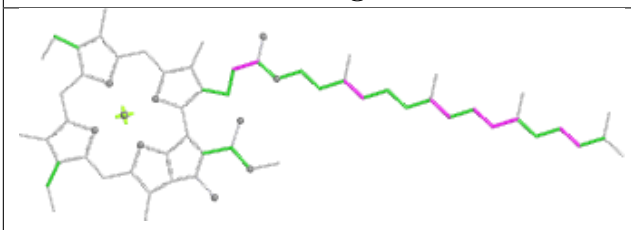
Ligand CLA cA 838



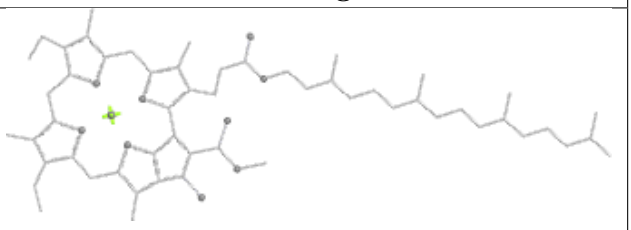
Bond lengths



Bond angles

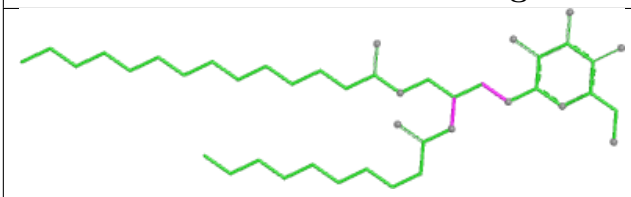


Torsions



Rings

Ligand LMG bB 947



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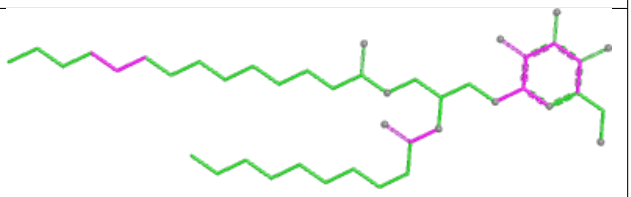
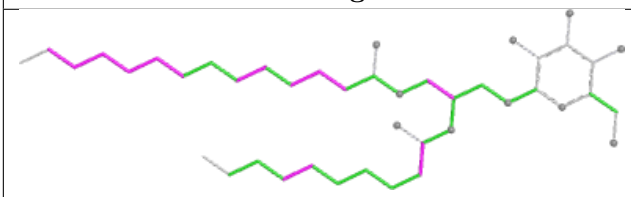
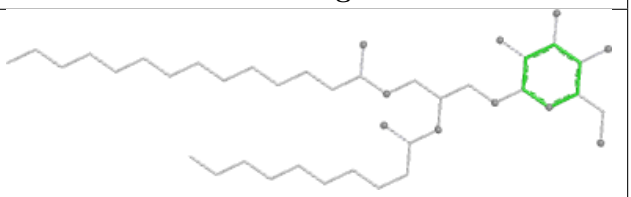


Bond angles

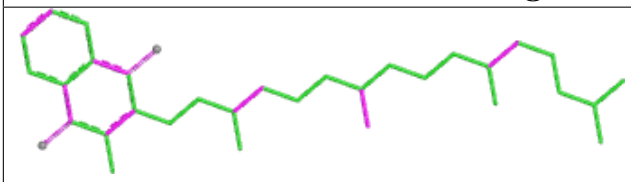


Torsions

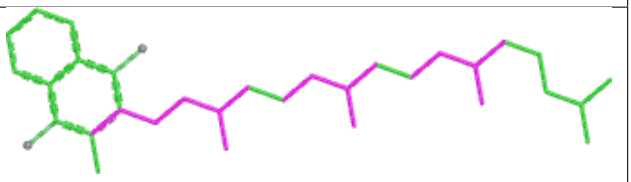


Rings

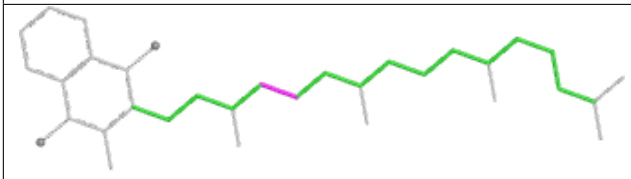
Ligand 1L3 aB 940



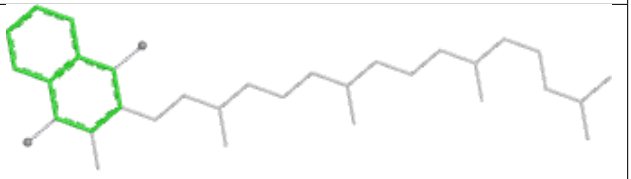
Bond lengths



Bond angles

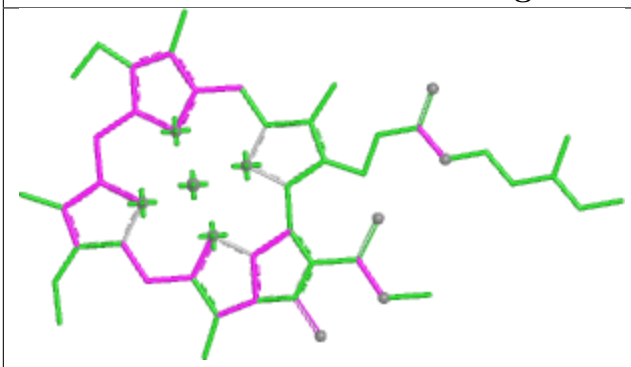


Torsions



Rings

Ligand CLA bB 903



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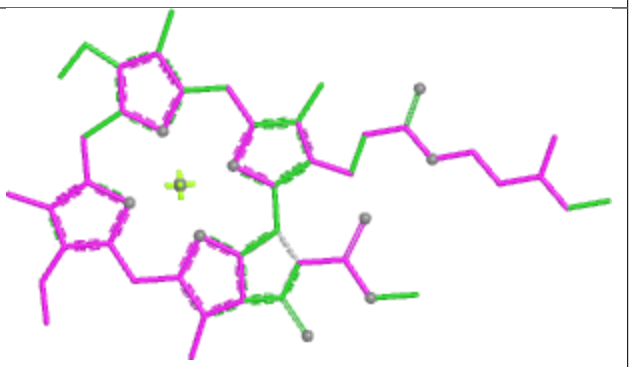
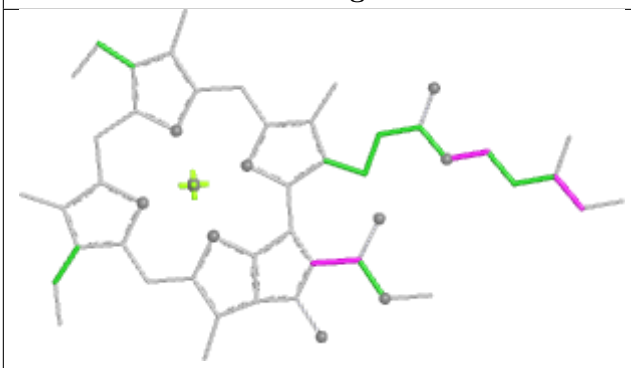
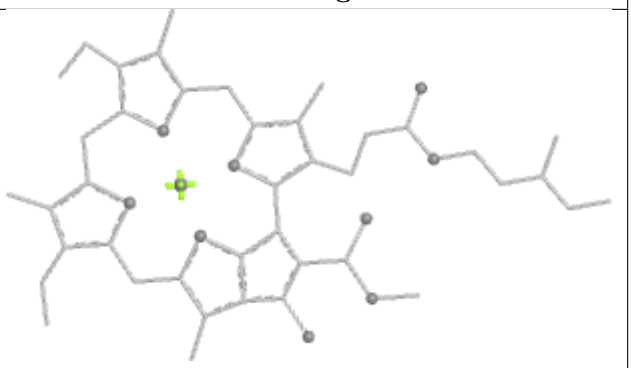


Bond angles

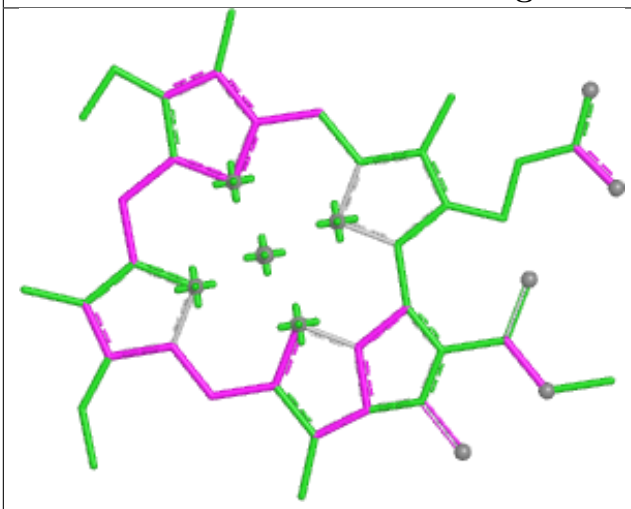


Torsions



Rings

Ligand CLA cA 815



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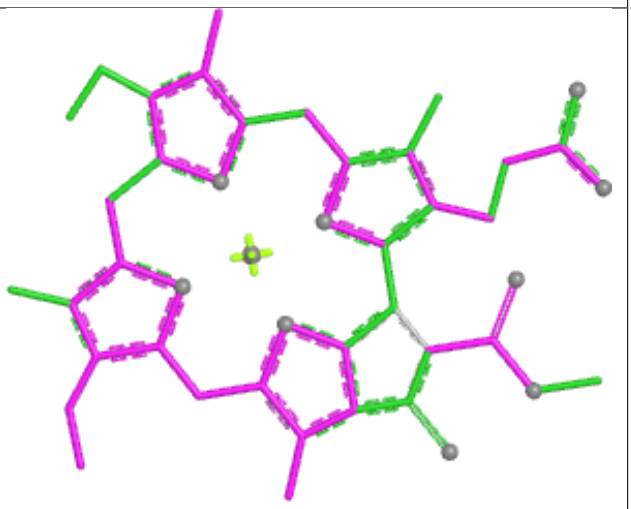
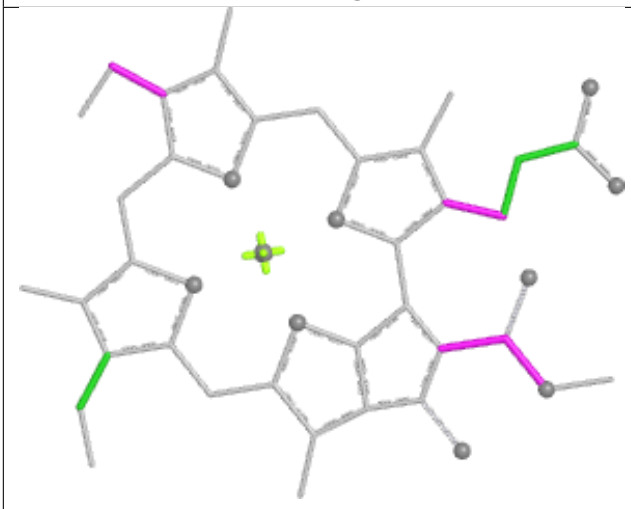


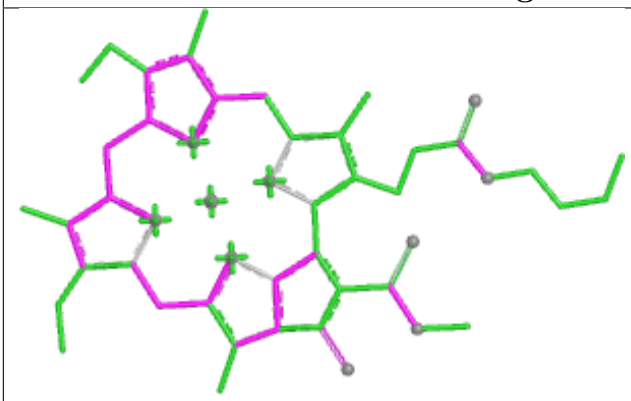
Bond angles



Torsions

Rings

Ligand CLA cB 930



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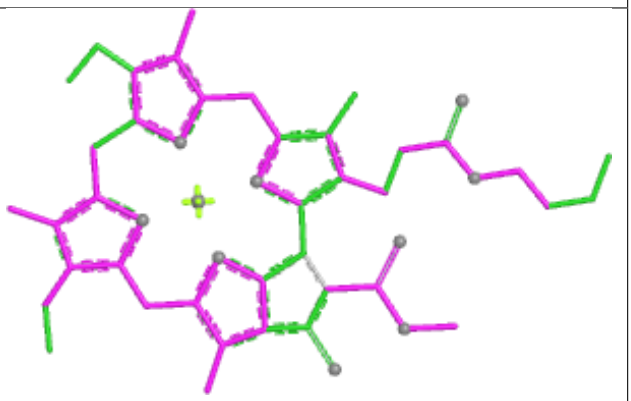
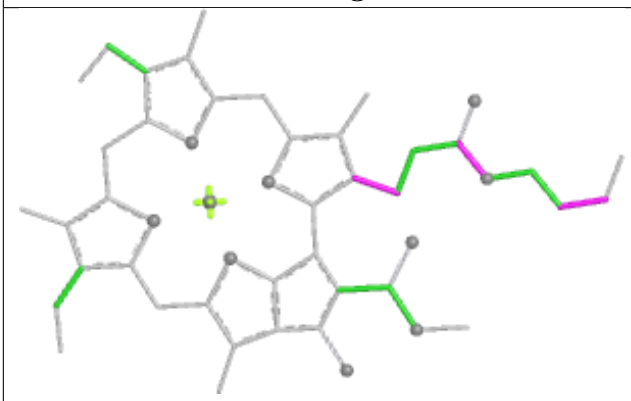
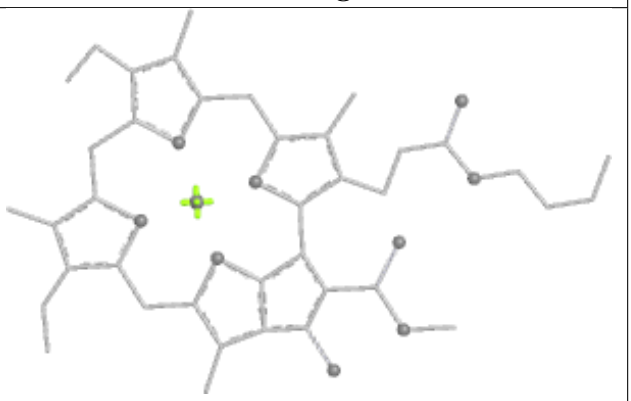


Bond angles

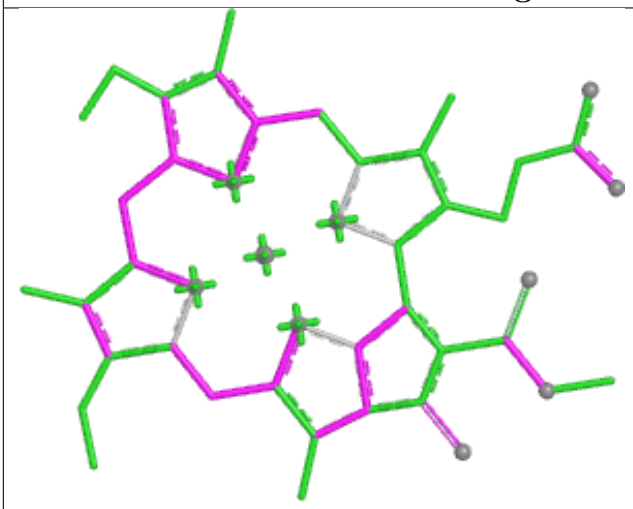


Torsions



Rings

Ligand CLA bB 939



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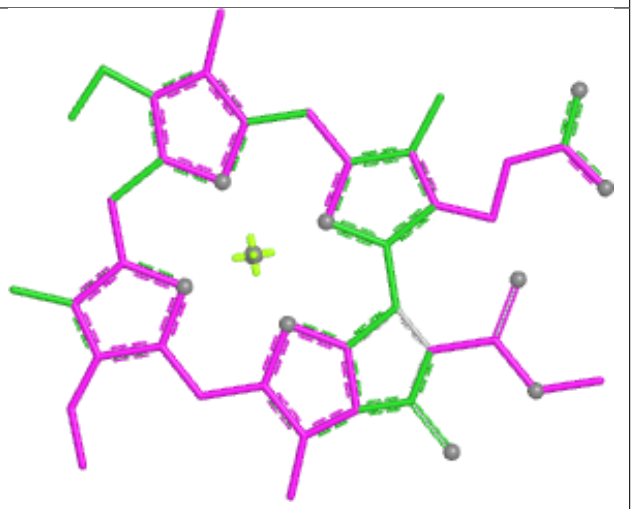
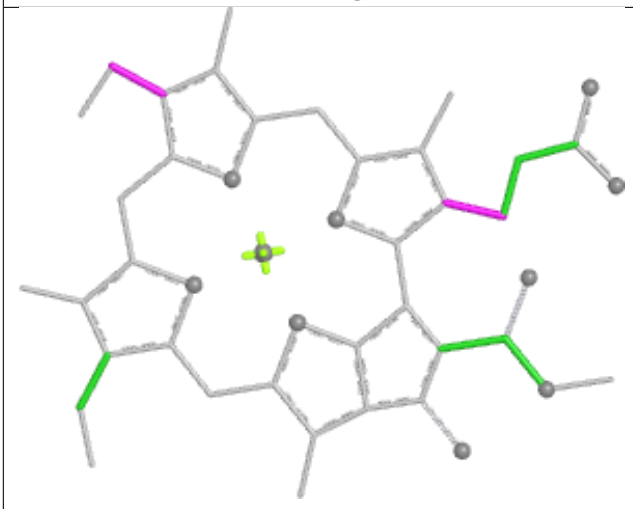


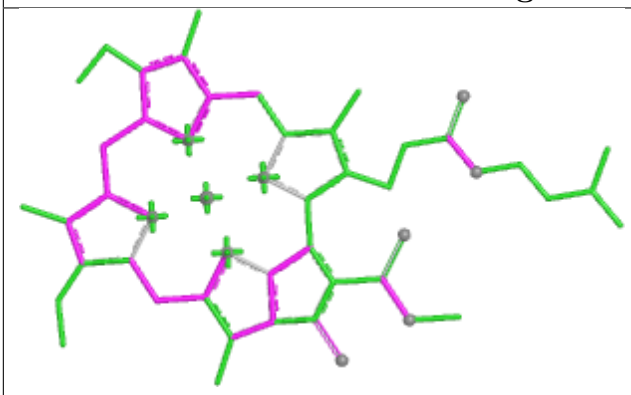
Bond angles



Torsions

Rings

Ligand CLA cB 935



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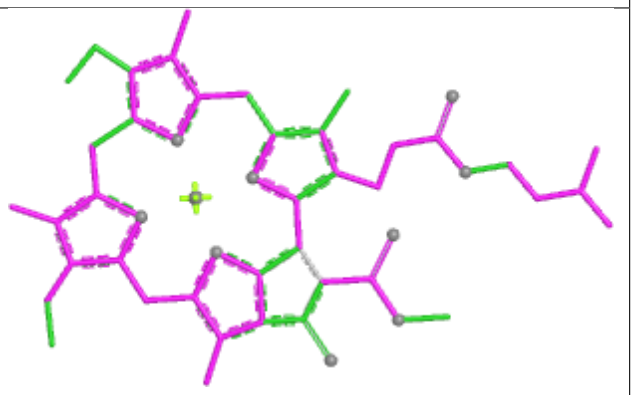
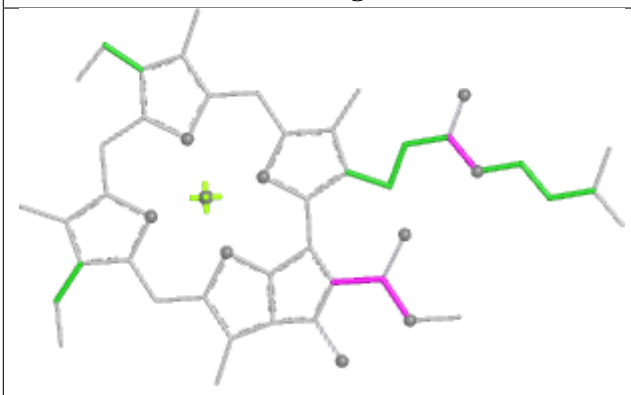
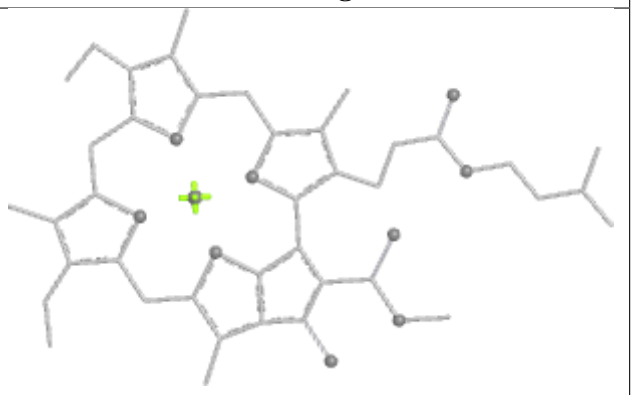


Bond angles

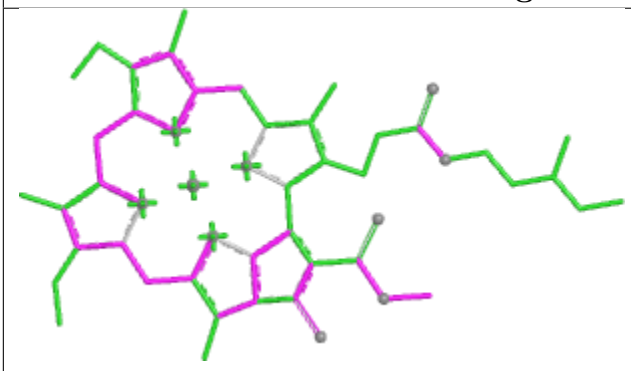


Torsions



Rings

Ligand CLA cA 837



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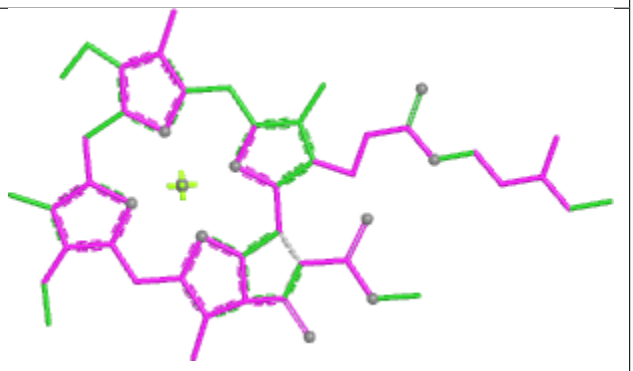
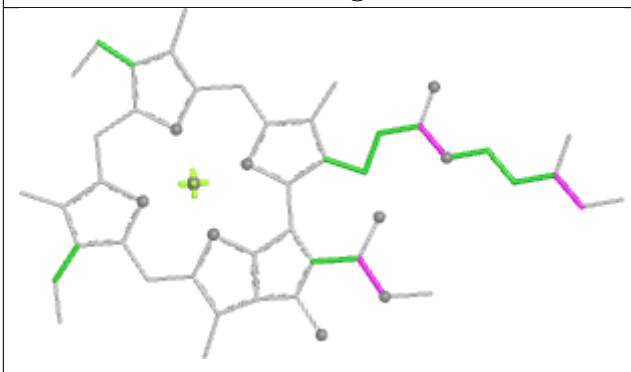
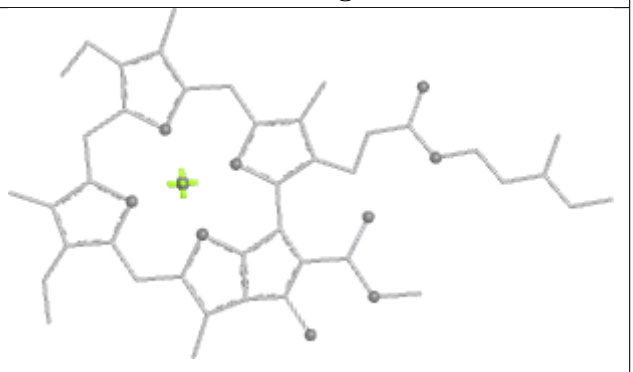


Bond angles

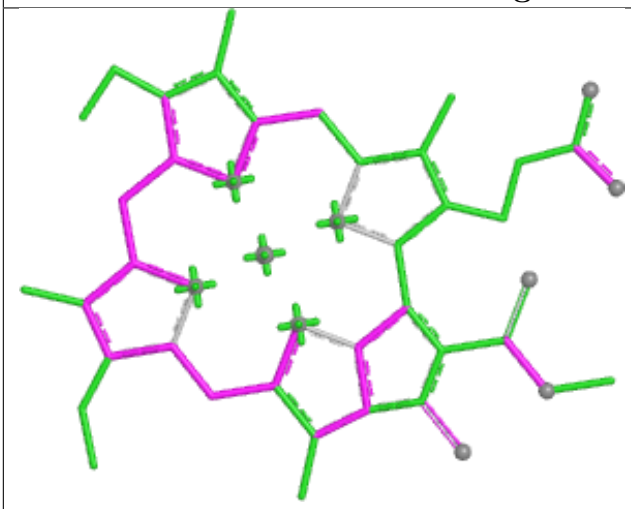


Torsions

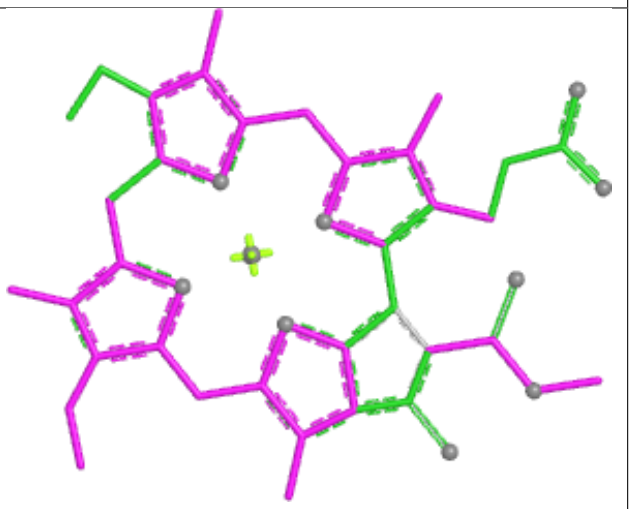


Rings

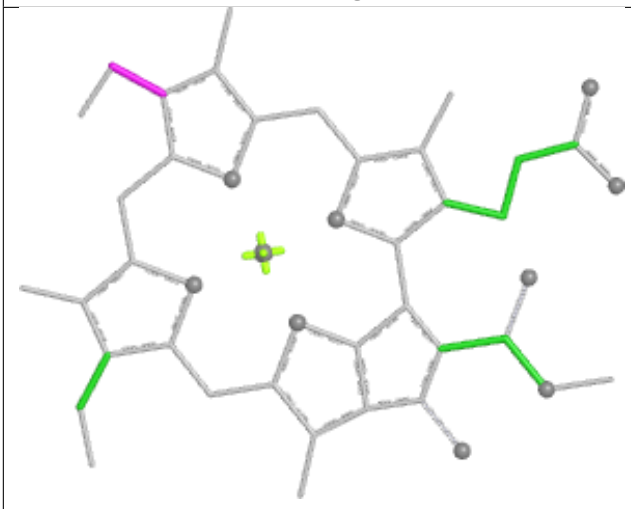
Ligand CLA bA 835



Bond lengths



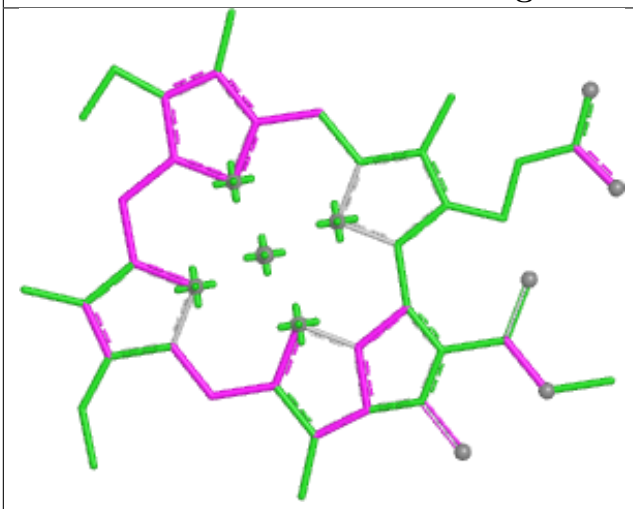
Bond angles



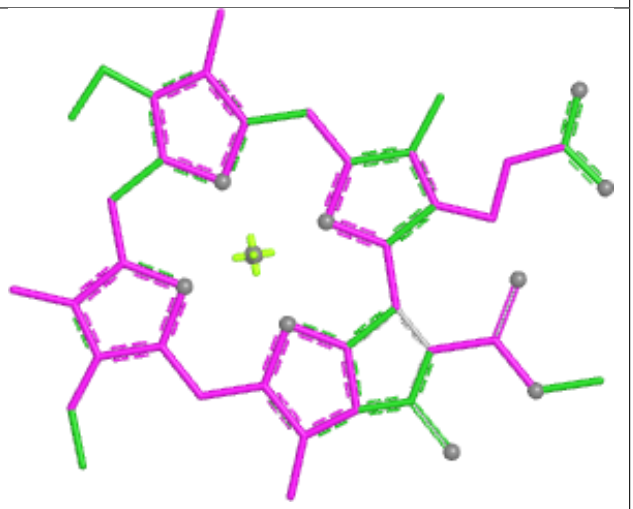
Torsions

Rings

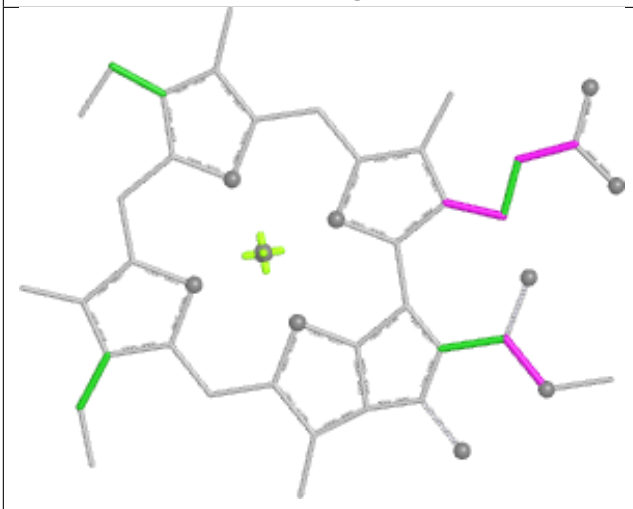
Ligand CLA cA 839



Bond lengths



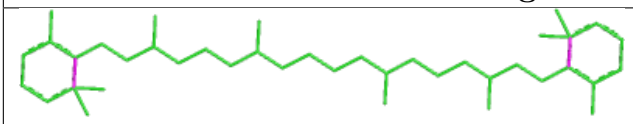
Bond angles



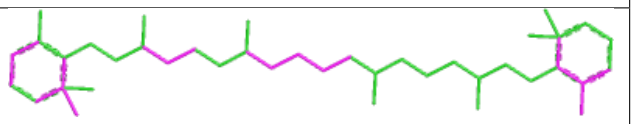
Torsions

Rings

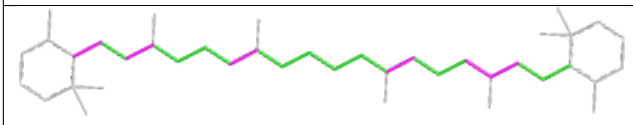
Ligand BCR bI 101



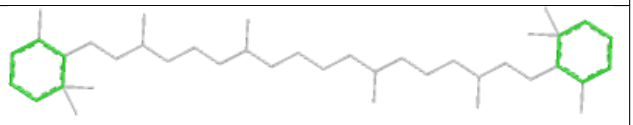
Bond lengths



Bond angles

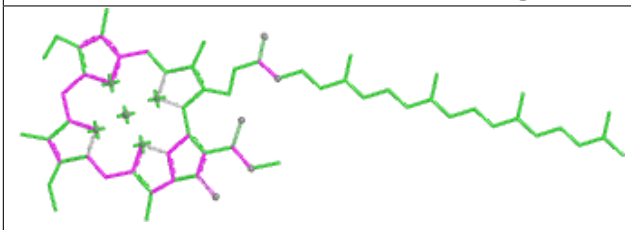


Torsions



Rings

Ligand CLA bB 926



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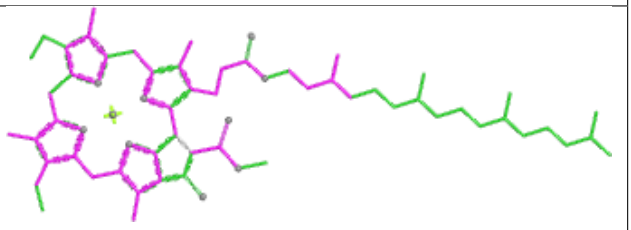
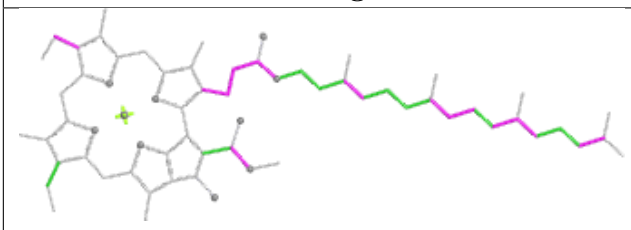
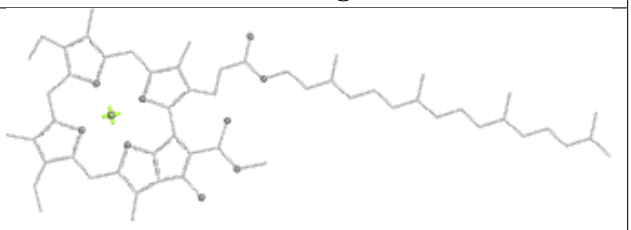


Bond angles

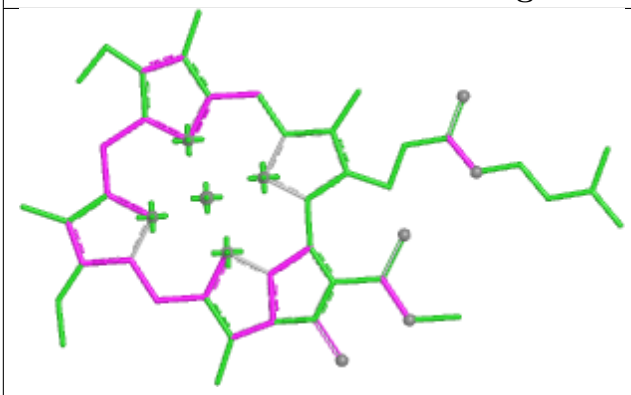


Torsions



Rings

Ligand CLA cB 928



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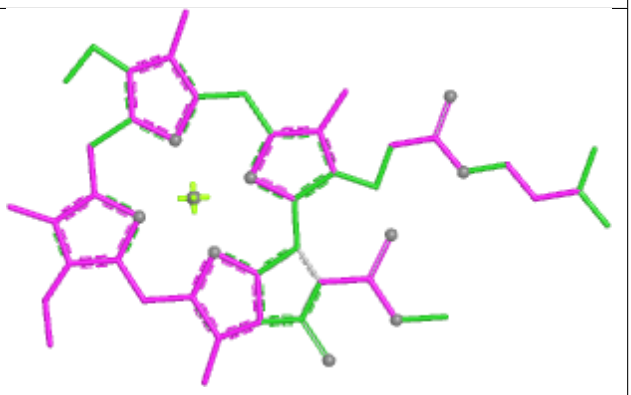
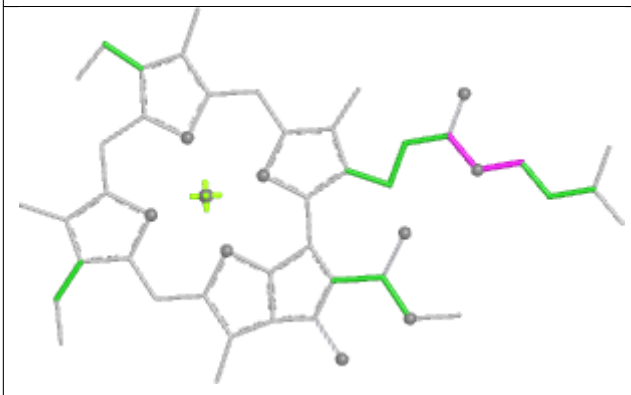


Bond angles



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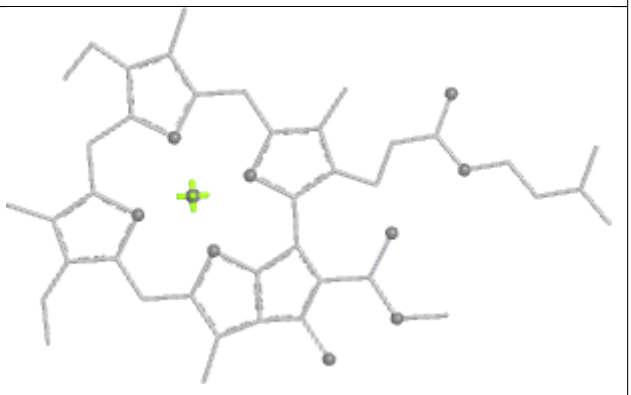
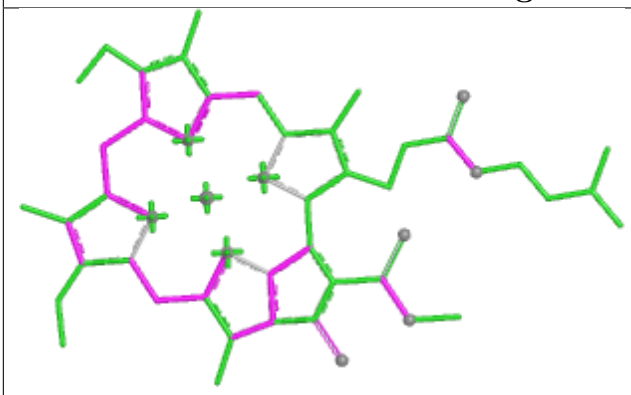


Rings

Ligand CLA cA 821



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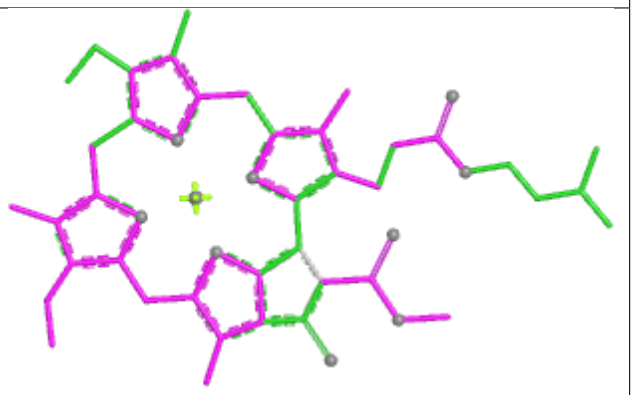
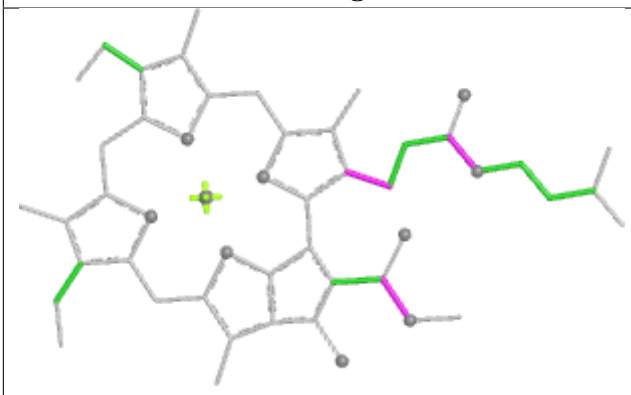


Bond angles



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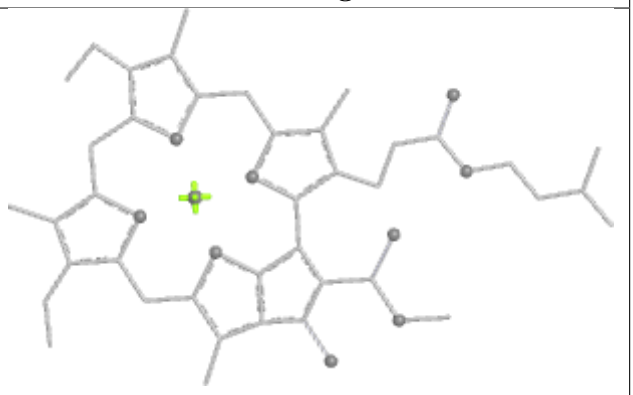
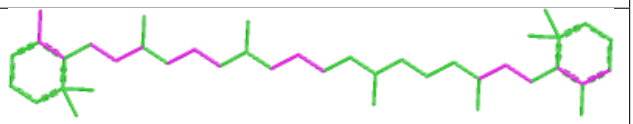


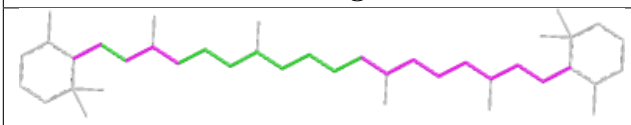
Rings

Ligand BCR aM 101

Bond lengths



Bond angles



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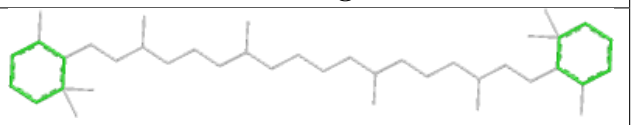
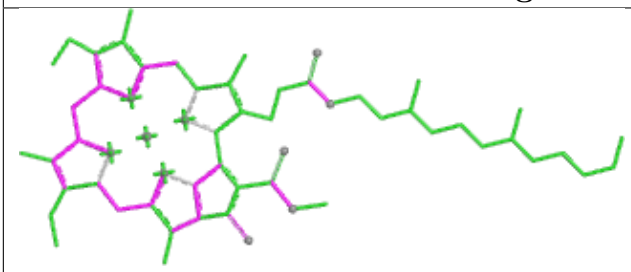


Rings

Ligand CLA aB 916



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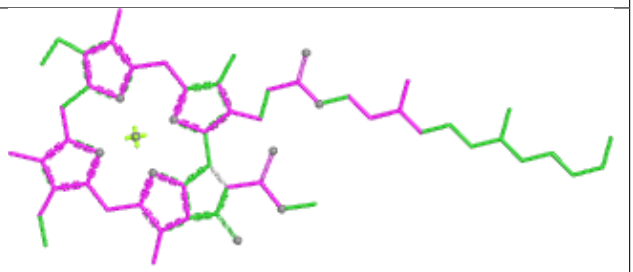
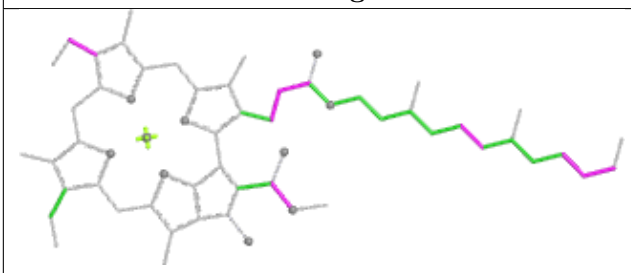


Bond angles



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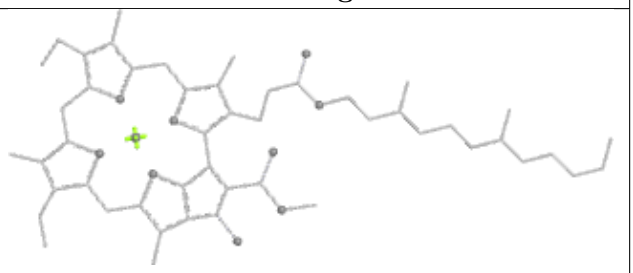
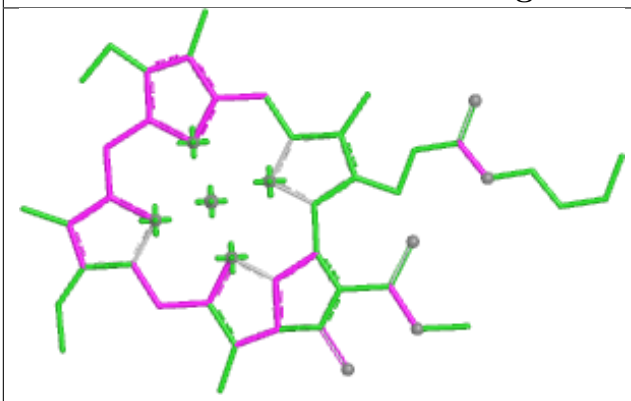


Rings

Ligand CLA cA 822



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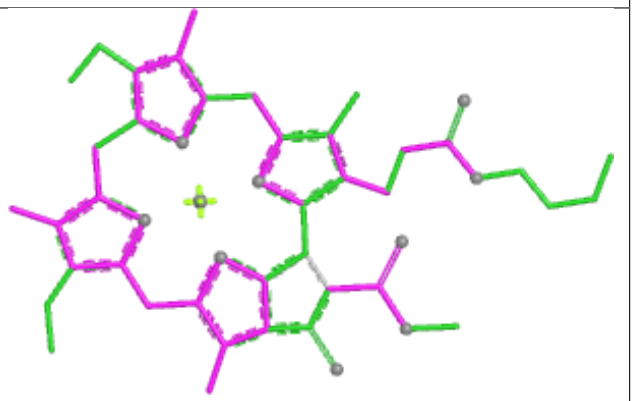
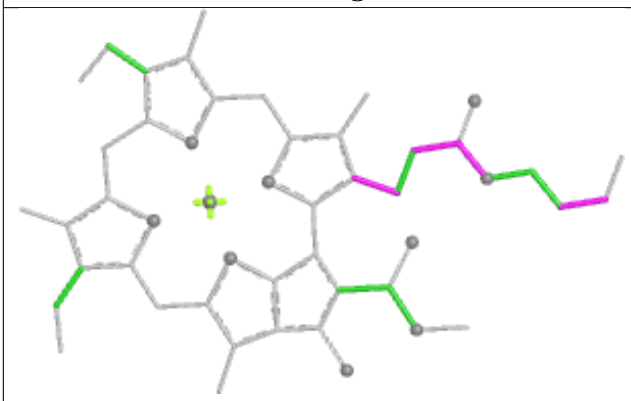


Bond angles



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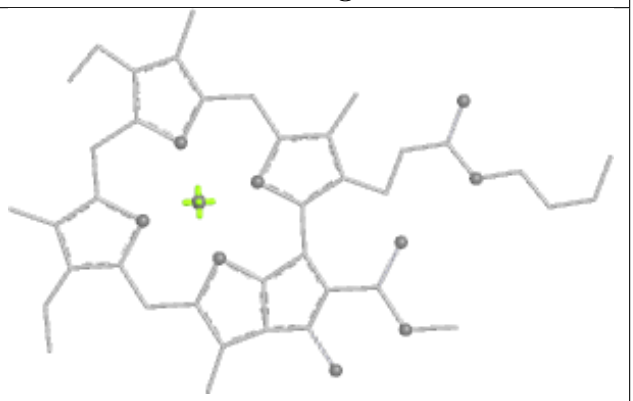
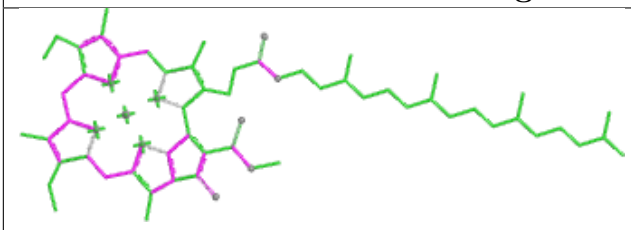


Rings

Ligand CLA aA 828



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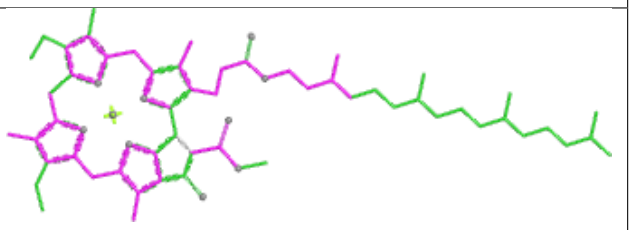
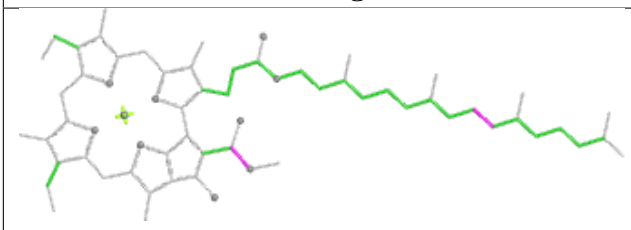
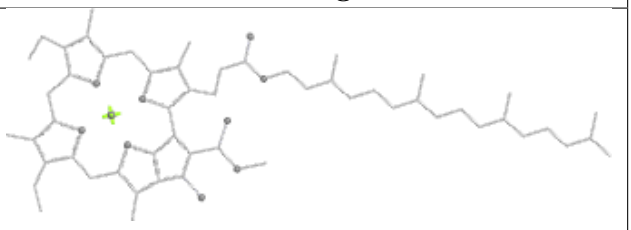


Bond angles

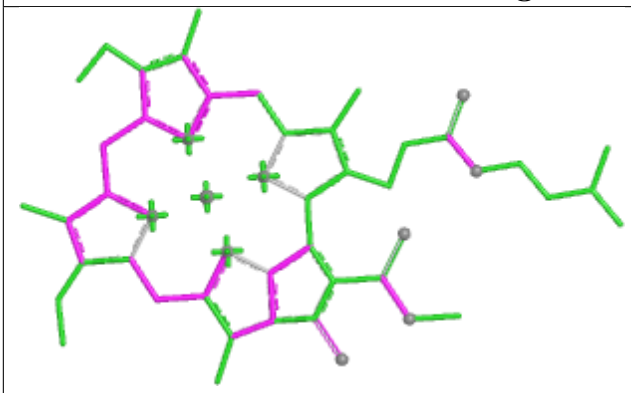


Torsions



Rings

Ligand CLA cA 831



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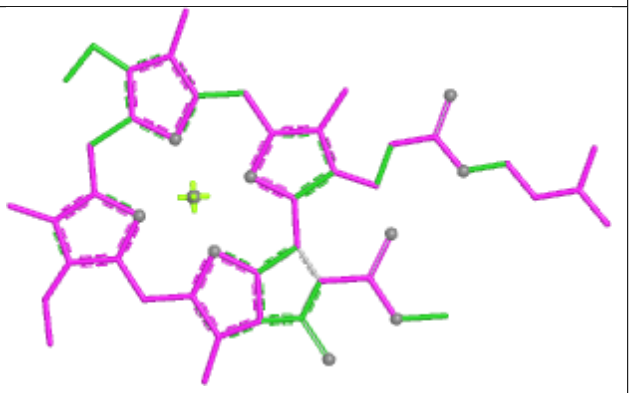
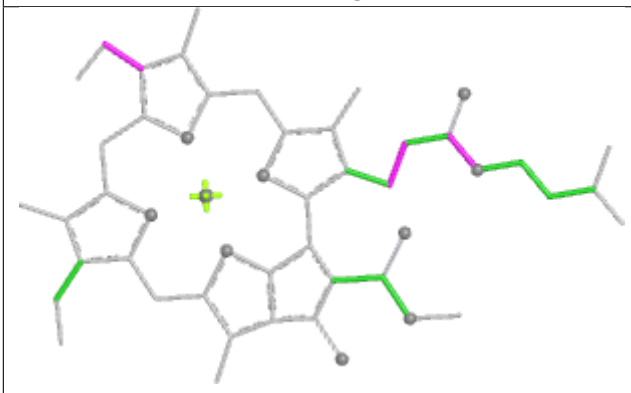
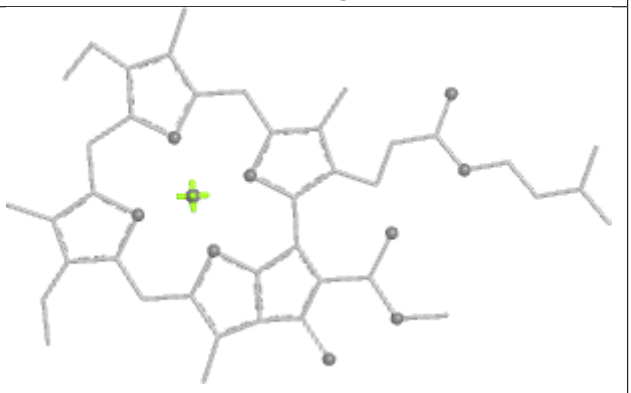


Bond angles

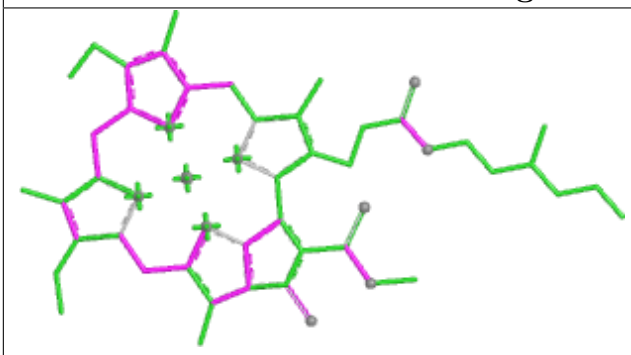


Torsions



Rings

Ligand CLA cB 915



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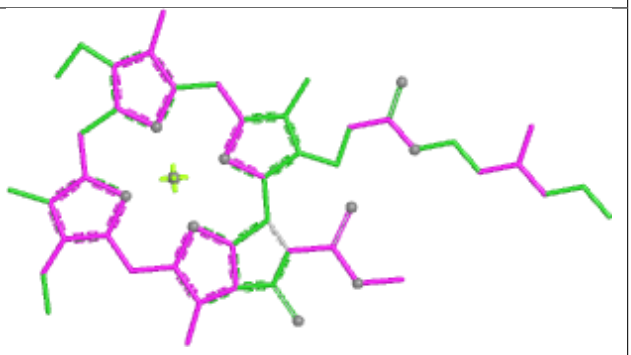
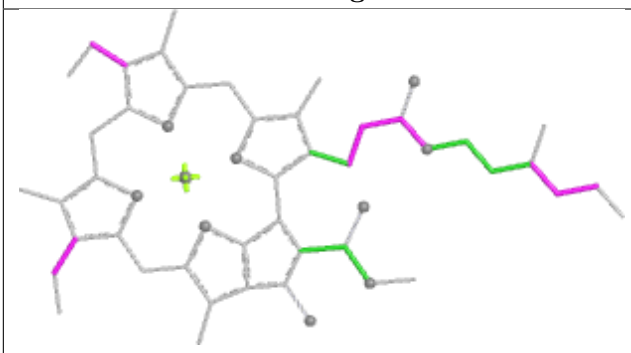
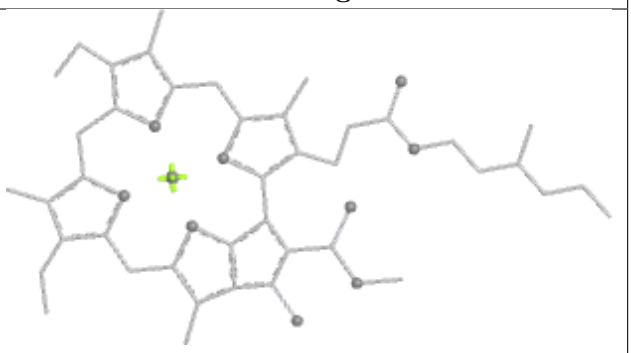


Bond angles

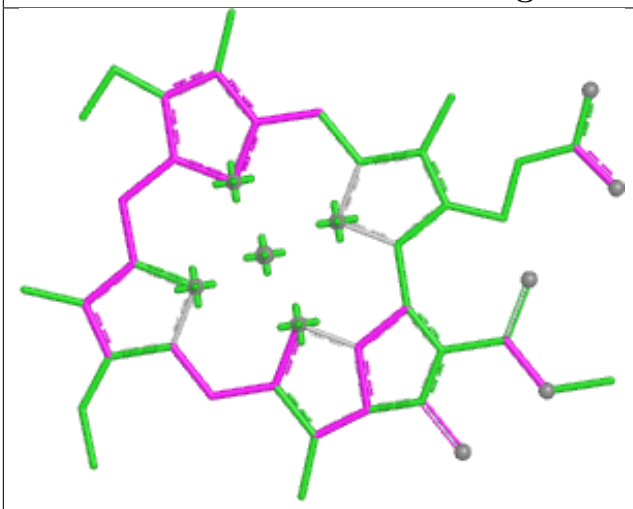


Torsions



Rings

Ligand CLA cB 920



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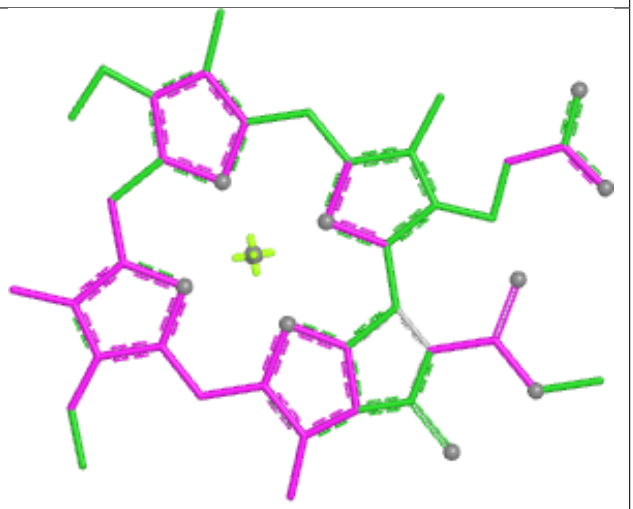
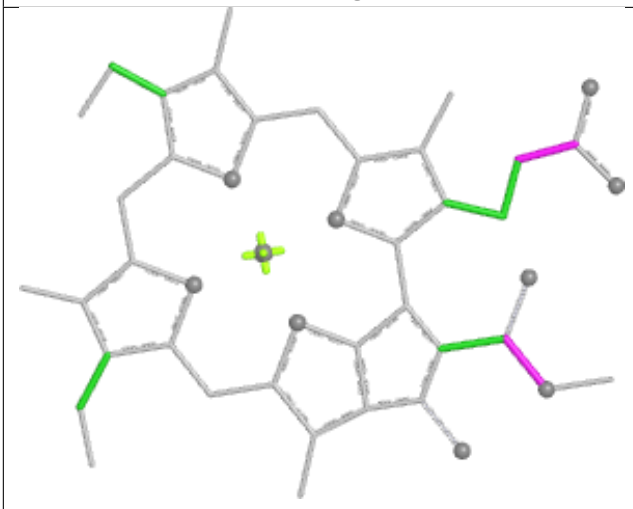


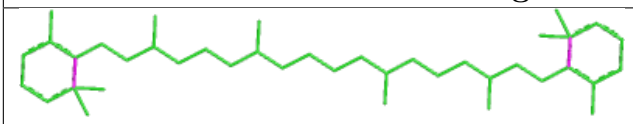
Bond angles



Torsions

Rings

Ligand BCR bA 846



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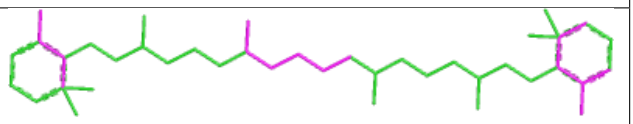
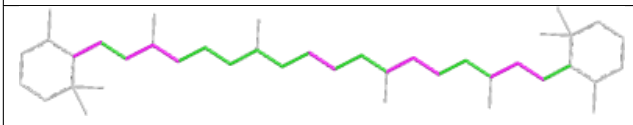
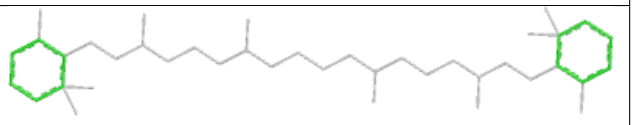


Bond angles

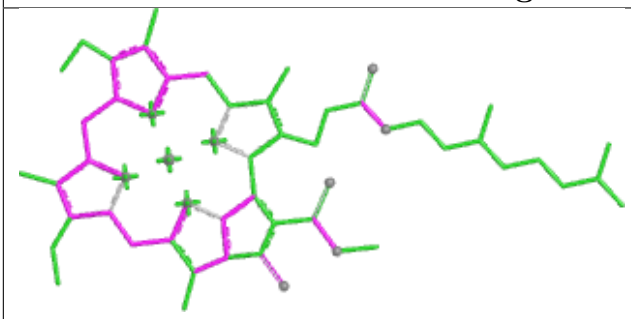


Torsions



Rings

Ligand CLA aB 906



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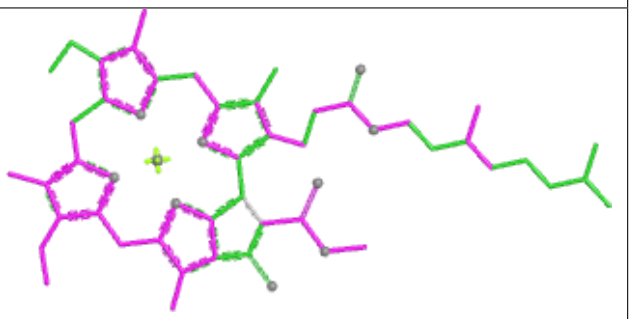
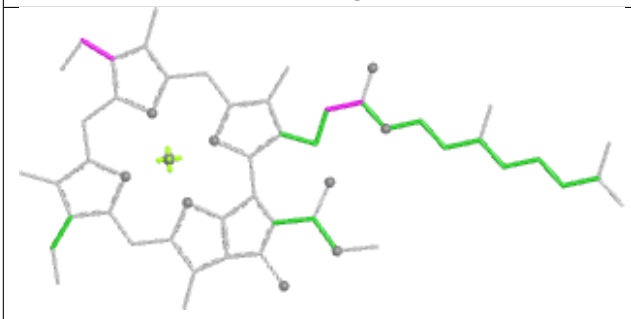
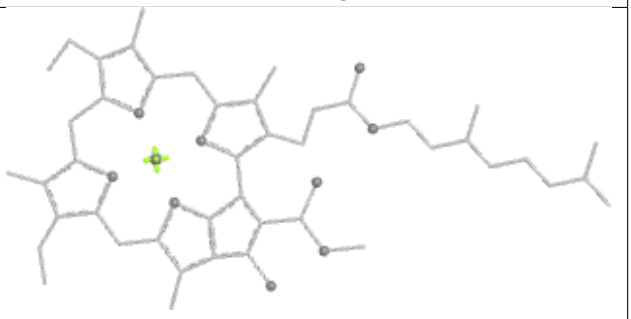


Bond angles

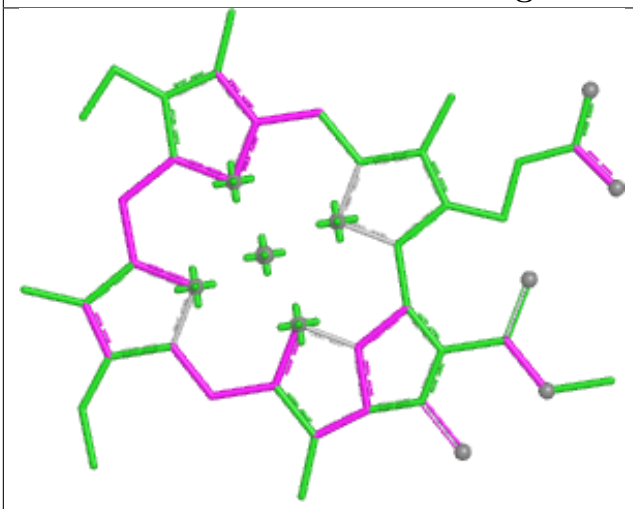


Torsions

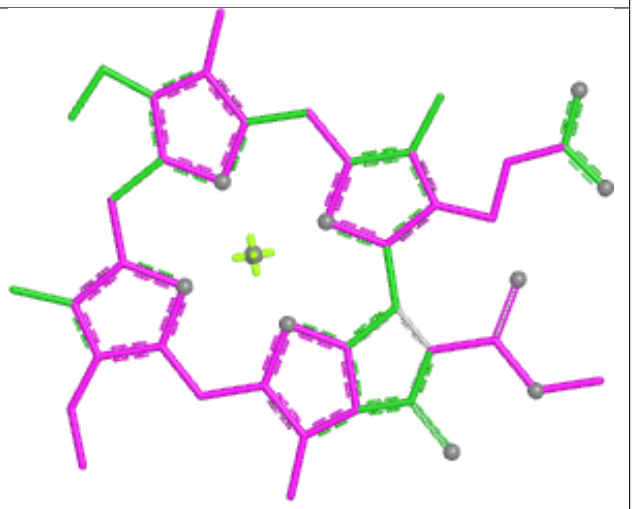


Rings

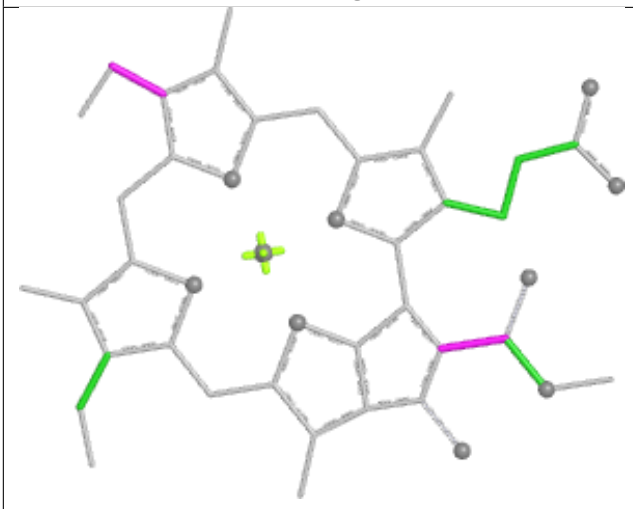
Ligand CLA aB 932



Bond lengths



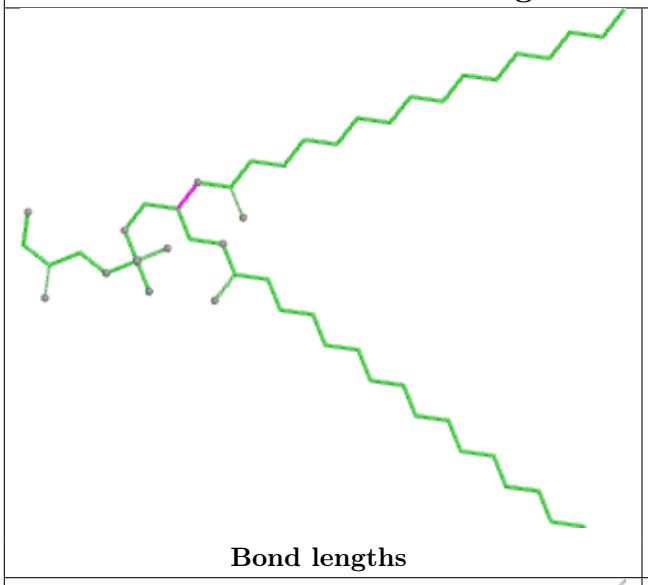
Bond angles



Torsions

Rings

Ligand LHG cA 851



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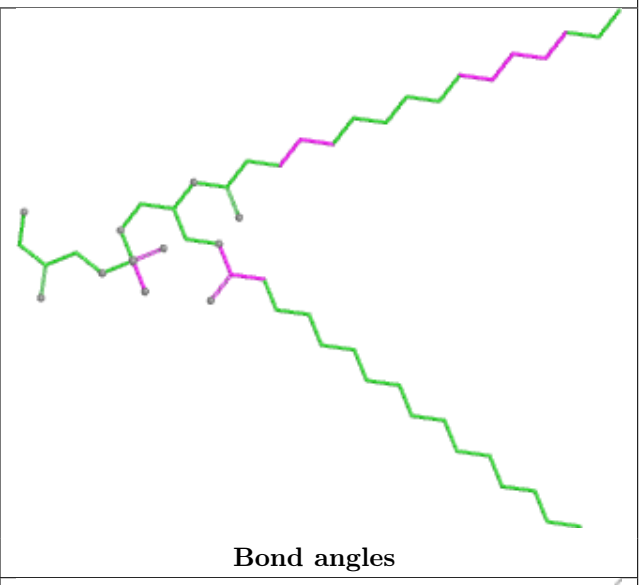
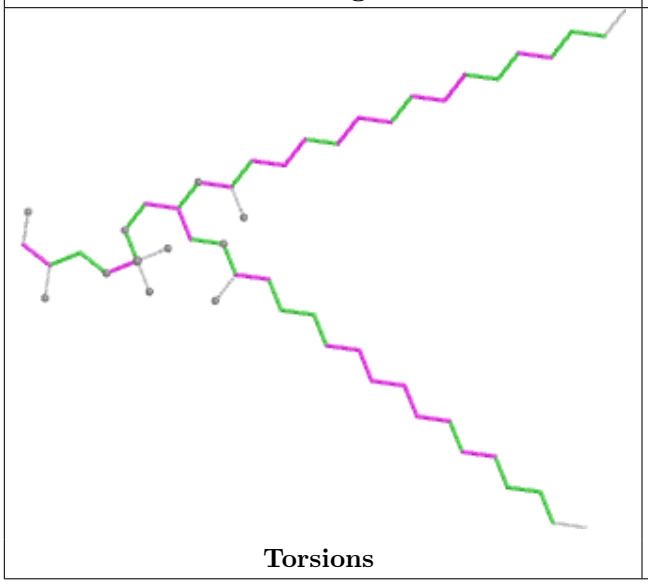
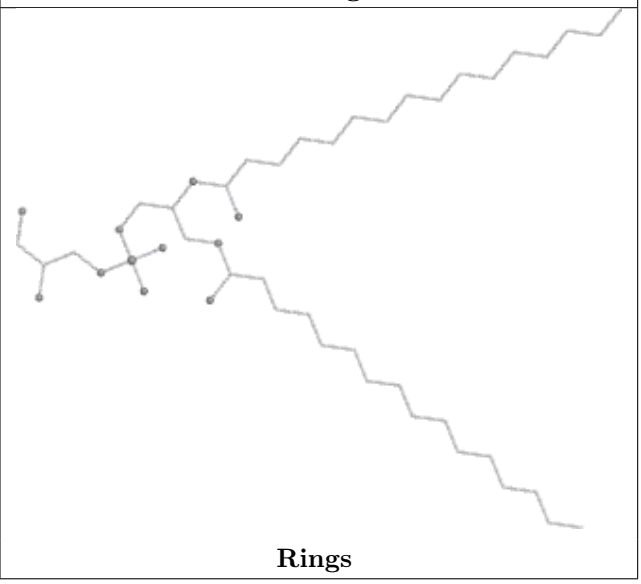


Bond angles

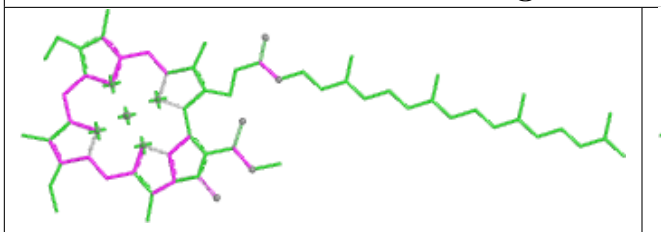


Torsions

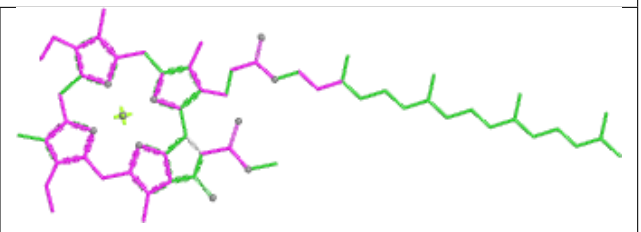


Rings

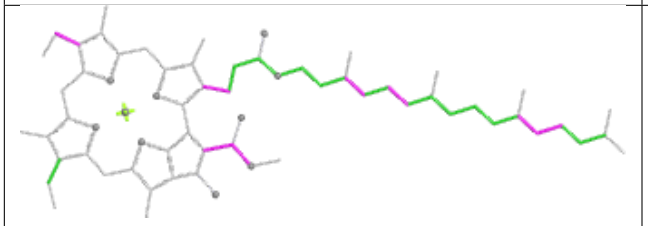
Ligand CLA cA 834



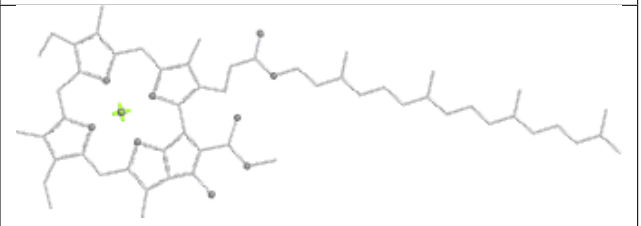
Bond lengths



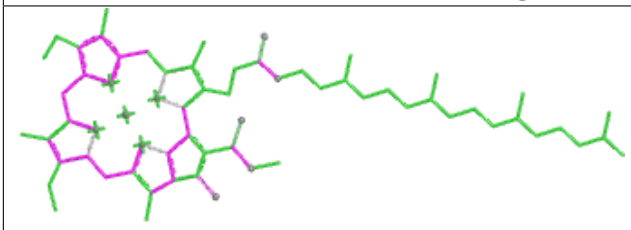
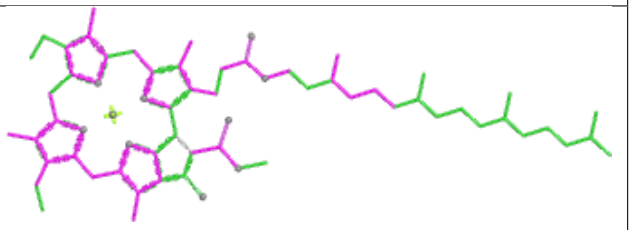
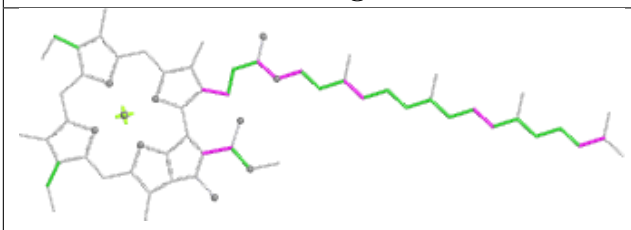
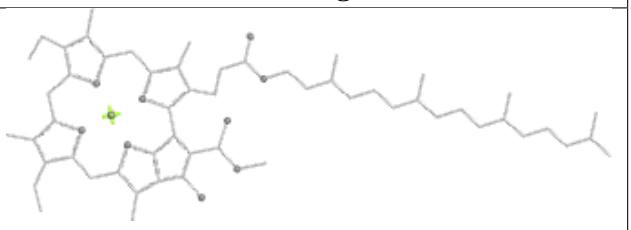
Bond angles

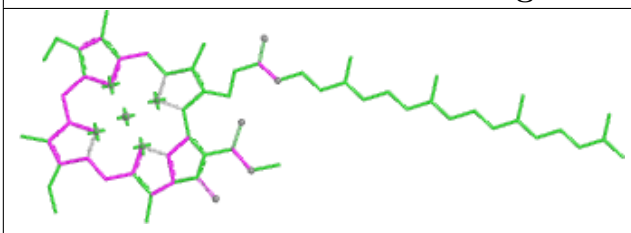
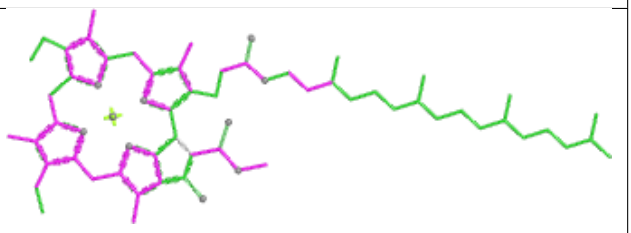
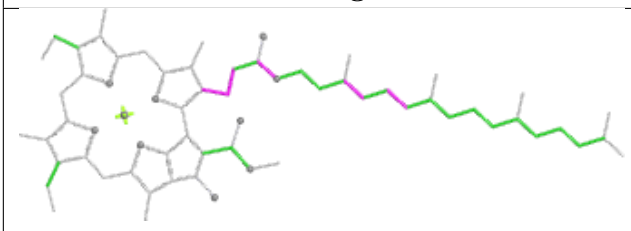
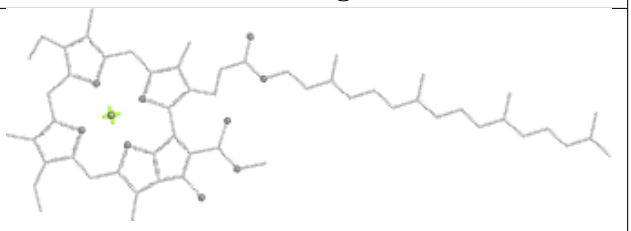


Torsions

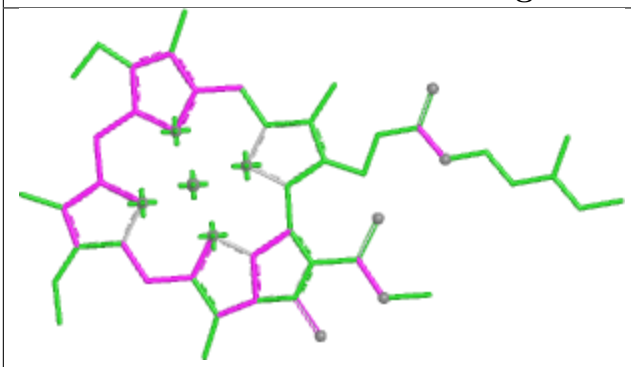


Rings

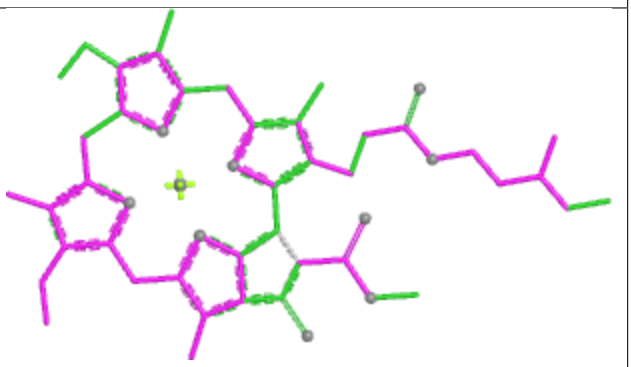
Ligand CLA bA 812	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA cB 927	
	
Bond lengths	Bond angles
	
Torsions	Rings

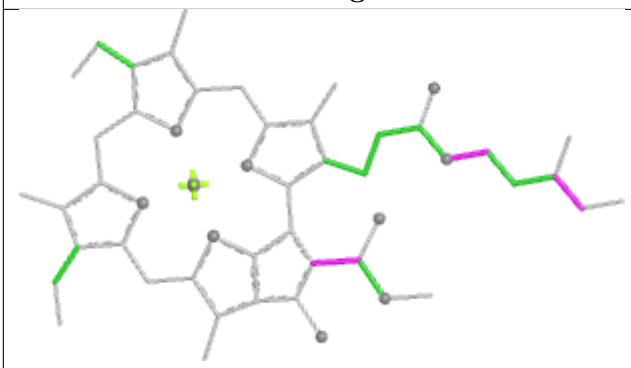
Ligand CLA aB 903



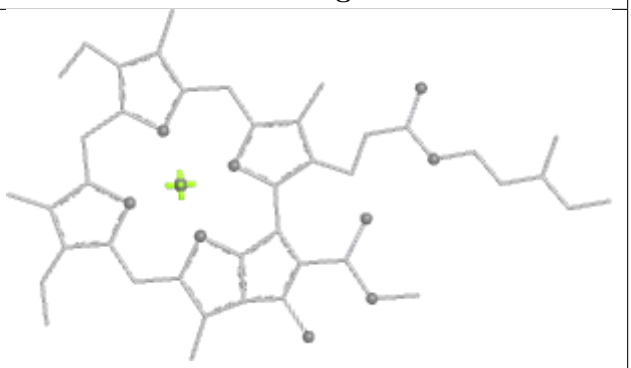
Bond lengths



Bond angles

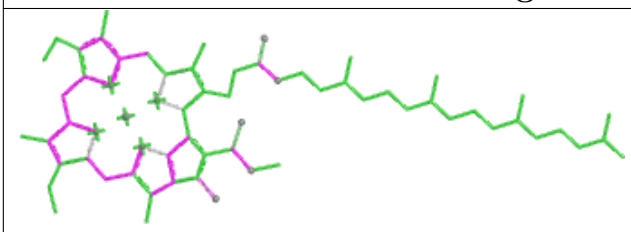


Torsions

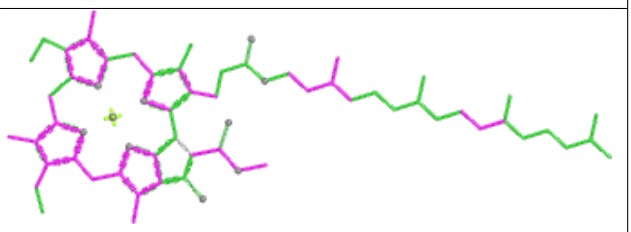


Rings

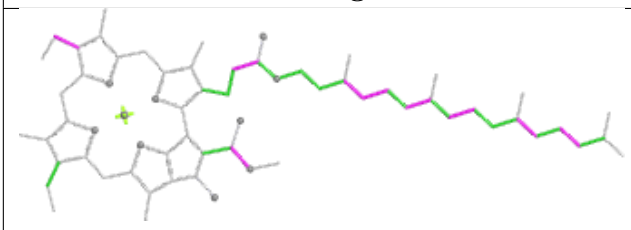
Ligand CLA cB 905



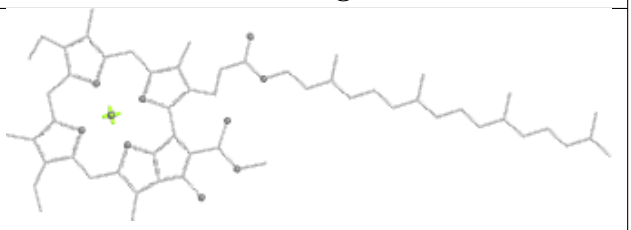
Bond lengths



Bond angles

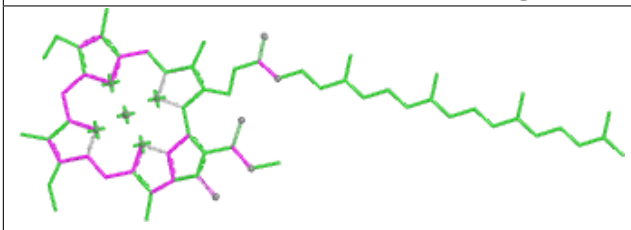


Torsions

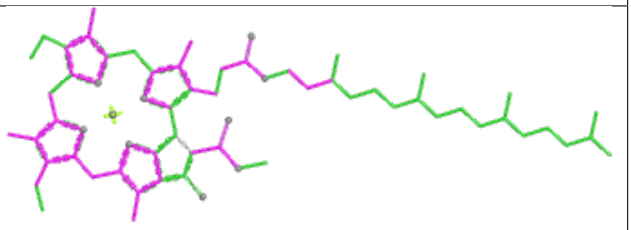


Rings

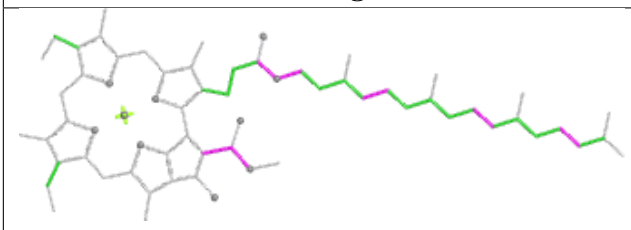
Ligand CLA aA 830



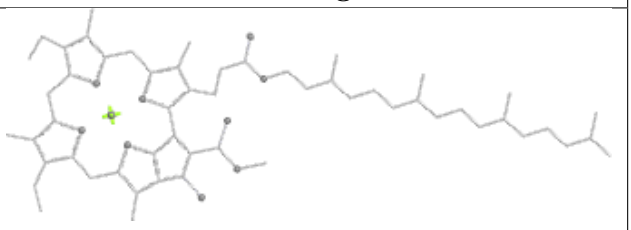
Bond lengths



Bond angles



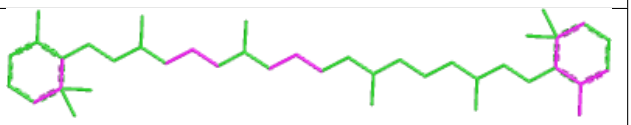
Torsions



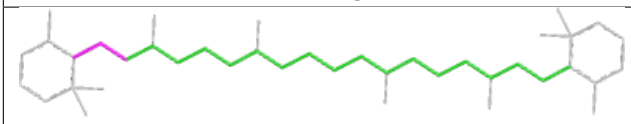
Rings

Ligand BCR bB 946

Bond lengths



Bond angles



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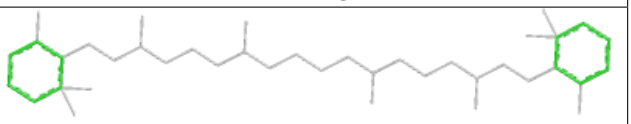
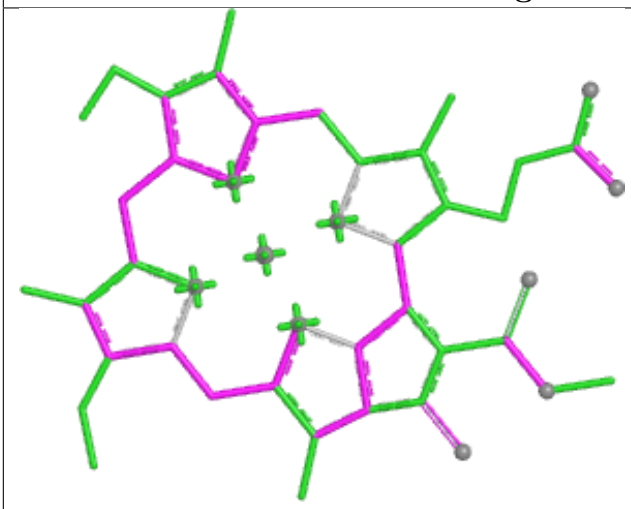


Rings

Ligand CLA aA 836



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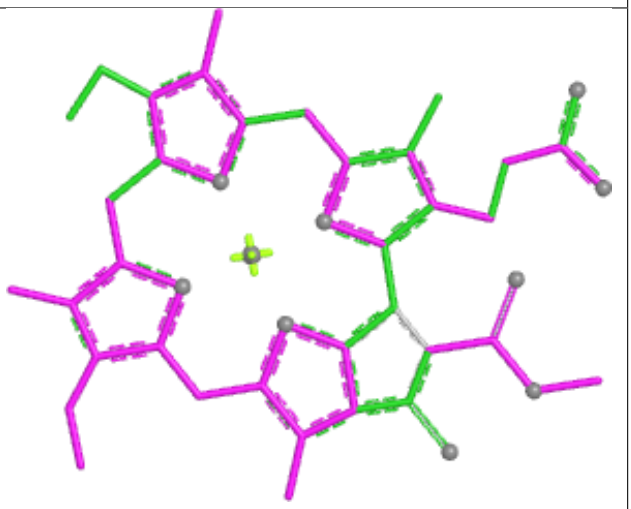
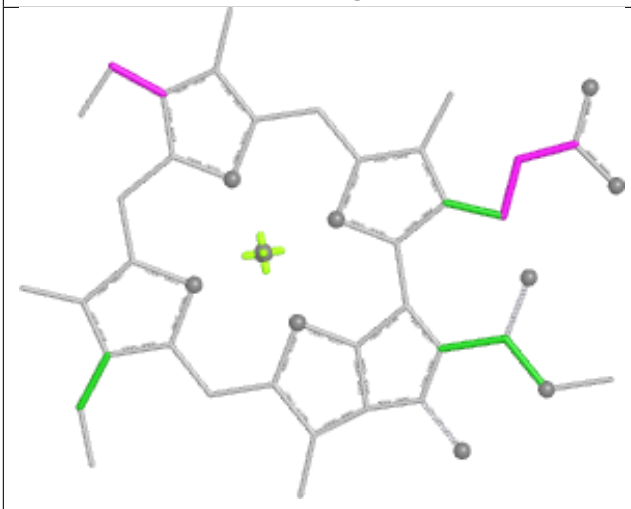


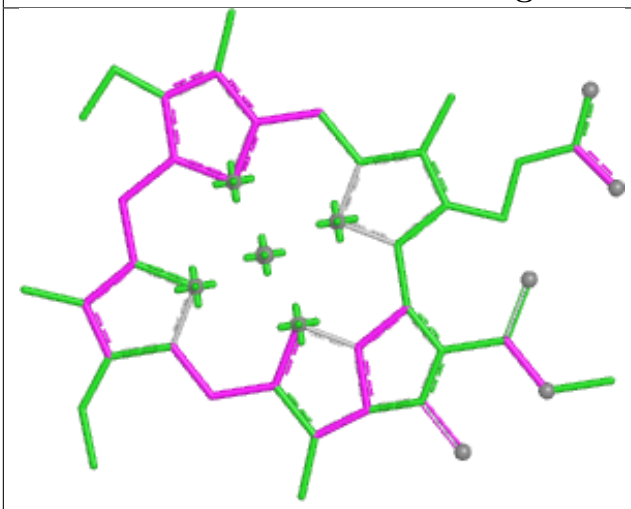
Bond angles



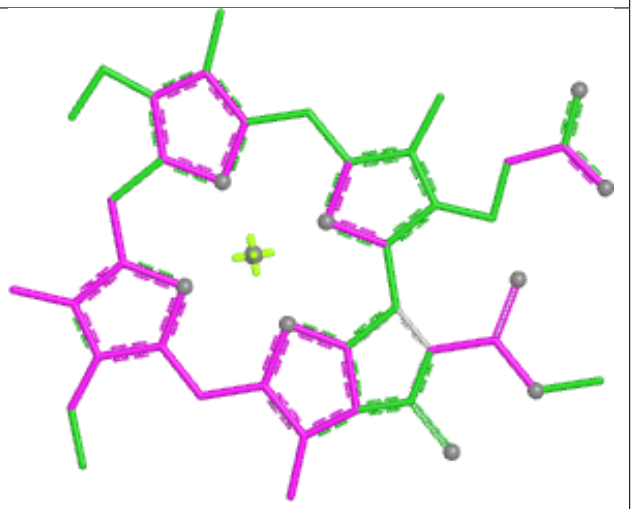
Torsions

Rings

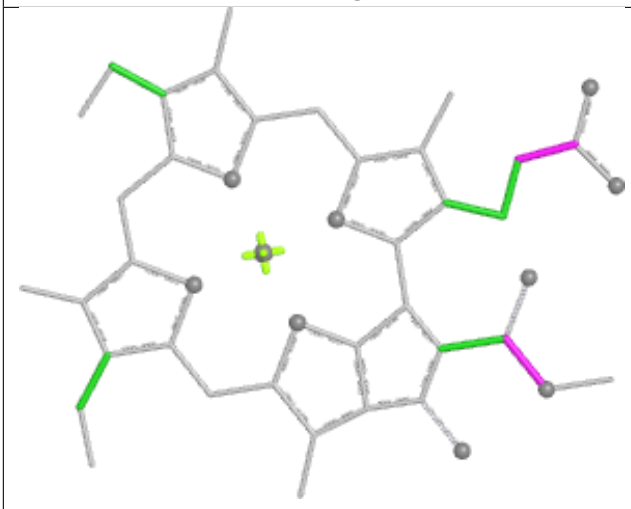
Ligand CLA aB 920



Bond lengths



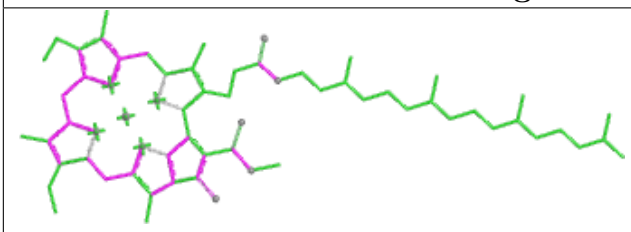
Bond angles



Torsions

Rings

Ligand CLA bA 838



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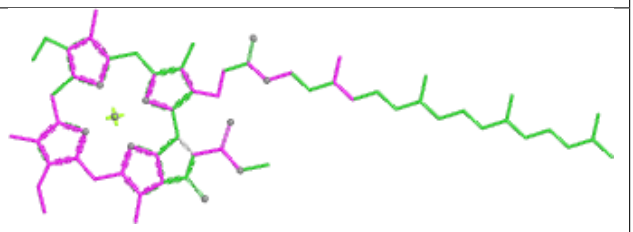
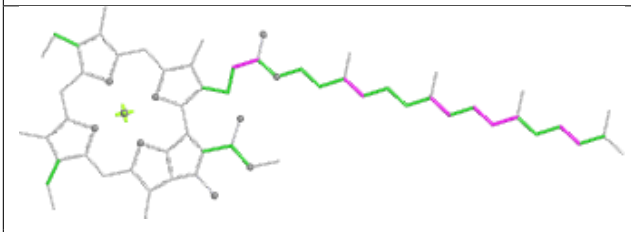
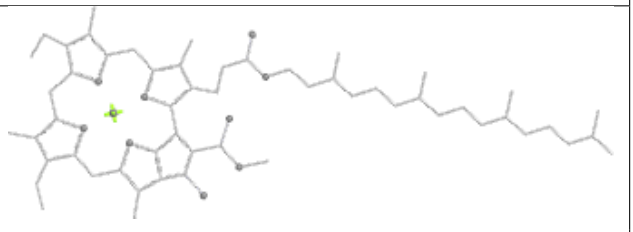


Bond angles

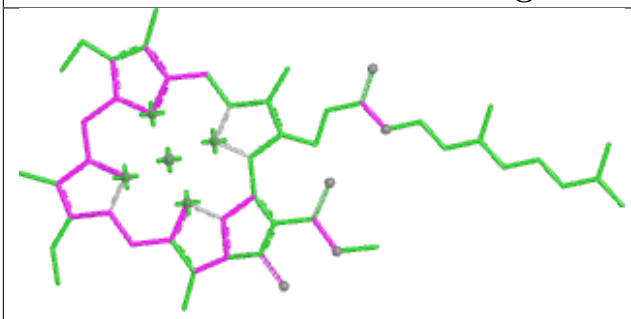


Torsions

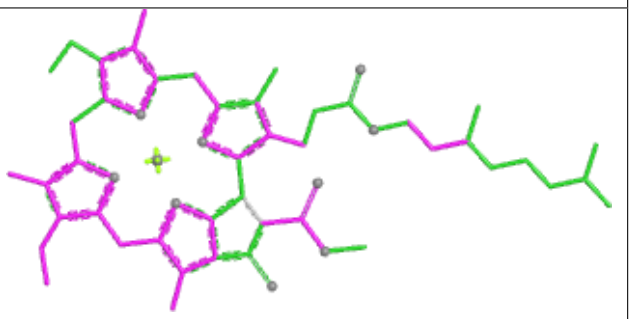


Rings

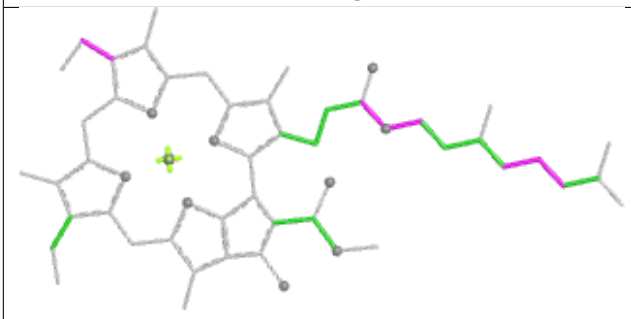
Ligand CLA cA 826



Bond lengths



Bond angles



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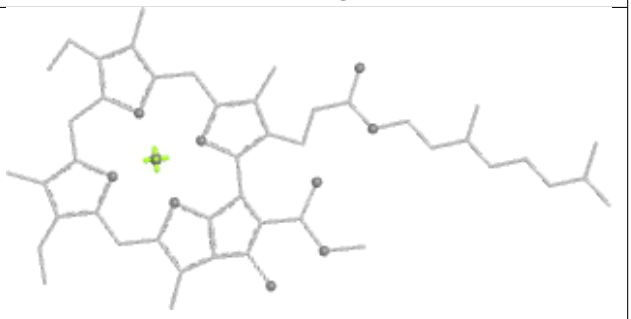
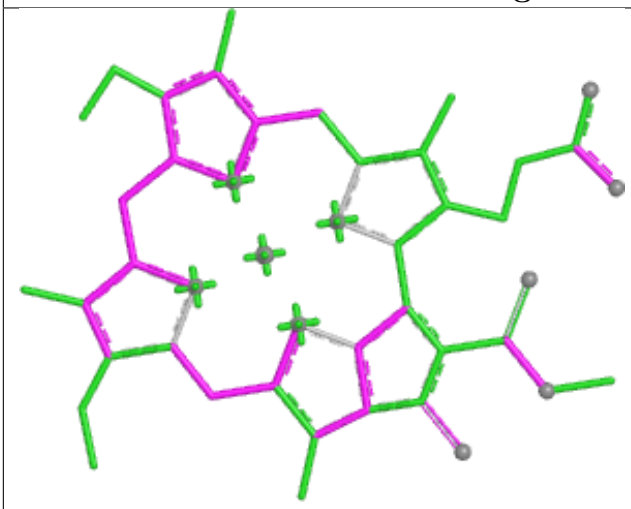
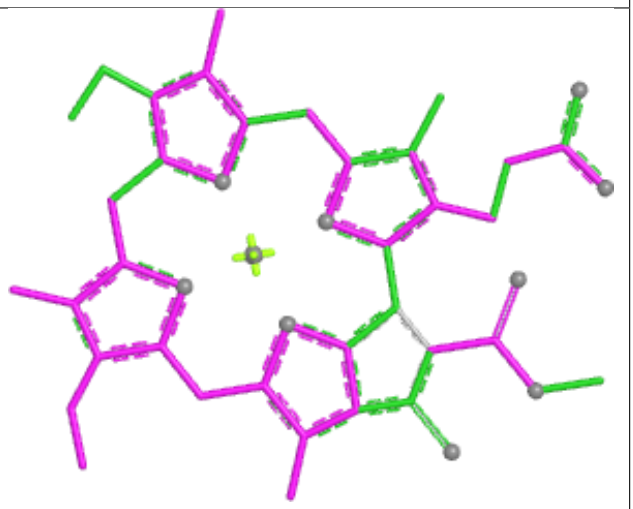


Rings

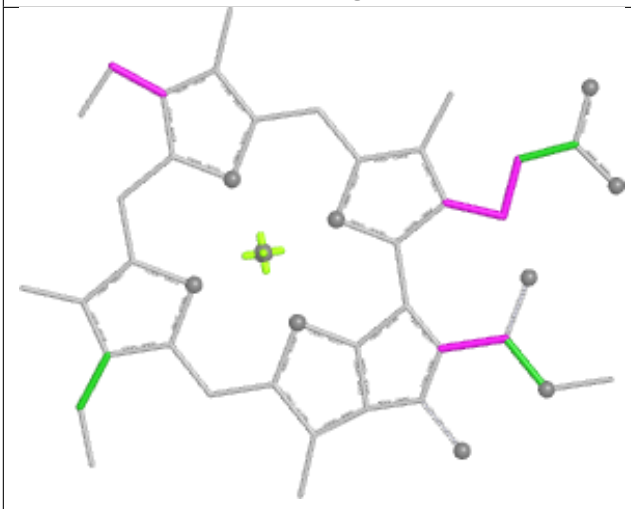
Ligand CLA bA 809



Bond lengths



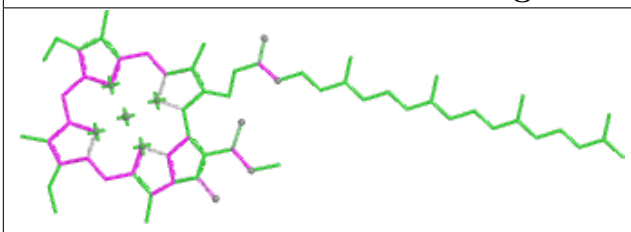
Bond angles



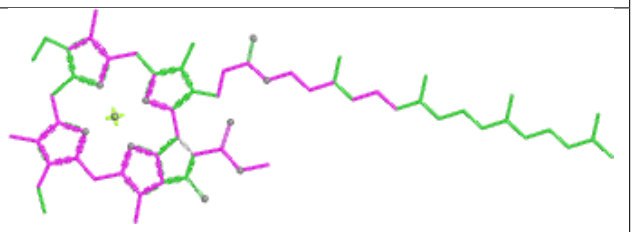
Torsions

Rings

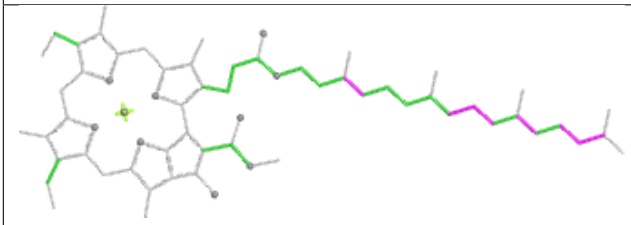
Ligand CLA bA 825



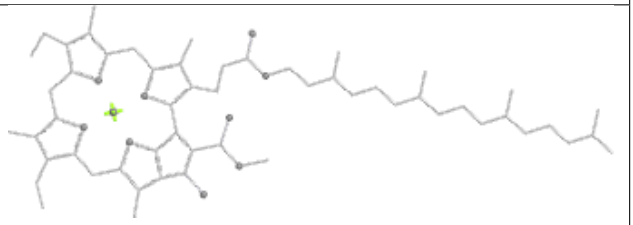
Bond lengths



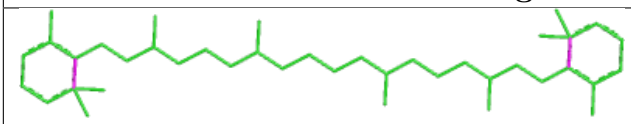
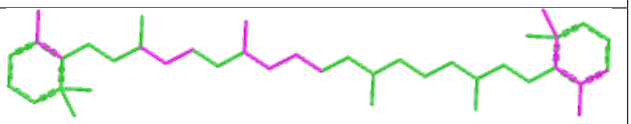
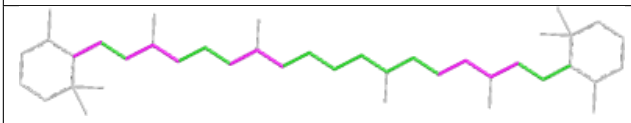
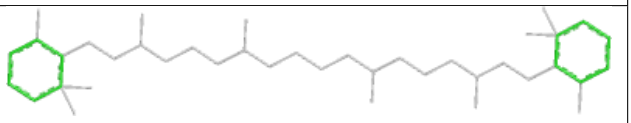
Bond angles

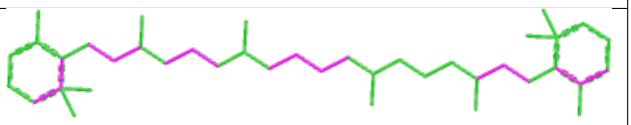
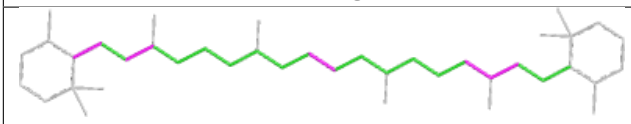
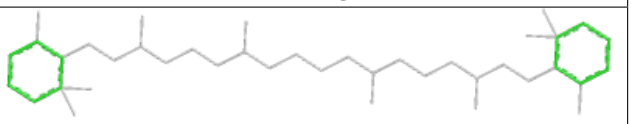


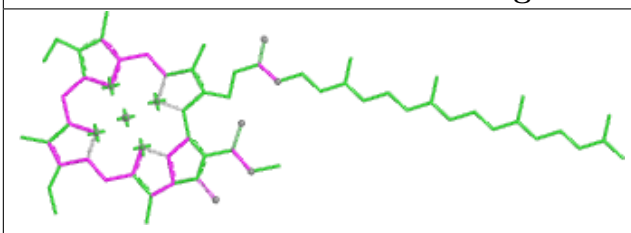
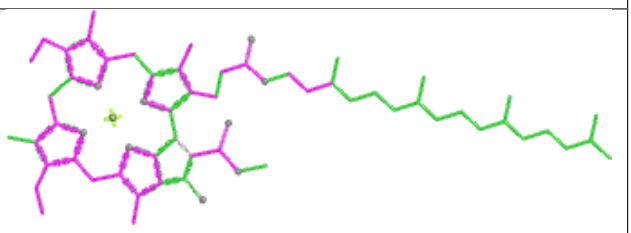
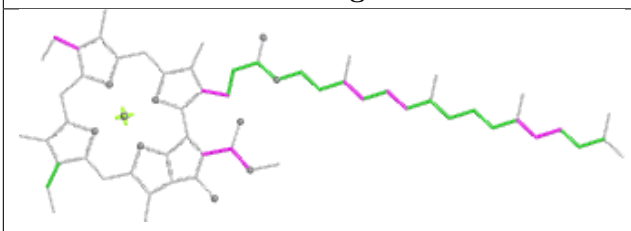
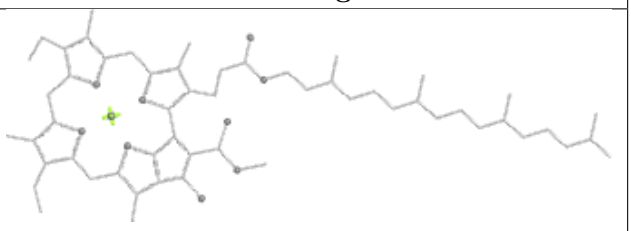
Torsions



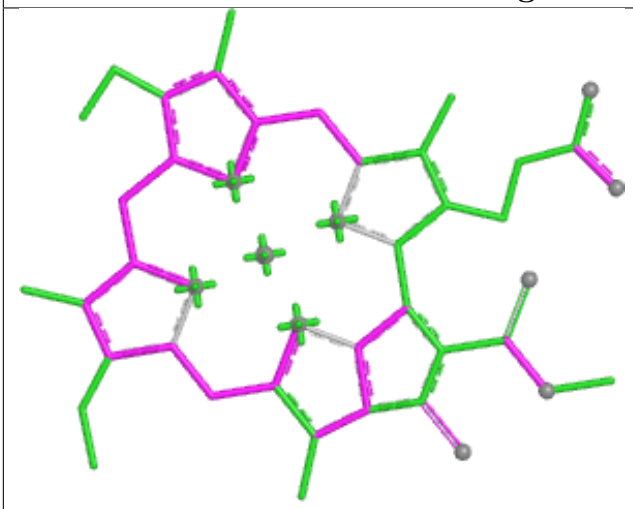
Rings

Ligand BCR aF 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

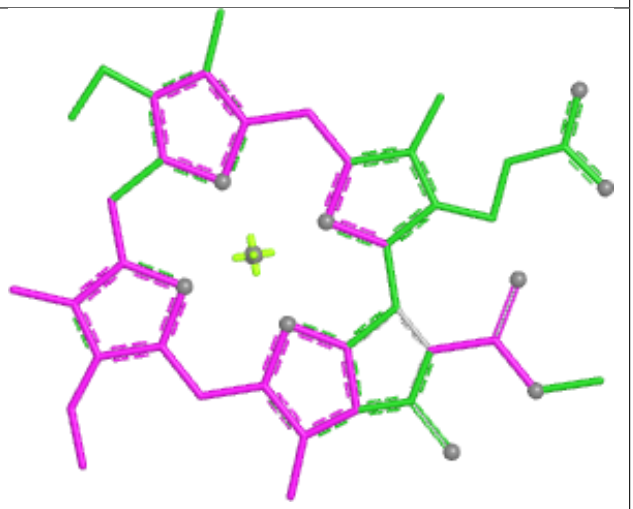
Ligand BCR aF 201	
Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA bA 834	
 Bond lengths	 Bond angles
 Torsions	 Rings

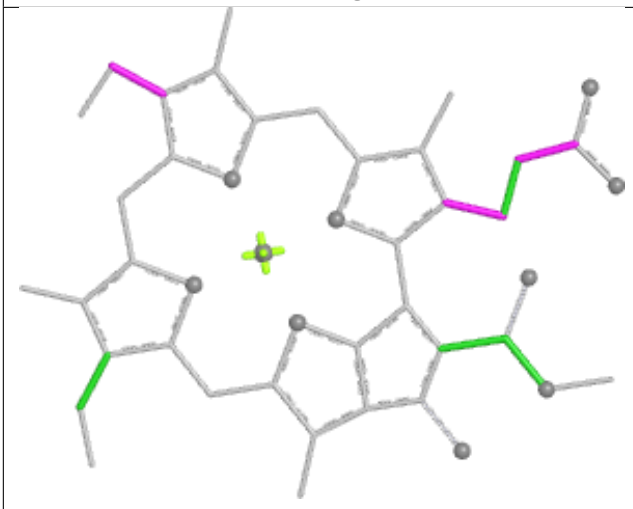
Ligand CLA aL 203



Bond lengths



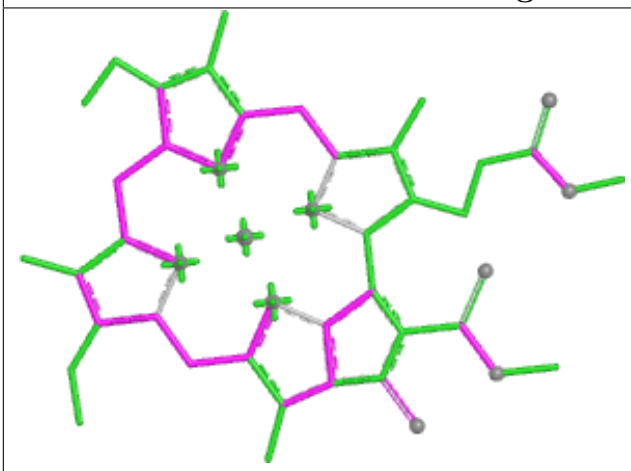
Bond angles



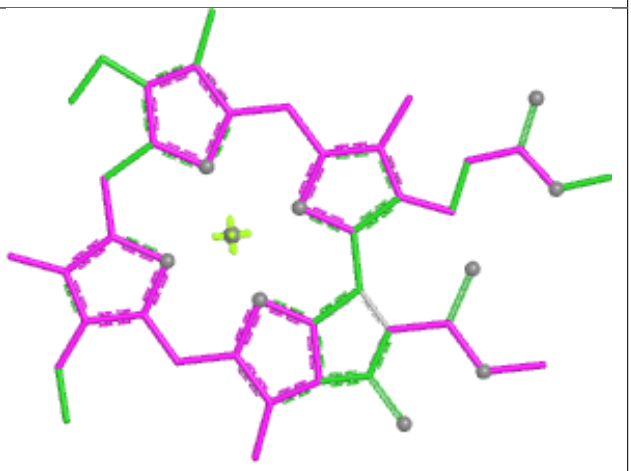
Torsions

Rings

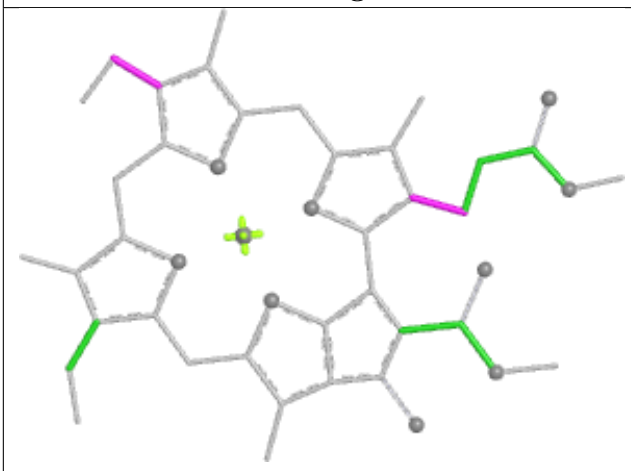
Ligand CLA cB 918



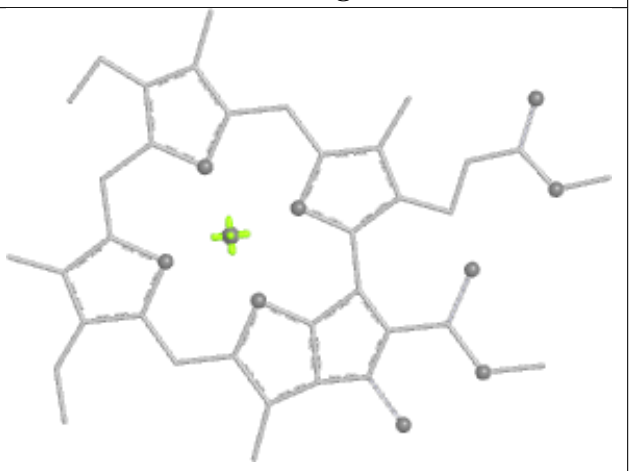
Bond lengths



Bond angles

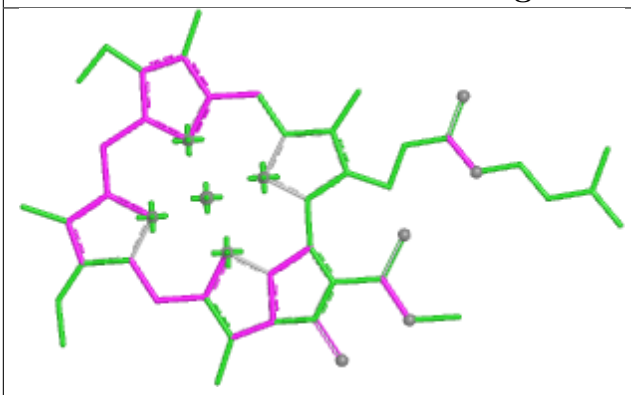


Torsions

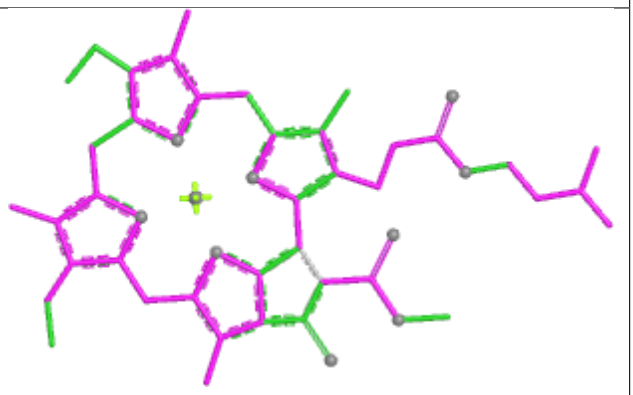


Rings

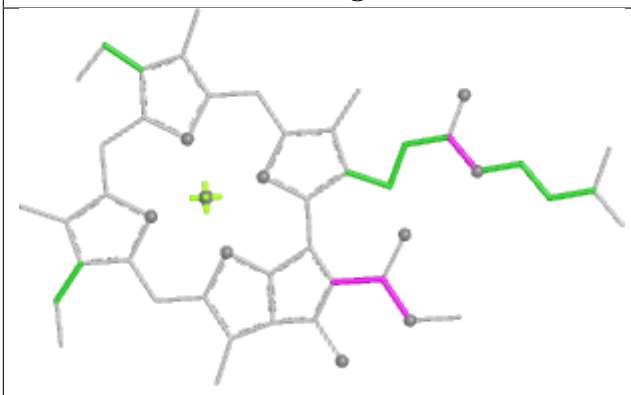
Ligand CLA bB 935



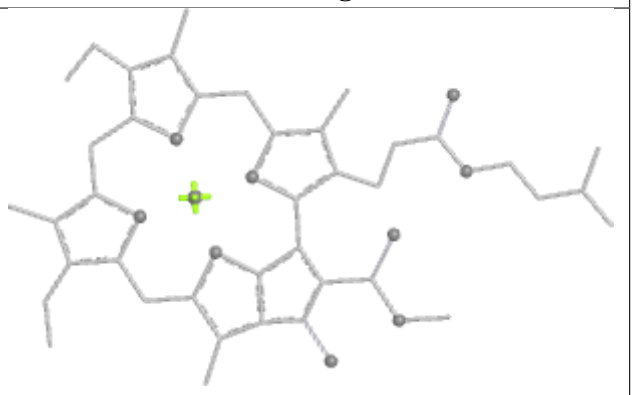
Bond lengths



Bond angles



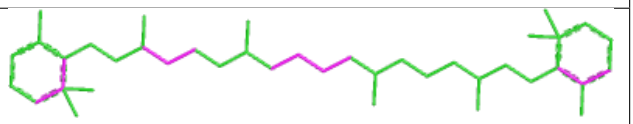
Torsions



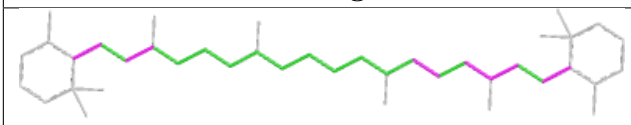
Rings

Ligand BCR aL 205

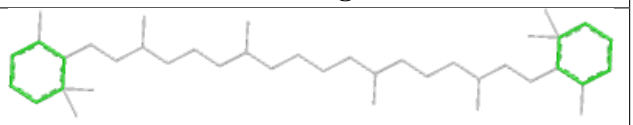
Bond lengths



Bond angles

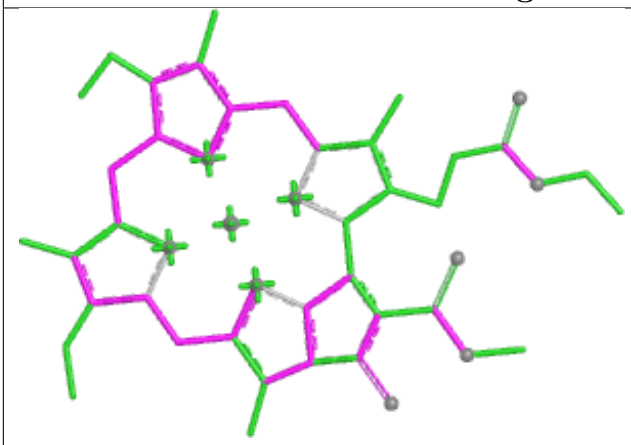


Torsions

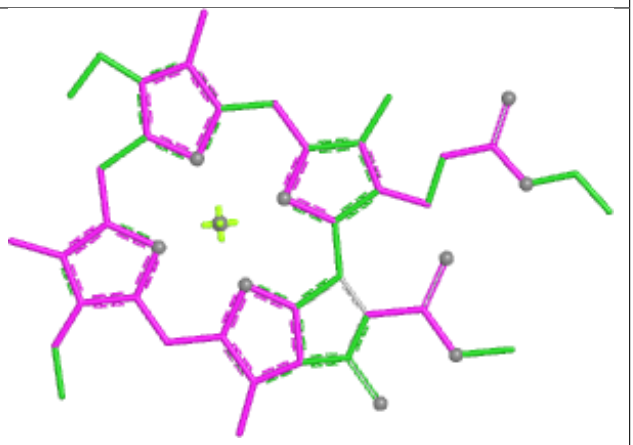


Rings

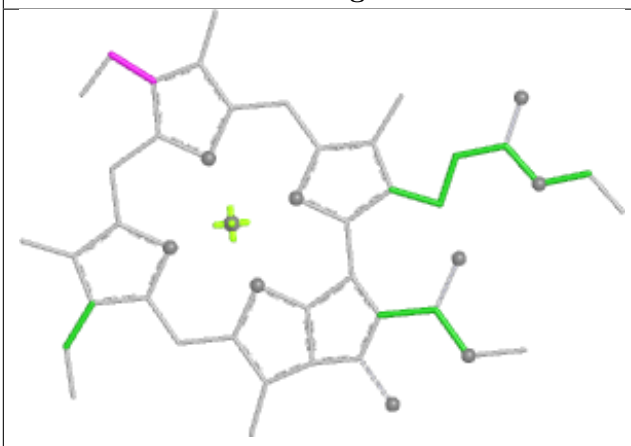
Ligand CLA cB 937



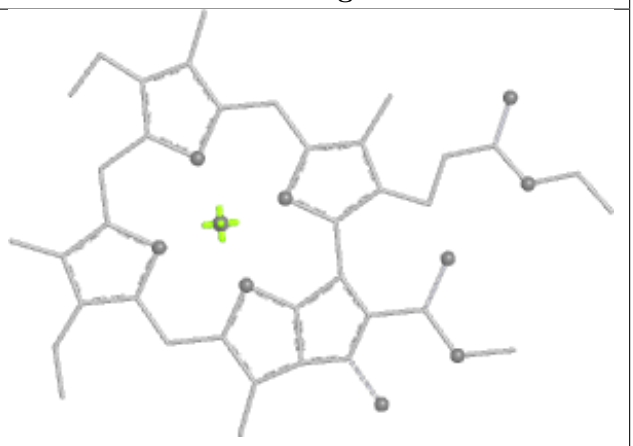
Bond lengths



Bond angles

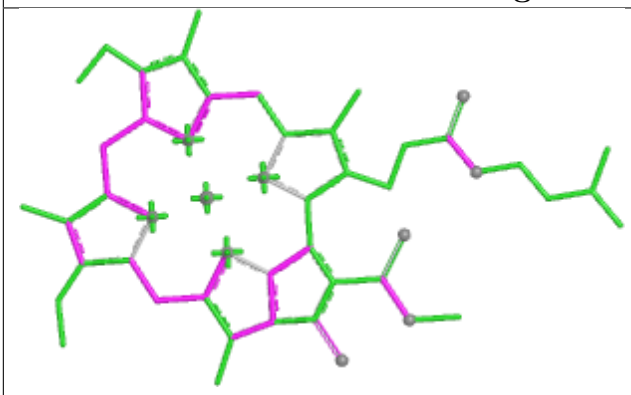


Torsions

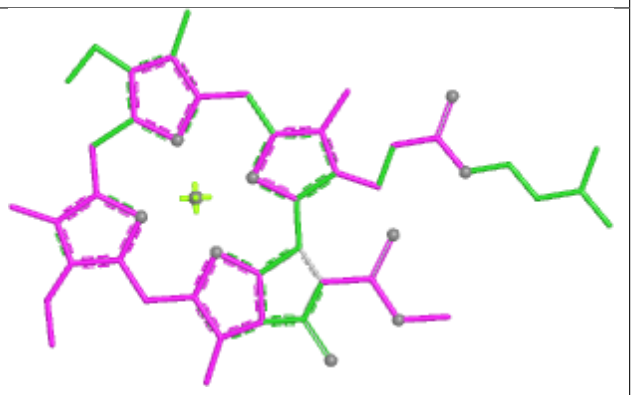


Rings

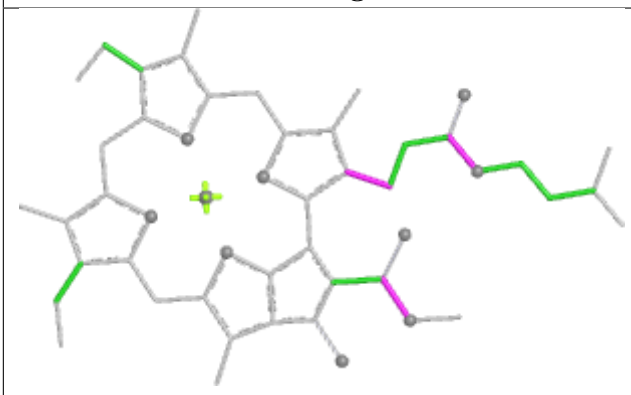
Ligand CLA bA 821



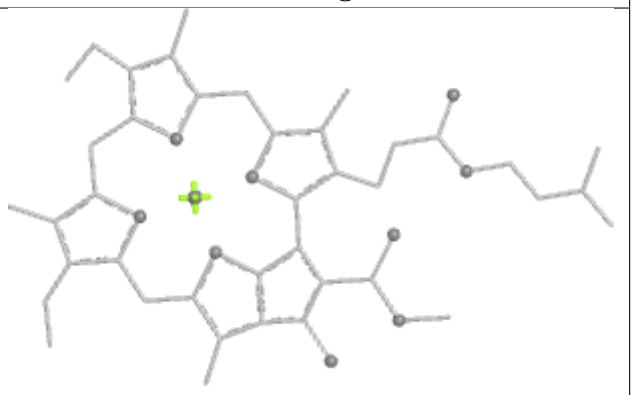
Bond lengths



Bond angles



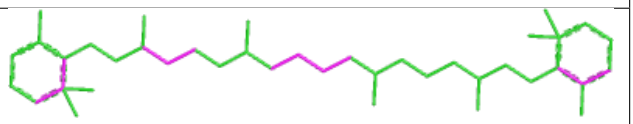
Torsions



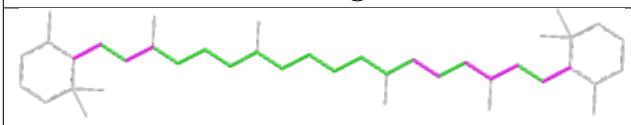
Rings

Ligand BCR cL 205

Bond lengths



Bond angles



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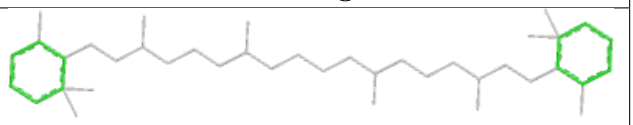
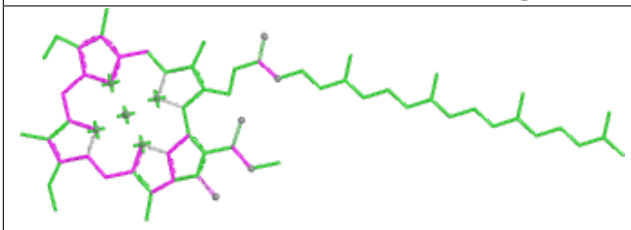
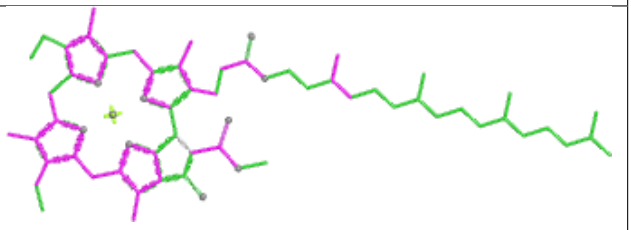


Rings

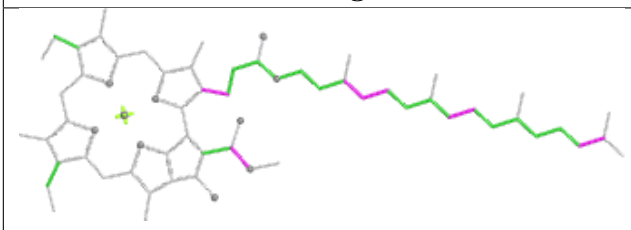
Ligand CLA cA 806



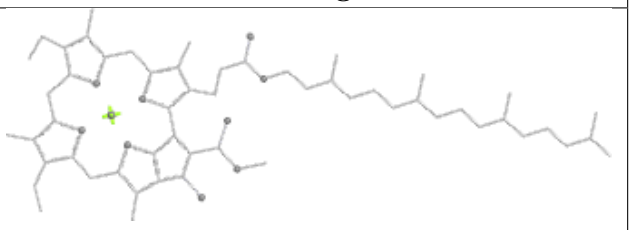
Bond lengths



Bond angles

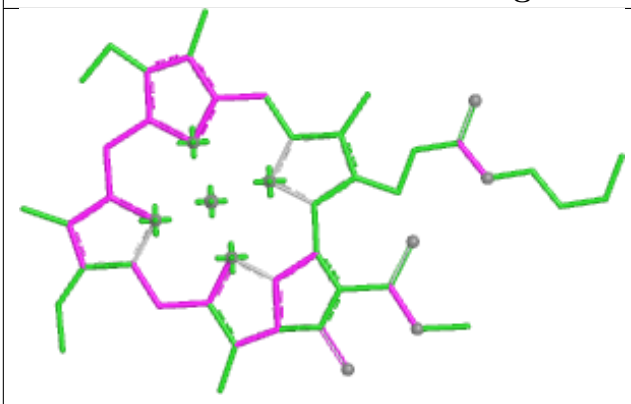


Torsions

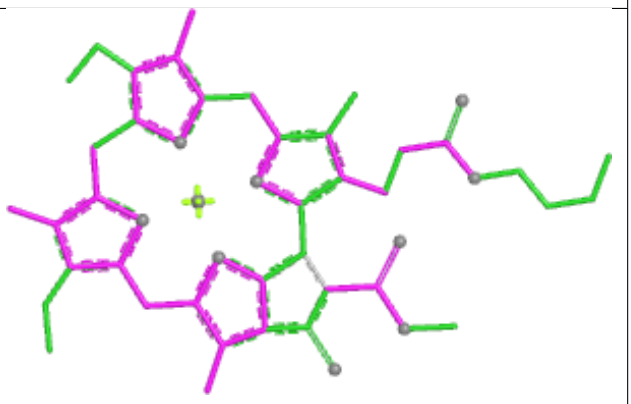


Rings

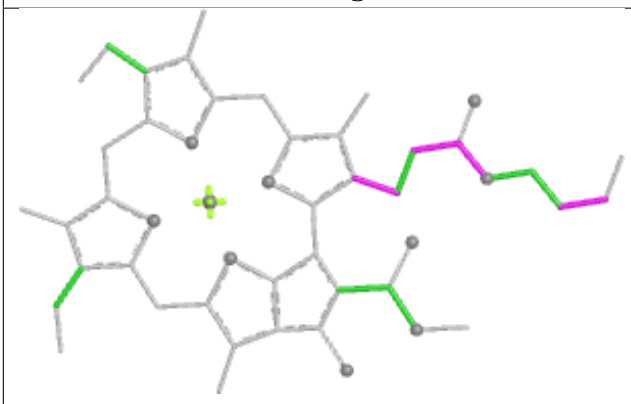
Ligand CLA bA 822



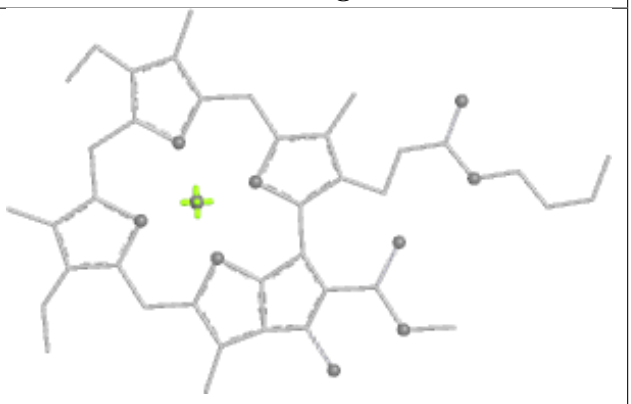
Bond lengths



Bond angles

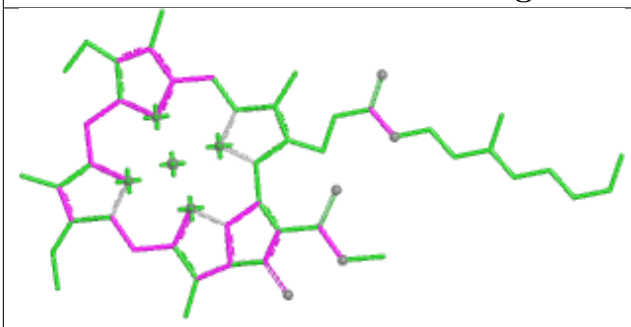


Torsions

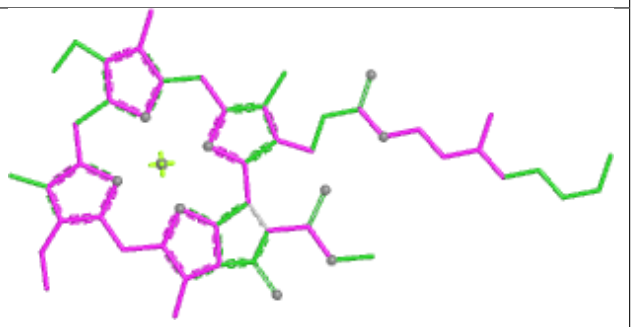


Rings

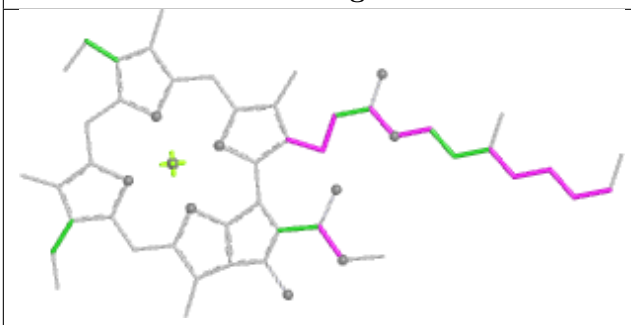
Ligand CLA aA 818



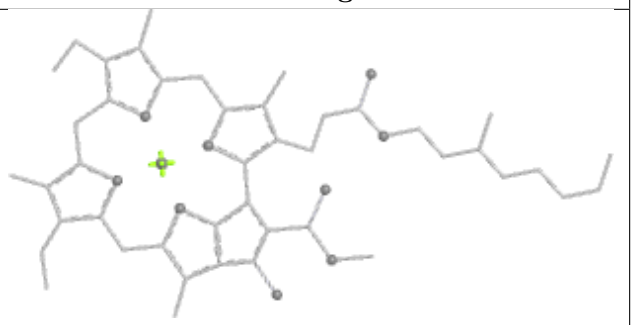
Bond lengths



Bond angles

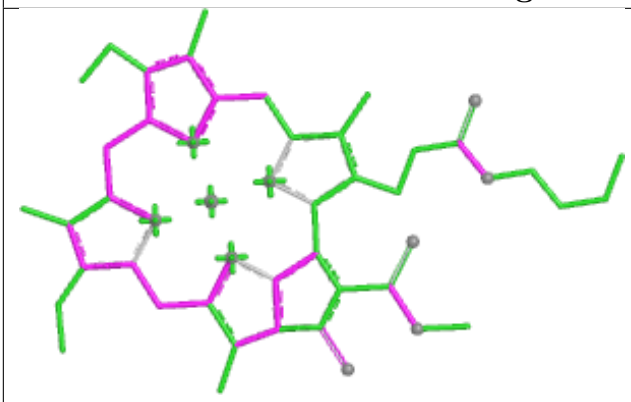


Torsions

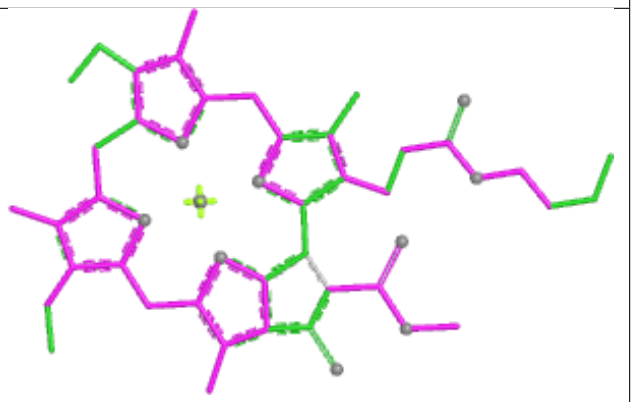


Rings

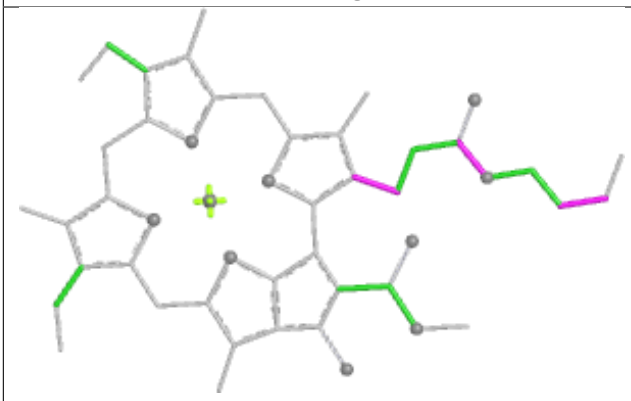
Ligand CLA aB 930



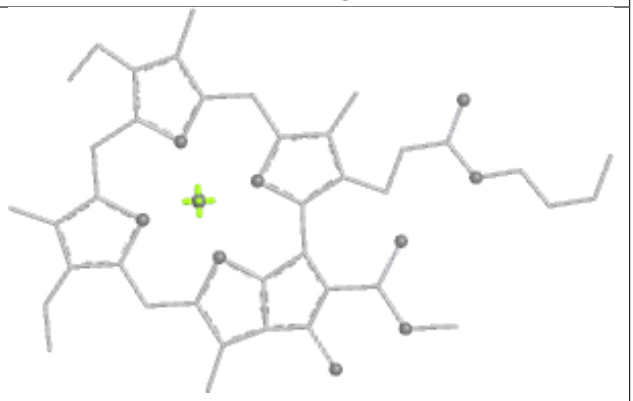
Bond lengths



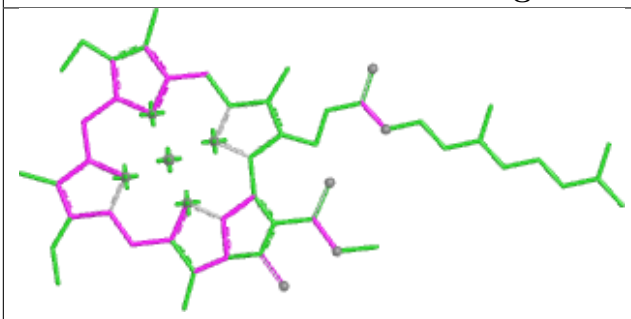
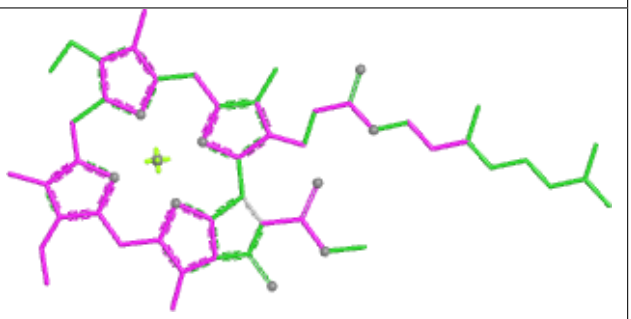
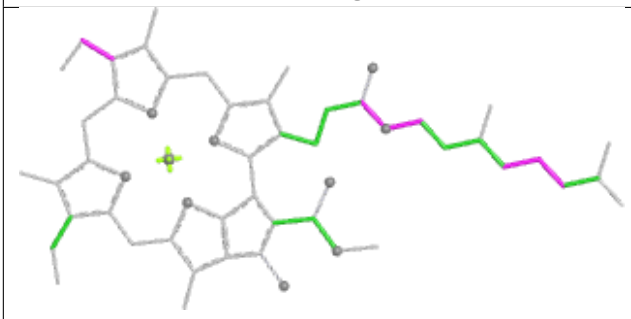
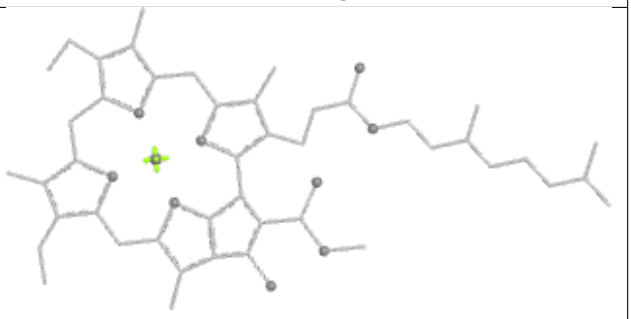
Bond angles

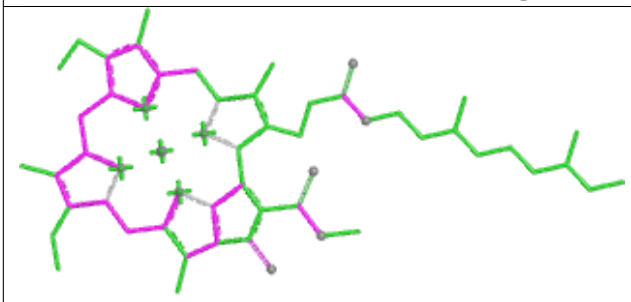
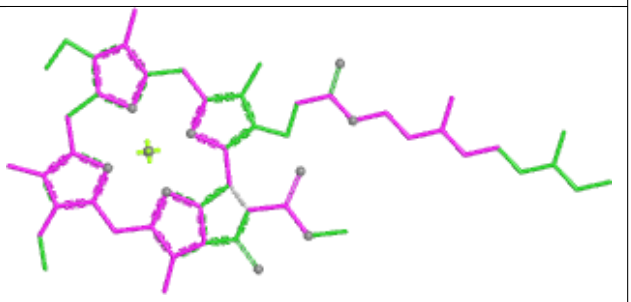
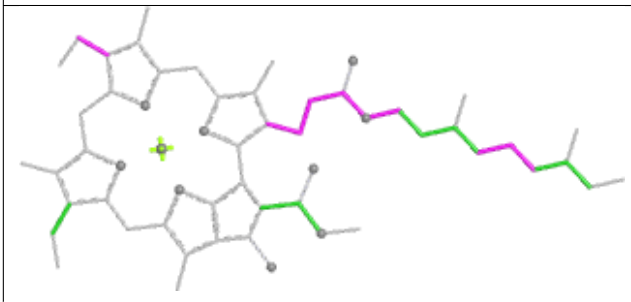
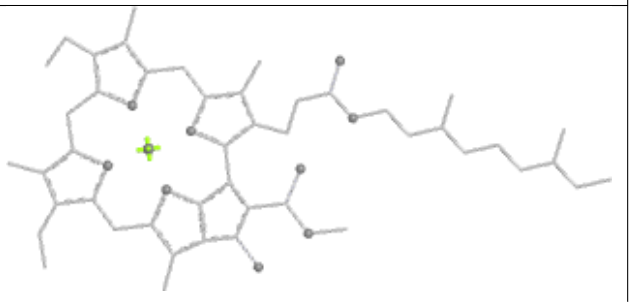


Torsions

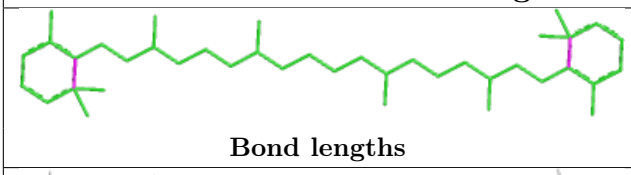


Rings

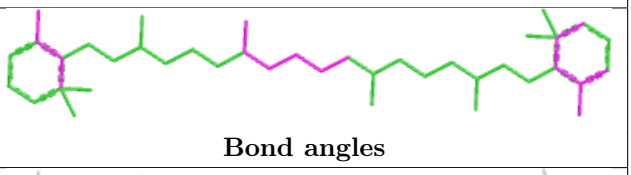
Ligand CLA bA 826	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA aA 820	
 Bond lengths	 Bond angles
 Torsions	 Rings

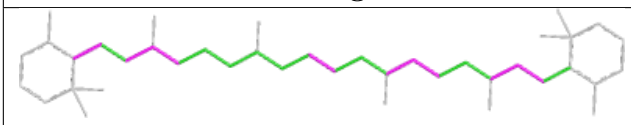
Ligand BCR aA 847



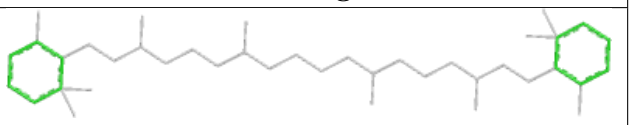
Bond lengths



Bond angles

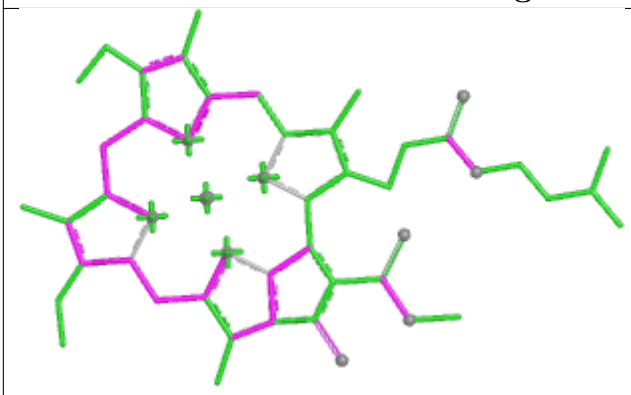


Torsions



Rings

Ligand CLA bB 928



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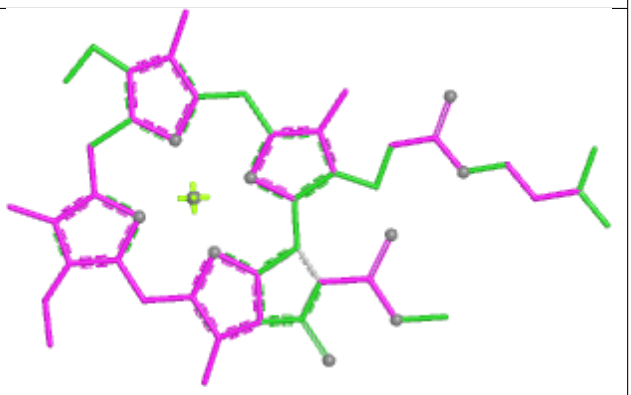
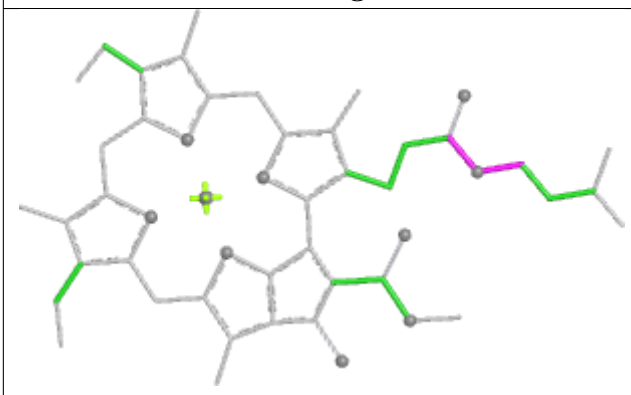


Bond angles



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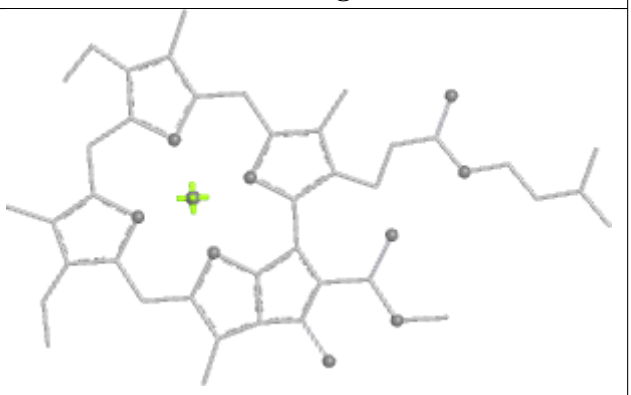
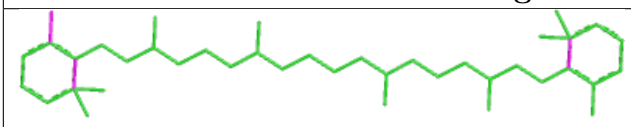


Rings

Ligand BCR aB 942



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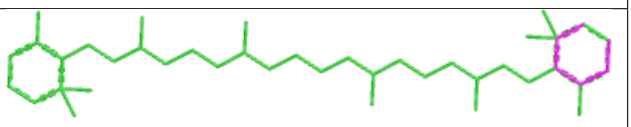
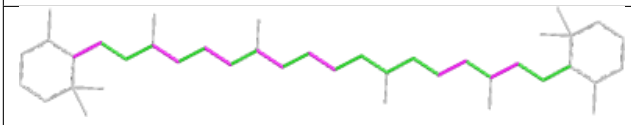


Bond angles



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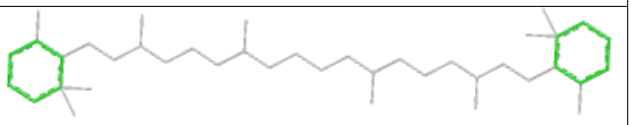
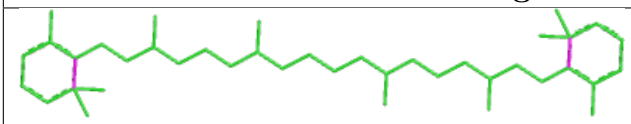


Rings

Ligand BCR aA 848



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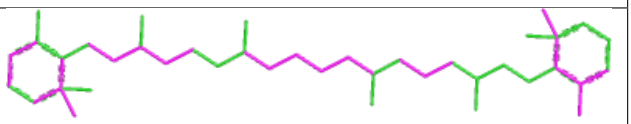
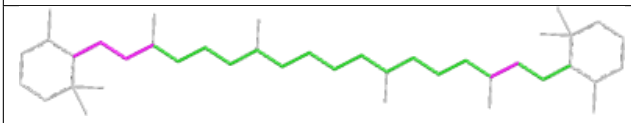


Bond angles



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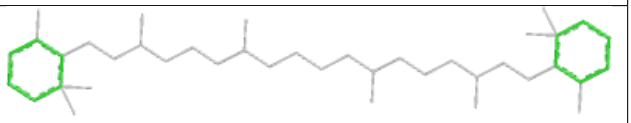
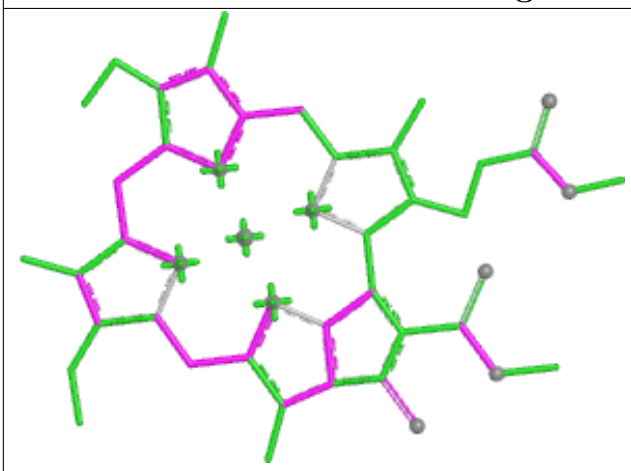


Rings

Ligand CLA cA 827



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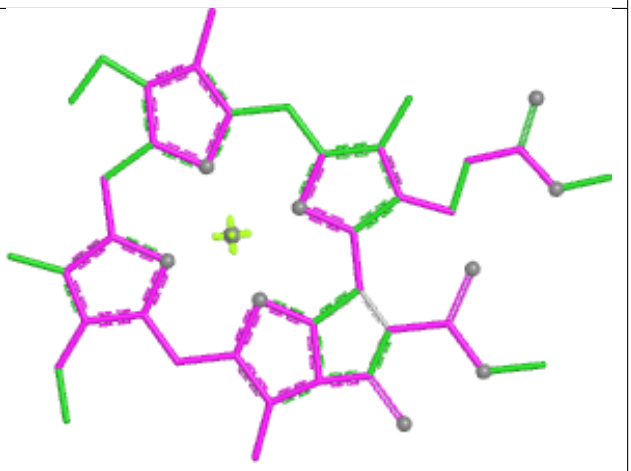
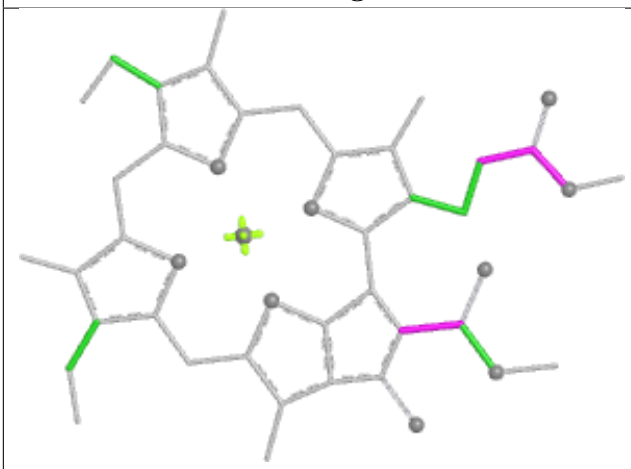


Bond angles



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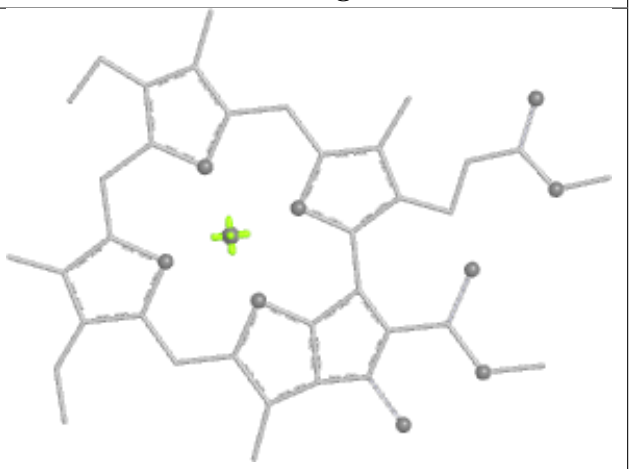
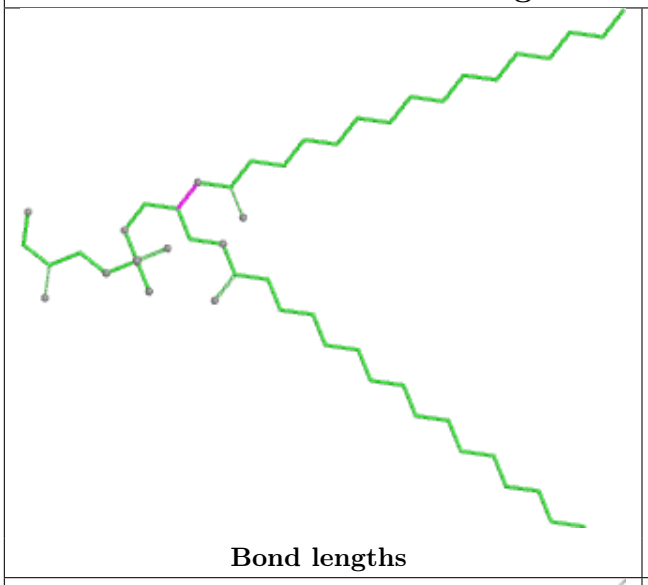


Rings

Ligand LHG aA 852



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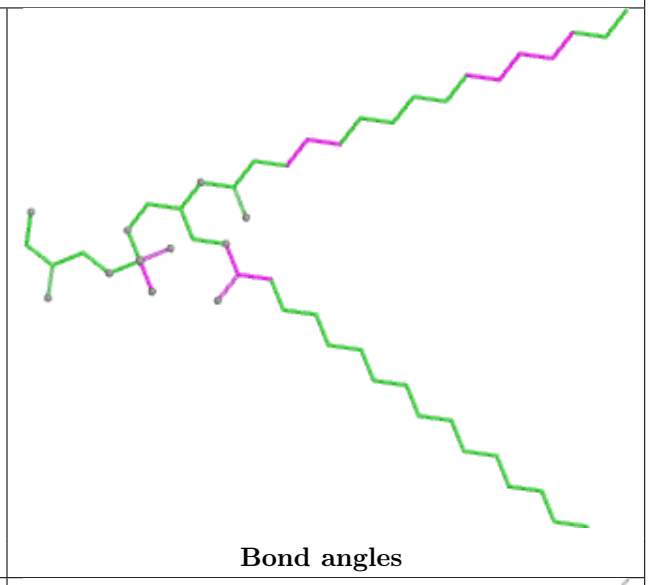

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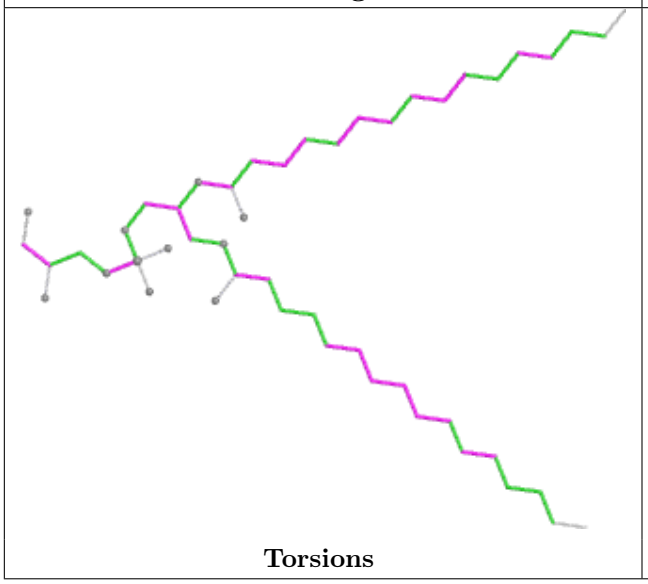

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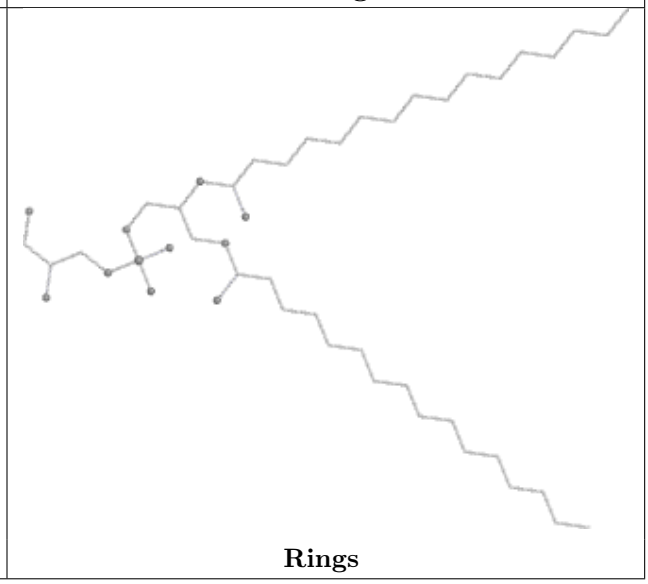
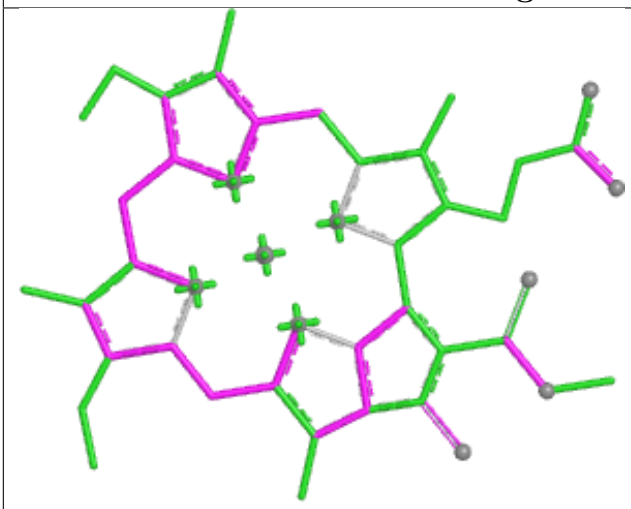


Rings

Ligand CLA cB 933



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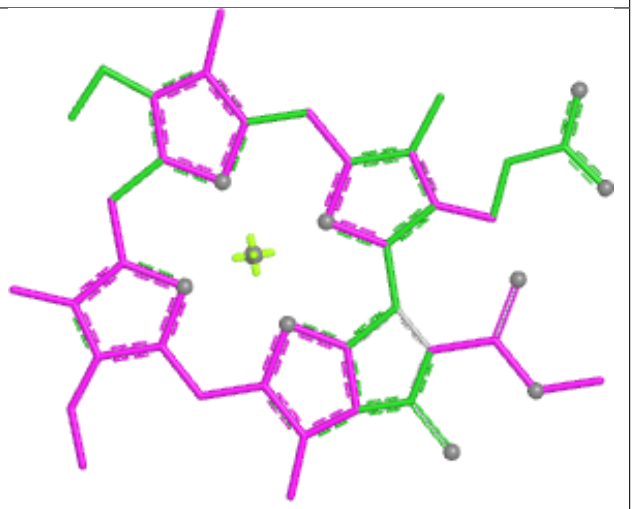

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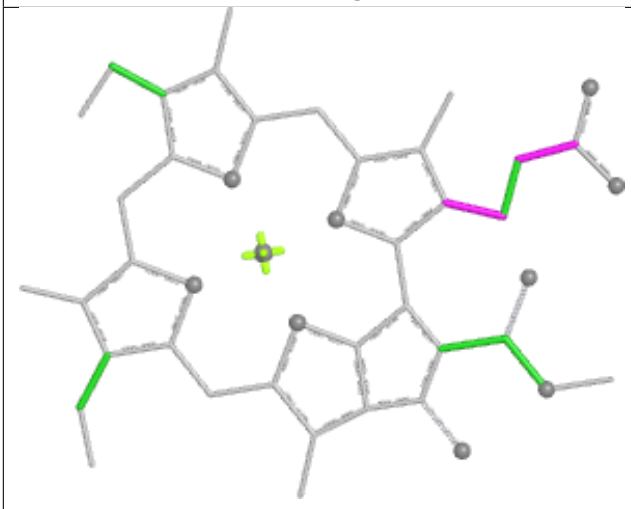
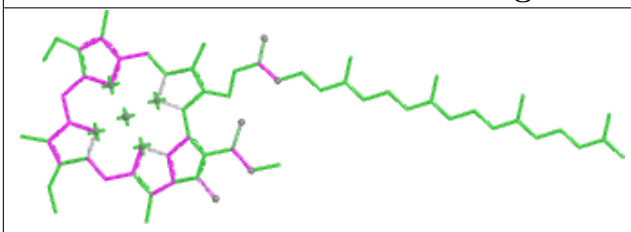


Torsions

Rings

Ligand CLA bB 905



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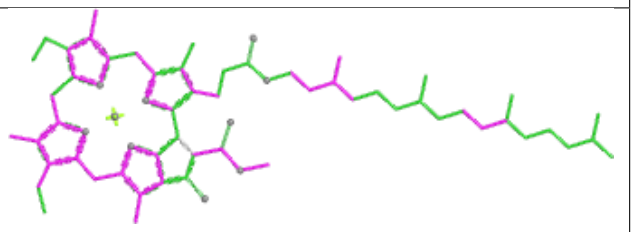

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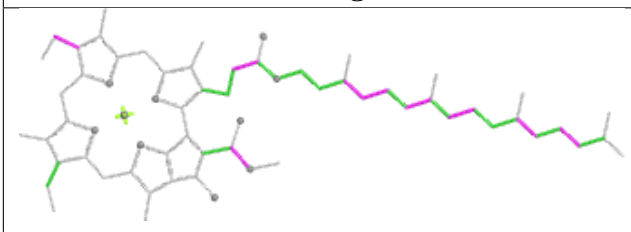

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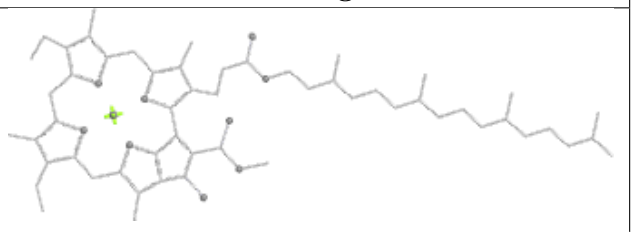
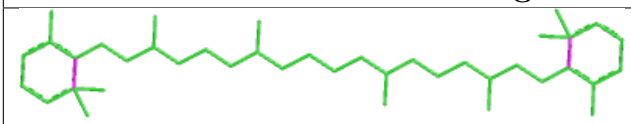


Rings

Ligand BCR aB 943



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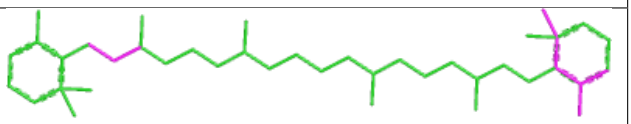

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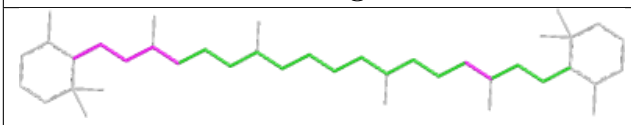

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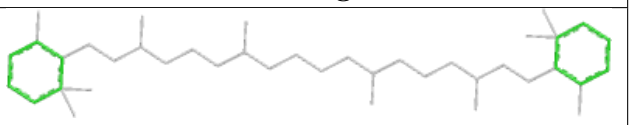
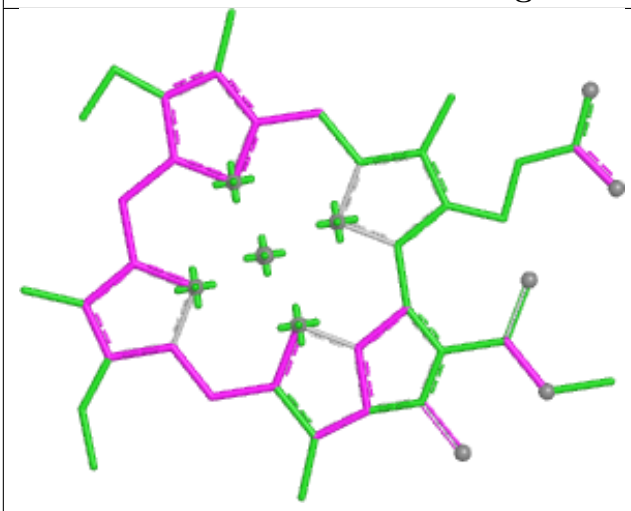


Rings

Ligand CLA aA 816



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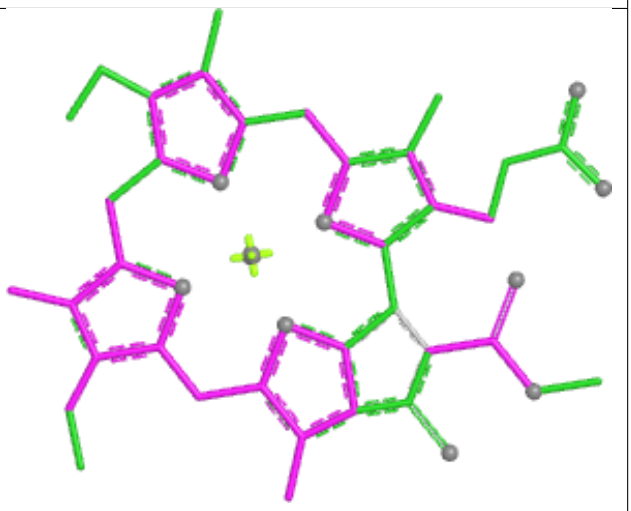

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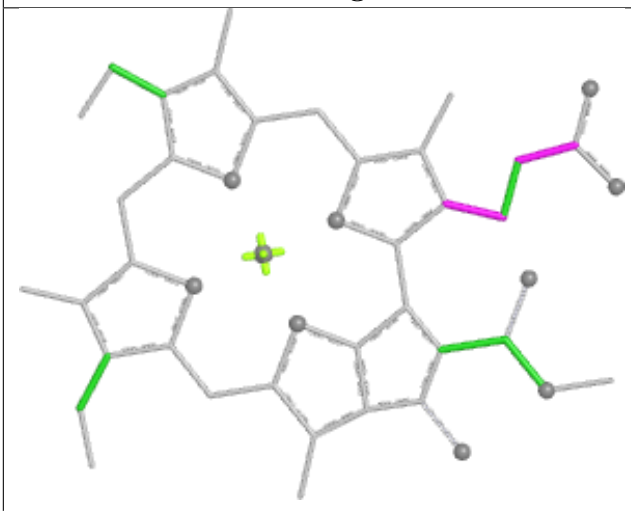
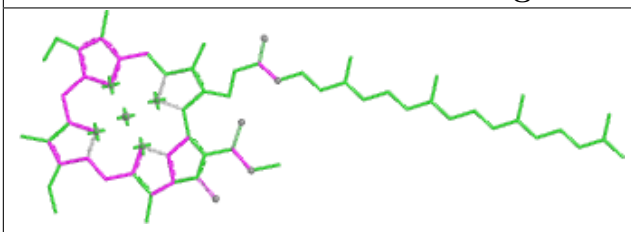


Torsions

Rings

Ligand CLA bA 843



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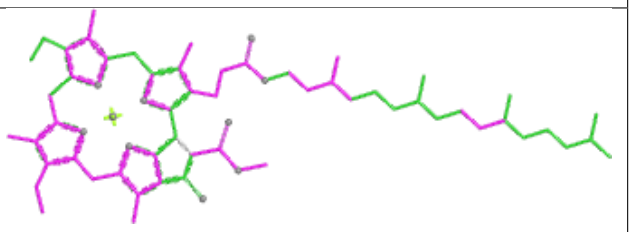

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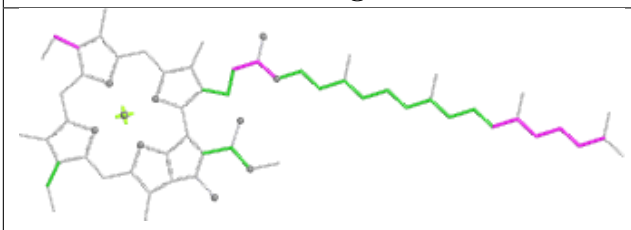

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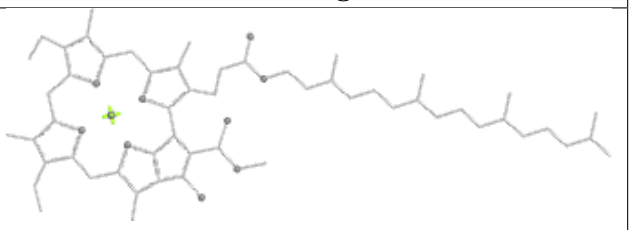
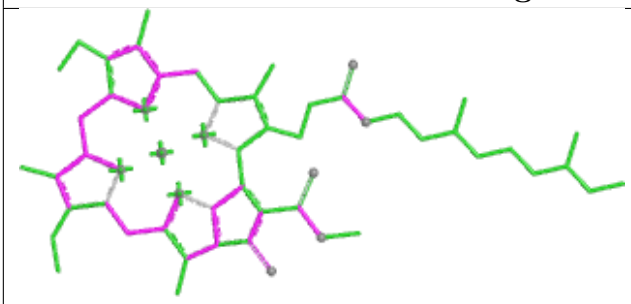


Rings

Ligand CLA bB 913



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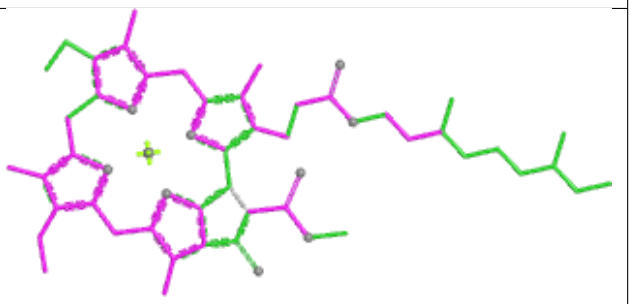
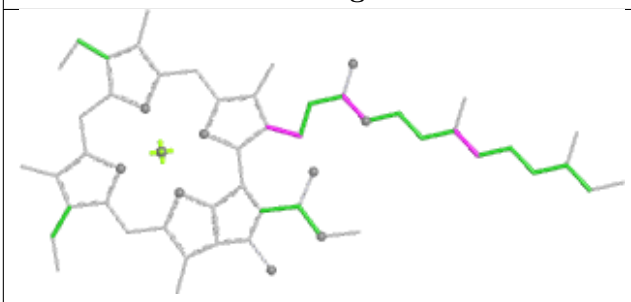


Bond angles



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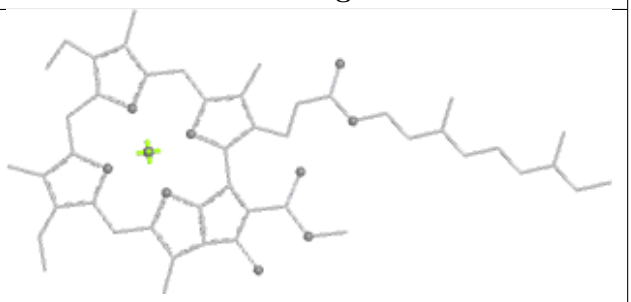
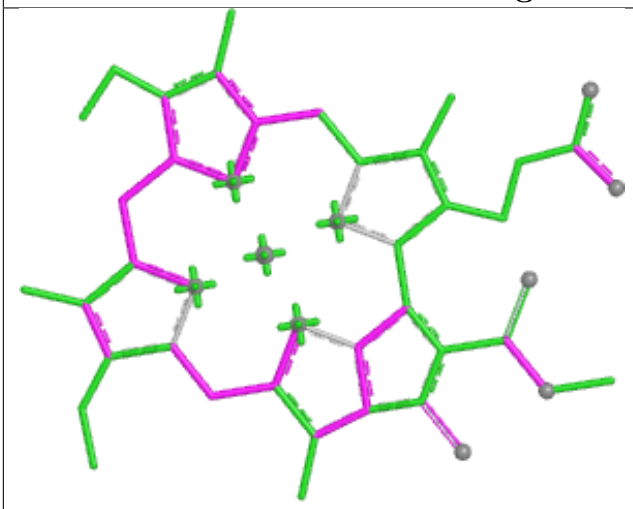


Rings

Ligand CLA aB 911



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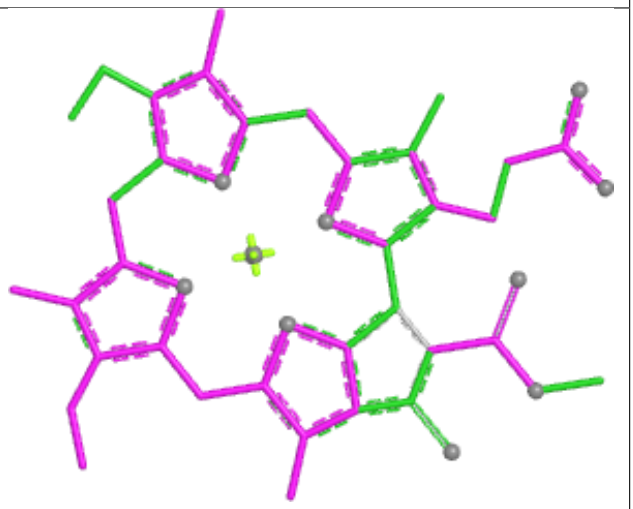
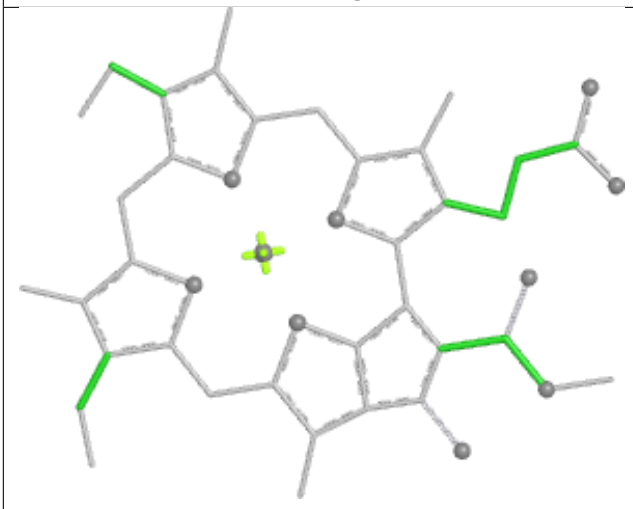
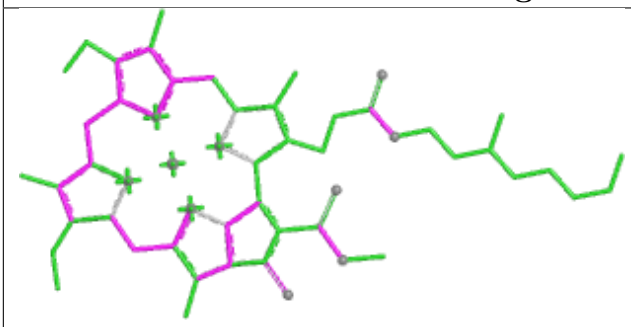
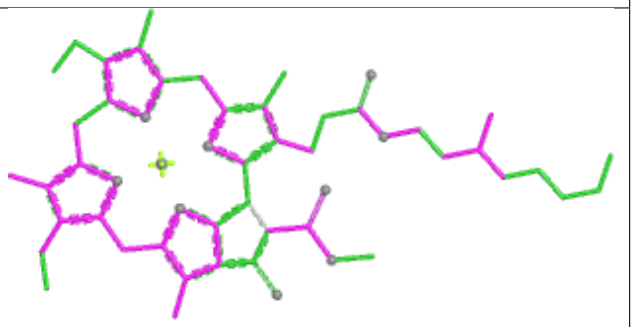


Bond angles



Torsions

Rings

Ligand CLA aA 817	
	
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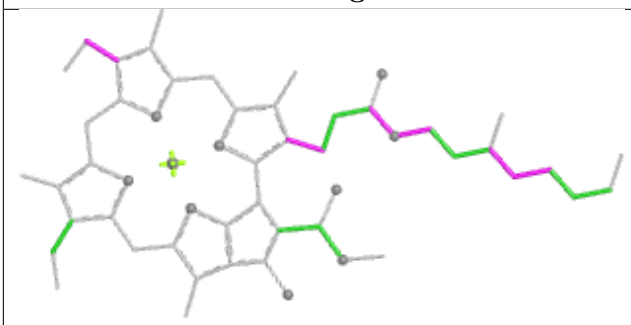
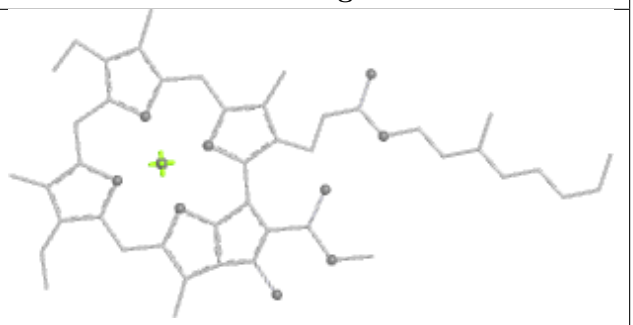
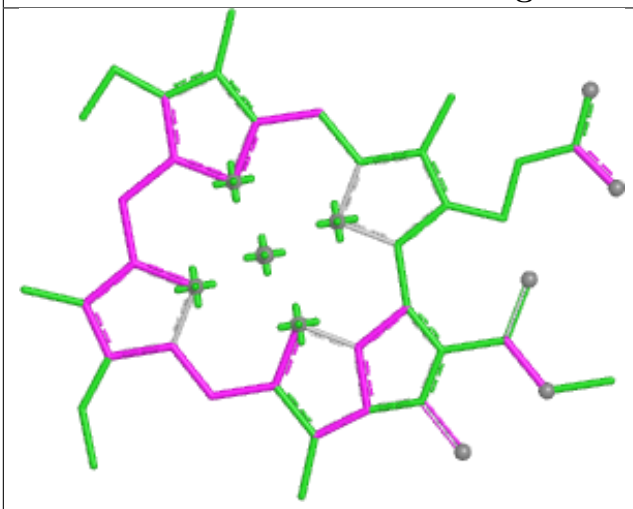
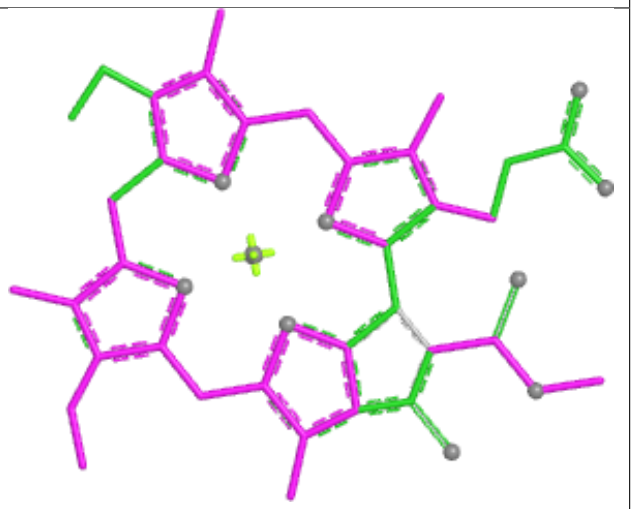
	
Torsions	**Rings**

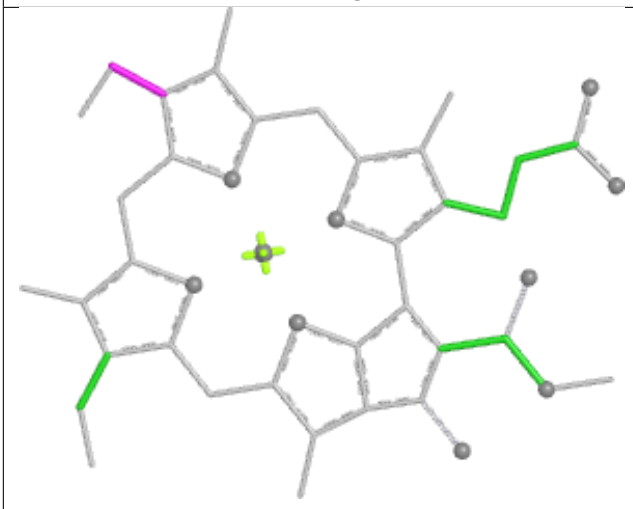
Ligand CLA cA 835



Bond lengths



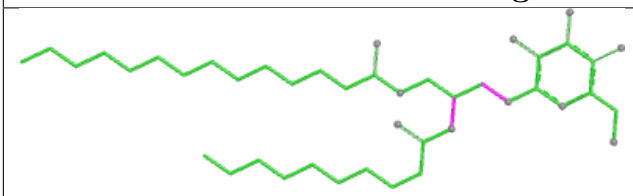
Bond angles



Torsions

Rings

Ligand LMG cB 947



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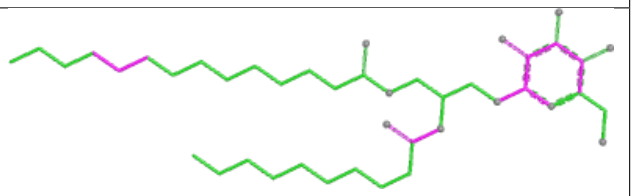
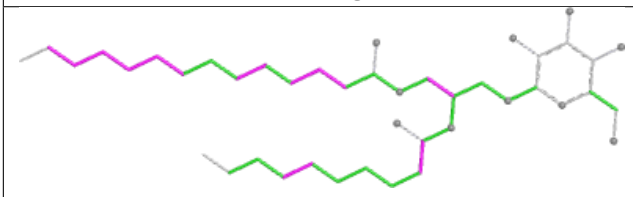
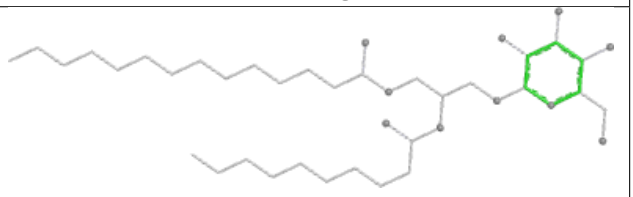


Bond angles

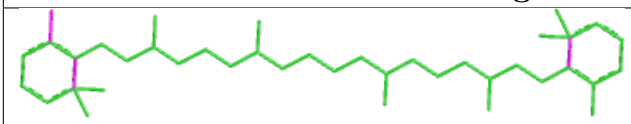


Torsions



Rings

Ligand BCR aA 850



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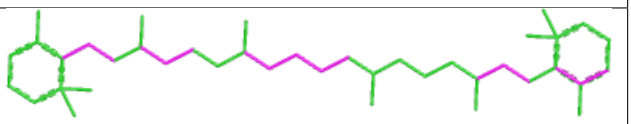
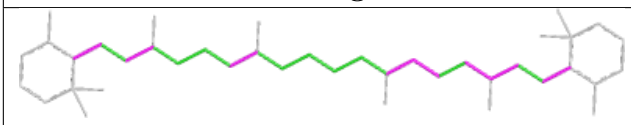
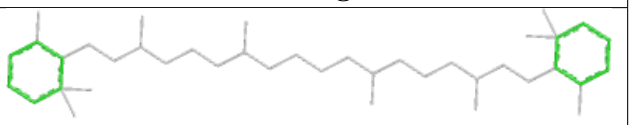


Bond angles

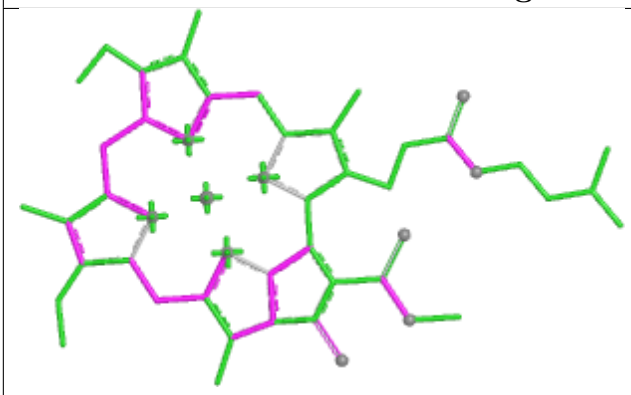


Torsions



Rings

Ligand CLA aA 821



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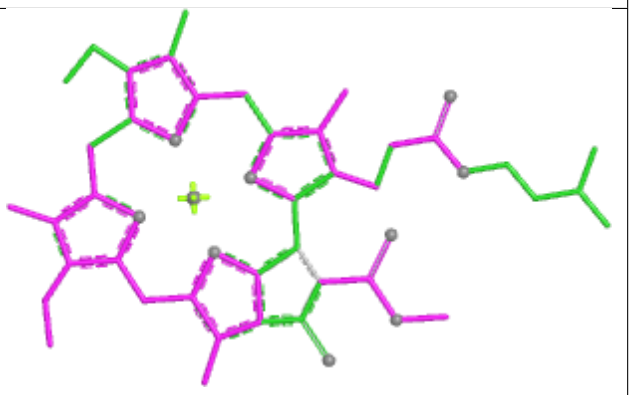
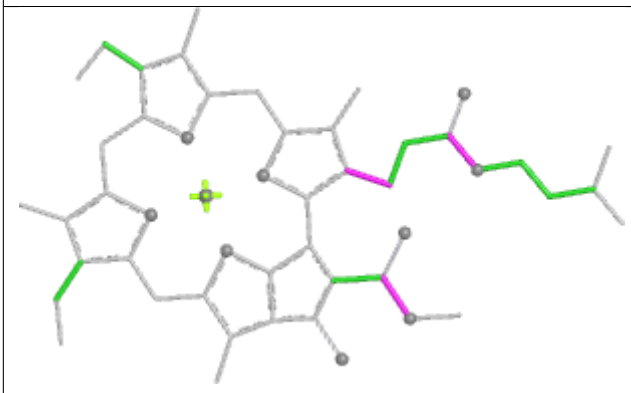
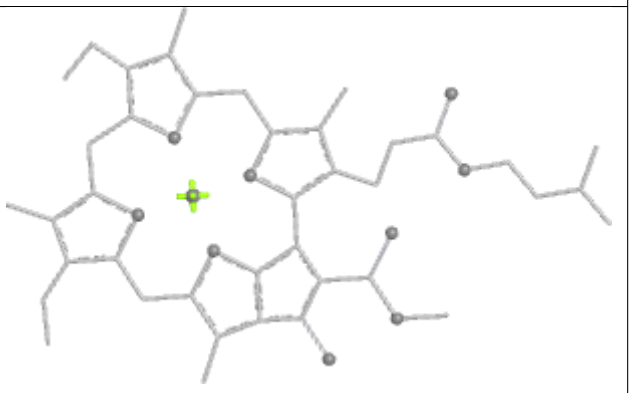


Bond angles

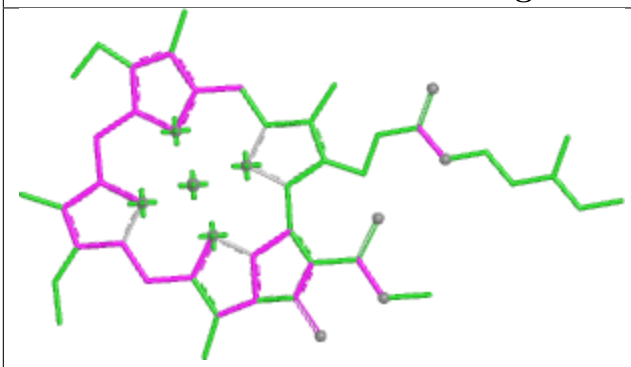


Torsions



Rings

Ligand CLA aA 841



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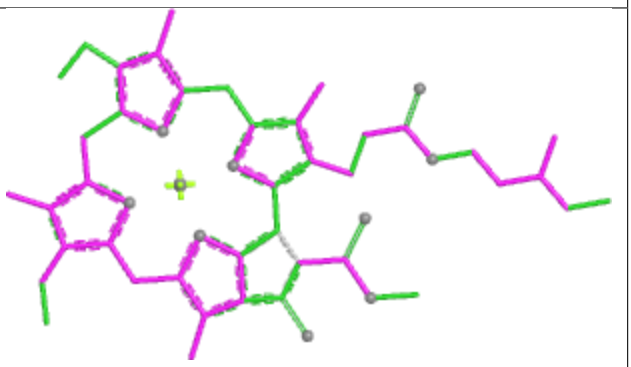
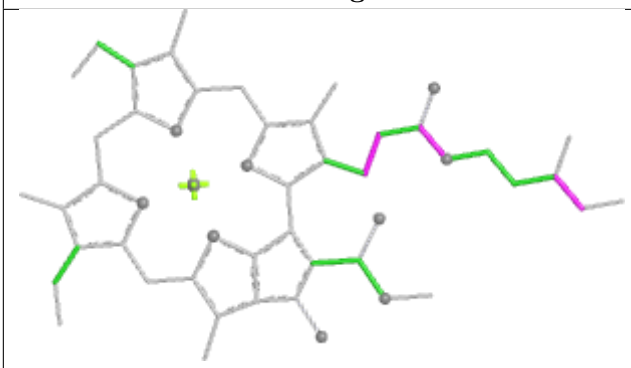
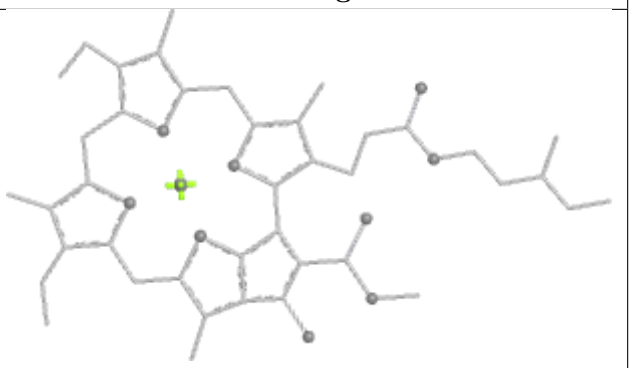


Bond angles

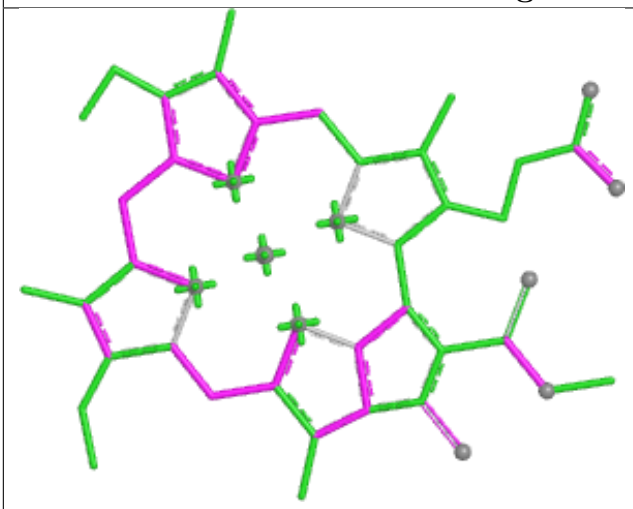


Torsions



Rings

Ligand CLA cB 932



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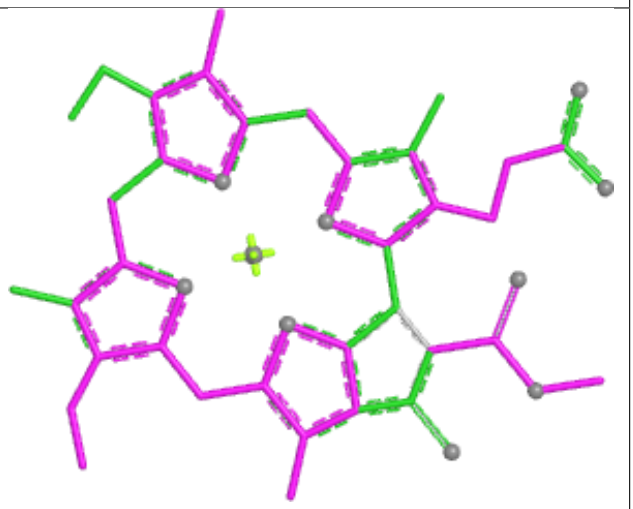
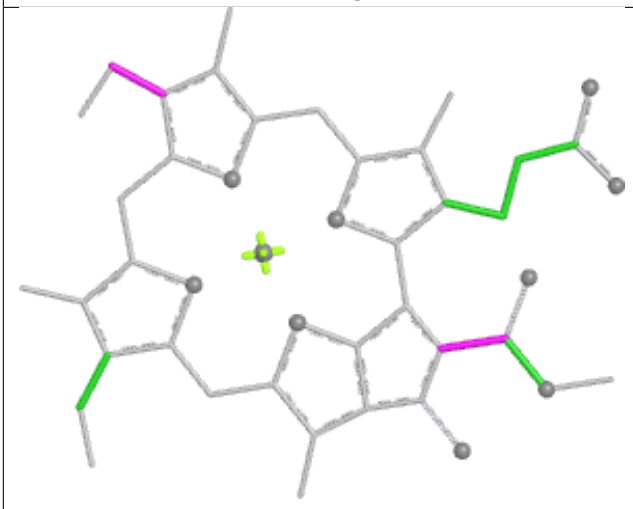


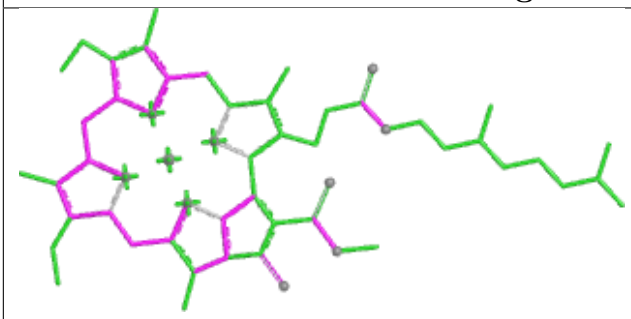
Bond angles



Torsions

Rings

Ligand CLA aB 909



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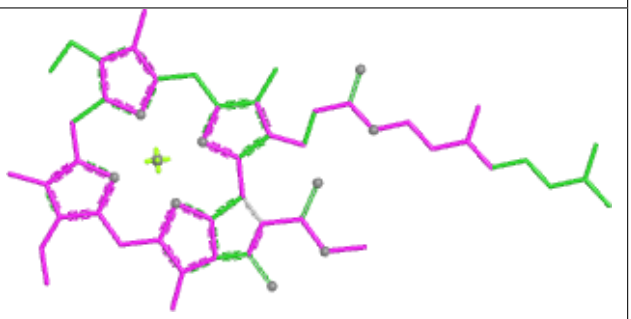
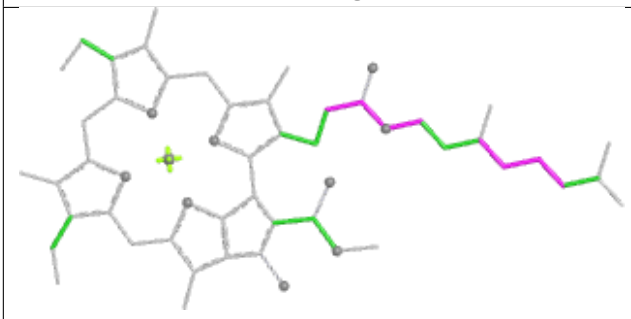
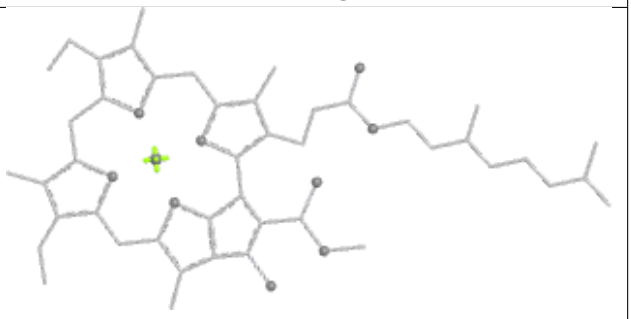


Bond angles

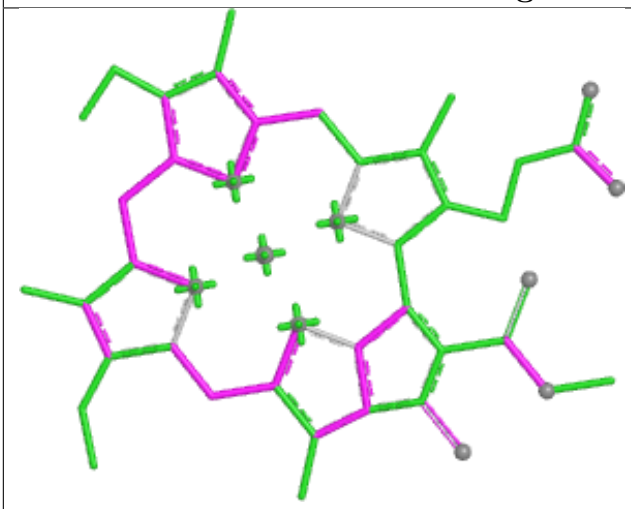


Torsions



Rings

Ligand CLA cB 911



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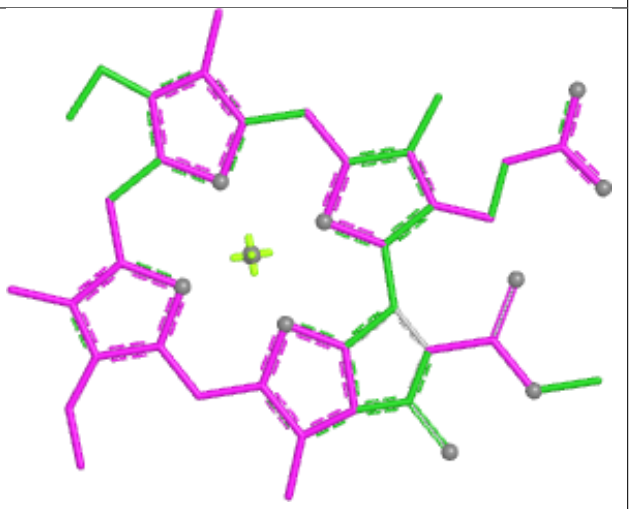
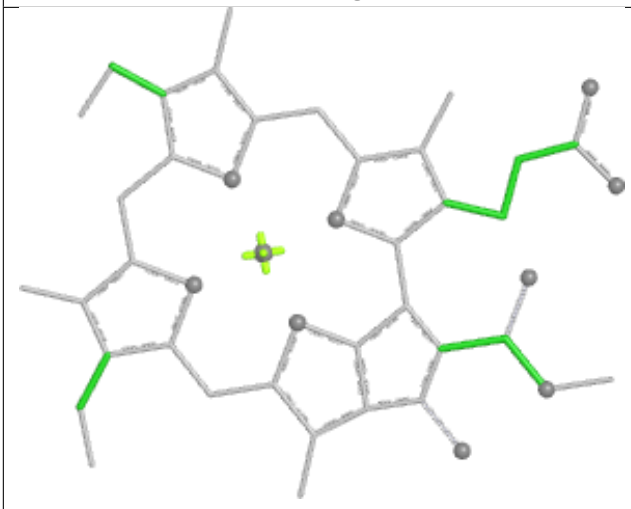


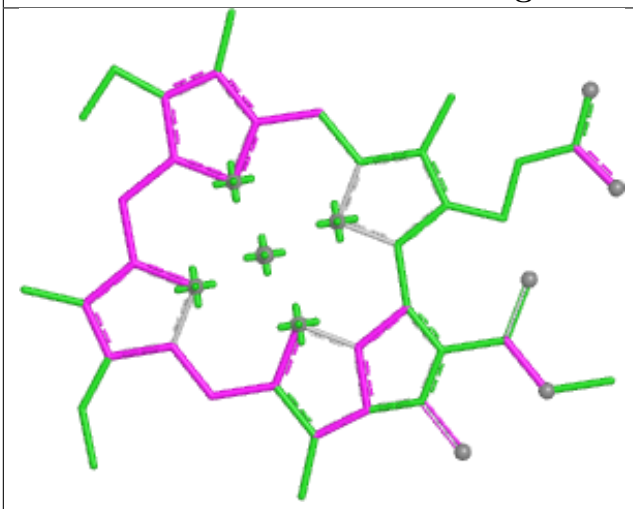
Bond angles



Torsions

Rings

Ligand CLA aA 813



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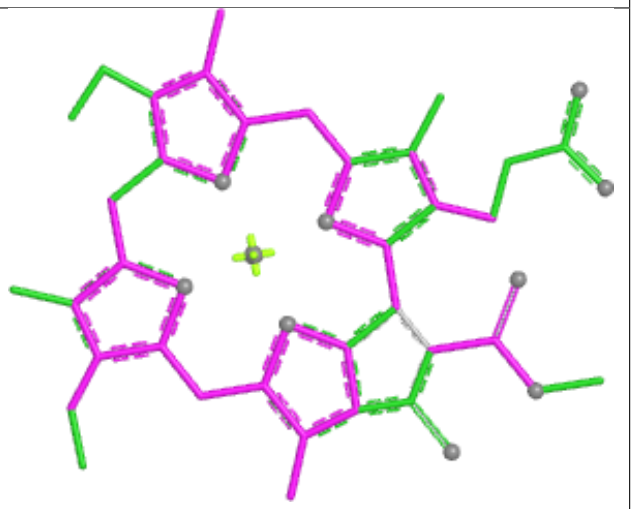
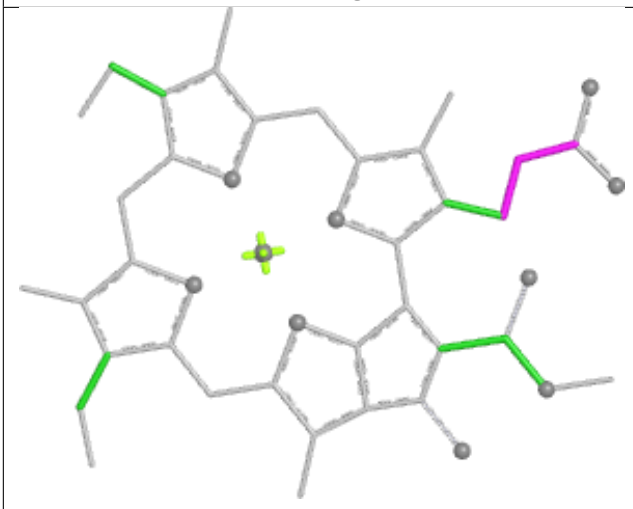


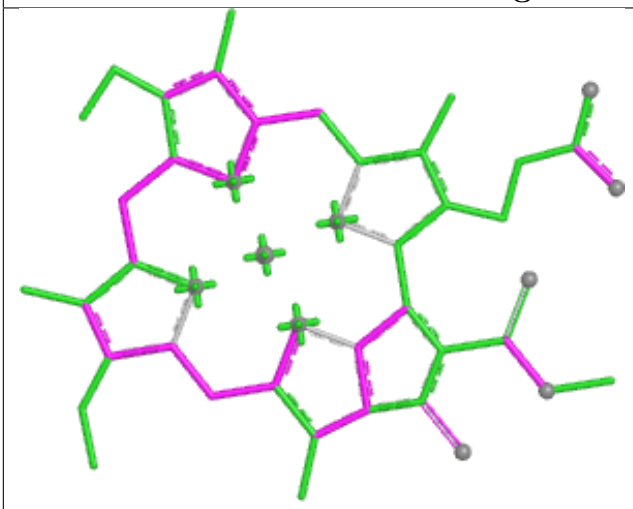
Bond angles



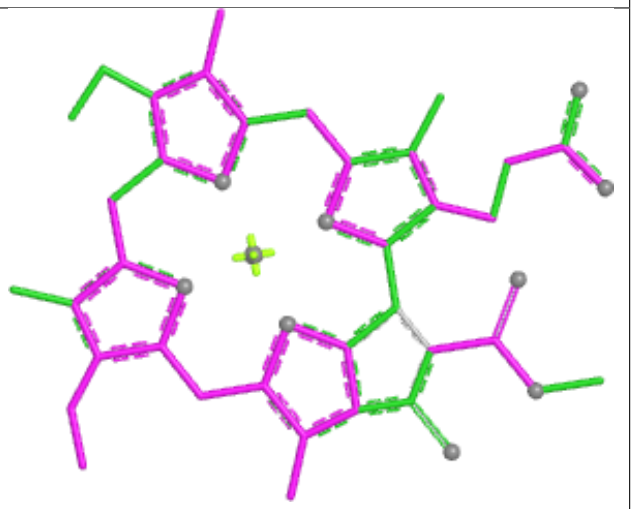
Torsions

Rings

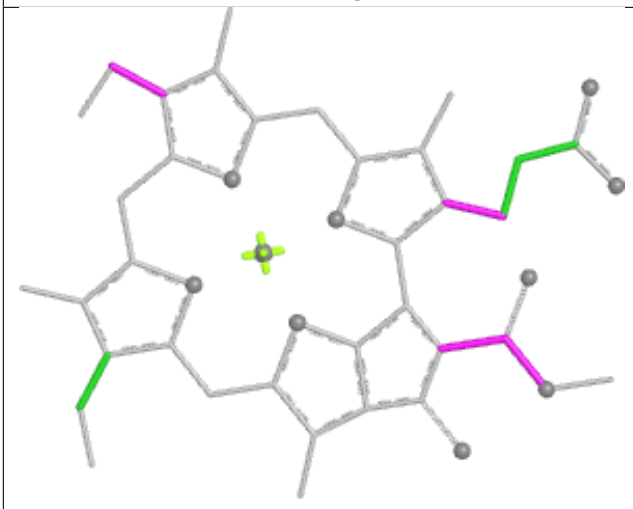
Ligand CLA bA 815



Bond lengths

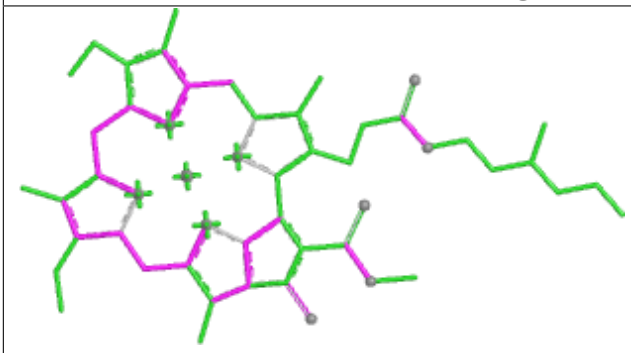
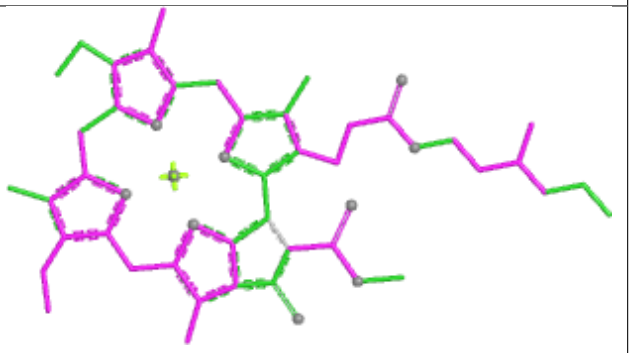
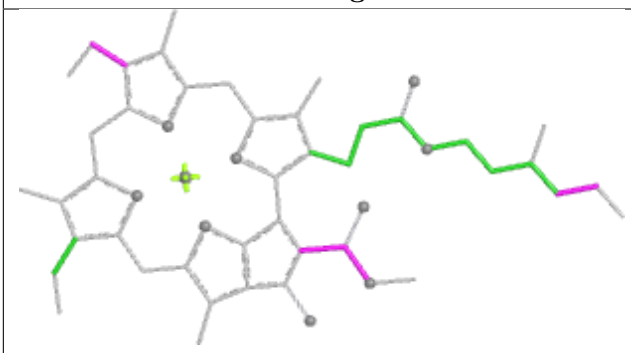
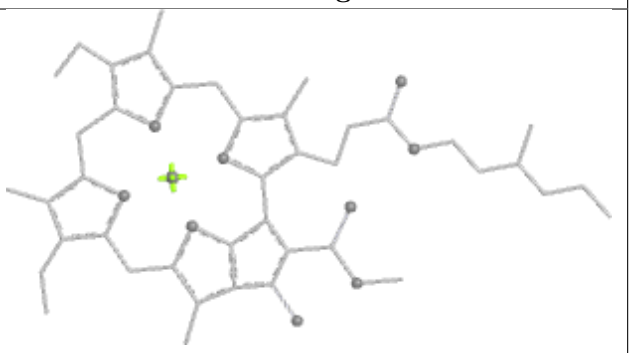


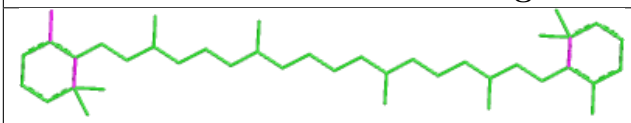
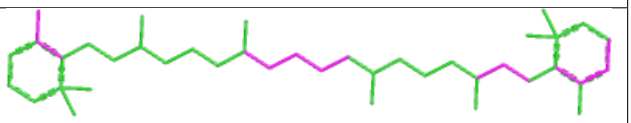
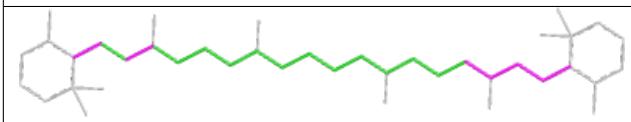
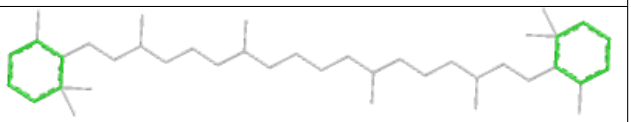
Bond angles



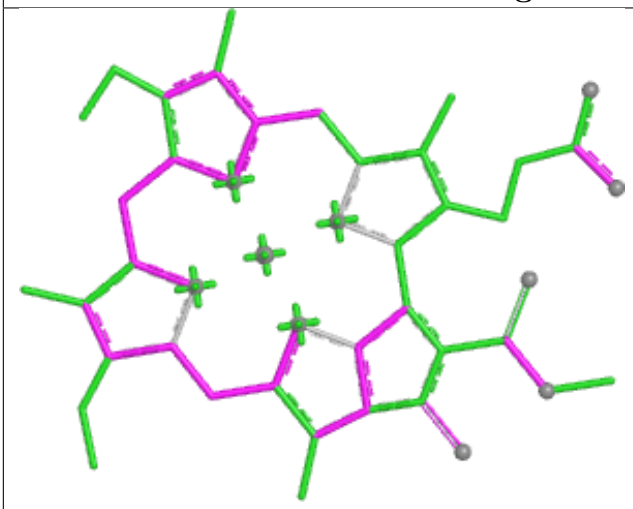
Torsions

Rings

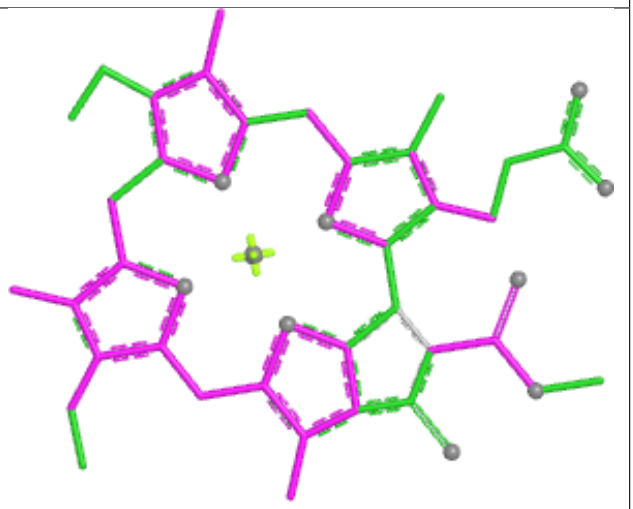
Ligand CLA bB 907	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR cB 941	
	
Bond lengths	Bond angles
	
Torsions	Rings

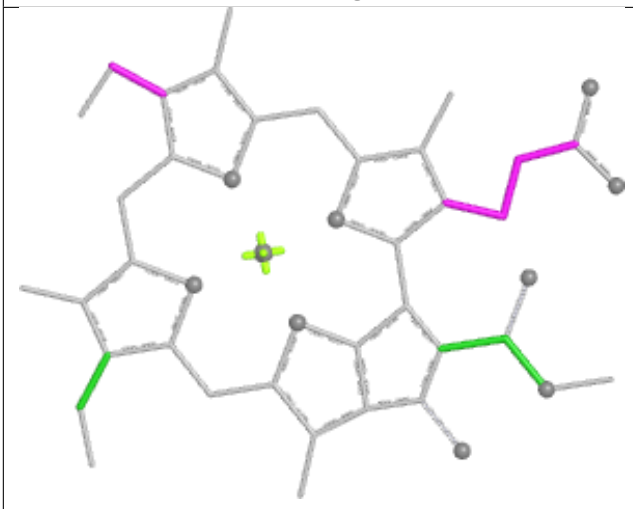
Ligand CLA aA 814



Bond lengths



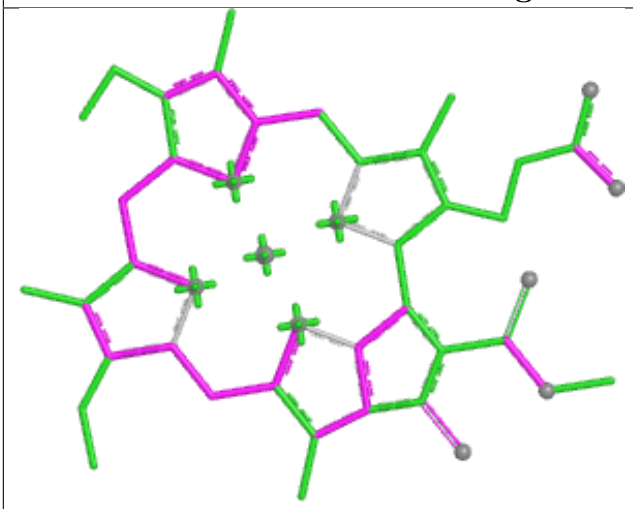
Bond angles



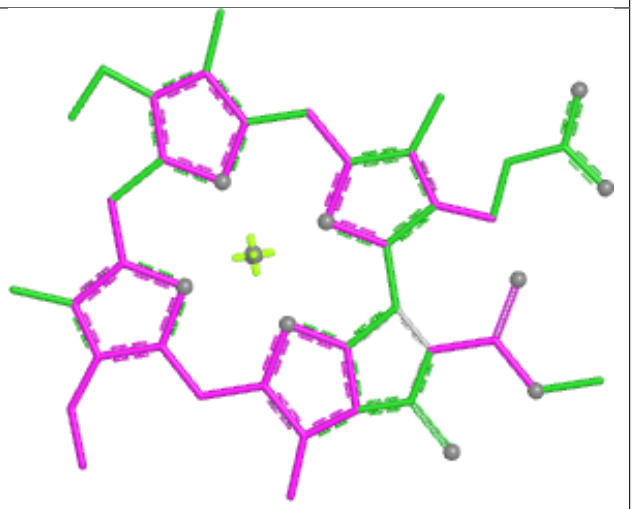
Torsions

Rings

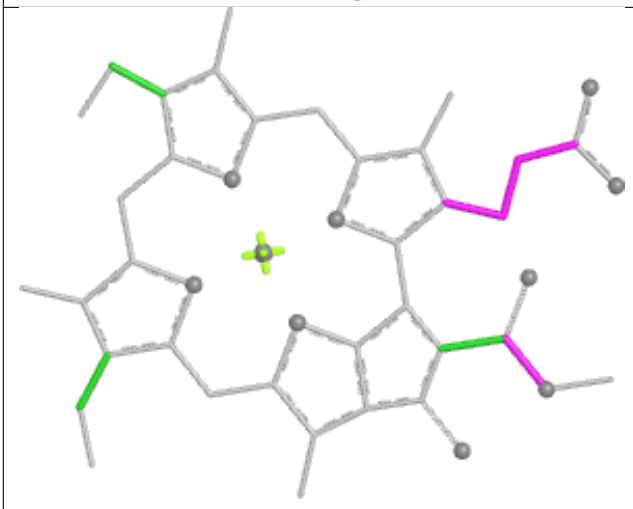
Ligand CLA aA 844



Bond lengths



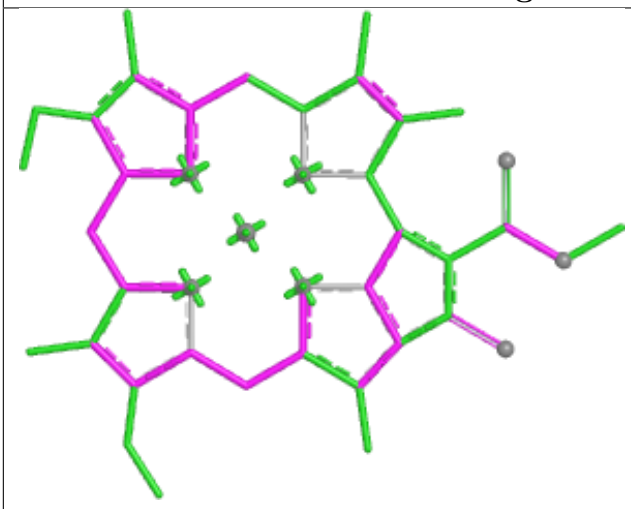
Bond angles



Torsions

Rings

Ligand CLA aB 949



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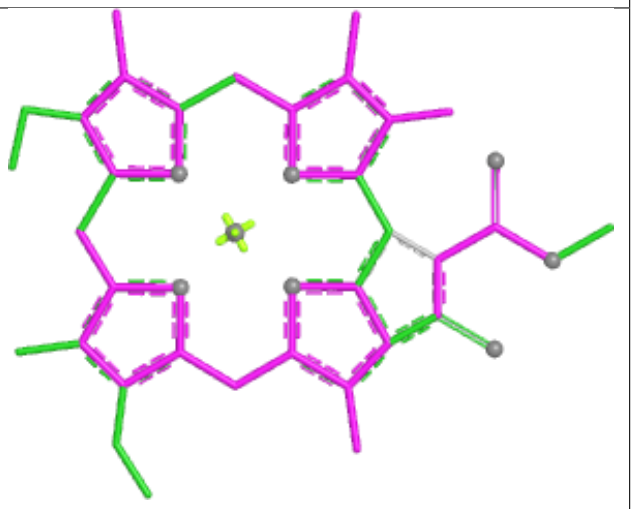
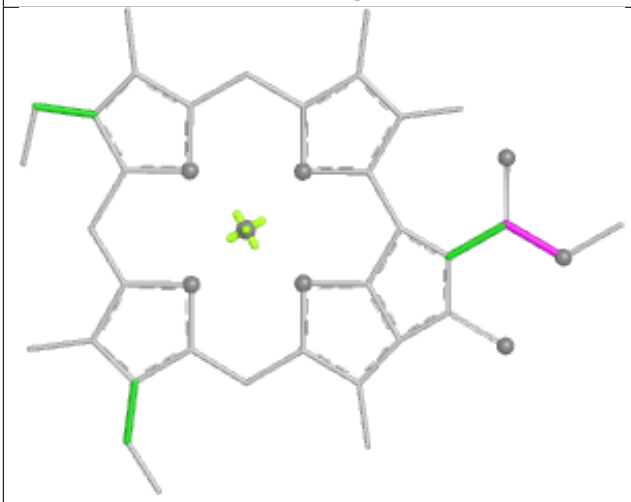
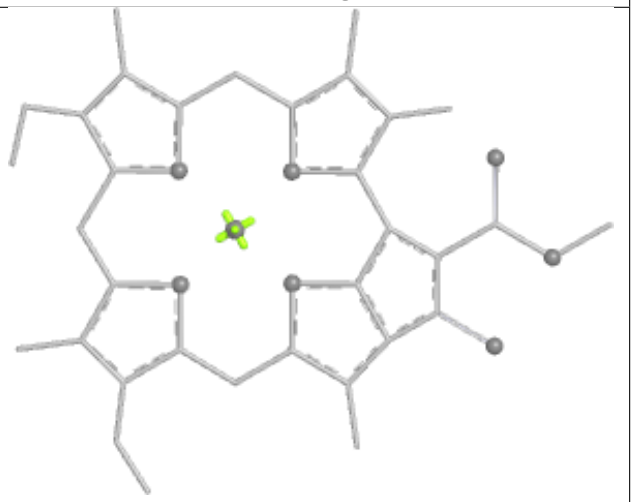


Bond angles

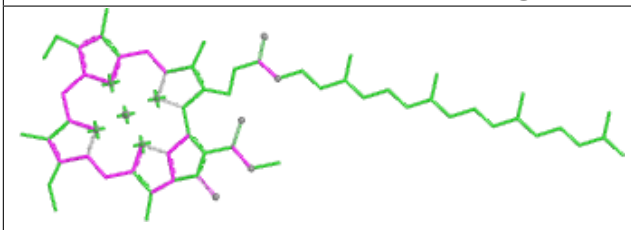


Torsions

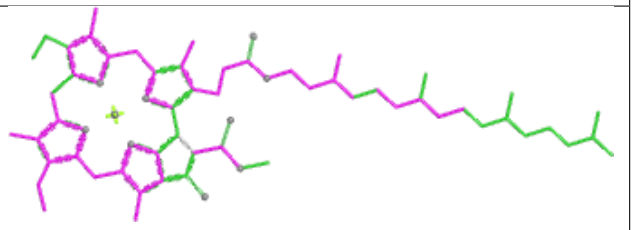


Rings

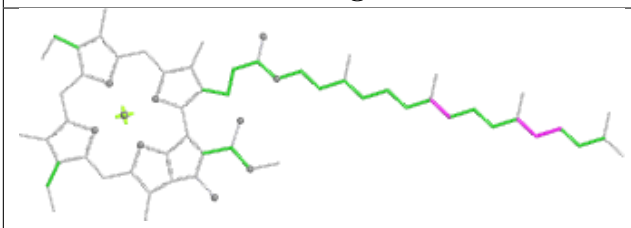
Ligand CLA aA 803



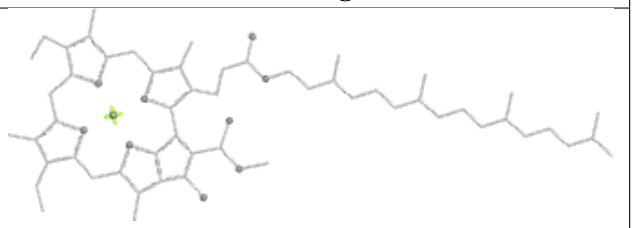
Bond lengths



Bond angles

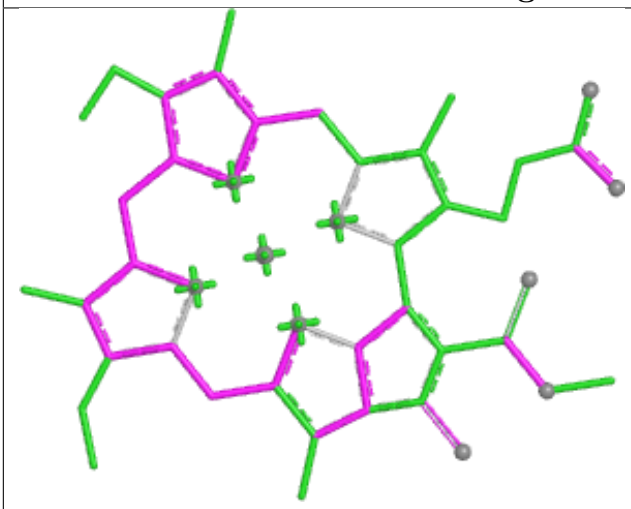


Torsions

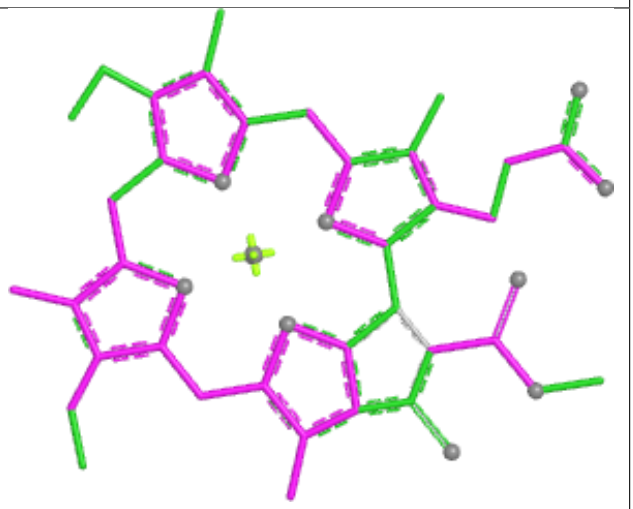


Rings

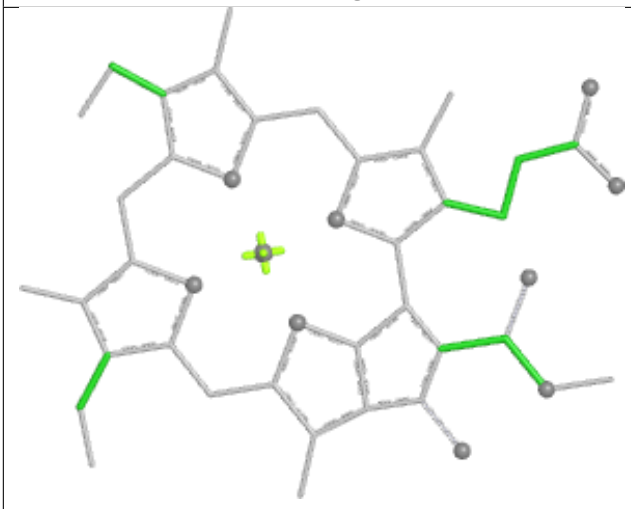
Ligand CLA aL 204



Bond lengths



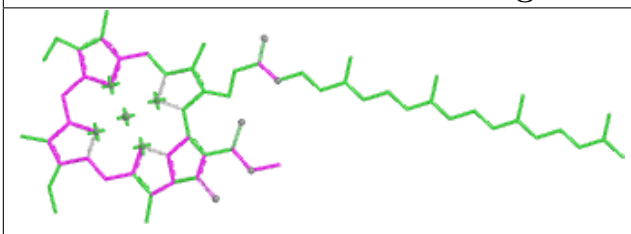
Bond angles



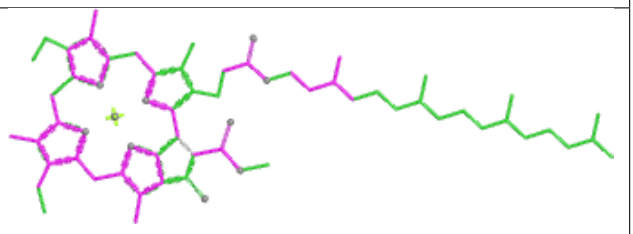
Torsions

Rings

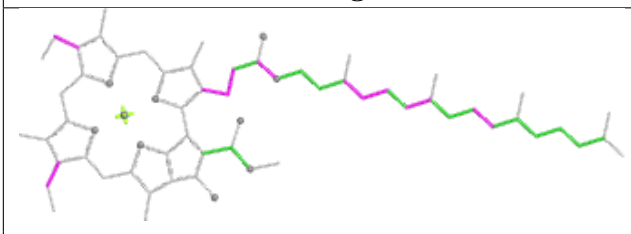
Ligand CLA cB 912



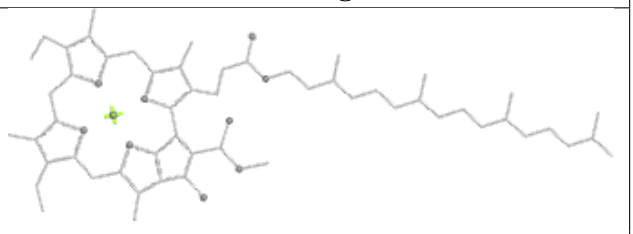
Bond lengths



Bond angles

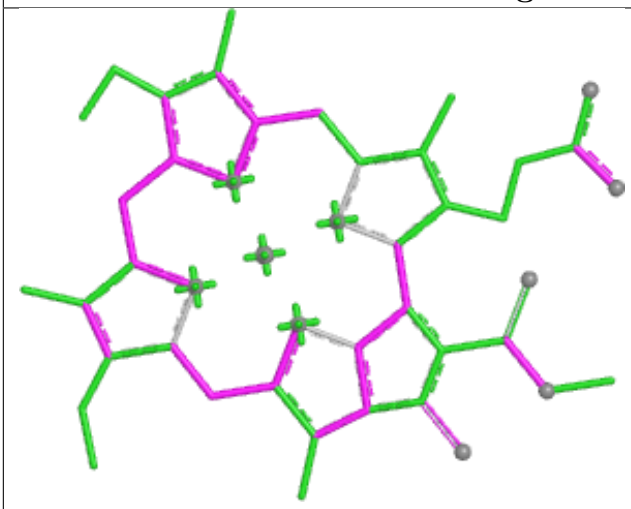


Torsions



Rings

Ligand CLA cB 939



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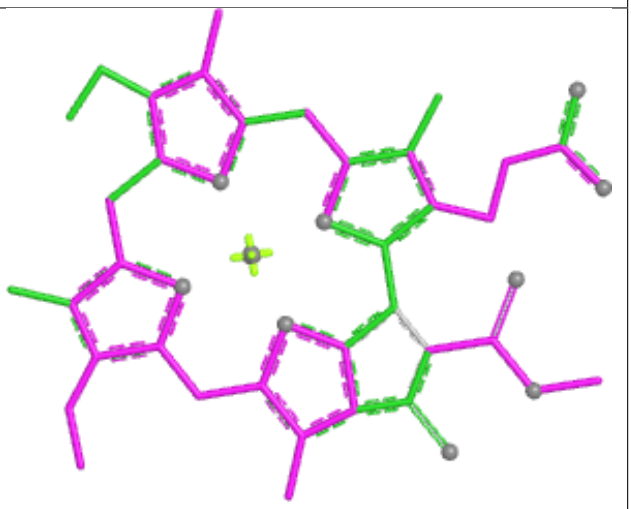
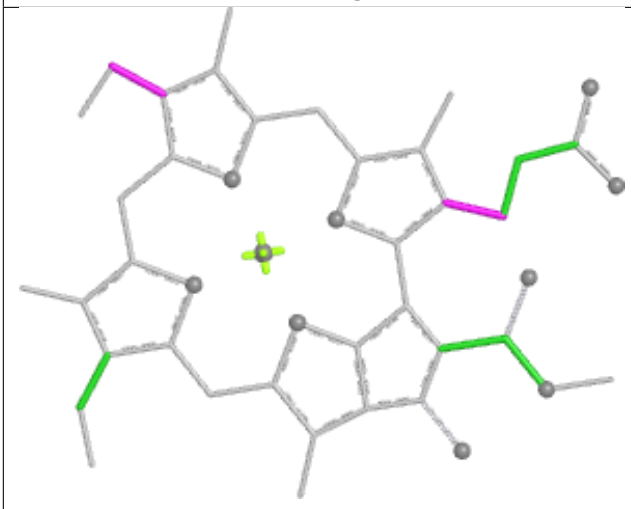


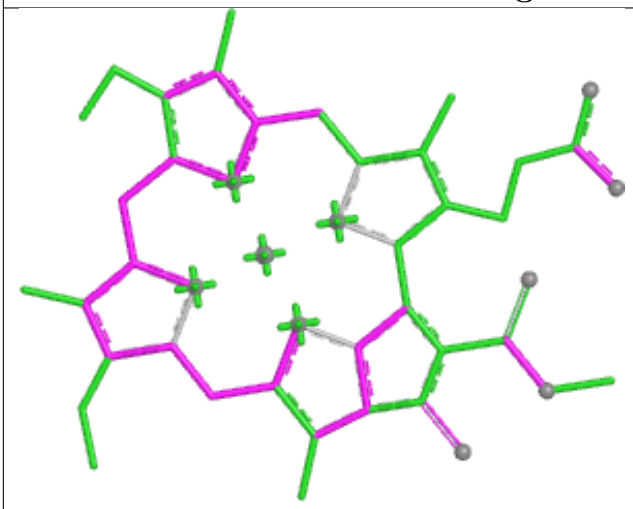
Bond angles



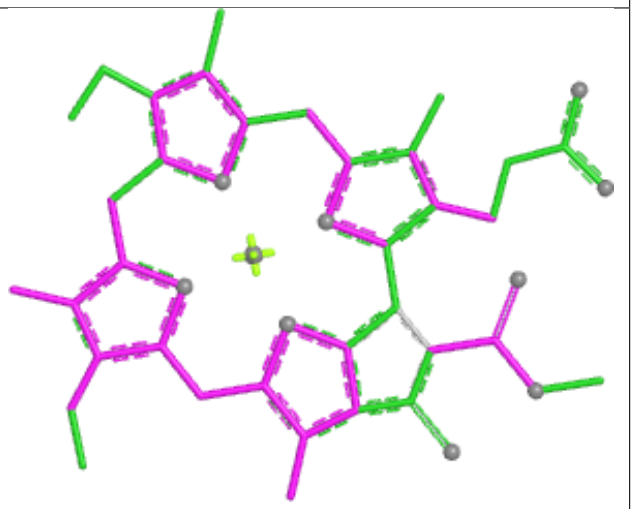
Torsions

Rings

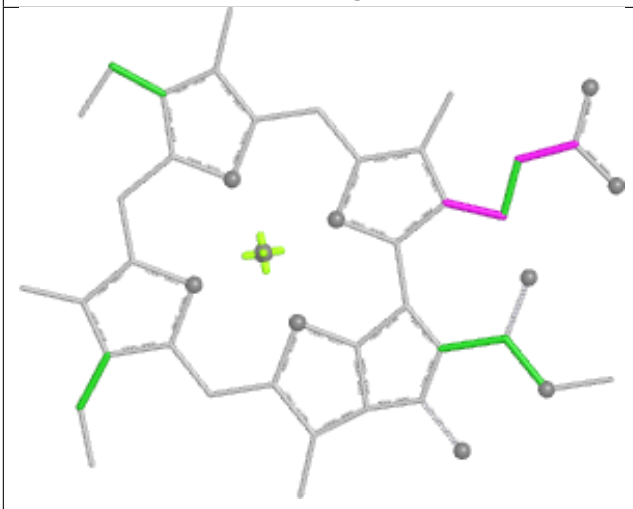
Ligand CLA cA 816



Bond lengths



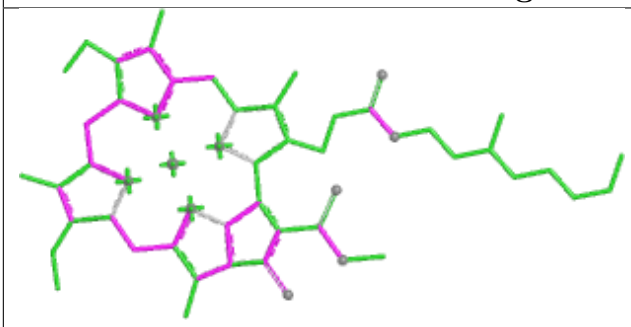
Bond angles



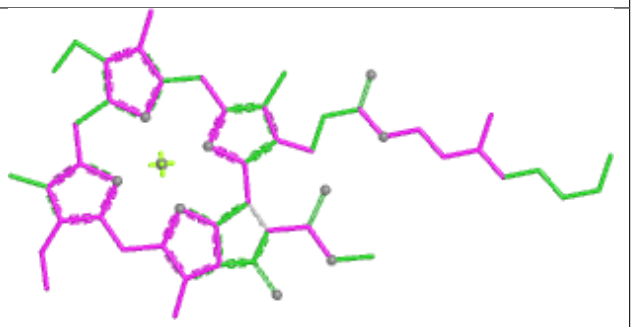
Torsions

Rings

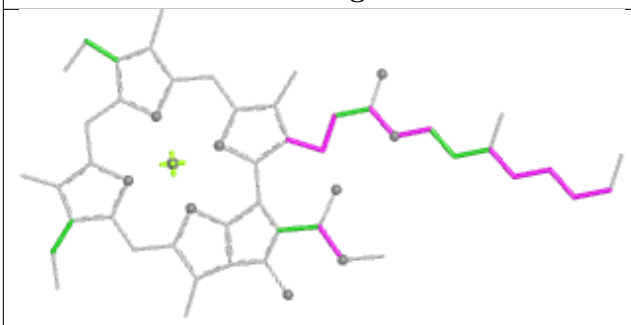
Ligand CLA cA 818



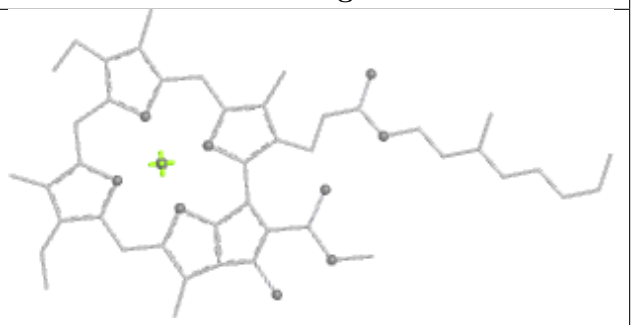
Bond lengths



Bond angles



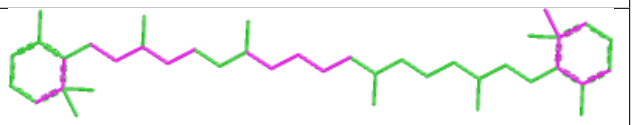
Torsions



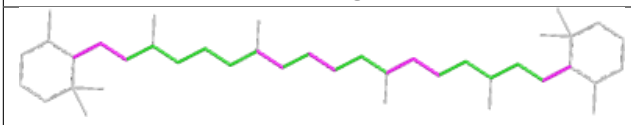
Rings

Ligand BCR aB 945

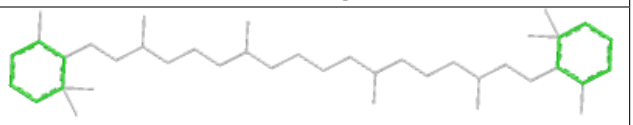
Bond lengths



Bond angles

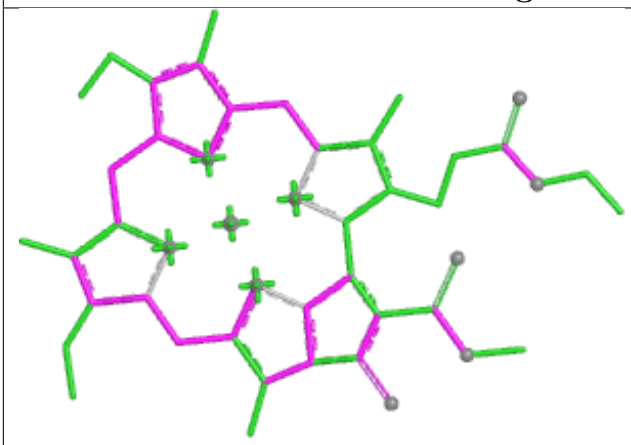


Torsions

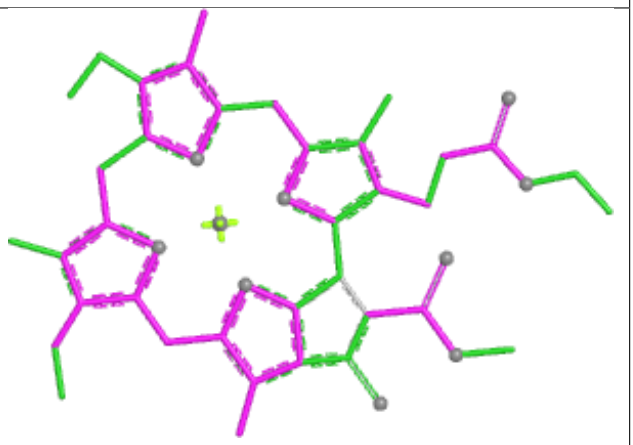


Rings

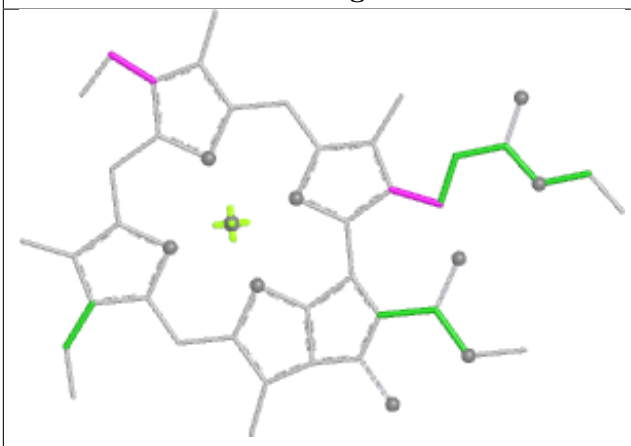
Ligand CLA aB 937



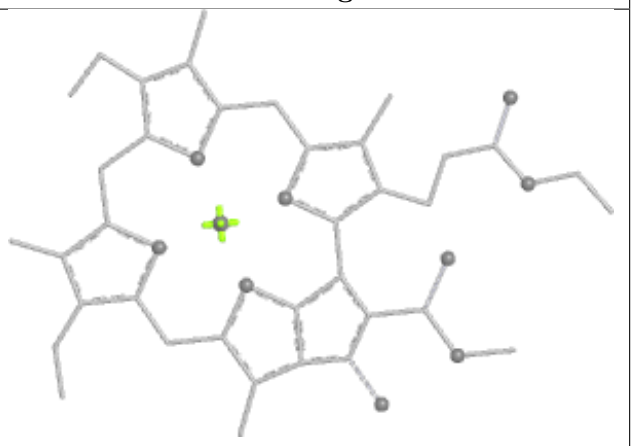
Bond lengths



Bond angles

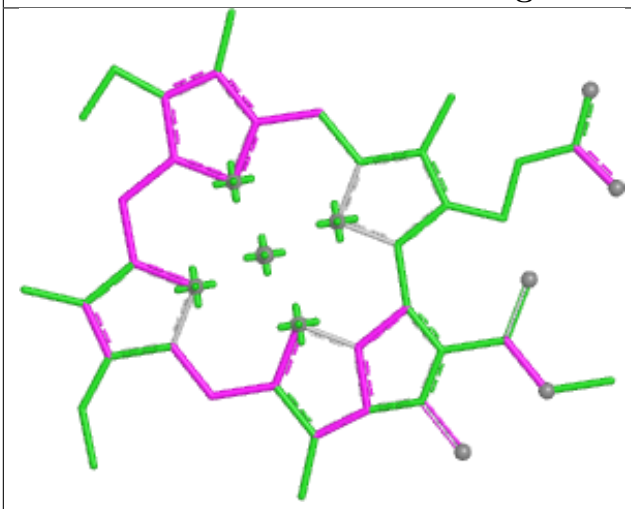


Torsions



Rings

Ligand CLA aB 922



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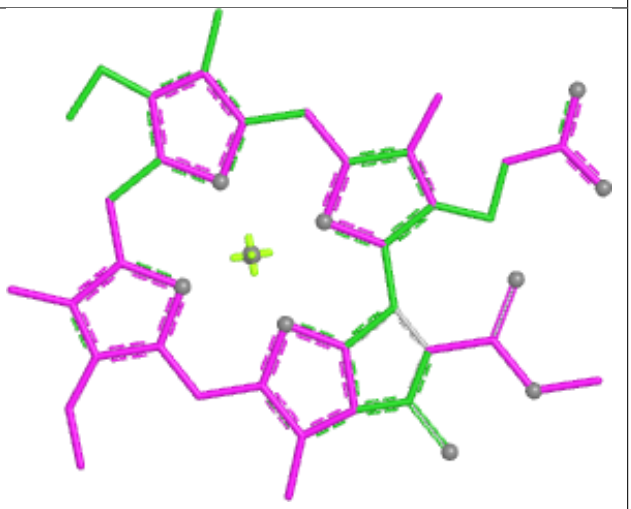
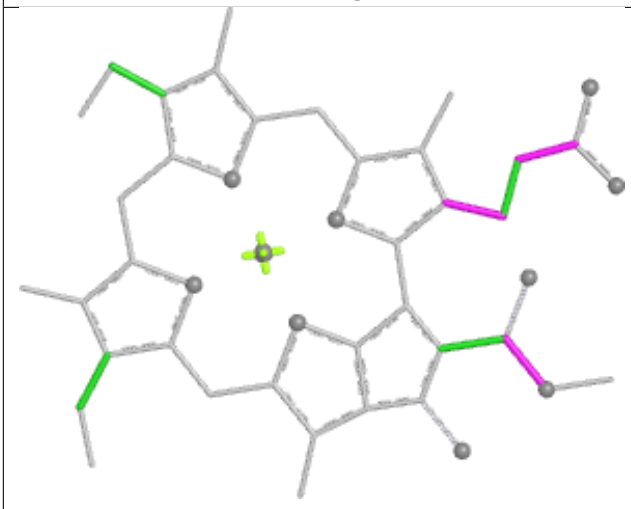


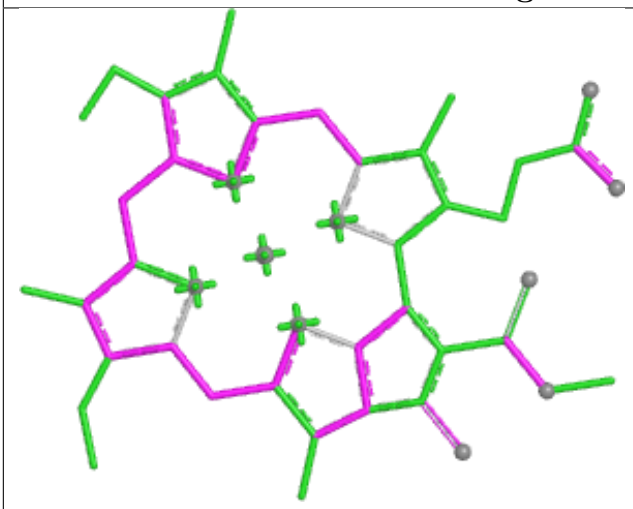
Bond angles



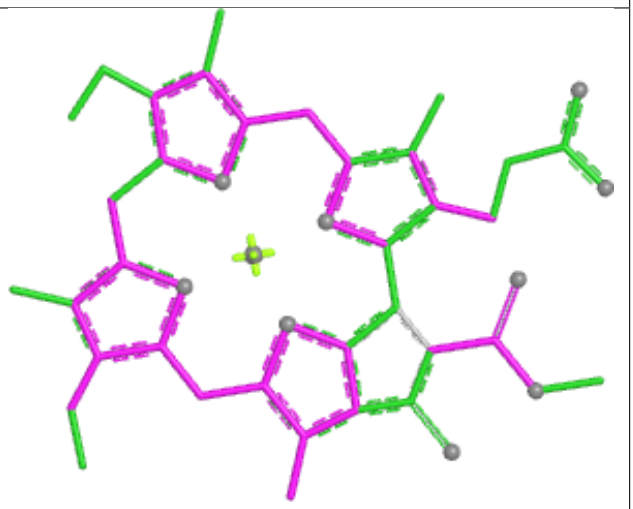
Torsions

Rings

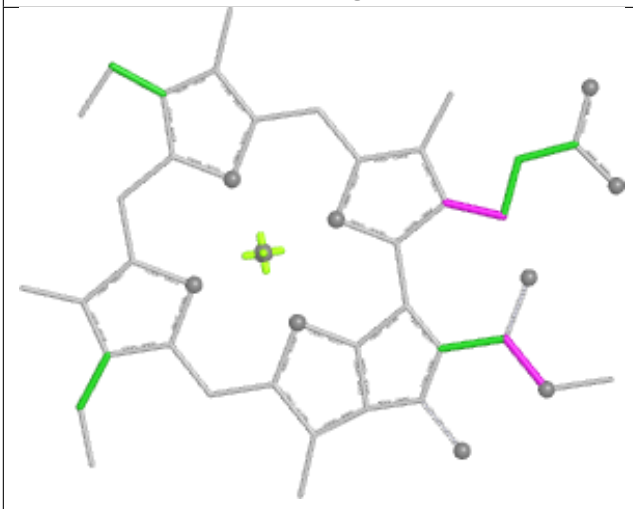
Ligand CLA cB 934



Bond lengths



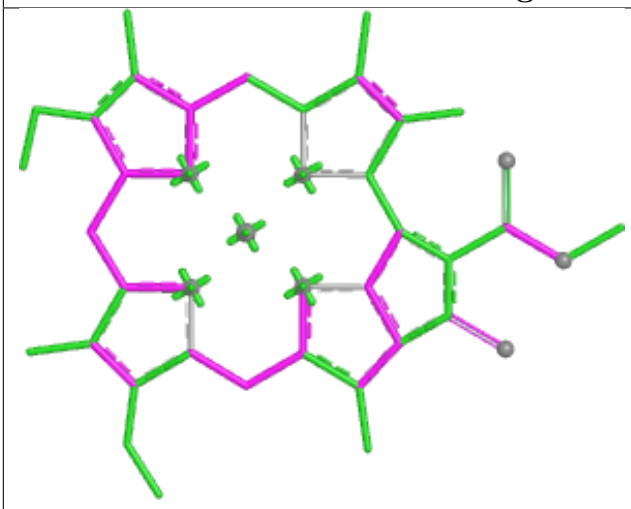
Bond angles



Torsions

Rings

Ligand CLA cB 949



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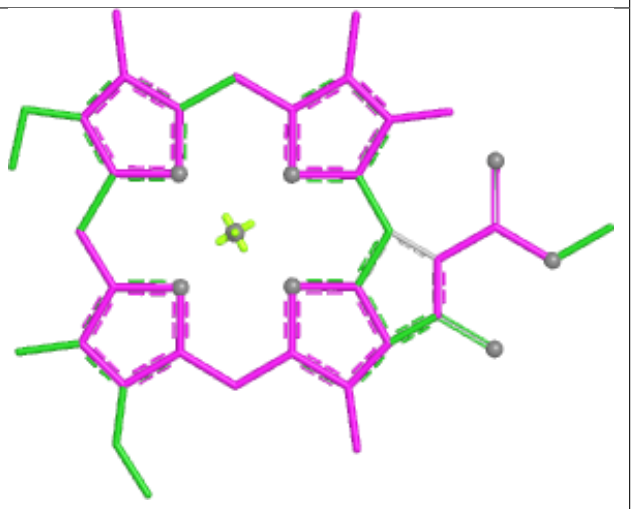
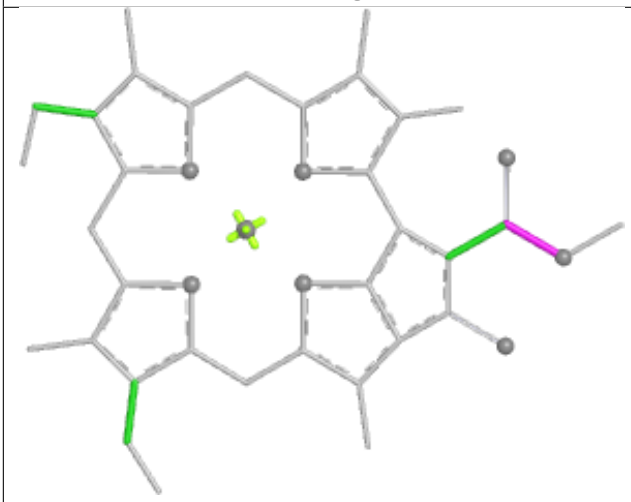


Bond angles



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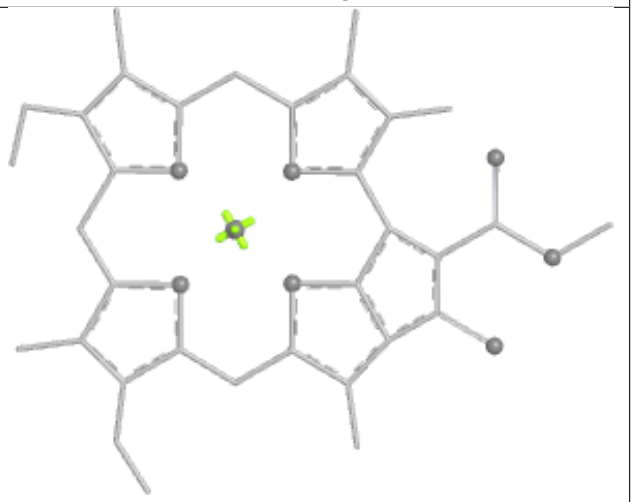
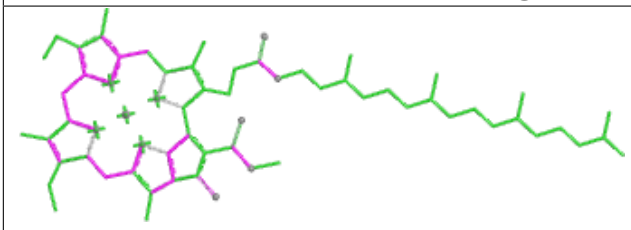


Rings

Ligand CLA cA 842



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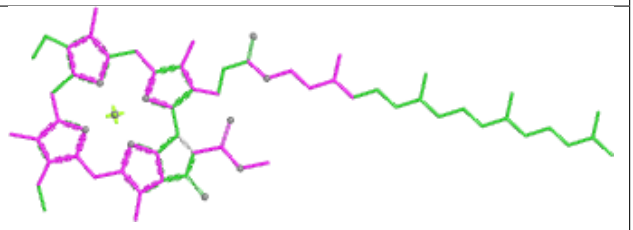
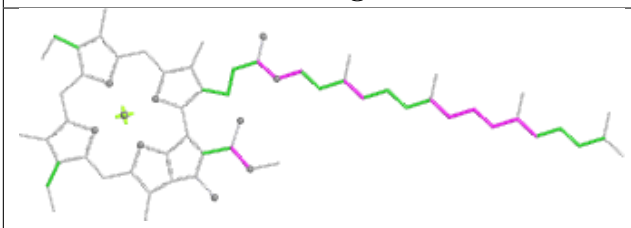


Bond angles



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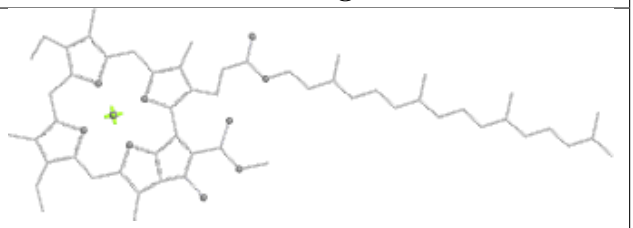
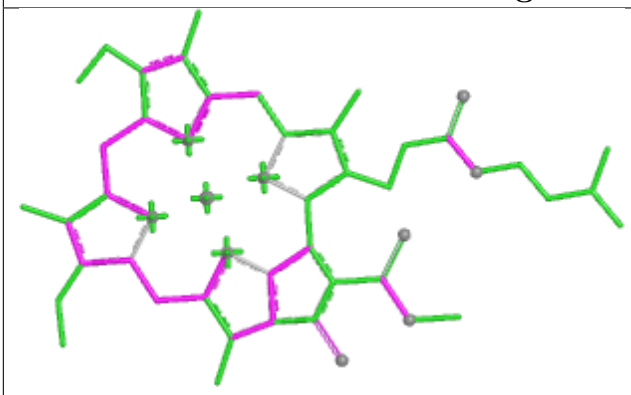


Rings

Ligand CLA aB 928



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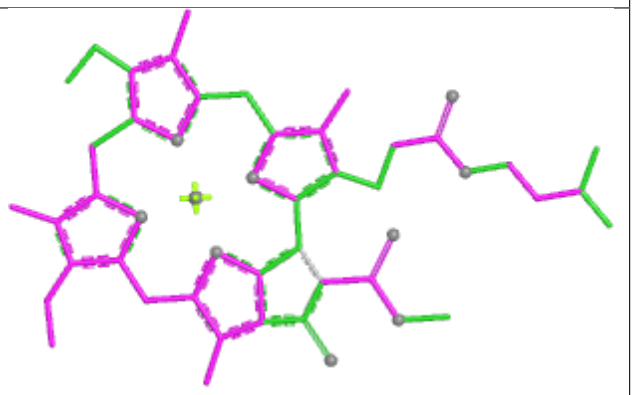
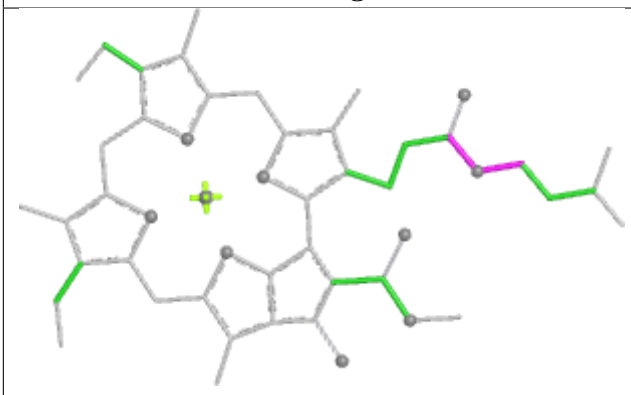
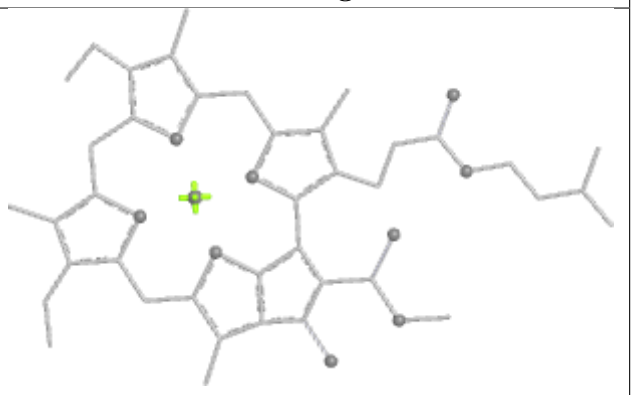


Bond angles



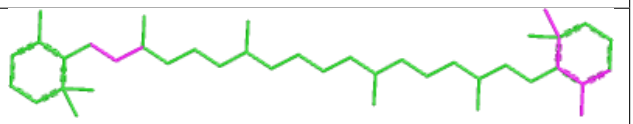
Torsions



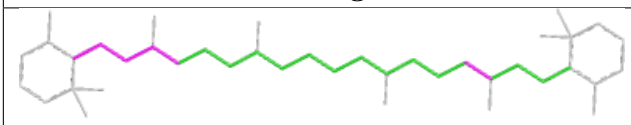
Rings

Ligand BCR cB 943

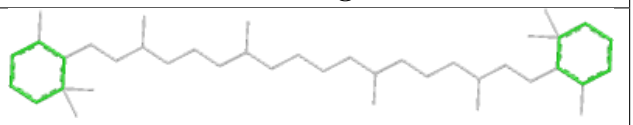
Bond lengths



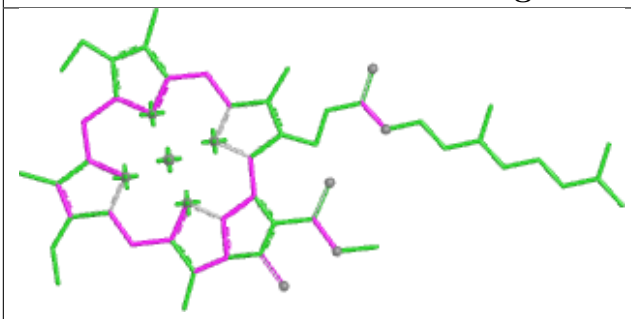
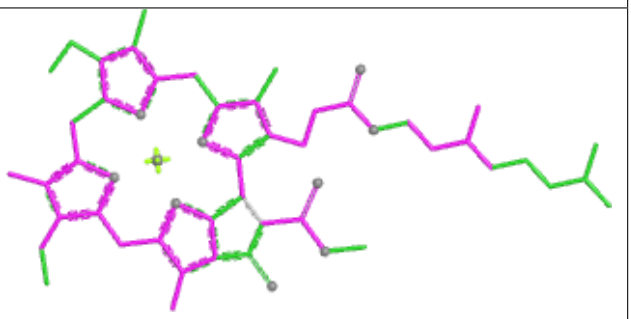
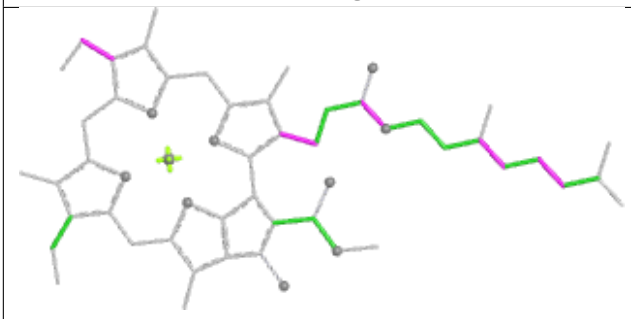
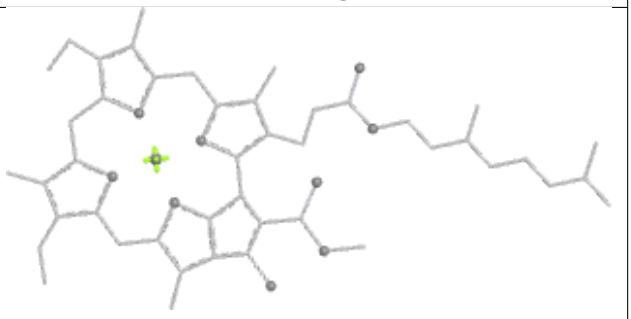
Bond angles

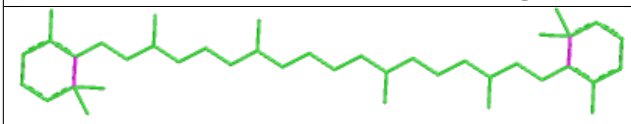
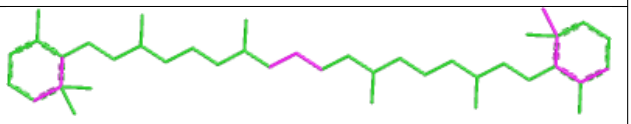
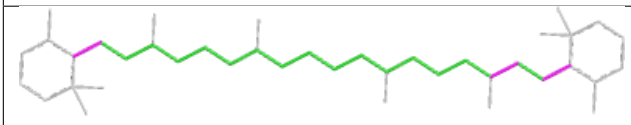
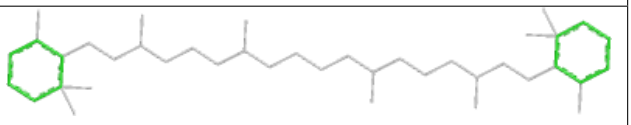


Torsions

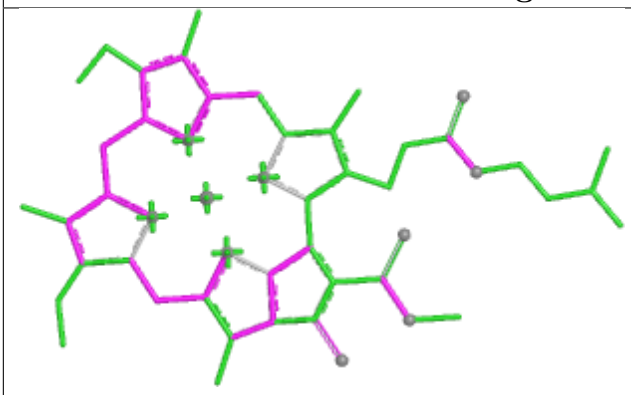


Rings

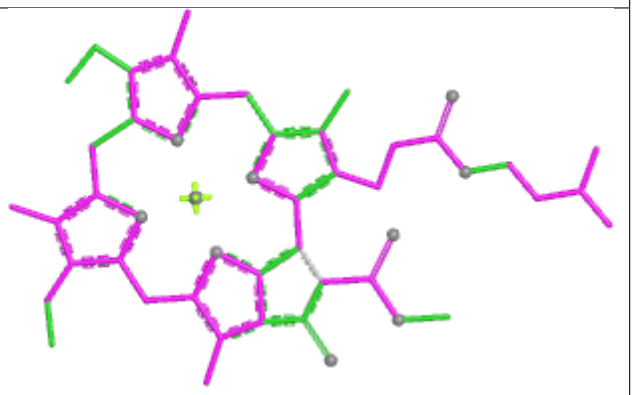
Ligand CLA bB 917	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR aL 206	
	
Bond lengths	Bond angles
	
Torsions	Rings

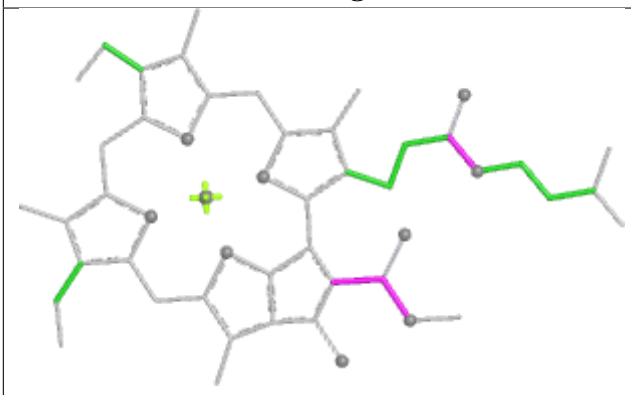
Ligand CLA aB 935



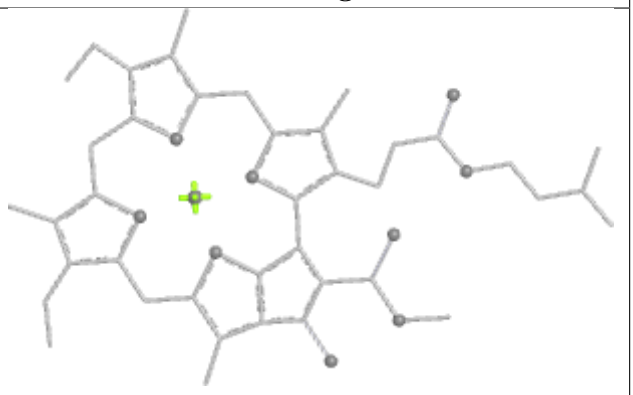
Bond lengths



Bond angles

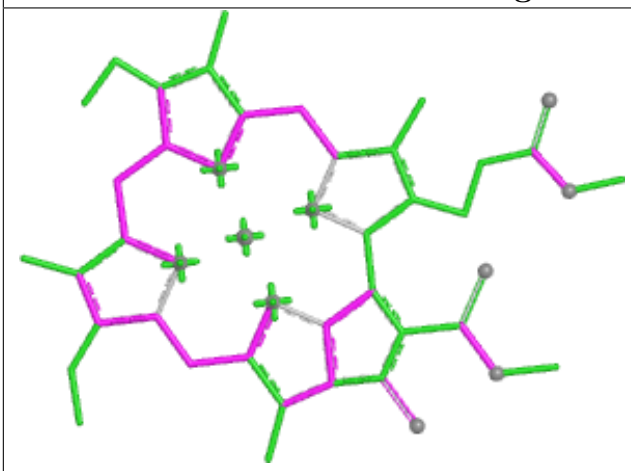


Torsions

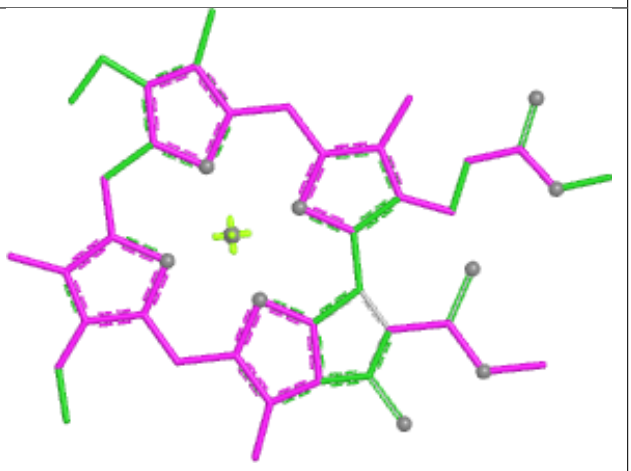


Rings

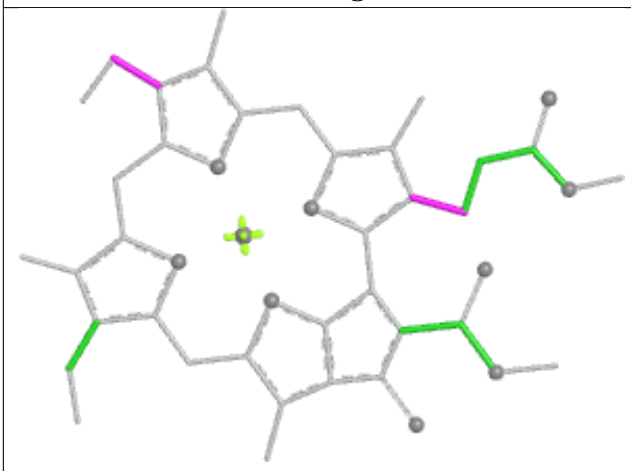
Ligand CLA bB 918



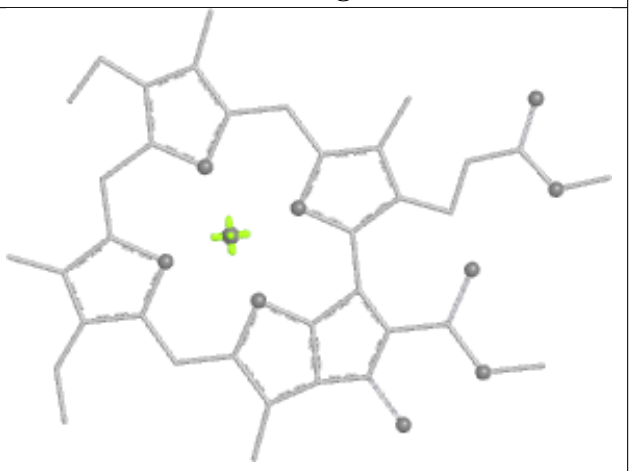
Bond lengths



Bond angles

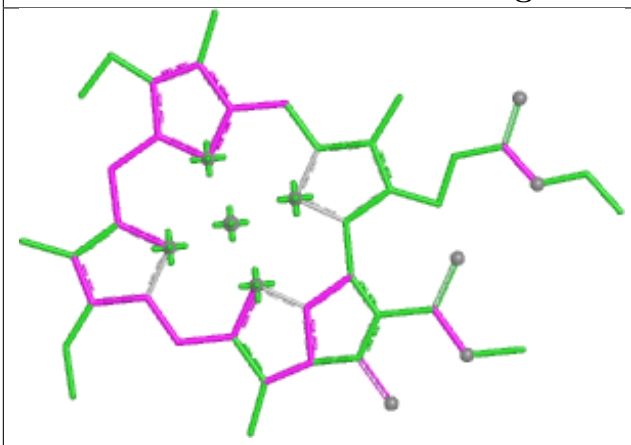


Torsions

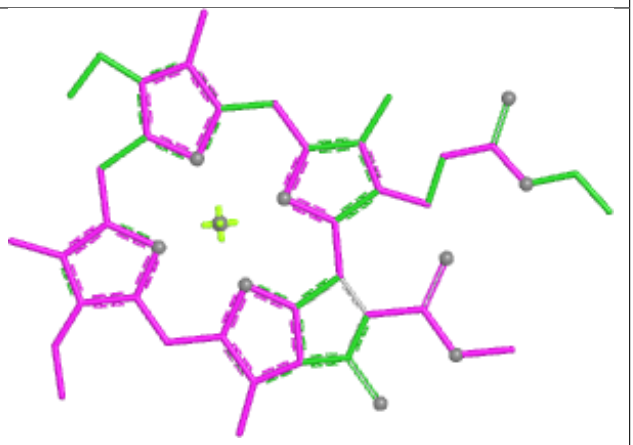


Rings

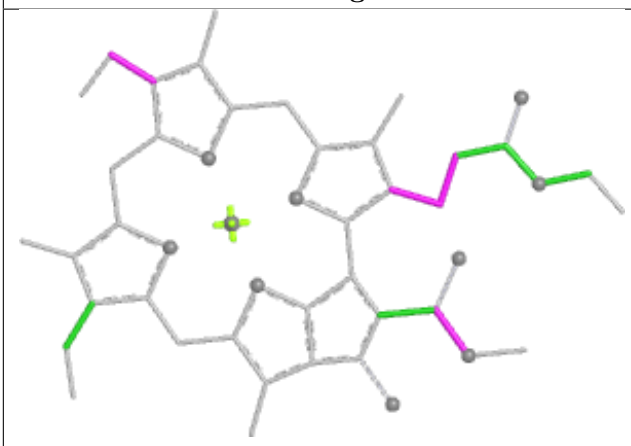
Ligand CLA aA 824



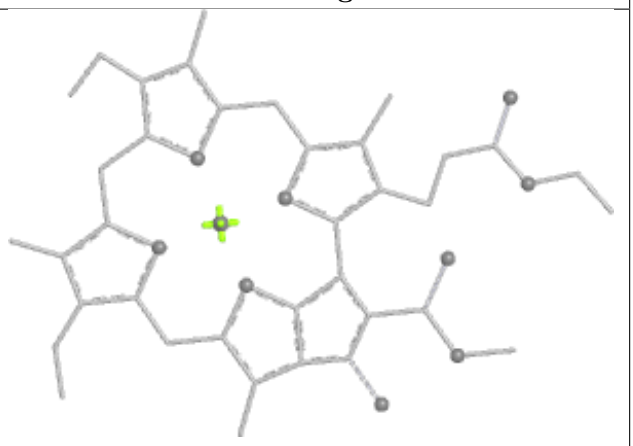
Bond lengths



Bond angles



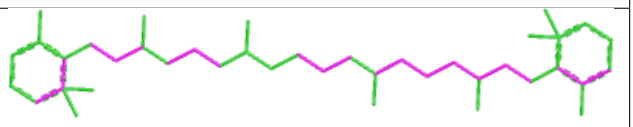
Torsions



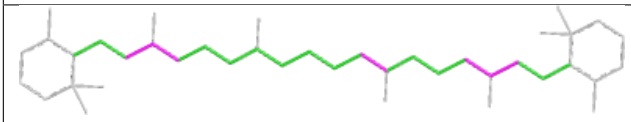
Rings

Ligand BCR aA 851

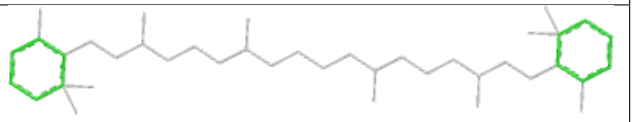
Bond lengths



Bond angles

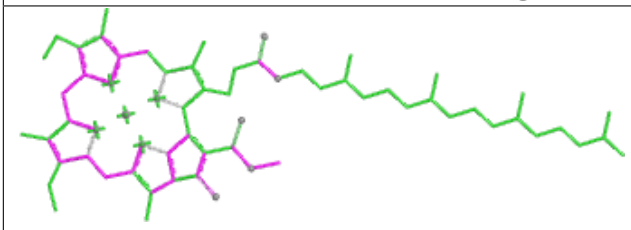


Torsions

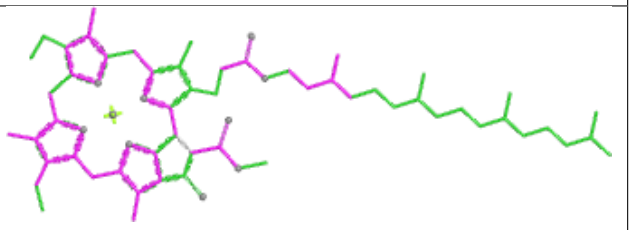


Rings

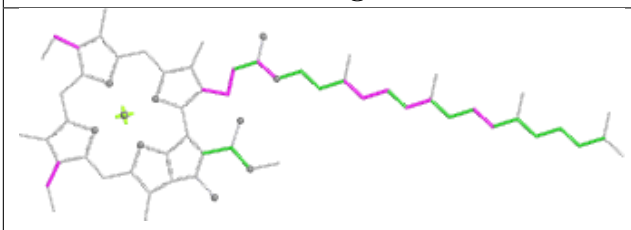
Ligand CLA bB 912



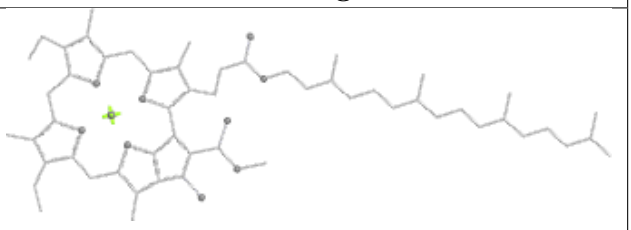
Bond lengths



Bond angles

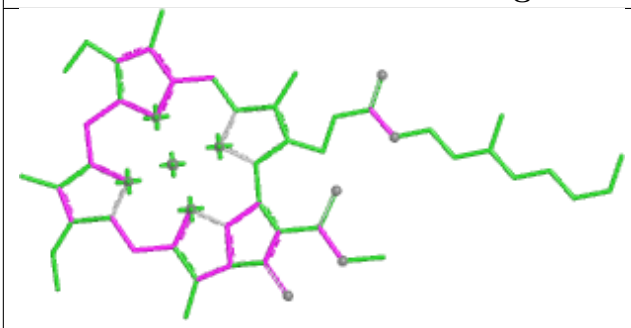


Torsions



Rings

Ligand CLA bA 818



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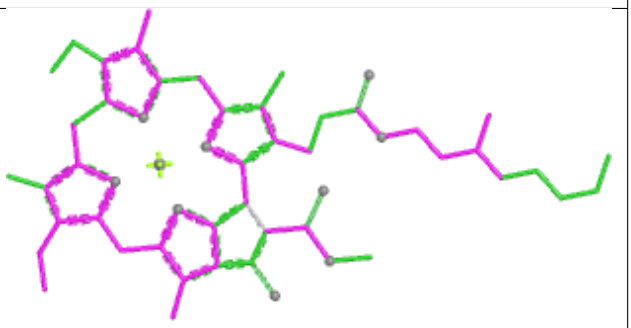
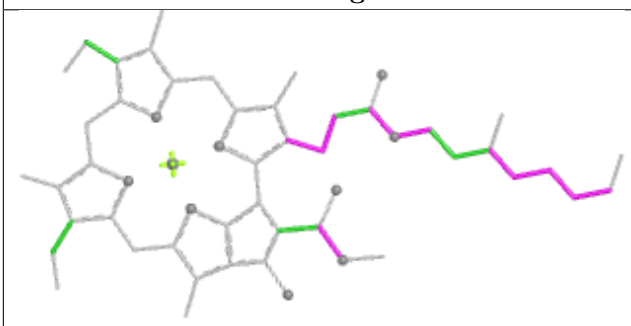
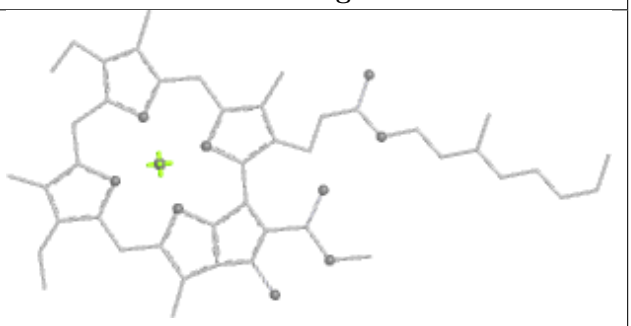


Bond angles

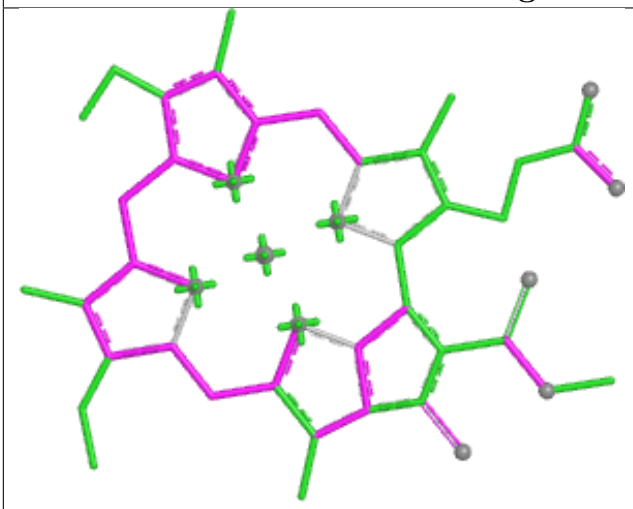


Torsions

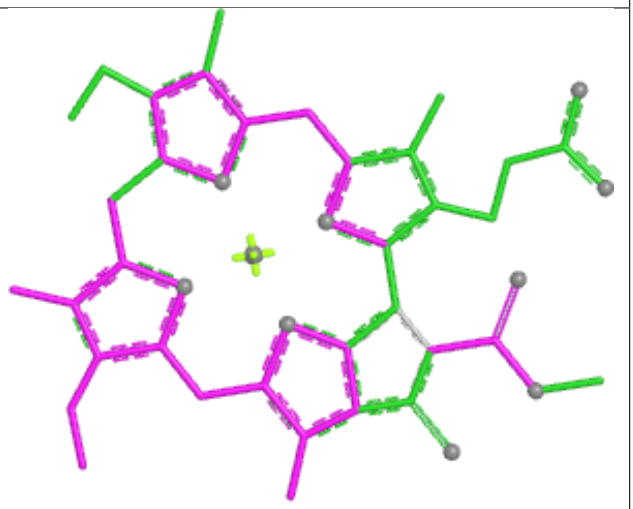


Rings

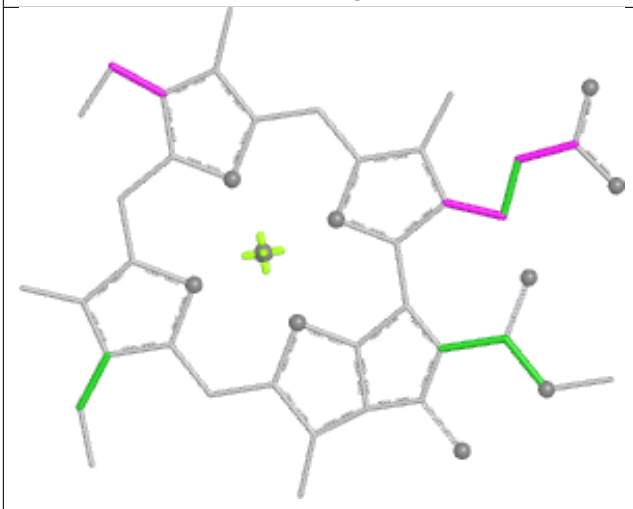
Ligand CLA cL 203



Bond lengths



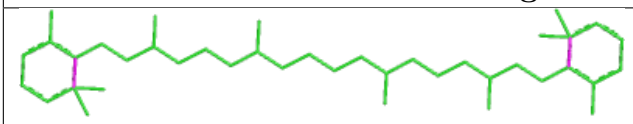
Bond angles



Torsions

Rings

Ligand BCR aI 101



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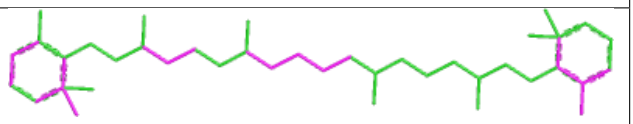
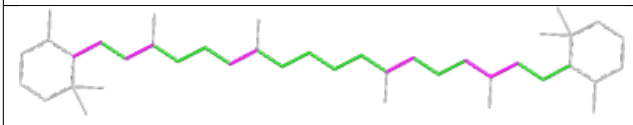
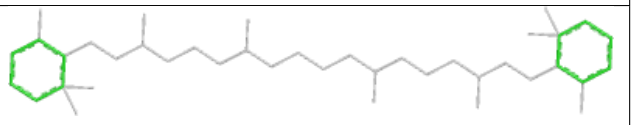


Bond angles

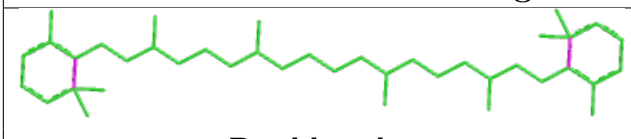


Torsions

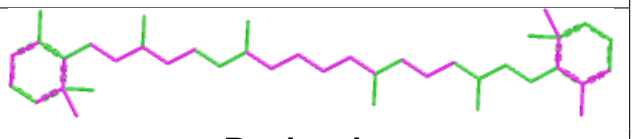


Rings

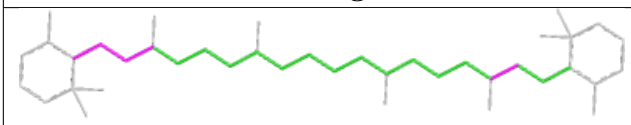
Ligand BCR cA 847



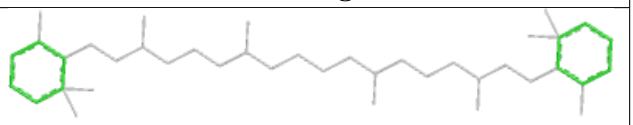
Bond lengths



Bond angles

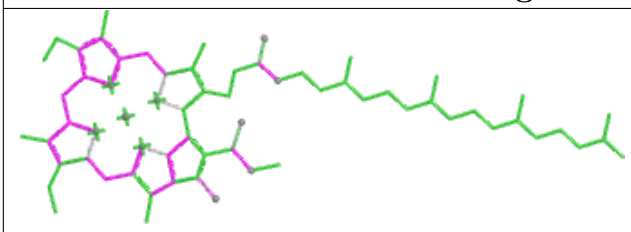


Torsions

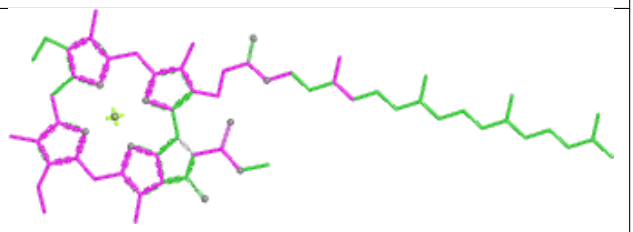


Rings

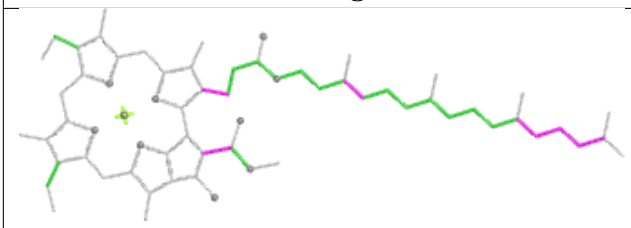
Ligand CLA aB 904



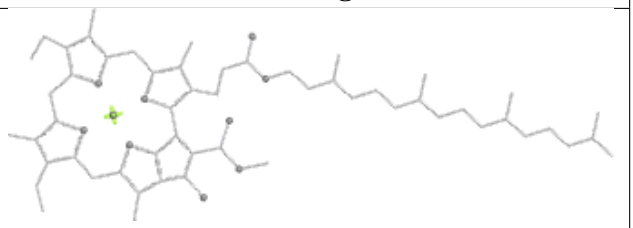
Bond lengths



Bond angles

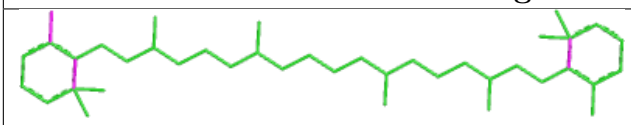


Torsions



Rings

Ligand BCR aB 941



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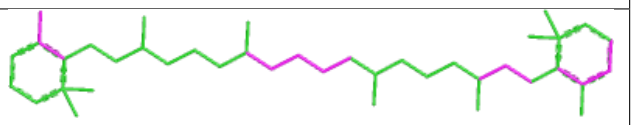
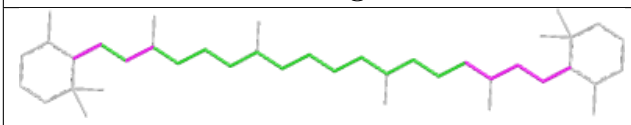
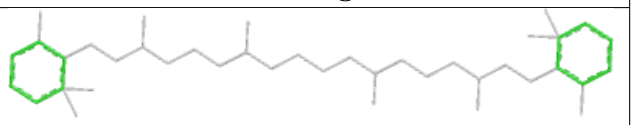


Bond angles

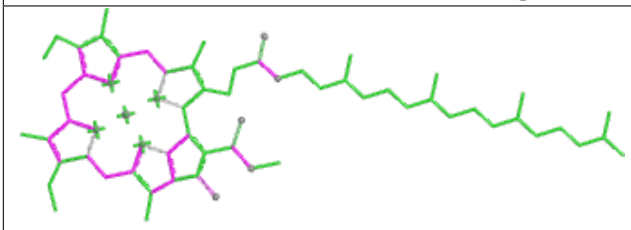


Torsions

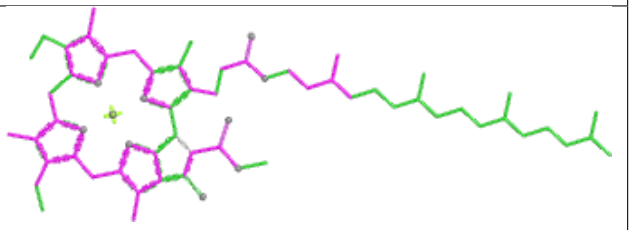


Rings

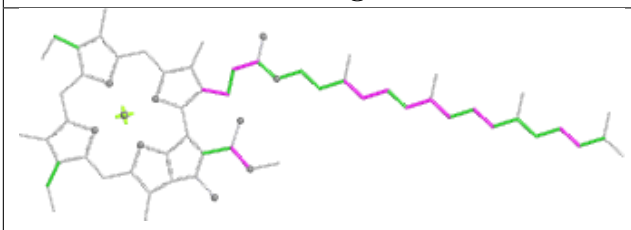
Ligand CLA bB 931



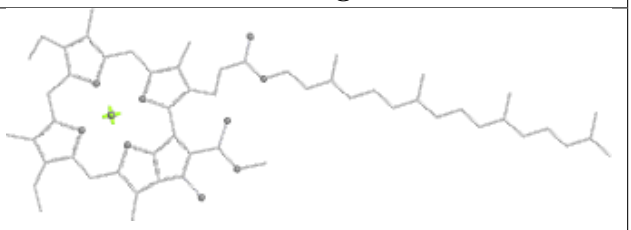
Bond lengths



Bond angles

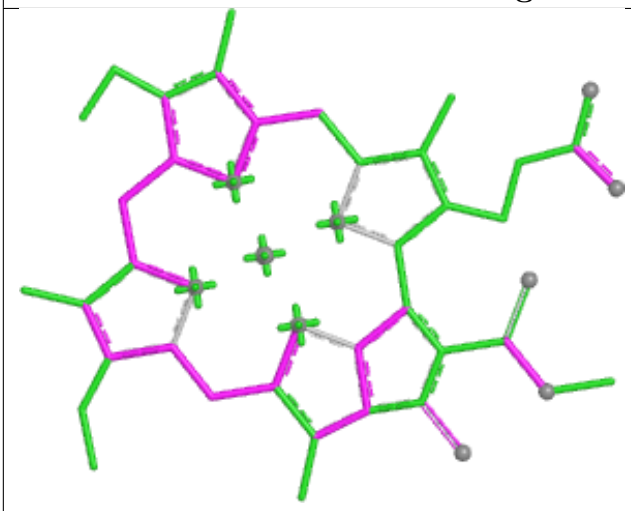


Torsions

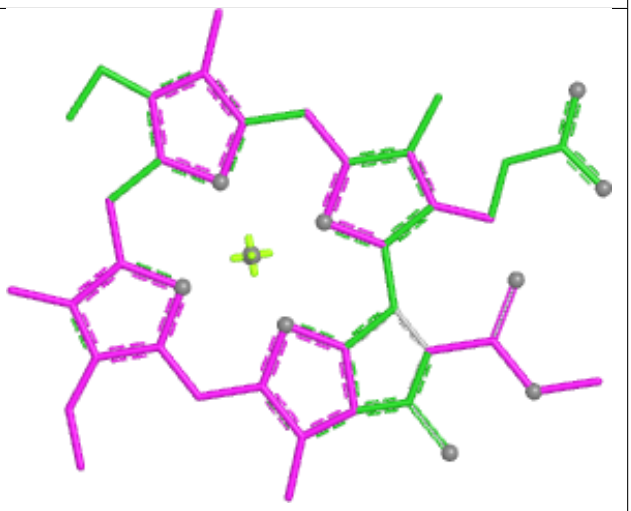


Rings

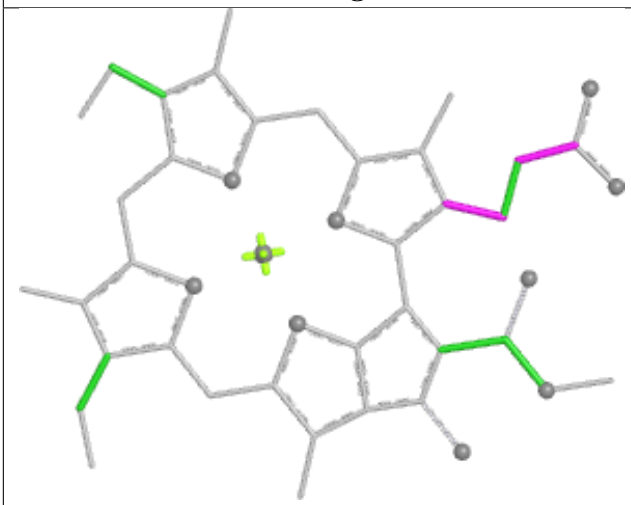
Ligand CLA aB 933



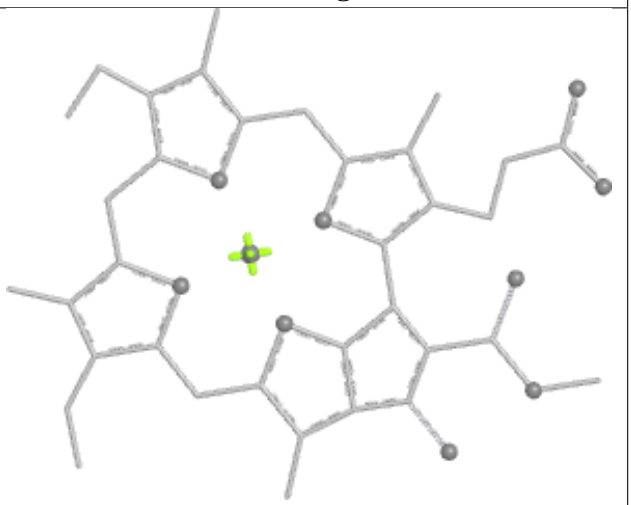
Bond lengths



Bond angles

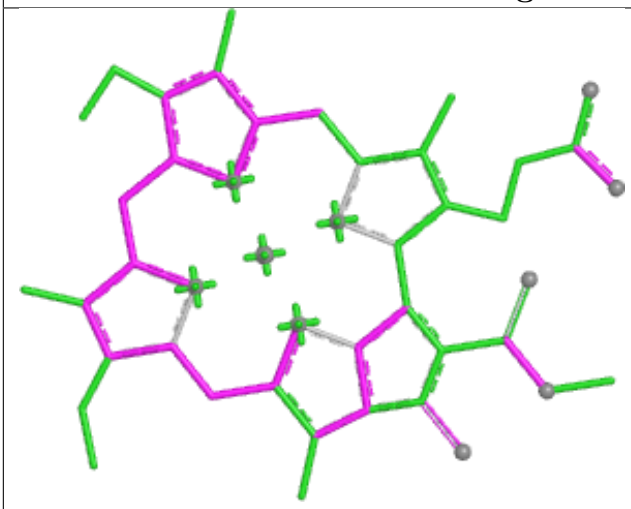


Torsions

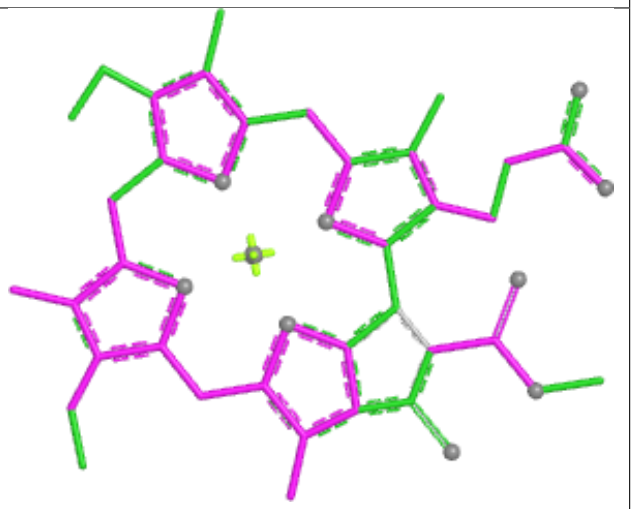


Rings

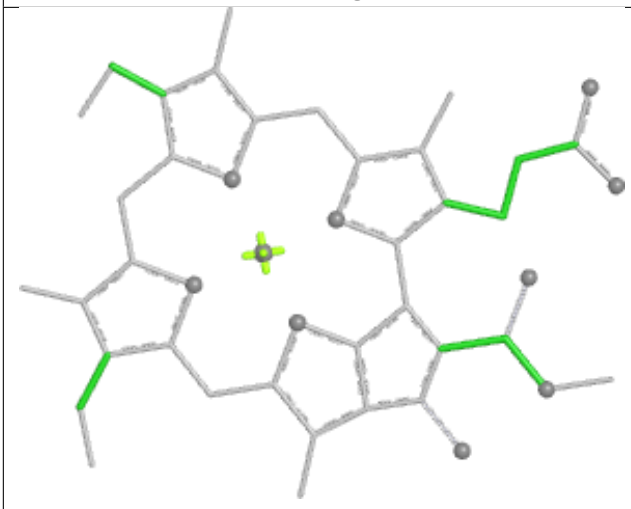
Ligand CLA bL 204



Bond lengths



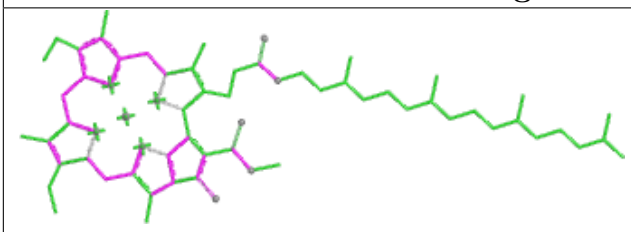
Bond angles



Torsions

Rings

Ligand CLA bA 807



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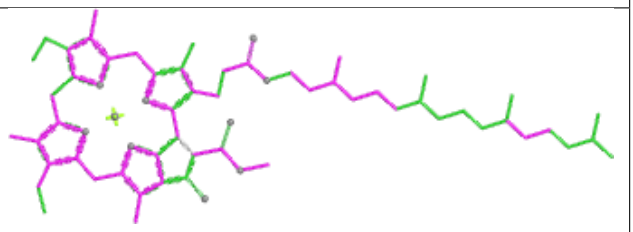
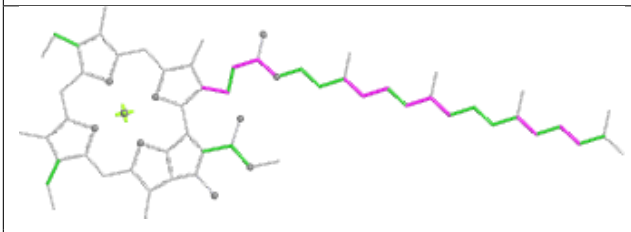
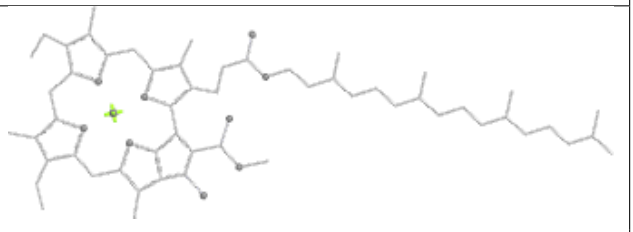


Bond angles

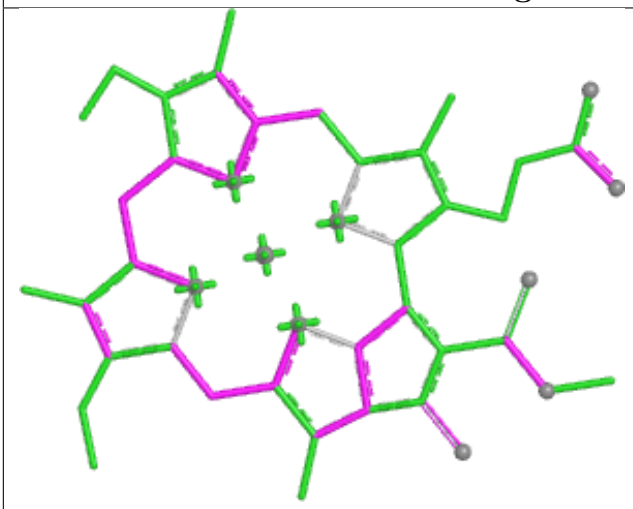


Torsions

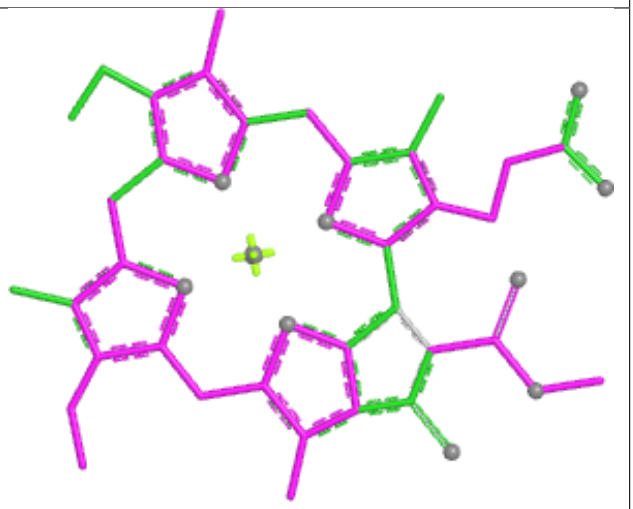


Rings

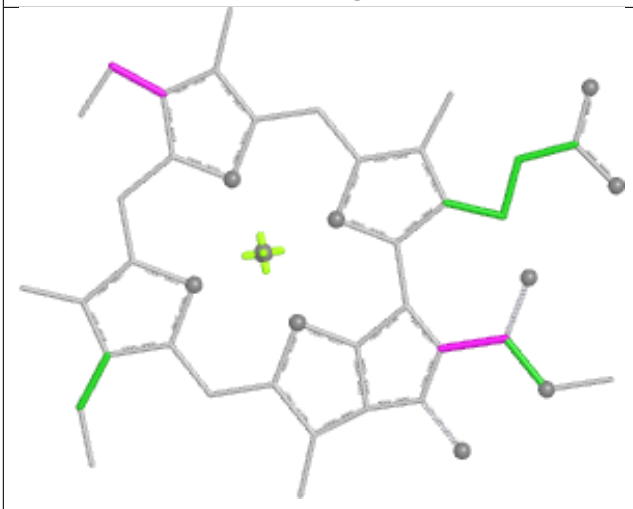
Ligand CLA bB 932



Bond lengths



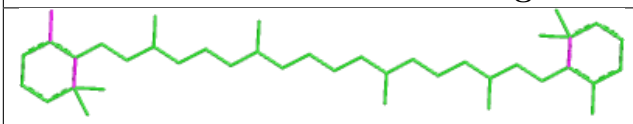
Bond angles



Torsions

Rings

Ligand BCR bL 201



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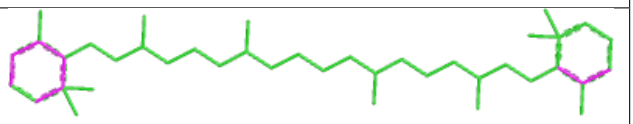
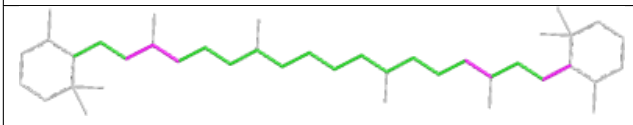
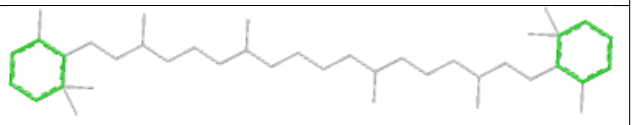


Bond angles

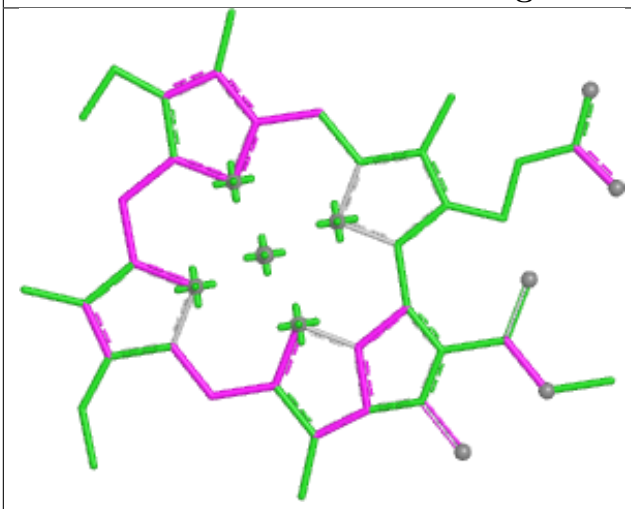


Torsions



Rings

Ligand CLA cA 810



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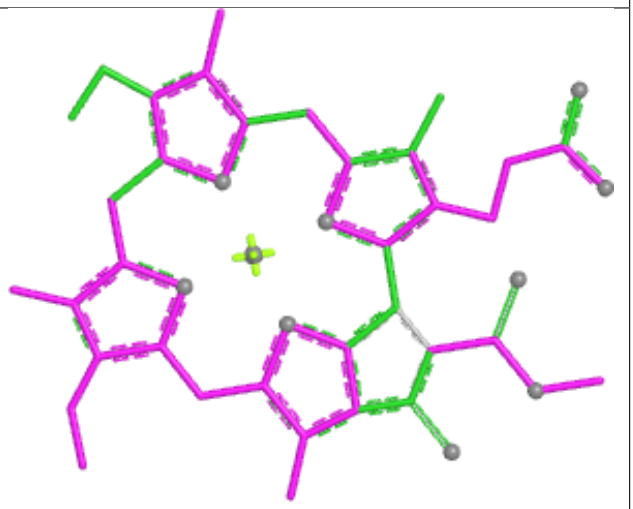
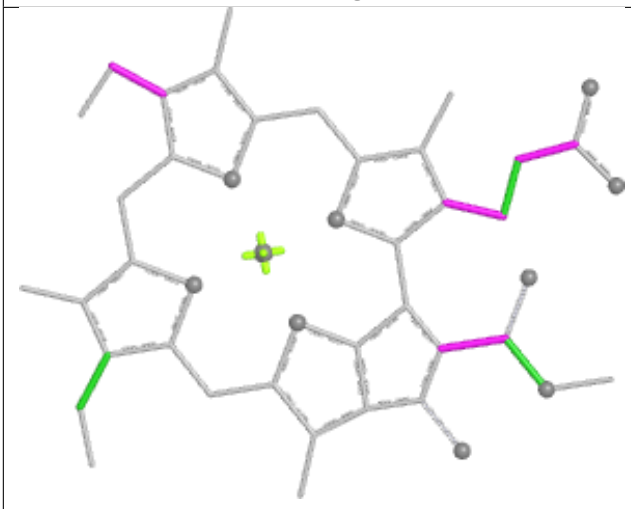


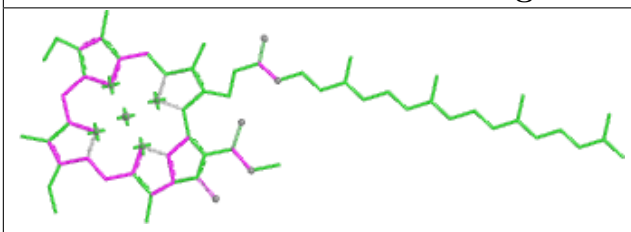
Bond angles



Torsions

Rings

Ligand CLA cA 830



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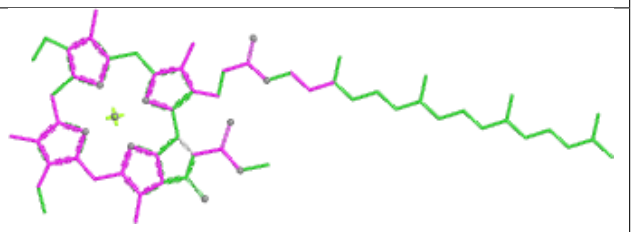
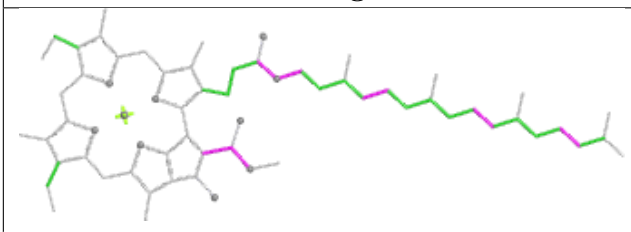
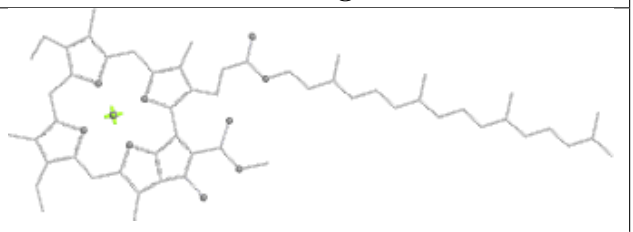


Bond angles

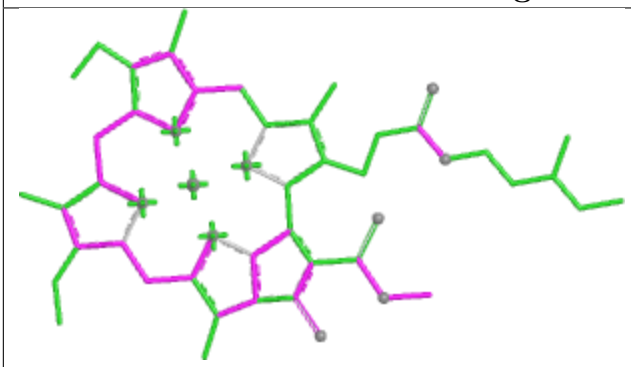


Torsions



Rings

Ligand CLA bA 837



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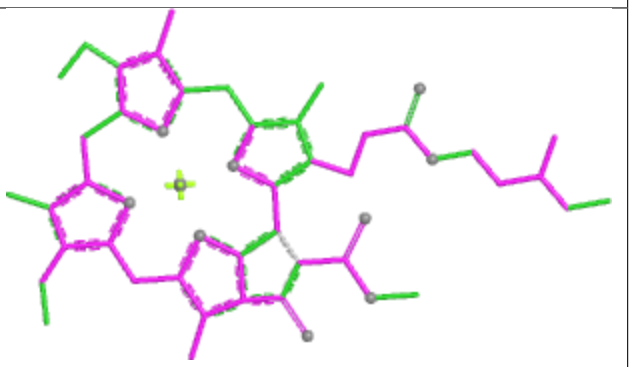
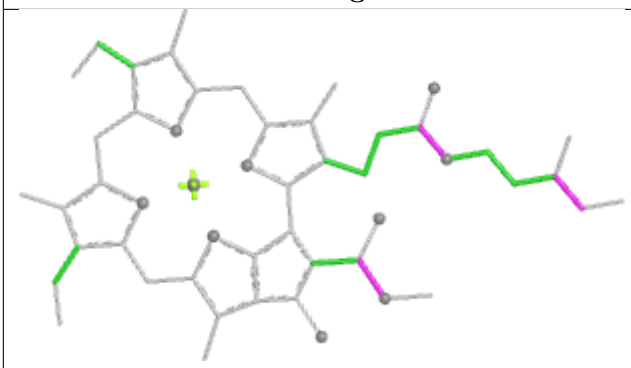
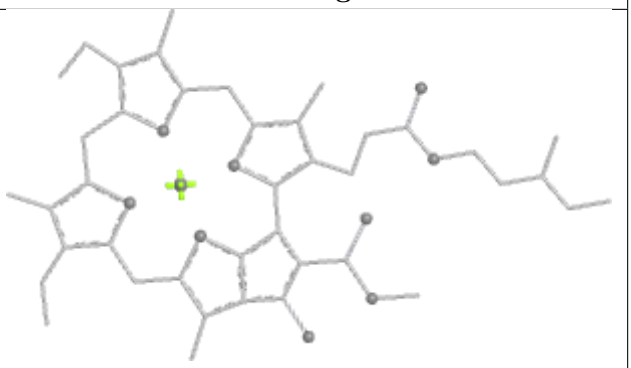


Bond angles

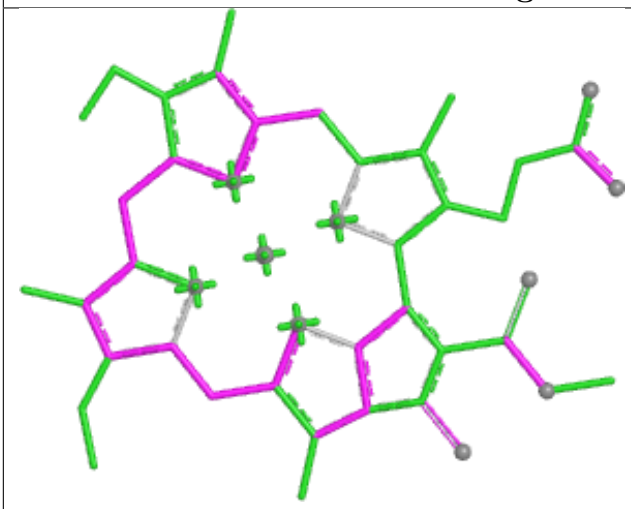


Torsions



Rings

Ligand CLA cB 929



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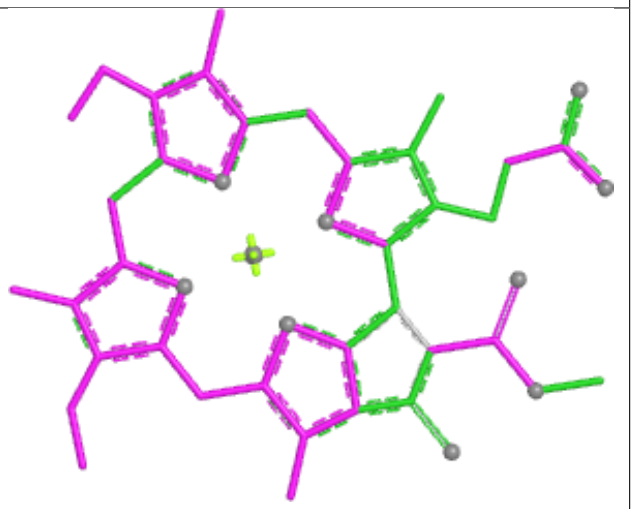

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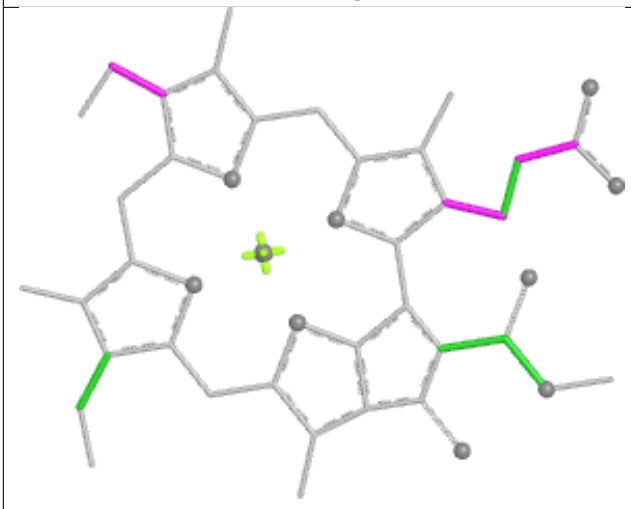
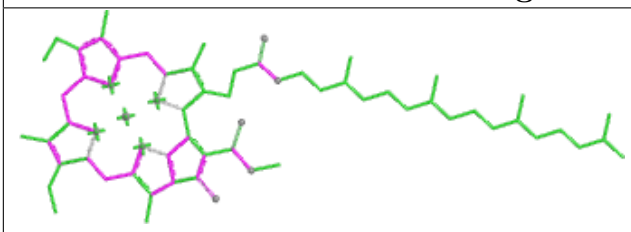


Torsions

Rings

Ligand CLA cA 807



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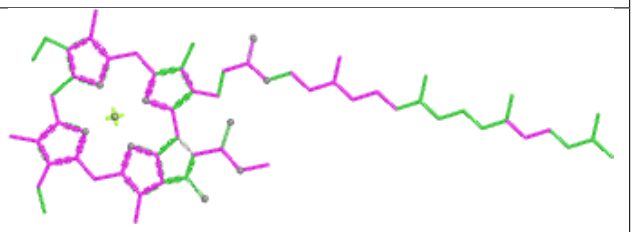
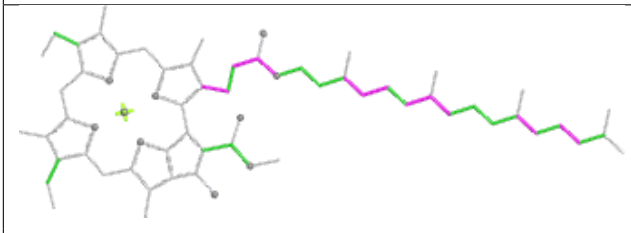


Bond angles



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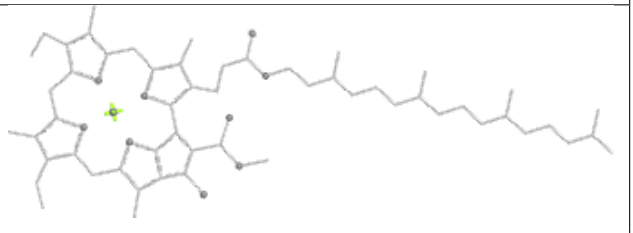
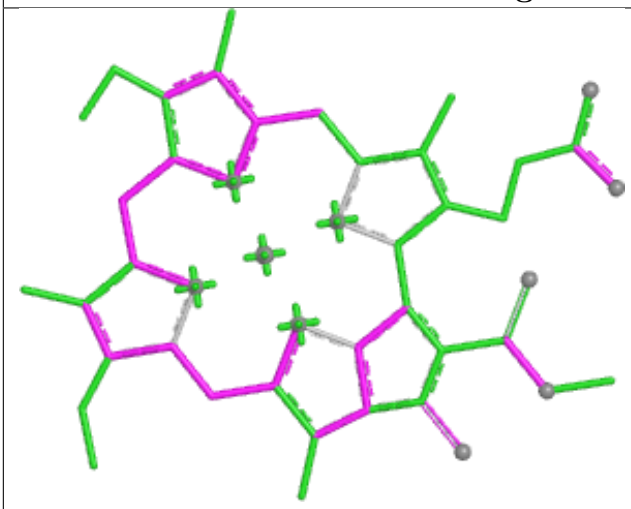


Rings

Ligand CLA cA 814



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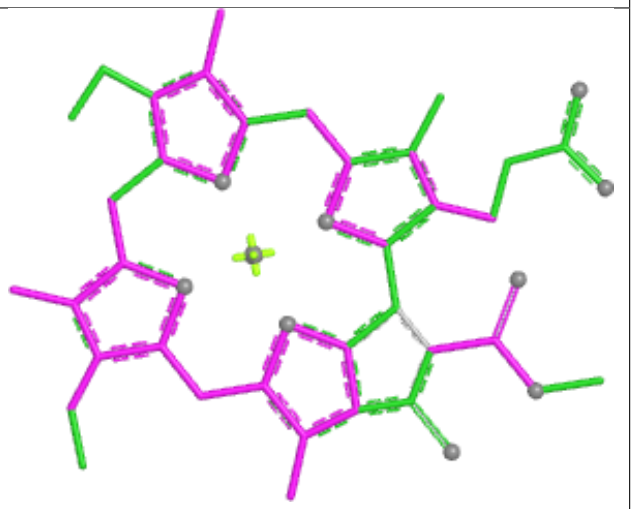
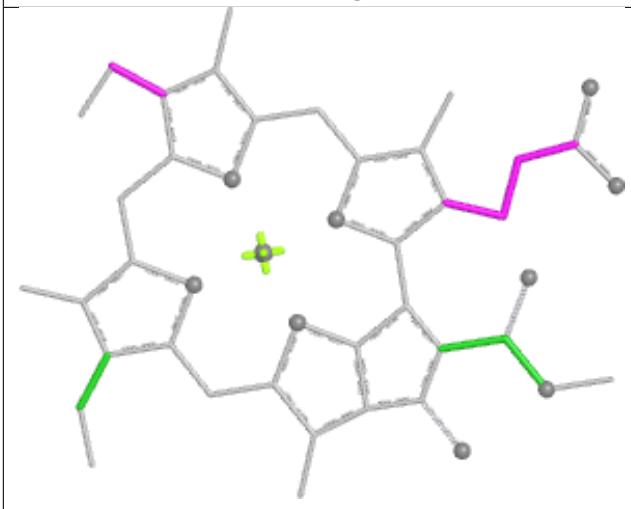
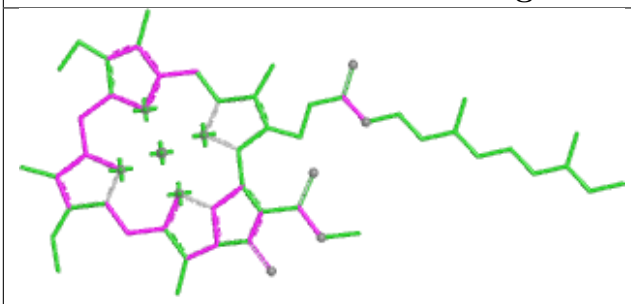
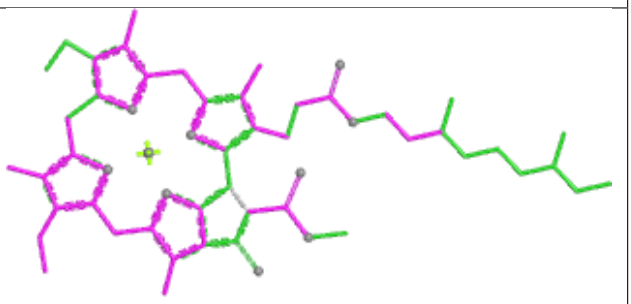
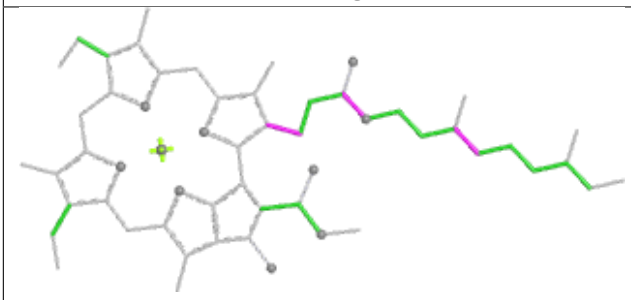
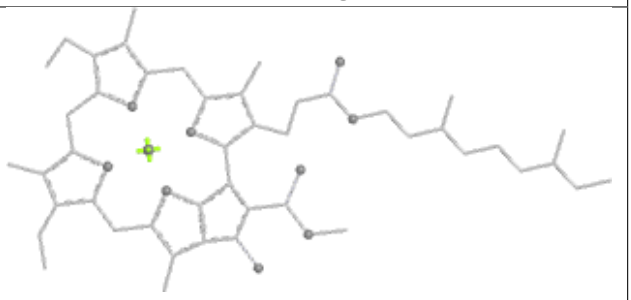


Bond angles

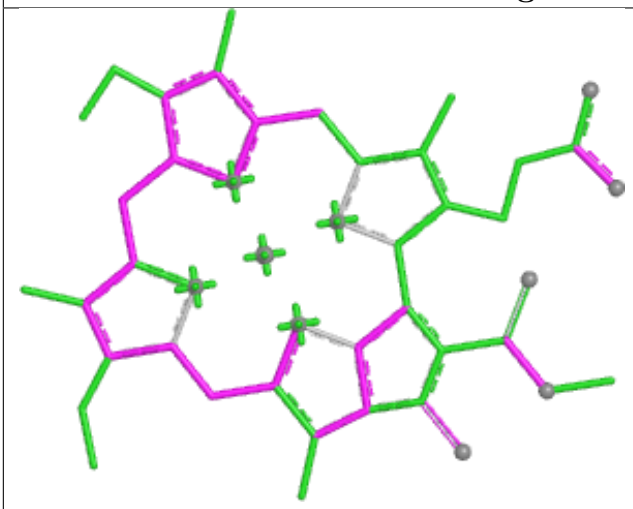


Torsions

Rings

Ligand CLA aB 913	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA aF 202



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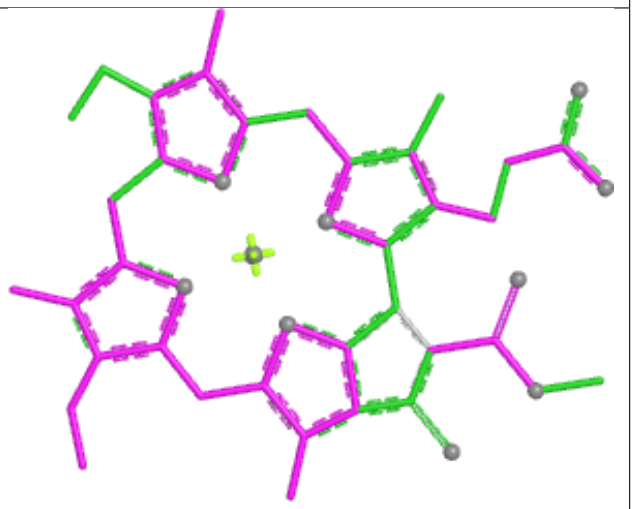
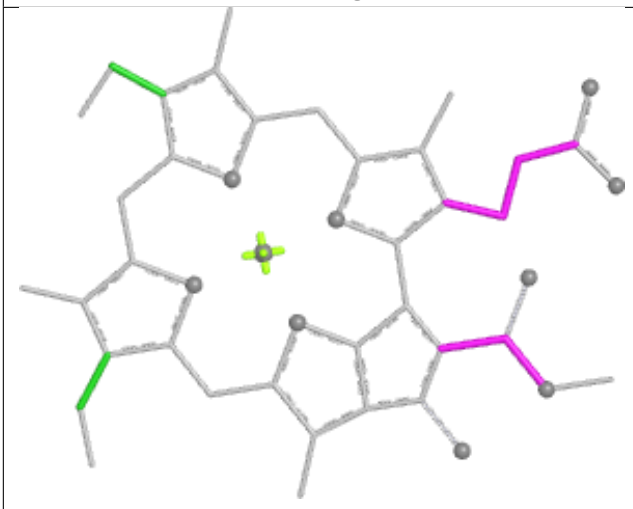


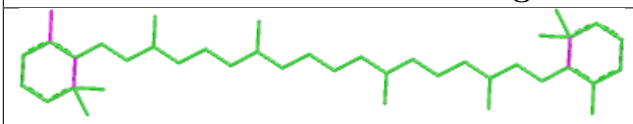
Bond angles



Torsions

Rings

Ligand BCR aA 849



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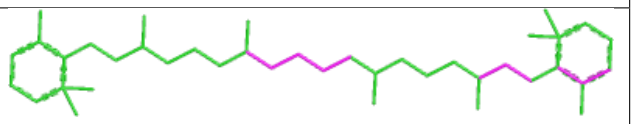
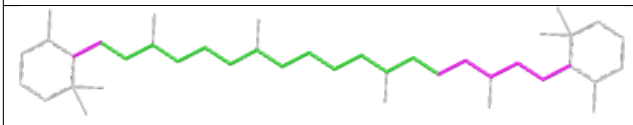


Bond angles



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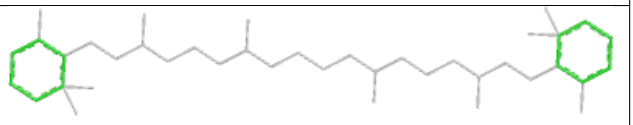
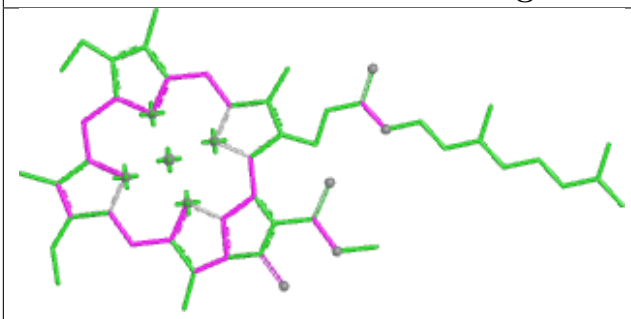


Rings

Ligand CLA cB 917



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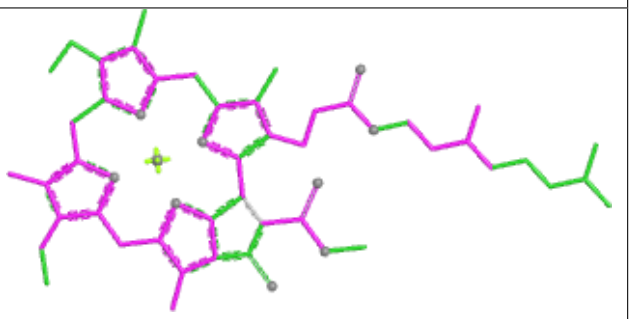
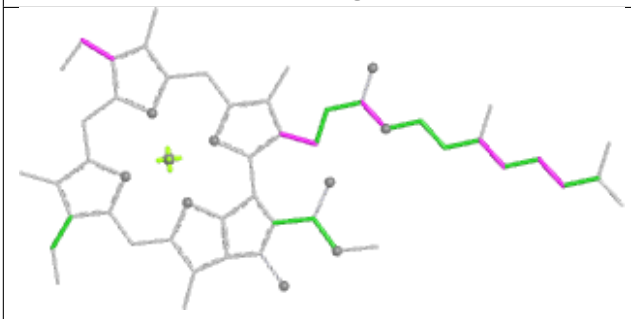
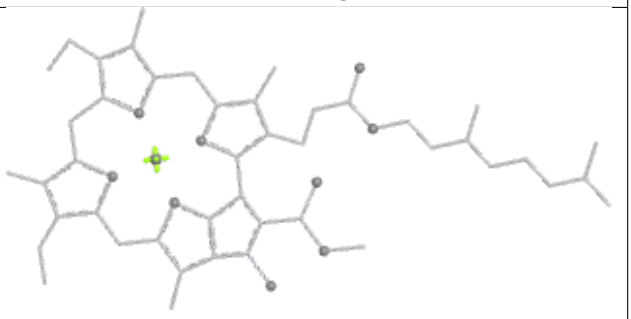


Bond angles

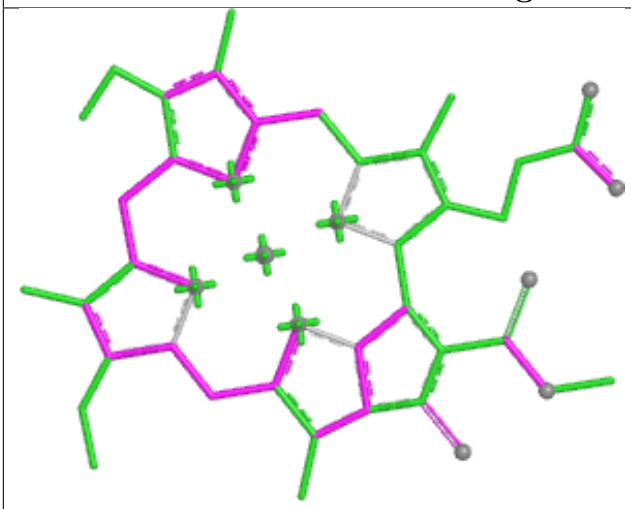


Torsions

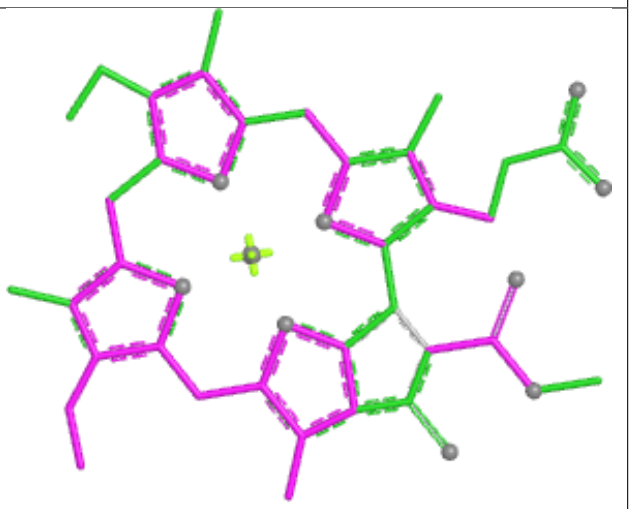


Rings

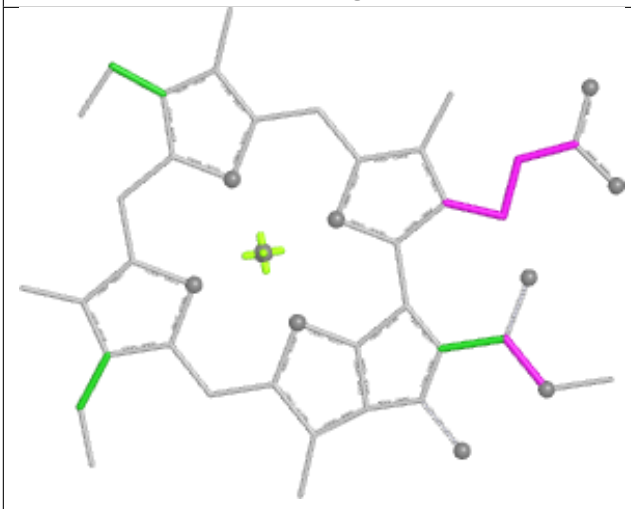
Ligand CLA aB 950



Bond lengths



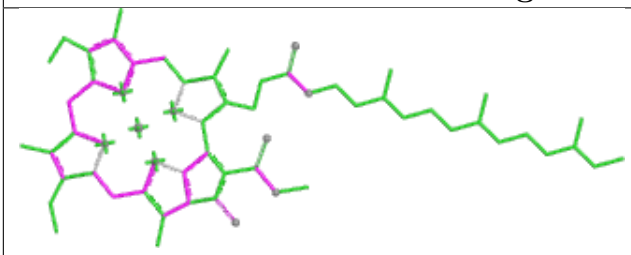
Bond angles



Torsions

Rings

Ligand CLA cB 902



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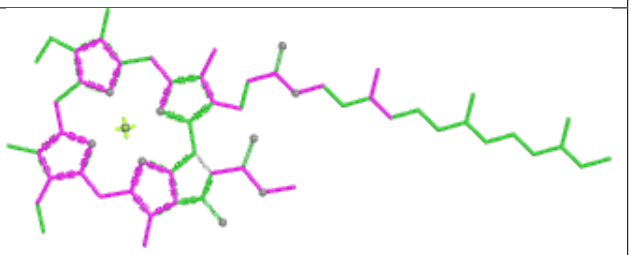
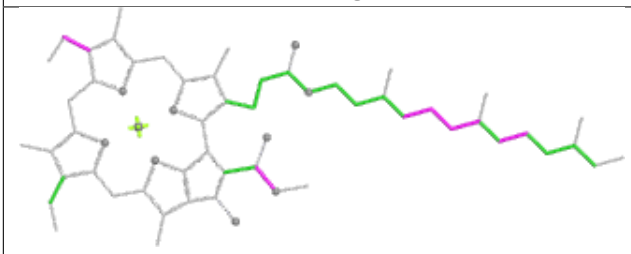
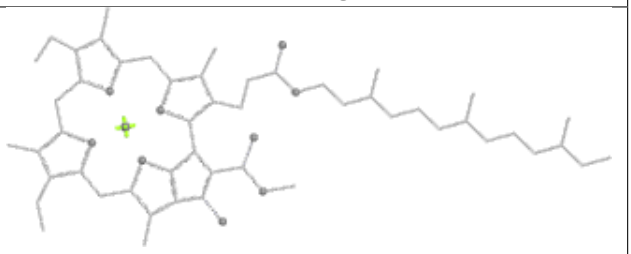


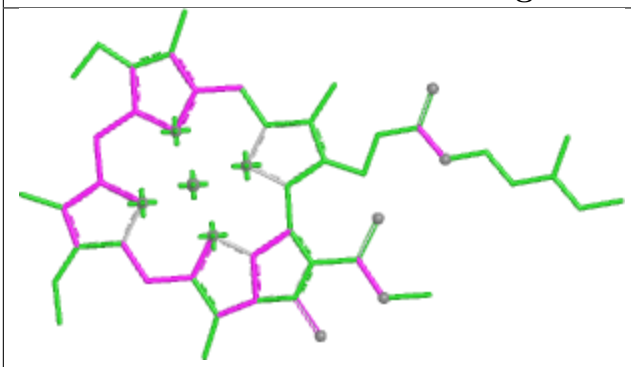
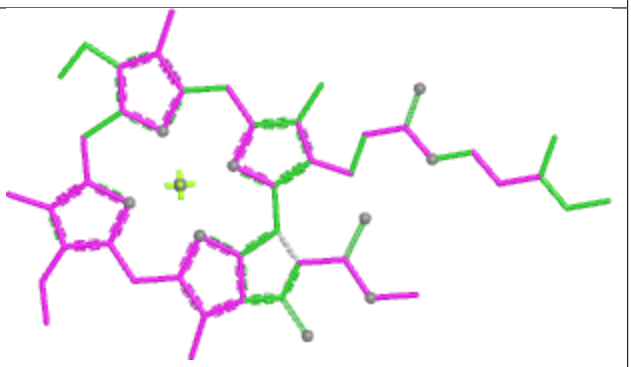
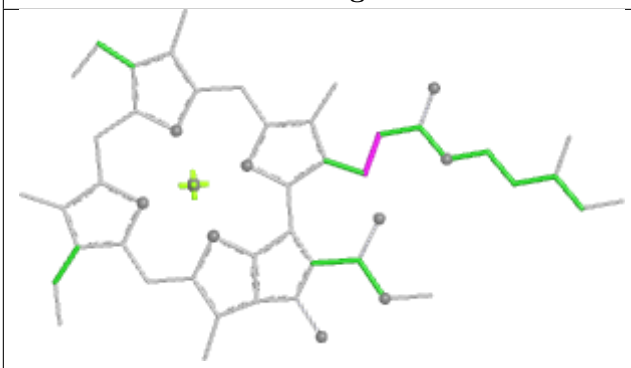
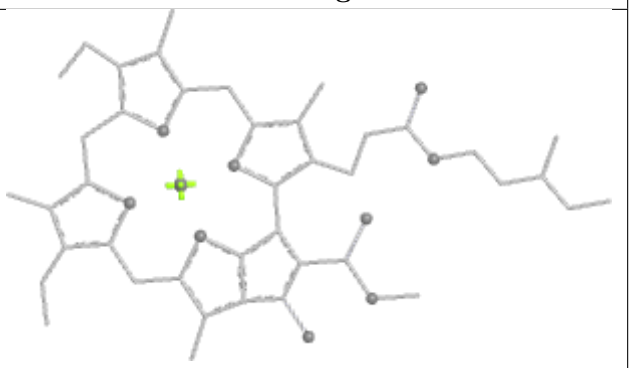
Bond angles

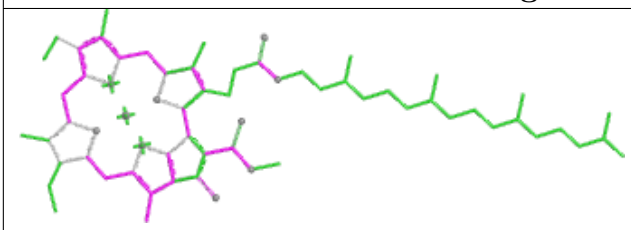
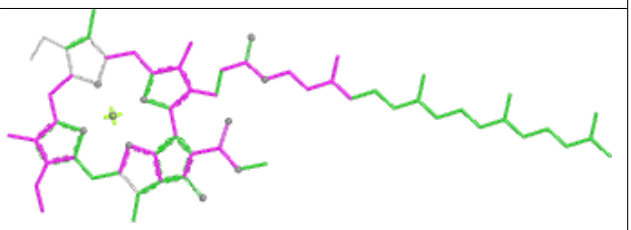
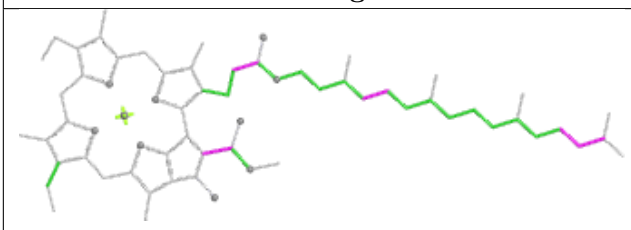
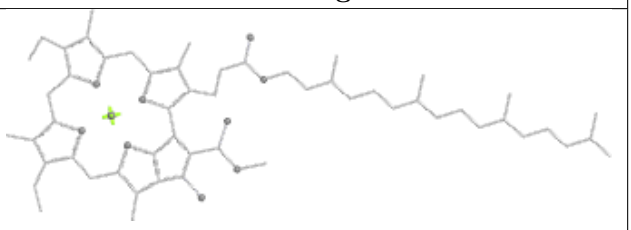


Torsions

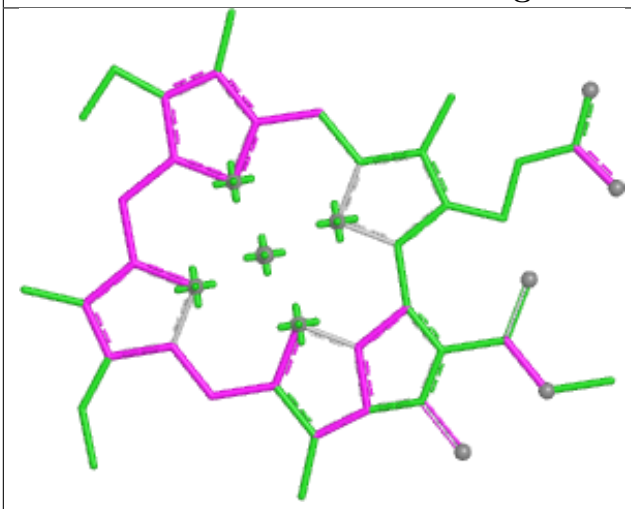


Rings

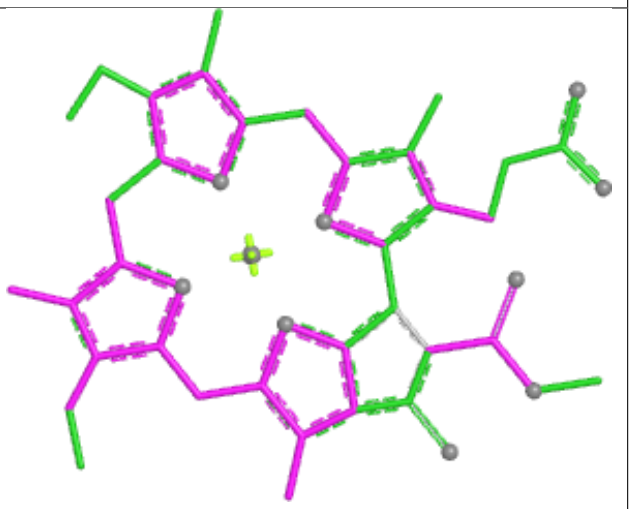
Ligand CLA aB 938	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CL0 cA 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

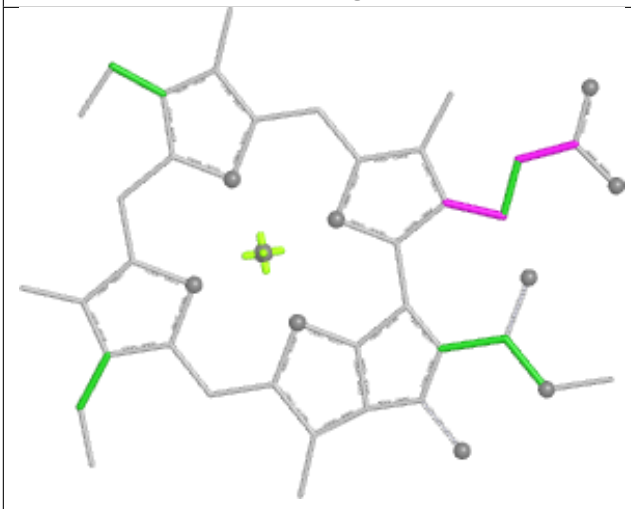
Ligand CLA bA 816



Bond lengths



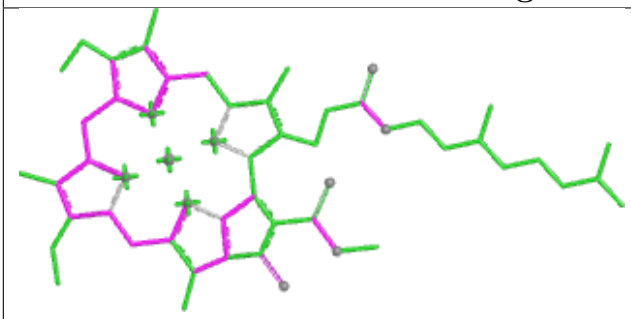
Bond angles



Torsions

Rings

Ligand CLA cB 909



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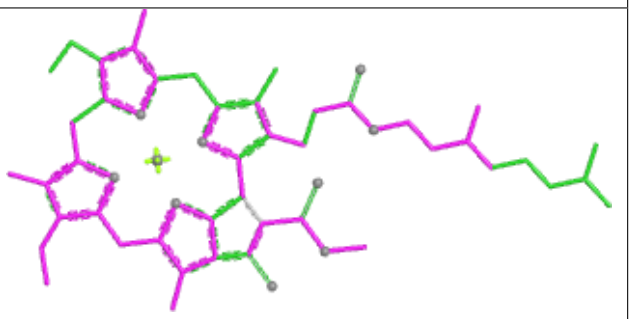
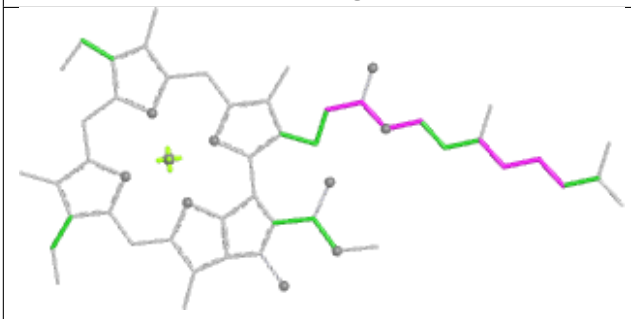
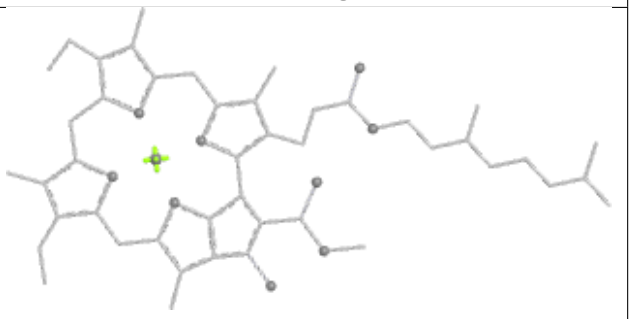


Bond angles

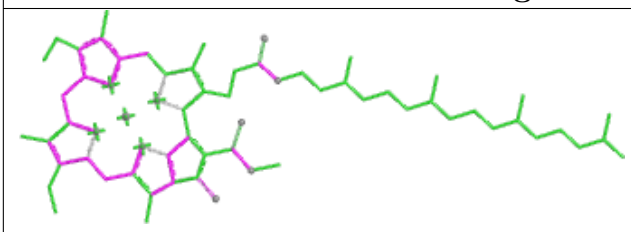


Torsions

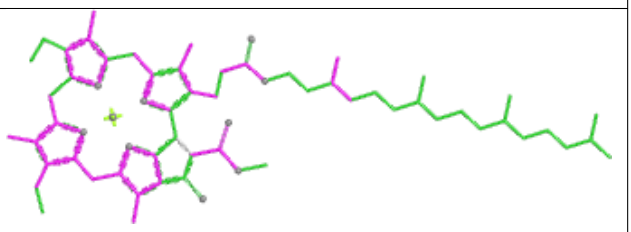


Rings

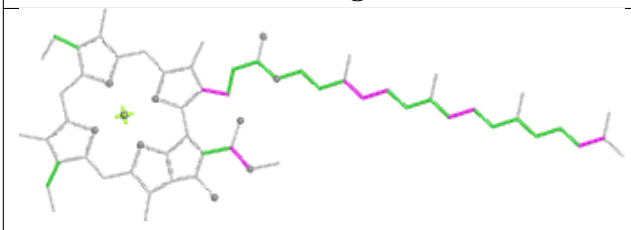
Ligand CLA bA 806



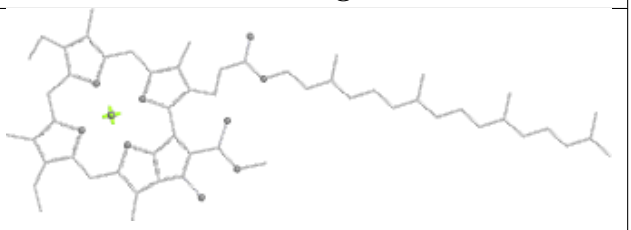
Bond lengths



Bond angles

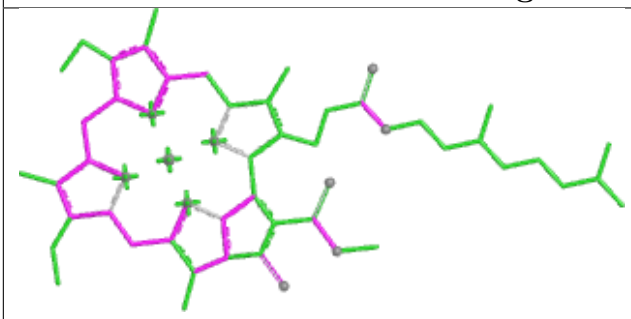


Torsions



Rings

Ligand CLA cB 906



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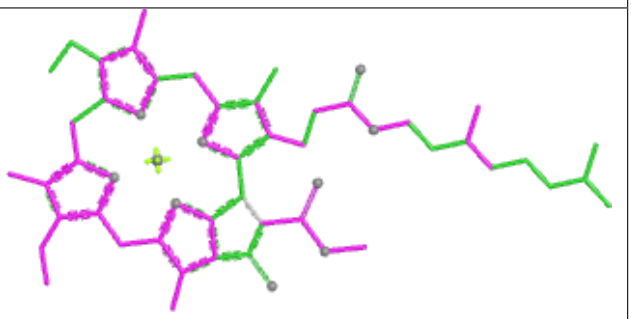
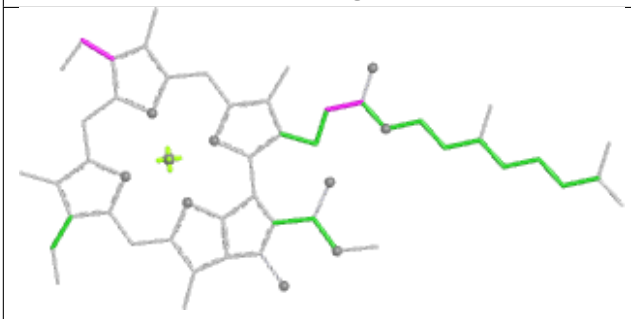
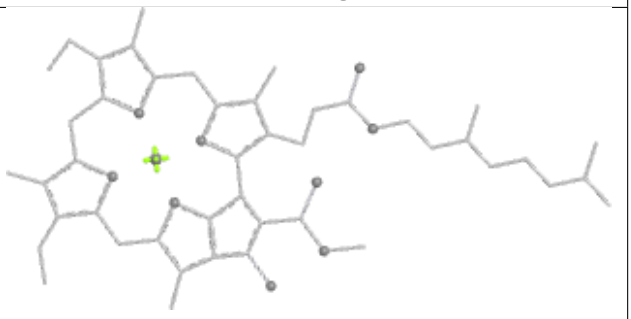


Bond angles

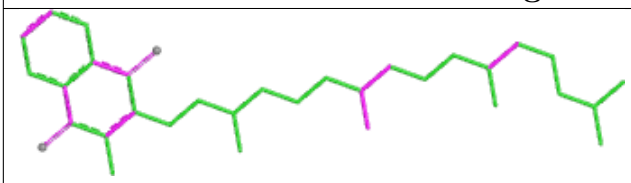


Torsions



Rings

Ligand 1L3 aA 845



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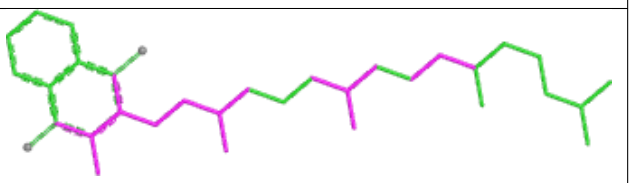
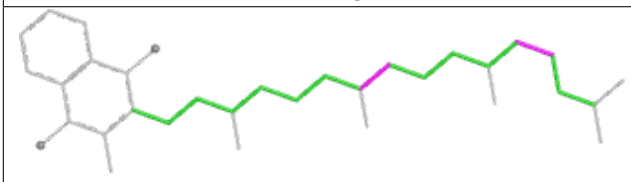


Bond angles



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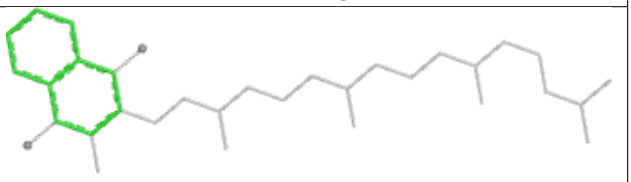
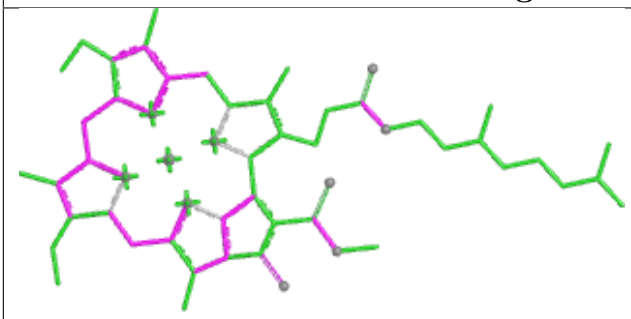


Rings

Ligand CLA cA 832



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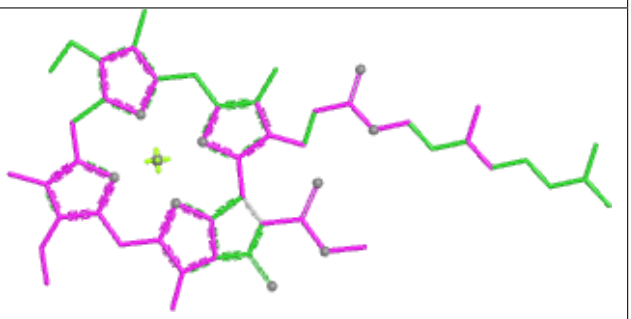
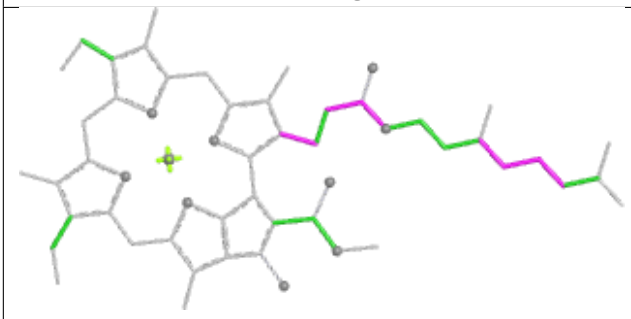


Bond angles



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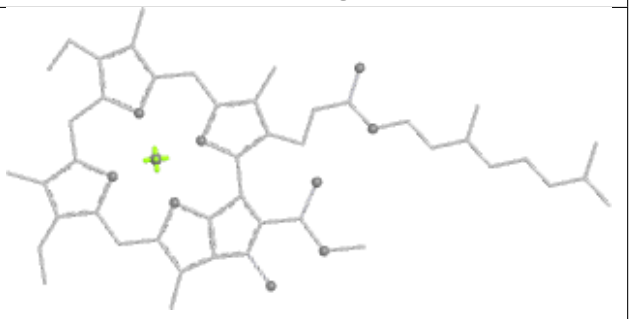
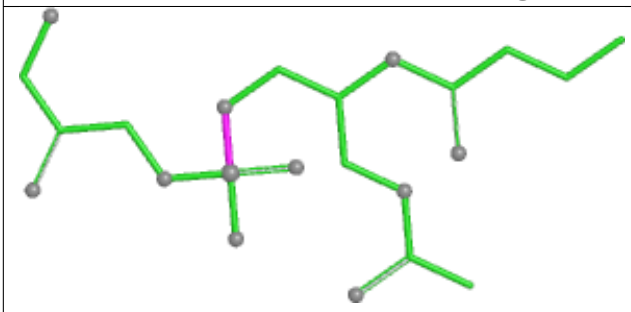


Rings

Ligand LHG aB 948



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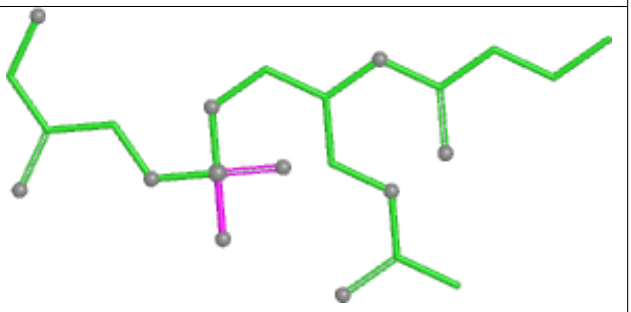
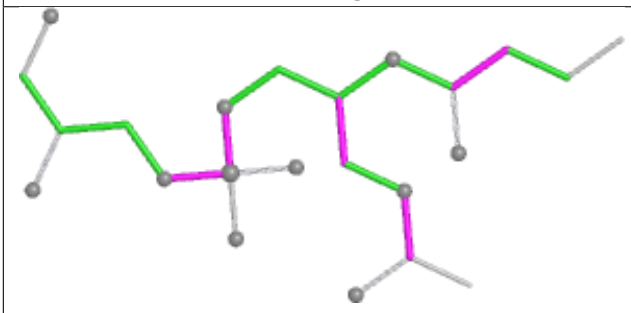


Bond angles



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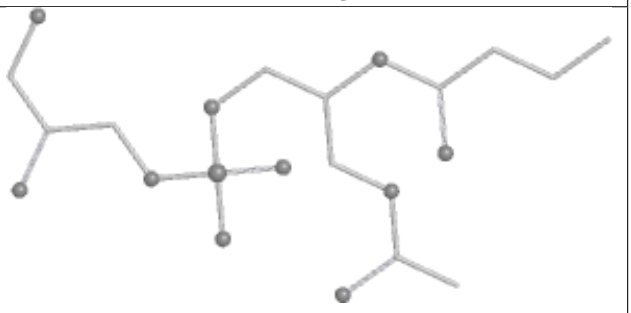
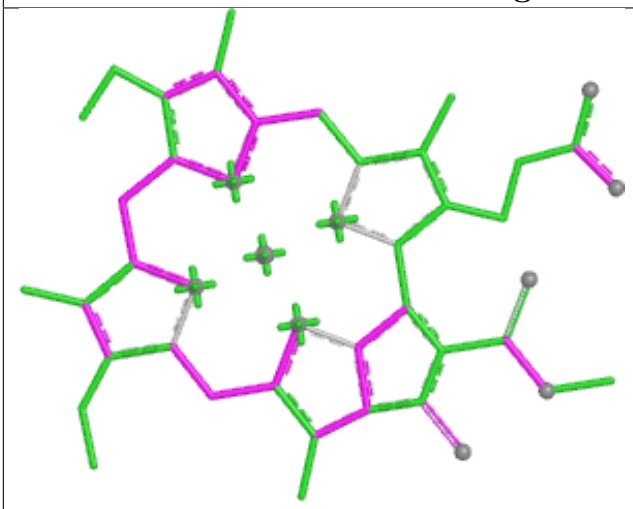


Rings

Ligand CLA bA 810



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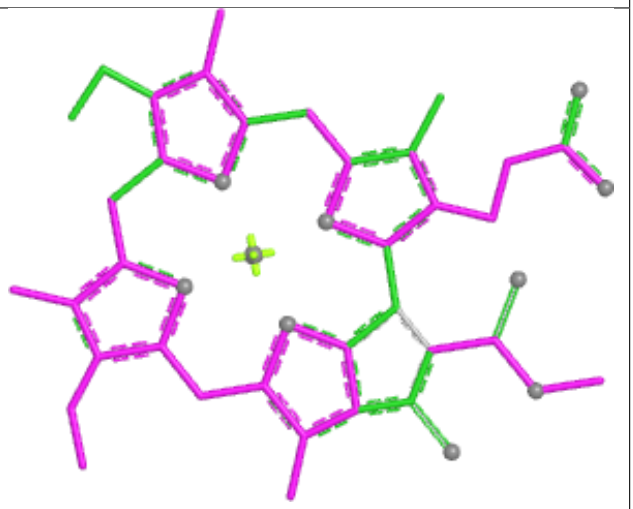
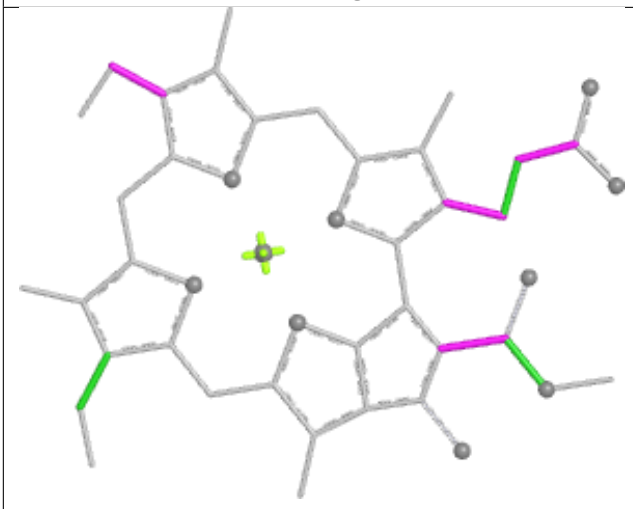


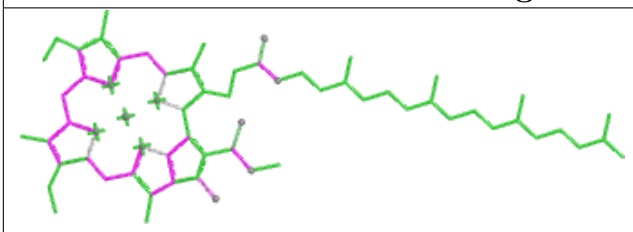
Bond angles



Torsions

Rings

Ligand CLA aB 931



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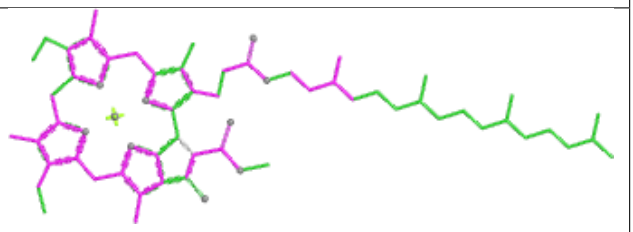
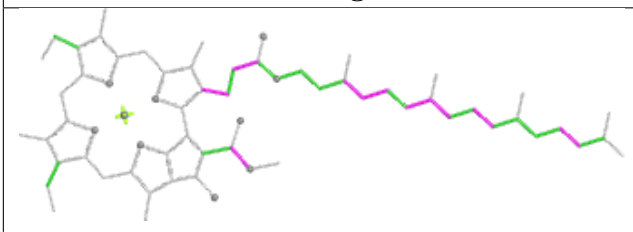
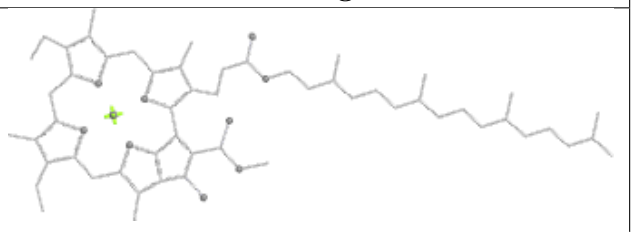


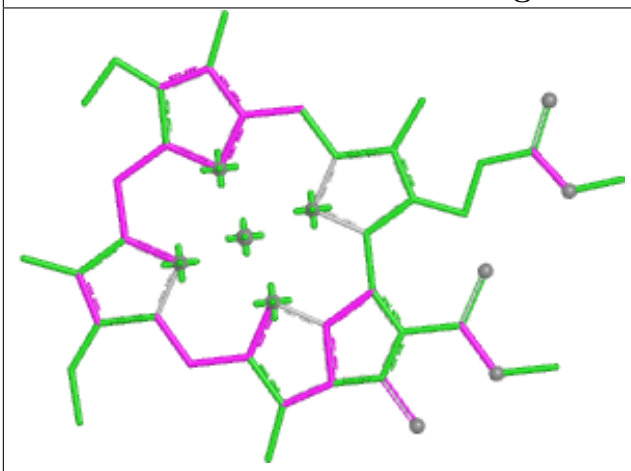
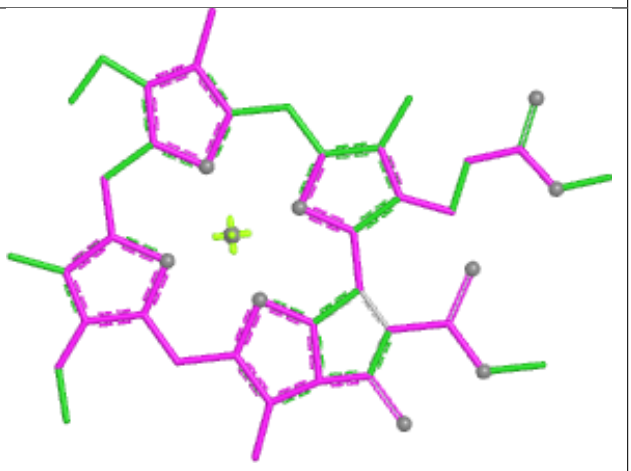
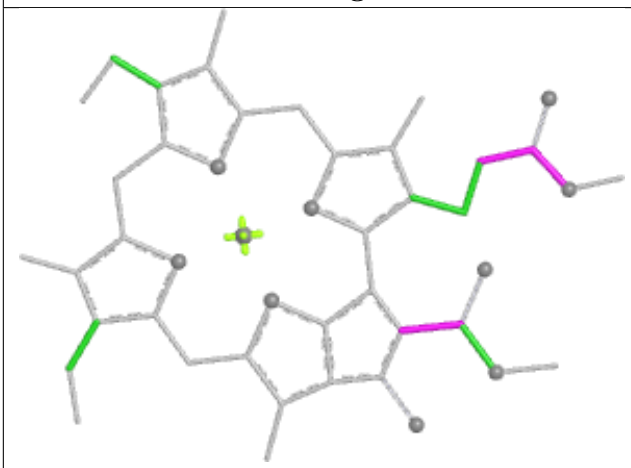
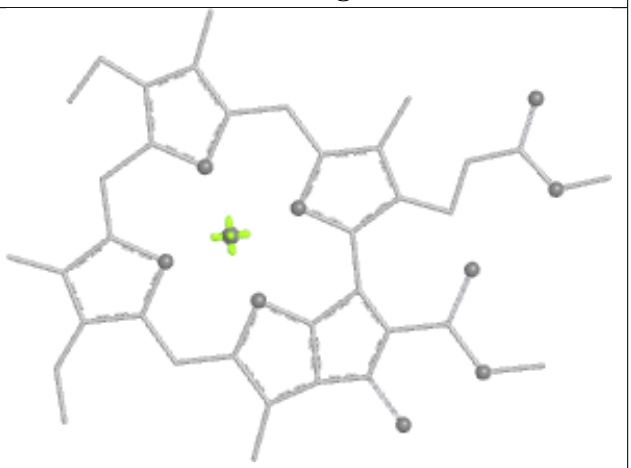
Bond angles

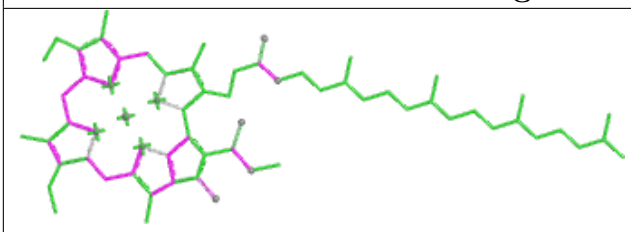
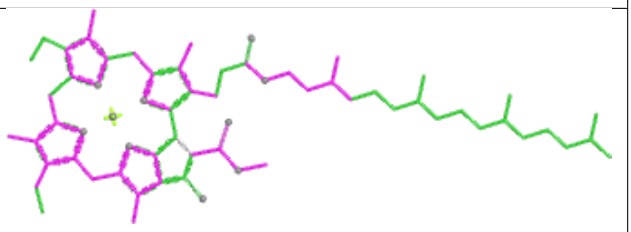
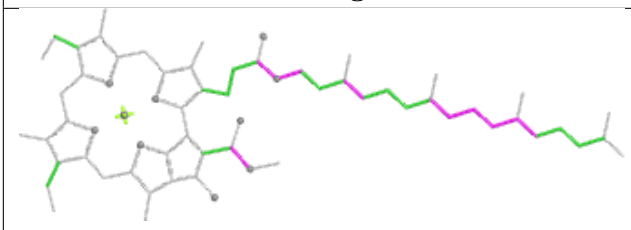
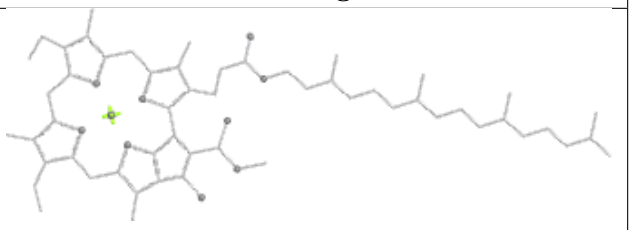


Torsions

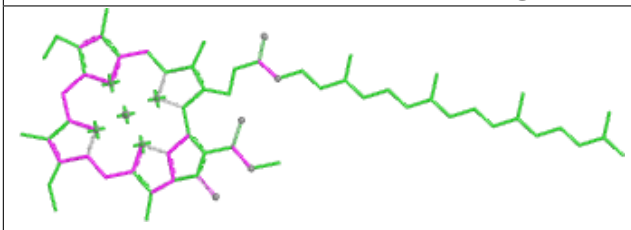


Rings

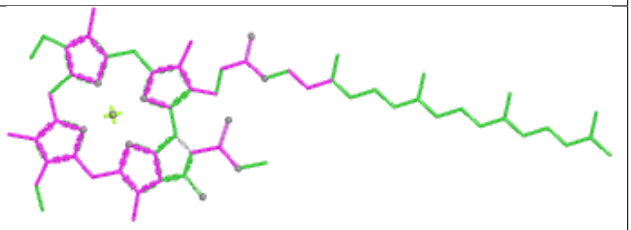
Ligand CLA bA 827	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA bA 842	
	
Bond lengths	Bond angles
	
Torsions	Rings

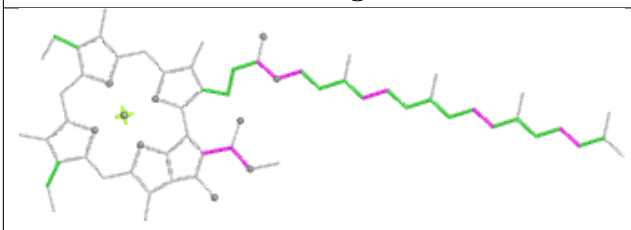
Ligand CLA bA 830



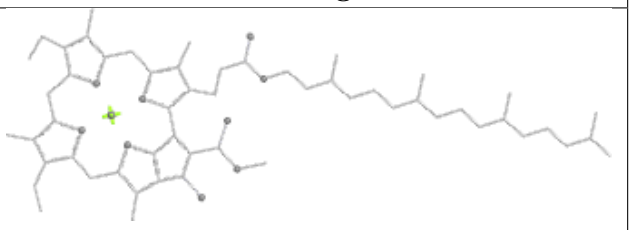
Bond lengths



Bond angles

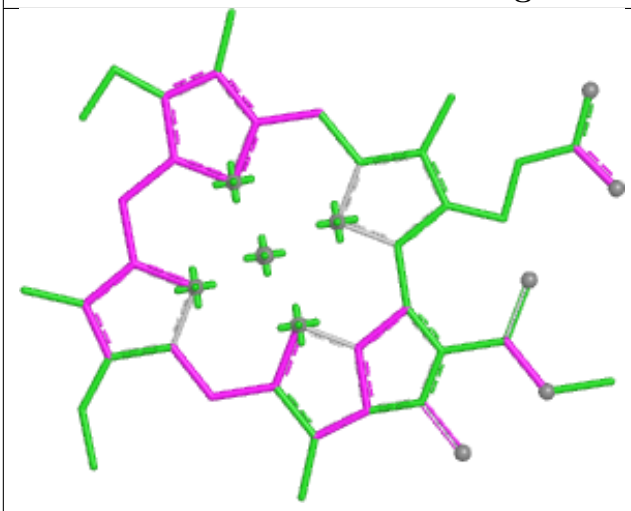


Torsions

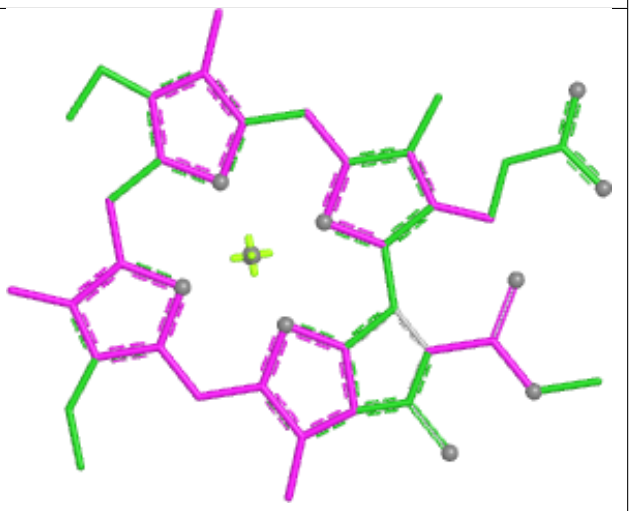


Rings

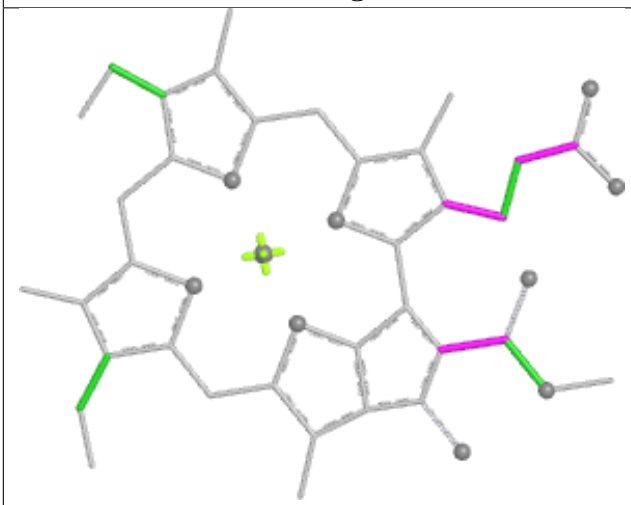
Ligand CLA bB 914



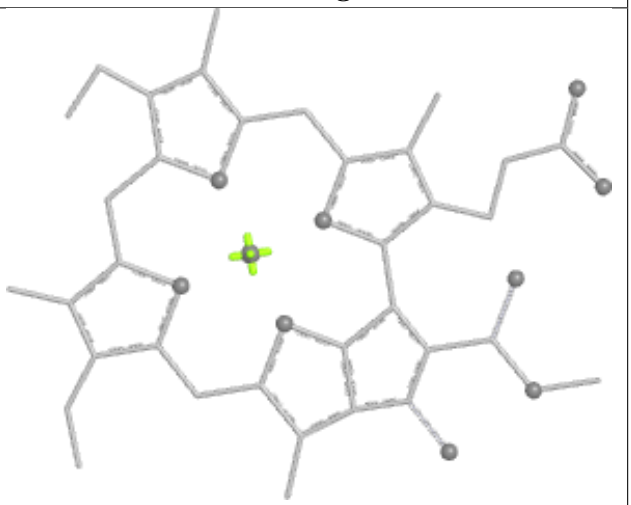
Bond lengths



Bond angles

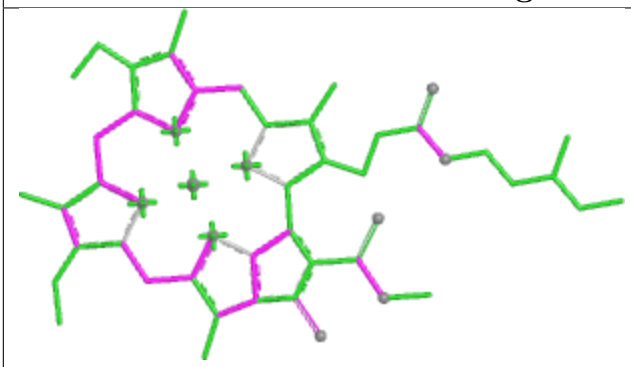


Torsions

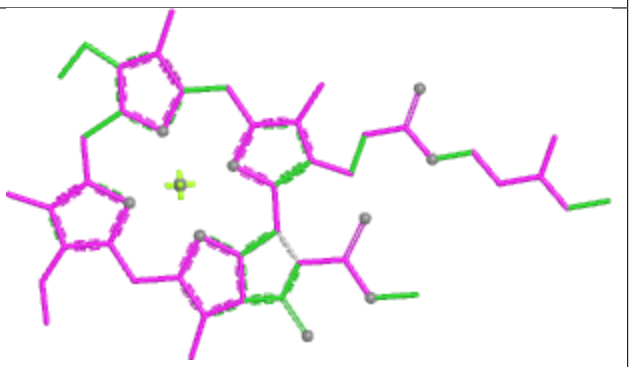


Rings

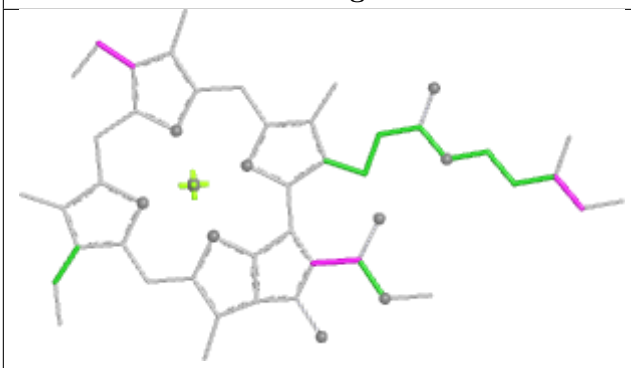
Ligand CLA cA 833



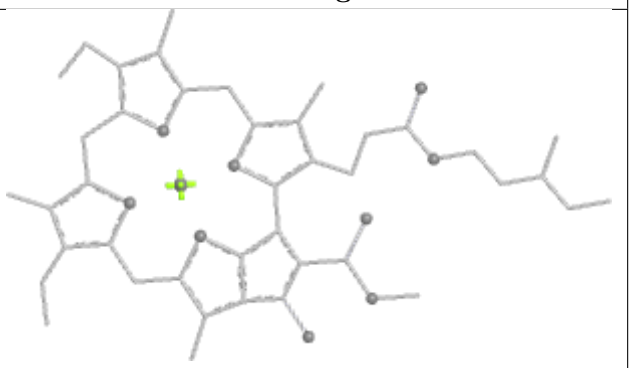
Bond lengths



Bond angles

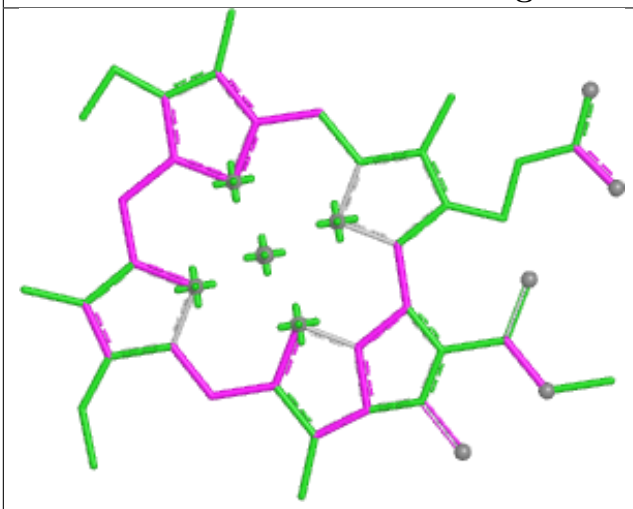


Torsions

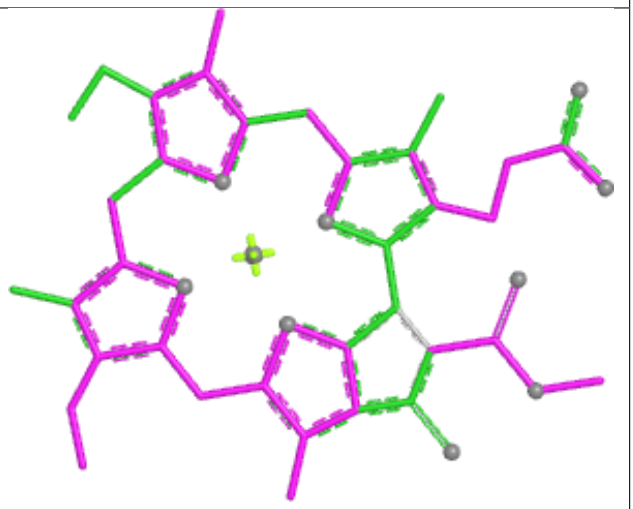


Rings

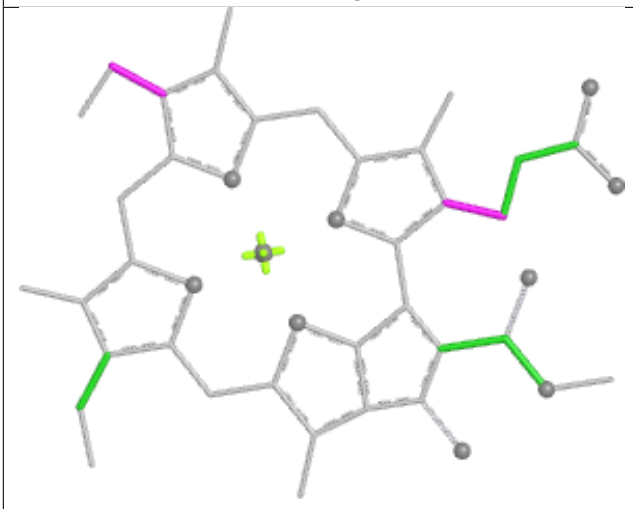
Ligand CLA aB 939



Bond lengths

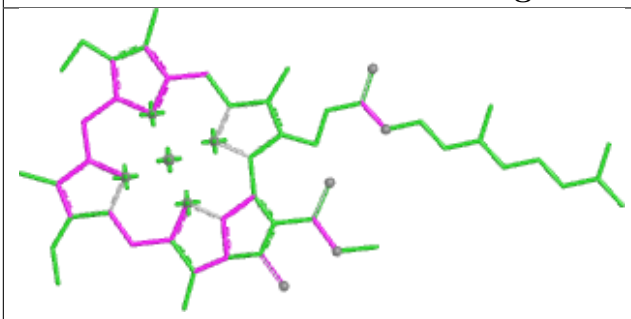
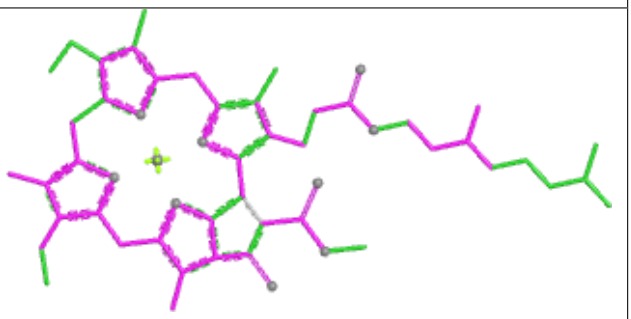
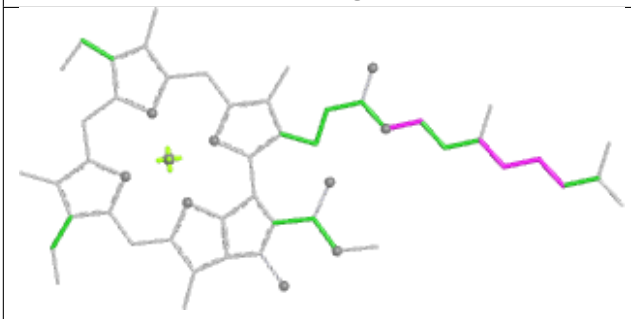
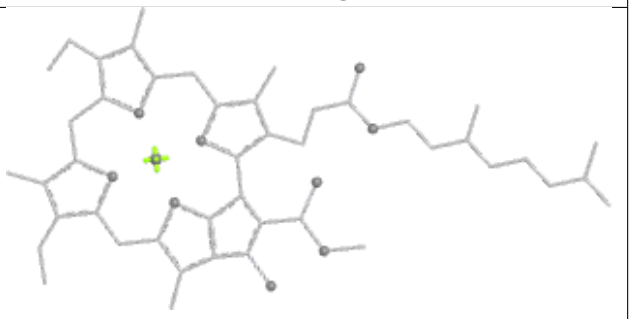


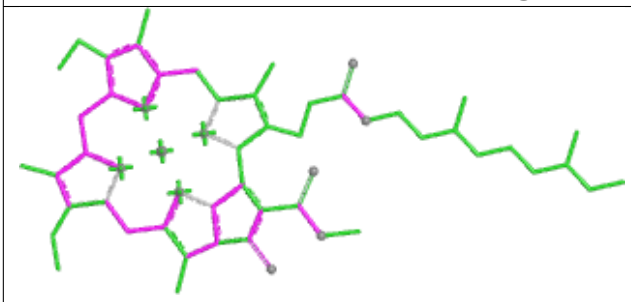
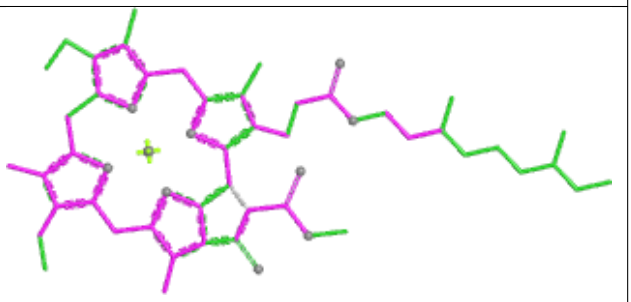
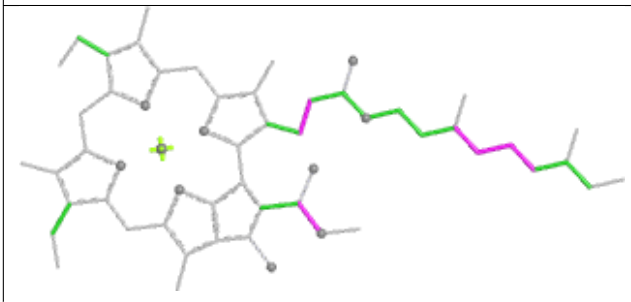
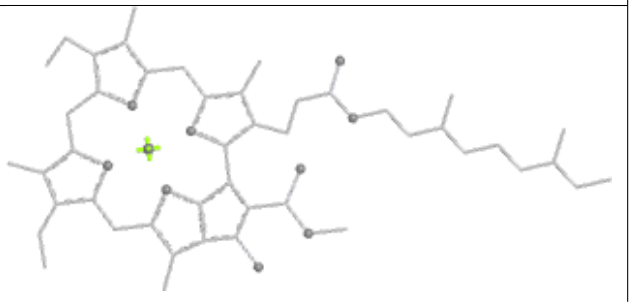
Bond angles



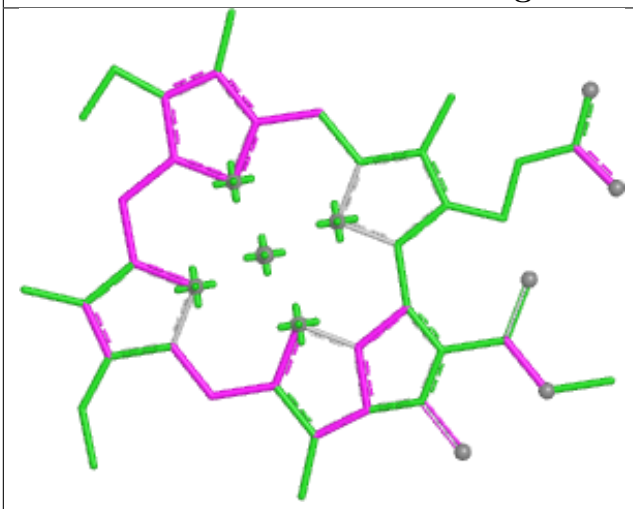
Torsions

Rings

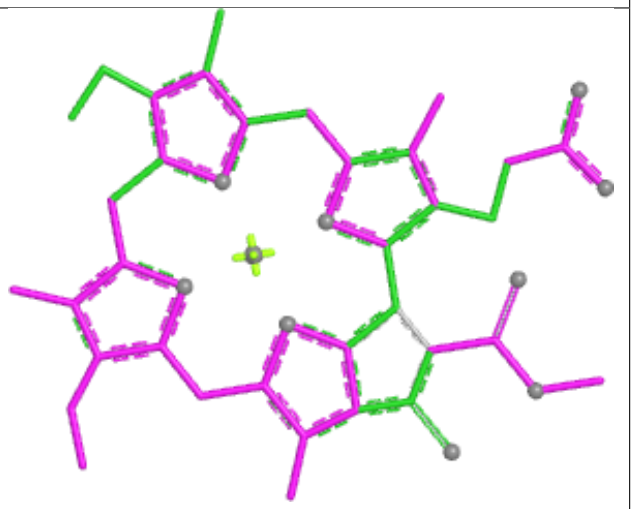
Ligand CLA bB 925	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA aA 854	
 Bond lengths	 Bond angles
 Torsions	 Rings

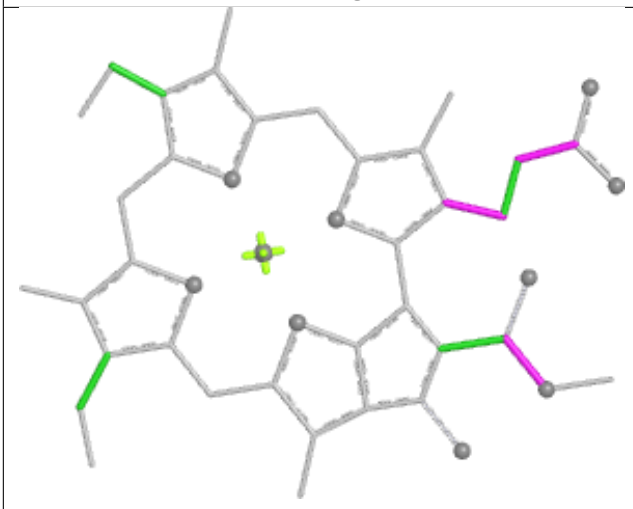
Ligand CLA bB 922



Bond lengths



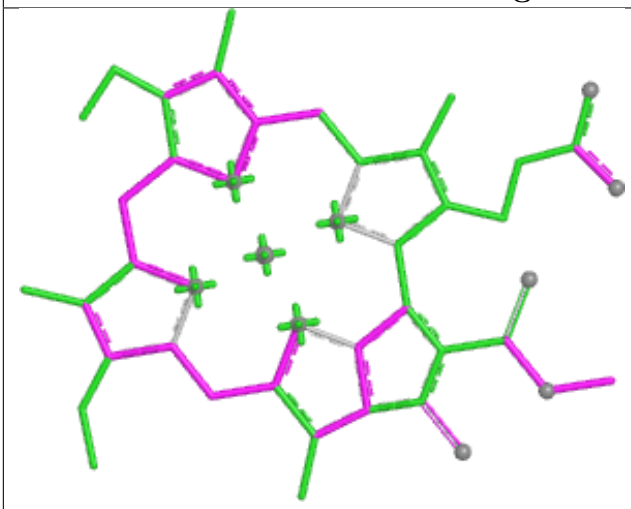
Bond angles



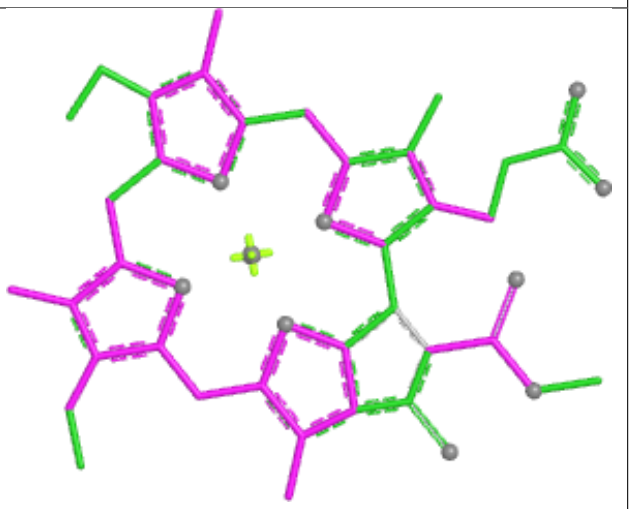
Torsions

Rings

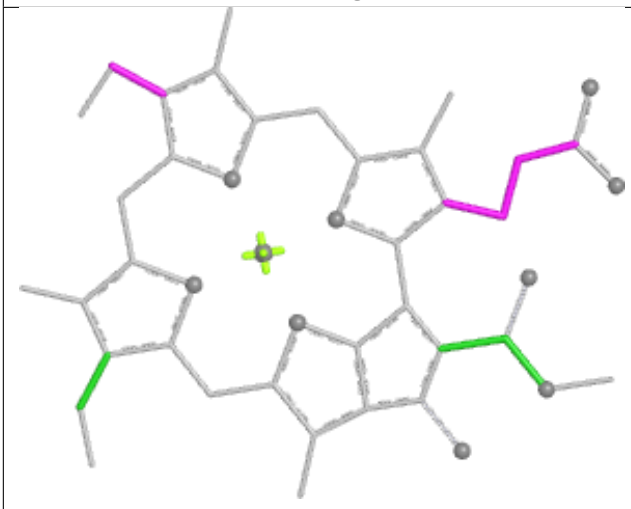
Ligand CLA bA 814



Bond lengths



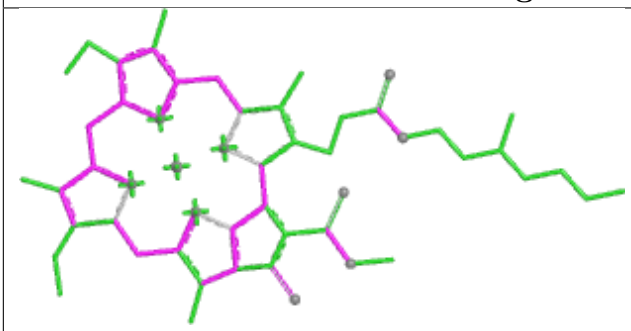
Bond angles



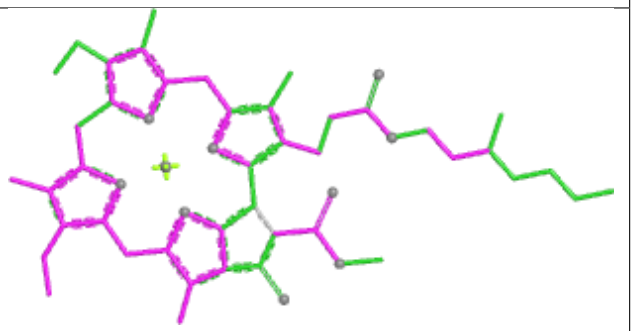
Torsions

Rings

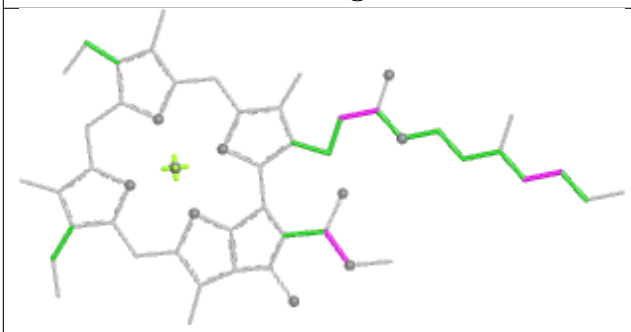
Ligand CLA cA 805



Bond lengths



Bond angles



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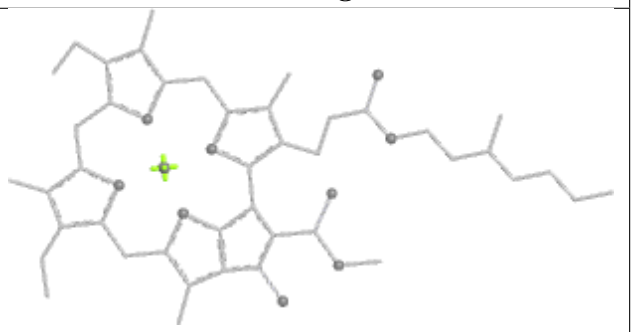
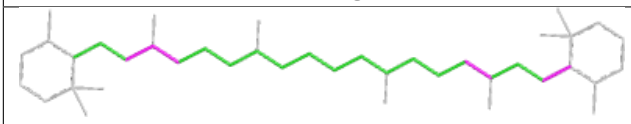


Rings

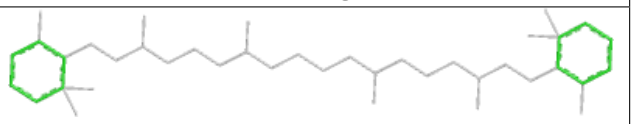
Ligand BCR aL 201

Bond lengths

Bond angles

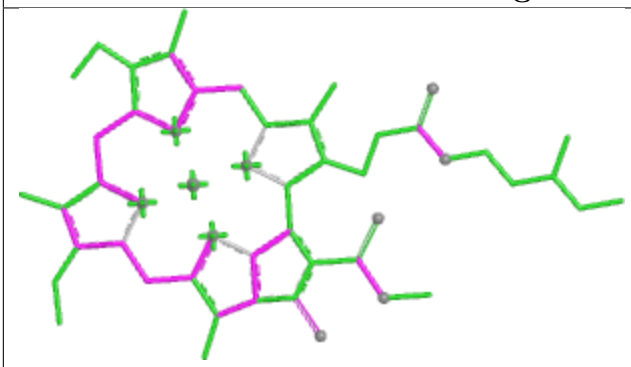


Torsions



Rings

Ligand CLA bA 833



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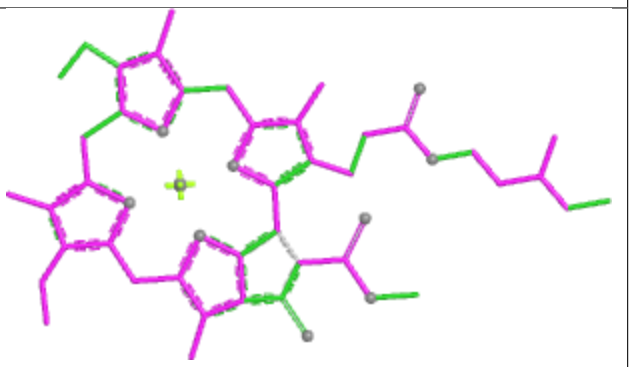
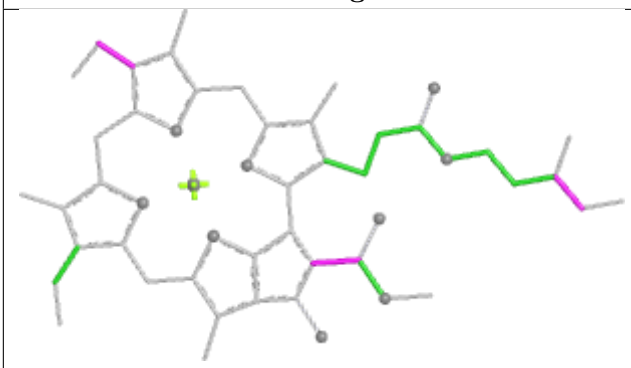


Bond angles



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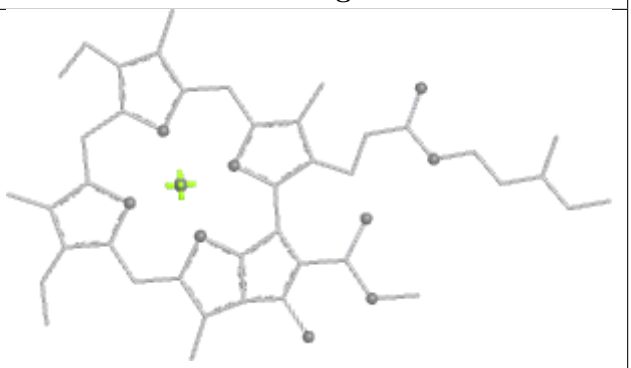
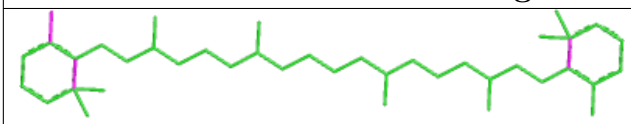
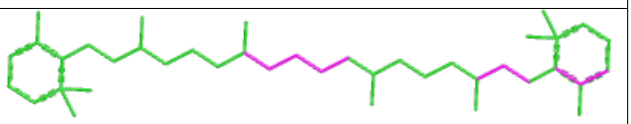


Rings

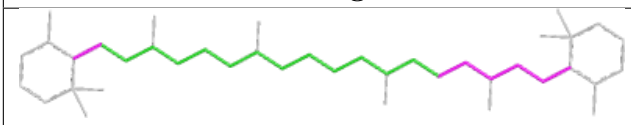
Ligand BCR cA 848



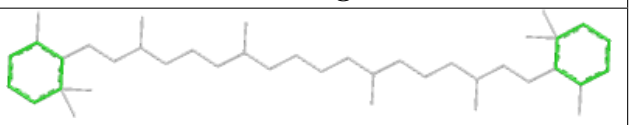
Bond lengths



Bond angles

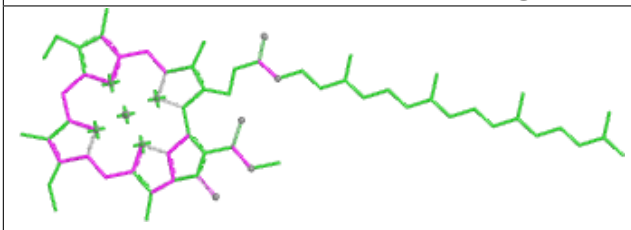


Torsions



Rings

Ligand CLA aA 834



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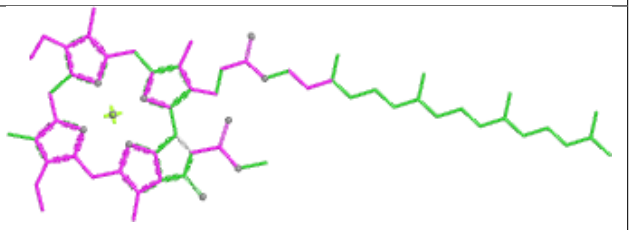
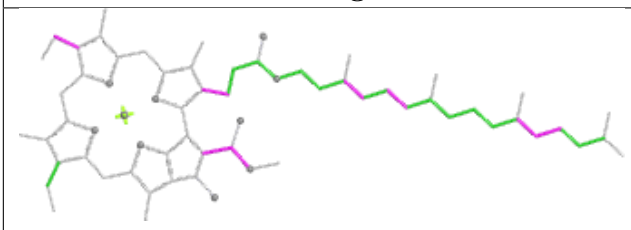
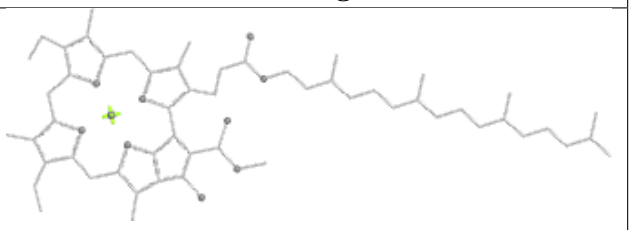


Bond angles

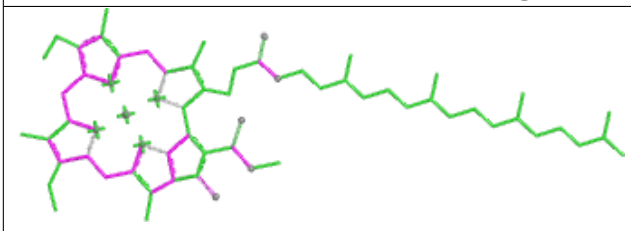


Torsions



Rings

Ligand CLA cA 803



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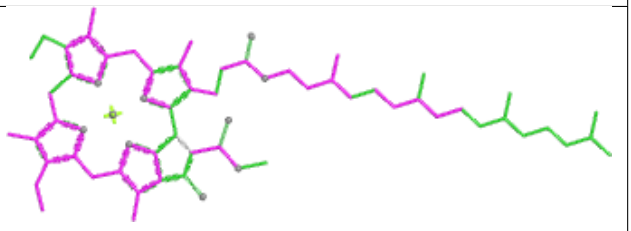
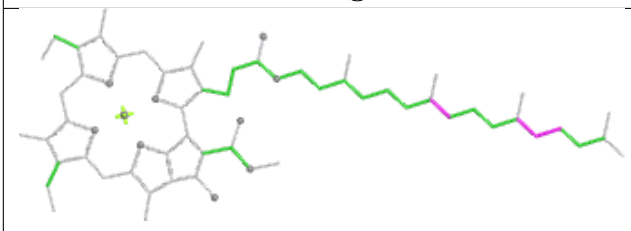
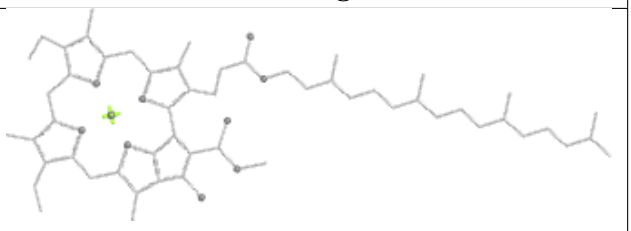


Bond angles

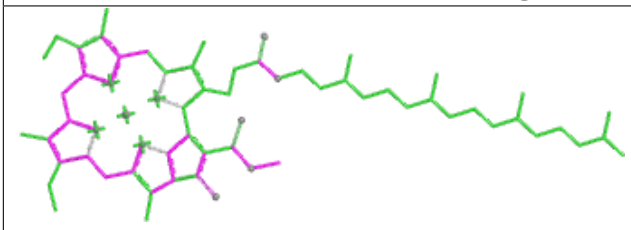


Torsions



Rings

Ligand CLA aB 912



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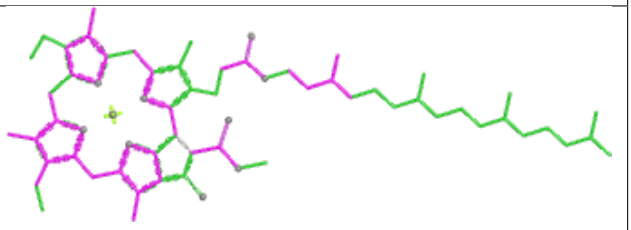
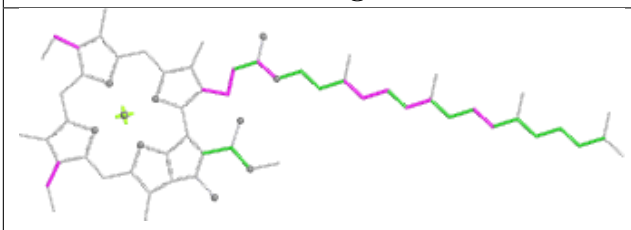
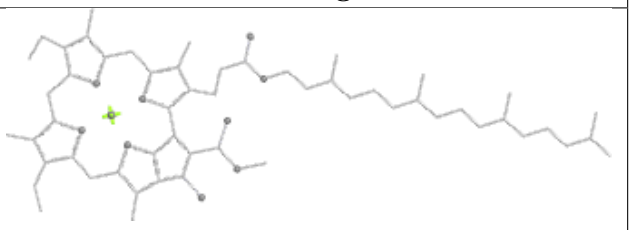


Bond angles

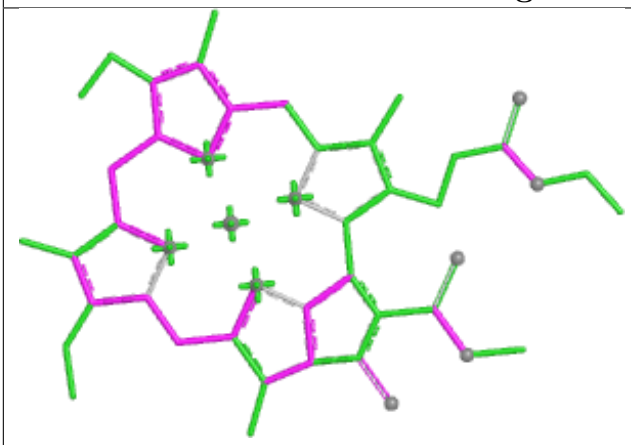


Torsions



Rings

Ligand CLA cA 824



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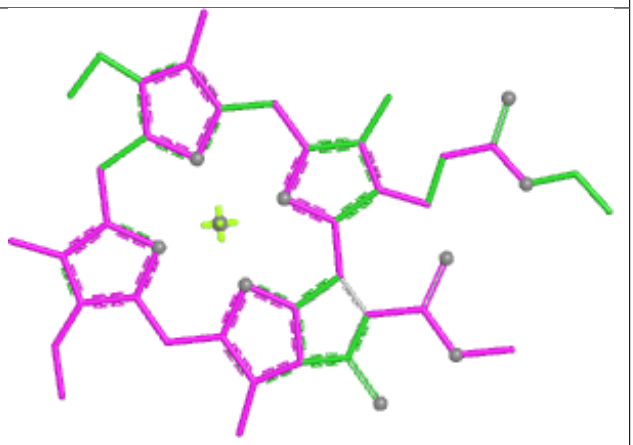
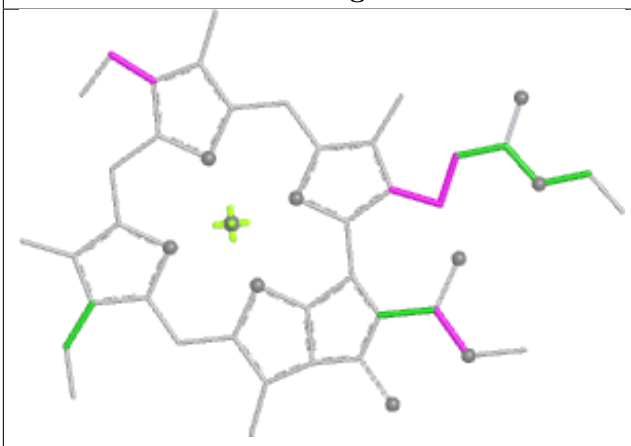
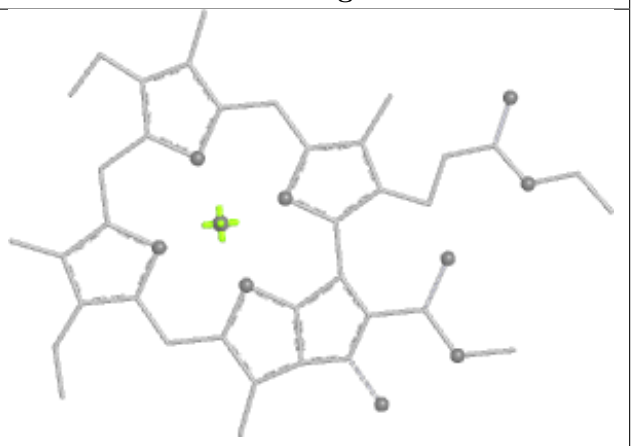


Bond angles

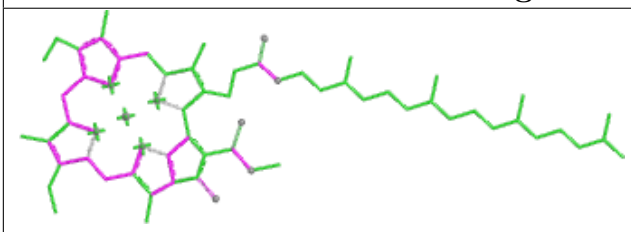


Torsions

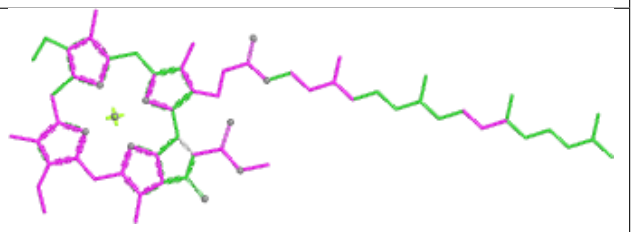


Rings

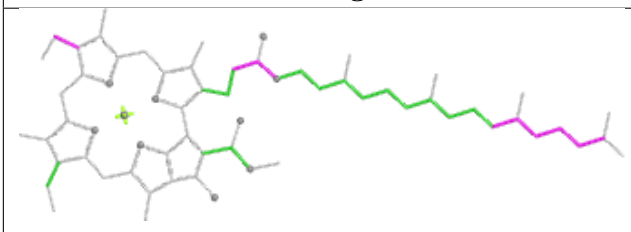
Ligand CLA aA 843



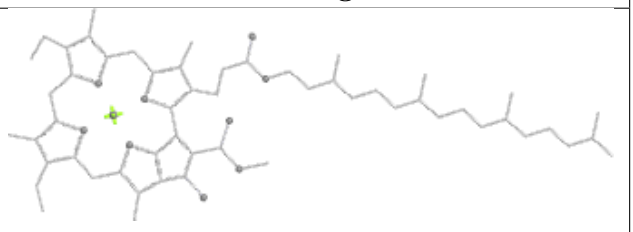
Bond lengths



Bond angles

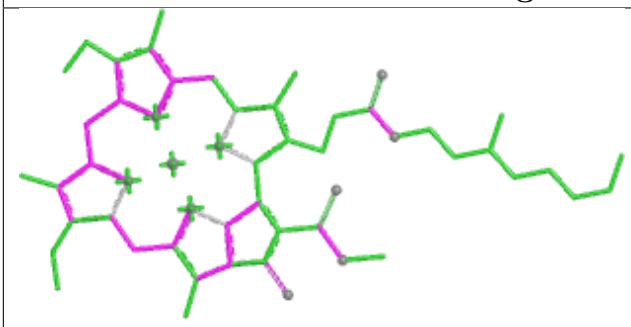


Torsions

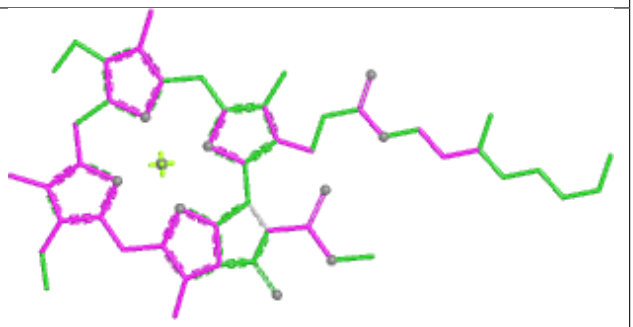


Rings

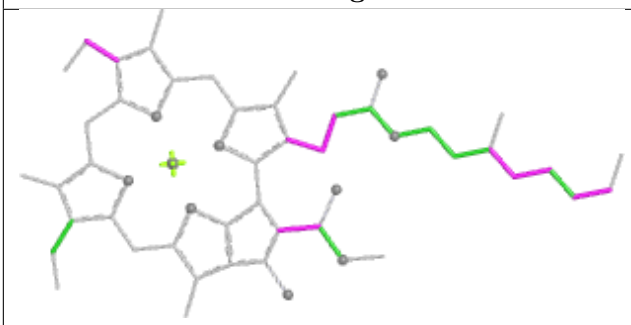
Ligand CLA cB 923



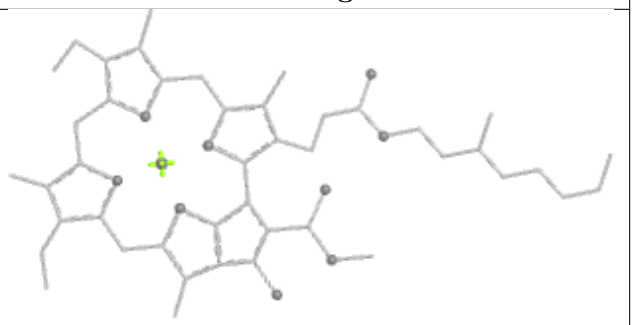
Bond lengths



Bond angles

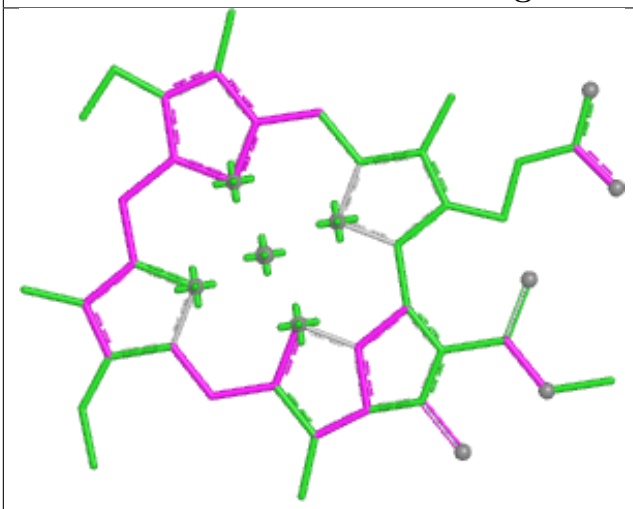


Torsions

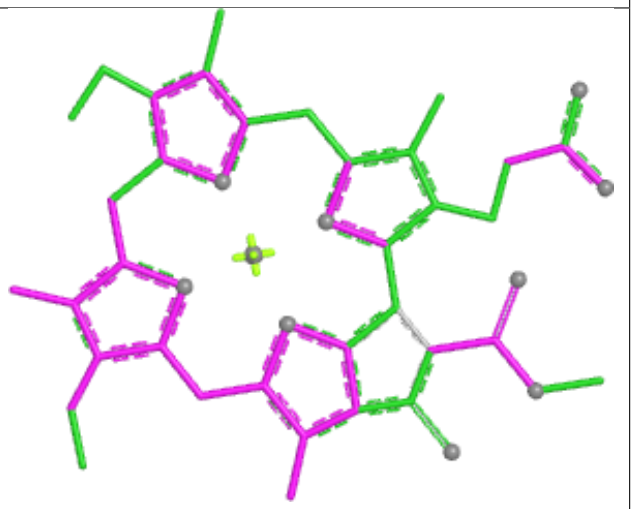


Rings

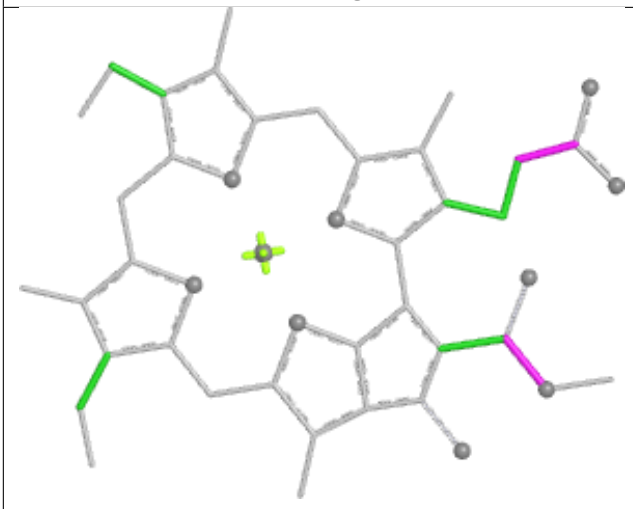
Ligand CLA bB 920



Bond lengths



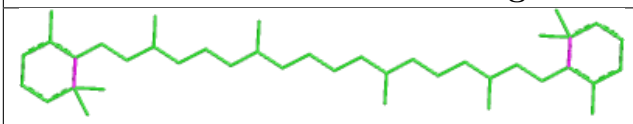
Bond angles



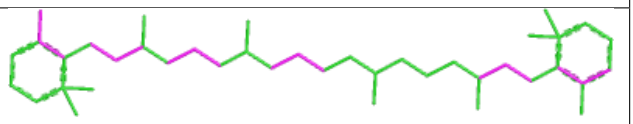
Torsions

Rings

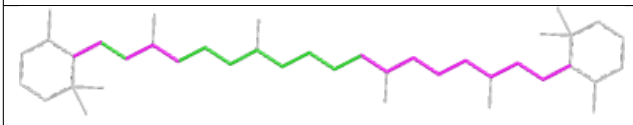
Ligand BCR bM 101



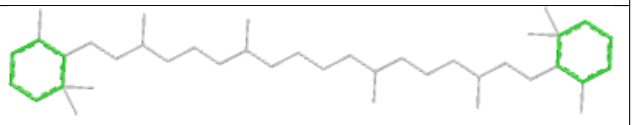
Bond lengths



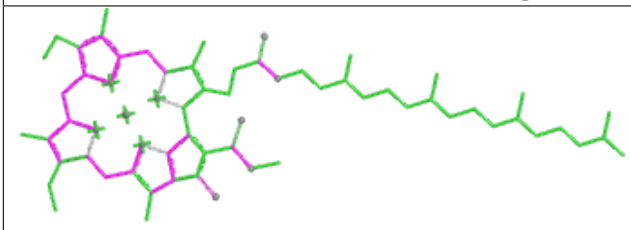
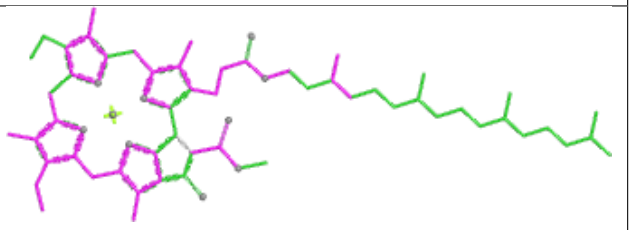
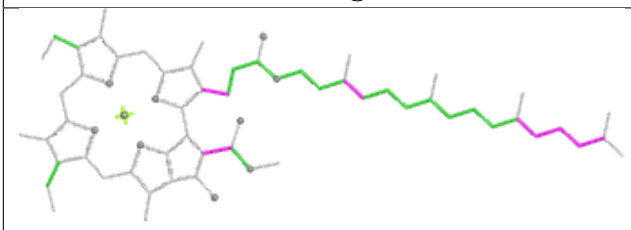
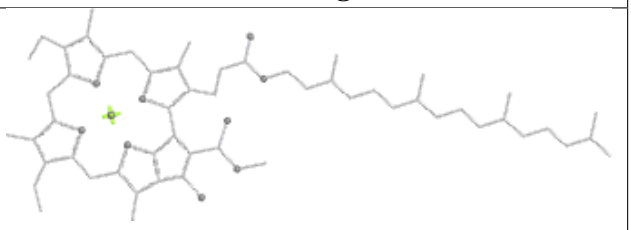
Bond angles

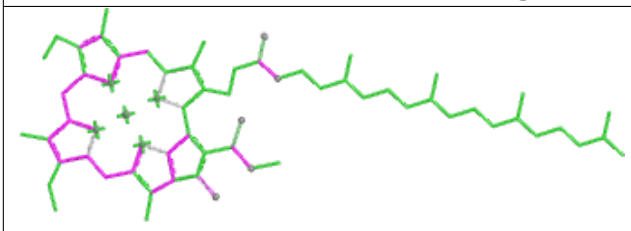
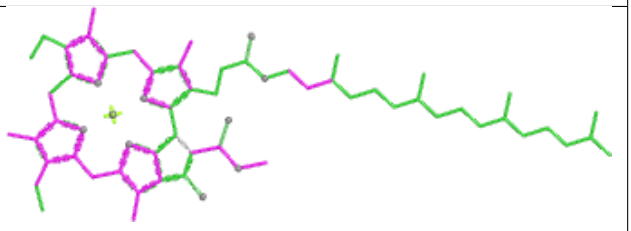
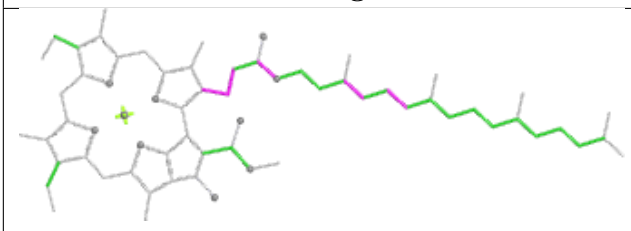
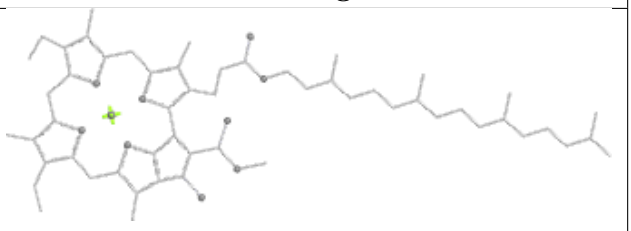


Torsions

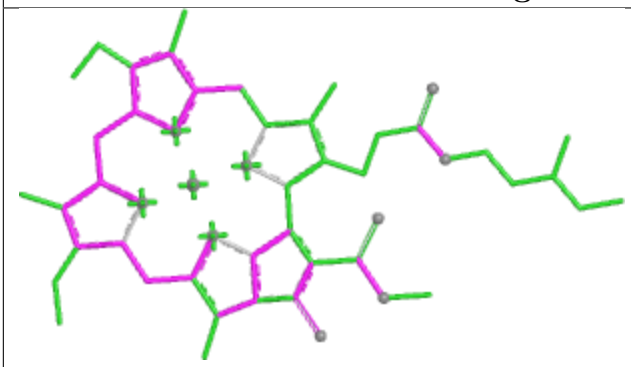


Rings

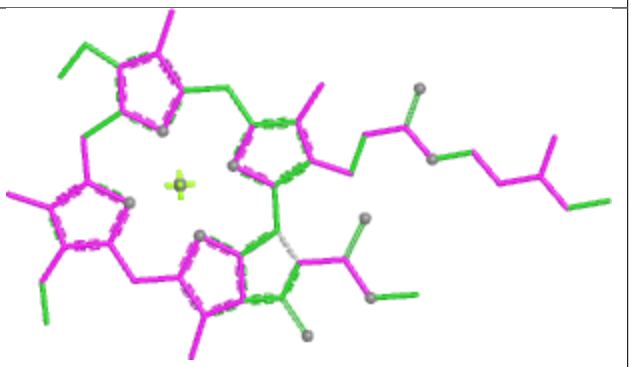
Ligand CLA cB 904	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA bB 927	
	
Bond lengths	Bond angles
	
Torsions	Rings

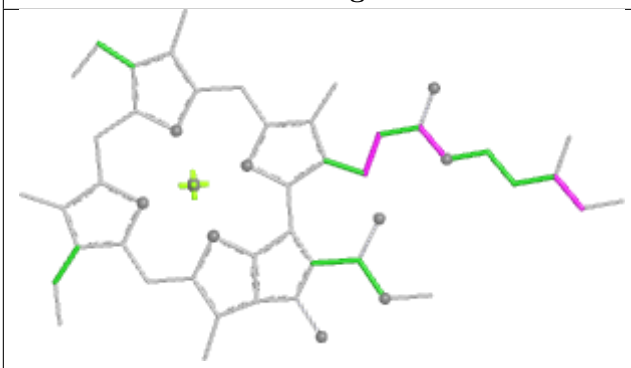
Ligand CLA bA 841



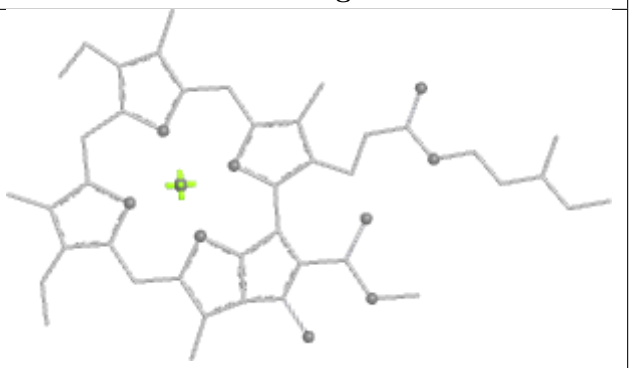
Bond lengths



Bond angles

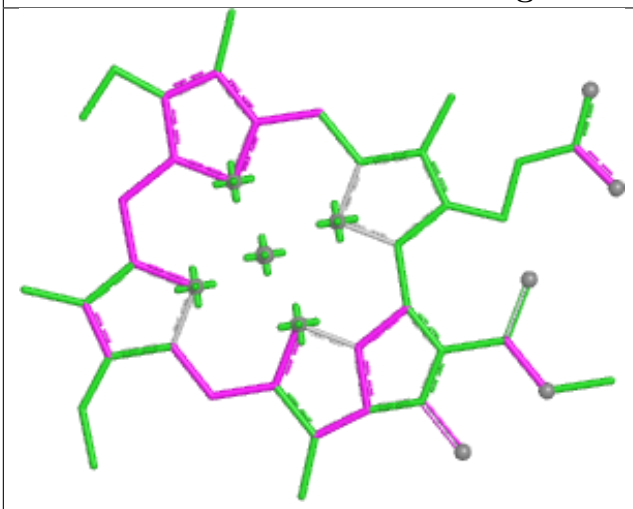


Torsions

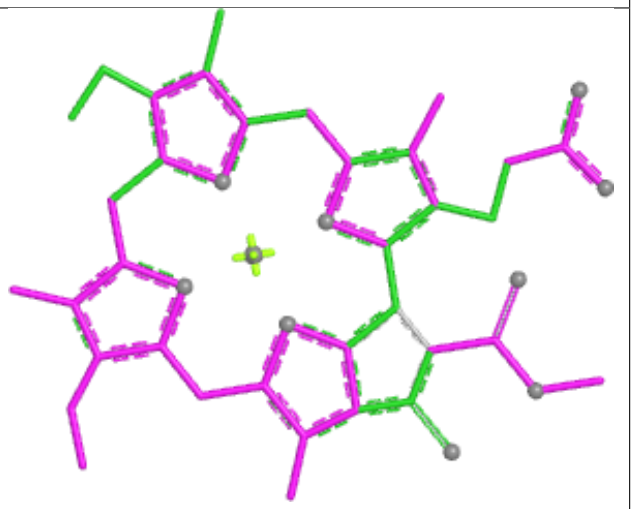


Rings

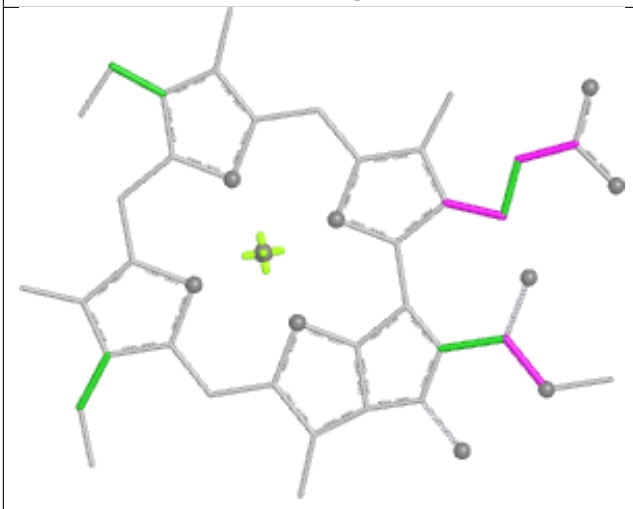
Ligand CLA cB 922



Bond lengths



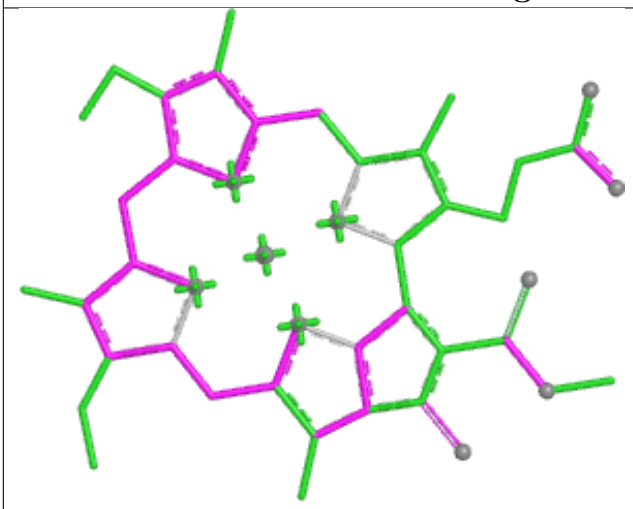
Bond angles



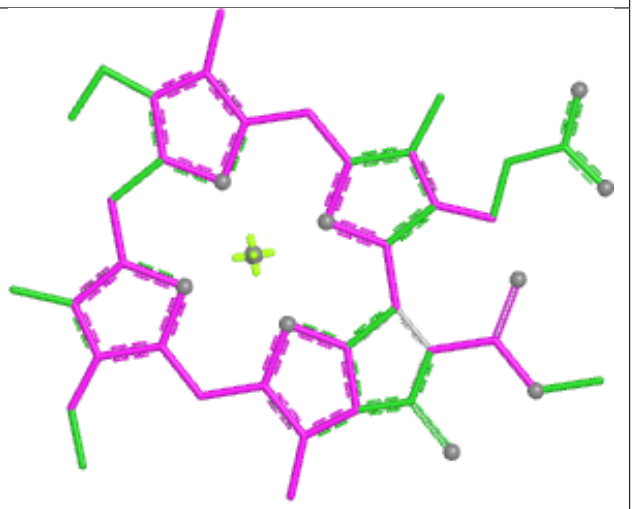
Torsions

Rings

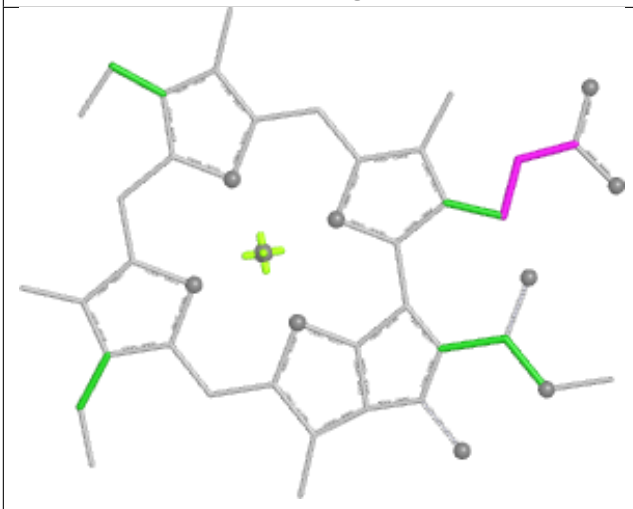
Ligand CLA bA 813



Bond lengths

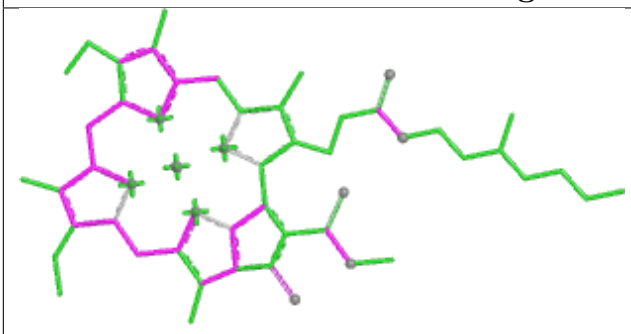
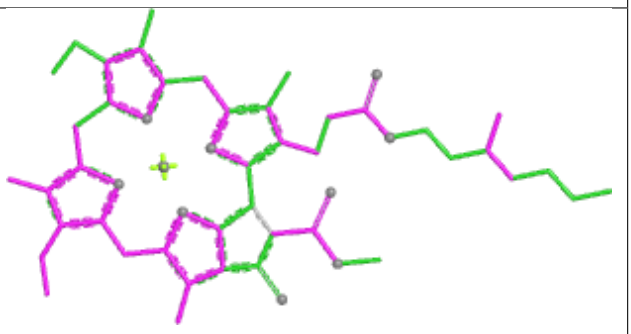
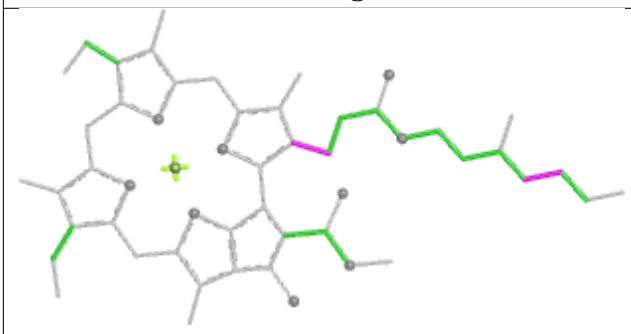
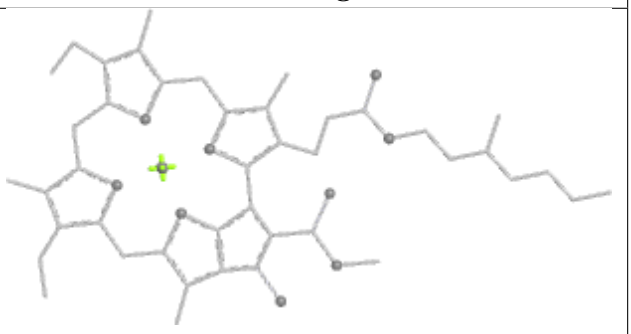


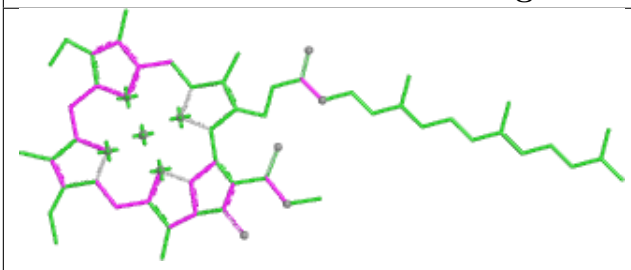
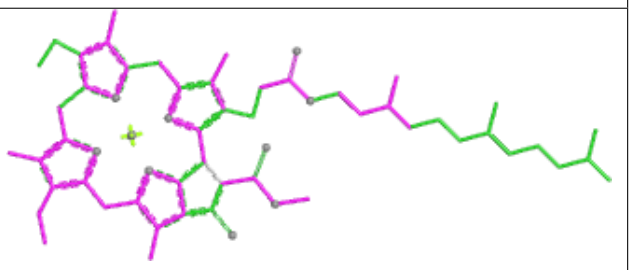
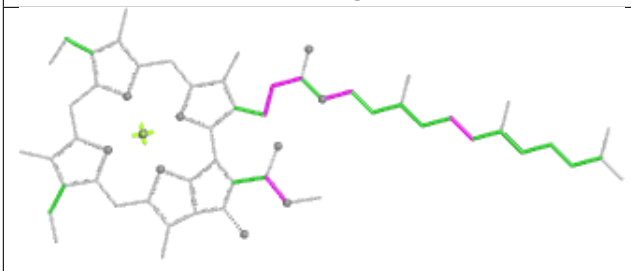
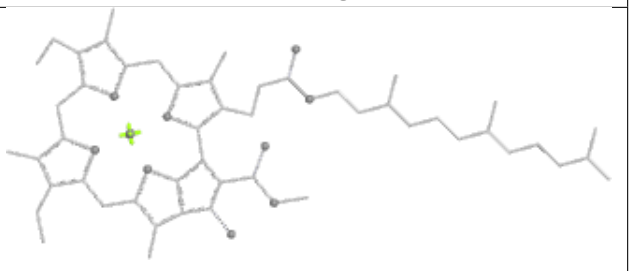
Bond angles



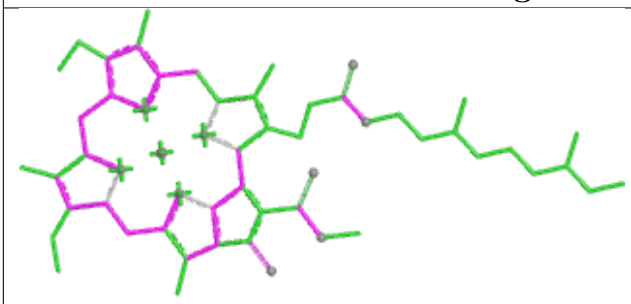
Torsions

Rings

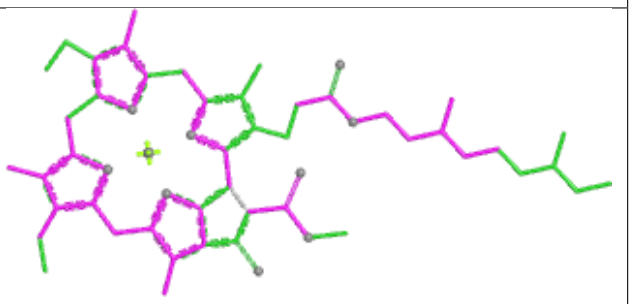
Ligand CLA aL 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA cA 829	
	
Bond lengths	Bond angles
	
Torsions	Rings

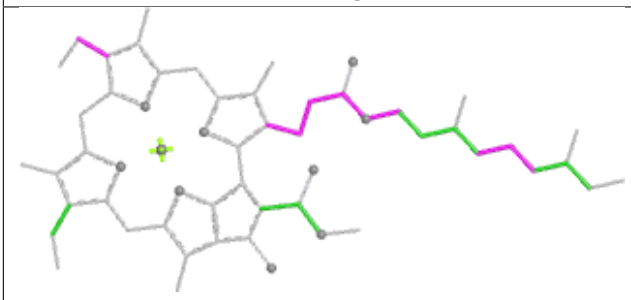
Ligand CLA bA 820



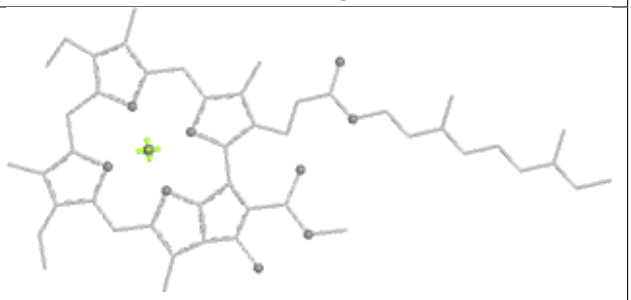
Bond lengths



Bond angles

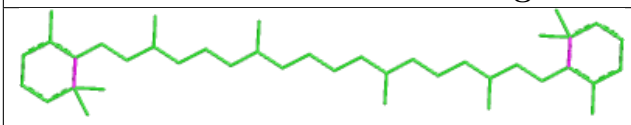


Torsions

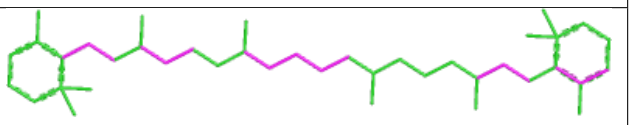


Rings

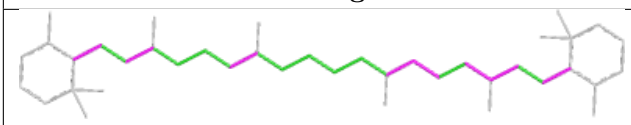
Ligand BCR cA 849



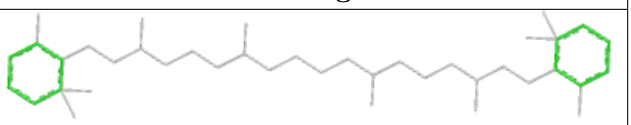
Bond lengths



Bond angles



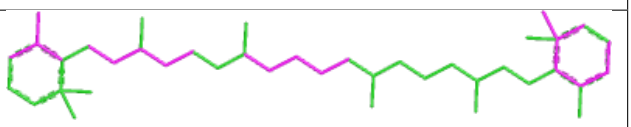
Torsions



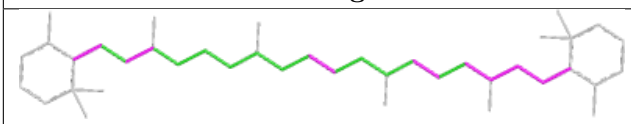
Rings

Ligand BCR cJ 101

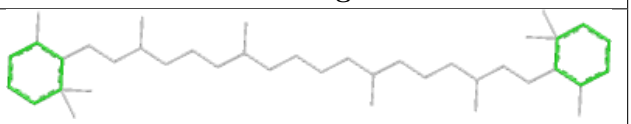
Bond lengths



Bond angles

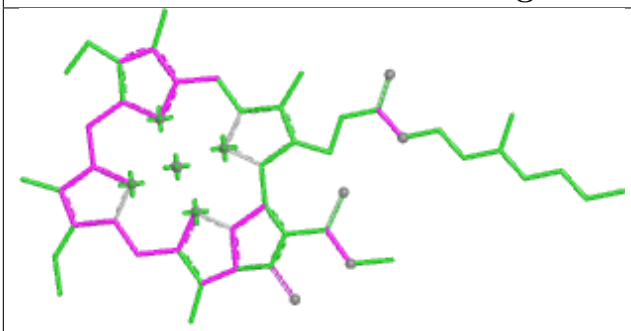


Torsions

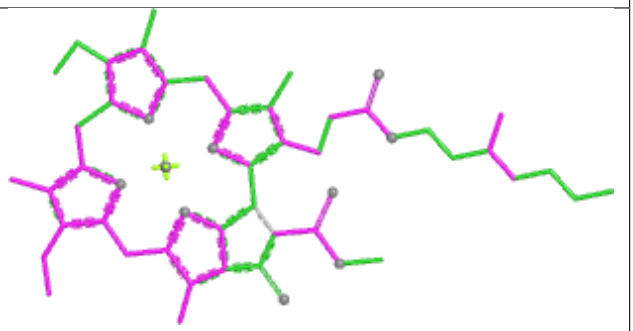


Rings

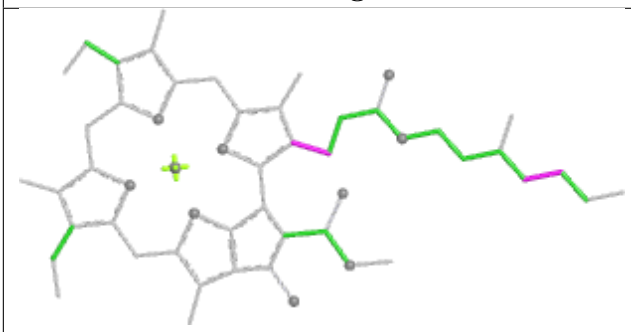
Ligand CLA bL 202



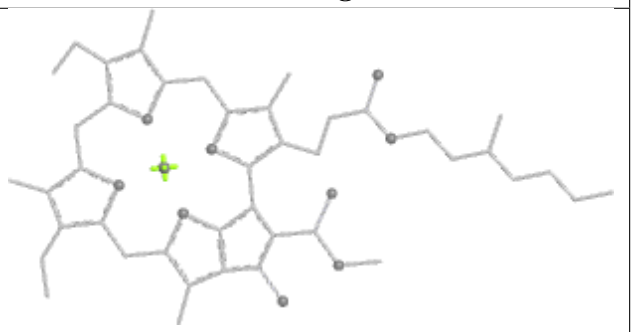
Bond lengths



Bond angles

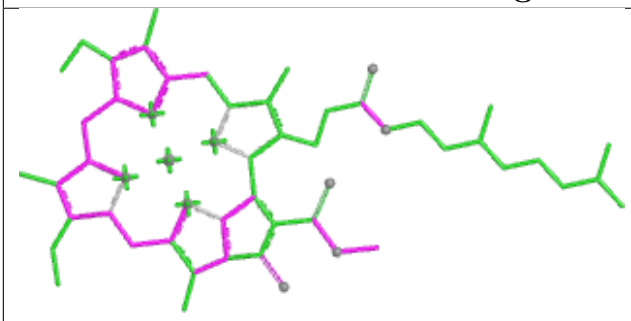


Torsions

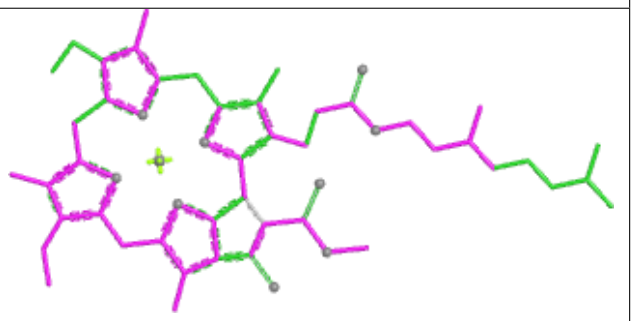


Rings

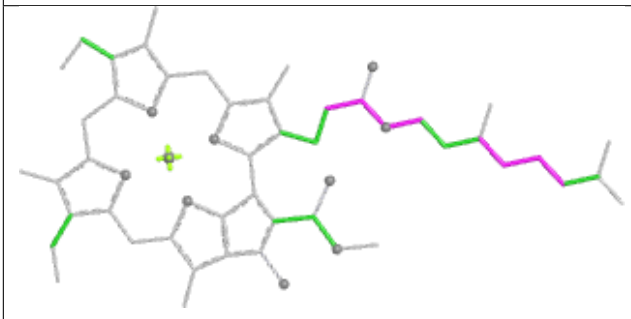
Ligand CLA bB 909



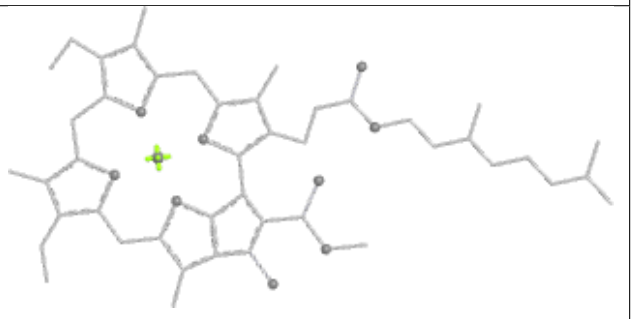
Bond lengths



Bond angles

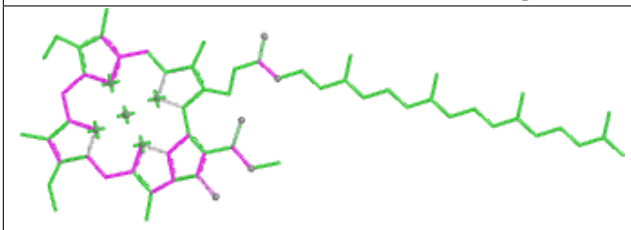


Torsions

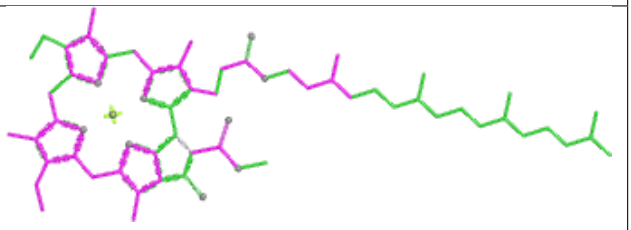


Rings

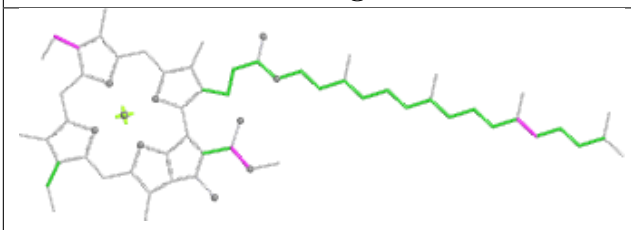
Ligand CLA cB 901



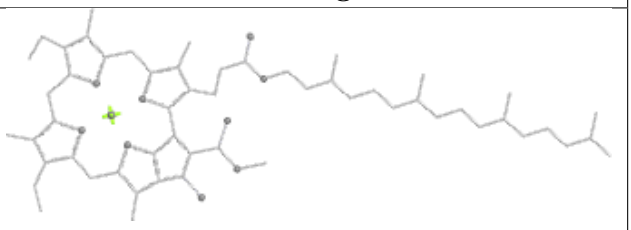
Bond lengths



Bond angles

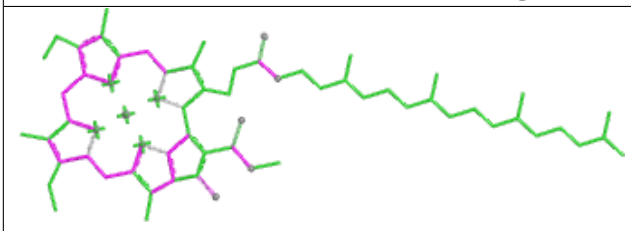


Torsions

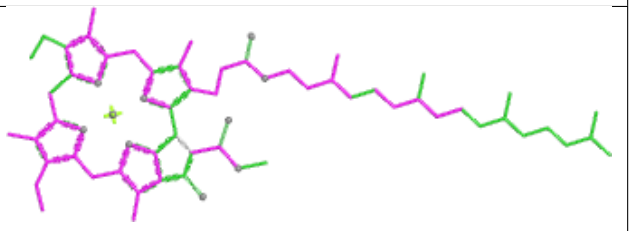


Rings

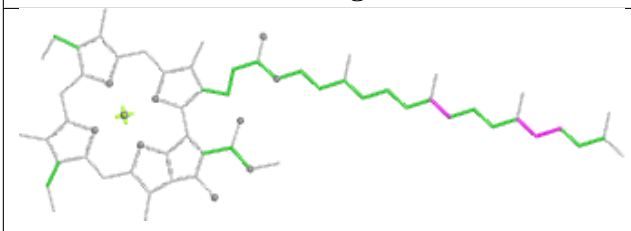
Ligand CLA bA 803



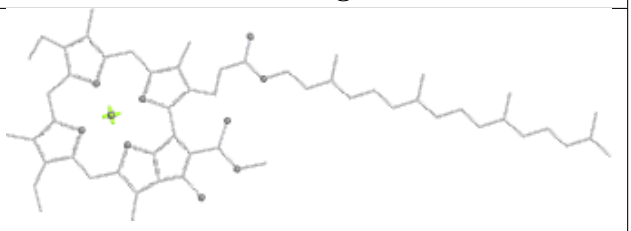
Bond lengths



Bond angles

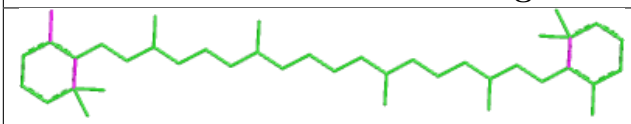


Torsions



Rings

Ligand BCR cB 942



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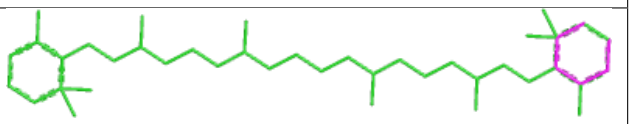
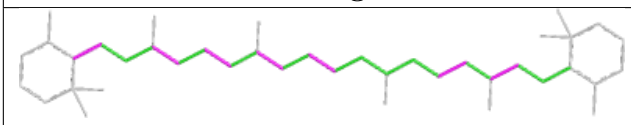
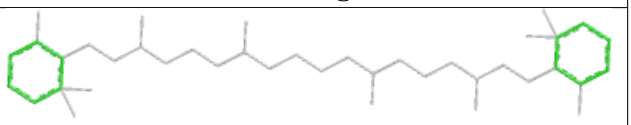


Bond angles

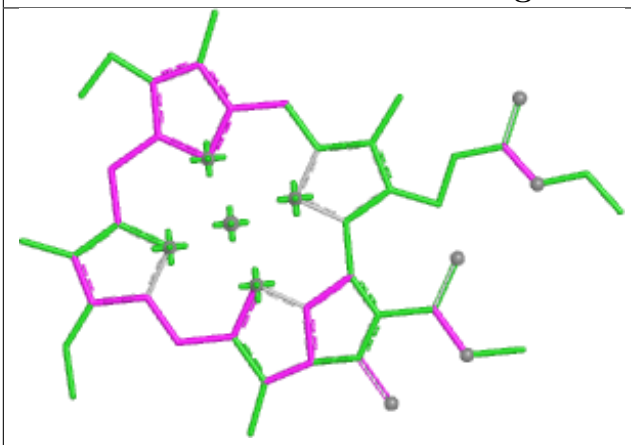


Torsions

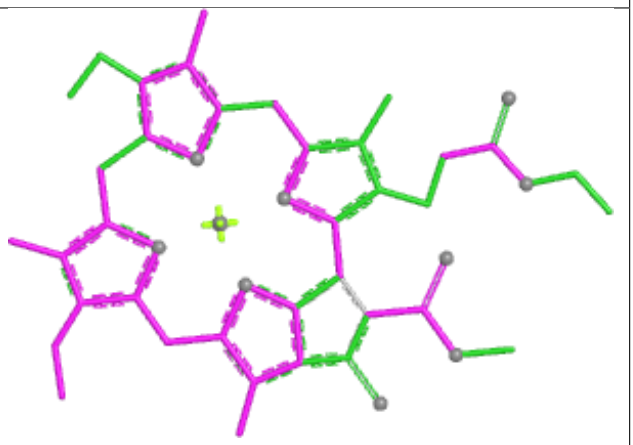


Rings

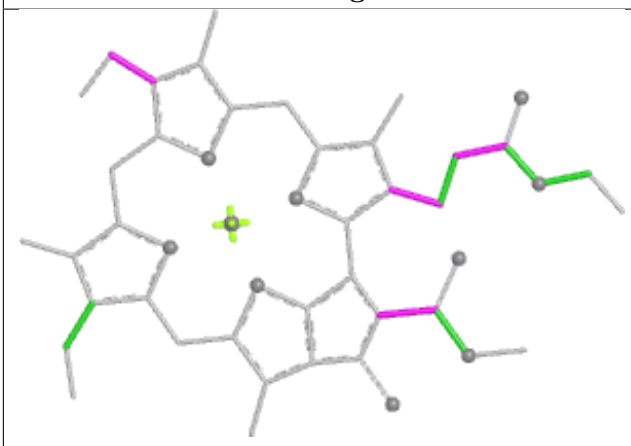
Ligand CLA bB 919



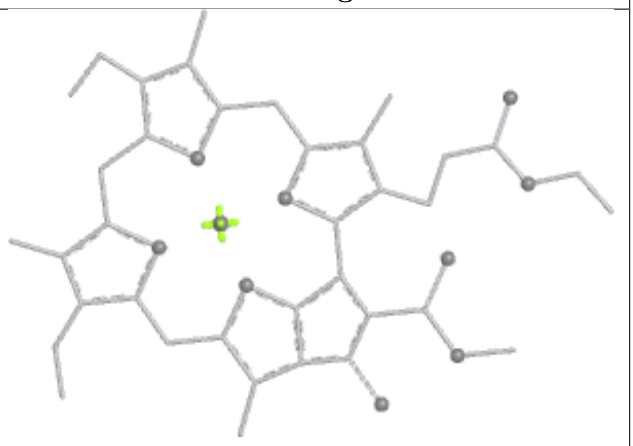
Bond lengths



Bond angles

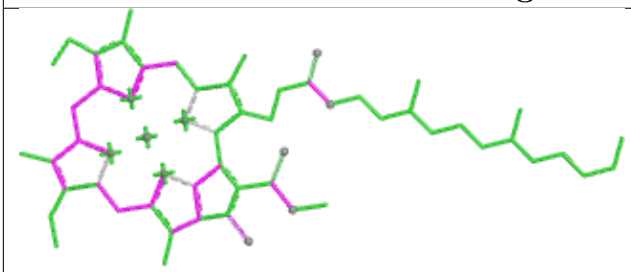


Torsions



Rings

Ligand CLA cB 916



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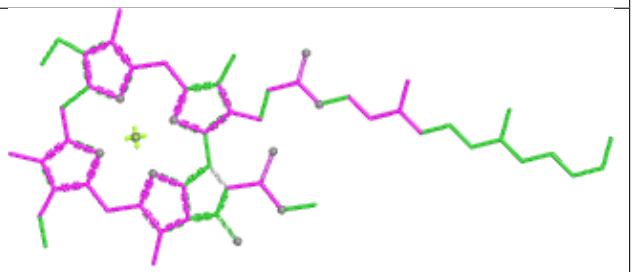
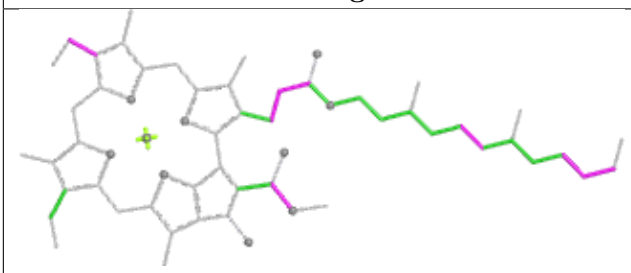


Bond angles



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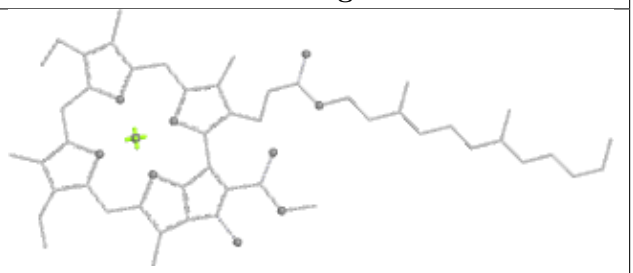
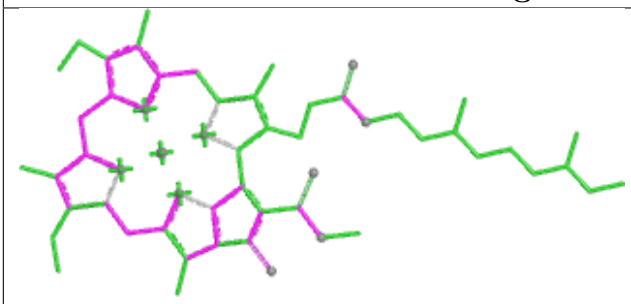


Rings

Ligand CLA bA 853



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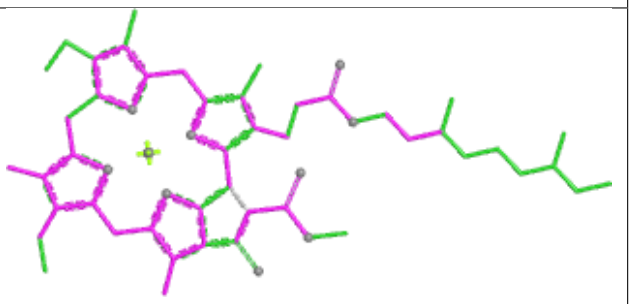
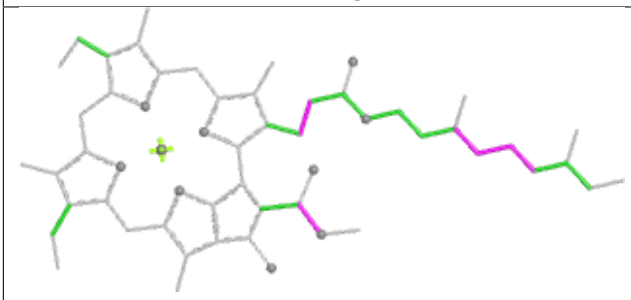
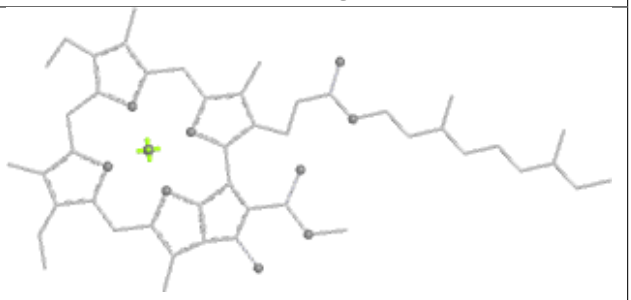


Bond angles

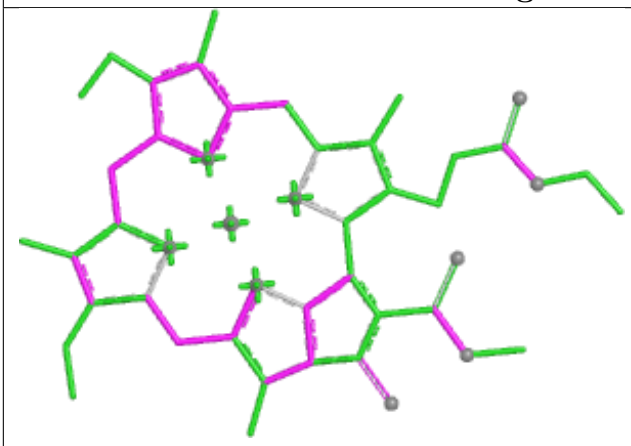


Torsions



Rings

Ligand CLA cB 919



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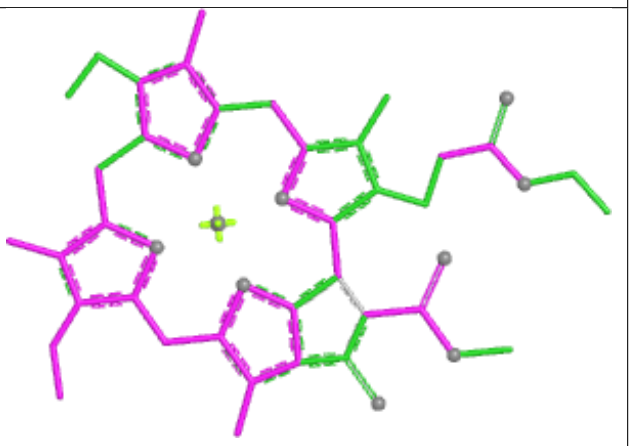
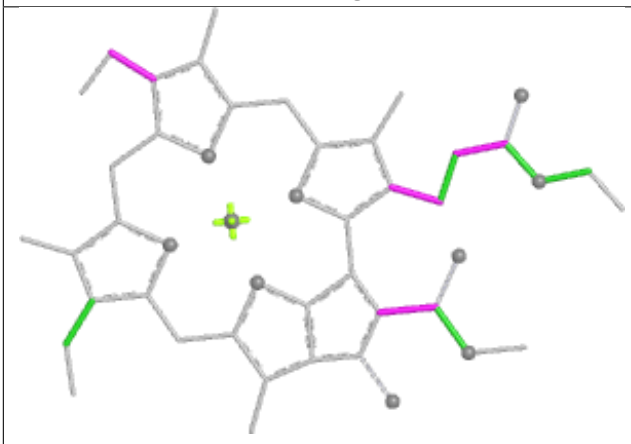
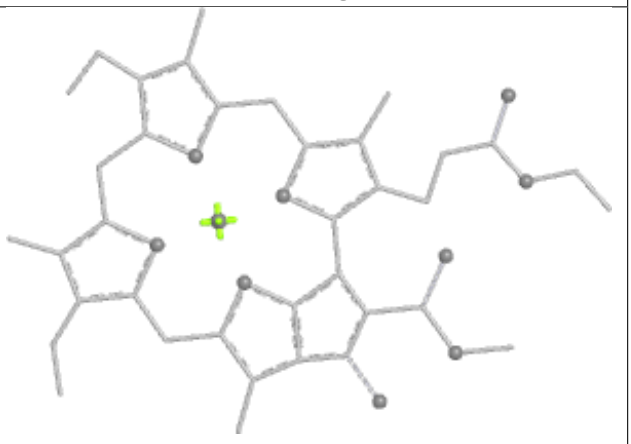


Bond angles

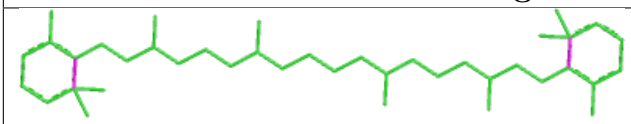


Torsions

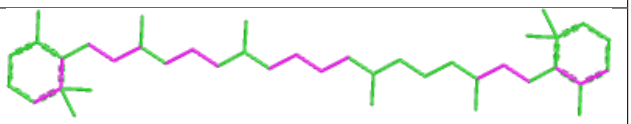


Rings

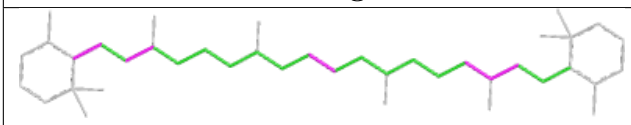
Ligand BCR bF 201



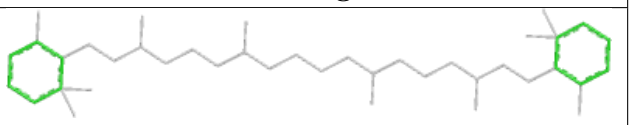
Bond lengths



Bond angles

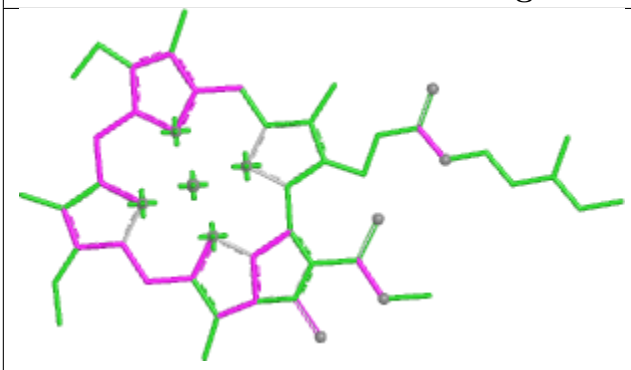


Torsions

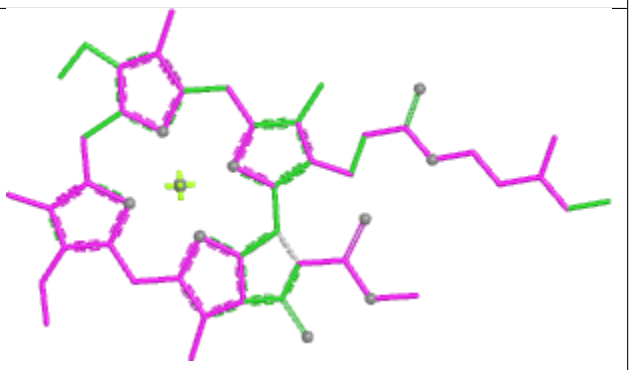


Rings

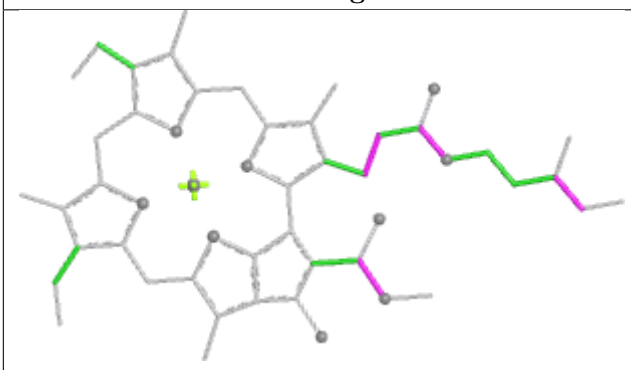
Ligand CLA cA 808



Bond lengths



Bond angles



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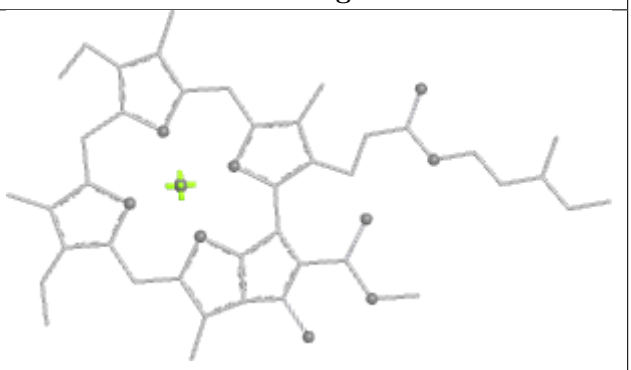
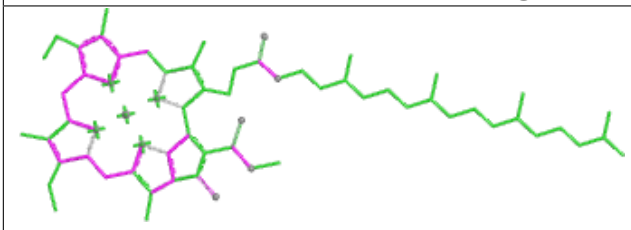


Rings

Ligand CLA aA 806



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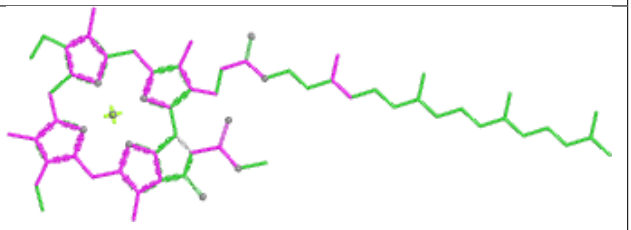
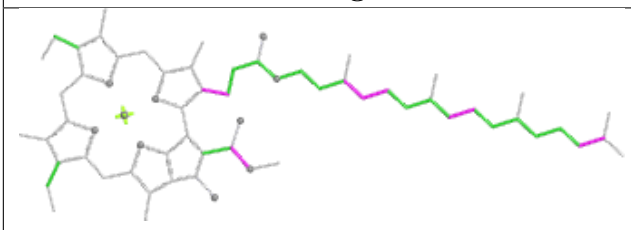
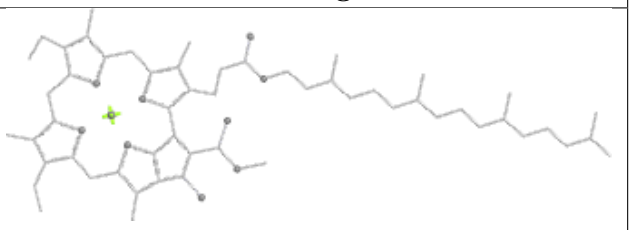


Bond angles

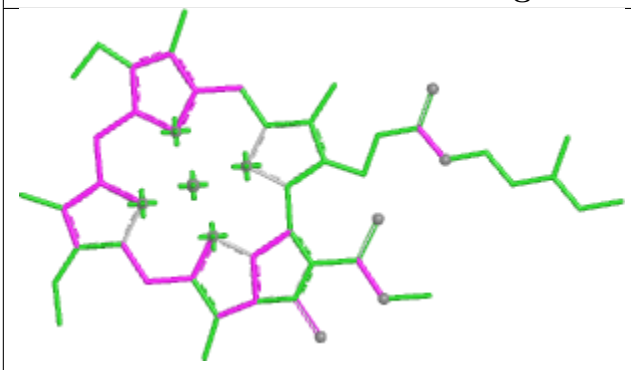


Torsions



Rings

Ligand CLA bA 823



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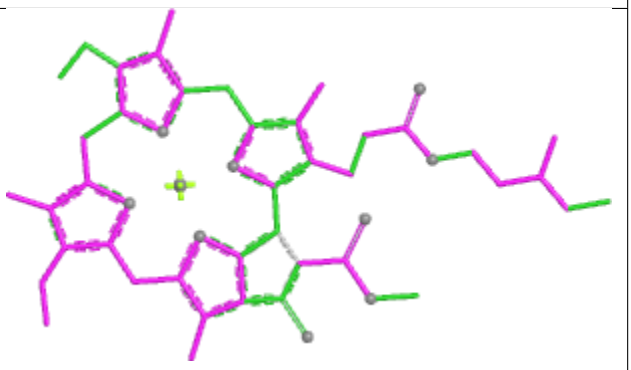
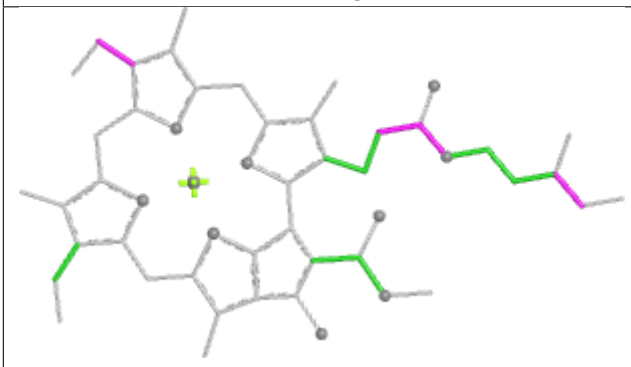


Bond angles



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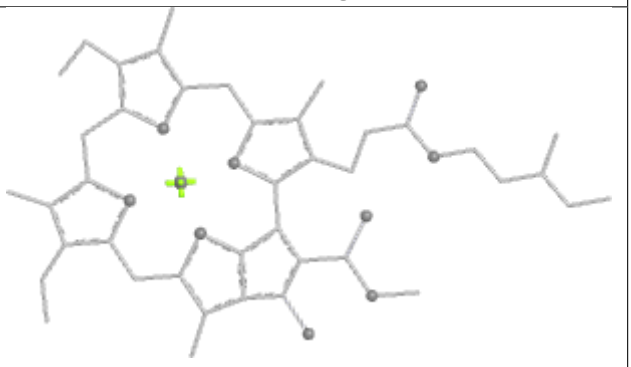
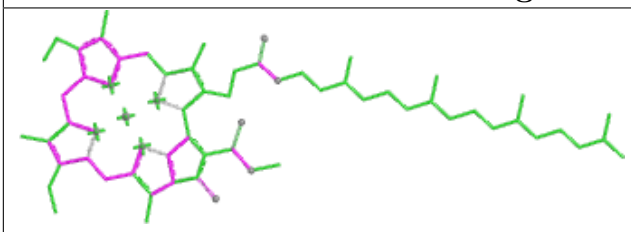


Rings

Ligand CLA cA 843



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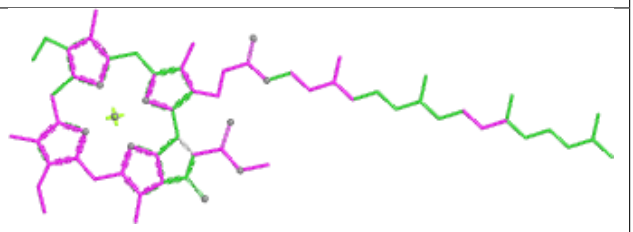
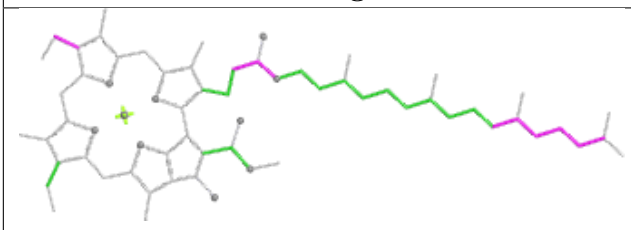
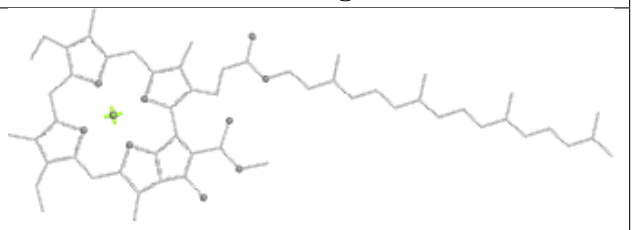


Bond angles



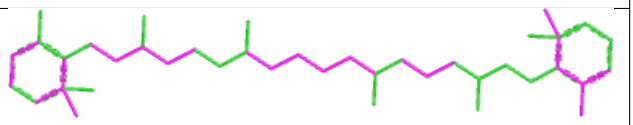
Torsions



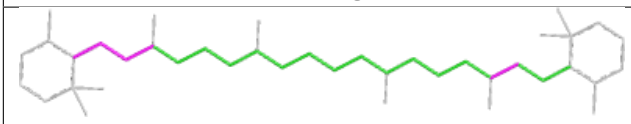
Rings

Ligand BCR bA 847

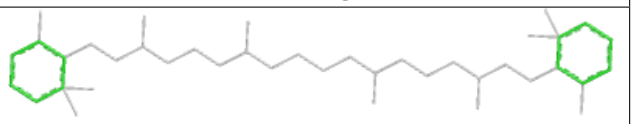
Bond lengths



Bond angles

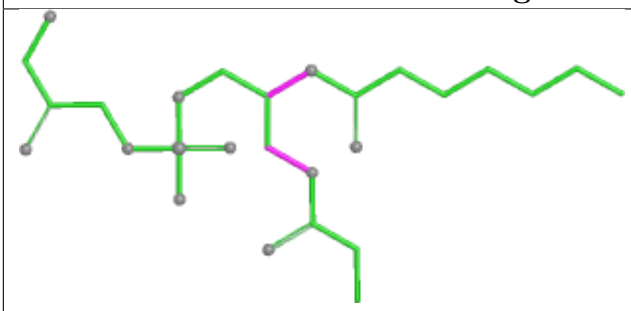


Torsions



Rings

Ligand LHG aA 853



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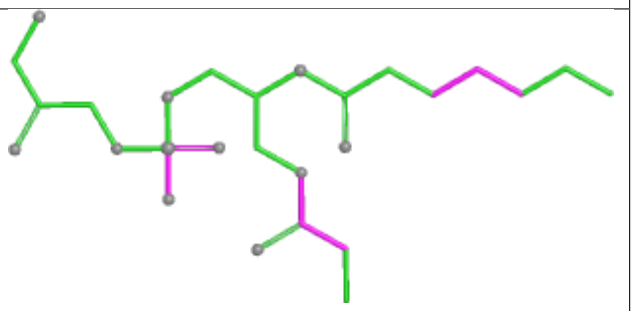
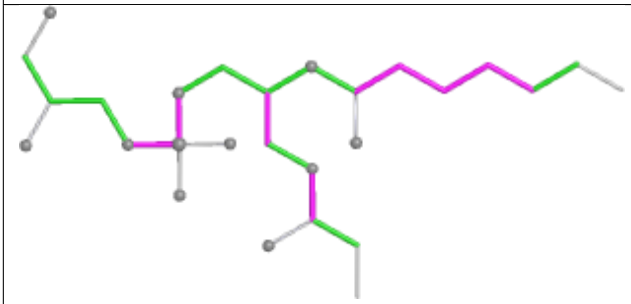
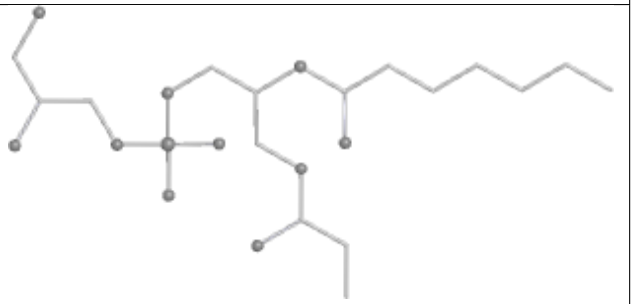


Bond angles

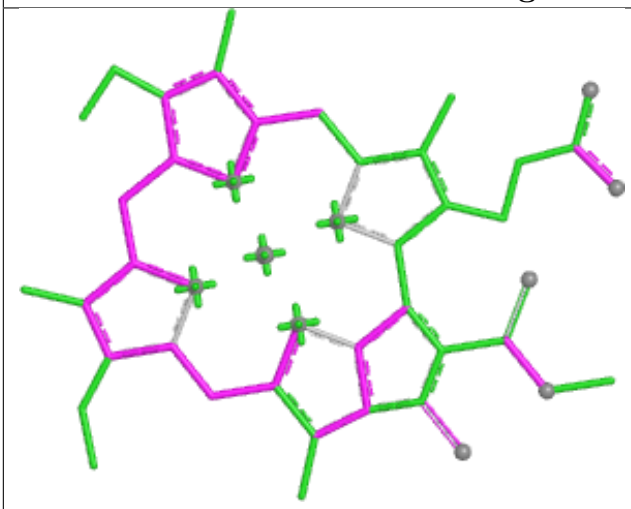


Torsions

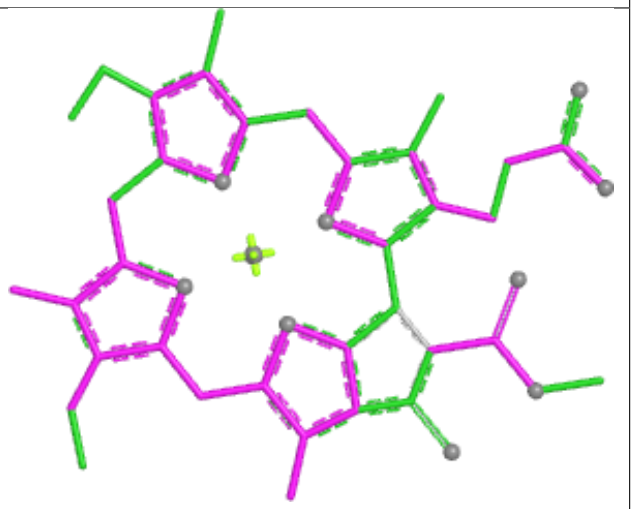


Rings

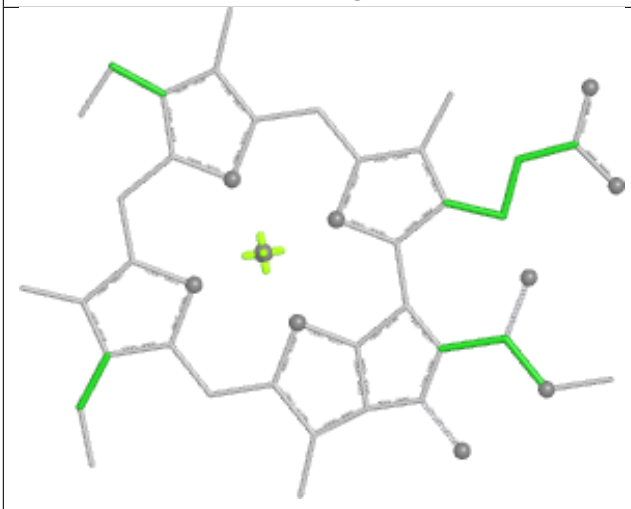
Ligand CLA cL 204



Bond lengths



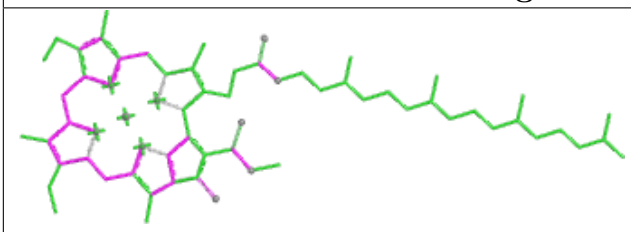
Bond angles



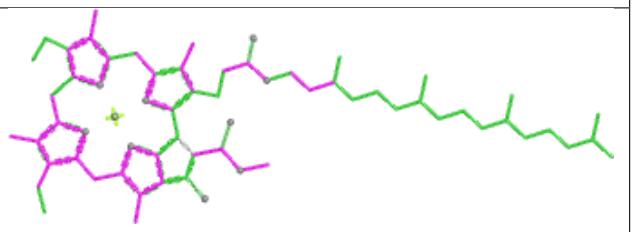
Torsions

Rings

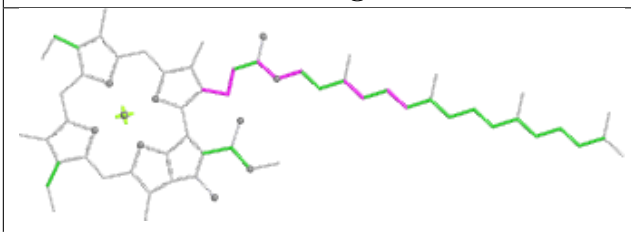
Ligand CLA aB 927



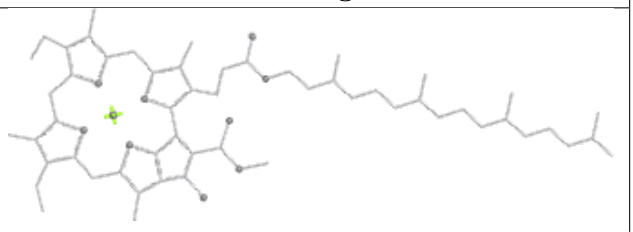
Bond lengths



Bond angles

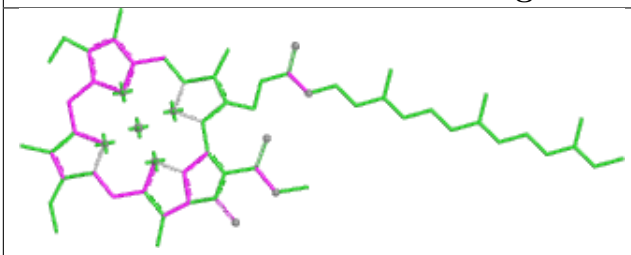


Torsions

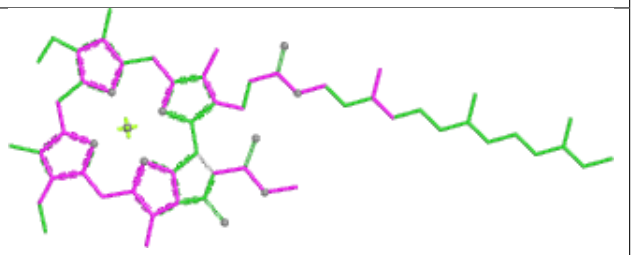


Rings

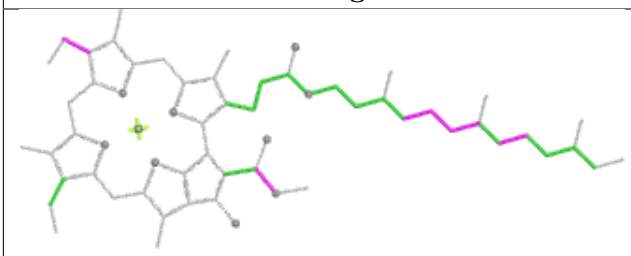
Ligand CLA aB 902



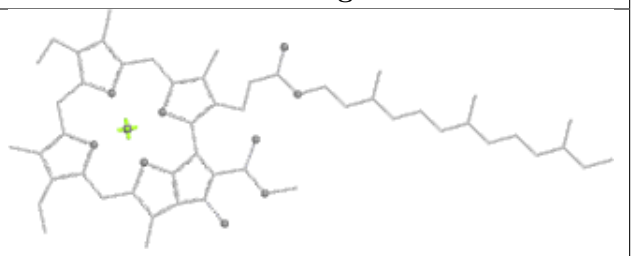
Bond lengths



Bond angles

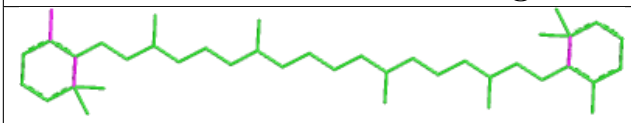


Torsions

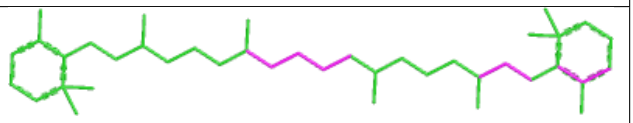


Rings

Ligand BCR bA 848

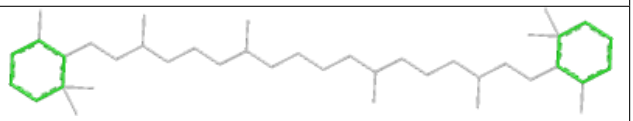


Bond lengths



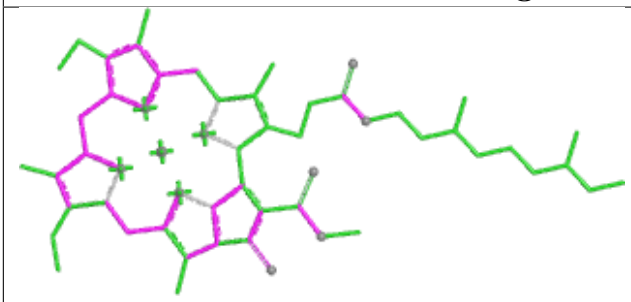
Bond angles

Torsions

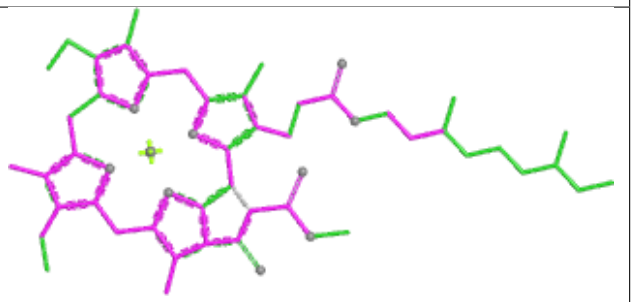


Rings

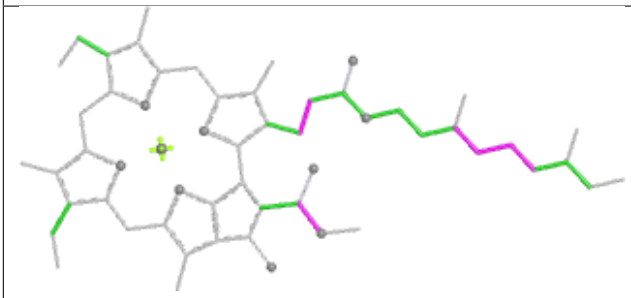
Ligand CLA cA 853



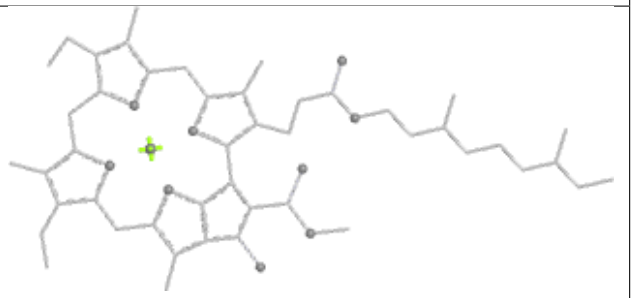
Bond lengths



Bond angles

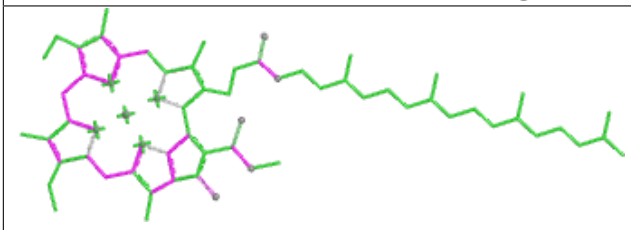


Torsions

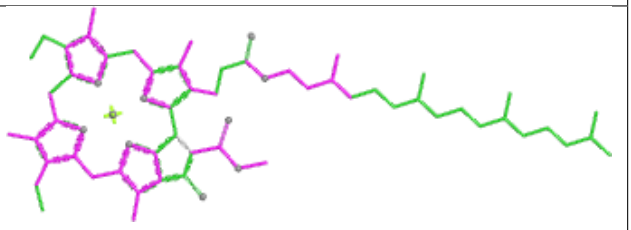


Rings

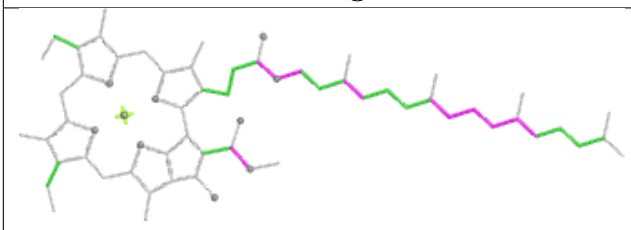
Ligand CLA aA 842



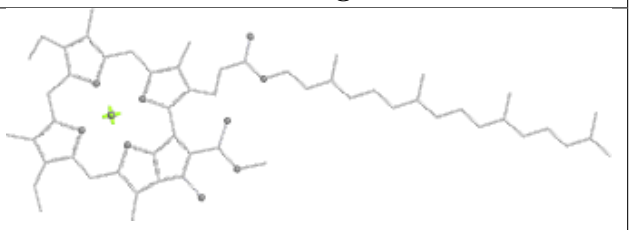
Bond lengths



Bond angles

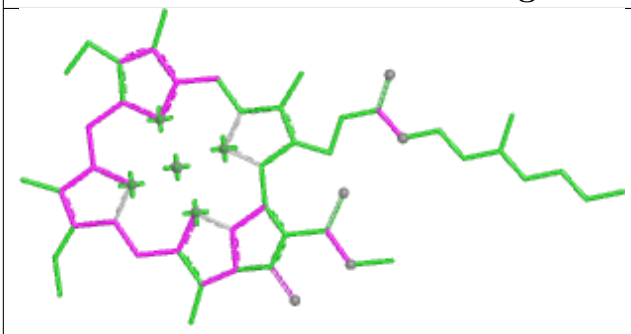


Torsions

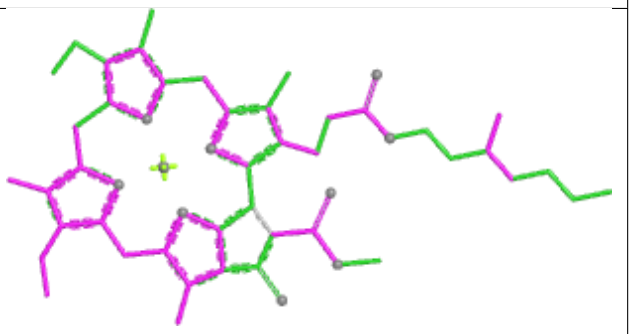


Rings

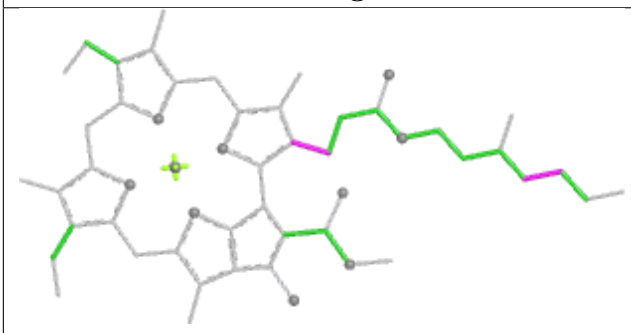
Ligand CLA cL 202



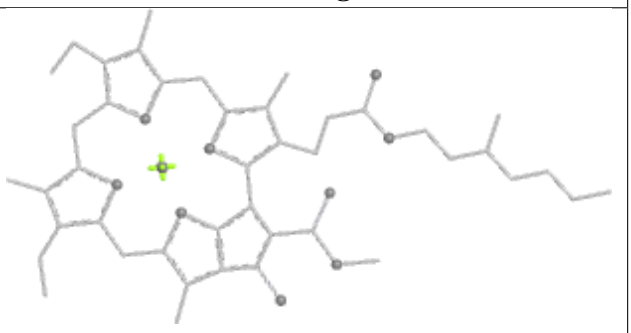
Bond lengths



Bond angles

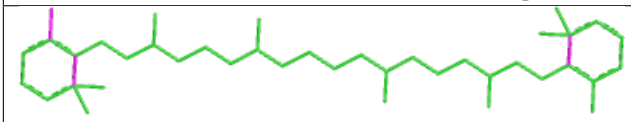


Torsions

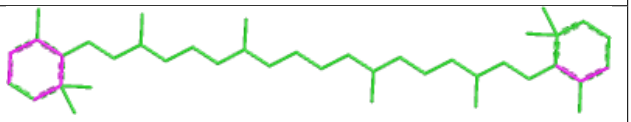


Rings

Ligand BCR cL 201

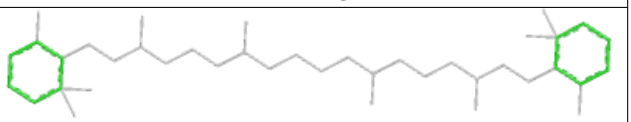


Bond lengths



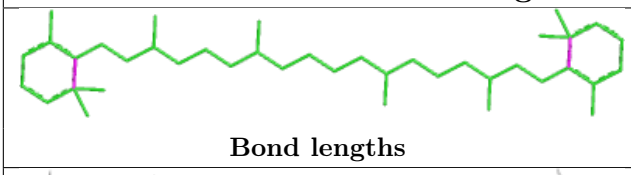
Bond angles

Torsions

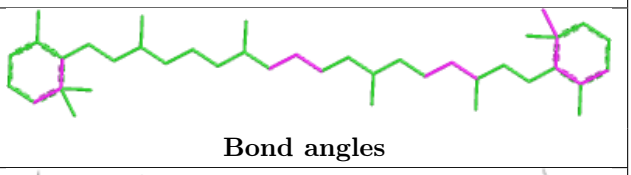


Rings

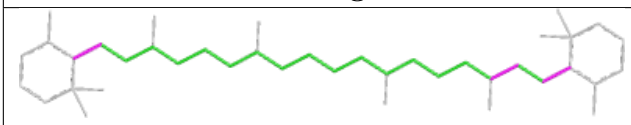
Ligand BCR bL 206



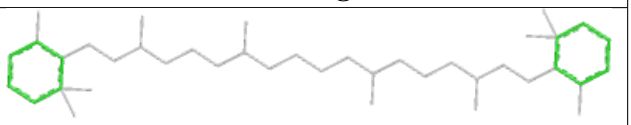
Bond lengths



Bond angles

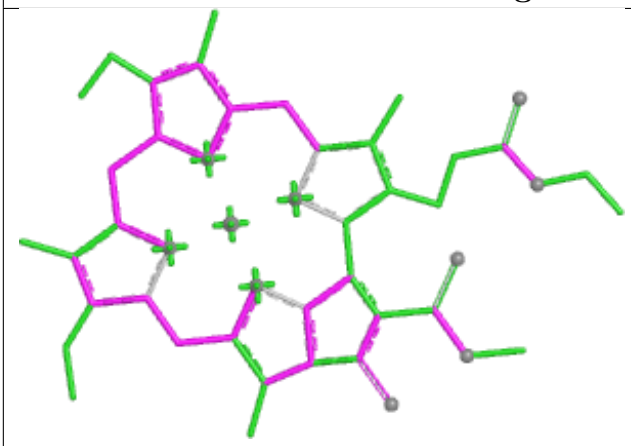


Torsions

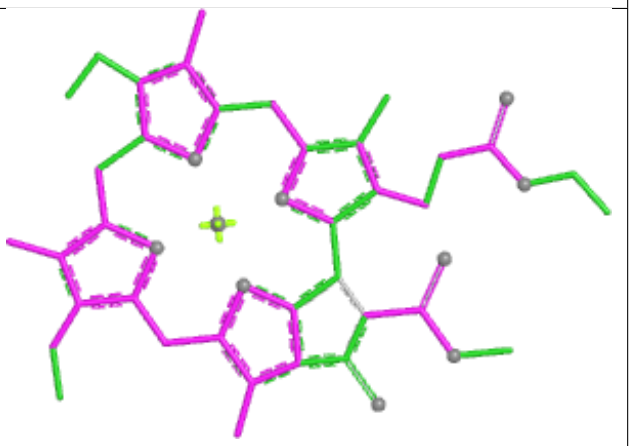


Rings

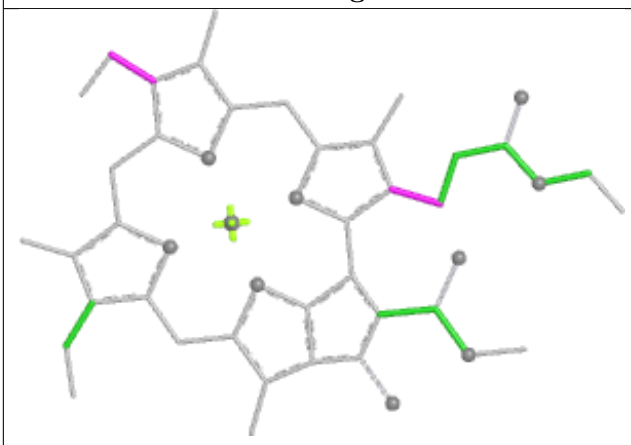
Ligand CLA bB 937



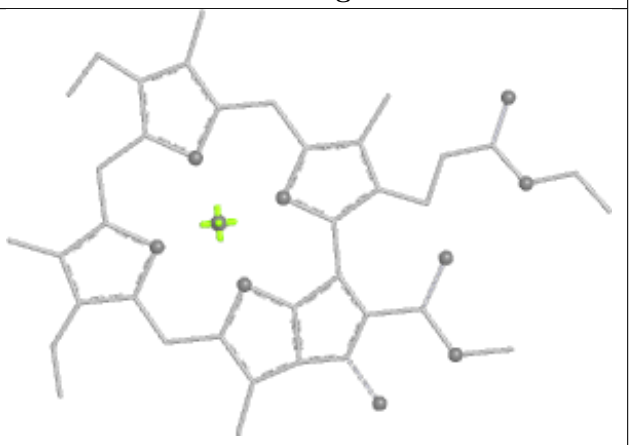
Bond lengths



Bond angles

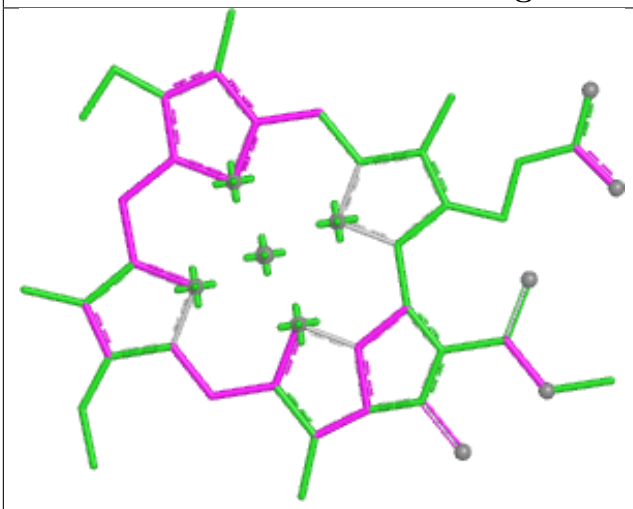


Torsions



Rings

Ligand CLA aA 839



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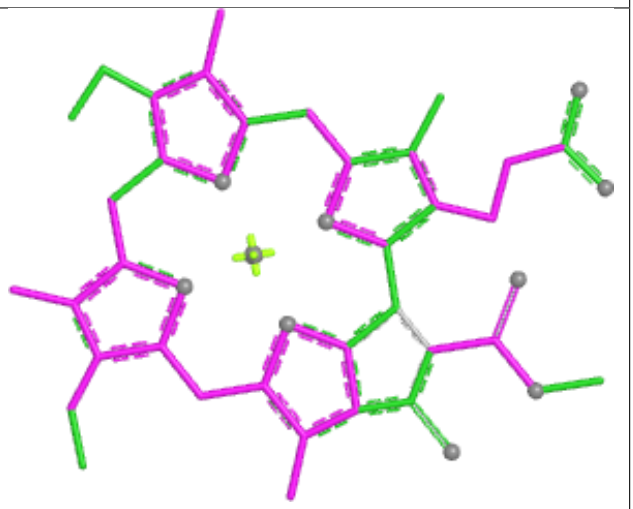
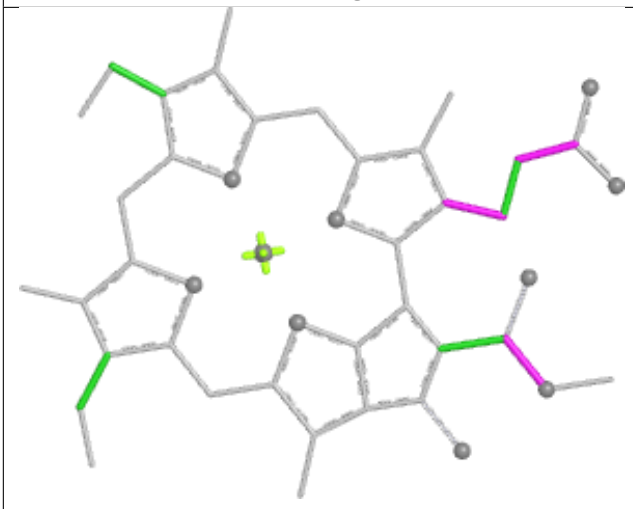


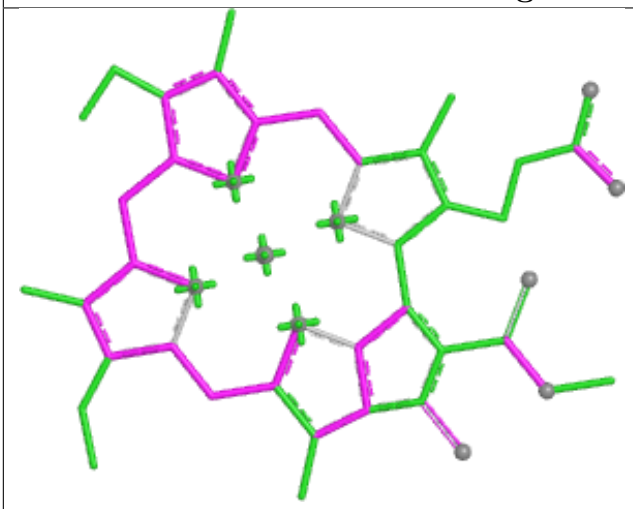
Bond angles



Torsions

Rings

Ligand CLA bL 203



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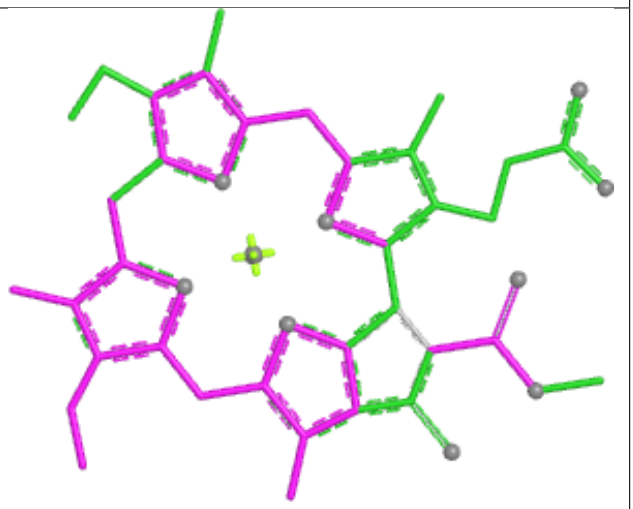
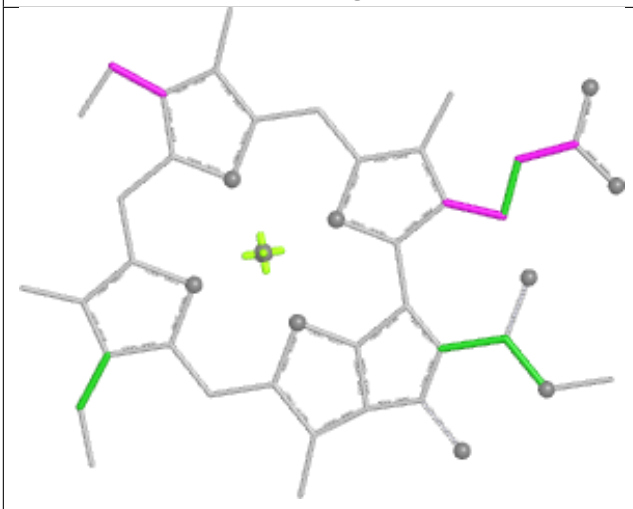


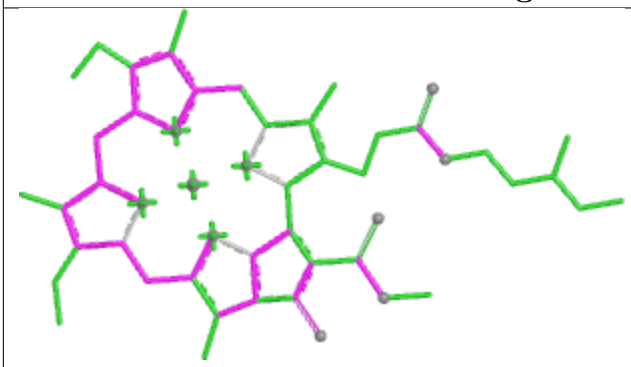
Bond angles



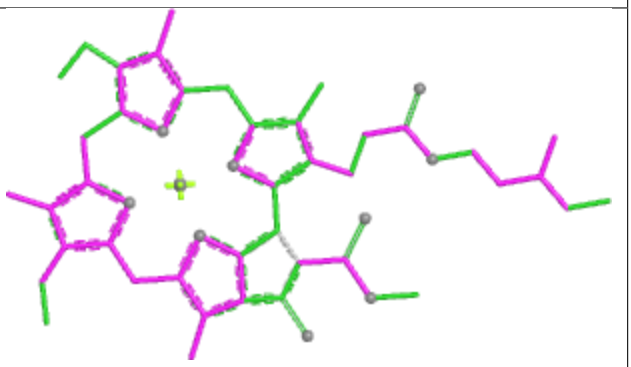
Torsions

Rings

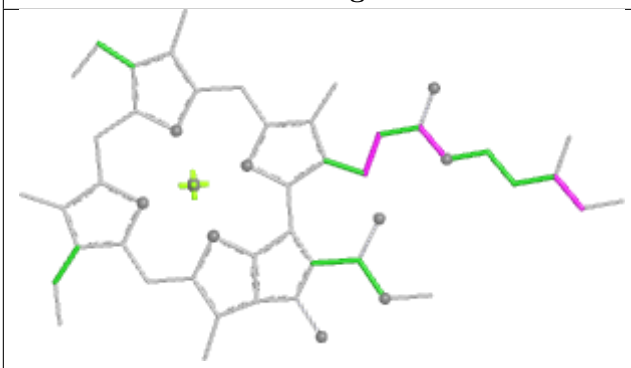
Ligand CLA cA 841



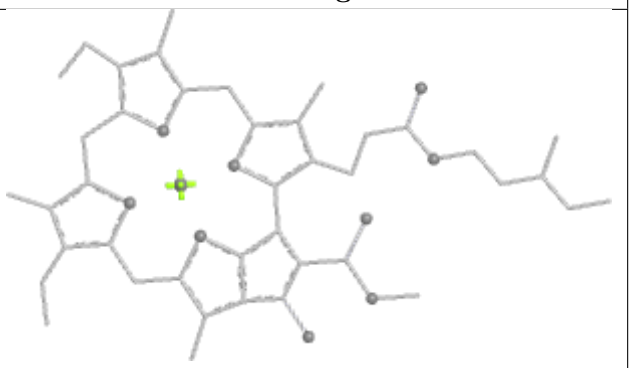
Bond lengths



Bond angles

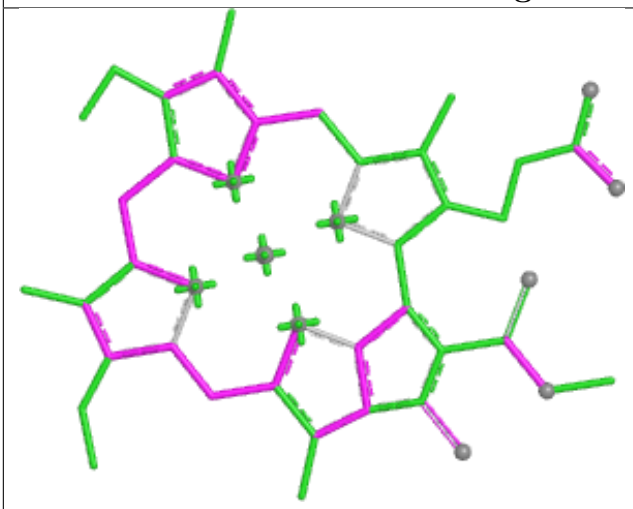


Torsions

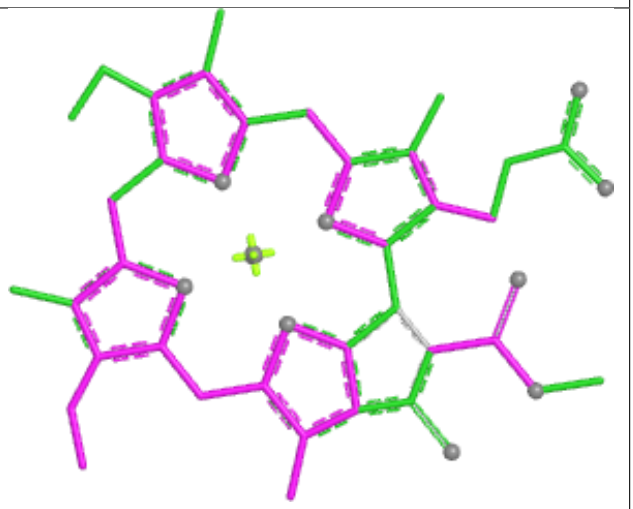


Rings

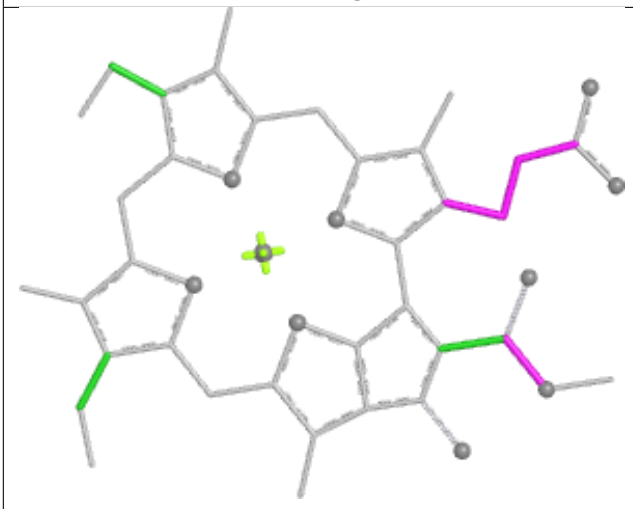
Ligand CLA bB 950



Bond lengths



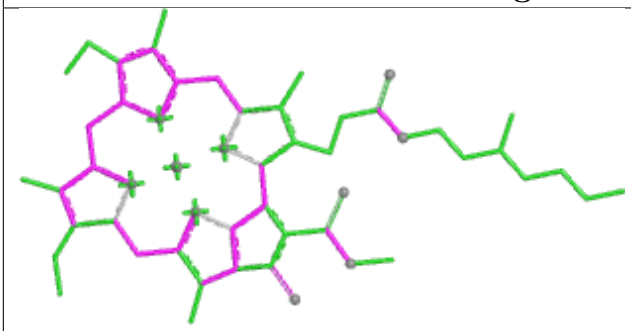
Bond angles



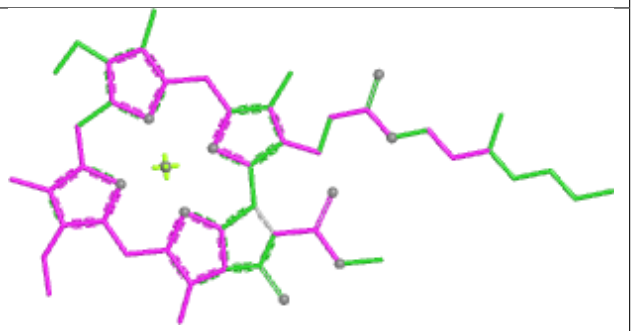
Torsions

Rings

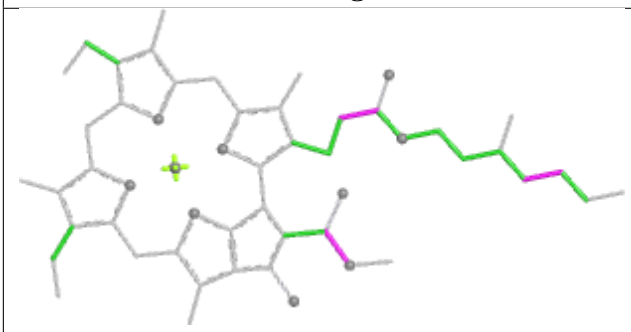
Ligand CLA bA 805



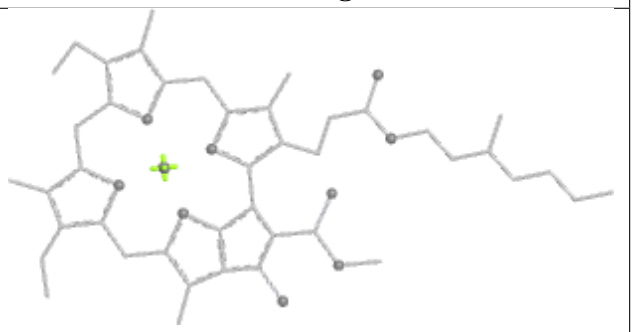
Bond lengths



Bond angles

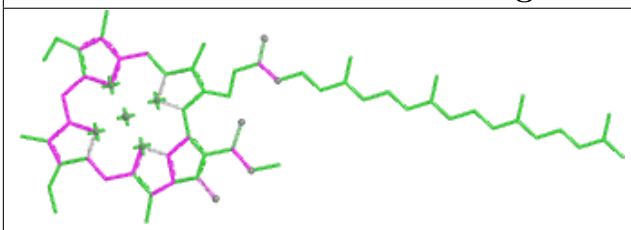


Torsions

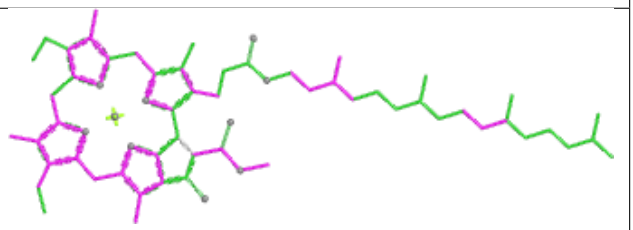


Rings

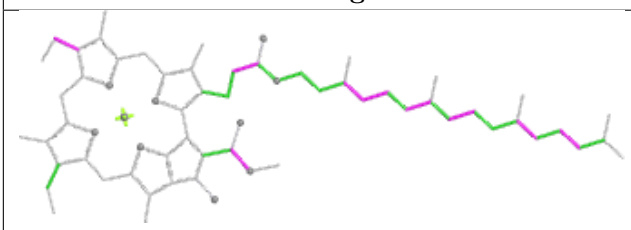
Ligand CLA aB 905



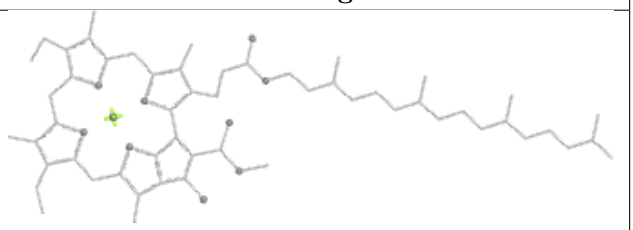
Bond lengths



Bond angles

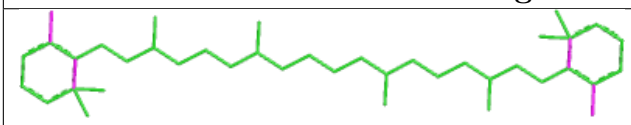


Torsions

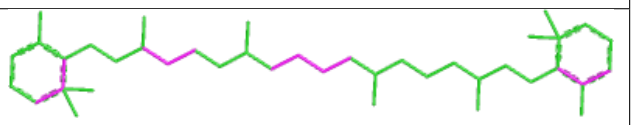


Rings

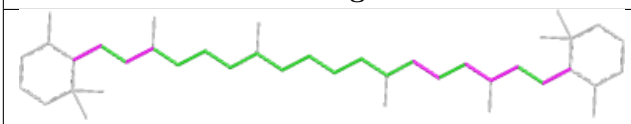
Ligand BCR bL 205



Bond lengths



Bond angles



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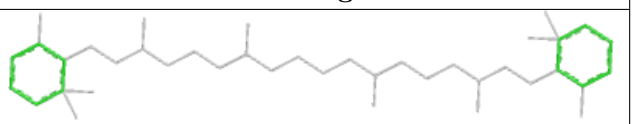
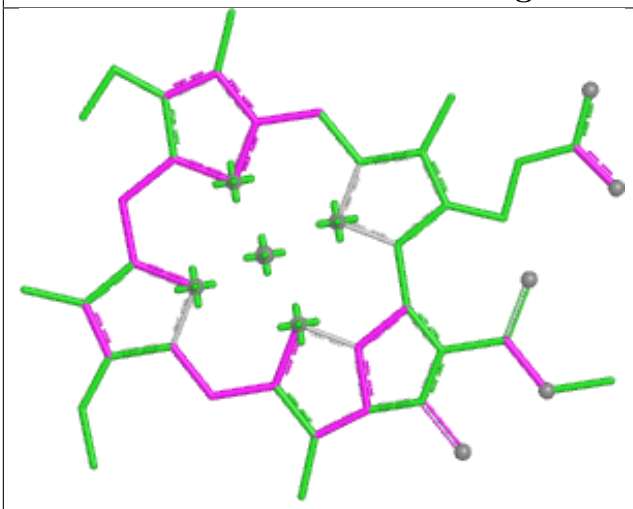
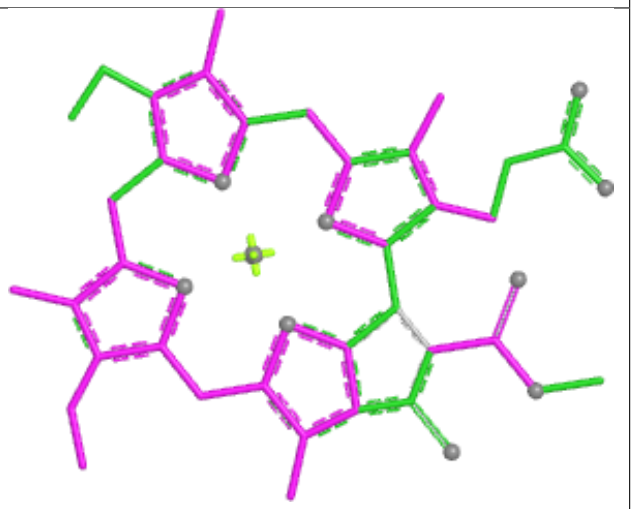


Rings

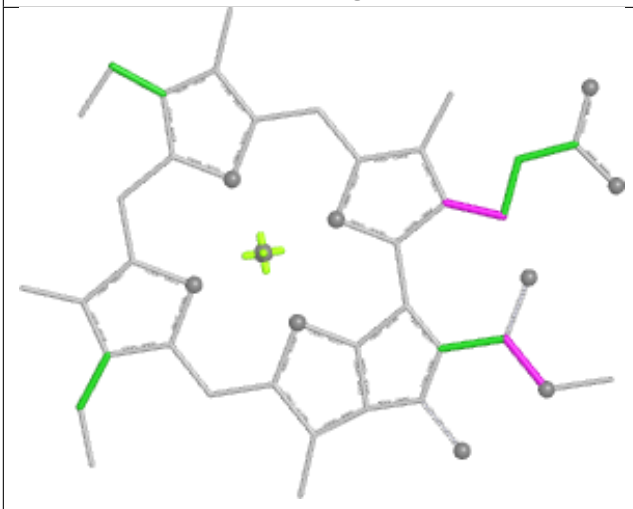
Ligand CLA aA 811



Bond lengths



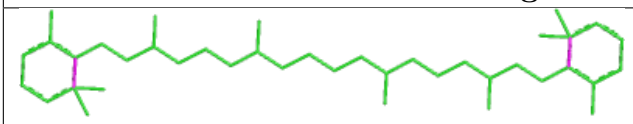
Bond angles



Torsions

Rings

Ligand BCR cI 101



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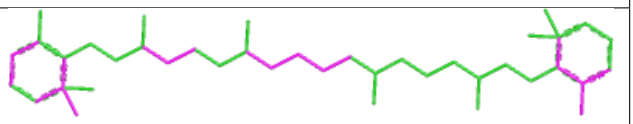
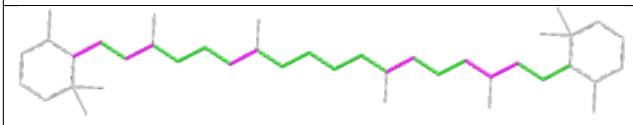
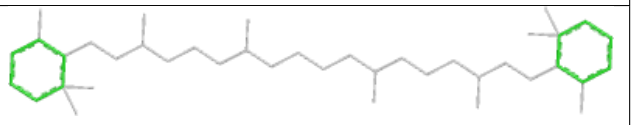


Bond angles

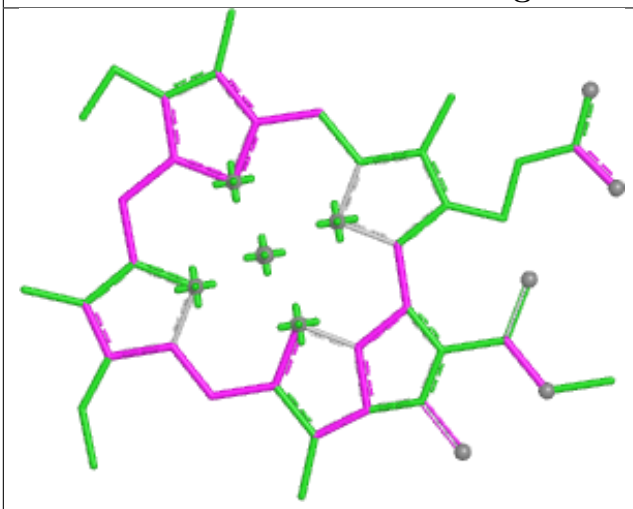


Torsions

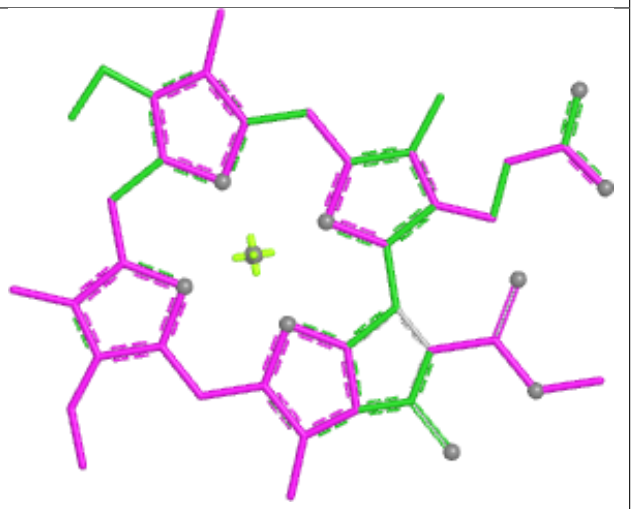


Rings

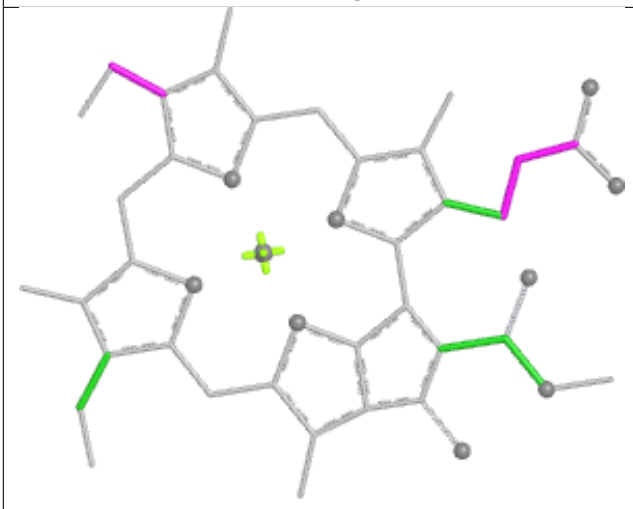
Ligand CLA bA 836



Bond lengths



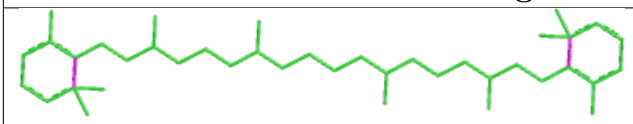
Bond angles



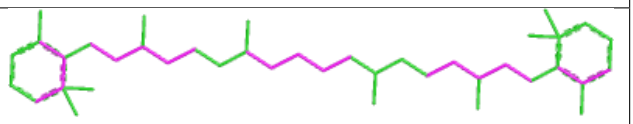
Torsions

Rings

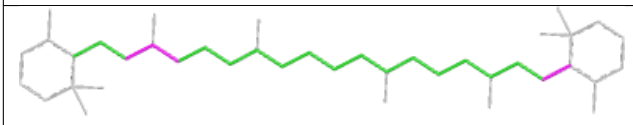
Ligand BCR aF 204



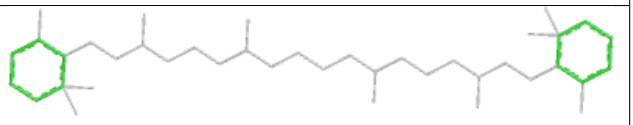
Bond lengths



Bond angles

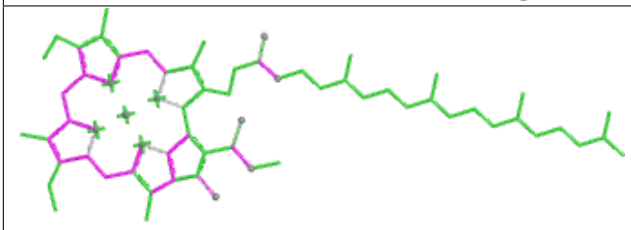


Torsions



Rings

Ligand CLA aA 825



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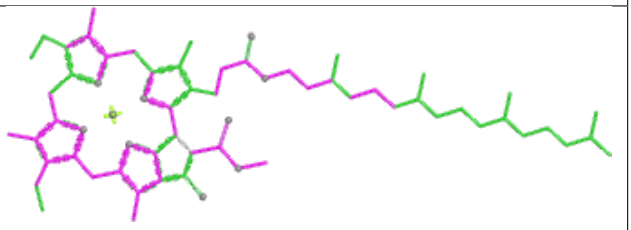
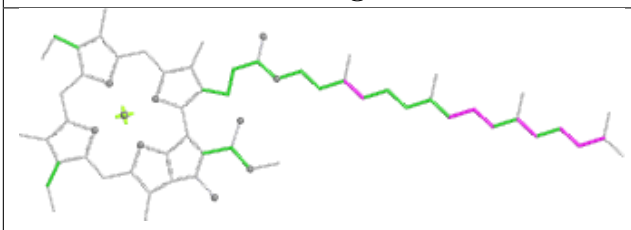
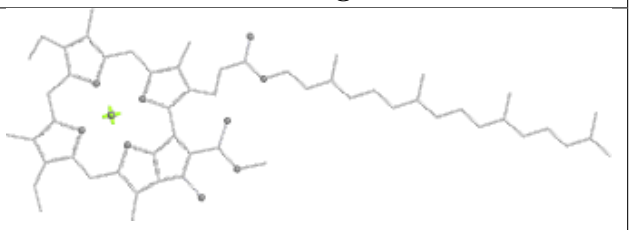


Bond angles

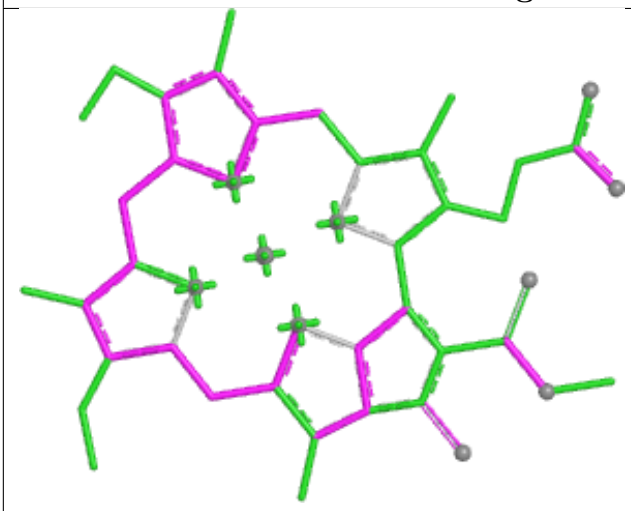


Torsions

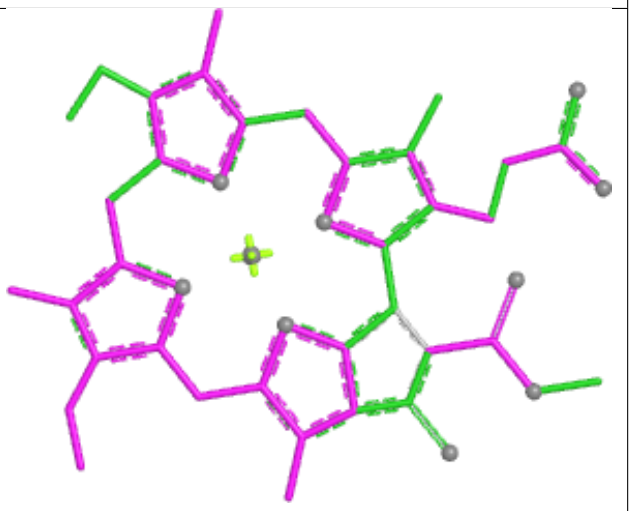


Rings

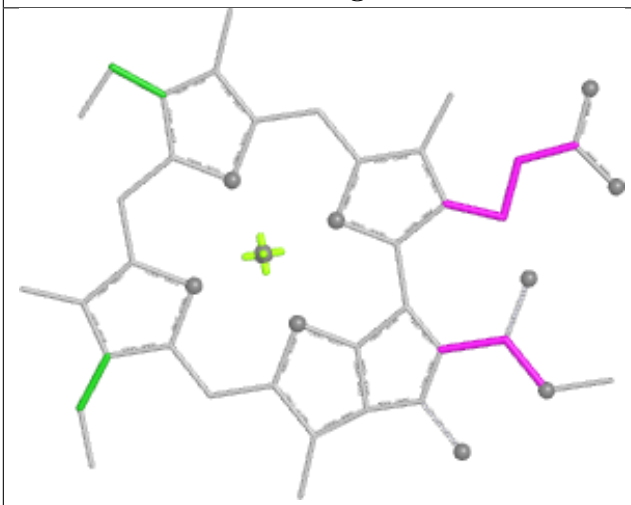
Ligand CLA bF 202



Bond lengths



Bond angles



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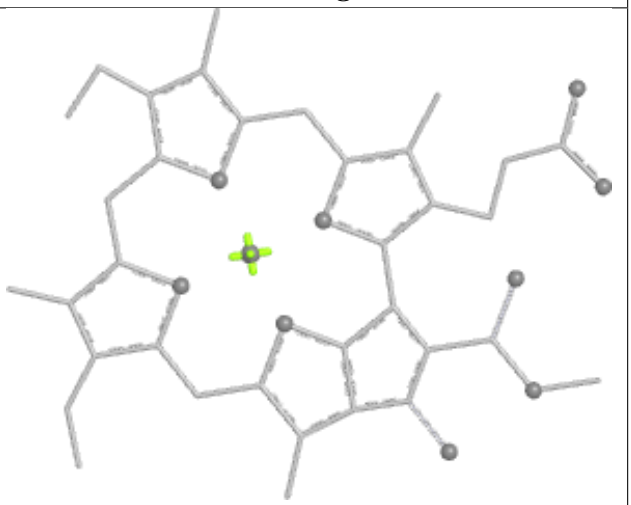
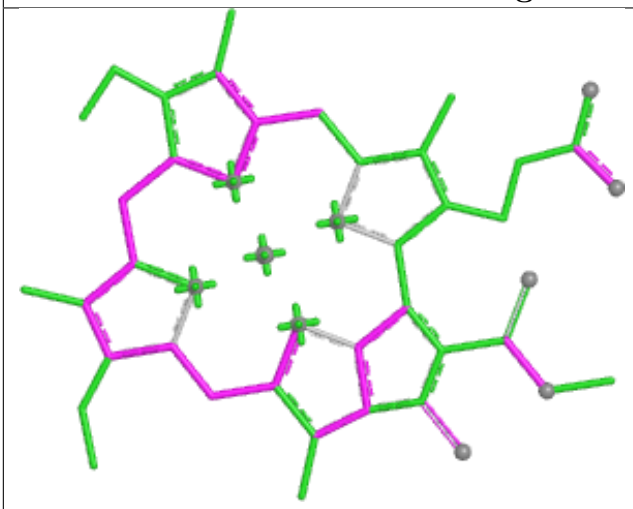


Rings

Ligand CLA aB 910



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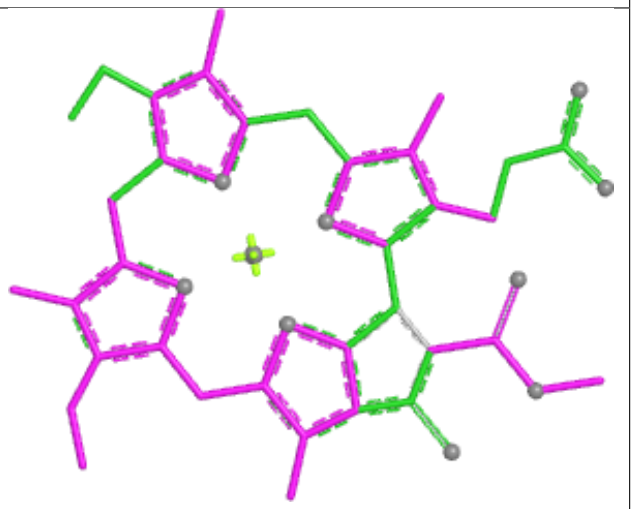
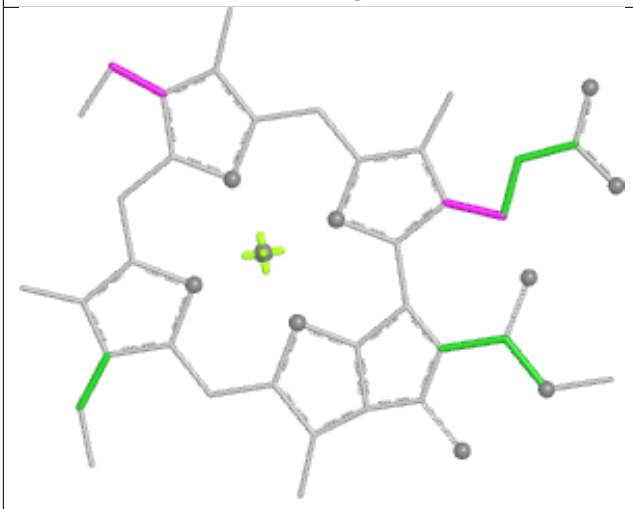


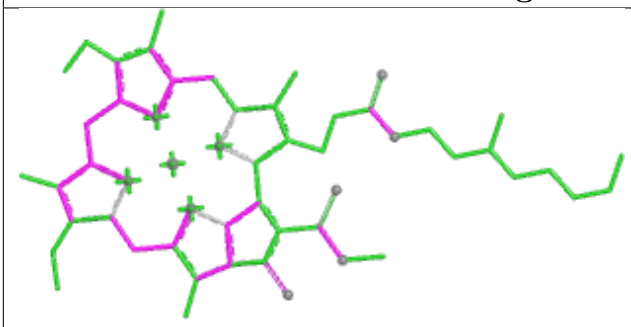
Bond angles



Torsions

Rings

Ligand CLA aB 923



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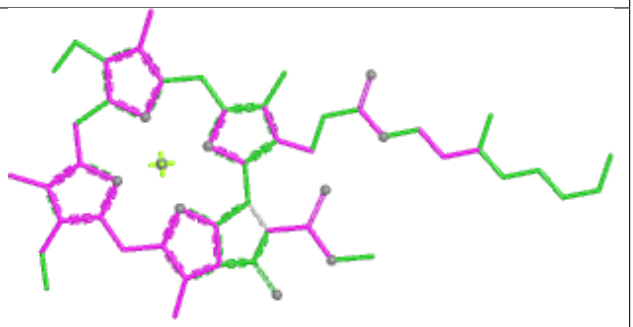
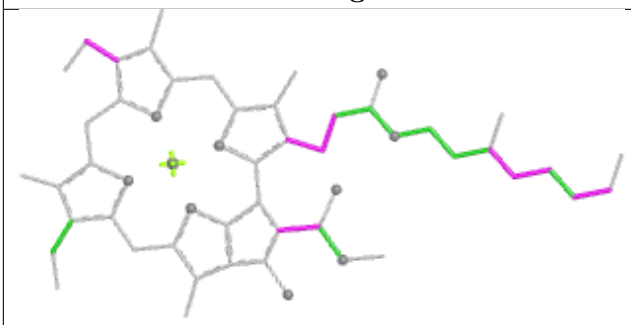
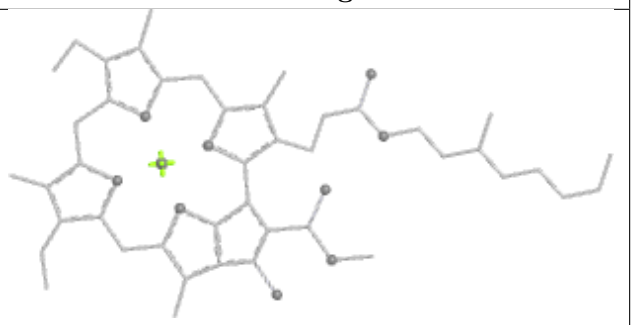


Bond angles

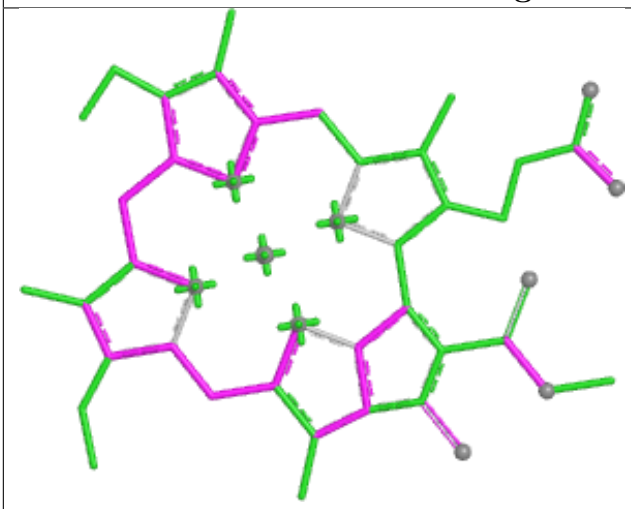


Torsions



Rings

Ligand CLA bB 933



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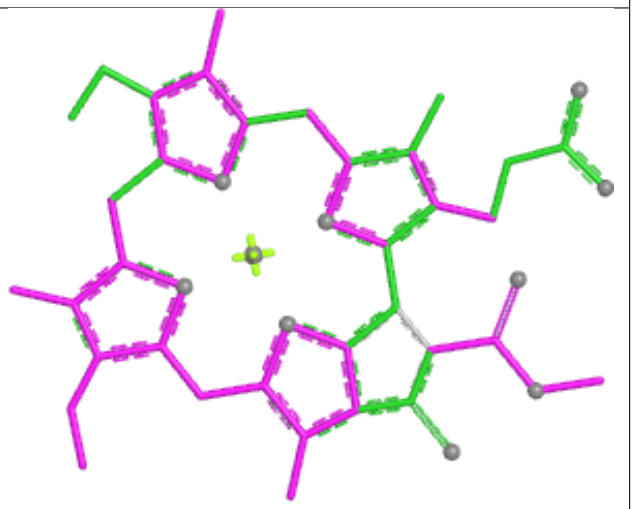
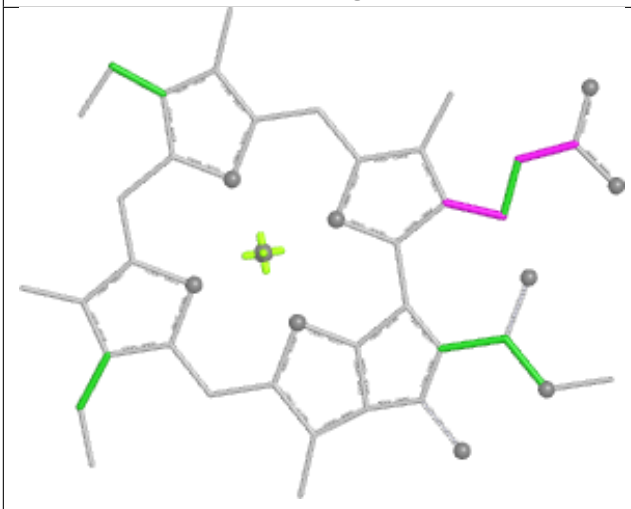


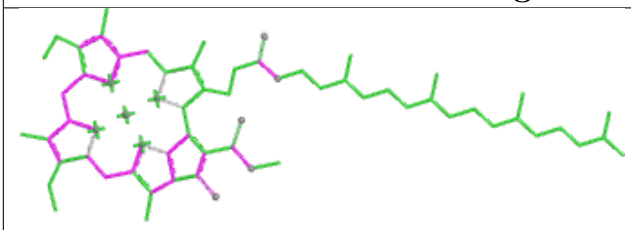
Bond angles



Torsions

Rings

Ligand CLA bA 828



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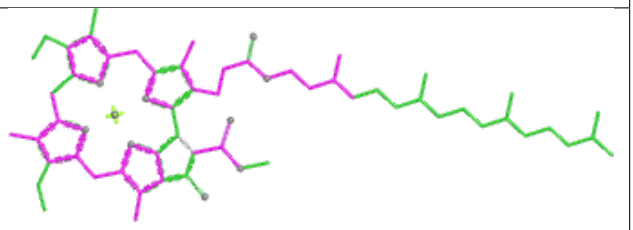
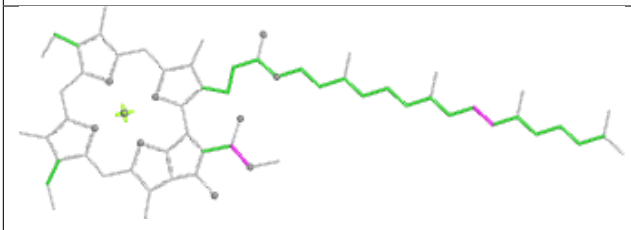


Bond angles



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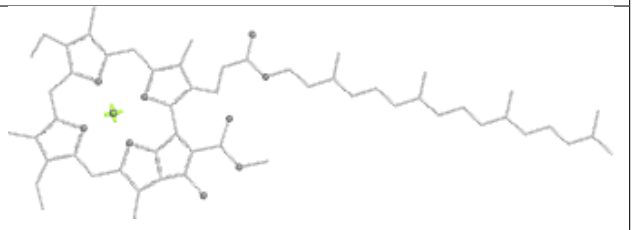
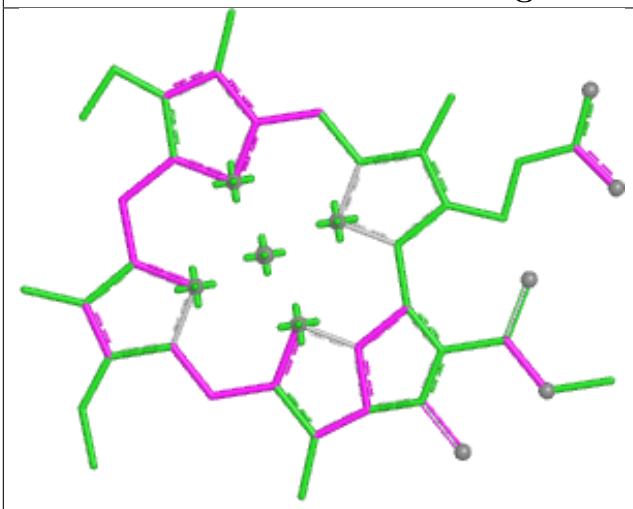


Rings

Ligand CLA cA 811



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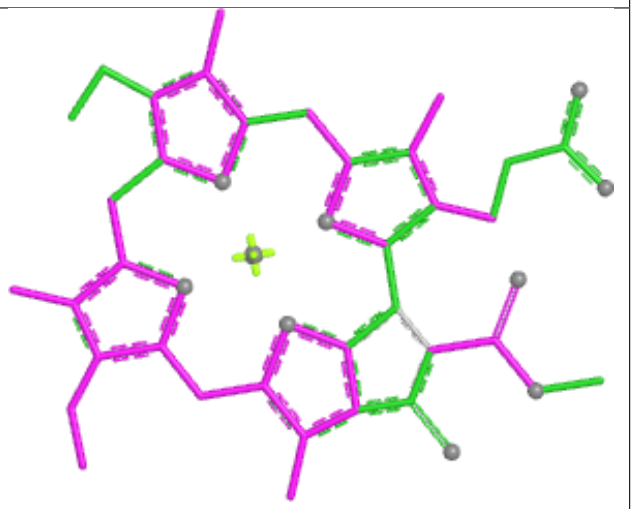
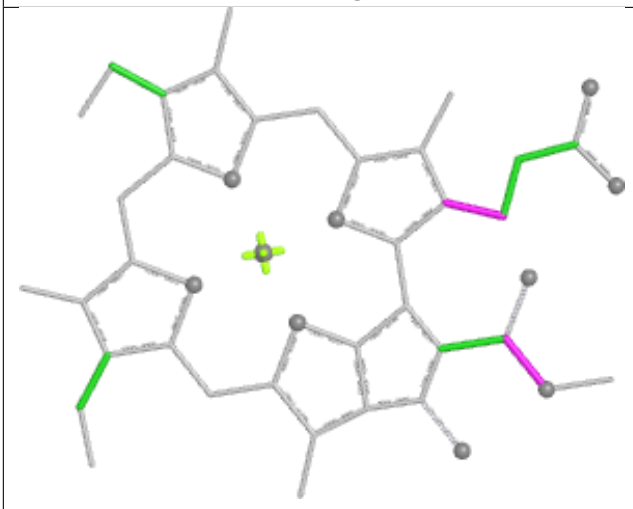
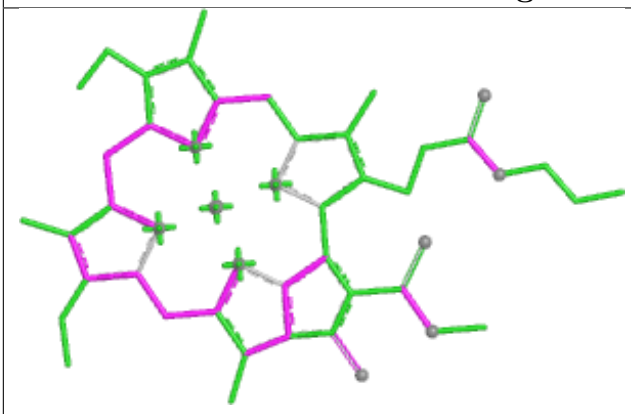
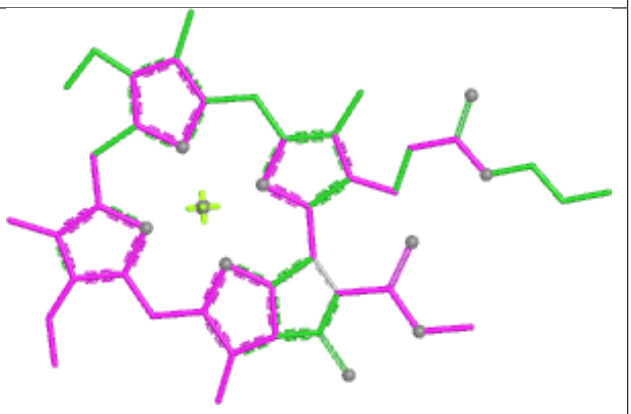
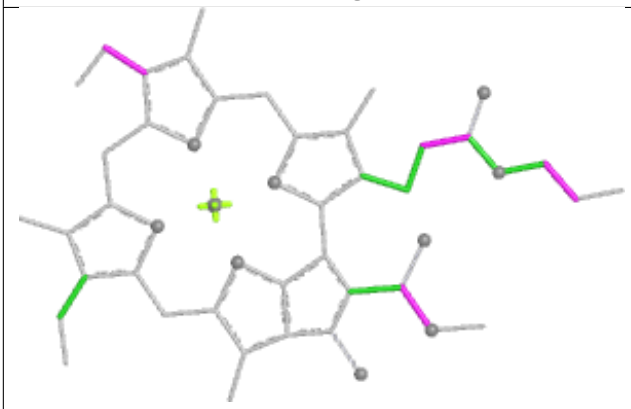
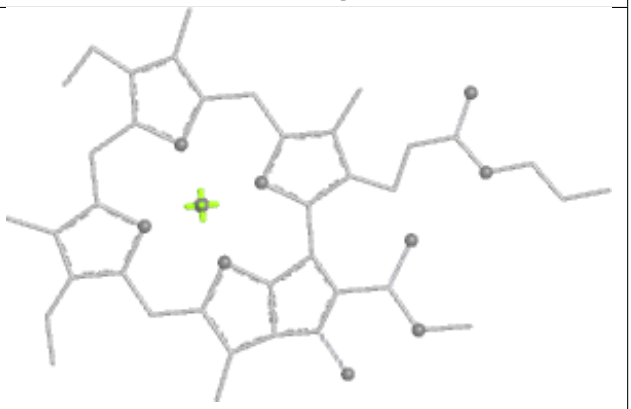


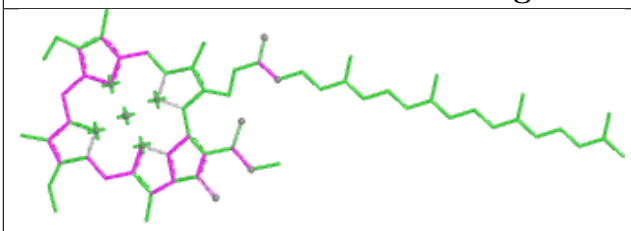
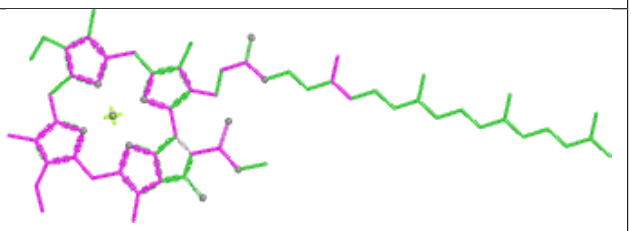
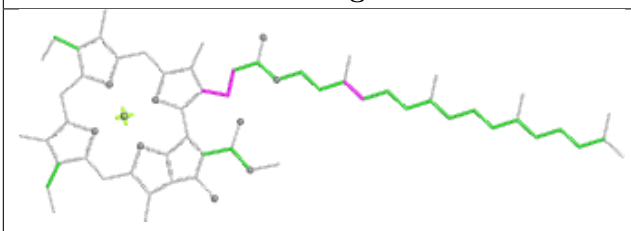
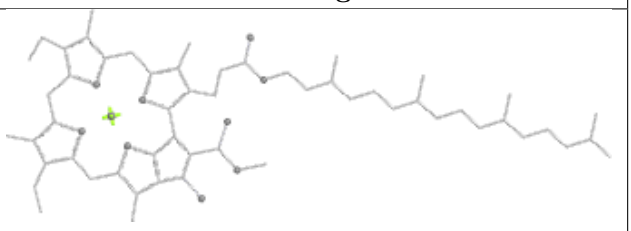
Bond angles



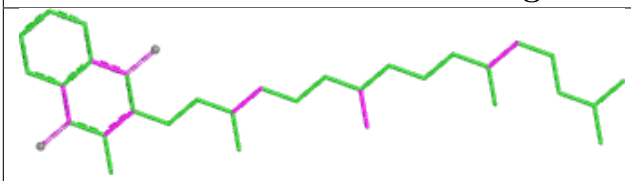
Torsions

Rings

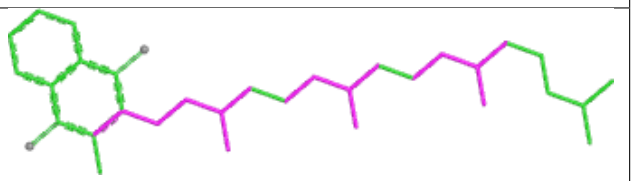
Ligand CLA cB 908	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA bA 802	
	
Bond lengths	Bond angles
	
Torsions	Rings

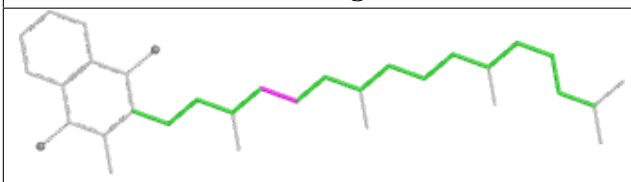
Ligand 1L3 bB 940



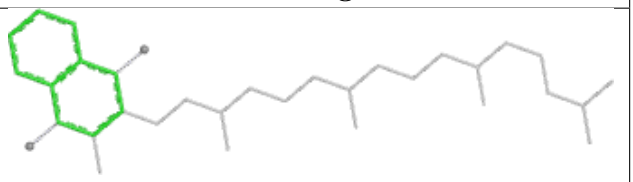
Bond lengths



Bond angles

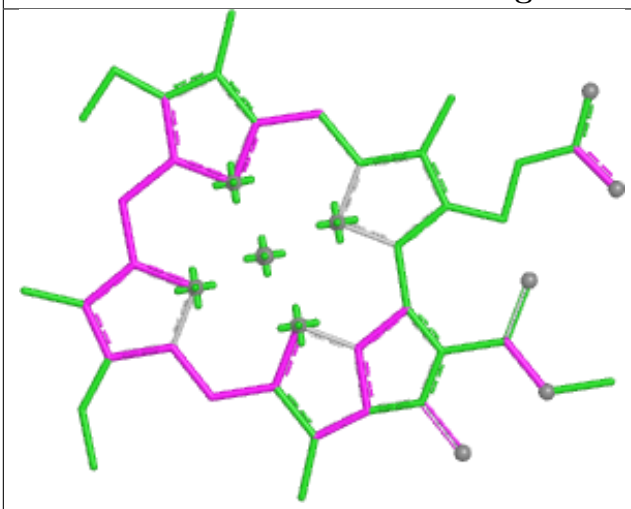


Torsions

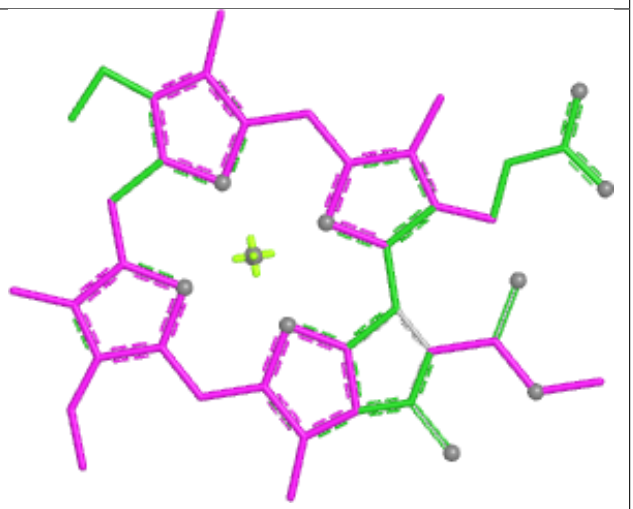


Rings

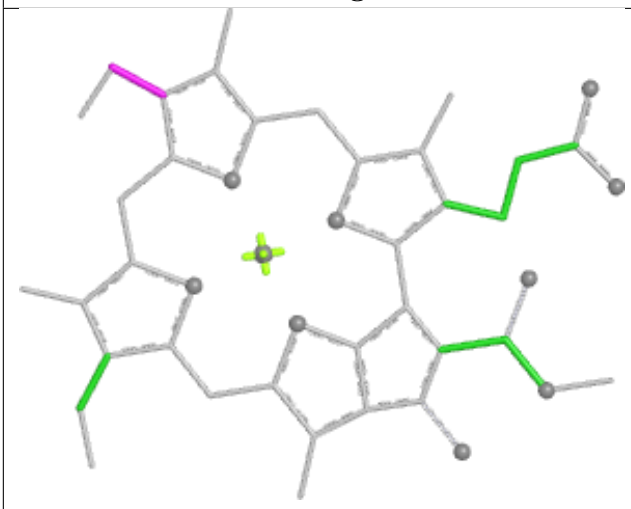
Ligand CLA aA 835



Bond lengths



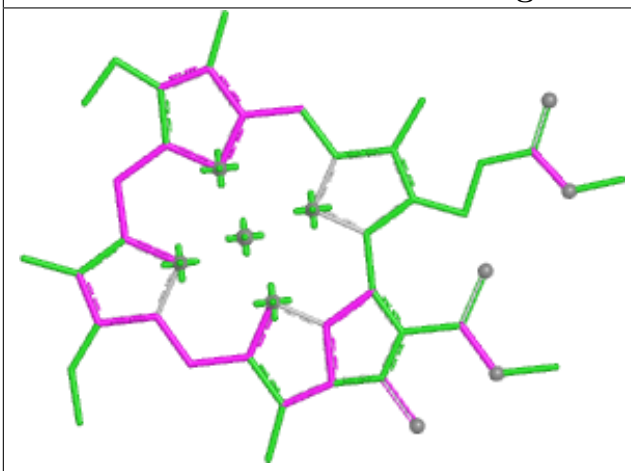
Bond angles



Torsions

Rings

Ligand CLA cB 924



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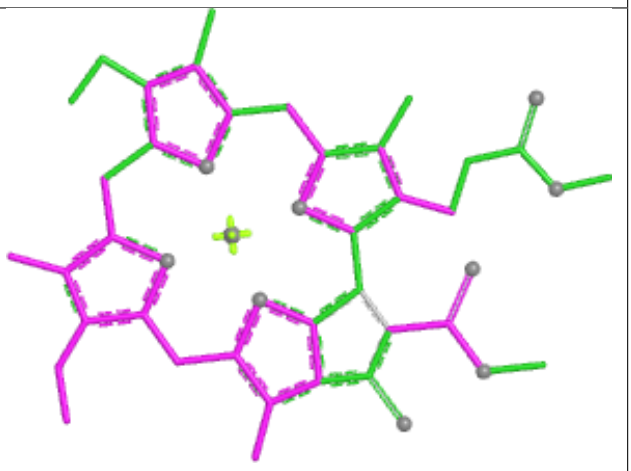
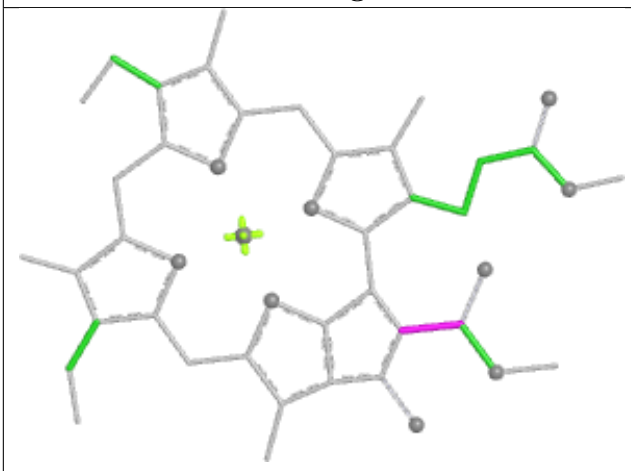
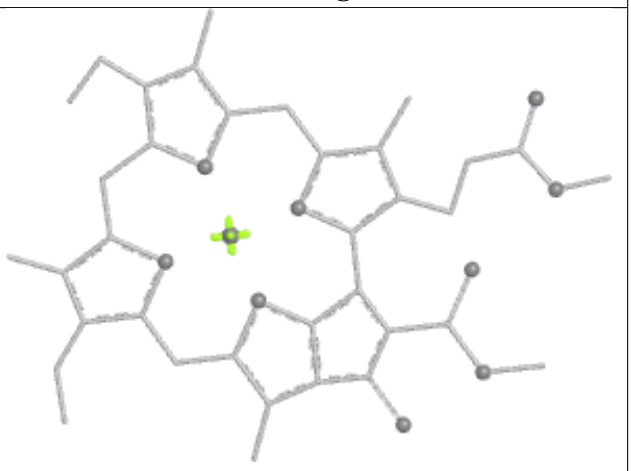


Bond angles

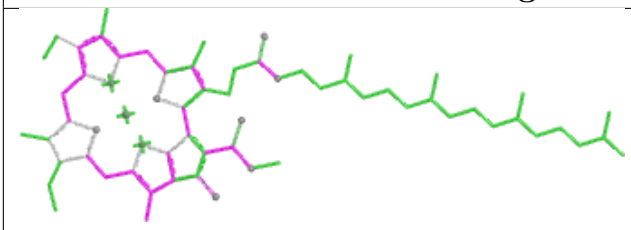


Torsions



Rings

Ligand CL0 bA 801



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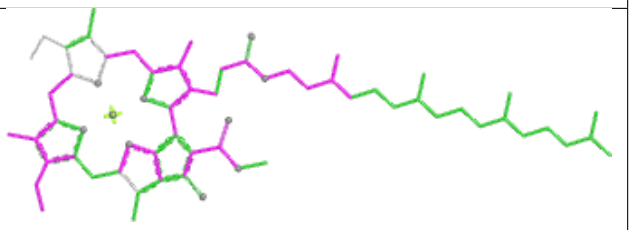
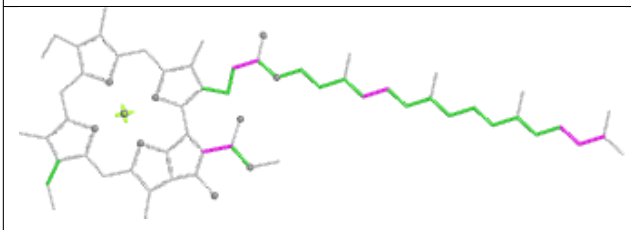
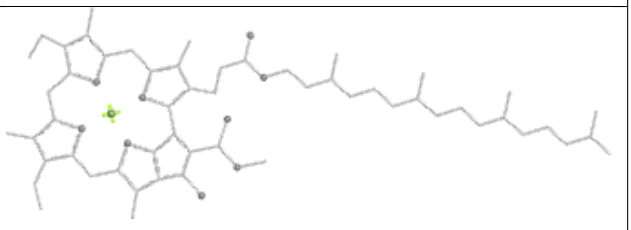


Bond angles

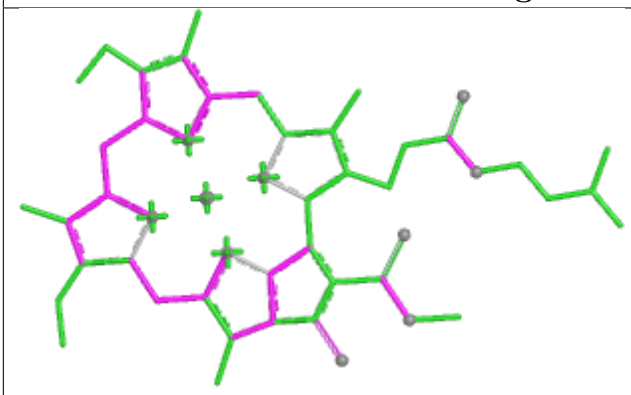


Torsions

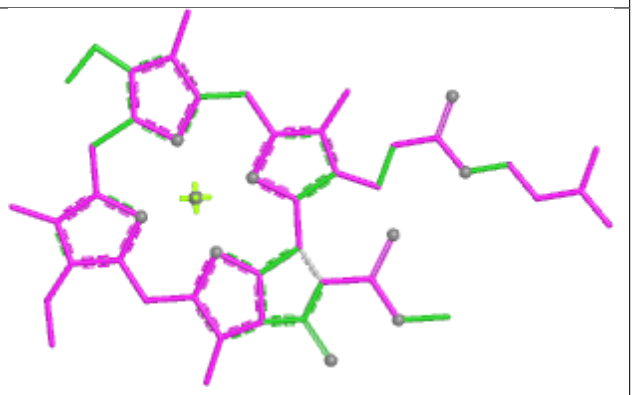


Rings

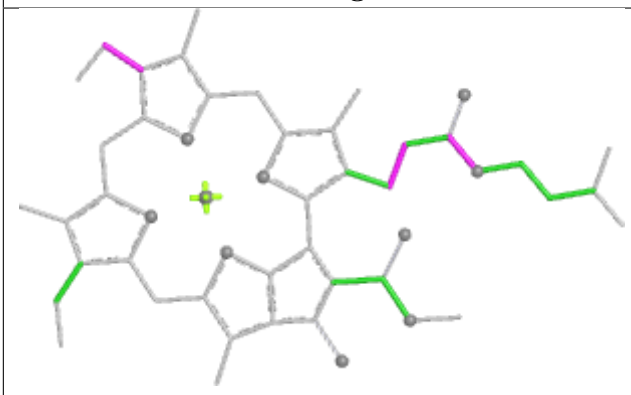
Ligand CLA aA 831



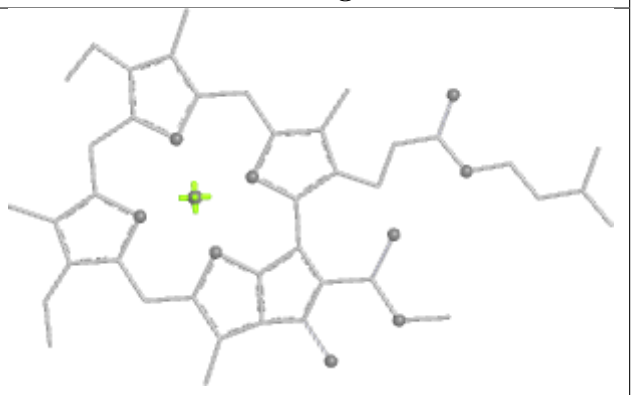
Bond lengths



Bond angles

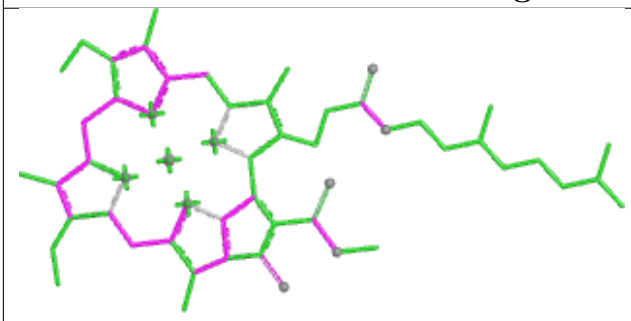


Torsions

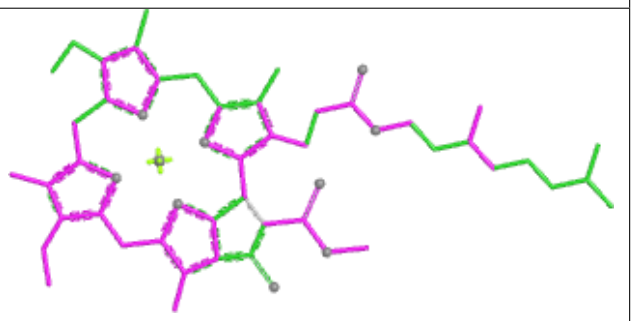


Rings

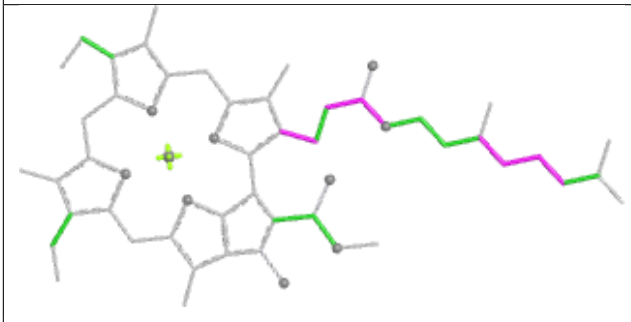
Ligand CLA bA 832



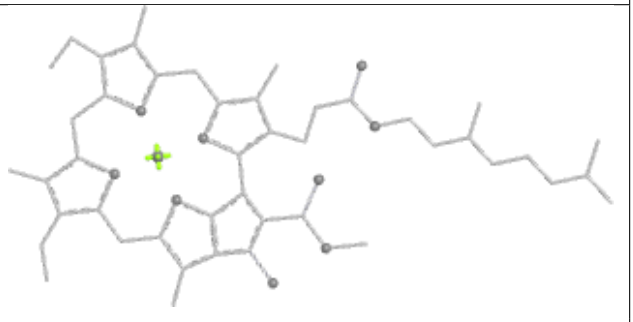
Bond lengths



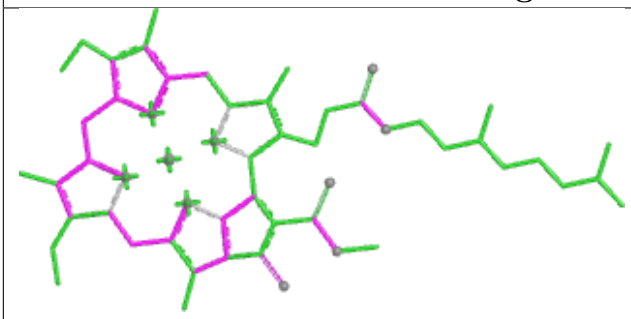
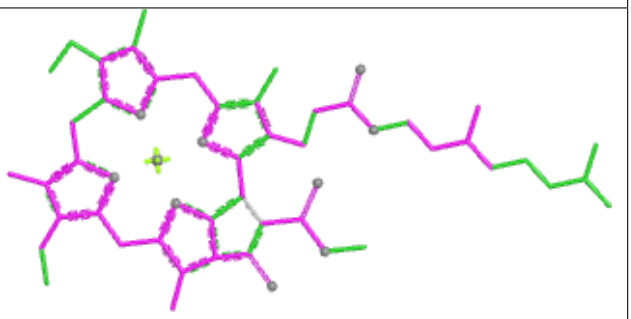
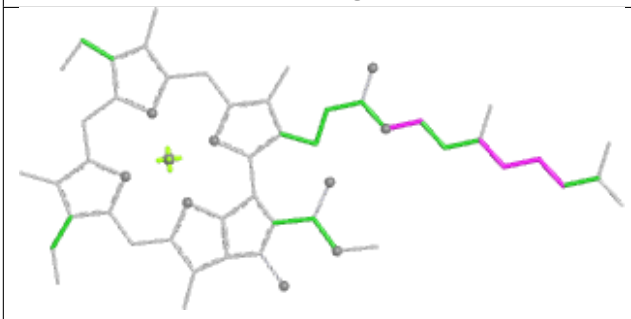
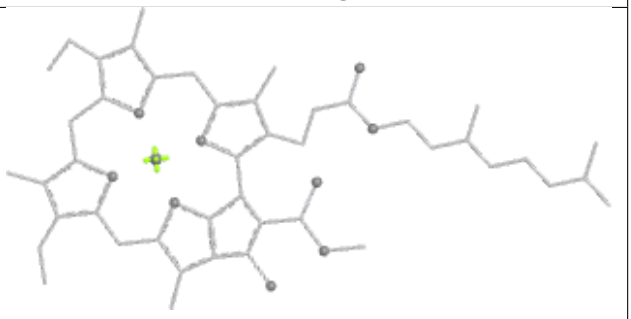
Bond angles

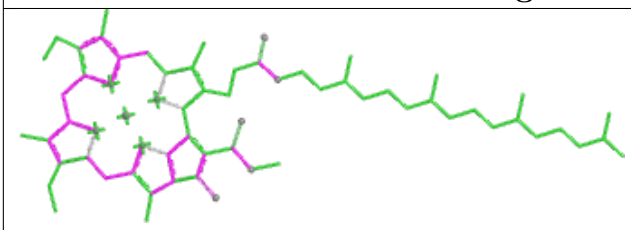
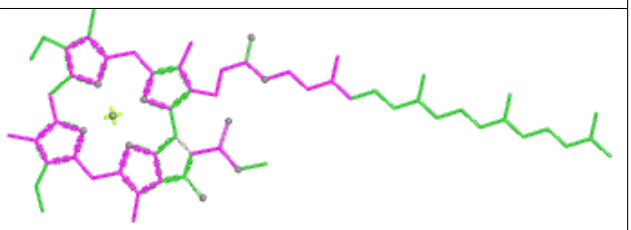
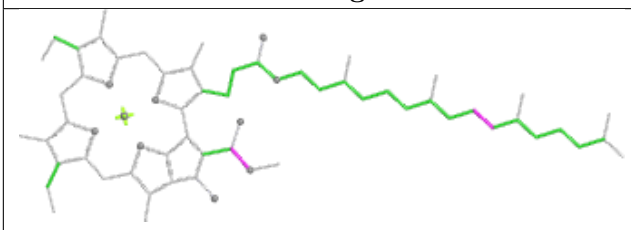
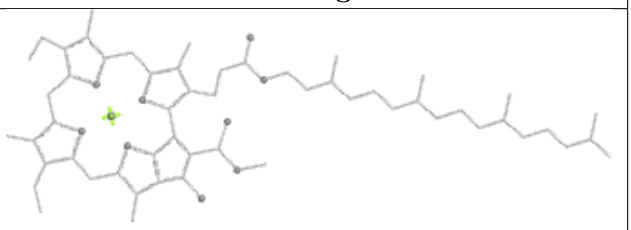


Torsions

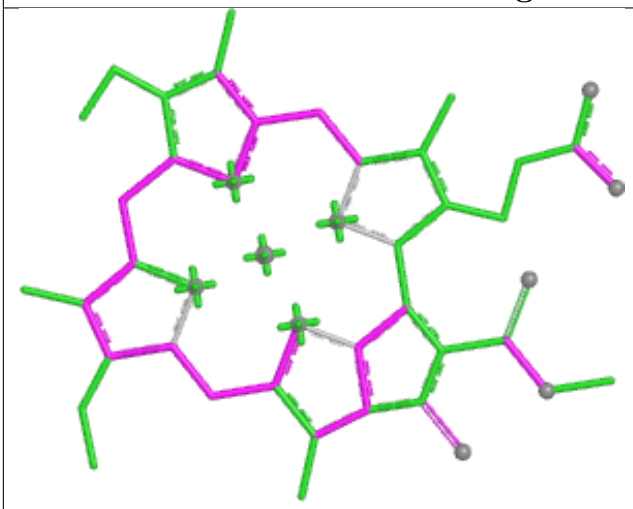


Rings

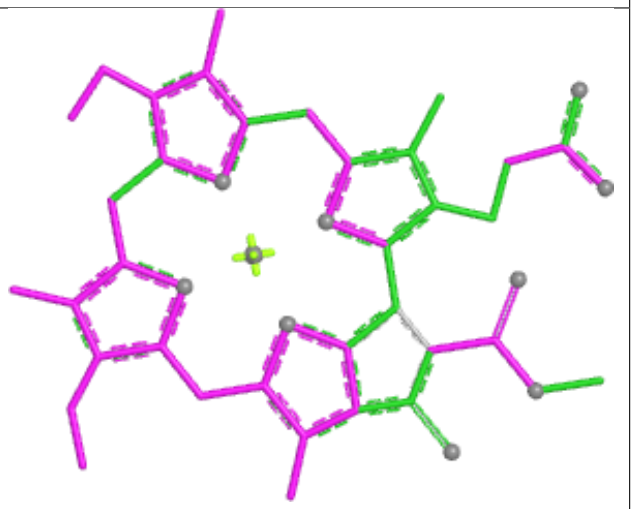
Ligand CLA aB 925	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA cA 828	
	
Bond lengths	Bond angles
	
Torsions	Rings

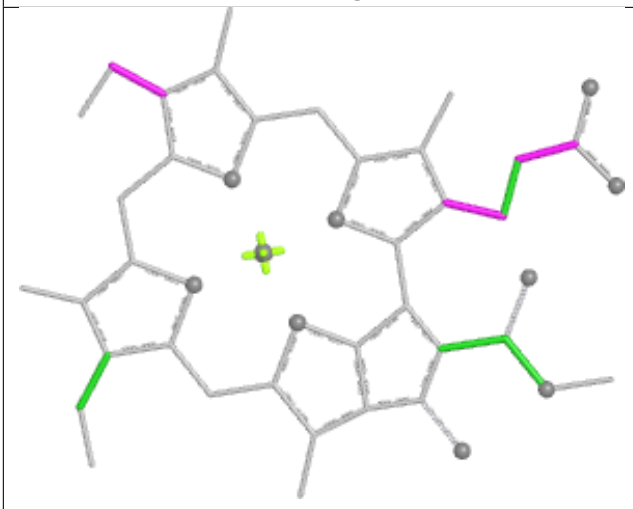
Ligand CLA aB 929



Bond lengths



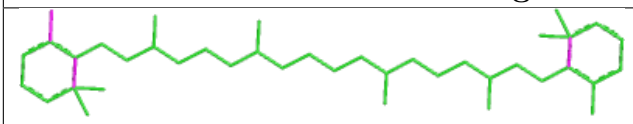
Bond angles



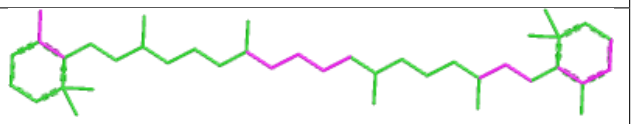
Torsions

Rings

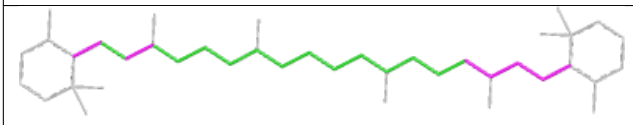
Ligand BCR bB 941



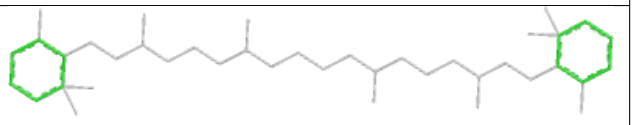
Bond lengths



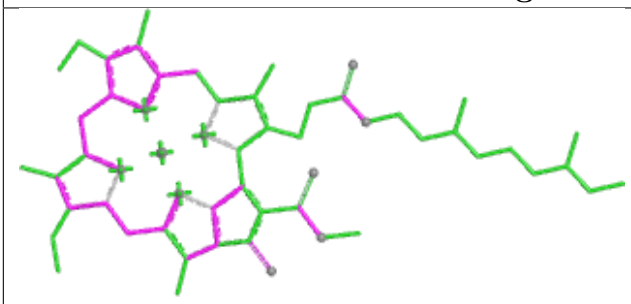
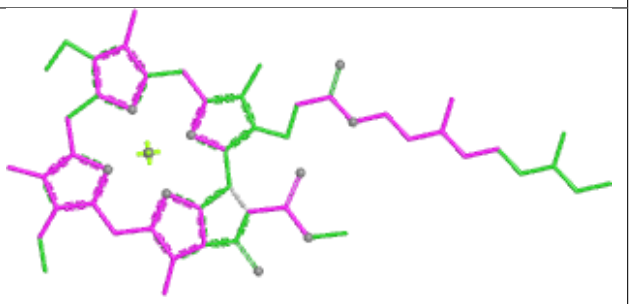
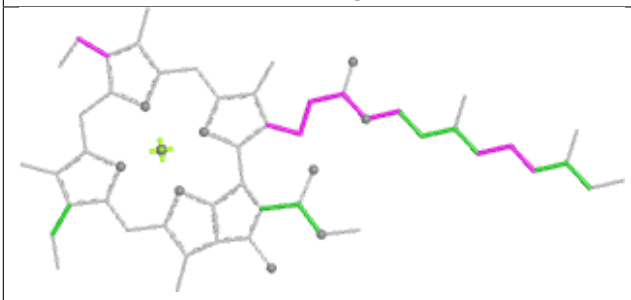
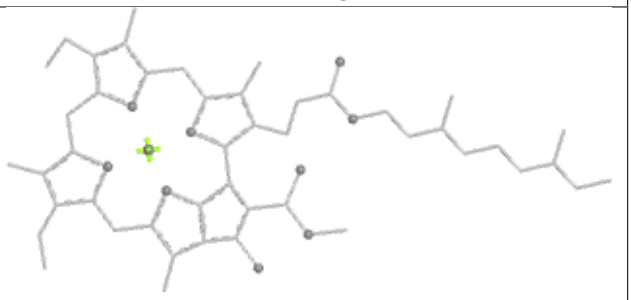
Bond angles



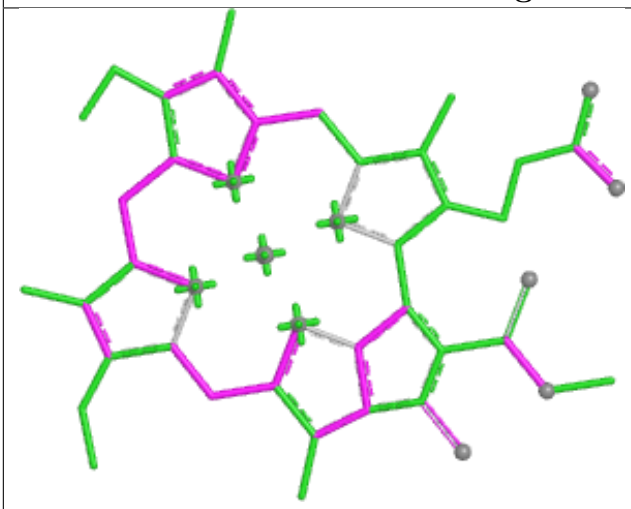
Torsions



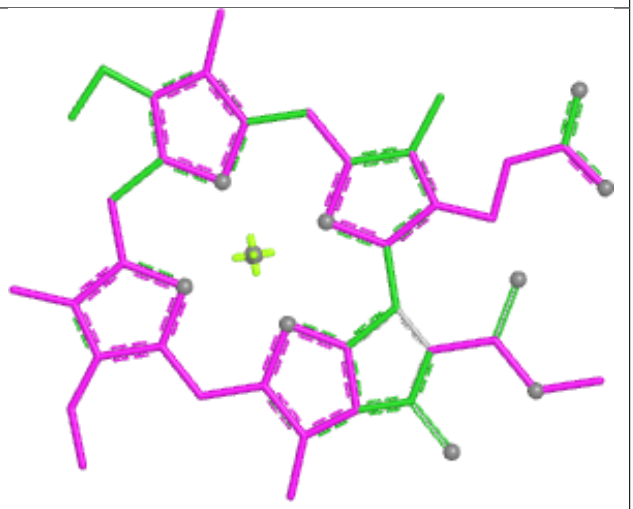
Rings

Ligand CLA cA 820	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

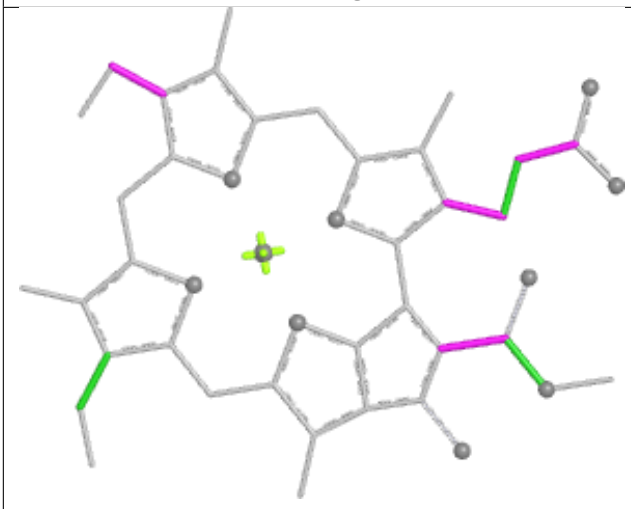
Ligand CLA aA 810



Bond lengths



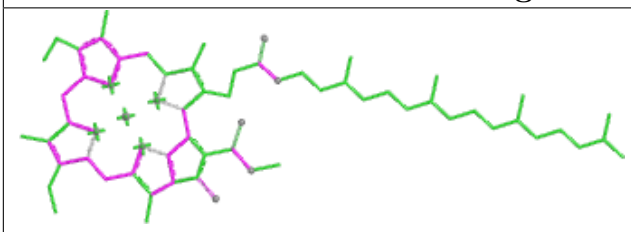
Bond angles



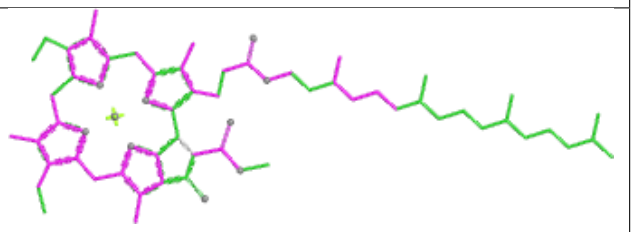
Torsions

Rings

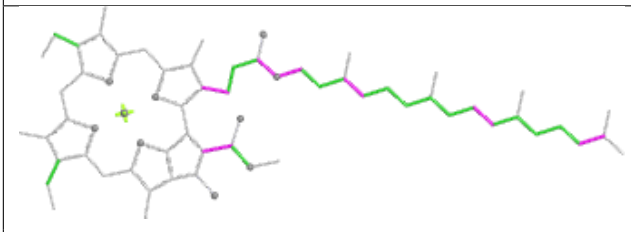
Ligand CLA aA 812



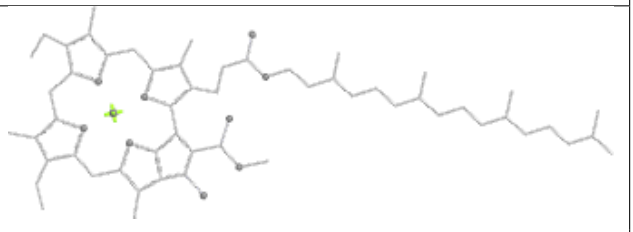
Bond lengths



Bond angles

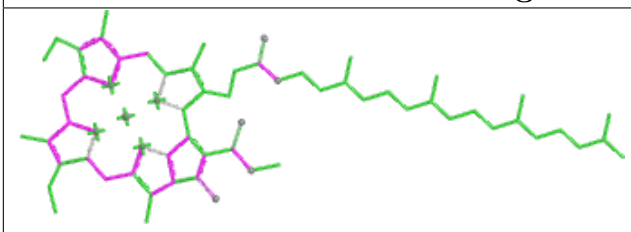


Torsions

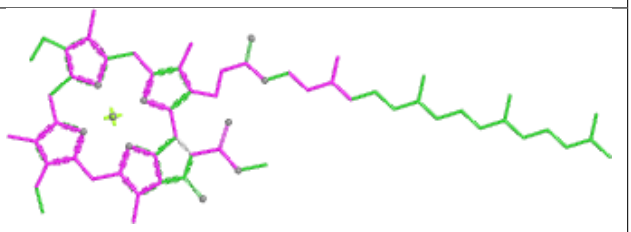


Rings

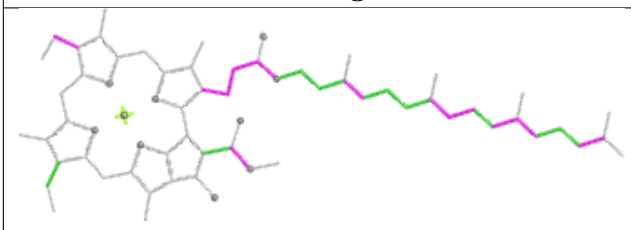
Ligand CLA aB 926



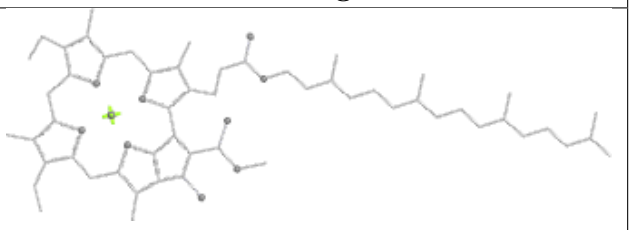
Bond lengths



Bond angles

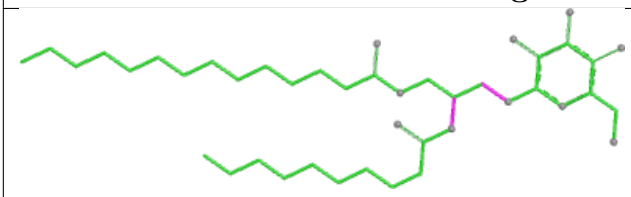


Torsions

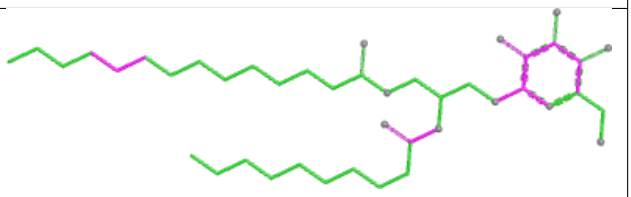


Rings

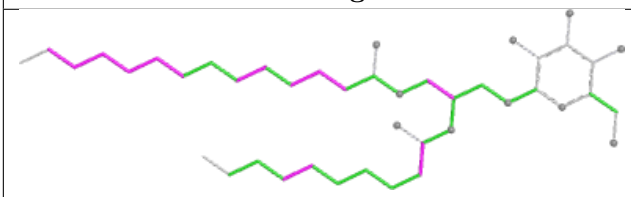
Ligand LMG aB 947



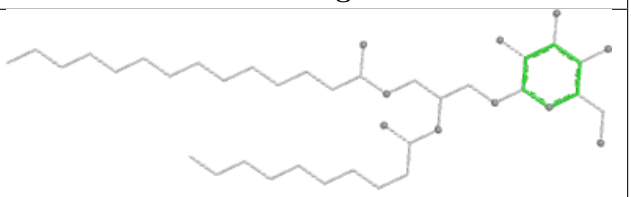
Bond lengths



Bond angles

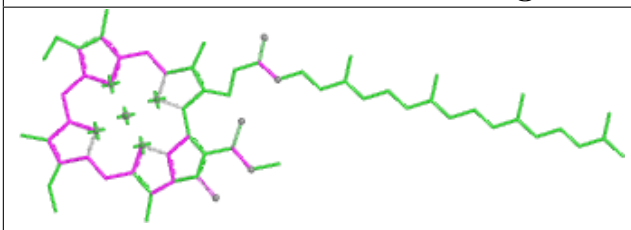


Torsions

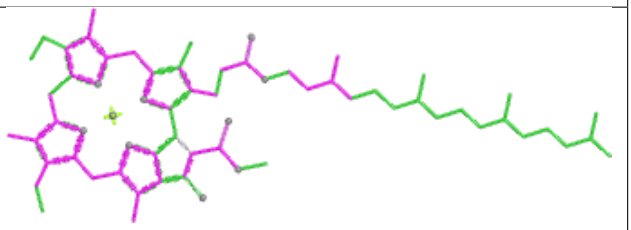


Rings

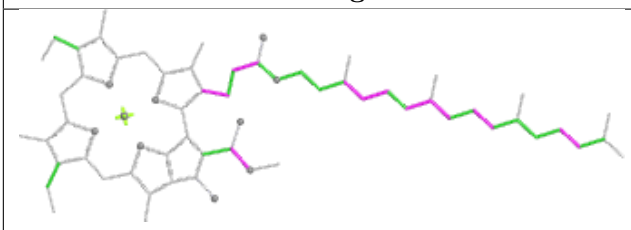
Ligand CLA cB 931



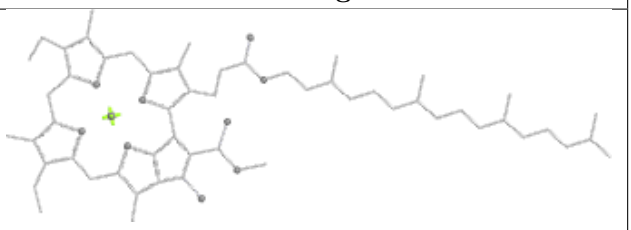
Bond lengths



Bond angles

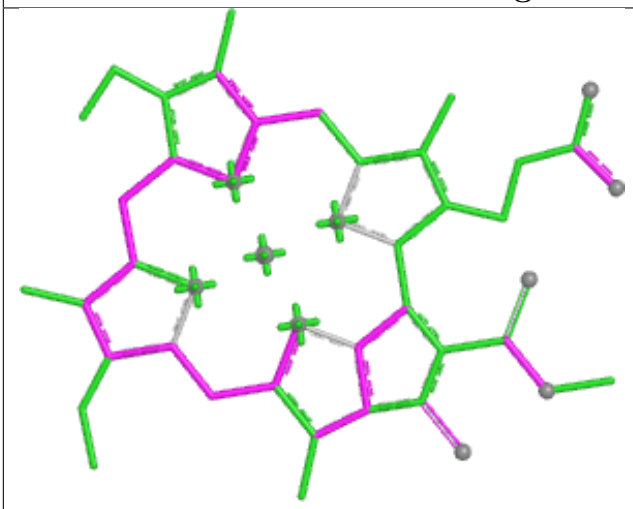


Torsions

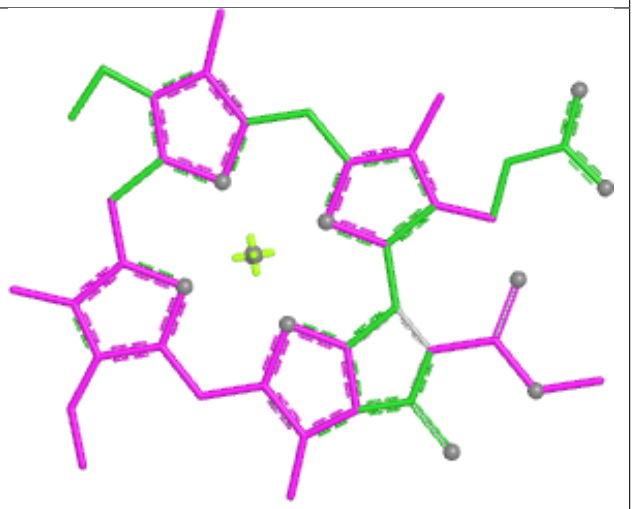


Rings

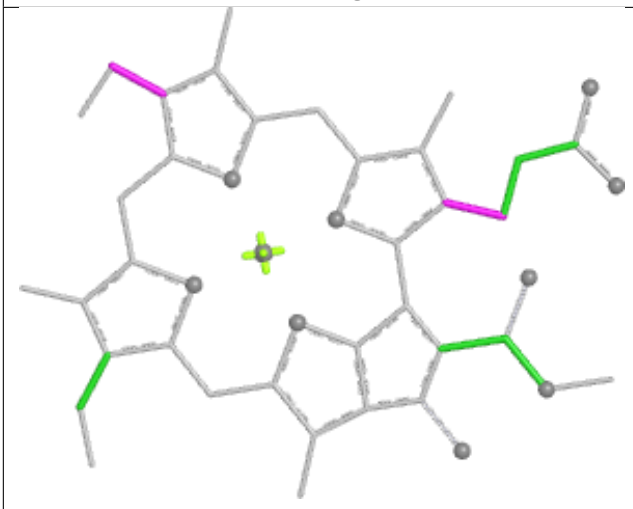
Ligand CLA bB 910



Bond lengths



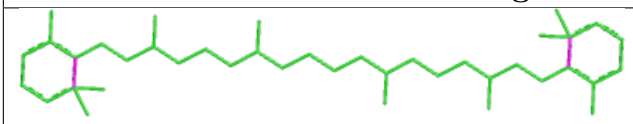
Bond angles



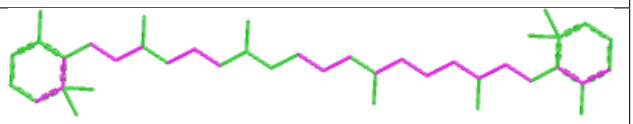
Torsions

Rings

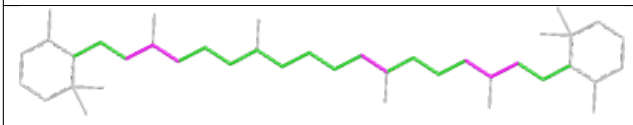
Ligand BCR bA 850



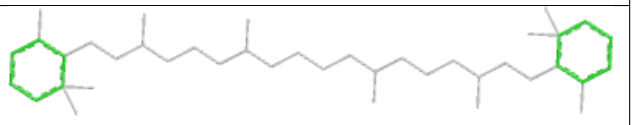
Bond lengths



Bond angles

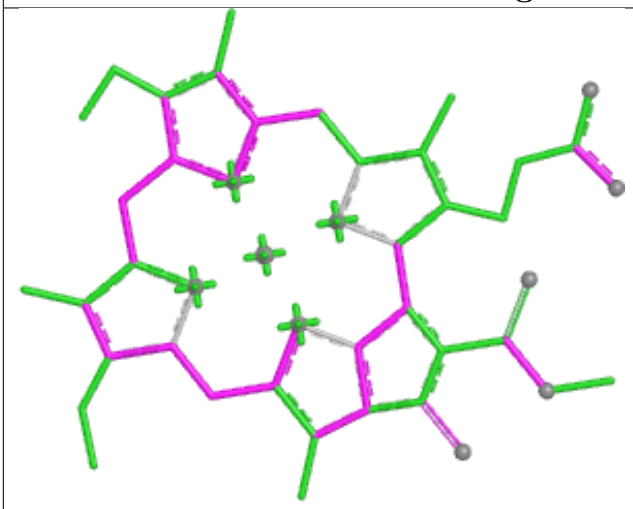


Torsions

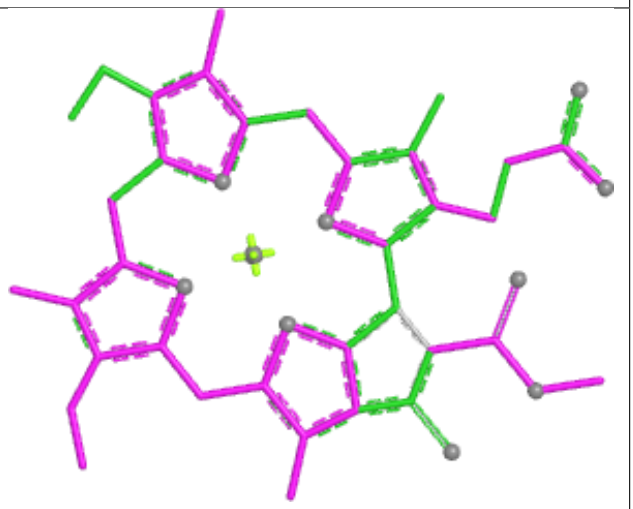


Rings

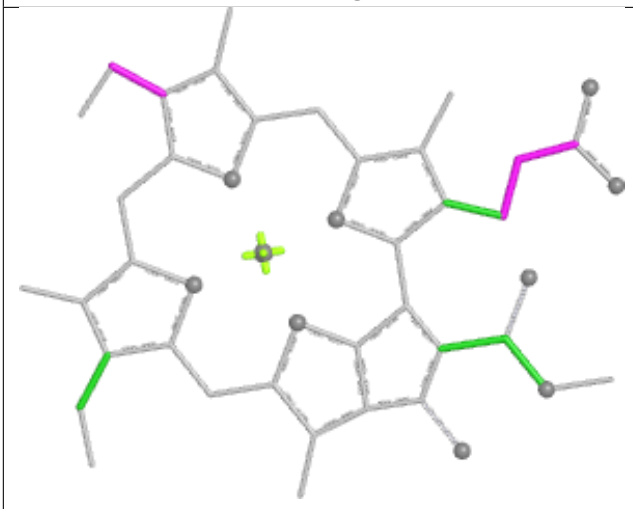
Ligand CLA cA 836



Bond lengths



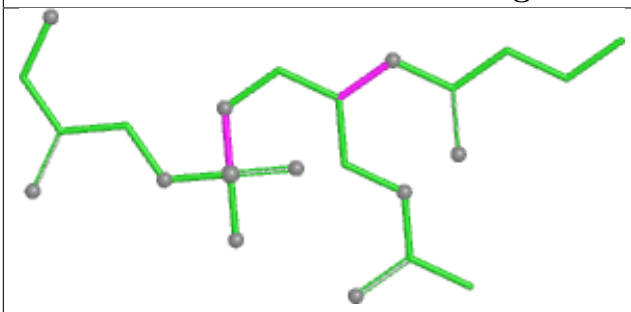
Bond angles



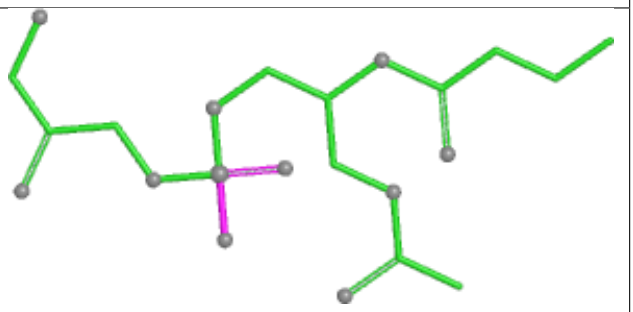
Torsions

Rings

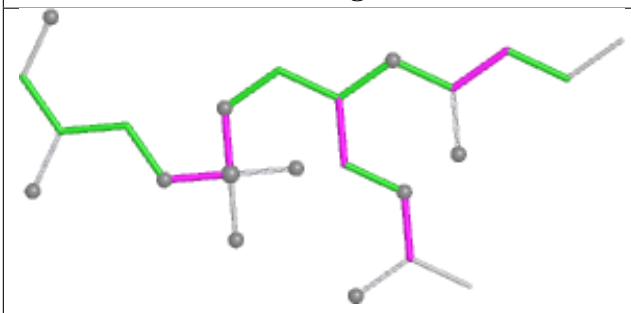
Ligand LHG bB 948



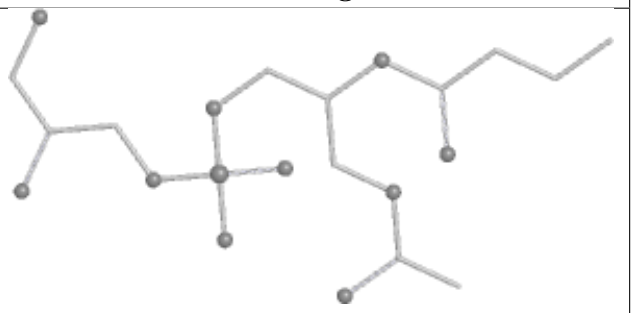
Bond lengths



Bond angles

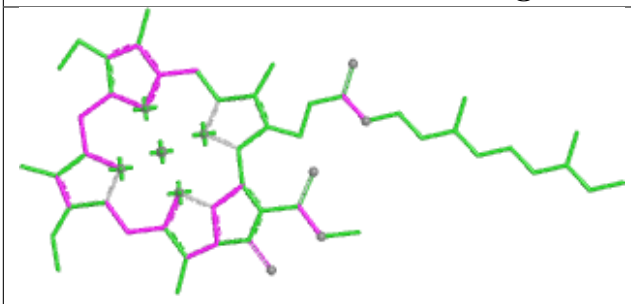


Torsions

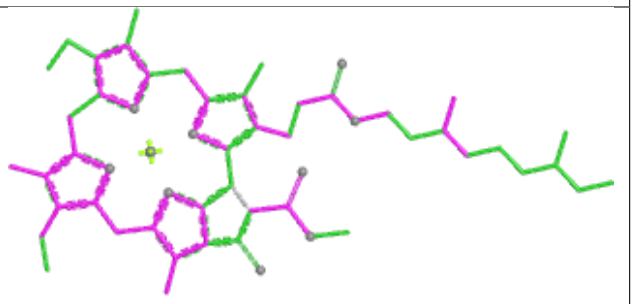


Rings

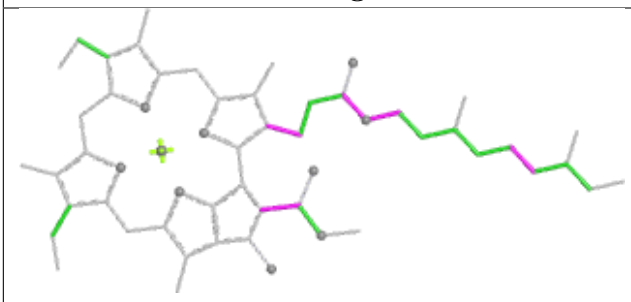
Ligand CLA aA 804



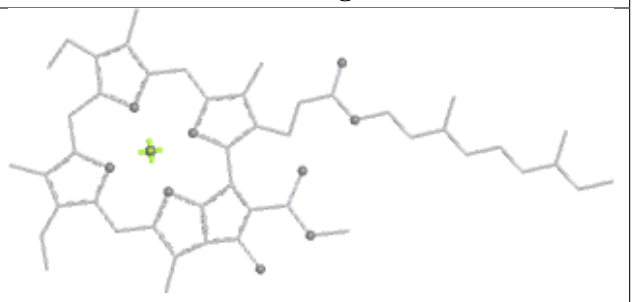
Bond lengths



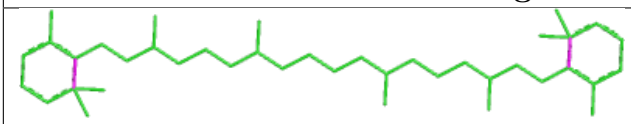
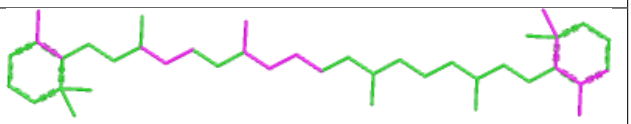
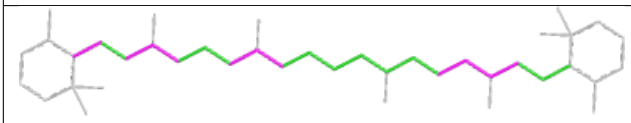
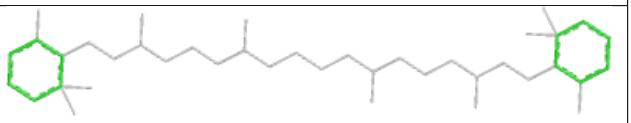
Bond angles

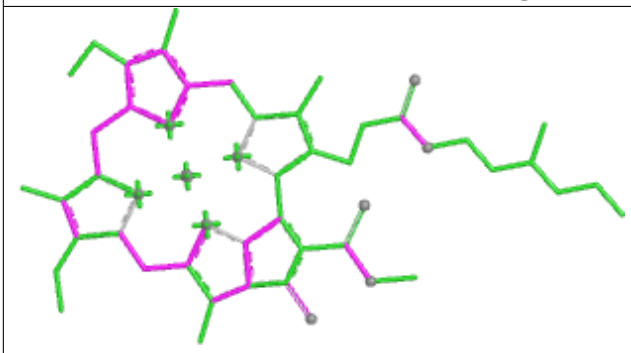
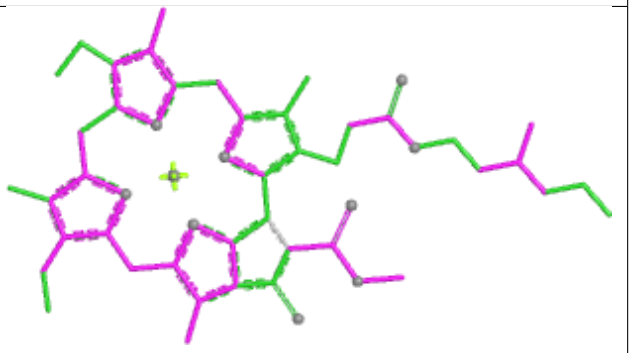
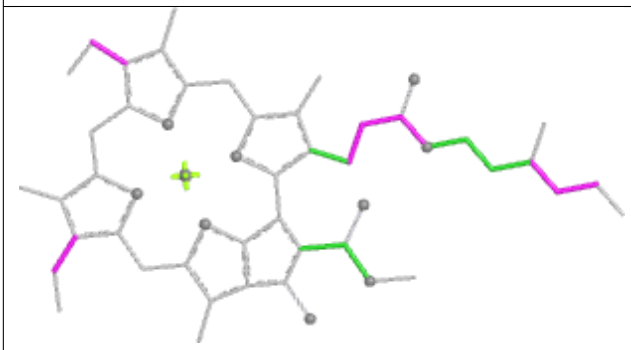
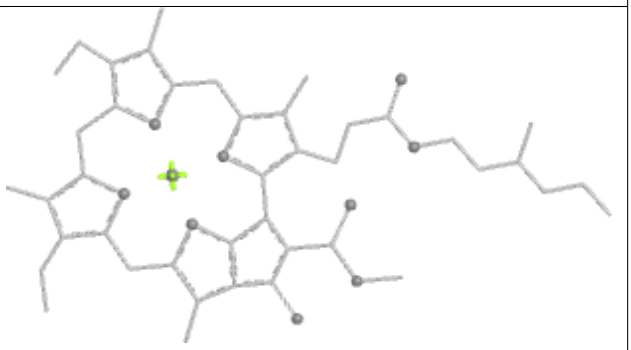


Torsions

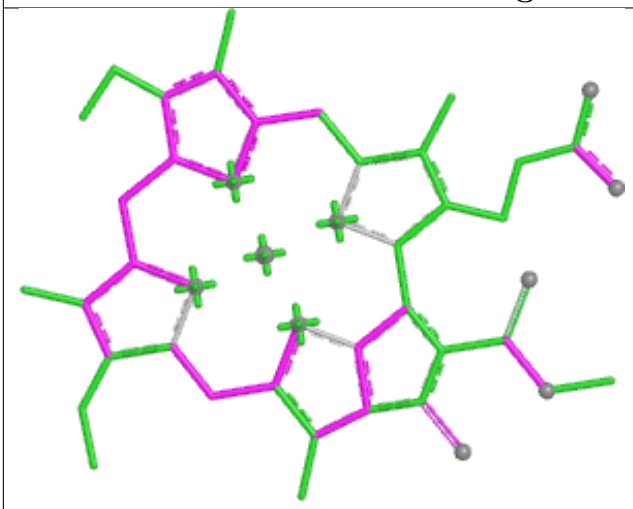


Rings

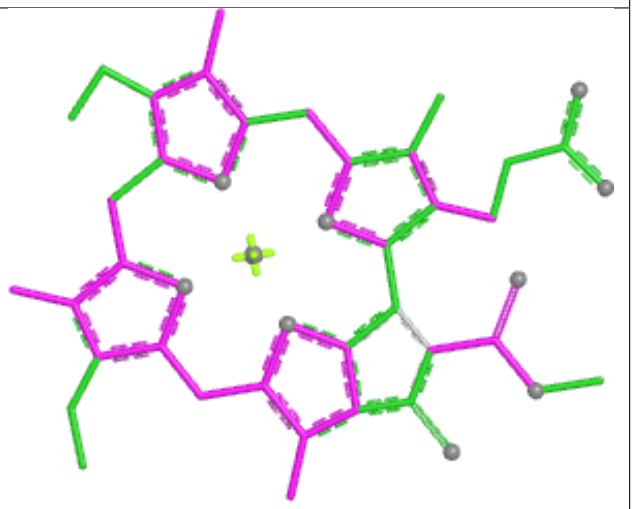
Ligand BCR bF 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA aB 915	
 Bond lengths	 Bond angles
 Torsions	 Rings

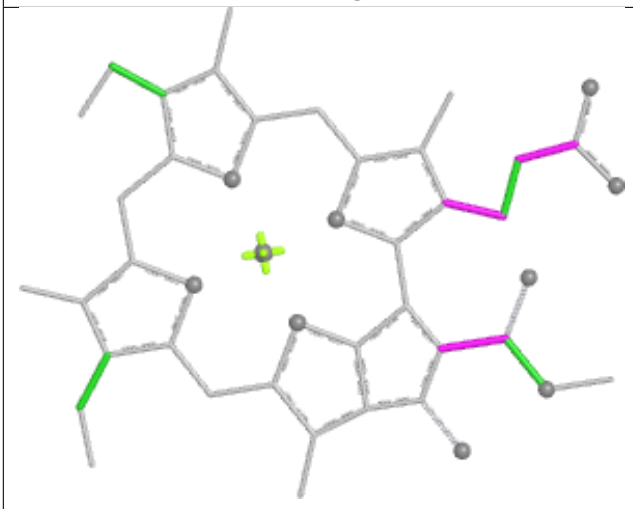
Ligand CLA cB 914



Bond lengths



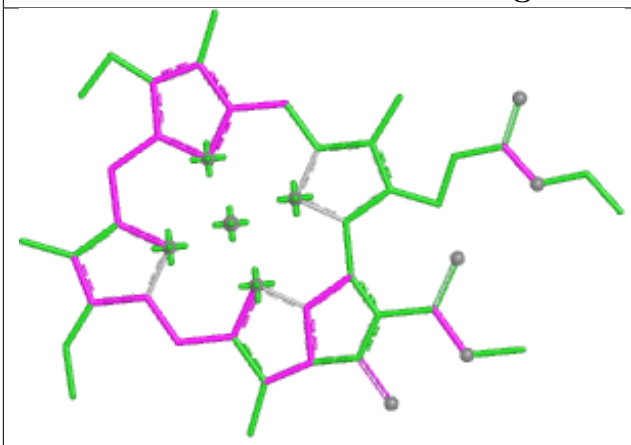
Bond angles



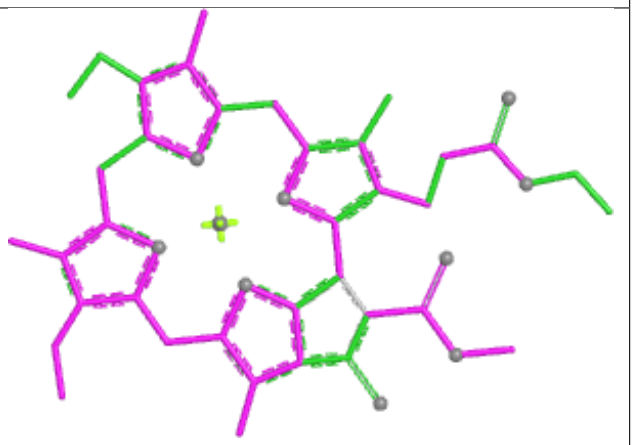
Torsions

Rings

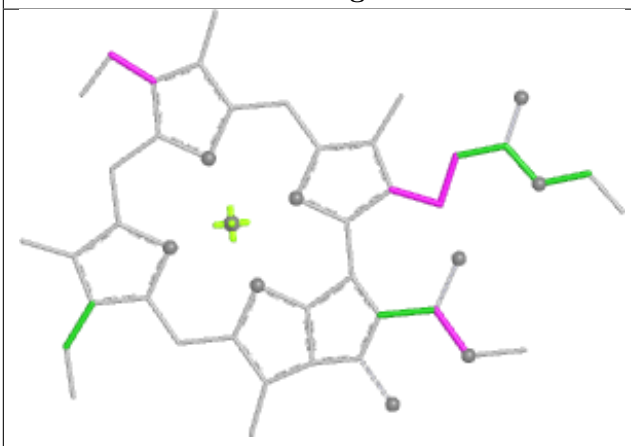
Ligand CLA bA 824



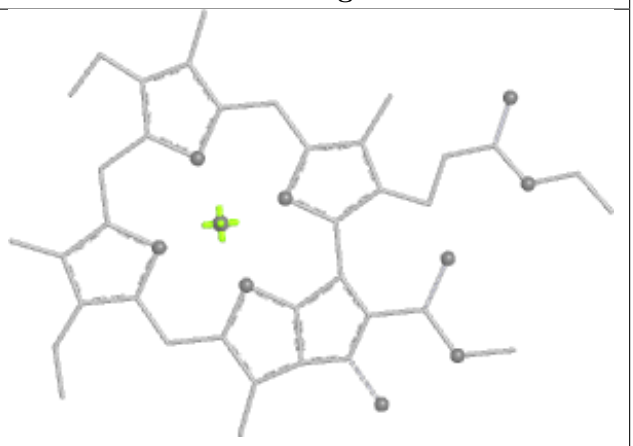
Bond lengths



Bond angles

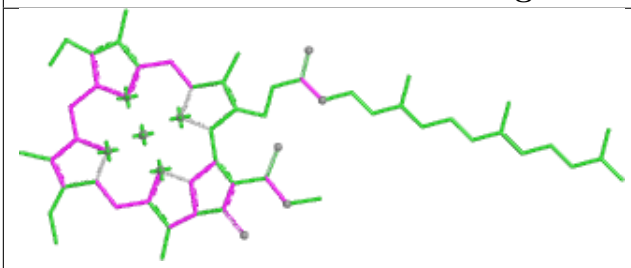


Torsions

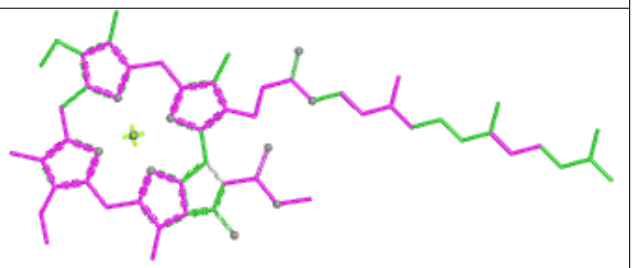


Rings

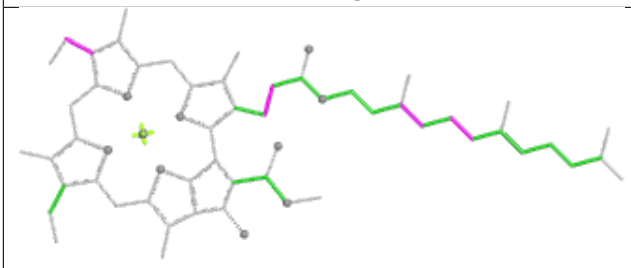
Ligand CLA aA 819



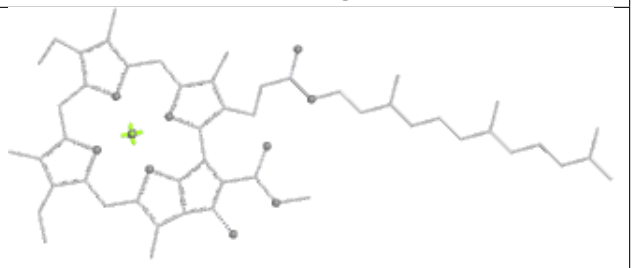
Bond lengths



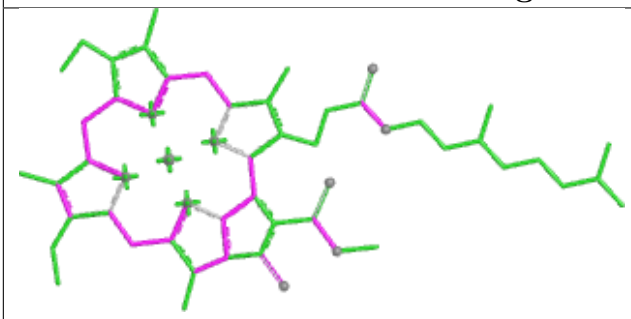
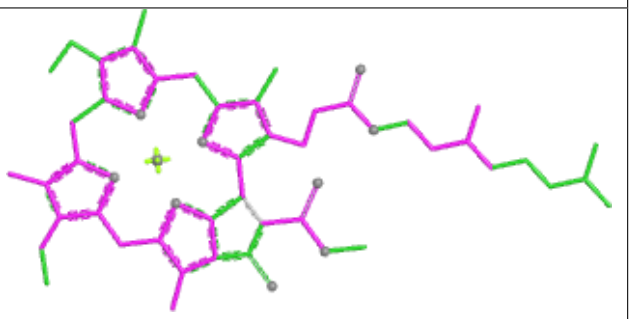
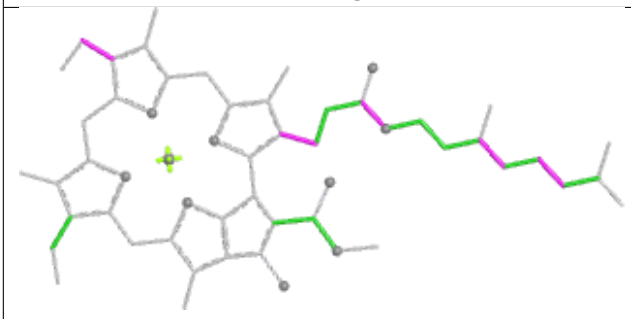
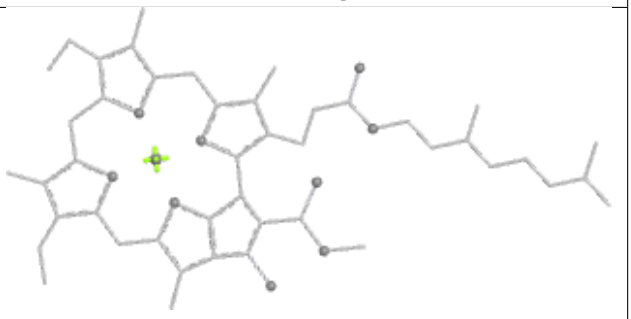
Bond angles

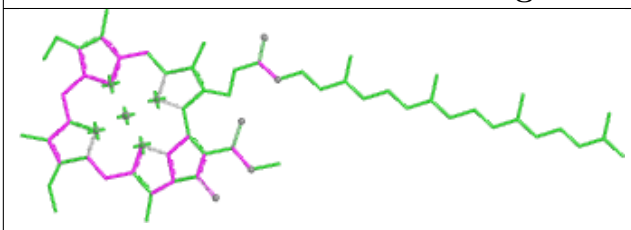
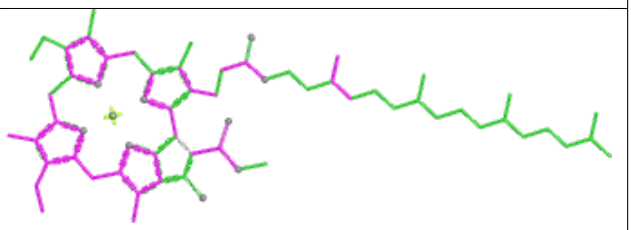
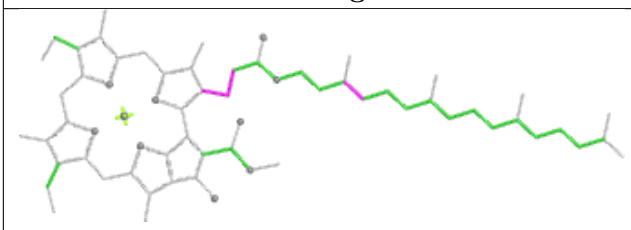
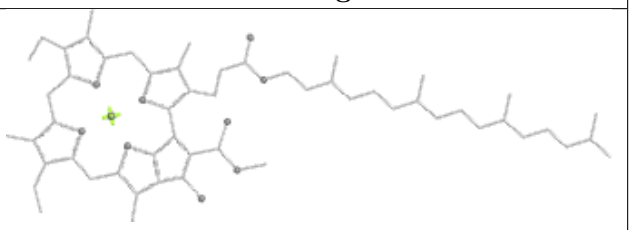


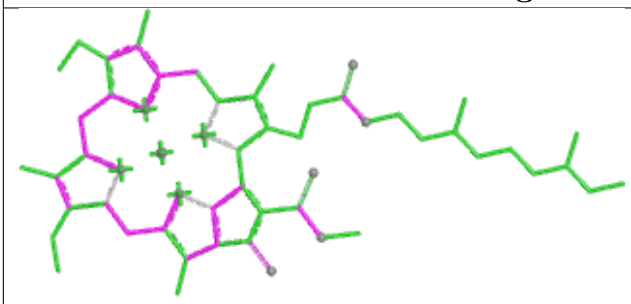
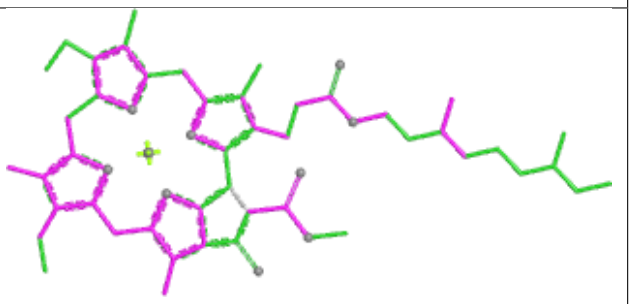
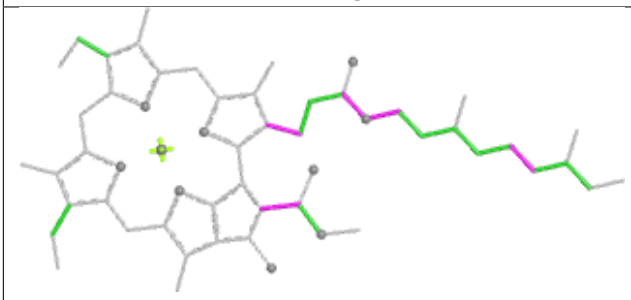
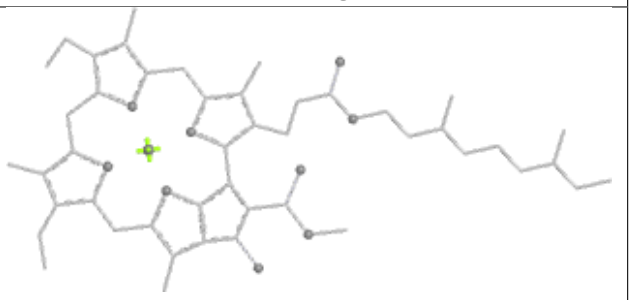
Torsions

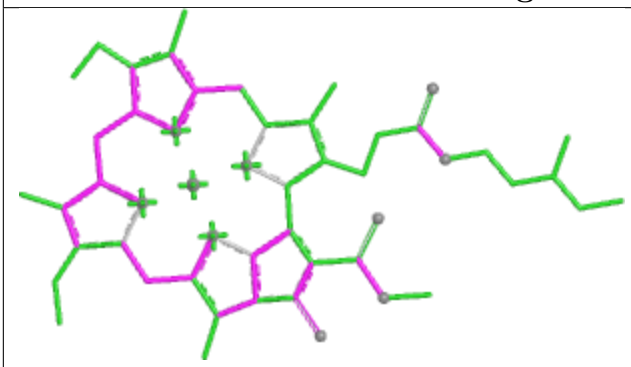
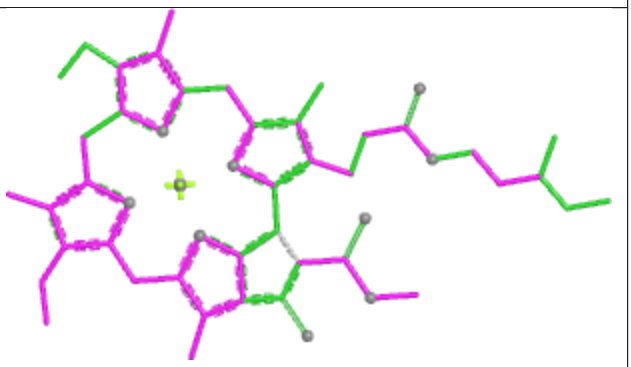
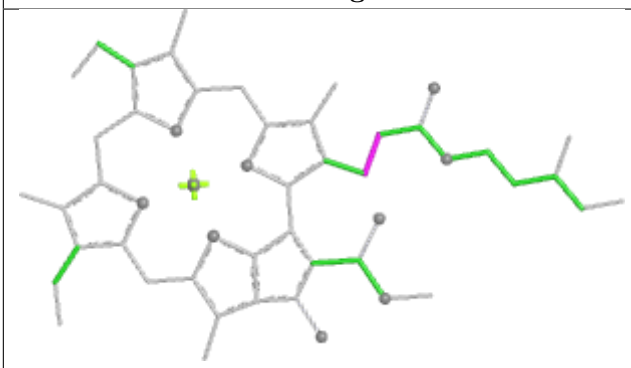
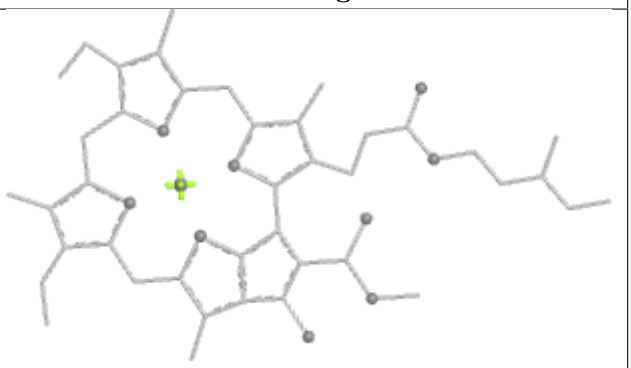


Rings

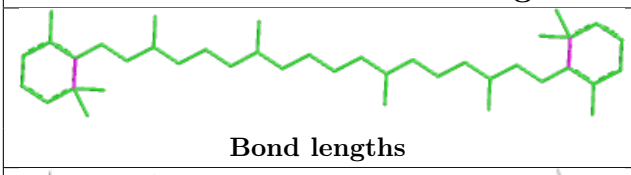
Ligand CLA aB 917	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA cA 802	
	
Bond lengths	Bond angles
	
Torsions	Rings

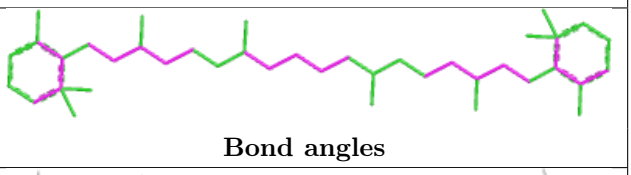
Ligand CLA cA 804	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA cB 938	
	
Bond lengths	Bond angles
	
Torsions	Rings

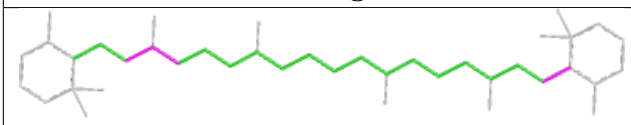
Ligand BCR bF 204



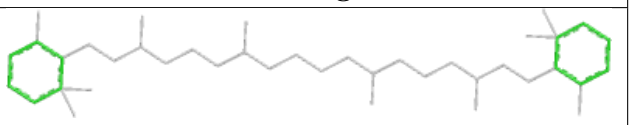
Bond lengths



Bond angles

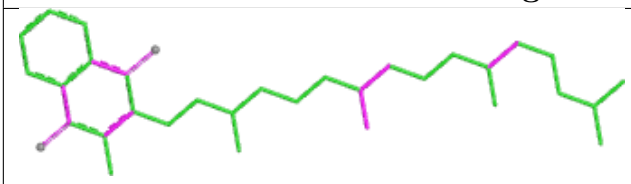


Torsions



Rings

Ligand 1L3 bA 844



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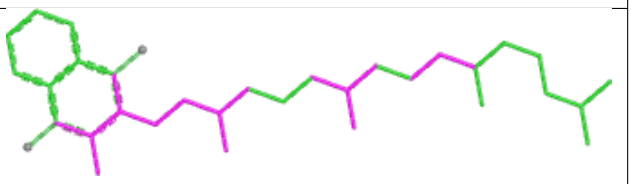
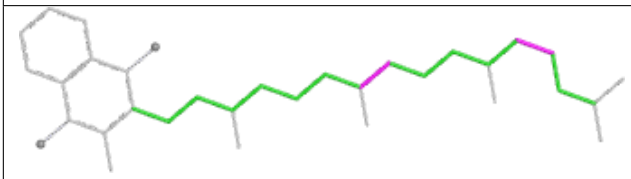


Bond angles



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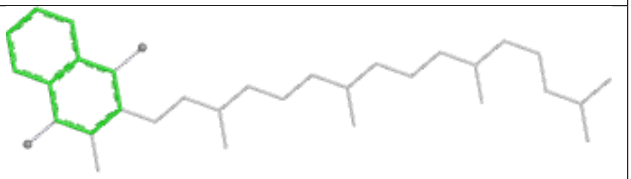
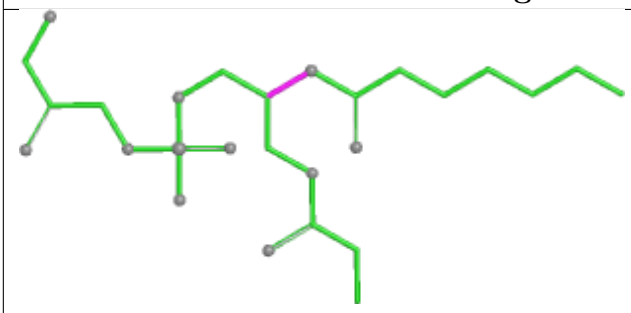


Rings

Ligand LHG cA 852



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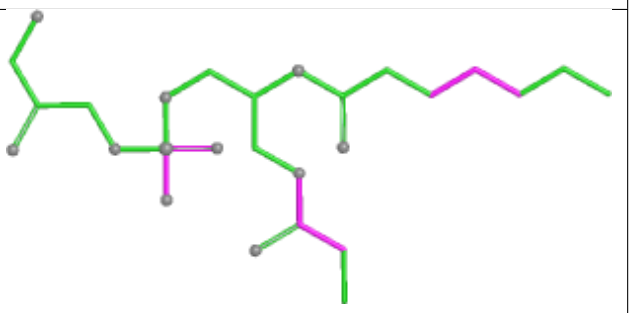
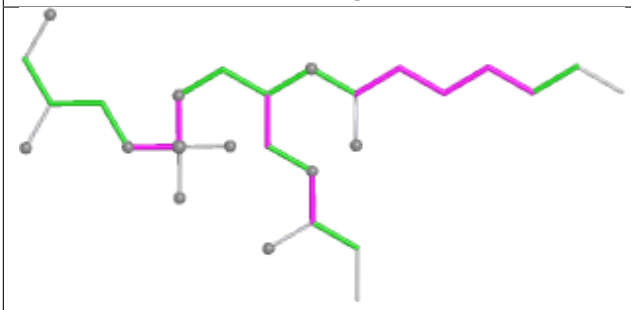


Bond angles



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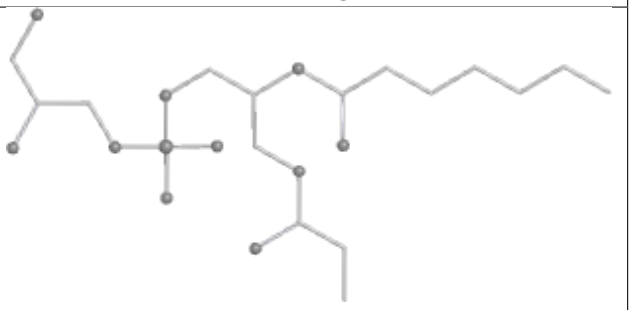
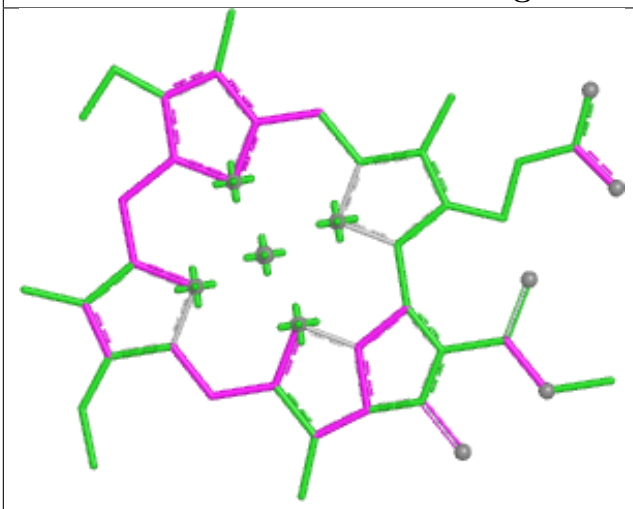


Rings

Ligand CLA bA 839



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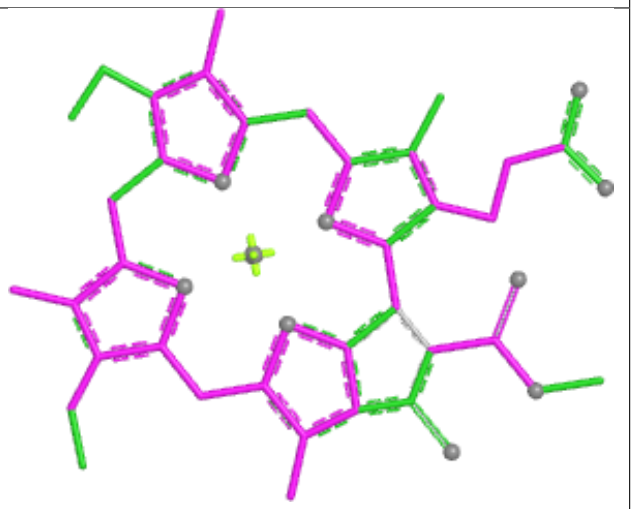
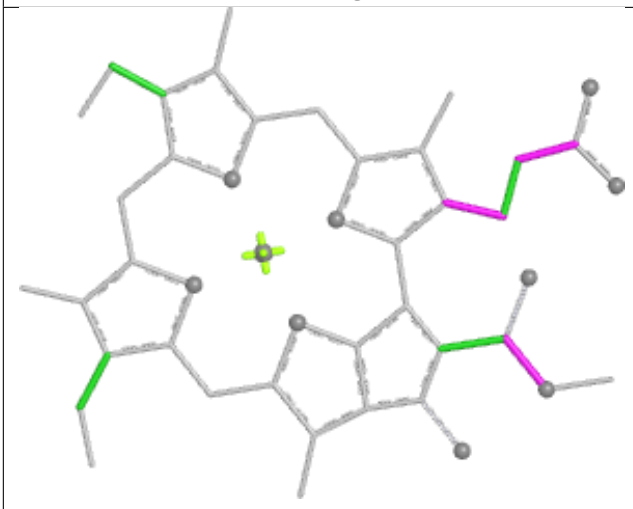


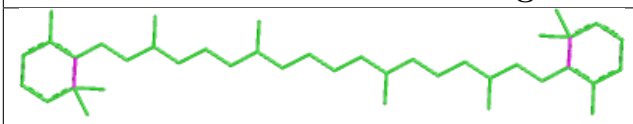
Bond angles



Torsions

Rings

Ligand BCR cL 206



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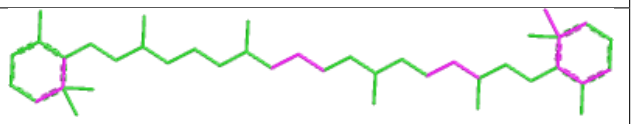

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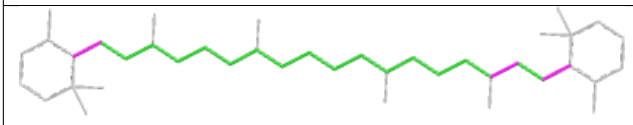

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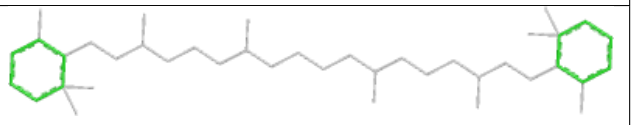
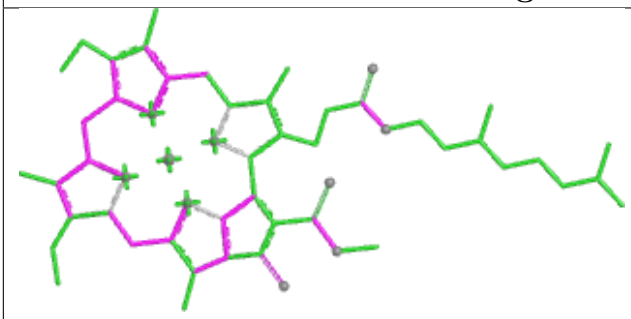


Rings

Ligand CLA cB 925



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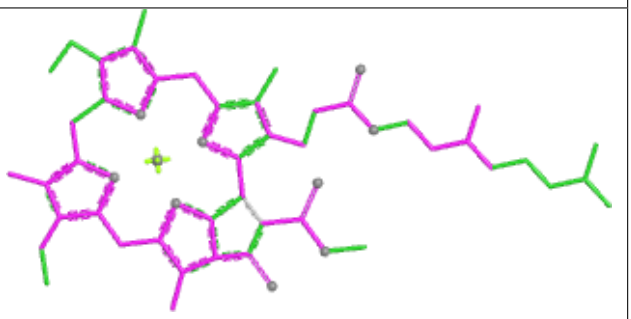

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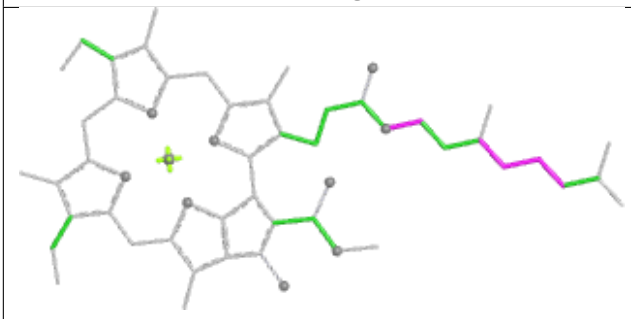

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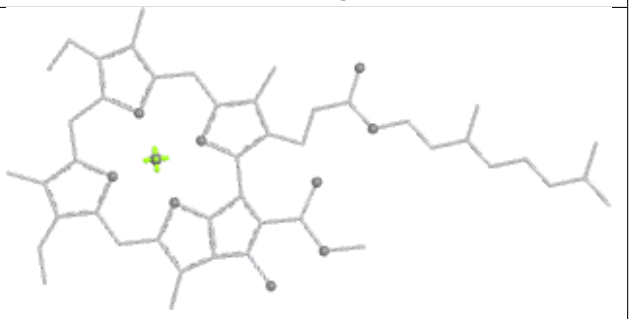
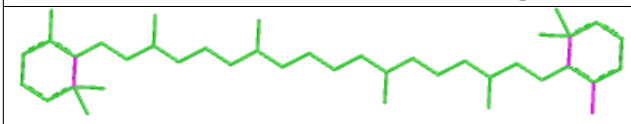


Rings

Ligand BCR aB 946



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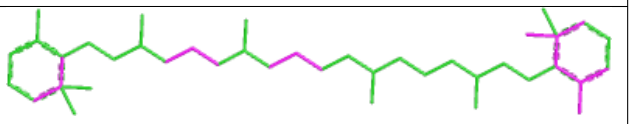

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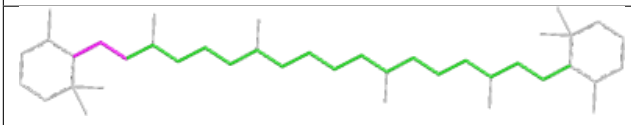

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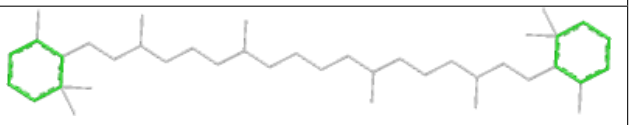
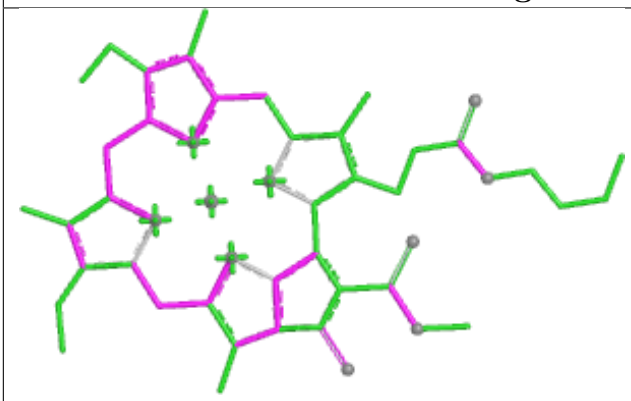


Rings

Ligand CLA bB 930



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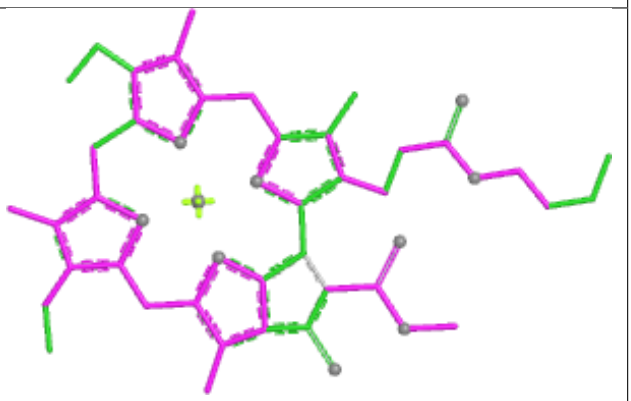
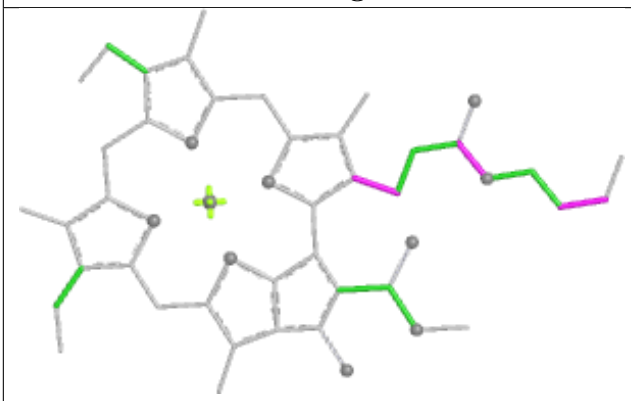


Bond angles



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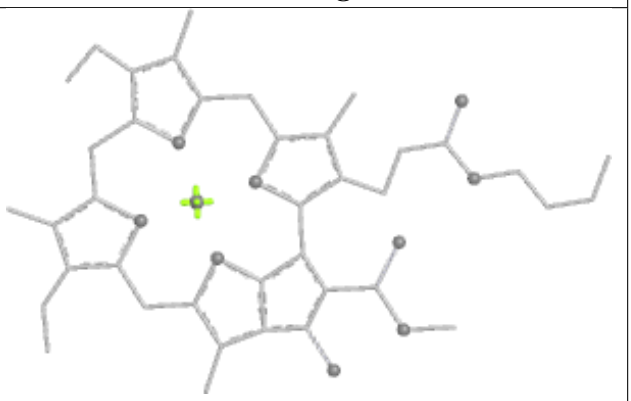
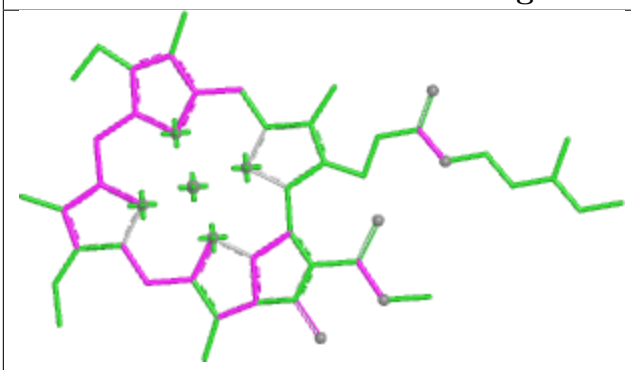


Rings

Ligand CLA cB 903



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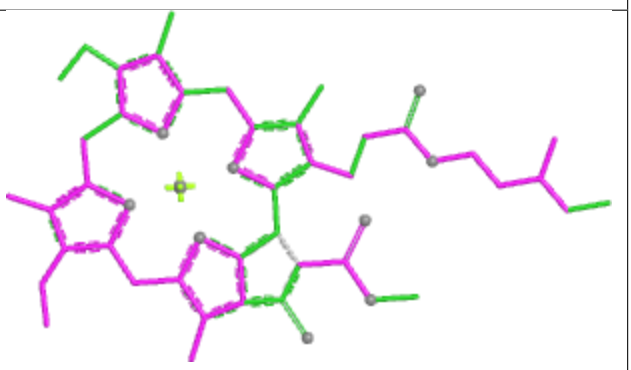
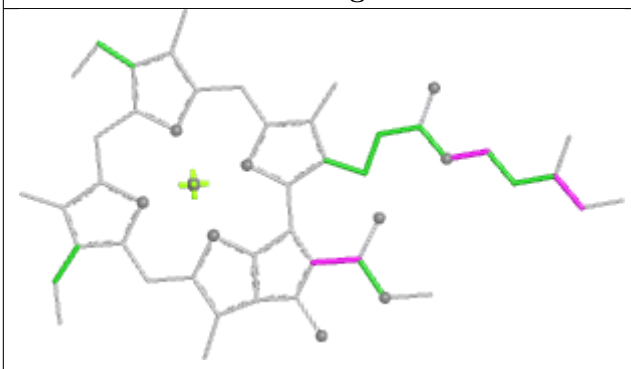
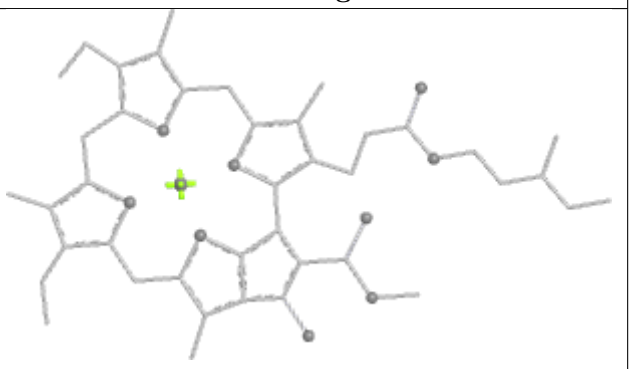


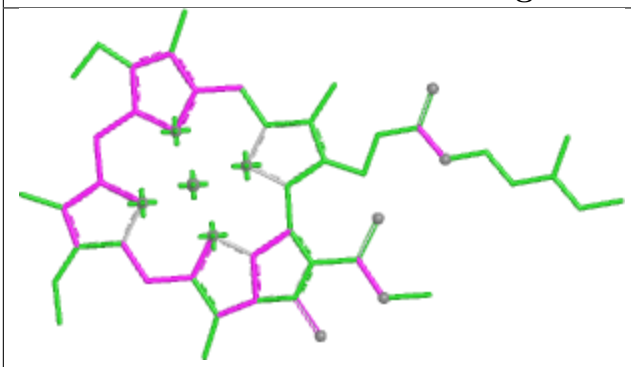
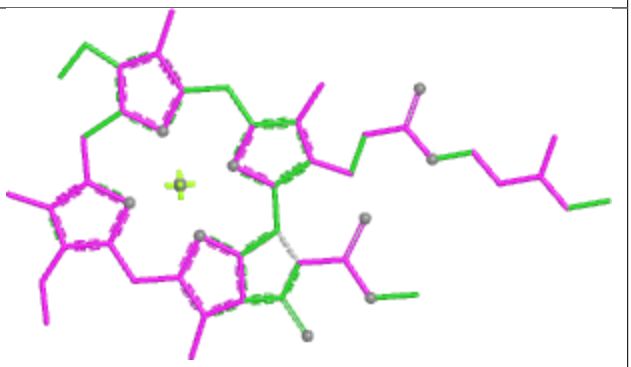
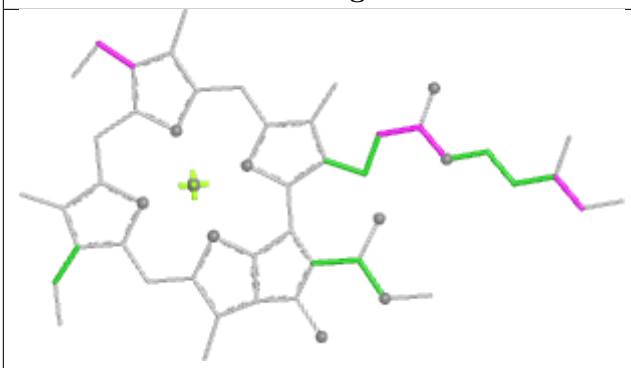
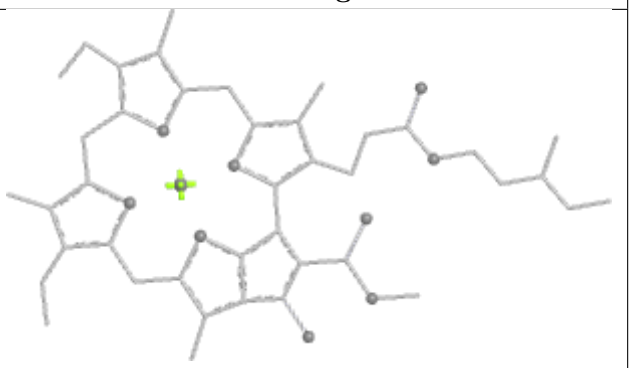
Bond angles

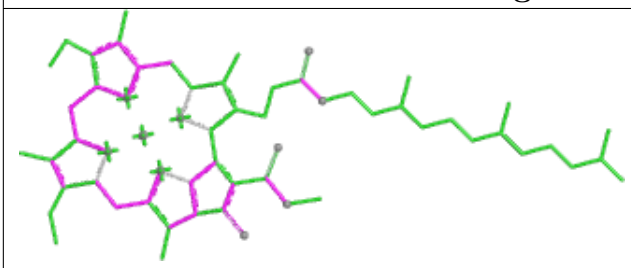
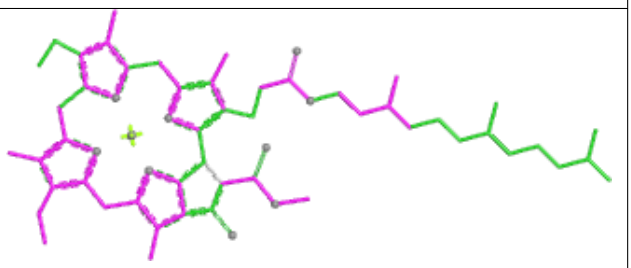
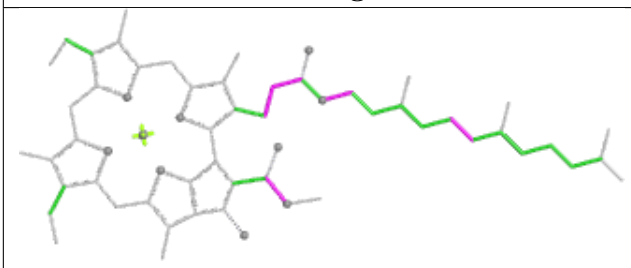
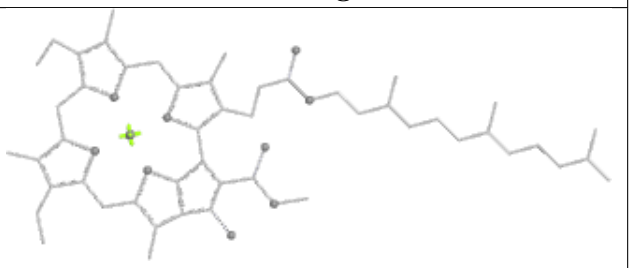


Torsions

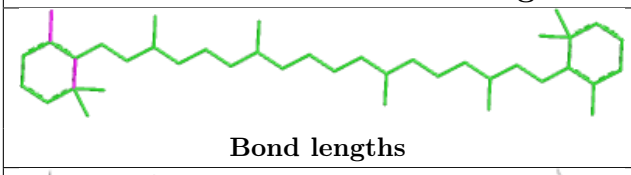


Rings

Ligand CLA cA 823	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA bA 829	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR aJ 101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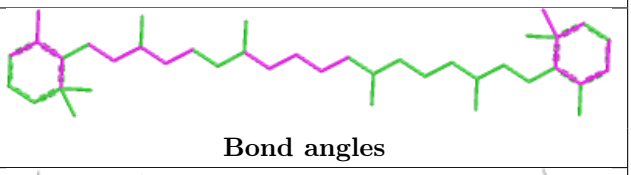
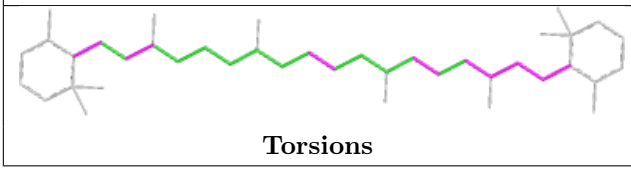
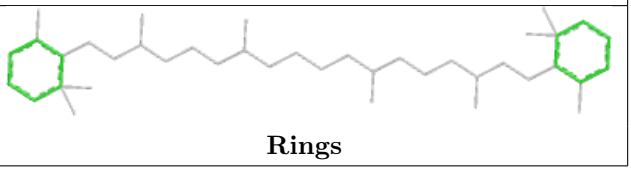
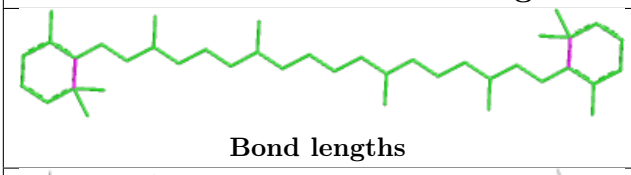
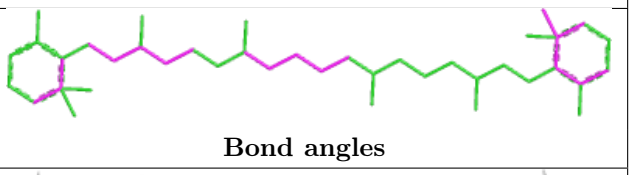

Bond angles

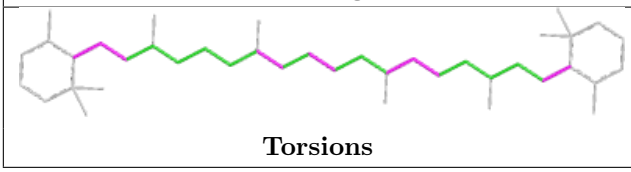

Torsions

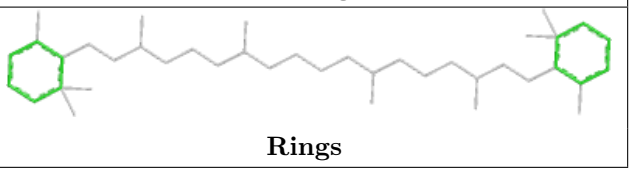

Rings

Ligand BCR cB 945

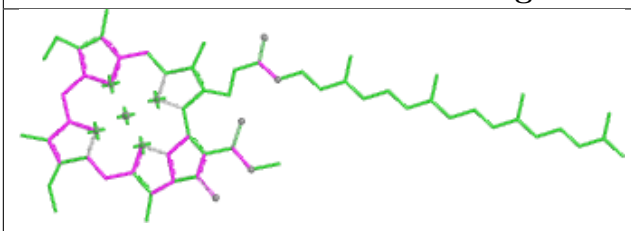

Bond lengths

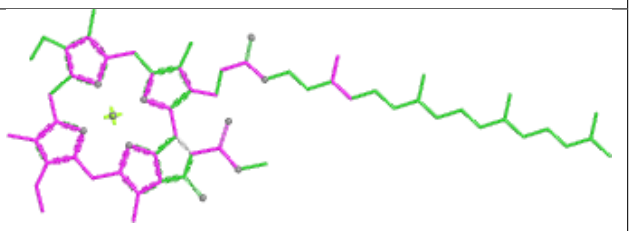

Bond angles

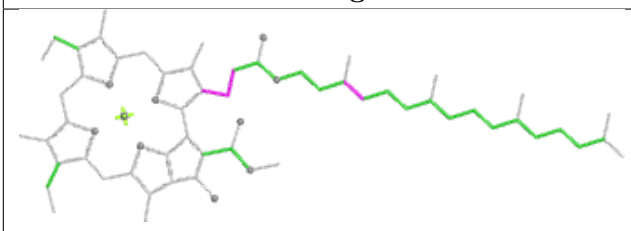

Torsions

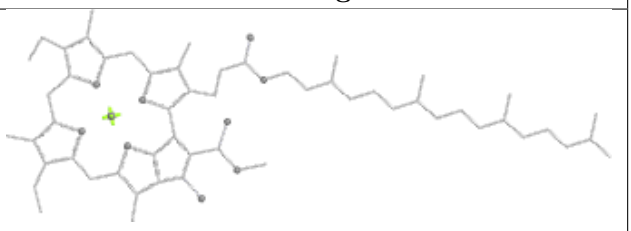

Rings

Ligand CLA aA 802

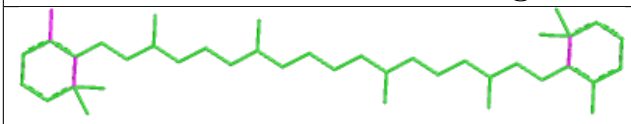

Bond lengths

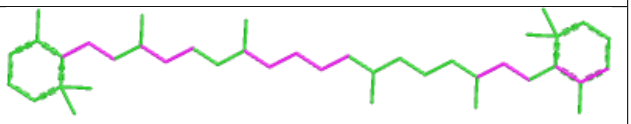

Bond angles

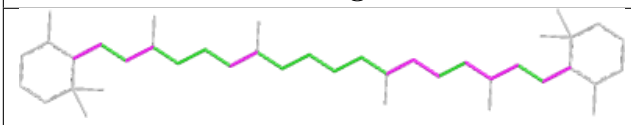

Torsions

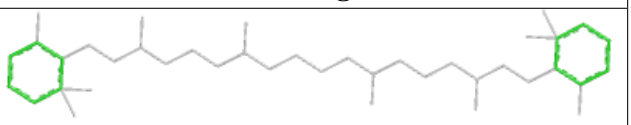

Rings

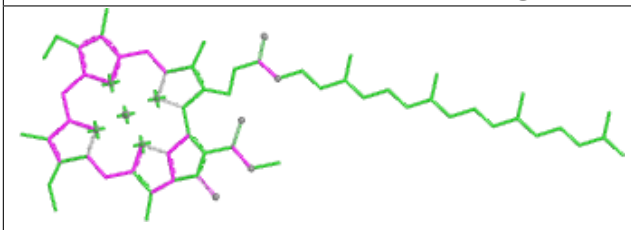
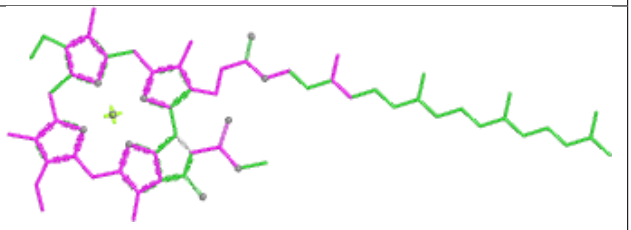
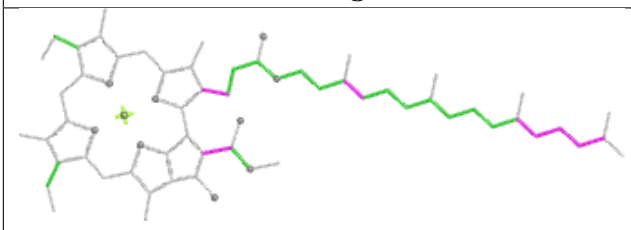
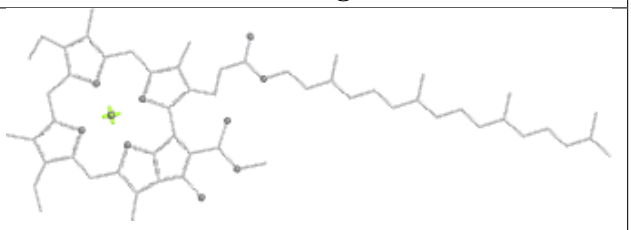
Ligand BCR bA 849

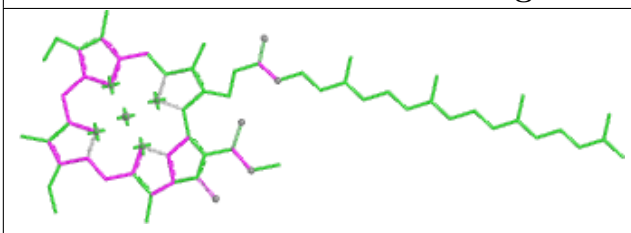
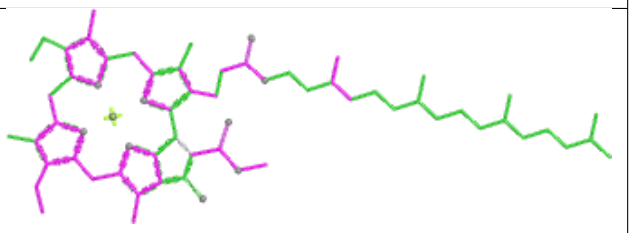
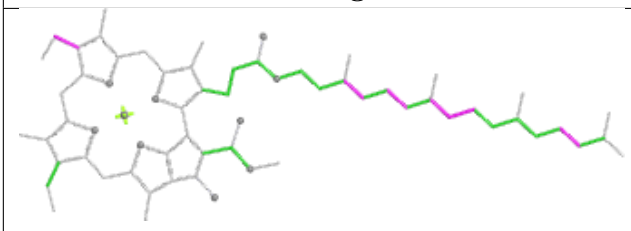
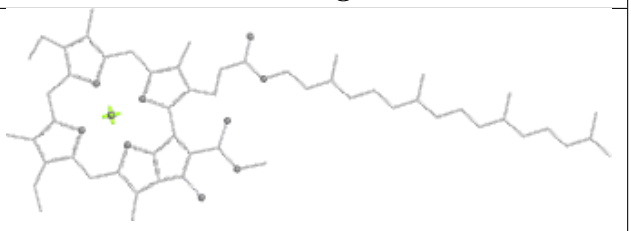

Bond lengths


Bond angles

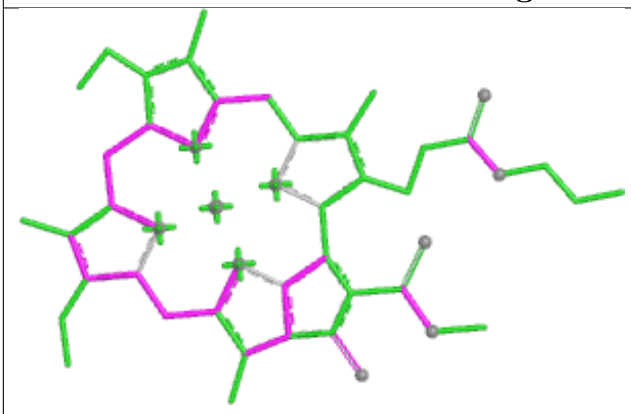

Torsions


Rings

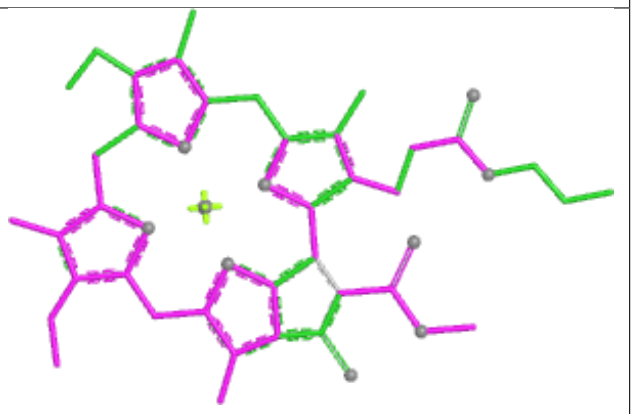
Ligand CLA bB 904	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA aA 840	
 Bond lengths	 Bond angles
 Torsions	 Rings

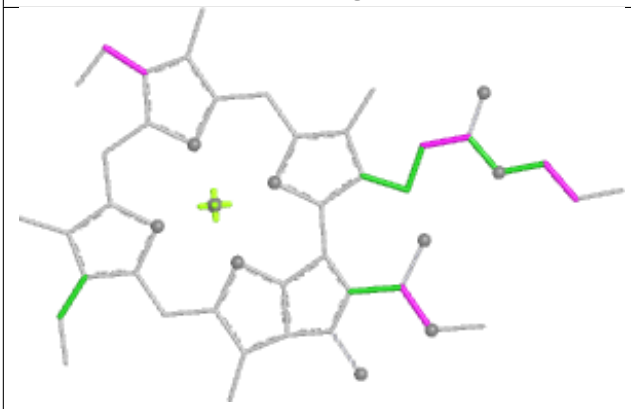
Ligand CLA aB 908



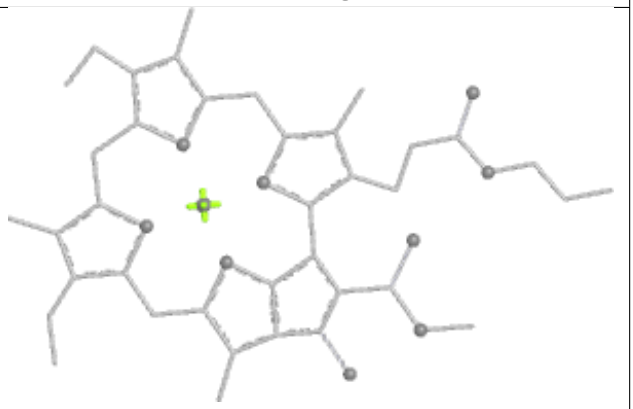
Bond lengths



Bond angles

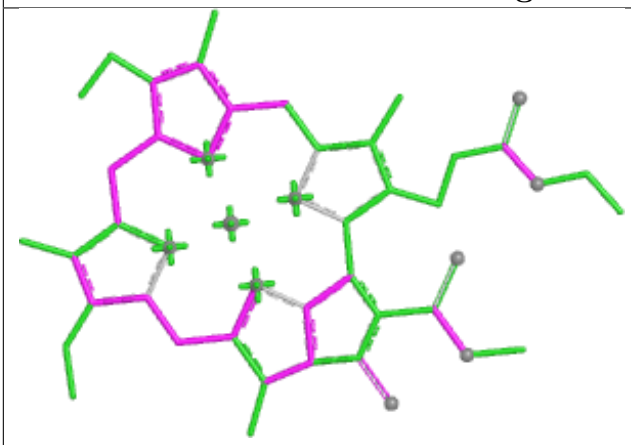


Torsions

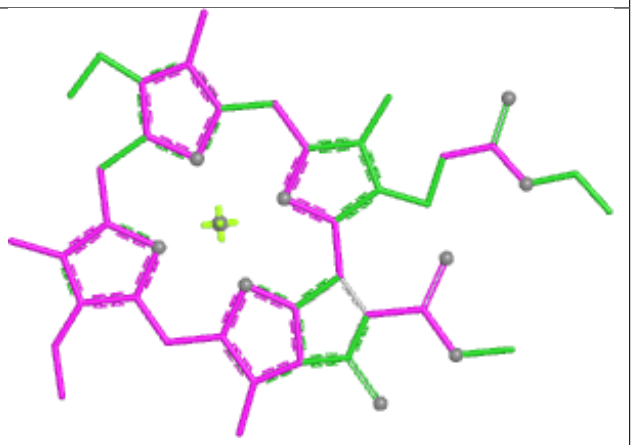


Rings

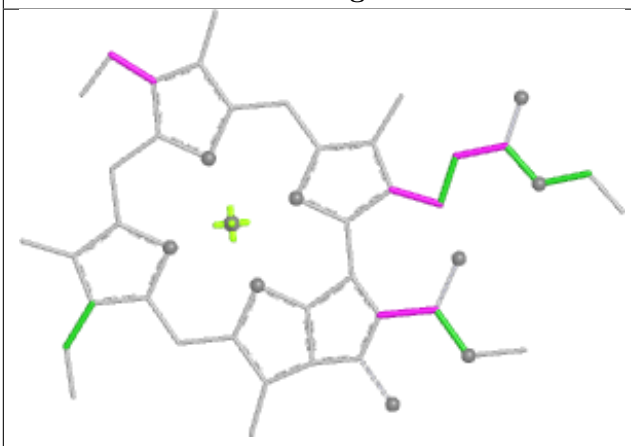
Ligand CLA aB 919



Bond lengths



Bond angles



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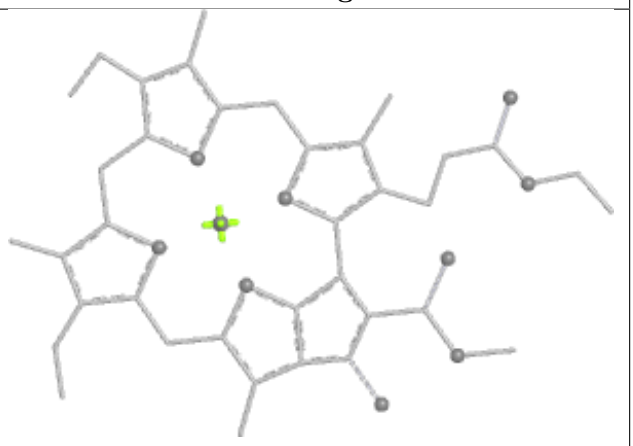
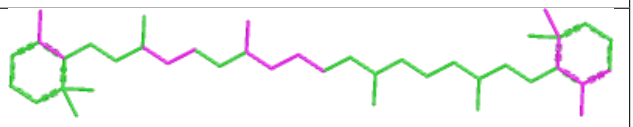


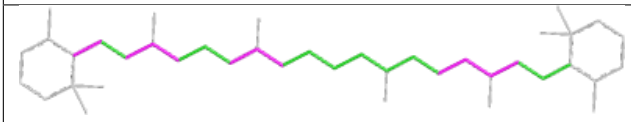
Rings

Ligand BCR cF 203

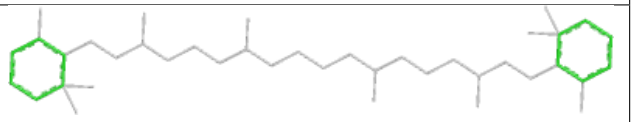
Bond lengths



Bond angles

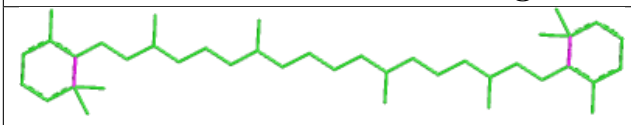


Torsions

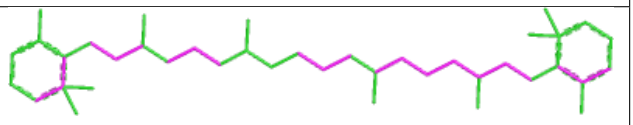


Rings

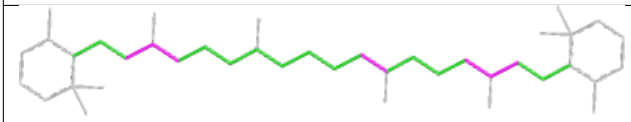
Ligand BCR cA 850



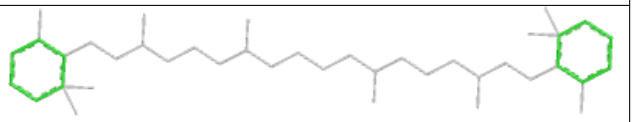
Bond lengths



Bond angles

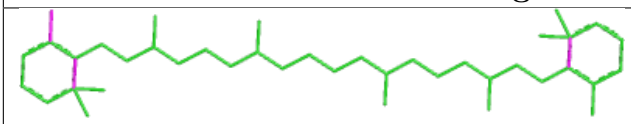


Torsions



Rings

Ligand BCR bB 942



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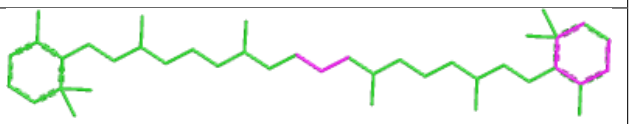
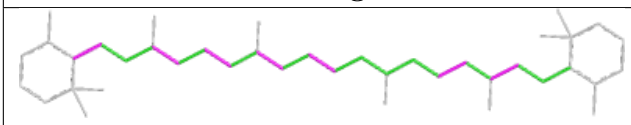
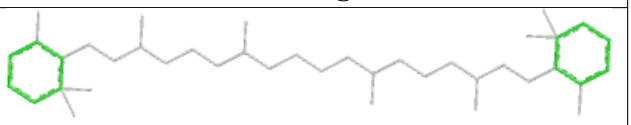


Bond angles

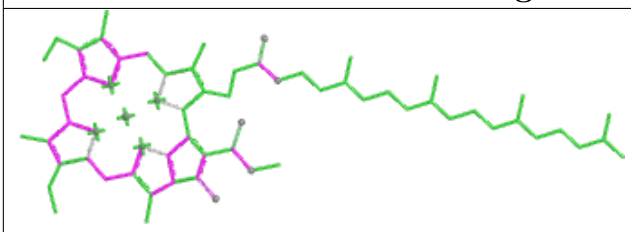


Torsions



Rings

Ligand CLA aA 838



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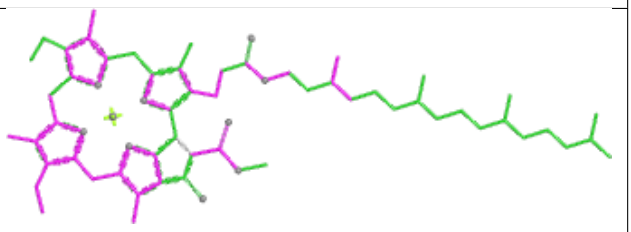
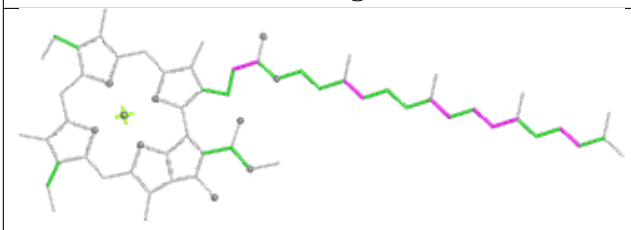
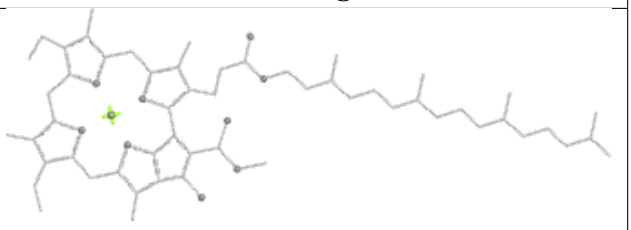


Bond angles

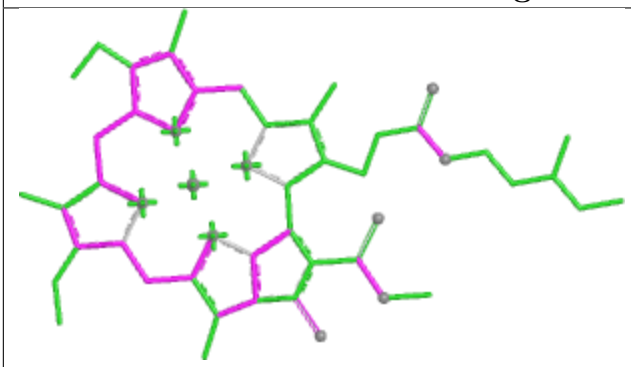


Torsions



Rings

Ligand CLA bA 808



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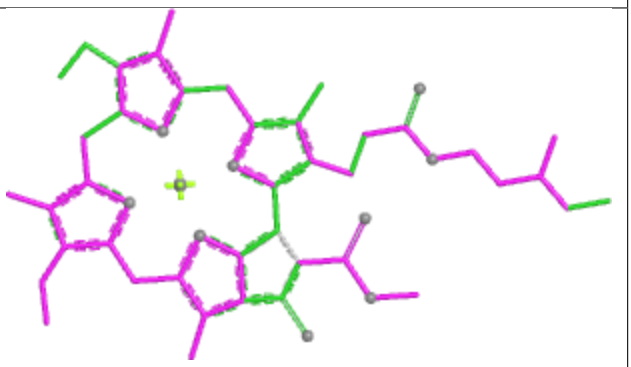
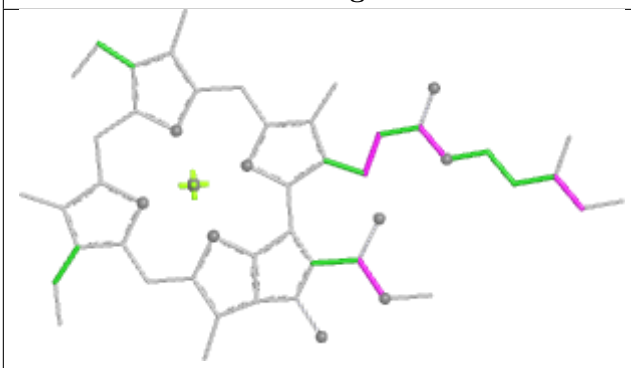
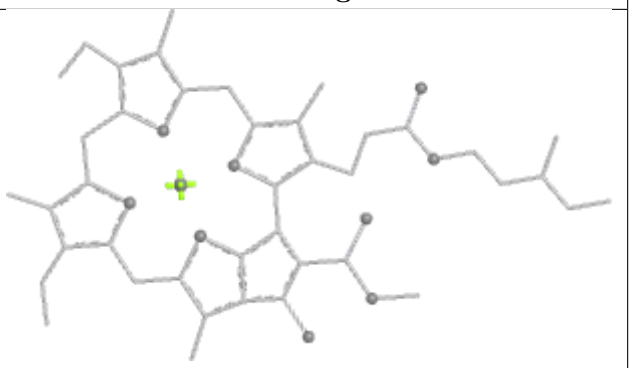


Bond angles

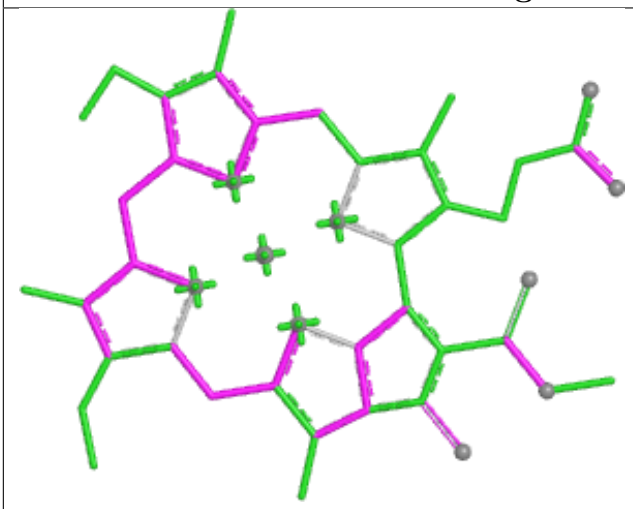


Torsions



Rings

Ligand CLA aA 809



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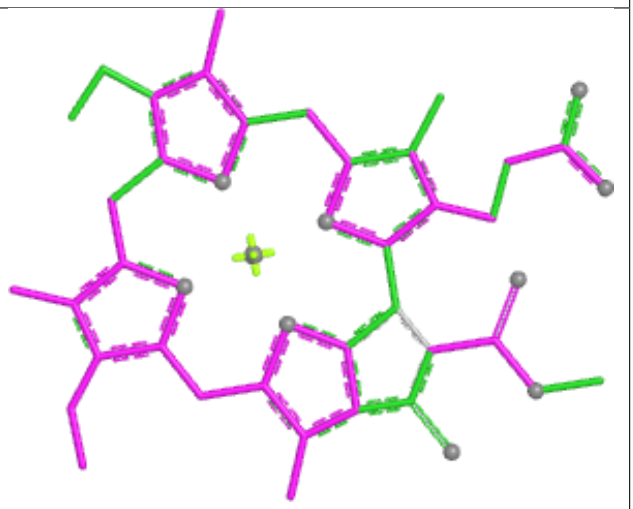
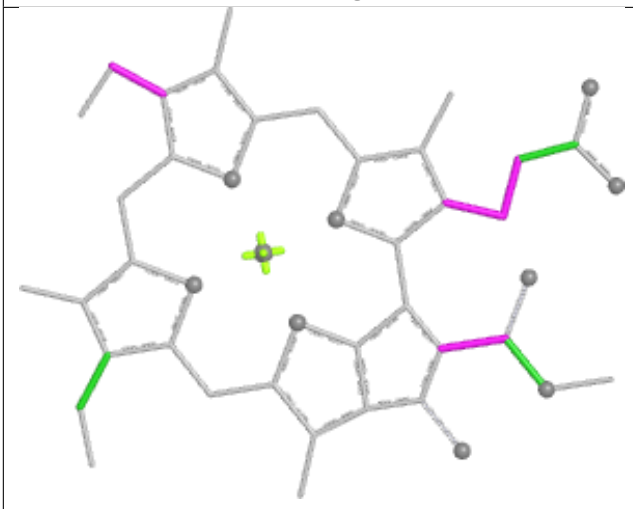


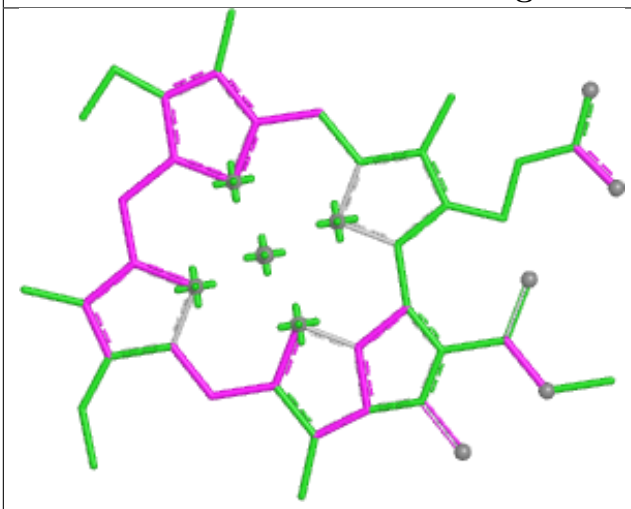
Bond angles



Torsions

Rings

Ligand CLA aB 914



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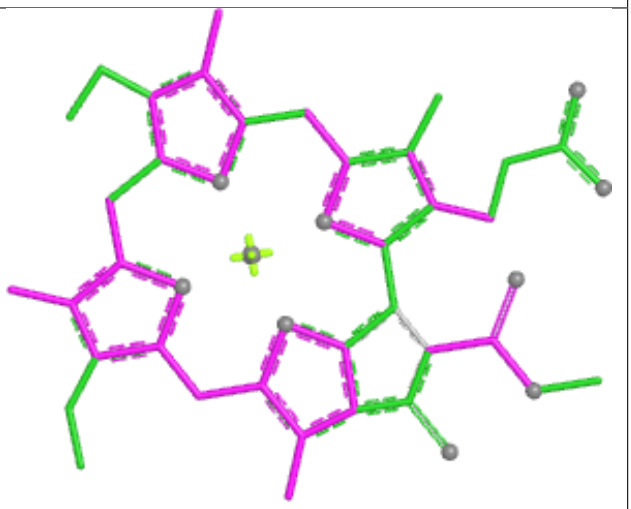
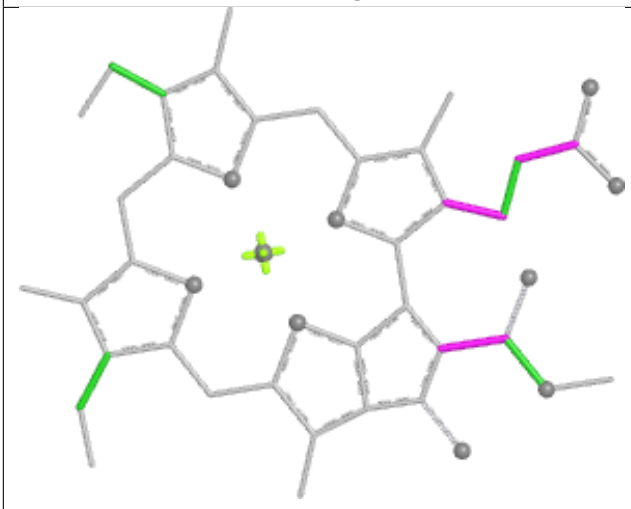


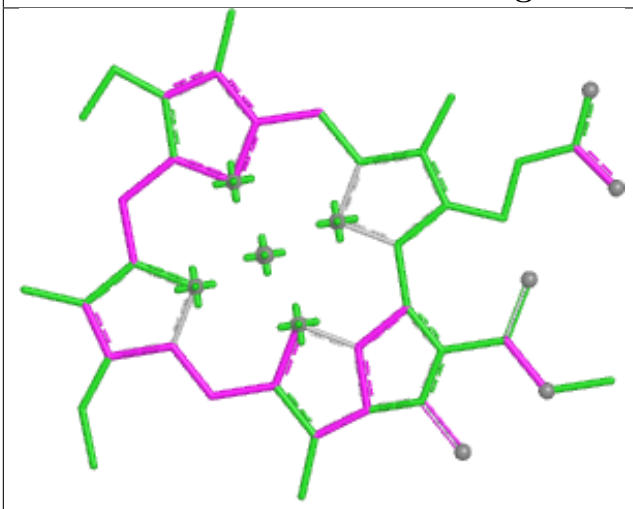
Bond angles



Torsions

Rings

Ligand CLA aA 815



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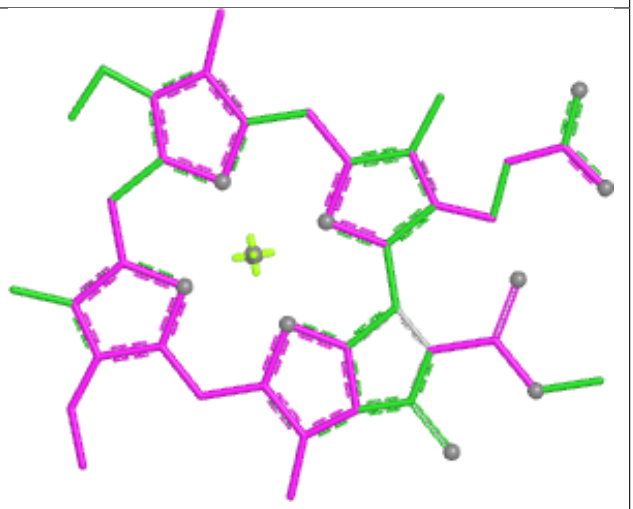
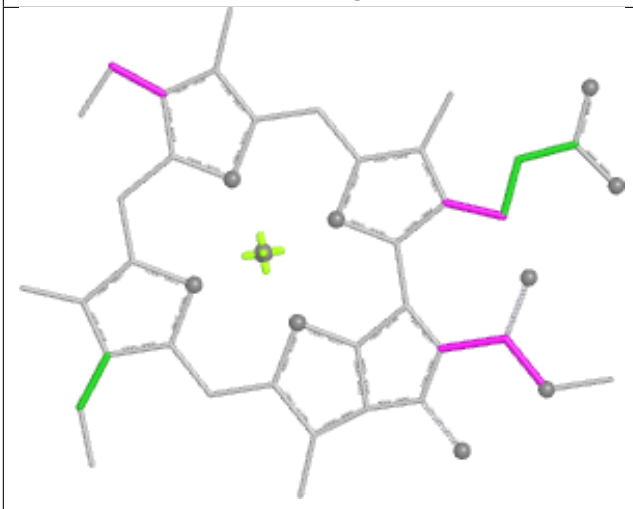


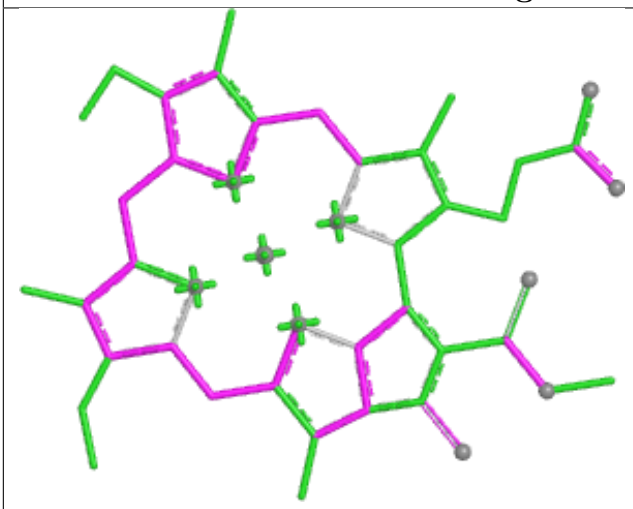
Bond angles



Torsions

Rings

Ligand CLA aB 934



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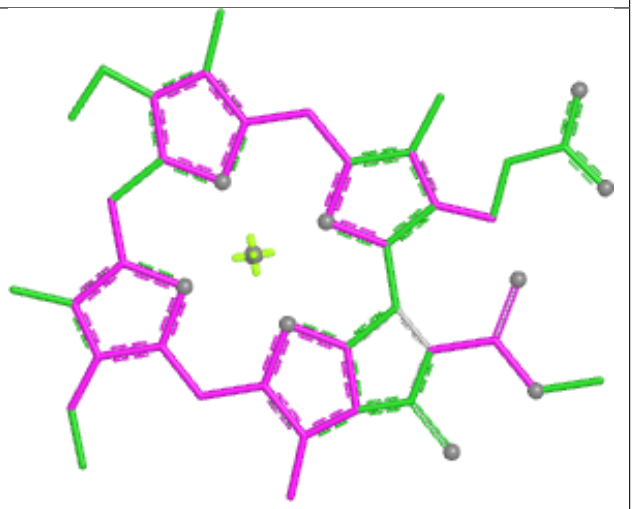
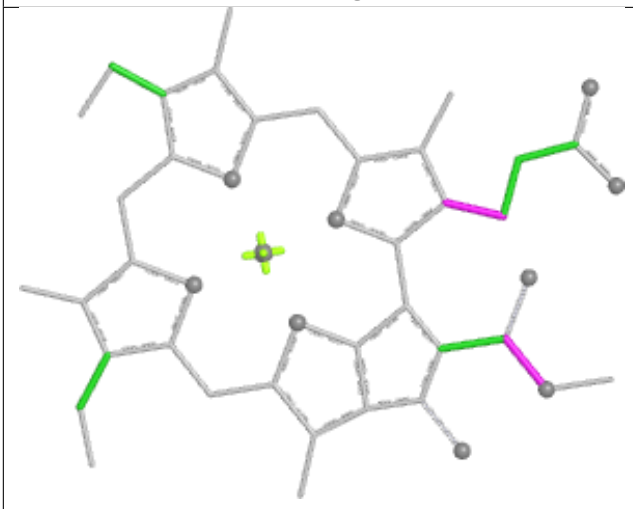


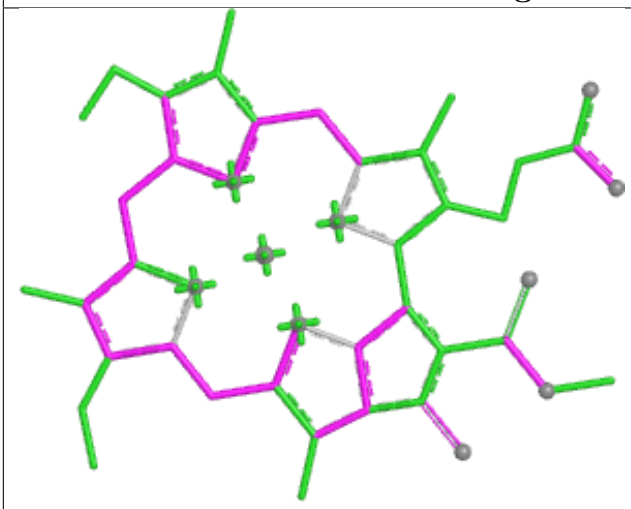
Bond angles



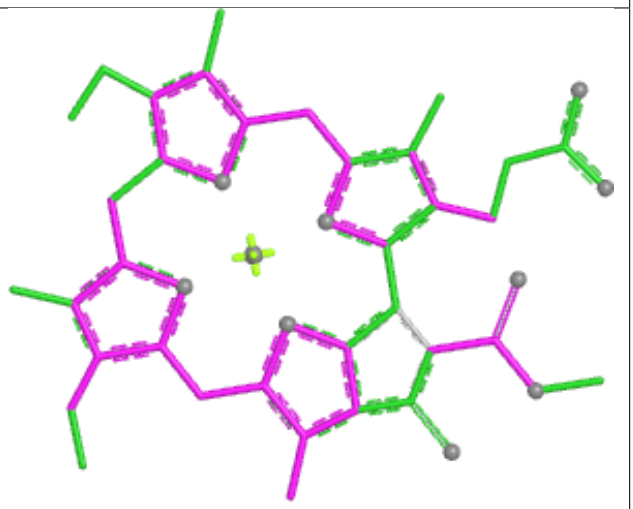
Torsions

Rings

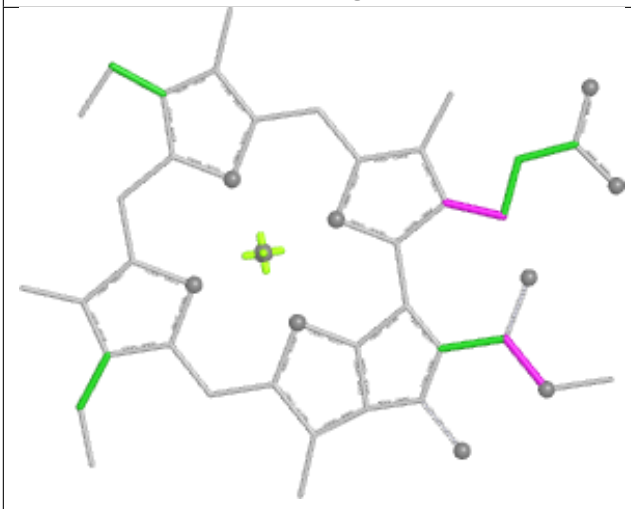
Ligand CLA bB 934



Bond lengths



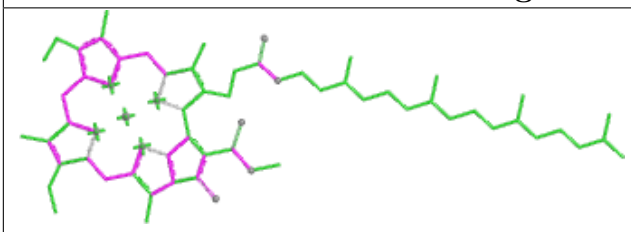
Bond angles



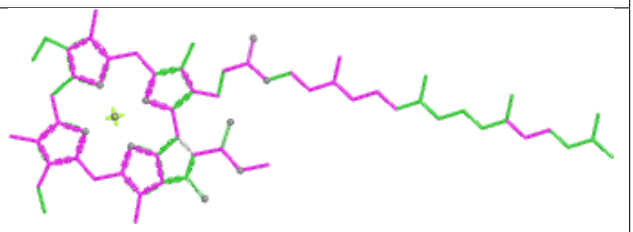
Torsions

Rings

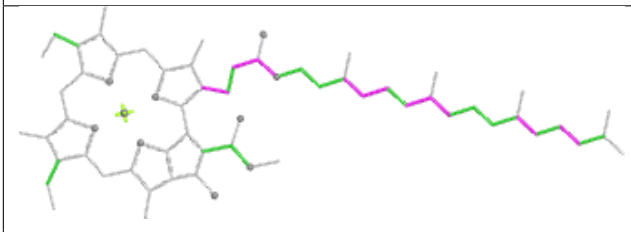
Ligand CLA aA 807



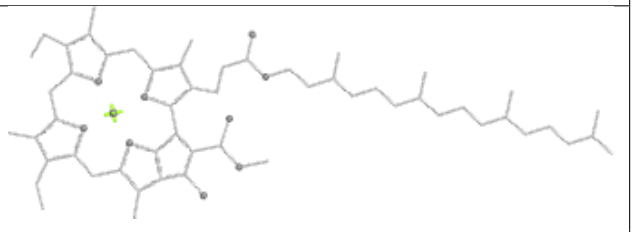
Bond lengths



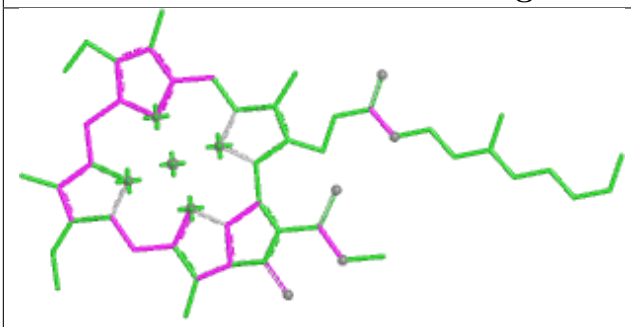
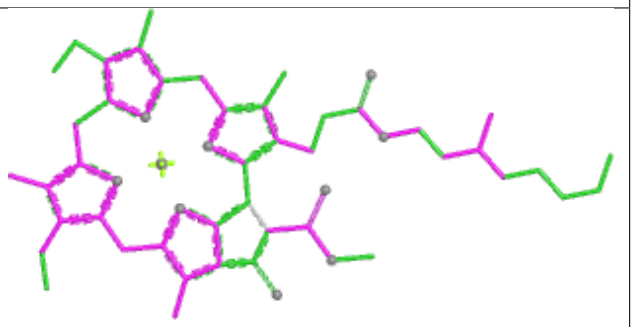
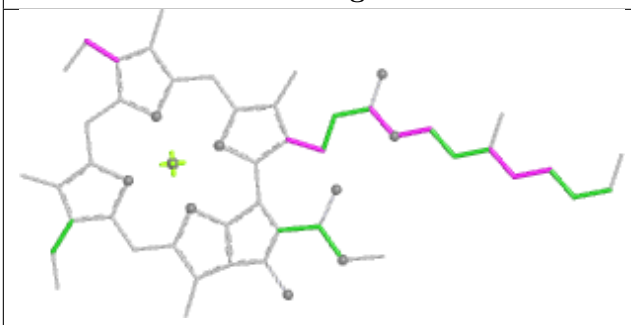
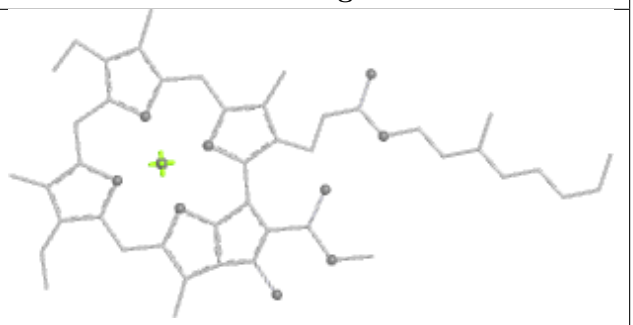
Bond angles

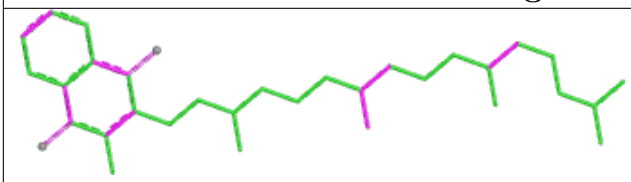
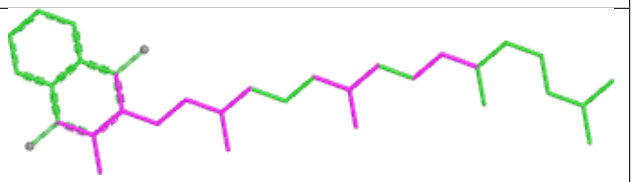
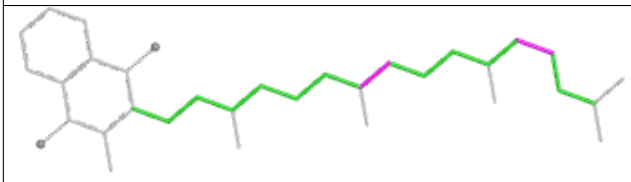
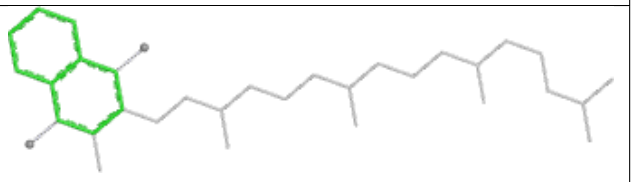


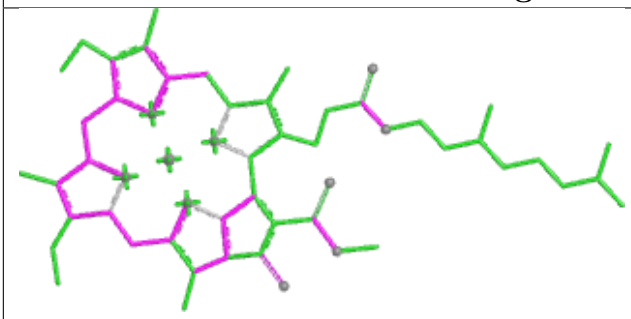
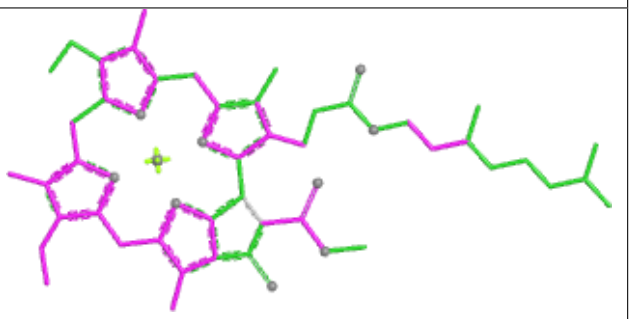
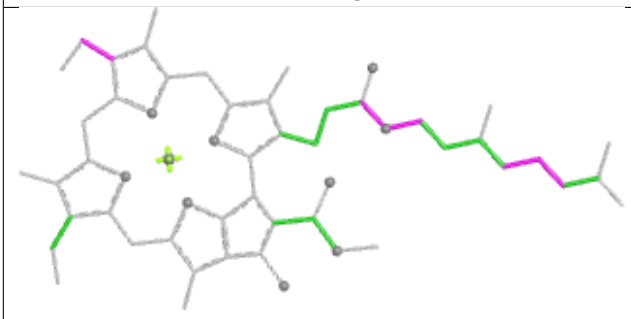
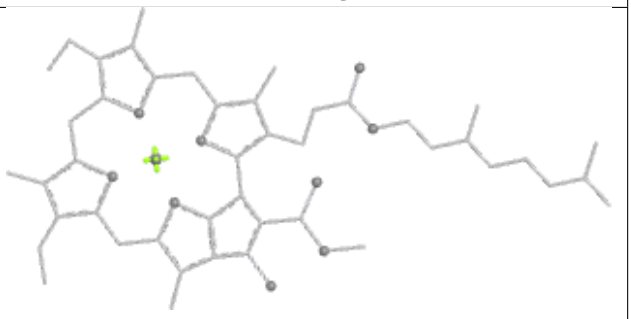
Torsions

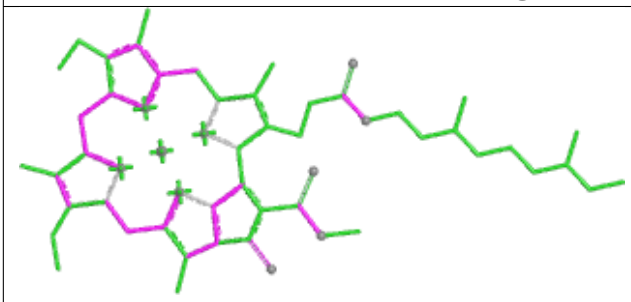
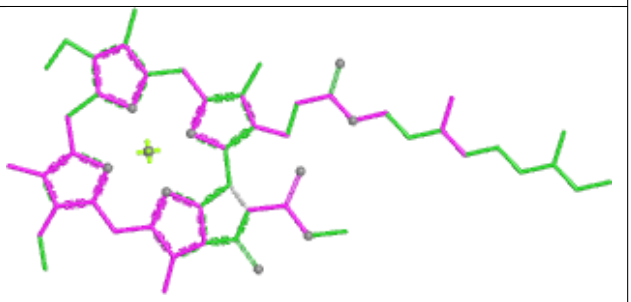
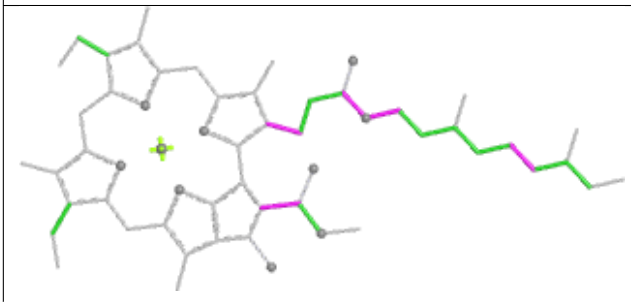
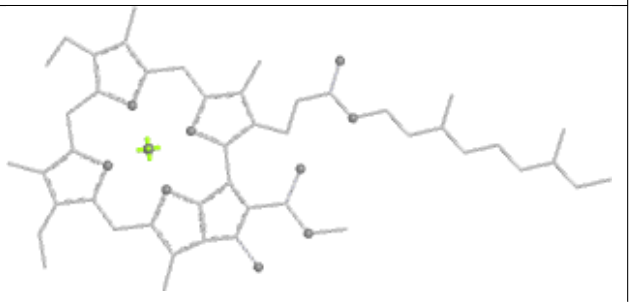


Rings

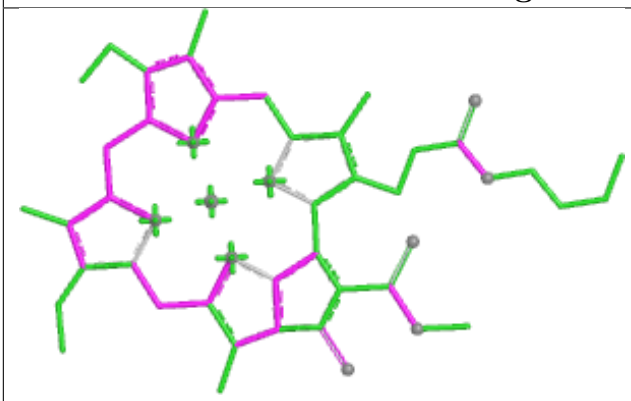
Ligand CLA cA 817	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand 1L3 cA 844	
	
Bond lengths	Bond angles
	
Torsions	Rings

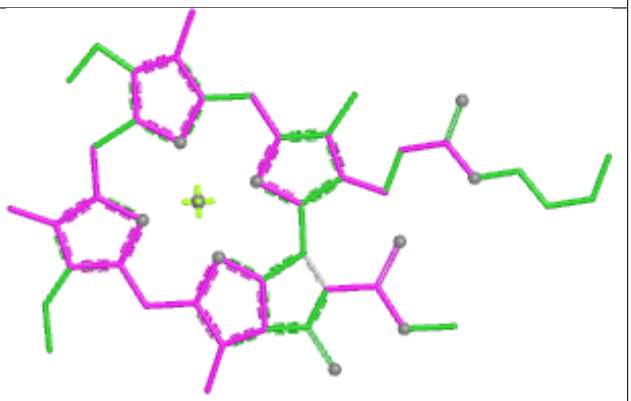
Ligand CLA aA 826	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA bA 804	
	
Bond lengths	Bond angles
	
Torsions	Rings

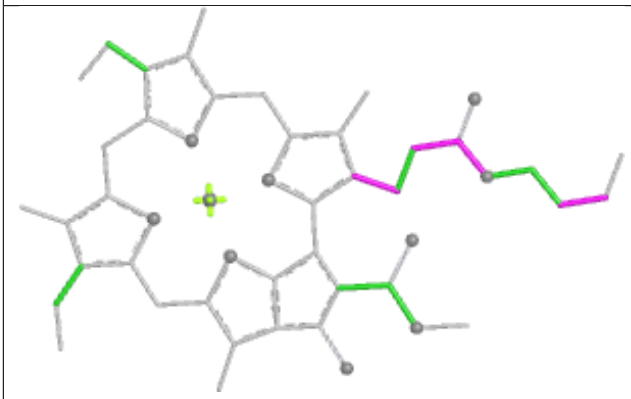
Ligand CLA aA 822



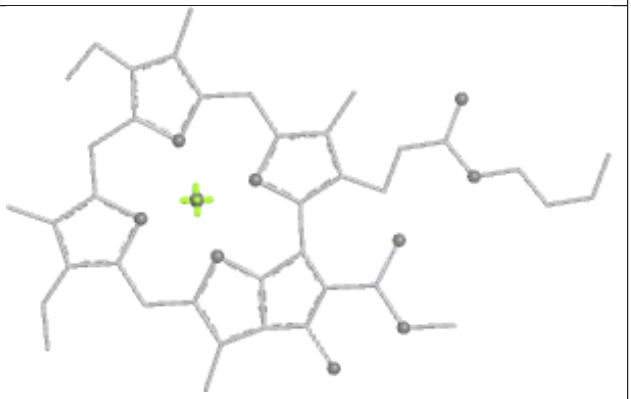
Bond lengths



Bond angles

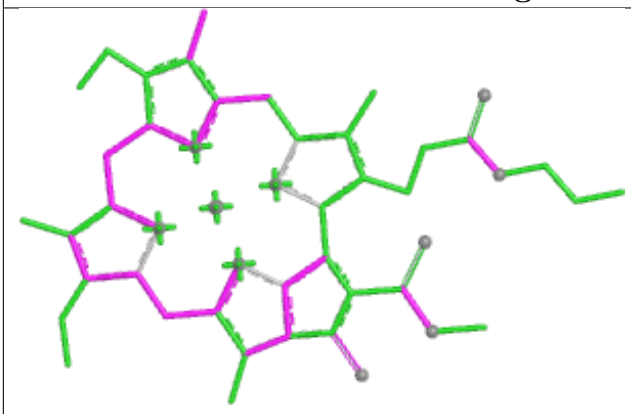


Torsions



Rings

Ligand CLA bB 908



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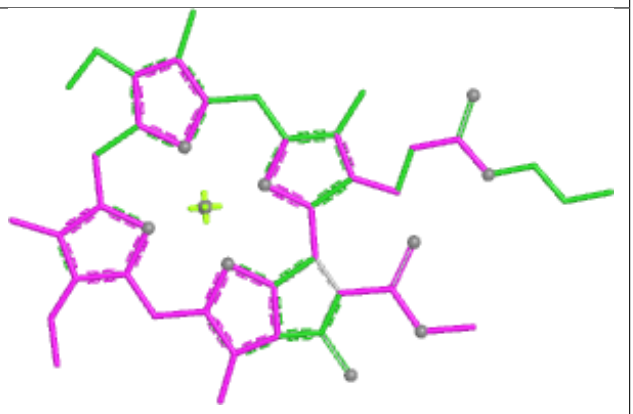
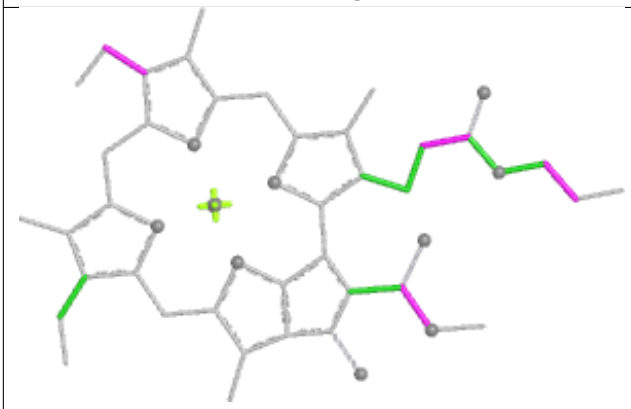


Bond angles



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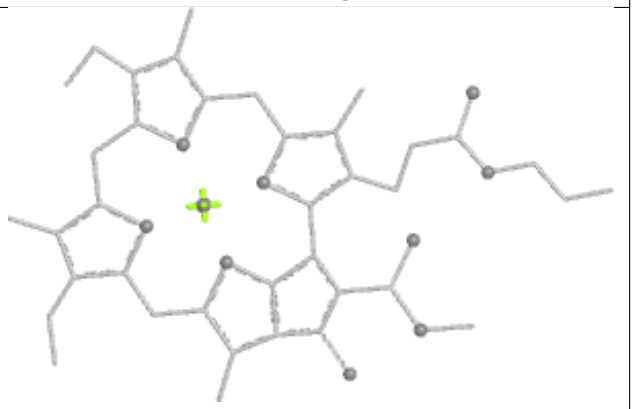
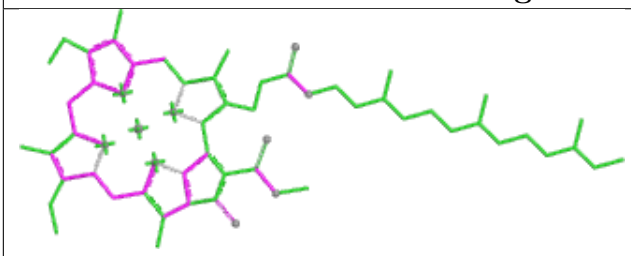
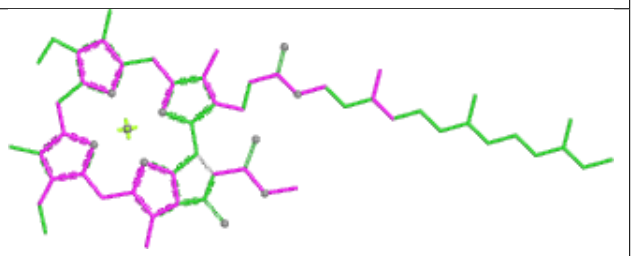


Rings

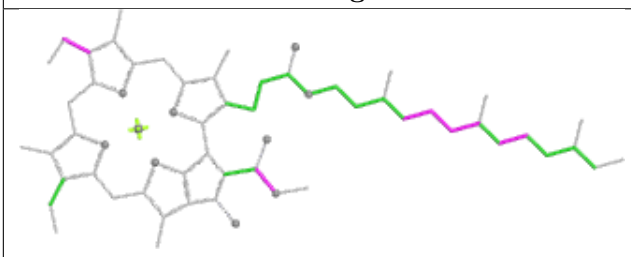
Ligand CLA bB 902



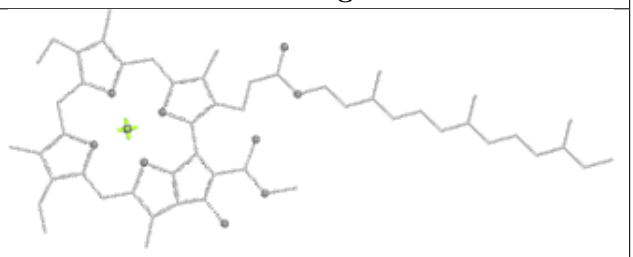
Bond lengths



Bond angles

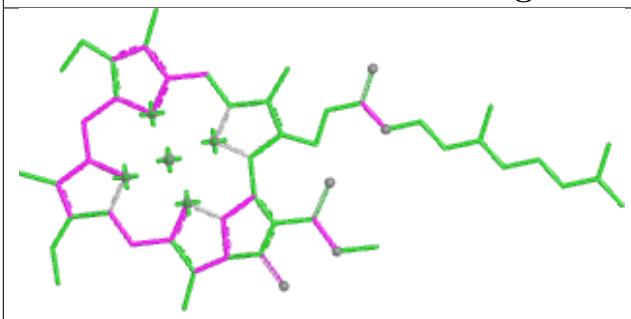


Torsions



Rings

Ligand CLA aA 832



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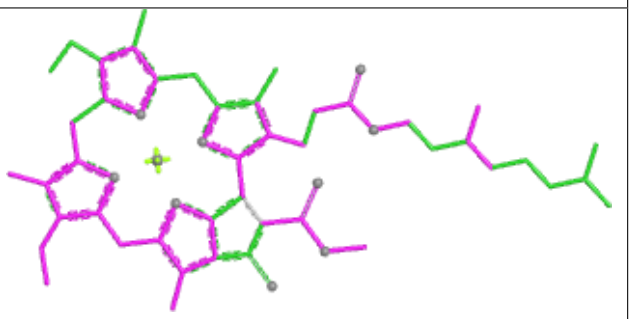
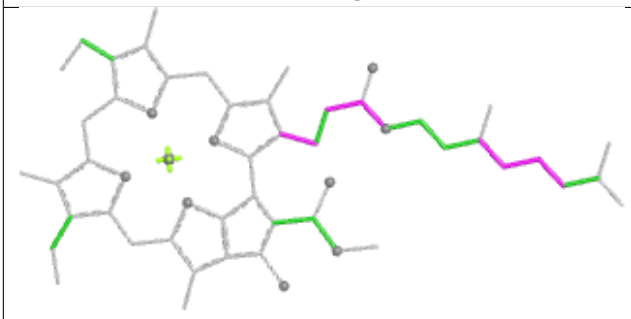
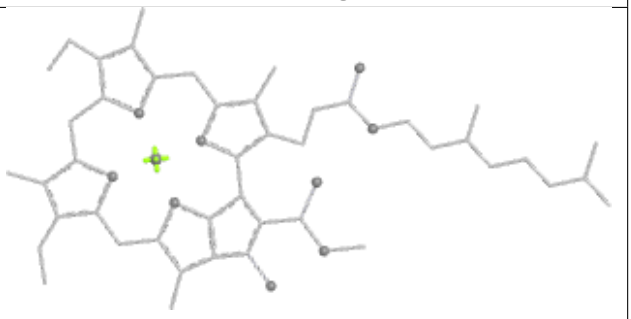


Bond angles

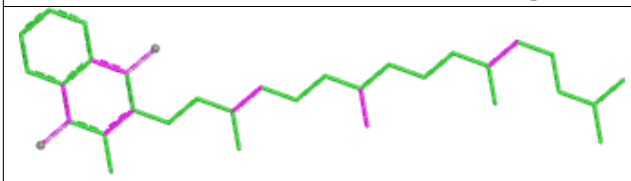


Torsions

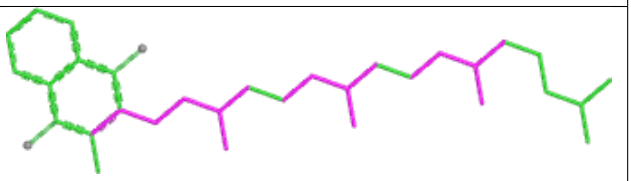


Rings

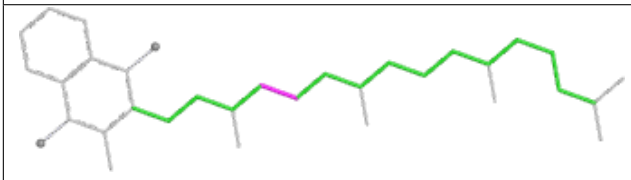
Ligand 1L3 cB 940



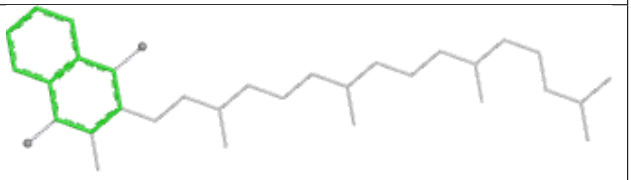
Bond lengths



Bond angles

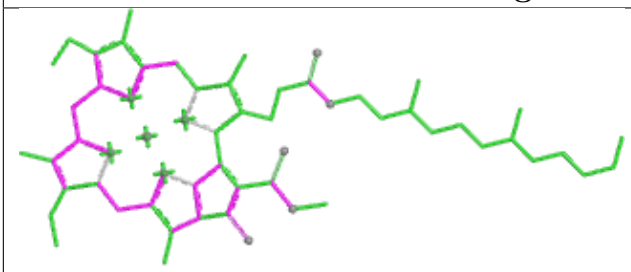


Torsions

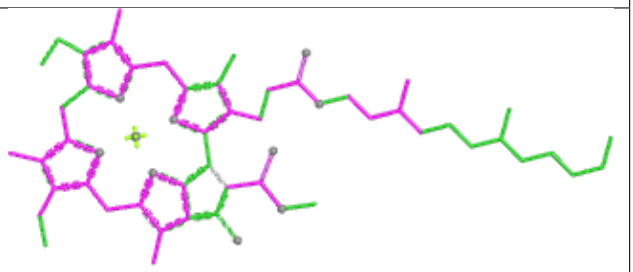


Rings

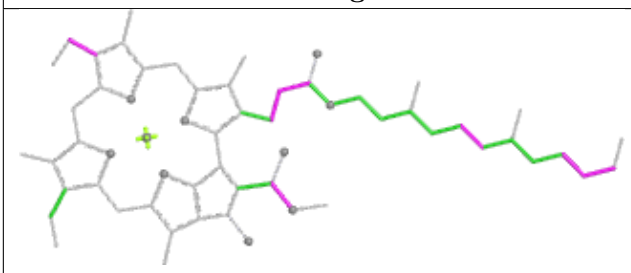
Ligand CLA bB 916



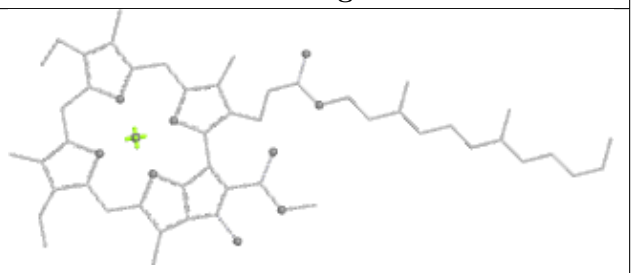
Bond lengths



Bond angles

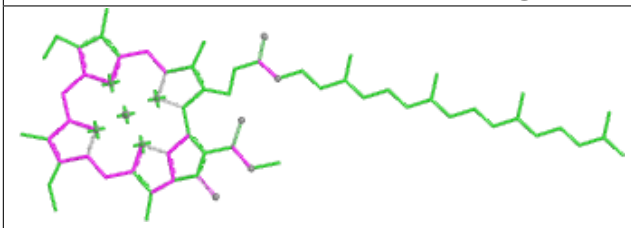


Torsions

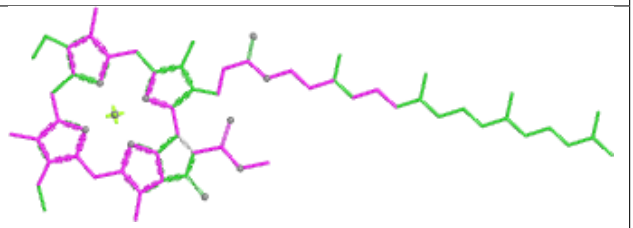


Rings

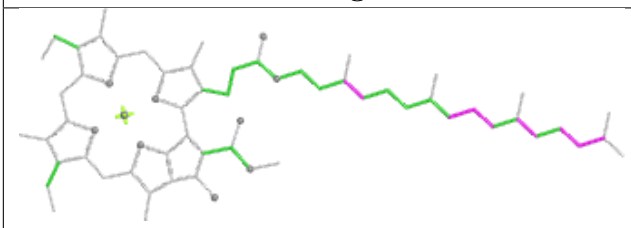
Ligand CLA cA 825



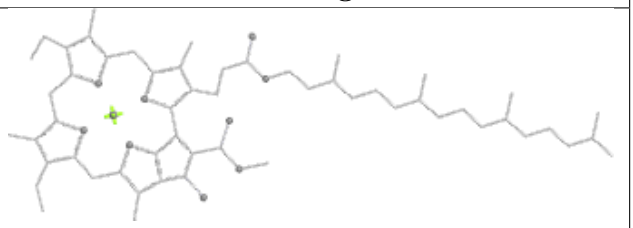
Bond lengths



Bond angles



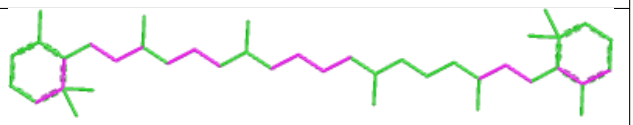
Torsions



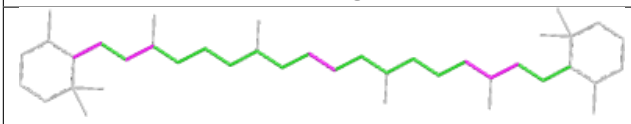
Rings

Ligand BCR cF 201

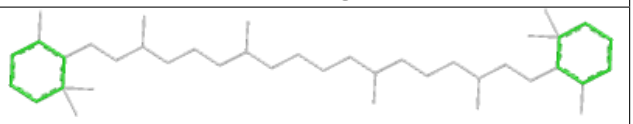
Bond lengths



Bond angles

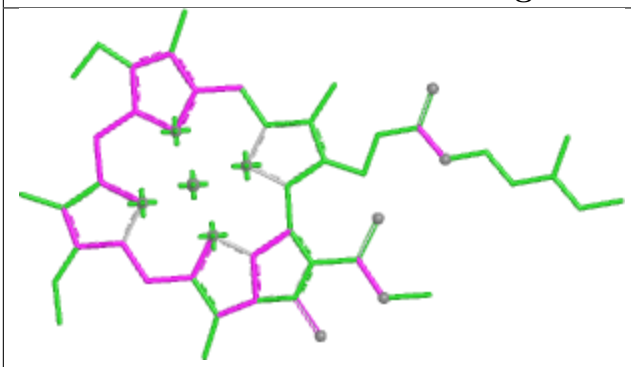


Torsions

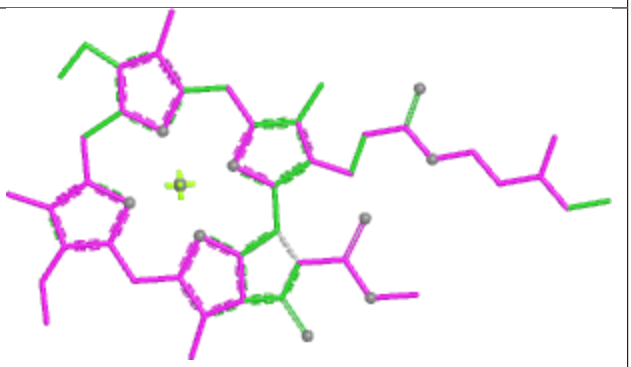


Rings

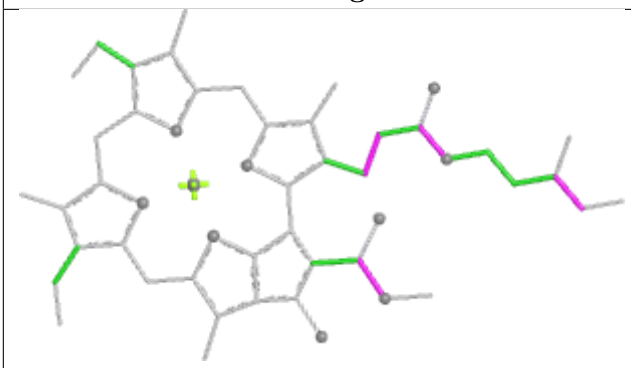
Ligand CLA aA 808



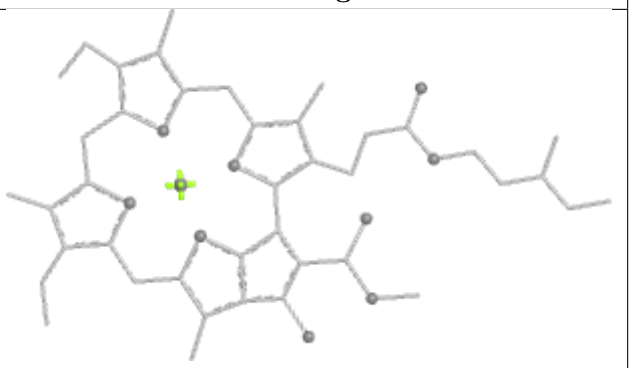
Bond lengths



Bond angles

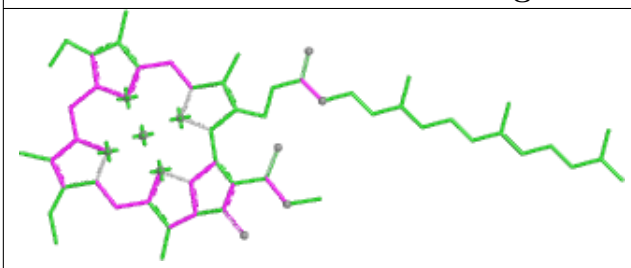


Torsions

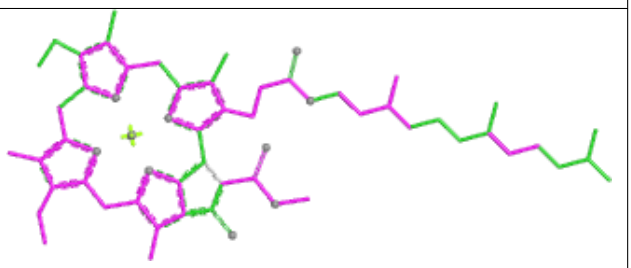


Rings

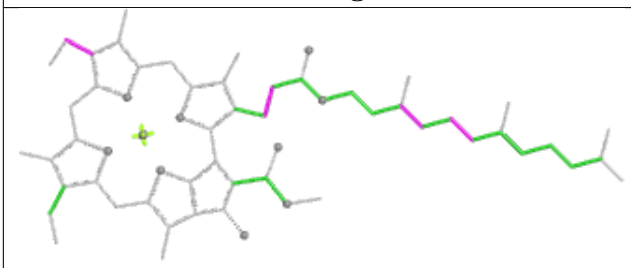
Ligand CLA bA 819



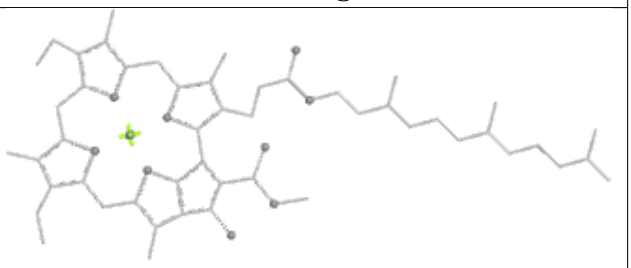
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

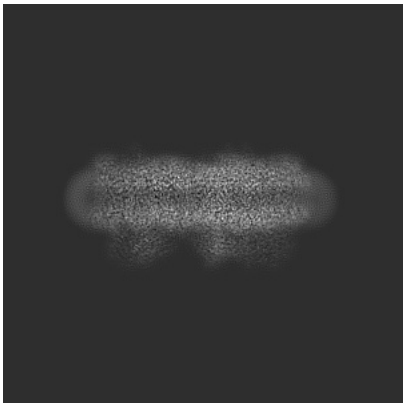
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31455. These allow visual inspection of the internal detail of the map and identification of artifacts.

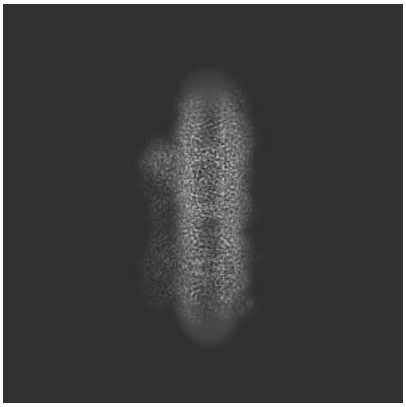
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

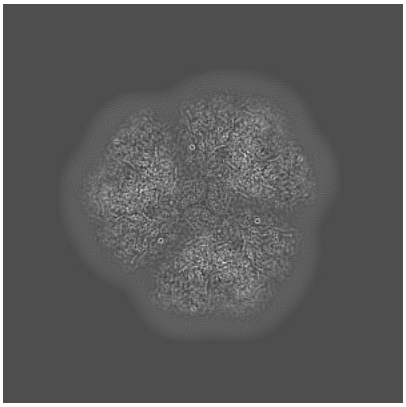
6.1.1 Primary map



X



Y



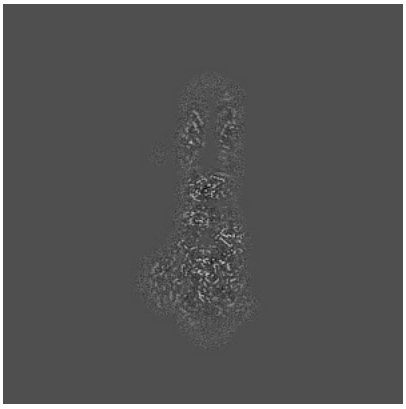
Z

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

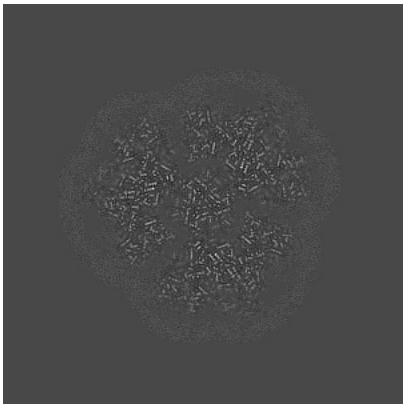
6.2 Central slices

6.2.1 Primary map

X Index: 200



Y Index: 200



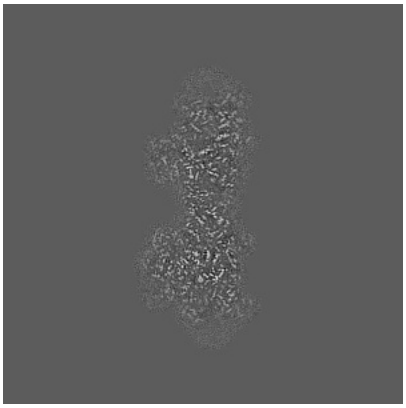
Z Index: 200

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

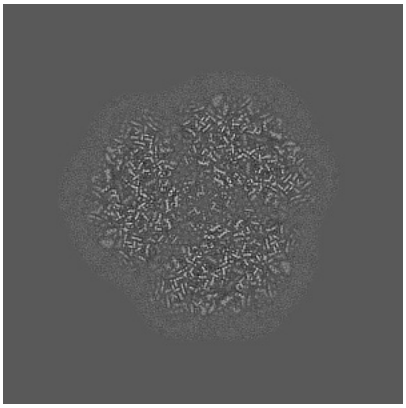
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 245



Y Index: 216

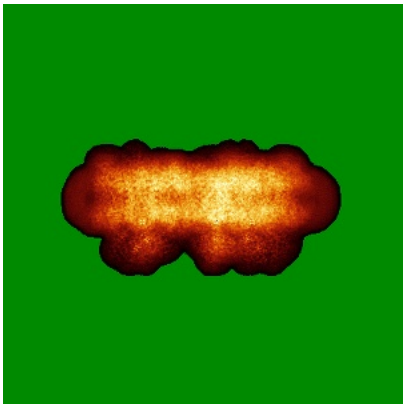


Z Index: 219

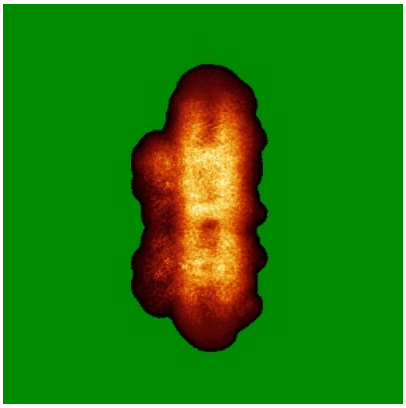
The images above show the largest variance slices of the map in three orthogonal directions.

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

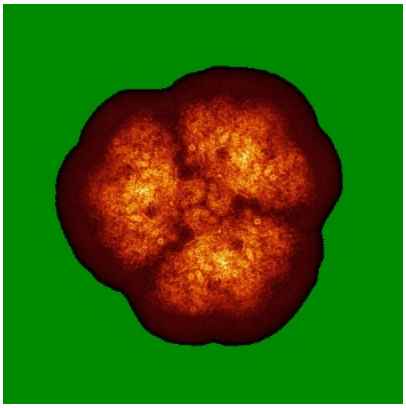
6.4.1 Primary map



X



Y

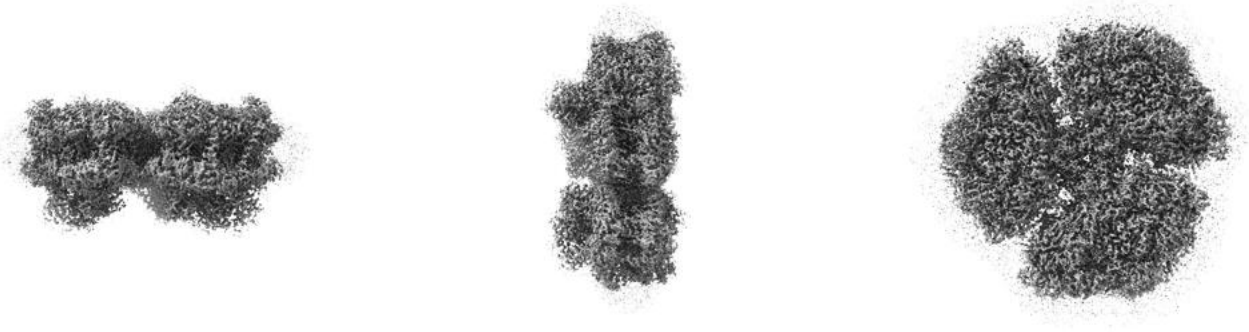


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

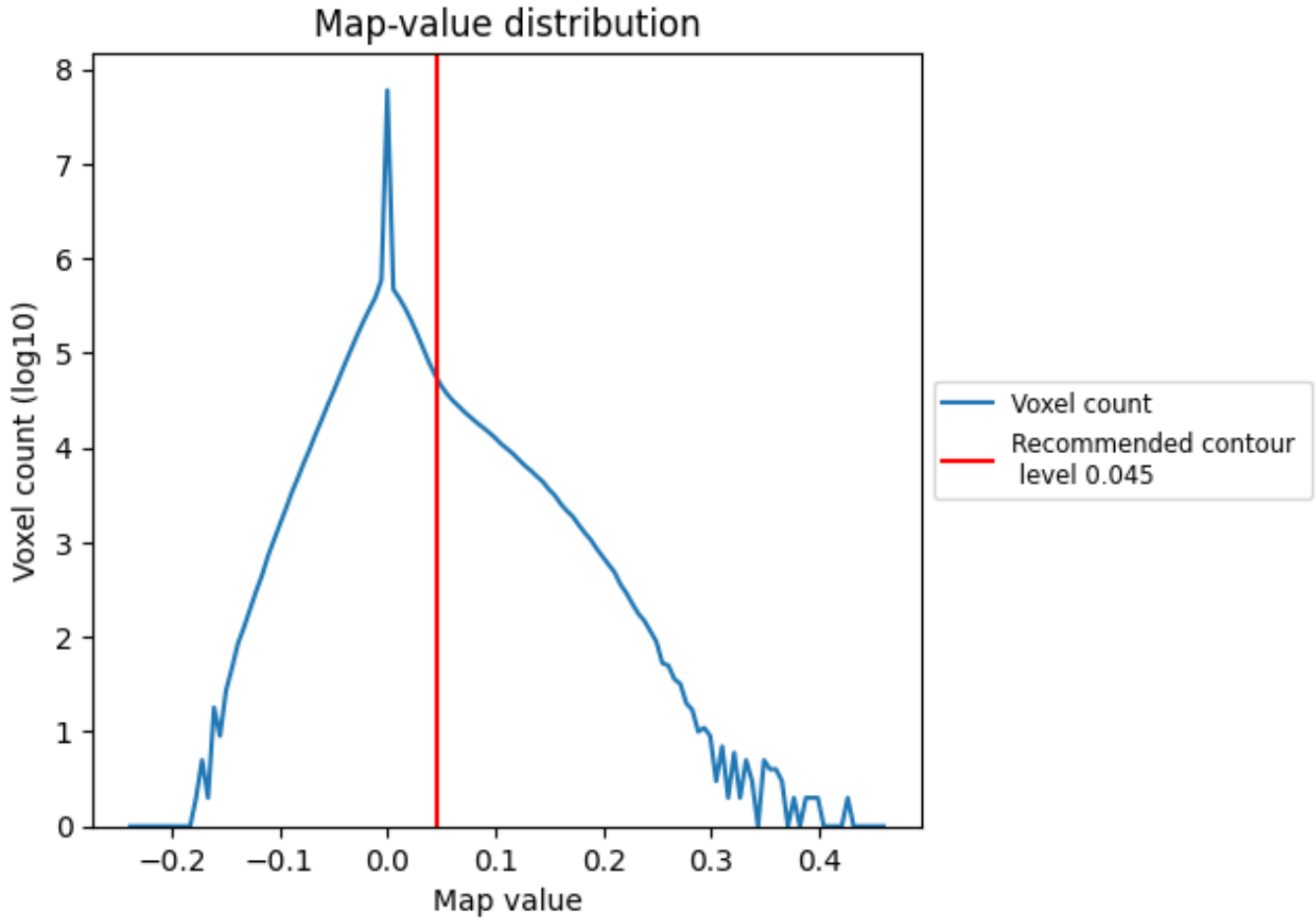
6.6 Mask visualisation (i)

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

7 Map analysis

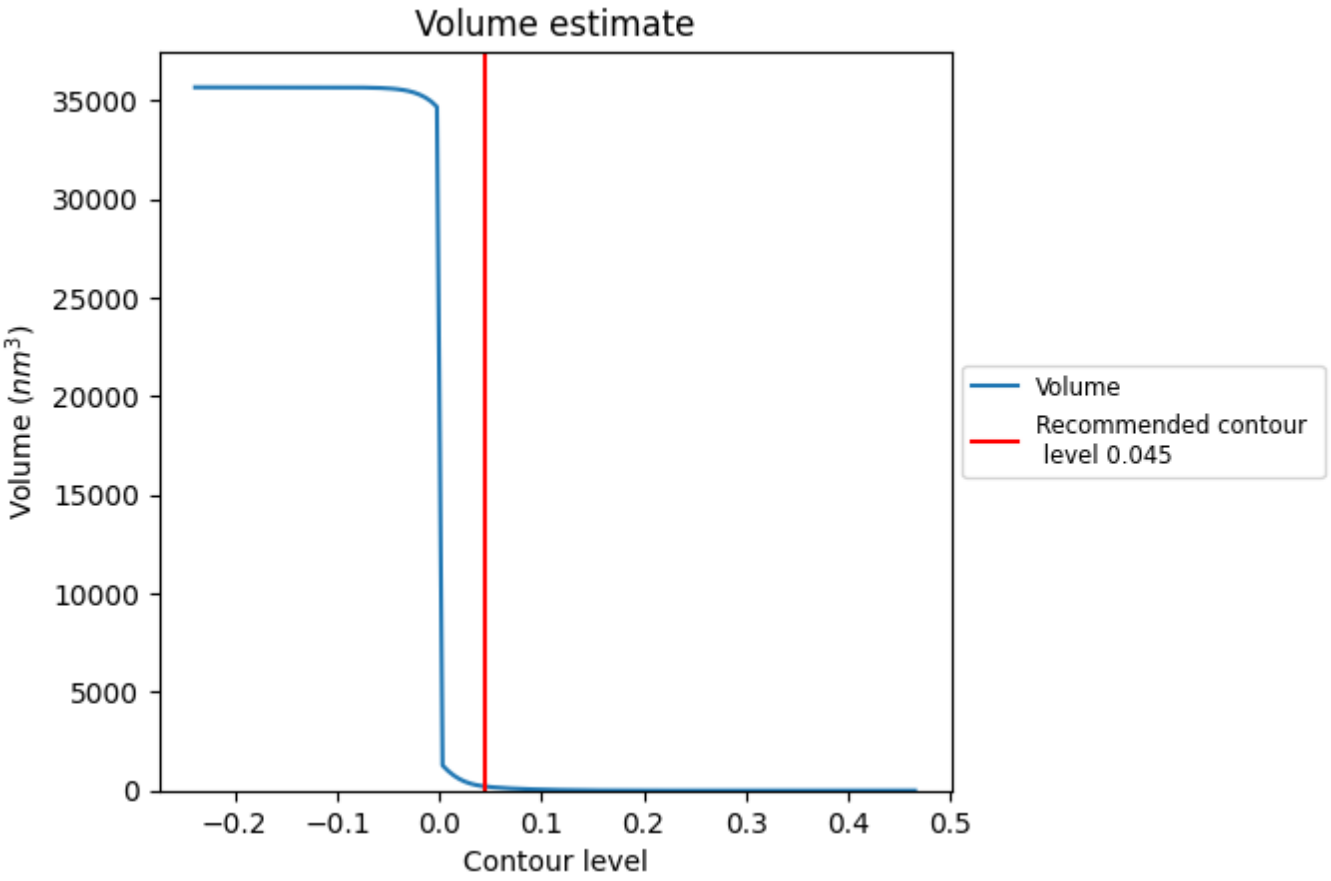
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

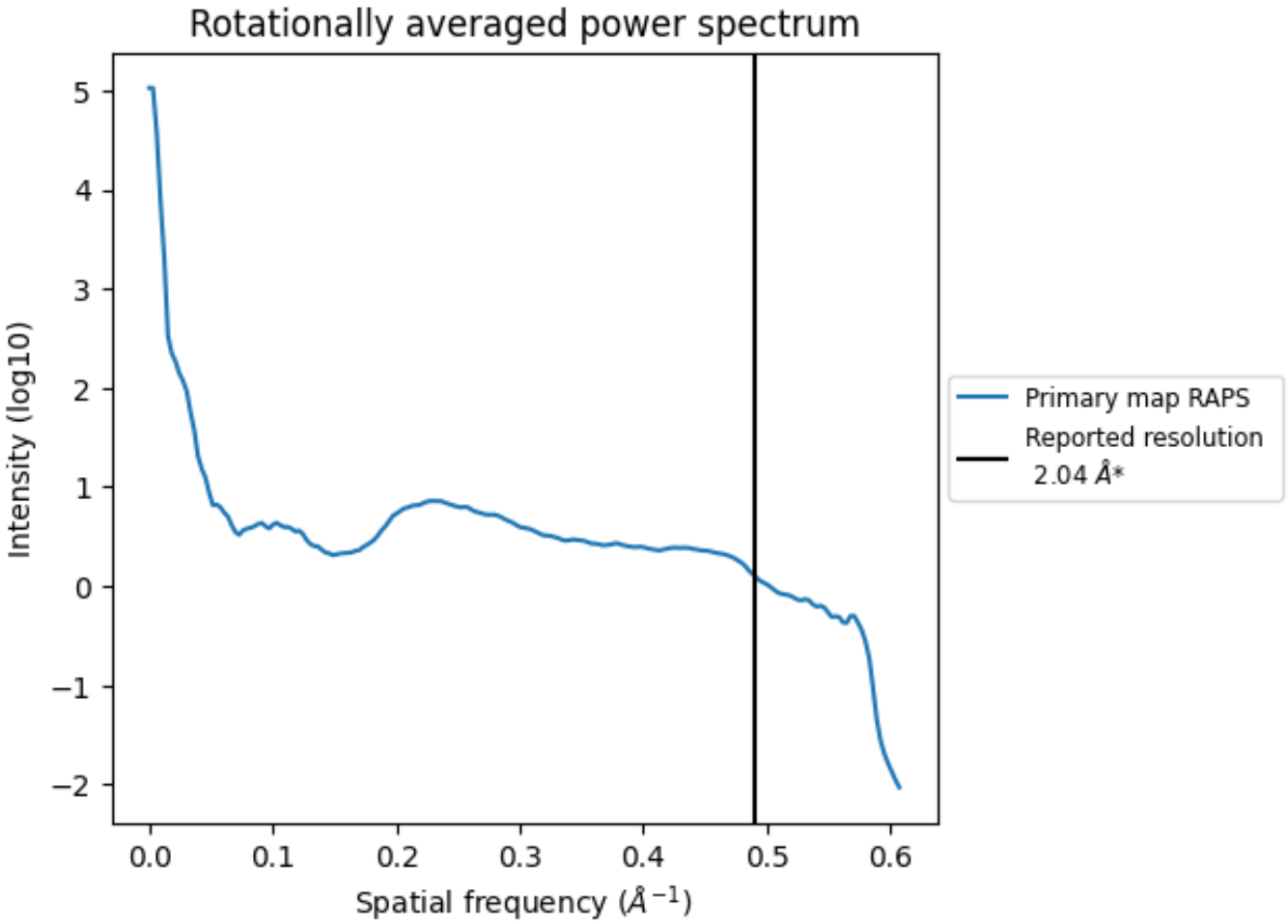
7.2 Volume estimate



The volume at the recommended contour level is 209 nm^3; this corresponds to an approximate mass of 189 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)

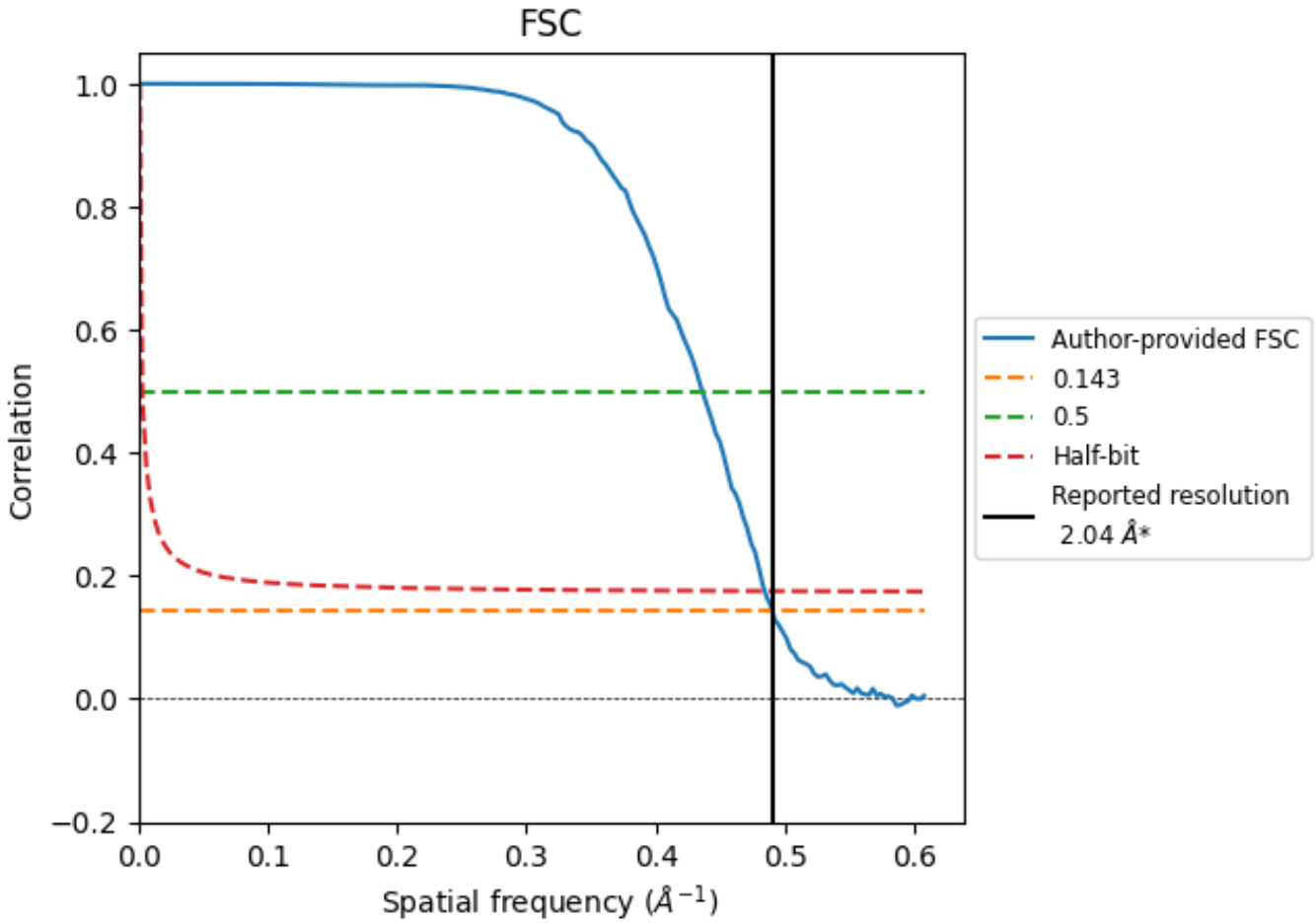


*Reported resolution corresponds to spatial frequency of 0.490 Å^{-1}

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 0.490 $Å^{-1}$

8.2 Resolution estimates (i)

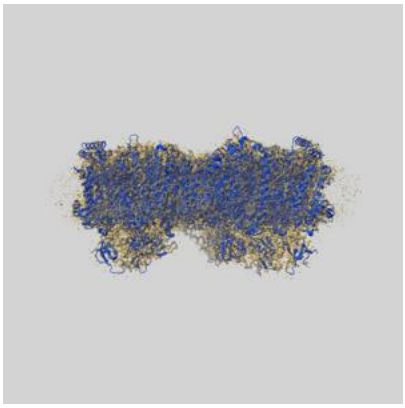
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.04	-	-
Author-provided FSC curve	2.04	2.29	2.06
Unmasked-calculated*	-	-	-

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

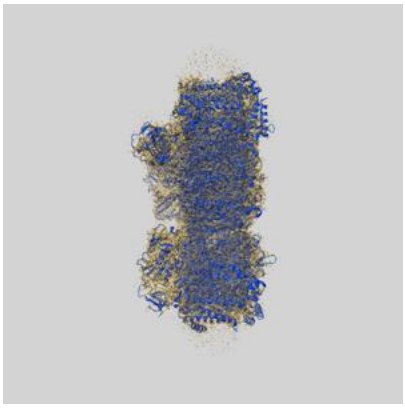
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31455 and PDB model 7F4V. Per-residue inclusion information can be found in section 3 on page 34.

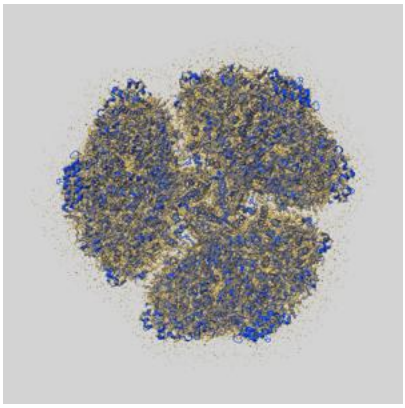
9.1 Map-model overlay



X



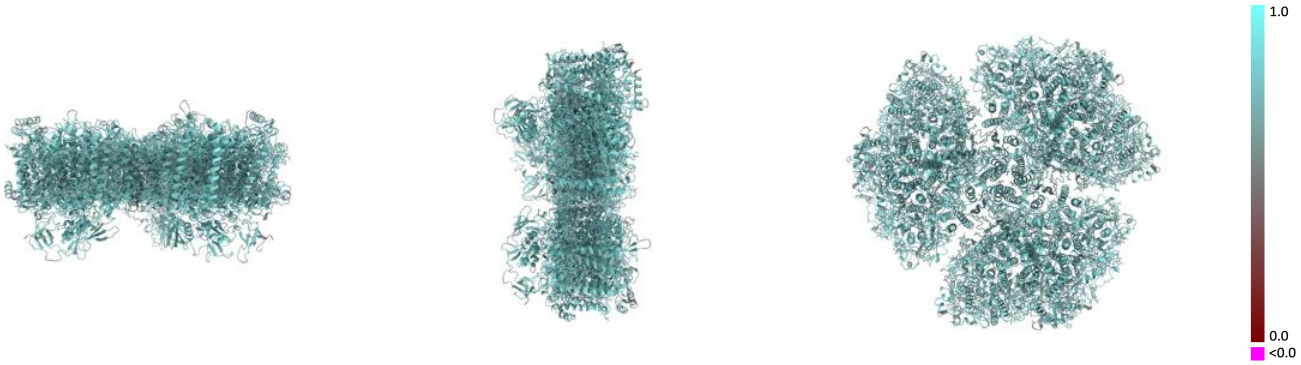
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

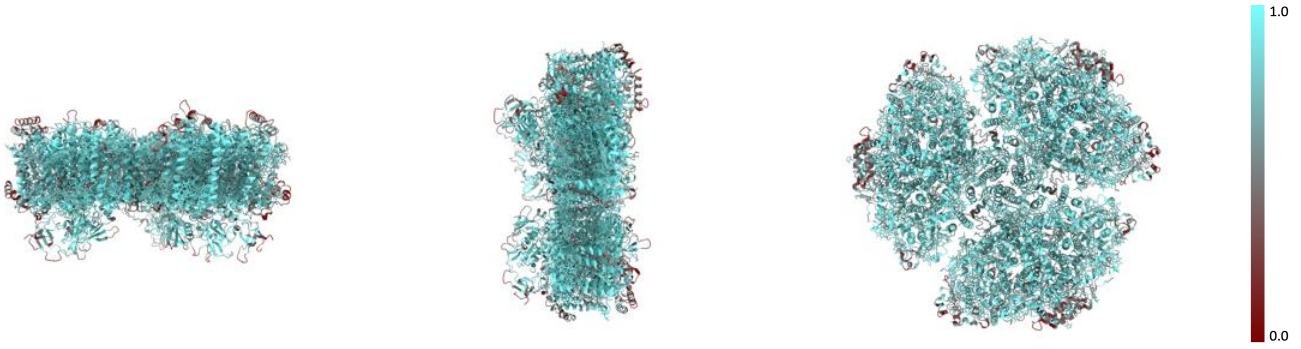
9.2 Q-score mapped to coordinate model



X Y Z

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

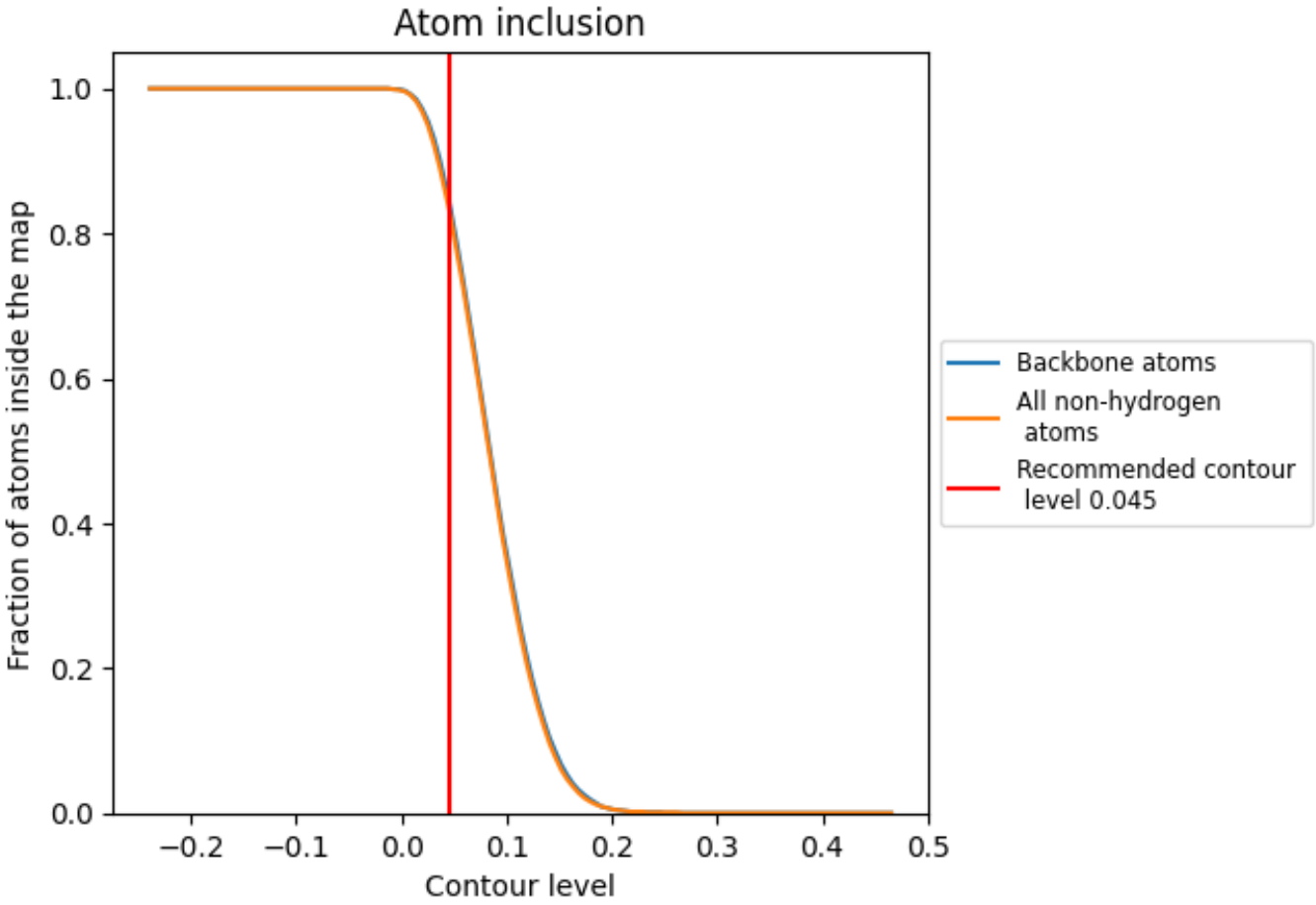
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.045).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 84% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8360	0.7520
aA	0.8580	0.7580
aB	0.8960	0.7710
aC	0.9170	0.7710
aD	0.6990	0.7180
aE	0.6140	0.6720
aF	0.5440	0.6770
aI	0.8340	0.7470
aJ	0.7450	0.7110
aL	0.8460	0.7570
aM	0.8480	0.7480
bA	0.8530	0.7560
bB	0.8940	0.7690
bC	0.9180	0.7680
bD	0.6930	0.7150
bE	0.5960	0.6670
bF	0.5280	0.6720
bI	0.8340	0.7450
bJ	0.7500	0.7120
bL	0.8400	0.7540
bM	0.8390	0.7460
cA	0.8500	0.7550
cB	0.8920	0.7690
cC	0.9320	0.7690
cD	0.6880	0.7150
cE	0.6020	0.6650
cF	0.5300	0.6720
cI	0.8300	0.7480
cJ	0.7450	0.7060
cL	0.8380	0.7500
cM	0.8480	0.7470